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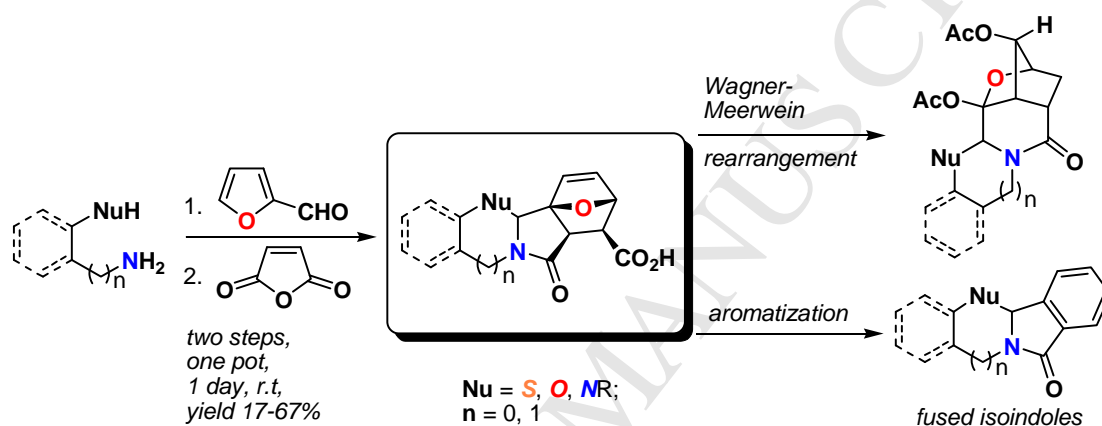
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General synthetic approach towards annelated 3a,6-epoxyisoindoles by tandem acylation/IMDAF reaction of furylazaheterocycles. Scope and limitations.

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An efficient and versatile one-pot synthesis of 3,6a-epoxyisoindoles annelated with oxazine, oxazole, thiazine, thiazole, pyrimidine fragments and with their benzoannelated analogues is presented. The method is based on tandem *N*-acylation/intramolecular cycloaddition (the intramolecular Diels–Alder reaction of furan, IMDAF) reaction between α,β -unsaturated acid anhydrides and α -furyl substituted azaheterocycles. The latter can be easily prepared by condensation of diverse furfurals and 1,2- or 1,3-*N,X*-binucleophiles (aminoalcohols, aminothiols, diamines). The observed IMDAF reaction is stereoselective: *exo*-adducts are formed exclusively with large prevalence of one of the diastereoisomers. In most cases, the condensation/*N*-acylation/IMDAF reaction sequence may be carried out *via* a one pot domino protocol. The scope and limitations of the proposed approach are thoroughly investigated. The obtained Diels–Alder adducts are attractive and useful substrates for further transformations. Fused isoindoles can be prepared from them in one step by aromatization of the 7-oxabicyclo[2.2.1]heptene ring. Other transformations, including halogenation, ring cleavage, and Wagner–Meerwein skeletal rearrangement, are also demonstrated. The spatial structures of the obtained compounds have been established by X-ray diffraction analyses.

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1. Introduction

Furyl amines are common building-blocks for the preparation of nitrogen-containing heterocyclic compounds and are often utilized for the formation of indole rings in particular. Electrophilic recyclization¹ and intramolecular [4+2] cycloaddition reactions² are used for this purpose. Intramolecular Diels-Alder reactions of furfurylamines towards isoindoles, on the other hand, have been investigated less comprehensively. The present work is aimed at demonstrating the possibility of construction of diverse isoindole-containing heterocyclic systems using this method.

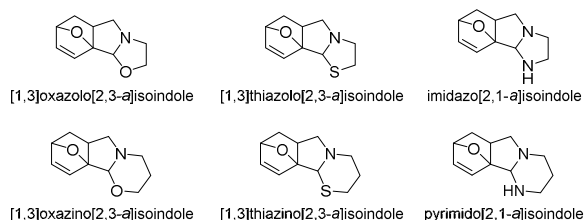


Fig. 1. Target objects.

A vast amount of research and many publications have been devoted to the synthesis and chemical transformations of isoindoles³ and isoindoles annelated with various azaheterocycles: 1,3-oxazolidine,⁴ 1,3-oxazine,^{4a-c,4f,4g,5} 1,3-thiazolidine,^{4a,5d,5f,6} 1,3-thiazine,^{5f,6b,6d,6e,7} pyrimidine.^{5b,5f,8} Similar epoxyisoindoles (Figure 1) have been studied significantly less well,^{5a,9} and there is only sparse and not always reliable information^{9b,10} (see Results and Discussion) on 3a,6-epoxyisoindoles annelated with the above mentioned heterocyclic fragments. Given the limited number of available methods of preparation of partially hydrogenated isoindoles, as well as the high synthetic potential of the 7-oxabicyclo[2.2.1]heptane (heptene) fragment and its immediate availability *via* IMDAF from furans bearing unsaturated substituents in the side chain,¹¹ we propose an effective and versatile method of synthesis of epoxy-containing [1,3]oxazo-, [1,3]oxazino-, [1,3]thiazolo-, [1,3]thiazino[2,3-*a*]isoindoles and pyrimido[2,1-*a*]isoindoles, as well as their benzoannellated analogues (Figure 2).

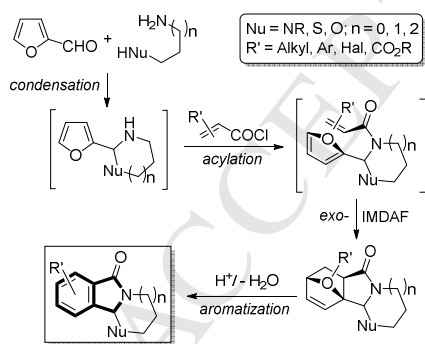


Fig. 2. General approach to the synthesis of isoindoles using IMDAF reaction

We demonstrate that such epoxy-containing adducts are useful precursors for further transformations, one of them being a one-step approach towards fused isoindoles. The only known general approach towards isoindoles annelated with various heterocycles was proposed by a Hungarian research group^{4a,4c,5a,5b,5d,5e,6a,6c,8d,9a} led by P. Sohár and is based on condensation of 2-oxocarboxylic acids with various 1,2-(1,3-, 1,4-)aminoalcohols (thioalcohols

and diamines). In many cases the authors were able to achieve satisfactory yields of target heterocycles, however, in general, the key step of the transformation – *retro*-Diels-Alder reaction required high temperature (over 170 °C) and often led to mixtures of isomeric products. Also, the Pedrosa group in their 1998–2000 publications^{10a–10c} utilized a similar IMDAF-based approach for the preparation of optically active decahydroisoquinolines and tetrahydroisoindolines. Synthetic approaches to heterocycle-fused isoindoles were recently reviewed.¹²

It should be noted also, that a large number of heteroannellated isoindoles possess biological activity¹³; some representative examples are given in Figure 3. Excellent activities against gram-positive bacteria of compounds **A** (X = O)^{14a} and **B**^{14b} and an activity against gram-negative bacteria of **A** (X = O, S, NH)^{14a} have been reported. Compound **C** has been proposed to protect sunflower shoots against adverse effects of 2,4-dichlorophenoxyacetic acid herbicide.¹⁵ Sub-structures **D** and **E** are useful as antiviral drugs.^{6e,16} Particularly, some thiazolo[2,3-*a*]isoindol-5-ones **D**^{6e} and 10b-phenyl-1,3,4,10b-tetrahydropyrimidino[2,1-*a*]isoindol-6(2*H*)-one¹⁶ inhibited human immunodeficiency virus reverse transcriptase with an IC₅₀ of 2.2 × 10⁻⁶ M. Heterocycles **F** increase the blood level of GLP-1 (glucagon-like peptide 1) and are useful as remedies for diabetes, preventives for chronic complications of diabetes, and antiobesity agents.¹⁷

We could not find any information regarding bioactivity of heterocycle-annellated epoxyisoindoles and their derivatives.

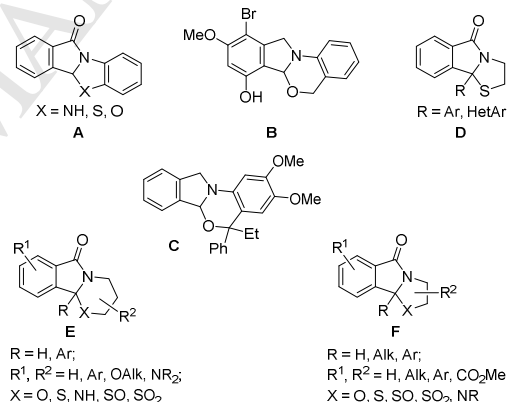


Fig. 3. Selected examples of bioactive isoindoles annelated with various five- and six-membered *O,S,N*-heterocycles

This work is a development of our approach towards annelated isoindoles and isoquinolines *via* epoxyisoindoles by IMDAF¹⁸ and proposes a short preparative methodology for design of isoindoles fused with two heteroatom containing five- and six-membered heterocyclic fragments and their benzoannellated analogues. The approach is based on substituted furfurals and involves a sequence of transformations including condensation/ acylation/ intramolecular [4+2] cycloaddition. Subsequent aromatization of the cycloaddition adducts may lead to fused isoindoles (Figure 2).

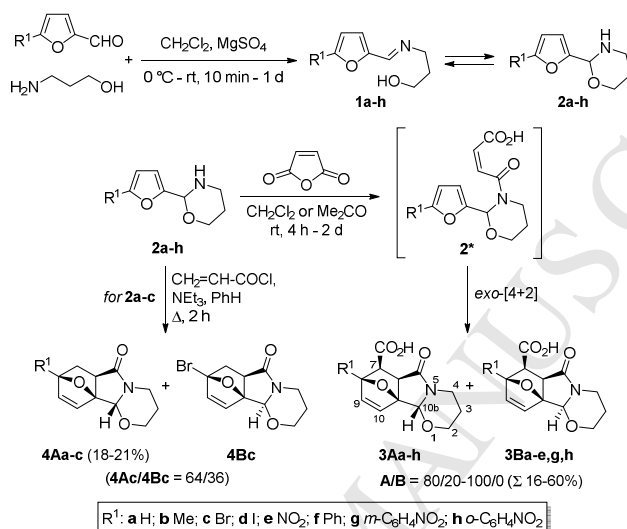
Given that the general strategy of synthesis of isoindoles using the IMDAF reaction has already been widely utilized,¹⁹ we believe that the experimental simplicity of the method, availability of starting materials and the synthetic diversity of the final products will promote wide application of the presented approach to preparation of fused epoxyisoindoles.

2. Results and discussion

2.1. Epoxyisoindoles fused with oxazoles and oxazines

Schiff bases **1**, the products of condensation of aromatic aldehydes (including furfural) with 1,2- and 1,3-aminoalcohols, are known to exist in tautomeric equilibrium with 1,3-oxazolines^{20a-f} and 1,3-oxazinanes **2**, respectively.^{20a,20c,21,22} The equilibrium position depends on the solvent, temperature and on the nature of the Ar-2 substituent. When ethanolamine is treated with aromatic aldehydes, the equilibrium usually shifts towards the open chain form – azomethine. The presence of a bulky substituent in the 1,2-aminoalcohol leads to a shift towards the

ring form – up to 70% of 2-aryl-1,3-oxazolines can be observed. 2-Phenyl-1,3-oxazinanes are usually more stable than the corresponding chain tautomers: the mixture may contain up to 98% of the former.²² However, the tautomeric mixture of products of condensation of furfural with 1,3-aminopropanol contains only 23% of the cyclic form – 2-furyl-1,3-oxazinane (**2a**)^{20a} (Scheme 1). Also, direct *N*-acylation of imines has been demonstrated.^{20g-j} Nevertheless, the presence of the ring form **2** in the tautomeric mixtures allows access to epoxyisoindoles-containing heterocycles *via* tandem acylation/IMDAF reaction¹⁸ (Figure 2), which has been the main topic of our research in recent years.



Scheme 1. Synthesis of 8,10a-epoxy[1,3]oxazino[2,3-*a*]isoindoles **4** and their 7-carboxy derivatives **3**.

First, we investigated the reaction of aliphatic aminoalcohols with substituted furfurals. The condensation of 3-aminopropanol with 5- R^1 -furfurals occurred at room temperature in the presence of a dehydrating agent (MgSO_4) and resulted in formation of the equilibrium **1** \rightleftharpoons **2** mixtures in almost quantitative yields. The position of the ring-chain tautomeric equilibrium **1** \rightleftharpoons **2** was determined by the ratio of the ^1H NMR integral intensities of the $\text{N}=\text{CH}$ (8.0–8.3 ppm, chain form) and $\text{H}-2$ (5.2–6.0 ppm, ring form) protons for reaction mixture solutions in CDCl_3 . In most cases, the reaction mixture contained 12–27% of the ring tautomer **2**. The rate of formation of the tautomeric mixtures depends on the electronic effects of the substituent R^1 : the reaction of 5-nitrofurfural was complete in 10 min at 0°C and it took about 1 day at room temperature for the condensation to proceed in case of 5-arylfurfurals. We failed to carry out the condensation of 5-methoxyfurfural,²³ bearing a strongly electron-donating methoxy group, with propanolamine in these conditions.

The next step of the proposed protocol is the acylation of furfurylamines (ring tautomers **2**) with α,β -unsaturated acid anhydrides. As was shown before,^{11a,18,19} the reaction of furfurylamines with anhydrides and chlorides of α,β -unsaturated acids does not stop at the *N*-acylation products (similar to **2***) formation step, instead, it is immediately followed by intramolecular *exo*-Diels–Alder cyclization with the furan ring (IMDAF). In general, the last step of this transformation requires heating up to 80–110 $^\circ\text{C}$, but in a recent short communication^{18a} we showed, that reaction of 2-furyl-1,3-oxazinane **2a** with maleic anhydride occurs at room temperature, which allows performing the transformation of furfurals to 8,10a-epoxy[1,3]oxazino[2,3-*a*]isoindole **3a** in a single synthetic procedure (Scheme 1).

From a preparative point of view, the procedure is exceptionally simple. A solution of maleic anhydride and the

tautomeric mixture **1** \rightleftharpoons **2** in CH_2Cl_2 was stirred at room temperature for 4 h – 2 days. The slightly colored adducts **3** were isolated by filtration and were used for most practical purposes without further purification. Oxazino[2,3-*a*]isoindoles (**3**) can also be obtained by carrying out the acylation/[4+2] cycloaddition in acetone (room temperature, 4–24 h). In this case the obtained samples were more than 98% pure. Only the adduct obtained by acylation of 2-(5-phenyl-2-furyl)-1,3-oxazinane (**2f**) could not be isolated by simple filtration, probably due to the low content of the ring form **2f** (14%) in the tautomeric equilibrium mixture **1f** \rightleftharpoons **2f**, and the low crystallization propensity of the product. Therefore, column chromatography was used to isolate the adduct **3Af**.

The reaction of Schiff bases **1a–c** with acryloyl chloride, a weaker dienophile compared to maleic anhydride, led to 8,10a-epoxy[1,3]oxazino[2,3-*a*]isoindoles **4a–c** *via* a similar acylation/cycloaddition domino reaction but in somewhat lower yields (Scheme 1). Similar to the case of maleic anhydride, the intermediate *N*-acyl derivatives (analogous to **2***), were neither detected nor isolated.

The IMDAF reaction in both cases was essentially stereoselective:^{11a} only *exo*-adducts were formed with a large prevalence of the **3A**, **4A** diastereoisomers. Individual isomers **3A** were easily isolated by crystallization from an *i*-PrOH/DMF mixture (individual diastereoisomers **3A**, **4A** were used for further transformations). Only for product **4c** ($\text{R}^1 = \text{Br}$) a low diastereoselectivity was observed – the **4Ac/4Bc** ratio was 64/36.

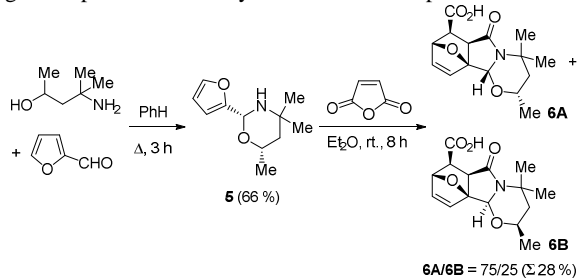
Similar IMDAF reaction conditions were used to obtain adducts discussed below (Schemes 5, 8, 9, 11, 12, 15, 16, 18) and the experimental data are summarized in Table 1.

We tried to determine the relative configuration of the H-10b proton in the adducts **3c,d** (for samples with the highest content

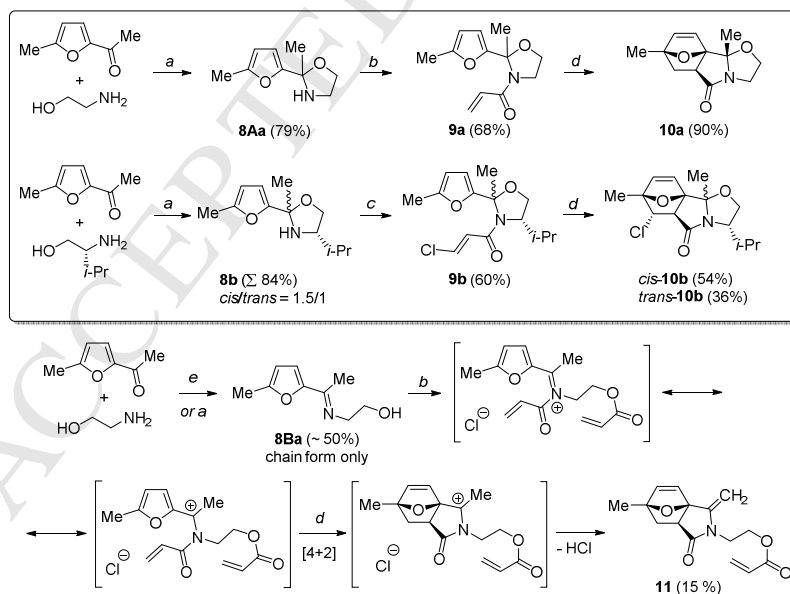
Tetrahedron

of the minor isomer **3B**) on the basis of 1D nOe experiments. When the H-10b proton in **3Ac,d** was irradiated, small changes in the integrated signal intensity were observed in H-6a. Somewhat higher but comparable intensities were observed for the minor isomers **3Bc,d**. Therefore, we employed a more reliable structural determination method for these adducts (see Scheme 13 and corresponding text below).

The sensitivity of the condensation/acylation/cycloaddition tandem reaction to steric hindrance by substituents in the α -position to the nitrogen atom of the amino binucleophile was then probed (Scheme 2). Readily available 4-amino-4-methylpentan-2-ol²⁴ was selected as a model compound. Due to the Thorpe-Ingold effect,²⁵ the tautomeric equilibrium in this case completely shifted towards the ring form – oxazinane **5** (furyl and Me-6 occupy equatorial positions in the six-membered cycle). The ring tautomer **5** readily reacted with maleic anhydride at 25 °C in ether, but the reaction led to formation of a large amount of by-products. Diastereomers **6** were isolated in rather low yields (Scheme 2) with the **6A/6B** ratio of ~ 3/1. When acetone, benzene or dichloromethane were used as reaction solvents, the diastereoselectivity was higher by comparison with ether, but the overall yield decreased (for instance, a single isomer **6A** was isolated in 12% yield after 1 h reflux in benzene). Thus, the bulky α -4,4-dimethyl fragment in oxazinane **5** led to lower yields of target compounds caused by formation of side products.



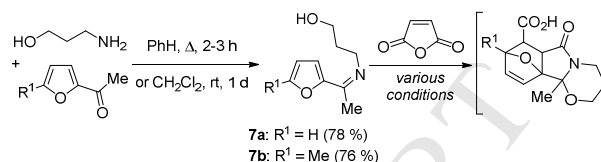
Scheme 2. Bulky 1,3-aminopropanol in the tandem reaction



Reagents and conditions: (a) CH(OEt)₃/TsOH (cat.); (b) CH₂=CH-COCl/NEt₃/CH₂Cl₂; (c) CHCl=CH-COCl/NEt₃/CH₂Cl₂; (d) PhMe/ Δ /1.5–4 h; (e) MeOH/rt/1 d.

Scheme 4. IMDAF reaction of 3-acryloyl-2-(2-furyl)-2-methyl-1,3-oxazolidines (**8**) reported earlier by M. Jung and L. Street^{10d-f} (top in frame) and the results of this work.

The reaction of 1,3-aminopropanol with 2-furyl ketones could be anticipated to give rise to a ring-chain tautomeric mixture similar to reaction with furfural, but the products of condensation of 1,3-propanolamine and 2-furylketones – 2-acetylfuran and 5-methylacetylfuran – were found only in the open chain forms **7** ($\delta_{C=N} \sim 157$ ppm, Scheme 3).



Scheme 3. 2-Furylketones in the target transformation

Schiff bases **7** readily reacted with maleic anhydride or CH₂=CH-COCl/NEt₃ at room temperature in acetone, dichloromethane or benzene. However, instead of crystalline products, only dark viscous poorly soluble in acetone or dichloromethane oils were formed. ¹H NMR spectra of the reaction mixtures revealed complex mixtures of products with no signals of the target 10b-methyloxazino[2,3-*a*]isoindoles. When acryloyl chloride was used, peaks responsible for the presence of the alkenyl fragment (C_q=CH₂) in adducts similar to **11** (see Scheme 4 below) were observed. In this case, the separation of the reaction products was not performed.

After investigation of the reaction of 1,3-aminoalcohols and furfurals towards oxazino[2,3-*a*]isoindoles, we turned to exploration of transformations of 1,2-aminoalcohols, expecting to obtain oxazolo[2,3-*a*]isoindoles similar to **10** (Scheme 4).

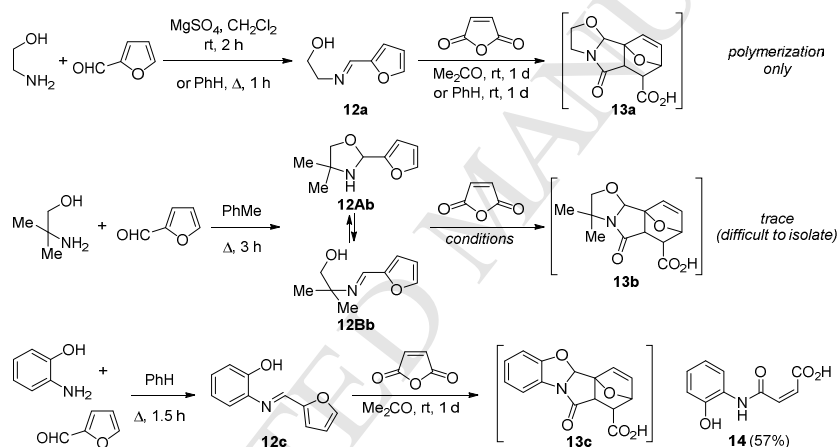
A literature review revealed a successful intramolecular [4+2]-cycloaddition of 3-acryloyl-2-(2-furyl)-2-methyl-1,3-oxazolidines **9** (Scheme 4) as a step of a newly developed route to dihydroxyhexahydrobenzofuran unit in avermectins (macrocyclic lactones with potent antihelmintic and insecticidal properties).^{10d-10f} 7,9a-Epoxy[1,3]oxazolo[2,3-*a*]isoindol-5-ones **10** were isolated in these 3-step syntheses in moderate to good yields. Unfortunately, we could not reproduce the **8a**→**9a**→**10a** sequence of steps as shown in Scheme 4. According to the ¹³C NMR data ($\delta_{C=N}$ 158.1 ppm), the product of condensation of 5-methyl-2-acetylfuran with ethanolamine obtained was the chain tautomer, azomethine, 2-[1-(5-methyl-2-furyl)ethylidene]aminoethanol (**8Ba**), which reacted with acryloyl chloride giving rise to a mixture of products, whose major component was (3-methylene-3a,6-epoxyisoindol-2-yl)ethyl acrylate (**11**). According to ¹H NMR (4.75 and 4.72, two d, ²*J* = 2.3 Hz, C(3)=CH₂), the reaction mixture contained about 20% of compound **11**, which was isolated by column chromatography in 15% yield (relative to the starting azomethine **8Ba**).

A plausible mechanism of formation of the adduct **11** is presented in Scheme 4. In the one-step synthesis (1.5 eq of acryloyl chloride/ 2 eq of NEt₃/PhMe/ Δ , 4 h) deprotonation of the methyl group is probably facilitated by NEt₃. A more detailed

study of this interesting transformation is outside the scope of this work.

Perplexed by this outcome, we tried to carry out the condensation/acylation/[4+2]-cycloaddition transformation using the simplest reactants: unsubstituted furfural and 1,2-aminoalcohols – 2-aminoethanol and 2-amino-2-methylpropan-1-ol (Scheme 5). According to the NMR data (CDCl₃, $\delta_{CH=N}$ 151.6, $\delta_{C=N}$ 8.07 ppm), the condensation product of 2-aminoethanol and furfural was azomethine 2-(2-furylmethylene)aminoethanol (**12a**) with no signals corresponding to the tautomeric 2-furyl-1,3-oxazolidine observed. The reaction of 2-amino-2-methylpropan-1-ol with furfural led (due to the Thorpe–Ingold effect) to a tautomeric mixture **12b**, consisting of 1,3-oxazolidine (**12Ab**) and imine (**12Bb**) in the ratio of 38/62.^{20a} The reaction of compound **12a** or tautomeric mixture **12b** with maleic anhydride gave rise to multicomponent reaction mixtures. The target cycloaddition adducts **13a,b** could not be isolated.

The reaction of aromatic *ortho*-aminoalcohol with constrained “*cis*”-conformation of the functional groups gave no positive results either. The only product of condensation of 2-aminophenol with furfural was aldimine – 2-[(2-furylmethylene)amino]phenol (**12c**), which when reacted with maleic anhydride, gave *N*-maleinamide **14** instead of 2,4a-epoxyisoindolo[1,2-*b*][1,3]benzoxazole-1-carboxylic acid (**13c**).



Scheme 5. Attempted synthesis of 7,9a-epoxy[1,3]oxazolo[2,3-*a*]isoindoles **13**

Thus, according to our results, furyl ketones and 1,2-aminoalcohols cannot be used in the presented transformation for the synthesis of oxazino[2,3-*a*]isoindoles (**3**, **4**) and oxazolo[2,3-*a*]isoindoles (**10**), respectively.

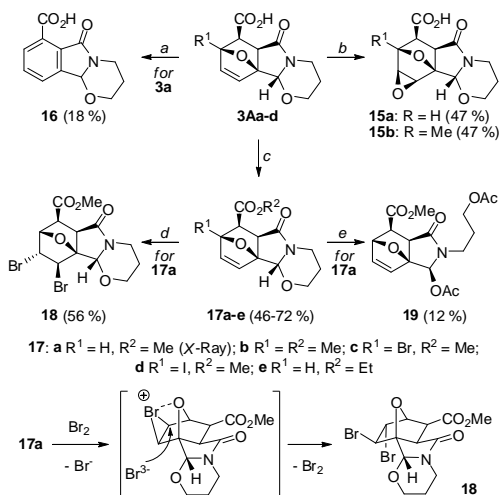
Very limited information^{10a-c} was found on the chemical transformations of epoxy[1,3]oxazino[2,3-*a*]isoindoles **3**. Some possible directions of modification of the obtained isoindolic acids **3** are presented in Scheme 6. Depending on the reaction conditions, the oxazine ring can be preserved: oxidation of the olefinic fragment (diepoxides **15**) and esterification of the carboxylic group (esters **17**); or aromatization of the 7-oxabicycloheptene fragment can be carried out to obtain isoindolone **16**. We tried to perform halogenation of **3Aa** (NBS in CHCl₃, Br₂/NaOH in H₂O or MeOH; dioxane dibromide or Me₂N⁺HCOMe·Br₃⁻·Me₂NCOMe²⁶ in CHCl₃) but could not isolate any individual products. Probably, in this case, bromination of the double bond was complicated by a skeletal rearrangement (see Scheme 13 below).

Esters **17** are more attractive for further transformations than [1,3]oxazino[2,3-*a*]isoindole carboxylic acids **3**. The acids are powders with very low solubility in organic solvents (almost insoluble in CHCl₃ and Me₂CO), and high solubility in basic

aqueous solutions, which leads to difficulties for syntheses and low yields of the final products. The esters **17**, on the other hand, are soluble in organic solvents. Moreover, the esters **17a,b** crystallized in well-formed prisms. This allowed using X-ray analysis for determination of their structures, thus, the spatial configuration of the H-10b proton in both the esters **17** and the *major* isomers of the acids **3A** was unambiguously determined. It was shown (see Supporting information) that the proton H-10b in **3A**, **15**, **17**, **18** is *cis*-oriented to the 8,10a-oxo bridge.

Unlike oxazino[2,3-*a*]isoindole carboxylic acids **3**, methyl ester **17a** was successfully transformed to *trans*-dibromide **18** with Me₂N⁺HCOMe·Br₃⁻·Me₂NCOMe.²⁶ This mild bromination agent gave better results than any other we tried (see above). Stereoselectivity of addition of bromine to the 7-oxaheptene fragment of the ester **17a** is governed by the steric factor: Br₃⁻ attacks the least hindered C-9 carbon atom (see Scheme 6) in the intermediate bromonium ion. This direction of bromination was established based on the spin-spin coupling constants of the H-8 – H-10 protons (³*J*_{9,10} = 5.4, ³*J*_{8,9} = 2.2 Hz) in the vicinal dibromide **18**. The moderate yields of the products **15**, **16**, **18**, presented in Scheme 6, are compensated by the ready availability

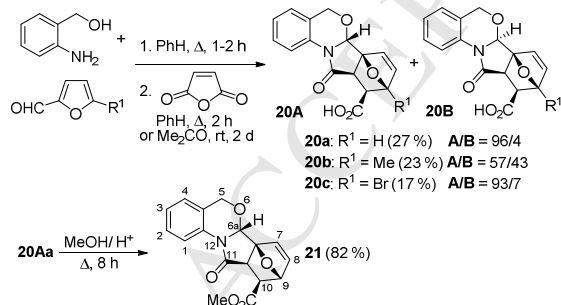
of the starting reagents and simplicity of the reaction and isolation procedures (see Experimental Section).



Reagents and conditions: (a) NaOH (10%), Δ , 2 h; (b) H₂O₂ (30%)/HCO₂H/CHCl₃, Δ , 12 h; (c) R²OH/H⁺, Δ , 5–25 h; (d) Me₂N⁺HCOMe⁻Br⁻·Me₂NCOMe/CHCl₃/ Δ , 12 h; (e) BF₃·OEt₂/Ac₂O, -5→25 °C, 24 h.

Scheme 6. Some examples of chemical transformations of 8,10a-epoxy[1,3]oxazino[2,3-a]isoindole-7-carboxylic acids **3Aa–d** and their methyl esters **17**

Benzoannulated 1,3-aminopropanols – 2-(hydroxymethyl)aniline (Scheme 7) and 2-(aminomethyl)phenol²⁷ (Scheme 8) can also be used as starting reagents for construction of the isoindole containing heterocycles. The condensation of *o*-aminobenzyl alcohol with 5-R¹-furfurals and follow-up reaction of the formed 2-(2-furyl)-1,3-benzoxazines with maleic anhydride was performed in situ (Method A, see Experimental Section) in benzene (Scheme 7). 6b,9-Epoxyisoindolo[2,1-a][3,1]benzoxazine-10-carboxylic acids **20** were isolated as diastereomeric pairs **20A** and **20B**. Isomers **20A** with the *cis*-oriented oxygen bridge and H-6a proton were more abundant and in these cases, the *major* components **20Aa** and **20Ac** were easily isolated by crystallization from an *i*-PrOH/DMF mixture. The presence of a substituent R¹ in the 5-position of the furan ring decreased the yields of adducts **20b,c**.



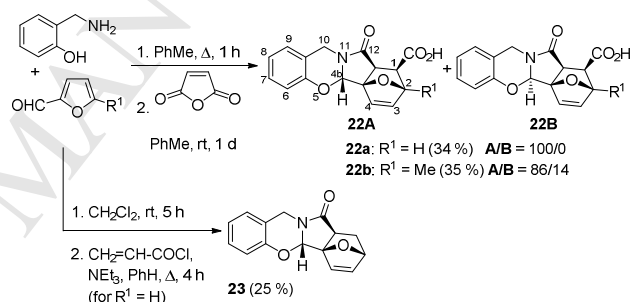
Scheme 7. One-pot synthesis of 6b,9-epoxyisoindolo[2,1-a][3,1]benzoxazine-10-carboxylic acids **20**

This transformation can also be carried out in two steps with isolation of the intermediate 2-furyl-1,3-benzoxazines (Method B). The yields of the adducts **20** obtained by methods A and B were comparable.

According to its ¹H NMR data, the ratio of tautomeric ring/chain forms in the equilibrium when furfural underwent condensation with *o*-aminobenzyl alcohol was ~ 78/22. The yields and the ratios of the isomers **20Aa** and **20Ba** for

cycloaddition reaction of this mixture with maleic anhydride in acetone or dichloromethane were similar. Esterification of carboxylic acid **20Aa** gave ester **21**, whose spatial structure was established by nOe. In the 1D nOe difference spectrum a low intensity peak, responsible for the spatial interaction of protons H-6a/H-10a (nOe $\eta_{\text{H-6a}}\{\text{H-10a}\} < 3\%$) was found. The nuclear Overhauser effect has an approximately similar value in the *major* isomer of acid **20Aa**. In the *minor* isomer **20Ba**, nOe is much higher on the same protons: $\eta_{\text{H-6a}}\{\text{H-10a}\} 9.0\%$. Based on these data and by analogy with esters **17**, *cis*-configuration of the proton H-6a relative to 6b,9-epoxy bridge was attributed to all *major* isomers **20A**.

The nucleophilicity of the nitrogen atom in the initial isomeric aminoalcohols (compare with Schemes 7 and 8) has no influence on the reaction. 2-(Aminomethyl)phenol,²⁷ when reacted with furfural and then anhydrides of α,β -unsaturated acids, underwent a similar transformation (Scheme 8). *Exo*-adducts of [4+2]-cycloaddition, 2,4a-epoxyisoindolo[1,2-*b*][1,3]benzoxazines (**22a**, **23**), were isolated with moderate yields as individual diastereomers. Adduct **22b** was isolated as a pair of isomers with a significant prevalence of the isomer **22Ab**. The relative configuration of the C-4b carbon in this series was established for isoindolo[1,2-*b*][1,3]benzoxazines **22a** and **23**, whose 2D ¹H NOESY NMR spectra showed only a weak cross-peak between the key protons H-4b/H-12a, but rather strong between H-4b/H-4 protons.



Scheme 8. Synthesis of 2,4a-epoxyisoindolo[1,2-*b*][1,3]benzoxazines **22** and **23**

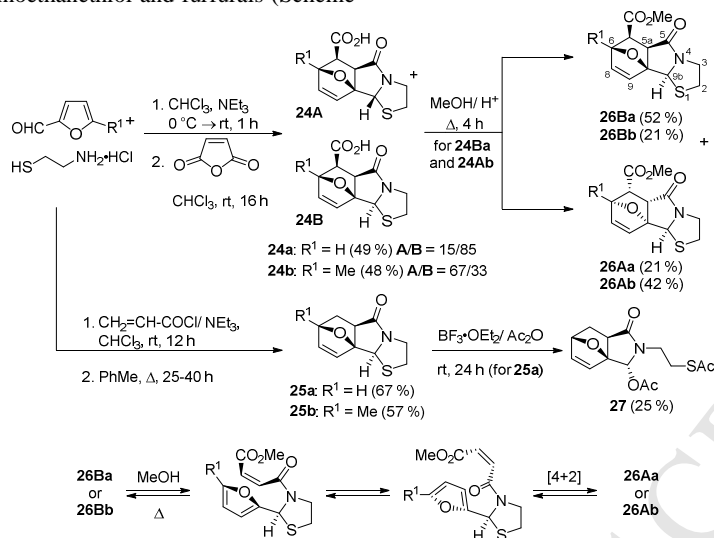
Extension of the distance between the reactive termini of the binucleophile to four carbon atoms leads to an increased influence of the entropic factor and prevents tandem transformation. Condensation of 1,4-aminobutanol with furfural gave rise to azomethine, 4-[(2-furylmethylene)amino]butan-1-ol, with no trace of the tautomeric 2-(2-furyl)-1,3-oxazepane. When this Schiff base was treated with maleic anhydride in various conditions (from Me₂CO, 24 °C to PhMe, Δ , 1 h) a mixture of unidentifiable compounds was formed.

The domino condensation/acylation/cycloaddition reaction between 1,3-aminoalcohols, furfurals and anhydrides of α,β -unsaturated carboxylic acids to give epoxyisoindoles **3**, **4**, **6**, **20–23** led us to pursue further studies of the scope of this transformation especially with regard to investigating whether sulfur and nitrogen analogues of 1,2- and 1,3-aminoalcohols could be involved in such transformation.

2.2. Epoxyisoindoles fused with thiazoles and thiazines

It is well known that 2-aminoethanethiols²⁸ and 3-aminopropane-1-thiols^{6d,29} readily react with aromatic aldehydes at room temperature with no catalyst giving the condensation products in yields close to quantitative. The products exist only in the ring form owing to high nucleophilicity of the sulfur atom.^{6d,28,29} The condensation/acylation/cycloaddition sequence of steps carried out in one pot enabled us to obtain the target

[1,3]thiazolo[2,3-*a*]isoindoles⁶ **24**, **25** in 48–67% overall yield (Scheme 9).



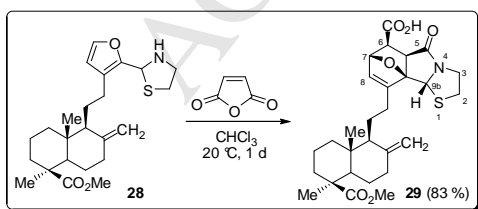
Scheme 9. One-pot synthesis and some transformations of 7,9a-epoxy[1,3]thiazolo[2,3-*a*]isoindoles **24** and **25**

Similarly to previous cases, the last step – the IMDAF reaction with maleic anhydride – is an *exo*-cycloaddition and gave a mixture of diastereoisomers **24A**/**24B** with a prevalence of the diastereomers **24B** (except **24b**) having a *trans* relative configuration of the C-9b proton and the 7,9a-epoxy bridge. Two fold recrystallization of these isomer mixtures from EtOH or EtOH/DMF allowed to obtain the *major* isomers **24Ba** and **24Ab** in 30–40% yield.

The cycloaddition of acryloyl chloride is more diastereoselective and led to isolation of a single isomer of adducts **25**.

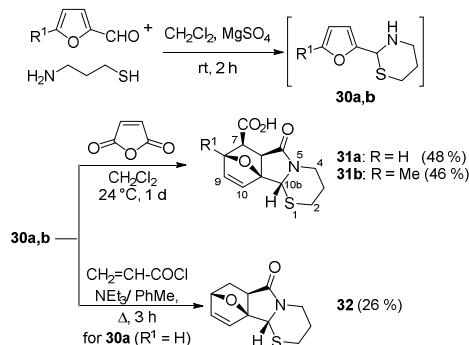
Some chemical transformations of the functional groups in isoindoles **24** and **25a** were performed. It was shown that transformations with conservation (ester **26**) and cleavage (3a,6-epoxyisoindol-3-yl acetate **27**) of the thiazole ring can be carried out. Unexpectedly, esterification of the individual diastereomers of acids **24Ba** and **24Ab** in boiling methanol led to the mixtures of diastereomers **26Aa,b**/**26Ba,b**, probably due to retro-Diels-Alder decomposition of adducts **26B** and follow-up recyclization to **26A** (or vice versa as shown in Scheme 9). This statement is substantiated by the fact that a long-term reflux in methanol of the individual isomer **26Ba** gave rise to the same mixture of **26Aa**/**26Ba**.

It should be noted here that the only analogous compound was reported in a recent work^{9b} which described a reaction of an optically active derivative of lambertianate – 2-(thiazolidinyl-2)-furyl-3 (**28**) with acryloyl chloride and maleic anhydride (Scheme 10).



Scheme 10. The cycloaddition of maleic anhydride to methyl 16-(thiazolidin-2-yl)lambertianate by Kharitonov and co-authors.^{9b} Only one of the two formed diastereoisomers **29** (in a 1:1 mixture) is presented in the scheme.

The authors^{9b} reported that the cycloaddition adduct **29** was formed in high yield and diastereoselectivity and stated, based on the 2D ¹H NOESY NMR analysis, that the H-9b proton in both of the diastereoisomers had a *cis*-orientation to 7,9a-epoxy bridge of the isoindole fragment. This conclusion does not agree with our results (Schemes 9, 12). In the 2D ¹H NOESY NMR spectra of the *major* isomer **24Ba**, the *major* isomer **24Ab**, adduct **25a**, and ester **26Ba** considerable cross-peaks are present. The features are responsible for spatial closeness of protons H-9b/H-5a. This spatial arrangement of the protons can be particularly clearly seen from the 2D ¹H NOESY NMR spectra of the **24Aa**/**24Ba** and **24Ab**/**24Bb** diastereomeric mixtures (the cross-peak between the H-9b/H-5a protons in isomers **24B** is significantly more intensive than that in isomers **24A**). Thus, the mentioned protons occupy the *cis*-position in the **B** series. This result is in agreement with the X-ray data for the rearrangement product **39b** (see Scheme 13 below). It should also be noted here, that the isomers of **24–26** can be attributed to **B** (*cis* H-9b and H-5a) or **A** (*trans* H-9b and H-5a) configurations without using nOe, but based solely on their ¹H NMR spectra. The singlet peak of the H-9b proton for **24–26B** is located in the lower field region (both in CDCl_3 and $\text{DMSO}-d_6$ δ 5.47–5.66 ppm) compared to the analogous peak in **24A**, **26A** (δ 5.16–5.23 ppm).



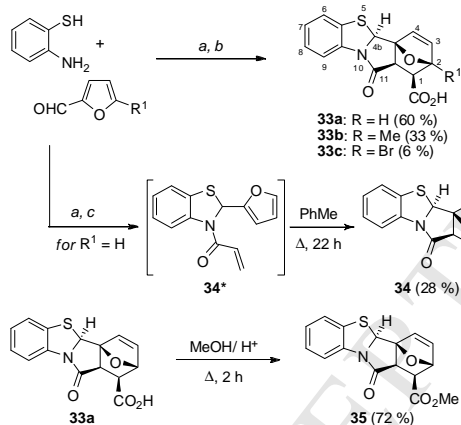
Scheme 11. One-pot synthesis of 8,10a-epoxy[1,3]thiazino[2,3-*a*]isoindole **32** and its 7-carboxy derivatives **31**

Tetrahedron

We would also like to note that a similar trend was observed for homologous compounds **31** and **32** (see Scheme 11), which could nominally be attributed to the **A** series (*trans* H-10b and H-6a), and whose H-10b proton is observed in the δ 5.04–5.26 ppm region.

3-Aminopropanethiol³⁰ reacted sequentially with furfural and anhydrides of α,β -unsaturated acids in a similar one-pot procedure (Scheme 11). No heating or use of dehydration agents were required for the formation of the intermediate 2-(furan-2-yl)-1,3-thiazinanes **30**. The latter can be introduced into the acylation/cycloaddition reaction with maleic anhydride or acryloyl chloride without isolation. In this case, the target [1,3]thiazino[2,3-*a*]isoindoles **31** and **32** were formed in moderate yields. According to the ¹H NMR data, the IMDAF reaction is diastereoselective. To our surprise, however, the configuration of H-10b in adducts **31**, **32** was found to be the opposite to that of H-9b in their five-membered analogues **24**, **25** (Scheme 9). No interaction between protons H-6a/H-10b was observed in the 2D ¹H NOESY NMR spectra of adducts **31a**, **32**, but in the same time cross-peaks H-2(*ax*)/H-10b(*ax*) and H-4(*ax*)/H-10b(*ax*) are present.

The behavior of 2-aminobenzenethiol in the studied transformations was similar to that of its aliphatic analogues, 2-aminoethanethiols. A one-pot synthesis of isoindo[1,2-*b*][1,3]benzothiazoles **33**, **34** is presented in Scheme 12. In the case of 5-bromofurfural, the reaction led to resinification: the adduct **33c** was isolated only in 6 % yield. This may be caused by a competitive nucleophilic substitution of the bromine atom in 5-bromofurfural by sulfur in the first step, followed by polymerization of the intermediate compounds.



Reagents and conditions: (a) MgSO₄/CH₂Cl₂, rt, 3 h; (b) maleic anhydride/Me₂CO, 25 °C, 12 h; (c) CH₂=CH-COCl/NEt₃/PhMe, Δ , 4 h.

Scheme 12. Synthesis of 11-oxo-2,4a-epoxyisoindo[1,2-*b*][1,3]benzothiazoles **33–35**

We were able to detect and isolate the intermediate *N*-acryloyl 2-furyl-1,3-benzothiazole **34*** in the course of the synthesis of isoindo[1,2-*b*][1,3]benzothiazole **34**: after 4 h heating under reflux in toluene, a mixture of compounds **34*** (15%) and **34** (20%) was isolated and separated by column chromatography. Longer reflux duration (22 h) allowed increasing the yield of **34** to 28 %.

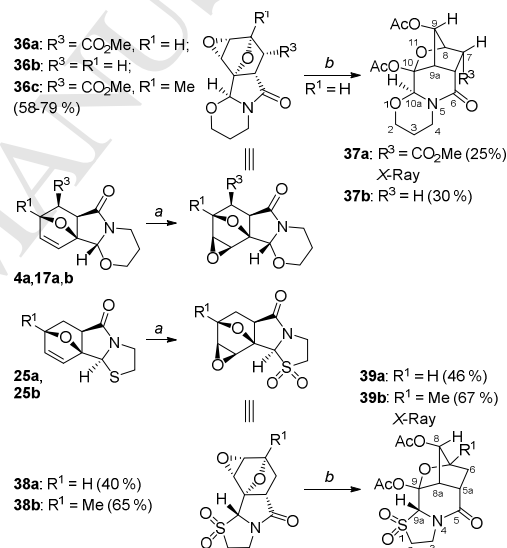
Esterification of acid **33a** by methanol gave the corresponding ester **35** (Scheme 12). No isomerization similar to **26A** \rightleftharpoons **26B** (see Scheme 9) was observed for **35**. Similar to the congeneric compounds **24**, **25** (Scheme 9) and based on the 2D ¹H NOESY NMR spectrum of the most soluble tetracyclic compound **35**, we attributed a *trans*-orientation of the H-4b proton relative to the

2,4a-epoxy bridge (interaction H-4b/H-11a was observed) in isoindo[1,2-*b*][1,3]benzothiazoles **33–35**.

The singlet peak of the H-4b proton in benzothiazoles **33–35** was observed in a significantly lower field (δ 6.52–6.99 ppm) compared to the analogous **24–26** (Scheme 9) and **31–32** (Scheme 11) compounds.

2.3. Wagner–Meerwein rearrangements of fused diepoxyisoindoles

Only some of the possible routes of modification of epoxy[1,3]oxazino[2,3-*a*]isoindole-7-carboxylic acids **3** showing their synthetic potential are presented in Scheme 6. Here we present another unusual transformation of the studied compounds. 7-Oxabicyclo[2.2.1]heptenes, 3,8-dioxatricyclo[3.2.1.0^{2,4}]octanes and their annelated derivatives are known to undergo sigmatropic rearrangements when treated with electrophilic agents, leading to significant and often unpredictable alterations in their carbon skeleton.^{10e,18b,18d,31–33} In order to investigate the possibility of the Wagner–Meerwein type³¹ rearrangements, we selected the tetracycles **4a**, **17** and **25a,b** with different positions of the nodal hydrogen atom, H-10b and H-9b, respectively (Scheme 13).



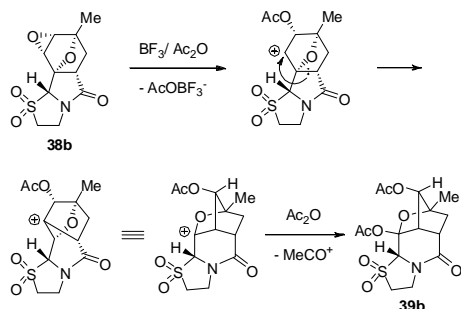
Reagents and conditions: (a) H₂O₂/HCO₂H/CH₂Cl₂, rt, 16 h or *m*-CPBA/CHCl₃, rt, 4–14 h; (b) BF₃·OEt₂/Ac₂O, 0 → 25 °C, 1–2 h.

Scheme 13. Wagner–Meerwein rearrangement of diepoxides **36** and **38**

Starting diepoxides **36**, **38** are readily available by the Prilezhaev reaction³¹ of the oxabicyclo[2.2.1]heptene fragment of isoindoles **4a**, **17a,b**, **25a,b** (both *m*-CPBA and HCO₂H can be used). When sulfur-containing compounds **25a,b** underwent this reaction, oxidation of the S(II) atom to sulfone took place, in addition to the oxidation of the double bond to the oxirane ring.^{34,35}

The cation-assisted skeletal rearrangements of hydrogenated 6,8a;7,8-diepoxyisoquinolines and 3a,6;4,5-isoindoles can occur in the presence of various electrophilic agents (I₂/AgOAc, NBS/H₂O/DMSO, LA/Ac₂O),³⁵ but likely the best and the most predictable results are achieved when Ac₂O/BF₃·OEt₂ system is utilized. This reagent allowed to obtain the unusual target 4,6-epoxycyclopenta[*c*]pyridines (similar to **37**, **39**) in mild conditions with satisfactory yields and no by-products formation.

A plausible mechanism of catalytic action of $\text{BF}_3 \cdot \text{OEt}_2$ is presented in Scheme 14 for the transformation of diepoxide **38b** to 7,9-epoxycyclopenta[*d*][1,3]thiazolo[3,2-*a*]pyridine **39b**. Interestingly, the 1,3-thiazolidine and 1,3-thiazinane fragments were preserved in the presented reaction conditions.



Scheme 14. Plausible mechanism of the Wagner–Meerwein rearrangement of the diepoxisoindole **38b**

The NMR spectra of diacetates **37**, **39** are rather complicated. In particular, it was difficult to establish the configurations of C-10a (for **37a,b**) and C-9a (for **39a,b**). X-ray analysis was performed for **37a** and **39b** in order to determine the spatial structure of the rearrangement products. In addition to the structures of compounds **37**, **39**, the X-ray data allowed us to unequivocally establish the structures of diepoxides **36**, **38**, and the starting isoindolones **4**, **17**, **25**. A detailed X-ray description of structures **17a**, **37a** and **39b** is given in the Supporting Information, here we only point out that the single crystals of **37a** and **39b** are racemic, while the crystal of **17a** is chiral. Evidently, this substance crystallizes as a conglomerate and is capable of spontaneous enantiomeric separation by the Pasteur method. Nevertheless, it is impossible to determine unambiguously the absolute configuration of the asymmetric centers in the single crystal of **17a** due to the absence of heavy atoms with $Z > 14$ (Si) in its structure.

2.4. Epoxyisoindoles fused with imidazoles and pyrimidines

In this part of our work we investigated the possibility of introducing 1,2- and 1,3-*N,N*-binucleophiles into the reaction and extension of the described protocol to the synthesis of isoindolones, condensed with imidazolidine and hexahydropyrimidine rings (Figure 4).

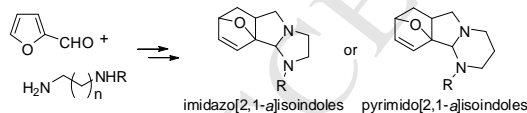
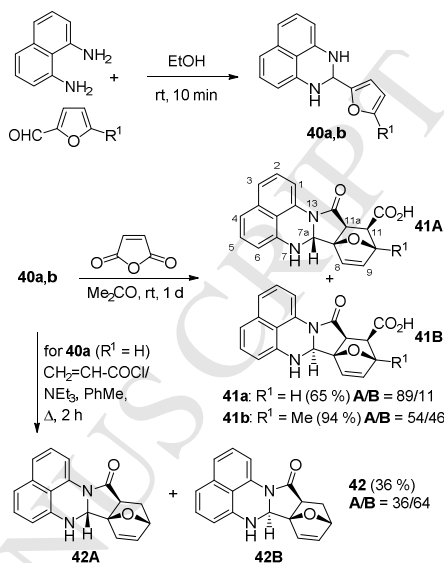


Figure 4. Extension of the method to the synthesis of isoindoles annulated with azaheterocycles.

It is well known, that 1,3-*N,N*-binucleophiles with a constrained “*cis*”-conformation of the amino groups readily (and often in quantitative yields) undergo condensation with aromatic aldehydes. Among such nucleophiles (2-aminobenzyl)amine and 1,8-diaminonaphthalene are the most readily available and we selected them for further study.

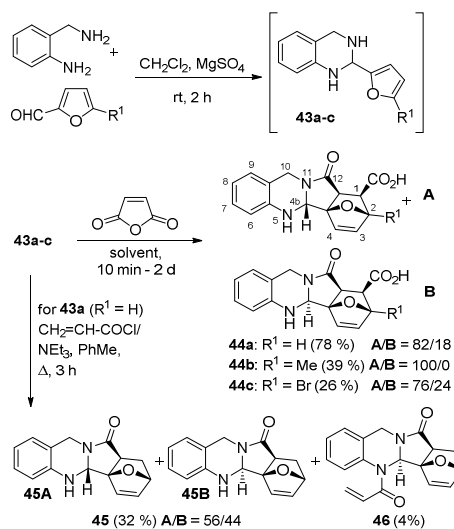
It was shown earlier,³⁶ that when dissolved in ethanol at room temperature, 1,8-diaminonaphthalene and furfural (or 5-methylfurfural) lead to 2-(2-furyl)-2,3-dihydro-1*H*-perimidines (**40**). The target products **40** exist entirely in the ring form.³⁶ After solvent replacement, the standard acylation/cycloaddition

procedure was performed on the intermediate dihydro-2-furylperimidines and adducts **41**, **42** were obtained in moderate-to-high yields as mixtures of isomers **A** and **B** (Scheme 15). When toluene was used as the reaction solvent in the last step (10 min reflux) the yield of the mixture of products **41a** increased to 95%. However, the diastereoselectivity was lower in this case – the **41Aa/41Ba** ratio decreased from 89/11 to 54/46.



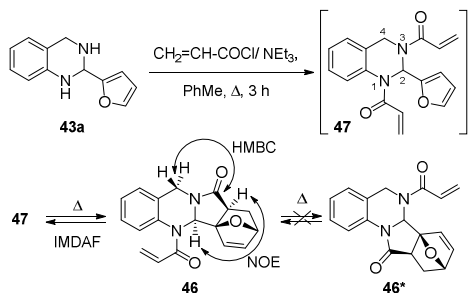
Scheme 15. Synthesis of 7b,10-epoxyisoindol[2,1-*a*]perimidines **41** and **42**

Spatial structures of the diastereoisomers **41A**, **41B** and **42A**, **42B** can easily be established by the 2D ^1H NOESY NMR spectra of their mixtures. The key *nOe* signals are interaction between protons H-7a/H-11a. In *minor* isomers **B** intensive cross-peaks were observed, whereas, in *major* isomers **A** these cross-peaks were hardly observable. *Major* isomers **41Aa** and **42B** were isolated as individual compounds by fractional recrystallization from *i*-PrOH/DMF mixture or by column chromatography, respectively.



Scheme 16. Synthesis of 2,4a-epoxyisoindol[1,2-*b*]quinazolines **44–46**

A similar approach towards isoindolo[1,2-*b*]quinazolinones (**44–46**) is presented in Scheme 16. The intermediate tetrahydroquinazolines **43** also exist only in the ring form and undergo chemoselective acylation by anhydrides of α,β -unsaturated acids predominantly at the more nucleophilic nitrogen atom (N-3). The yields and ratio of the isomers **44Aa/44Ba** depend strongly on the temperature. This was shown for reaction of quinazoline **43a** ($R^1=H$) with maleic anhydride: in dichloromethane or acetone at 25 °C the isomers **44Aa/44Ba** were formed in the 82/12 ratio (overall yields were 78 and 48%, respectively), whereas, when refluxed in toluene (10 min) a mixture with the **44Aa/44Ba** ratio of ~50/50 (33 %) was formed.



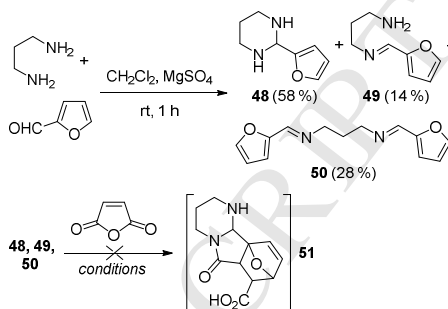
Scheme 17. Evidence of epoxyisoindolo[1,2-*b*]quinazoline structure (**46**)

In the case of acryloyl chloride, a side product of double acylation **46** was isolated in an insignificant yield. It was established from its NMR data that the N-3 acetyl fragment was involved in the Diels-Alder reaction (Scheme 17). When diamine **43a** was acylated, dialkyl derivative **47** was probably formed, which could theoretically exist in equilibrium with adducts **46** and **46***. The 2D 1H - ^{13}C HMBC NMR spectrum of isoindolo[1,2-*b*]quinazoline **46** displayed signals due to spin interaction H-10/C-12, which is impossible in the alternative product **46***. The structures of compounds **44** were established in a similar way. When isoindoloquinazolinone **45B** was treated with acryloyl chloride a product identical to amide **46** was formed.

Isomers of compounds **41**, **42**, **44**, **45** can also be attributed to either **A** or **B** series based only on the 1H NMR shift of the nodal

proton H-7a (H-4b) in their spectra: δ 5.01–4.24 ppm for **A** and δ 5.28–5.64 ppm for **B** series.

Aliphatic diamines undergo more complicated transformations. The presented condensation/acylation/IMDAF approach was tested for reaction of propanediamine, furfural and maleic anhydride. A multicomponent reaction mixture was obtained instead of the expected amino acid **51**. Therefore we performed a detailed study of the first step (condensation) products.



Scheme 18. Attempted synthesis of epoxypyrimido[2,1-*a*]isoindole **51**

We found out that condensation of propane-1,3-diamine with furfural leads to an equilibrium mixture of mainly three products (**48–50**). NMR of the mixture in $CDCl_3$ unequivocally established their structures and relative abundances. These results are in a good agreement with earlier work.³⁷ So far, we could not find the suitable conditions (solvents and temperature range we have tried are CH_2Cl_2 , Et_2O , PhMe and -70 °C - 110 °C) for a successful acylation of this mixture neither with maleic anhydride (Scheme 18) nor with acryloyl chloride. Viscous, dark brown multicomponent mixtures were formed in each case, which could not be separated into the components. Our preliminary attempts to perform the reaction with 1,4-diaminobutylene, ethane- and benzene-1,2-diamines were not successful either.

Table 1. Yields of the obtained isomeric mixtures of IMDAF adducts and the ratios of the isomers.

Compound	R ¹	R ²	R ³	R ⁴	R ⁵	X	n	A/B	Yield, % ^a
3a	H	CO ₂ H	H,H	H,H	H,H	O	1	94/6	60
3b	Me	CO ₂ H	H,H	H,H	H,H	O	1	95/5	58
3c	Br	CO ₂ H	H,H	H,H	H,H	O	1	83/17	42
3d	I	CO ₂ H	H,H	H,H	H,H	O	1	80/20	55
3e	NO ₂	CO ₂ H	H,H	H,H	H,H	O	1	89/11	35
3f	Ph	CO ₂ H	H,H	H,H	H,H	O	1	100/0	16
3g	<i>m</i> -C ₆ H ₄ NO ₂	CO ₂ H	H,H	H,H	H,H	O	1	91/9	46
3h	<i>o</i> -C ₆ H ₄ NO ₂	CO ₂ H	H,H	H,H	H,H	O	1	92/8	39
4a	H	H	H,H	H,H	H,H	O	1	100/0	18

4b	Me	H	H,H	H,H	H,H	O	1	100/0	19
4c	Br	H	H,H	H,H	H,H	O	1	64/36	21
13a	H	CO ₂ H	H,H	H,H	-	O	0	-	0
13b	H	CO ₂ H	Me,Me	H,H	-	O	0	-	0
13c	H	CO ₂ H	CH-CH=CH-CH	-	-	O	0	-	0
20a	H	CO ₂ H	CH-CH=CH-CH	H,H	-	O	1	96/4	27
20b	Me	CO ₂ H	CH-CH=CH-CH	H,H	-	O	1	57/43	23
20c	Br	CO ₂ H	CH-CH=CH-CH	H,H	-	O	1	93/7	17
22a	H	CO ₂ H	H,H	CH-CH=CH-CH	-	O	1	100/0	34
22b	Me	CO ₂ H	H,H	CH-CH=CH-CH	-	O	1	86/14	35
23	H	H	H,H	CH-CH=CH-CH	-	O	1	100/0	25
24a	H	CO ₂ H	H,H	H,H	-	S	0	15/85	49
24b	Me	CO ₂ H	H,H	H,H	-	S	0	67/33	48
25a	H	H	H,H	H,H	-	S	0	0/100	67
25b	Me	H	H,H	H,H	-	S	0	0/100	57
31a	H	CO ₂ H	H,H	H,H	H,H	S	1	100/0	48
31b	Me	CO ₂ H	H,H	H,H	H,H	S	1	100/0	46
32	H	H	H,H	H,H	H,H	S	1	100/0	26
33a	H	CO ₂ H	CH-CH=CH-CH	-	-	S	0	0/100	60
33b	Me	CO ₂ H	CH-CH=CH-CH	-	-	S	0	0/100	33
33c	Br	CO ₂ H	CH-CH=CH-CH	-	-	S	0	0/100	6
34	H	H	CH-CH=CH-CH	-	-	S	0	0/100	28
41a	H	CO ₂ H	CH-CH=CH-C-CH=CH-CH	-	-	NH	1	89/11	65
41b	Me	CO ₂ H	CH-CH=CH-C-CH=CH-CH	-	-	NH	1	54/46	94
42	H	H	CH-CH=CH-C-CH=CH-CH	-	-	NH	1	36/64	36
44a	H	CO ₂ H	CH-CH=CH-CH	H,H	-	NH	1	82/18	78
44b	Me	CO ₂ H	CH-CH=CH-CH	H,H	-	NH	1	100/0	39
44c	Br	CO ₂ H	CH-CH=CH-CH	H,H	-	NH	1	76/24	26
45	H	H	CH-CH=CH-CH	H,H	-	NH	1	56/44	32
51	H	CO ₂ H	H,H	H,H	H,H	NH	1	-	0
^b	H	CO ₂ H	H,H	H,H	H,H	NH	2	-	0
^c	H	CO ₂ H	CH-CH=CH-CH	-	-	NH	0	-	0
^d	H	CO ₂ H	CH-CH=CH-C-CH=CH-CH	-	-	S	1	-	0
^e	H	CO ₂ H	CH-CH=CH-C-CH=CH-CH	-	-	O	1	-	0

^aYields are given relative to the starting furfurals after two steps;

^bThe initial binucleophile is 1,4-diaminobutane;

^cThe initial binucleophile is 1,2-phenylenediamine;

^dThe initial binucleophile is 8-aminonaphthalene-1-thiol;

^eThe initial binucleophile is 8-aminonaphthalen-1-ol.

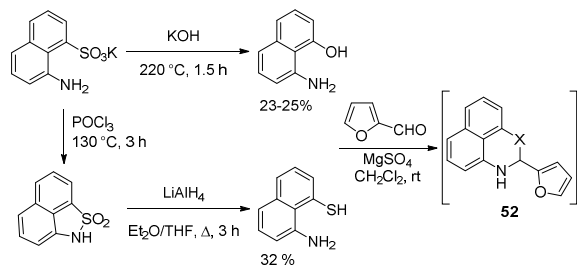
2.5. Attempted synthesis of naphtholo[1,3]oxazino- and naphtholo[1,3]thiazino[2,3-a]isoindoles

In order to show the synthetic potential of the method, in this work we used only two compounds as dienophiles: readily available maleic anhydride and acryloyl chloride. Given that in our previous works^{18a-d,31,38} we showed that a large range of dienophiles can be used in tandem acylation/IMDAF reaction (allyl halogenides, dihalogenomaleic, and citraconic anhydrides, as well as acryloyl, methacryloyl, crotonyl and cinnamoyl

chlorides and all were used as dienophiles), we believe that the two dienes are good representative reactants, demonstrating the advantages and limitations of the method. Similarly, we present only one example of aromatization of epoxyisoindole **3Aa** to isoindole **16** (Scheme 6), other examples of aromatization of 3,6a-isoindolones can be found in a recent publication.^{38c} It should be pointed out that aromatization of the 7-oxabicycloheptene fragment leads to elimination of all but one asymmetric centers in the molecules, thus, transforming

diastereomeric mixtures of adducts **A/B** to single aromatization products (**16**).

As stated above, not every system we tried worked out successfully (for example, furyl ketones do not provide oxazino- or oxazoloisoindoles in these conditions), and we should mention here another unsuccessful attempt of the fused epoxyisoindole synthesis. For generality, we tried to involve two rather complex aminonaphthalenes in the tandem reaction (Scheme 19).



Scheme 19. Attempts to involve 8-aminonaphthalene-1-thiol and 8-aminonaphthalen-1-ol in the IMDAF reaction

8-Aminonaphthalene-1-thiol³⁹ and 8-aminonaphthalen-1-ol⁴⁰ react fairly readily with furfural at room temperature (according to TLC, the initial compounds disappear completely and a new spot appears in 1 h). But probably due to instability of the solutions of both 8-aminonaphthalenes and compounds **52**, we could not isolate them (the mixture components were turned dark brown (for X = O) or violet (X = S) in an attempt of concentration). The one-pot approach - without isolation of the condensation products **52** - failed as well: no solid products were observed in the reaction of **52** with maleic anhydride at 24 °C in acetone. But nevertheless, we believe that the proposed methodology may be extended to a wide range of *N,X*-binucleophiles. For instance, our preliminary attempts to utilize it for the reaction anthranilamide and methyl cysteine were successful and will be presented in a follow-up publication.

3. Conclusions

In summary, in this work we propose a general strategy for construction of epoxyisoindoles annelated with saturated 5- and 6-membered heterocycles. We have tested our approach on many available *N,X*-binucleophiles and showed that 1,3-aminoalcohols, 1,2- and 1,3-aminothiols, their benzoannulated analogues and some 1,3-diamines react with furfural and α,β -unsaturated acid anhydrides in a one-pot tandem reaction sequence leading to isoindolones condensed with oxazolidine, oxazinane, thiazolidine, thiazinane, pyrimidine and perimidine fragments, respectively. Some attractive transformations of the epoxyisoindoles were also demonstrated, including a one-step approach to condensed isoindolones and skeletal rearrangements of the oxabicyclo[2.2.1]heptenes fragment.

The proposed approach compares favorably with literature methods owing to the availability of starting reagents and simplicity of the experiment, allowing to obtain attractive polyfunctional building blocks with isoindole scaffolds, containing a large set of functional groups: carboxyl, amide, *N,O*-, *N,S*-acetal fragments, multiple bonds and epoxy bridges.

4. Experimental Section

5. Experimental Section

All commercially available reagents and solvents were used without further purification. Melting points were determined with

SMP30 apparatus within 0.5 °C accuracy and are uncorrected. IR spectra were obtained in KBr pellets for solids or in thin films for oils using an IR-Fourier spectrometer. NMR spectra were recorded on NMR spectrometers with working frequency 400 or 600 MHz for ¹H and 100.6 or 150.9 MHz for ¹³C, for 2–5% solutions in CDCl₃, DMSO-*d*₆, D₂O (for compounds **3b–d**, **15b**) or C₆D₆ (for **37a**) at ~ 27 °C. Traces of chloroform (¹H NMR δ 7.26 ppm and ¹³C NMR δ 77.16 ppm) or DMSO-*d*₅H (¹H NMR δ 2.49 ppm and ¹³C NMR δ 39.43 ppm) were used as the internal standards. Assignments of ¹H and ¹³C signals were made with the aid of 2D COSY, TOCSY, NOESY, HSQC and HMBC NMR spectra where necessary. Mass spectra were taken either on a chromatography-mass (electron ionization, 70 eV, ion source temperature 200 °C, gas chromatographic inlet with a 5ms column) or a mass (electron ionization, 70 eV, ion source temperature 200 °C, direct inlet probe) spectrometer. High-resolution mass spectra (HRMS) were taken on a mass-spectrometer using direct analysis in real time (DART) ionization method (helium was used as DART gas, gas flow rate was 1 L/min, flow T 300 °C, discharge electrode was set to +4000 V, the mass scale was calibrated using PEG 600) or using a MALDI-TOF mass spectrometer, operated in positive reflectron mode (2,5-dihydroxybenzoic acid was used as matrix). These methods were used when no molecular ions were observed in the electron ionization mass spectra. The purity of the substances obtained and the composition of the reaction mixtures were monitored by TLC (SiO₂ plates) or, when possible, by GCMS. The purification of the final products was carried out by column chromatography on Al₂O₃ (activated, neutral, 50–200 mesh) or SiO₂ (40–100 mesh) or by fractional crystallization. Microanalyses were performed for C, H, N on a C,H,N,O,S-analyzer and were within $\pm 0.4\%$ of theoretical values. The detailed X-ray description of structures **17a**, **37a**, **39a** is given in the Supporting Information.

Multiscale synthesis of starting 5-arylfurfurals

5-Arylfurfurals (**f–h**) required for the synthesis of **1** (**2**) were obtained by the following procedures. Literature methods^{41,42} turned out to be either difficult to scale to multi-gram quantities^{41b,41d,42a–f} or hardly reproducible.^{41c,41g,42c,42i}

5-(2-Nitrophenyl)furan-2-carbaldehyde (h) and **5-(3-nitrophenyl)furan-2-carbaldehyde (g)**. **General experimental procedure.** A mixture of nitroaniline (28.0 g, 0.20 mol), water (80 mL) and concentrated hydrochloric acid (45 mL) was cooled (–5 °C) and a solution of NaNO₂ (14.8 g, 0.20 mol) in water (50 mL) was added dropwise to the stirred mixture keeping the temperature below +5 °C. After the addition of NaNO₂ was complete, a solution of furfural (24.8 mL, 0.30 mol) in Me₂CO (100 mL) was quickly added to the mixture. Powdered Cu₂Cl₂ was added in small portions at 20–30 °C until nitrogen evolution had ceased (in general it took 15–25 min for the reaction to complete and required 3–5 g of the catalyst). The mixture was stirred at room temperature for 10 min and cold water (400 mL) was then added. The mixture was kept overnight at +4 °C and on the next day the greenish water layer was decanted from the semi-crystalline precipitate. The precipitate was then washed with water (2 \times 200 mL) and suspended in Et₂O (100 mL). The crystals formed were separated by filtration, washed with water (2 \times 100 mL) and Et₂O (2 \times 30 mL). The crude products were further purified if necessary by recrystallization from *i*-PrOH/DMF mixtures affording 5.2–15.5 g of 5-arylfuran-2-carbaldehydes **h**, **g** as yellow crystals (12–35 % yield), m.p. 95–96 °C (**h**), 155–156 °C (**g**).

5-Phenylfuran-2-carbaldehyde (f). A solution of aniline (45.5 mL, 0.50 mol) in a mixture of concentrated HCl (100 mL) and water (100 mL) was diazotized with a solution of NaNO₂ (34.5 g, 0.50 mol) in water (100 mL) at 0 °C. A solution of furfural (41.4 mL, 0.50 mol) in Me₂CO (150 mL) was then added. The reaction mixture was brought to 20 °C and then a mixture consisting of 10 mol % CuCl₂·H₂O (7.60 g, 0.05 mol) and 10 mol % Cu₂Cl₂ (9.90 g, 0.05 mol) was added in small portions with intensive stirring during an ~ 1 h period and keeping the temperature within 25–35 °C (in general, no cooling was required). The mixture was stirred for another ~ 2 h until nitrogen evolution had ceased. Na₂CO₃ was added until the solution turned basic and the mixture was extracted with diethyl ether (1 × 100 and 1 × 180 mL). The combined organic layers were washed with a saturated NaHCO₃ solution (2 × 150 mL), dried (MgSO₄), filtered and the solvent was removed in *vacuo* and dark-yellow oil (b.p. 120–160/7 mm Hg, 20–25 g) was initially collected, then redistilled yielding 5-phenylfuran-2-carbaldehyde (**f**) (14.2–18.8 g, 16–21 % yield) as a yellow liquid (b.p. 147–153 °C/7 mm Hg or 130–134 °C/1 mm Hg).

Physical and spectroscopic data for 5-arylfurfurals **f–h** match the literature data.^{41,42}

General procedure for preparation of tautomeric mixtures of imines (1a–h) and 2-furyl-1,3-oxazinanes (2a–h) and their adducts with maleic anhydride (3a–h).

Anhydrous powdered MgSO₄ (12.1 g, 0.10 mol) was added to a solution of 3-amino-1-propanol (7.80 mL, 0.10 mol) and corresponding furaldehyde (0.10 mol) in CH₂Cl₂ (70 mL). The mixture was stirred at room temperature for 4–24 h (in case of 5-nitrofurfural the mixture was stirred at 0 °C for 10 min). MgSO₄ was filtered off and washed with CH₂Cl₂ (40 mL). The organic phases were combined and used in the next step or concentrated under reduced pressure to give a mixture of tautomers **1a–h/2a–h** as yellow or reddish yellow oils. The tautomers **1a–h/2a–h** (or their solutions in CH₂Cl₂) were used for the next step without further purification, assuming quantitative yield. Tautomeric equilibrium of the condensation products **1a** (**2a**) and **1f** (**2f**) was investigated by NMR.

Mixture of tautomers **1a/2a** in ratio ~ 77/23, yellow viscous oil; ν_{\max} (liquid film) 3390, 2939, 2857, 1647 cm⁻¹; GC-MS (EI, 70 eV) m/z 153 (1, M⁺), 152 (2), 124 (2), 123 (11), 109 (100), 108 (52), 96 (12), 95 (32), 94 (39), 93 (6), 81 (62), 80 (30), 67 (10), 53 (20), 51 (14), 41 (14), 39 (36%).

3-[(2-Furylmethylene)amino]propan-1-ol (1a). δ_{H} (400 MHz, CDCl₃) 8.07 (1 H, s, CH=N), 7.49 (1 H, dd, ³J_{5,4}: 1.8, ⁴J_{5,3}: 0.8 Hz, H-5'), 6.72 (1 H, br.d, ³J_{4,3}: 3.6 Hz, H-3'), 6.46 (1 H, dd, ³J_{4,3}: 3.6, ³J_{4,5}: 1.8 Hz, H-4'), 3.81 (2 H, t, ³J_{1,2}: 5.8 Hz, H-1), 3.72 (2 H, dt, ³J_{2,3}: 5.8, J : 1.2 Hz, H-3), 1.91–1.95 (2 H, m, H-2); δ_{C} (100.6 MHz, CDCl₃) 151.5 (C-2'), 150.0 (C=N), 144.9 (C-5'), 114.0 and 111.7 (C-3' and C-4'), 62.2 (C-1), 59.8 (C-3), 33.6 (C-2).

2-(Furan-2-yl)-1,3-oxazinane (2a). δ_{H} (400 MHz, CDCl₃) 7.35 (1 H, dd, ³J_{5,4}: 1.8, ⁴J_{5,3}: 0.8 Hz, H-5'), 6.33–6.30 (2 H, m, H-3' and H-4'), 5.21 (1 H, s, H-2), 4.18–4.22 (1 H, m, H-6^{eq}), 3.92 (1 H, dt, ²J_{6,6} ~ ³J_{6a,5a}: 11.9, ³J_{5e,6a}: 2.3 Hz, H-6^{ax}), 3.22–3.25 (1 H, m, H-4^{eq}), 3.06 (1 H, ddd, ²J_{4,4}: 15.6, ³J_{4a,5a}: 12.4, ³J_{4a,5a}: 3.7 Hz, H-4^{ax}), 1.85–1.88 (1 H, m, H-5^{ax}), 1.41–1.45 (1 H, m, H-5^{eq}); δ_{C} (100.6 MHz, CDCl₃) 148.1 (C-2'), 142.2 (C-5'), 112.7 and 110.2 (C-3' and C-4'), 83.8 (C-2), 67.9 (C-6), 44.1 (C-4), 27.1 (C-5).

Mixture of tautomers **1f/2f** in ratio ~ 86/14, yellow viscous oil.

3-[[5-Phenyl-2-furyl)methylene]amino]propan-1-ol (1f). δ_{H} (400 MHz, CDCl₃) 8.10 (1 H, s, CH=N), 7.75 (2 H, dd, ³J 7.8, ⁴J 1.3 Hz, H-Ph), 7.39 (2 H, dt, ³J 7.8, ⁴J 1.3 Hz, H-Ph), 7.30 (1 H,

br.t, ³J 7.8 Hz, H-Ph), 6.85 (1 H, d, ³J_{4,3}: 3.5 Hz, H-4'), 6.73 (1 H, d, ³J_{3,4}: 3.5 Hz, H-3'), 3.90 (2 H, t, ³J_{1,2}: 5.5 Hz, H-1), 3.80 (2 H, br.t, ³J_{2,3}: 5.5 Hz, H-3), 1.97 (2 H, p, ³J_{2,3} ~ ³J_{1,2}: 5.5 Hz, H-2); δ_{C} (100.6 MHz, CDCl₃) 156.3 (C-5'), 150.7 (C-2'), 150.1 (C=N), 128.6 (C-1'), 128.8 (C-3'' and C-5''), 128.5 (C-4''), 124.6 (C-2'' and C-6''), 116.4 (C-3'), 107.1 (C-4'), 61.9 (C-1), 59.8 (C-3), 33.5 (C-2).

2-(5-Phenyl-2-furyl)-1,3-oxazinane (2f). δ_{H} (400 MHz, CDCl₃) 7.67 (2 H, dd, ³J 7.7, ⁴J 1.2 Hz, H-Ph), 7.39–7.24 (3 H, m, H-Ph), 6.60 (1 H, d, ³J_{4,3}: 3.5 Hz, H-4'), 6.42 (1 H, d, ³J_{3,4}: 3.5 Hz, H-3'), 5.28 (1 H, s, H-2), 4.23–4.26 (1 H, m, H-6^{eq}), 3.96 (1 H, dt, ²J_{6,6} ~ ³J_{6a,5a}: 11.9, ³J_{5e,6a}: 2.3 Hz, H-6^{ax}), 3.29–3.32 (1 H, m, H-4^{eq}), 3.11 (1 H, br.dt, ²J_{4,4} ~ ³J_{4a,5a}: 12.4, ³J_{4a,5a}: 3.2 Hz, H-4^{ax}), 1.75–1.79 (1 H, m, H-5^{ax}), 1.45–1.48 (1 H, m, H-5^{eq}); δ_{C} (100.6 MHz, CDCl₃) 149.5 (C-2'), 144.7 (C-5'), 129.5 and 129.9 (C-1'' and C-4''), 127.5 (C-3'' and C-5''), 124.0 (C-2'' and C-6''), 108.7 (C-3'), 105.6 (C-4'), 83.8 (C-2), 67.9 (C-6), 44.1 (C-4), 27.0 (C-5).

Maleic anhydride (9.80 g, 0.10 mol) was added to a solution of the tautomeric mixture **1f/2f** (0.10 mol) in Me₂CO (100 mL) or CH₂Cl₂ (~ 100 mL). The mixture was stirred at 24 °C for 4–46 h. The precipitate formed was collected by filtration, washed with Me₂CO (2 × 30 mL) and Et₂O (2 × 30 mL) and dried in air until constant weight to give a diastereomeric pair of the title acids **3a–e.g.h** as white or slightly colored powders. Compound **3f** does not crystallize from the reaction mixture and thus was isolated by column chromatography on SiO₂. The yields were in general 5–7 % higher when the reactions were carried out in CH₂Cl₂. However, the products crystallized from Me₂CO were less tinted and did not require any purification after filtration and washing with Me₂CO. The yields of the mixtures of diastereomeric adducts **3** given below are for reactions in Me₂CO.

(6aRS,7SR,8RS,10aSR,10bRS)-6-Oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-*a*]isoindole-7-carboxylic acid (3Aa) and (6aRS,7SR,8RS,10aSR,10bSR)-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-*a*]isoindole-7-carboxylic acid (3Ba). Ratio of isomers **3Aa/3Ba** ~ 94/6, white powder (15.06 g, 60 %), m.p. 181–182 °C; [Found: C, 57.26; H, 5.34; N, 5.63. C₁₂H₁₃NO₅ requires C, 57.33; H, 5.22; N, 5.58%]; R_f (50% EtOH/DMF) 0.45; ν_{\max} (KBr) 3109, 3006, 2971, 1738, 1664, 1165, 1056, 917 cm⁻¹; δ_{H} (400 MHz, DMSO-*d*₆) (**3Aa**) 12.22 (1 H, br.s, CO₂H), 6.60 (1 H, d, ³J_{10,9}: 5.8 Hz, H-10), 6.46 (1 H, dd, ³J_{9,10}: 5.8, ³J_{9,8}: 1.7 Hz, H-9), 5.12 (1 H, s, H-10b), 5.08 (1 H, d, ³J_{8,9}: 1.7 Hz, H-8), 4.14–4.10 (1 H, m, ²J_{2,2}: 11.6, ³J_{2e,3a}: 4.6, ³J_{2e,3e} ~ ⁴J_{2e,4e}: 1.6 Hz, H-2^{eq}), 3.87–3.91 (1 H, m, H-4^{eq}), 3.86–3.91 (1 H, m, H-2^{ax}), 3.09 (1 H, ddd, ²J_{4,4}: 13.2, ³J_{4a,3a}: 12.3, ³J_{4a,3e}: 3.7 Hz, H-4^{ax}), 2.73 (1 H, dd, ³J_{6a,7}: 9.2, ⁵J_{6a,4}: 0.5 Hz, H-6a), 2.52 (1 H, d, ³J_{7,6a}: 9.2 Hz, H-7), 1.68–1.57 (1 H, m, H-3^{ax}), 1.53–1.47 (1 H, m, H-3^{eq}); (**3Ba**) 12.22 (1 H, br.s, CO₂H), 6.60 (1 H, d, ³J_{10,9}: 5.7 Hz, H-10), 6.44 (1 H, dd, ³J_{9,10}: 5.7, ³J_{9,8}: 1.7 Hz, H-9), 5.40 (1 H, s, H-10b), 5.01 (1 H, d, ³J_{8,9}: 1.7 Hz, H-8), 4.09–4.04 (1 H, m, H-2^{eq}), 3.88–3.84 (1 H, m, H-4^{eq}), 3.67 (1 H, dt, ²J_{2,2} ~ ³J_{2a,3a}: 11.6, ³J_{2a,3e}: 3.0 Hz, H-2^{ax}), 3.01–2.93 (1 H, m, H-4^{ax}), 2.76 (1 H, dd, ³J_{6a,7}: 9.2, ⁵J_{6a,4a}: 1.4 Hz, H-6a), 2.45 (1 H, d, ³J_{7,6a}: 9.2 Hz, H-7), 1.61–1.57 (2 H, m, H-3^{ax} and H-3^{eq}); δ_{C} (100.6 MHz, DMSO-*d*₆) (**3Aa**) 172.6 (s, CO₂H), 170.7 (s, C-6), 136.8 (d, J : 177.5 Hz, C-9), 133.8 (d, J : 179.5 Hz, C-10), 89.5 (s, C-10a), 85.1 (d, J : 165.0 Hz, C-10b), 82.3 (d, J : 169.0 Hz, C-8), 66.8 (t, J : 144.0 Hz, C-2), 49.3 (d, J : 137.5 Hz, C-6a), 44.0 (d, J : 139.0 Hz, C-7), 38.3 (t, J : 139.0 Hz, C-4), 25.1 (t, J : 129.5 Hz, C-3); (**3Ba**) 172.9 (s, CO₂H), 167.9 (s, C-6), 137.2 (d, J : 179.0 Hz, C-9), 134.6 (d, J : 179.0 Hz, C-10), 89.5 (s, C-10a), 82.8 (d, J : 160.0 Hz, C-

10b), 81.5 (d, J 169.0 Hz, C-8), 66.2 (t, J 144.5 Hz, C-2), 50.2 (d, J 138.5 Hz, C-6a), 44.4 (d, J 138.5 Hz, C-7), 37.4 (t, J 139.0 Hz, C-4), 23.4 (t, J 130.0 Hz, C-3); MS (EI, 70 eV) m/z 251 (2, M^+), 207 (22), 206 (20), 178 (13), 153 (10), 152 (100), 150 (11), 138 (18), 124 (26), 122 (18), 121 (27), 110 (11), 99 (20), 96 (19), 95 (57), 94 (18), 86 (69), 85 (13), 65 (15), 56 (18), 41 (12), 39 (19), 28 (12), 27 (11%).

Similar procedure carried out in CH_2Cl_2 (150 mL) leads to a diastereomeric mixture **3Aa/3Ba** in ratio of ~ 95/5 (44 % yield). When PhMe was used (150 mL, 10 min reflux), only the *major* isomer **3Aa** (m.p. 182 °C from an *i*-PrOH/DMF mixture) was obtained in 27 % yield.

(6aRS,7SR,8RS,10aSR,10bRS)-8-Methyl-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-*a*]isoindole-7-carboxylic acid (3Ab) and (6aRS,7SR,8RS,10aSR,10bSR)-8-methyl-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-*a*]isoindole-7-carboxylic acid (3Bb). Ratio of isomers **3Ab/3Bb** ~ 95/5, pale-yellow powder (15.3 g, 58 %), m.p. 148–155 °C (decomp.); [Found: C, 58.94; H, 5.77; N, 5.17. $\text{C}_{13}\text{H}_{15}\text{NO}_5$ requires C, 58.86; H, 5.70; N, 5.28%]; R_f (50% EtOH/DMF) 0.90; ν_{max} (KBr) 3083, 2985, 1741, 1661, 1450, 1170, 1075, 872 cm^{-1} ; δ_{H} (400 MHz, $\text{DMSO}-d_6$) (**3Ab**) 12.22 (1 H, br.s, CO_2H), 6.62 (1 H, br.d, $^3J_{9,10}$ 5.7 Hz, H-10), 6.30 (1 H, d, $^3J_{10,9}$ 5.7 Hz, H-9), 5.11 (1 H, s, H-10b), 4.11 (1 H, br.dd, $^2J_{2,2}$ 12.1, $^3J_{2e,3e}$ 4.0 Hz, H-2^{eq}), 3.92 (1 H, br.dd, $^2J_{4,4}$ 13.0, $^3J_{4e,3e}$ 5.0 Hz, H-4^{eq}), 3.88 (1 H, dt, $^2J_{2,2}$ ~ $^3J_{2a,3a}$ 12.1, $^3J_{2a,3e}$ 2.0 Hz, H-2^{ax}), 3.08 (1 H, br.dt, $^2J_{4,4}$ ~ $^3J_{4a,3a}$ 13.0, $^3J_{4a,3e}$ 4.1 Hz, H-4^{ax}), 2.76 (1 H, d, $^3J_{7,6a}$ 8.9 Hz, H-7), 2.55 (1 H, d, $^3J_{6a,7}$ 8.9 Hz, H-6a), 1.68–1.55 (1 H, m, H-3^{ax}), 1.51 (3 H, s, Me-8), 1.50–1.45 (1 H, m, H-3^{eq}); (**3Bb**) 12.22 (1 H, br.s, CO_2H), 6.62 (1 H, br.d, $^3J_{9,10}$ 5.7 Hz, H-10), 6.25 (1 H, d, $^3J_{10,9}$ 5.7 Hz, H-9), 5.32 (1 H, s, H-10b), 4.07 (1 H, br.dd, $^2J_{2,2}$ 12.1, $^3J_{2e,3e}$ 3.8 Hz, H-2^{eq}), 3.94–3.88 (1 H, m, H-4^{eq}), 3.66 (1 H, dt, $^2J_{2,2}$ ~ $^3J_{2a,3a}$ 12.1, $^3J_{2a,3e}$ 2.5 Hz, H-2^{ax}), 2.95 (1 H, br.dt, $^2J_{4,4}$ ~ $^3J_{4a,3a}$ 12.5, $^3J_{4a,3e}$ 4.5 Hz, H-4^{ax}), 2.74 (1 H, d, $^3J_{7,6a}$ 8.9 Hz, H-7), 2.47 (1 H, d, $^3J_{6a,7}$ 8.9 Hz, H-6a), 1.68–1.55 (1 H, m, H-3^{ax}), 1.52 (3 H, s, Me-8), 1.50–1.45 (1 H, m, H-3^{eq}); δ_{C} (100.6 MHz, $\text{D}_2\text{O}/\text{NaOD}$ (5 mol %)) (**3Ab**) 175.2 (CO_2H), 173.0 (C-6), 138.3 (C-9), 131.4 (C-10), 88.7 and 86.9 (C-10a and C-8), 84.4 (C-10b), 65.7 (C-2), 50.9 (C-7), 48.0 (C-6a), 36.9 (C-4), 22.7 (C-3), 13.4 (Me-8); δ_{C} (100.6 MHz, $\text{DMSO}-d_6$) (**3Ab**) 171.4 (CO_2H), 170.8 (C-6), 139.6 (C-9), 134.5 (C-10), 89.6 (C-8), 89.0 (C-10a), 85.2 (C-10b), 66.7 (C-2), 52.4 (C-7), 47.4 (C-6a), 38.1 (C-4), 25.0 (C-3), 15.6 (Me-8); (**3Bb**) 171.5 (CO_2H), 170.8 (C-6), 139.9 (C-9), 135.7 (C-10), 88.79 (C-8), 88.76 (C-10a), 83.1 (C-10b), 66.2 (C-2), 53.5 (C-7), 47.6 (C-6a), 37.5 (C-4), 23.3 (C-3), 15.6 (Me-8); MS (EI, 70 eV) m/z 265 (3, M^+), 221 (18), 220 (10), 219 (11), 204 (10), 167 (11), 166 (94), 152 (31), 138 (14), 137 (13), 136 (15), 135 (33), 123 (23), 122 (18), 111 (15), 110 (38), 109 (100), 108 (17), 99 (15), 95 (21), 86 (91), 79 (11), 58 (10), 56 (16), 55 (13), 54 (15), 53 (17), 43 (24), 41 (11), 28 (19), 27 (17), 26 (16%).

(6aRS,7RS,8SR,10aSR,10bRS)-8-Bromo-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-*a*]isoindole-7-carboxylic acid (3Ac) and (6aRS,7RS,8SR,10aSR,10bSR)-8-bromo-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-*a*]isoindole-7-carboxylic acid (3Bc). Ratio of isomers **3Ac/3Bc** ~ 83/17, (13.86 g, 42 %), yellow powder, m.p. 205–208 °C; [Found: C, 43.59; H, 3.55; N, 4.16; Br, 24.20%]; R_f (50% EtOH/DMF) 0.73; ν_{max} (KBr) 3136, 1751, 1670, 1449, 1162, 1056 cm^{-1} ; δ_{H} (600 MHz, $\text{DMSO}-d_6$) (**3Ac**) 12.60 (1 H, br.s, CO_2H), 6.73 and 6.55 (1 H and 1 H, two d, $^3J_{9,10}$ 5.5 Hz, H-9 and H-10), 5.18 (1 H, s, H-10b), 4.07 (1 H, br.dd,

$^2J_{2,2}$ 11.7, $^3J_{2e,3a}$ 4.1 Hz, H-2^{eq}), 3.90–3.86 (2 H, m, H-4^{eq} and H-2^{ax}), 3.09 (1 H, dt, $^2J_{4,4}$ ~ $^3J_{4a,3a}$ 12.4, $^3J_{4a,3e}$ 3.4 Hz, H-4^{ax}), 2.98 and 2.96 (1 H and 1 H, two d, $^3J_{6a,7}$ 8.9 Hz, H-7 and H-6a), 1.62–1.55 (1 H, m, H-3^{ax}), 1.46–1.48 (1 H, m, H-3^{eq}); (**3Bc**) 12.60 (1 H, br.s, CO_2H), 6.76 and 6.48 (1 H and 1 H, two d, $^3J_{9,10}$ 5.5 Hz, H-9 and H-10), 5.37 (1 H, s, H-10b), 4.07 (1 H, br.dd, $^2J_{2,2}$ 11.7, $^3J_{2e,3a}$ 4.1 Hz, H-2^{eq}), 3.85–3.82 (2 H, m, H-4^{eq} and H-2^{ax}), 3.66 (1 H, dt, $^2J_{4,4}$ ~ $^3J_{4a,3a}$ 11.7, $^3J_{4a,3e}$ 2.0 Hz, H-4^{ax}), 2.98 and 2.96 (1 H and 1 H, two d, $^3J_{6a,7}$ 8.9 Hz, H-7 and H-6a), 1.62–1.55 (1 H, m, H-3^{ax}), 1.55–1.51 (1 H, m, H-3^{eq}); δ_{C} (100.6 MHz, $\text{DMSO}-d_6$) (**3Ac**) 170.2 and 170.1 (CO_2H and C-6), 140.7 (C-9), 136.1 (C-10), 91.3 and 88.6 (C-10a and C-8), 84.8 (C-10b), 67.4 (C-2), 52.3 (br.s, C-7), 51.3 (C-6a), 38.8 (C-4), 25.5 (C-3); (**3Bc**) 170.13 and 170.07 (CO_2H and C-6), 140.8 (C-9), 137.5 (C-10), 91.4 and 88.1 (C-10a and C-8), 83.2 (C-10b), 67.0 (C-2), 53.4 (C-6a), 51.4 (br.s, C-7), 38.2 (C-4), 23.9 (C-3); δ_{C} (100.6 MHz, $\text{D}_2\text{O}/\text{NaOD}$ (5 mol %)) (**3Ac**) 173.1 and 171.6 (CO_2H and C-6), 138.6 (C-10), 132.4 (C-9), 86.2 and 81.2 (C-10a and C-8), 83.7 (C-10b), 66.0 (C-2), 51.4 (br.s, C-7), 51.1 (C-6a), 37.0 (C-4), 22.7 (C-3); MS (EI, 70 eV) m/z 331 (1, M^+ , for Br^{81}), 329 (1), 303 (3), 301 (5), 286 (7), 285 (7), 284 (7), 250 (10), 232 (25), 230 (25), 201 (11), 199 (11), 175 (13), 173 (11), 137 (18), 99 (12), 86 (100), 85 (18), 65 (15), 56 (24), 41 (18), 39 (19%).

(6aRS,7RS,8SR,10aSR,10bRS)-8-Iodo-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-*a*]isoindole-7-carboxylic acid (3Ad) and (6aRS,7RS,8SR,10aSR,10bSR)-8-iodo-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-*a*]isoindole-7-carboxylic acid (3Bd). Ratio of isomers **3Ad/3Bd** ~ 80/20, pale brown powder (20.75 g, 55 %), m.p. 178–182 °C (decomp.); [Found: C, 38.39; H, 3.29; N, 3.60. $\text{C}_{12}\text{H}_{12}\text{INO}_5$ requires C, 38.22; H, 3.21; N, 3.71%]; R_f (50% EtOH/DMF) 0.72; ν_{max} (KBr) 3153, 1747, 1678 cm^{-1} ; δ_{H} (400 MHz, $\text{DMSO}-d_6$) (**3Ad**) 12.54 (1 H, br.s, CO_2H), 6.62 and 6.57 (1 H and 1 H, two br.d, $^3J_{9,10}$ 5.7 Hz, H-9 and H-10), 5.18 (1 H, s, H-10b), 4.12 (1 H, br.dd, $^2J_{2,2}$ 11.4, $^3J_{3a,2e}$ 4.4 Hz, H-2^{eq}), 3.94–3.88 (2 H, m, H-2^{ax} and H-4^{eq}), 3.11 (1 H, br.dt, $^2J_{4,4}$ ~ $^3J_{4a,3a}$ 12.7, $^3J_{4a,3e}$ 3.8 Hz, H-4^{ax}), 2.91 (2 H, s, H-7 and H-6a), 1.68–1.58 (1 H, m, H-3^{ax}), 1.53–1.47 (1 H, m, H-3^{eq}); (**3Bd**) 12.54 (1 H, br.s, CO_2H), 6.77 and 6.58 (1 H and 1 H, two br.d, $^3J_{9,10}$ 5.7 Hz, H-9 and H-10), 5.21 (1 H, s, H-10b), 4.12 (1 H, br.dd, $^2J_{2,2}$ 11.4, $^3J_{3a,2e}$ 4.4 Hz, H-2^{eq}), 3.94–3.88 (2 H, m, H-2^{ax} and H-4^{eq}), 3.11 (1 H, br.dt, $^2J_{4,4}$ ~ $^3J_{4a,3a}$ 12.7, $^3J_{4a,3e}$ 3.8 Hz, H-4^{ax}), 3.02 and 3.00 (1 H and 1 H, two d, H-7 and H-6a), 1.68–1.58 (1 H, m, H-3^{ax}), 1.53–1.47 (1 H, m, H-3^{eq}); δ_{C} (100.6 MHz, $\text{DMSO}-d_6$) (**3Ad**) 170.3 and 169.7 (CO_2H and C-6), 143.3 (C-10), 134.7 (C-9), 88.9 (C-10a), 84.0 (C-10b), 66.8 (C-2), 65.5 (C-8), 52.5 (C-6a), 50.9 (C-7), 38.2 (C-4), 24.9 (C-3); (**3Bd**) 169.7 and 169.4 (CO_2H and C-6), 140.1 (C-10), 135.5 (C-9), 90.7 (C-10a), 84.2 (C-10b), 66.8 (C-2), 65.5 (C-8), 51.7 (C-6a), 50.7 (C-7), 38.2 (C-4), 24.9 (C-3); δ_{C} (100.6 MHz, $\text{D}_2\text{O}/\text{NaOD}$ (5 mol %)) (**3Ad**) 173.9 and 171.7 (CO_2H and C-6), 141.9 (C-10), 131.6 (C-9), 87.0 and 80.8 (C-10a and C-8), 83.4 (C-10b), 66.0 (C-2), 53.5 (br.s, C-7), 53.3 (C-6a), 37.0 (C-4), 22.7 (C-3); MS (EI, 70 eV) m/z 377 (1, M^+), 332 (12), 278 (100), 253 (11), 250 (34), 249 (47), 235 (65), 222 (50), 221 (68), 207 (21), 206 (31), 194 (17), 180 (28), 179 (42), 178 (62), 151 (29), 149 (36), 138 (24), 137 (47), 128 (46), 123 (49), 107 (59), 99 (50), 86 (77), 79 (38), 68 (32), 66 (35), 59 (54), 56 (79), 45 (19), 44 (28), 43 (35), 42 (37%).

(6aRS,7SR,8RS,10aSR,10bRS)-8-Nitro-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-*a*]isoindole-7-carboxylic acid (3Ae) and (6aRS,7SR,8RS,10aSR,10bSR)-8-nitro-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-*a*]isoindole-7-

carboxylic acid (3Be). The reaction was carried out following the general procedure above, but the condensation step was performed at $-5 - 0$ °C, 10 min. Ratio of isomers **3Ae/3Be** ~ 89/11, maize yellow powder (10.36 g, 35 %), m.p. > 229 °C (decomp.); [Found: C, 48.29; H, 4.30; N, 9.61. $C_{12}H_{12}N_2O_7$ requires C, 48.65; H, 4.08; N, 9.46%]; R_f (35% EtOAc/hexane) 0.35; ν_{max} (KBr) 3149, 1745, 1695, 1579, 1433, 1390 cm^{-1} ; δ_H (600 MHz, DMSO- d_6) (**3Ae**) 13.02 (1 H, s, CO₂H), 7.00 and 6.89 (1 H and 1H, two d, $^3J_{9,10}$ 5.5 Hz, H-9 and H-10), 5.32 (1 H, s, H-10b), 4.11 (1 H, br.dd, $^2J_{2,2}$ 12.2, $^3J_{2e,3a}$ 4.8 Hz, H-2^{eq}), 3.91 (1 H, br.dt, $^2J_{2,2}$ ~ $^3J_{2a,3a}$ 12.2, $^3J_{2a,3e}$ 2.1 Hz, H-2^{ax}), 3.88 (1 H, br.dd, $^2J_{4,4}$ 13.7, $^3J_{4e,3a}$ 5.5 Hz, H-4^{eq}), 3.34 and 3.24 (1 H and 1 H, two d, $^3J_{6a,7}$ 8.9 Hz, H-7 and H-6a), 3.14 (1 H, dt, $^2J_{4,4}$ ~ $^3J_{4a,3a}$ 13.7, $^3J_{4a,3e}$ 4.1 Hz, H-4^{ax}), 1.65–1.57 (1 H, m, H-3^{ax}), 1.51–1.49 (1 H, m, H-3^{eq}); (**3Be**) 13.02 (1 H, br.s, CO₂H), 7.03 and 6.81 (1 H and 1 H, two d, $^3J_{9,10}$ 5.5 Hz, H-9 and H-10), 5.47 (1 H, s, H-10b), 4.09 (1 H, br.dd, $^2J_{2,2}$ 11.7, $^3J_{2e,3a}$ 4.8 Hz, H-2^{eq}), 3.89–3.84 (2 H, m, H-4^{eq} and H-2^{ax}), 3.34 and 3.29 (1 H and 1 H, two d, $^3J_{6a,7}$ 8.9 Hz, H-7 and H-6a), 2.98 (1 H, dt, $^2J_{4,4}$ ~ $^3J_{4a,3a}$ 13.7, $^3J_{4a,3e}$ 4.1 Hz, H-4^{ax}), 1.65–1.57 (1 H, m, H-3^{ax}), 1.51–1.49 (1 H, m, H-3^{eq}); δ_C (150.9 MHz, DMSO- d_6) (**3Ae**) 169.6 and 169.2 (CO₂H and C-6), 137.1 and 135.8 (C-10 and C-9), 113.1 (C-8), 87.8 (C-10a), 84.4 (C-10b), 67.4 (C-2), 50.9 and 47.5 (C-6a and C-7), 38.8 (C-4), 25.5 (C-3); (**3Be**) 169.7 (CO₂H), 166.6 (C-6), 138.3 and 136.1 (C-10 and C-9), 113.0 (C-8), 88.3 (C-10a), 82.7 (C-10b), 66.8 (C-2), 51.9 and 48.0 (C-6a and C-7), 37.9 (C-4), 23.7 (C-3); MS (EI, 70 eV) m/z 296 (14, M⁺), 286 (4), 270 (3), 268 (5), 259 (3), 257 (6), 254 (9), 250 (68), 233 (16), 221 (15), 220 (24), 205 (22), 204 (38), 197 (78), 181 (25), 177 (33), 176 (56), 169 (38), 164 (10), 153 (11), 149 (17), 138 (41), 130 (15), 123 (26), 121 (41), 111 (20), 110 (38), 101 (16), 99 (100), 95 (56), 85 (57), 84 (67), 83 (70), 78 (55), 65 (69), 63 (74), 59 (25), 57 (50), 56 (80), 45 (30), 43 (35%).

The individual isomer **3Ae** was isolated by crystallization from Me₂CO/EtOH as a fine-crystalline yellow powder, m.p. 230–231 °C (decomp.).

(6aRS,7SR,8RS,10aSR,10bRS)-6-Oxo-8-phenyl-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-a]isoindole-7(10bH)-carboxylic acid (3Af). Acids **3f** (R Ph) could not be obtained by the general procedure due to their low crystallization propensity (after the reaction with maleic anhydride a brown oil soluble in Me₂CO or CH₂Cl₂ is formed). In this case, the solvent was evaporated, and the residue was purified by column chromatography (Al₂O₃, 3 × 14 cm) using hexane/EtOAc (5/1 → 1/1) as eluent. Compound **3Af** was obtained in 16 % yield (5.23 g) as white needles, m.p. 124.8–127.1 °C (decomp., from EtOAc/EtOH); [Found: C, 66.19; H, 5.14; N, 4.40. $C_{18}H_{17}NO_5$ requires C, 66.05; H, 5.23; N, 4.28%]; ν_{max} (KBr) 3195, 1753, 1682 cm^{-1} ; δ_H (400 MHz, DMSO- d_6) 11.84 (1 H, br.s, CO₂H), 7.41–7.27 (5 H, m, H-Ph), 6.77 (1 H, br.d, $^3J_{9,10}$ 5.7 Hz, H-9), 6.55 (1 H, d, $^3J_{10,9}$ 5.7 Hz, H-10), 5.31 (1 H, s, H-10b), 4.15 (1 H, br.dd, $^2J_{2,2}$ 11.4, $^3J_{2e,3e}$ 4.4 Hz, H-2^{eq}), 3.98–3.92 (2 H, m, H-2^{ax} and H-4^{eq}), 3.16 (1 H, dt, $^2J_{4,4}$ ~ $^3J_{4a,3a}$ 13.4, $^3J_{4a,3e}$ 3.8 Hz, H-4^{ax}), 3.03 and 2.96 (1 H and 1 H, two d, $^3J_{7,6a}$ 8.9 Hz, H-7 and H-6a), 1.71–1.62 (1 H, m, H-3^{ax}), 1.55–1.51 (1 H, m, H-3^{eq}); δ_C (100.6 MHz, DMSO- d_6) 170.7 and 170.4 (CO₂H and C-6), 140.0 (C-9), 136.4 (C-1'), 134.3 (C-10), 127.9 (2 C, C-2' and C-6'), 127.4 (C-4'), 125.3 (2 C, C-3' and C-5'), 93.6 and 89.2 (C-10a and C-8), 85.2 (C-10b), 66.8 (C-2), 52.3 (C-7), 48.6 (C-6a), 38.2 (C-4), 25.0 (C-3); MALDI-TOF HR: MH⁺, found 328.1192. $C_{18}H_{18}NO_5$ requires 328.1179.

(6aRS,7SR,8RS,10aSR,10bRS)-8-(3-Nitrophenyl)-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-

a]isoindole-7-carboxylic acid (3Ag) and (6aRS,7SR,8RS,10aSR,10bSR)-8-(3-nitrophenyl)-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-a]isoindole-7-carboxylic acid (3Bg). The synthesis was carried out following the general procedure above, but CHCl₃ was used as the reaction solvent because the starting 5-arylfurfural has a low solubility in CH₂Cl₂ and Me₂CO. Ratio of isomers **3Ag/3Bg** ~ 91/9, pale yellow powder (17.1 g, 46 %), m.p. > 169 °C (decomp.); [Found: C, 58.23; H, 4.67; N, 7.41. $C_{18}H_{16}N_2O_7$ requires C, 58.06; H, 4.33; N, 7.52%]; ν_{max} (KBr) 3413, 1730, 1692, 1531, 1348, 1195, 1056 cm^{-1} ; δ_H (600 MHz, DMSO- d_6) (**3Ag**) 12.05 (1 H, br.s, CO₂H), 8.17 (1 H, br.s, 1 H, H-2'), 8.16 (1 H, d, $^3J_{4',5'}$ 8.3 Hz, H-4'), 7.90 (1 H, d, $^3J_{6',5'}$ 7.7 Hz, H-6'), 7.68 (1 H, ddd, $^3J_{5',4'}$ 8.3, $^3J_{5',6'}$ 7.7, $^3J_{5',2'}$ 1.3 Hz, H-5'), 6.79 and 6.64 (1 H and 1 H, two d, $^3J_{9,10}$ 5.5 Hz, H-9 and H-10), 5.34 (1 H, s, H-10b), 4.13 (1 H, br.dd, $^2J_{2,2}$ 11.7, $^3J_{2e,3a}$ 4.1 Hz, H-2^{eq}), 3.94–3.90 (2 H, m, H-2^{ax} and H-4^{eq}), 3.15 (1 H, dt, $^2J_{4,4}$ ~ $^3J_{4a,3a}$ 13.1, $^3J_{4a,3e}$ 3.4 Hz, H-4^{ax}), 3.11 and 3.00 (1 H and 1 H, two d, $^3J_{7,6a}$ 8.9 Hz, H-7 and H-6a), 1.65–1.61 (1 H, m, H-3^{ax}), 1.51–1.49 (1 H, m, 3-H^{eq}); (**3Bg**) 12.05 (1 H, br.s, CO₂H), 8.28 (1 H, s, H-2'), 8.16 (1 H, d, $^3J_{4',5'}$ 8.3 Hz, H-4'), 7.90 (1 H, d, $^3J_{6',5'}$ 7.7 Hz, H-6'), 7.68 (1 H, ddd, $^3J_{5',4'}$ 8.3, $^3J_{5',6'}$ 7.7, $^3J_{5',2'}$ 1.3 Hz, H-5'), 6.81 and 6.54 (1 H and 1 H, two d, $^3J_{9,10}$ 5.5 Hz, H-9 and H-10), 5.45 (1 H, s, H-10b), 4.13 (1 H, dd, $^2J_{2,2}$ 11.7, $^3J_{2a,3e}$ 4.1 Hz, H-2^{eq}), 3.94–3.90 (2 H, m, H-2^{ax} and H-4^{eq}), 3.15 (1 H, dt, $^2J_{4,4}$ ~ $^3J_{4a,3a}$ 13.1, $^3J_{4a,3e}$ 3.4 Hz, 1 H, H-4^{ax}), 3.11 and 3.06 (1 H and 1 H, two d, $^3J_{7,6a}$ 8.9 Hz, H-7 and H-6a), 1.65–1.61 (1 H, m, H-3^{ax}), 1.51–1.49 (1 H, m, H-3^{eq}); δ_C (150.9 MHz, DMSO- d_6) (**3Ag**) 171.0 and 170.9 (CO₂H and C-6), 147.9 (C-3'), 139.6 and 138.9 (C-10 and C-9), 135.3 (C-1'), 132.7 (C-6'), 130.4 (C-5'), 123.2 (C-2'), 120.7 (C-4'), 93.2 (C-8), 90.0 (C-10a), 85.5 (C-10b), 67.3 (C-2), 52.6 and 49.1 (C-6a and C-7), 38.7 (C-4), 25.5 (C-3); (**3Bg**) 171.1 and 168.1 (CO₂H and C-6), 147.9 (C-3'), 140.0 and 139.8 (C-10 and C-9), 135.3 (C-1'), 132.7 (C-6'), 130.3 (C-5'), 123.2 (C-2'), 120.7 (C-4'), 92.6 (C-8), 89.9 (C-10a), 83.6 (C-10b), 66.9 (C-2), 53.7 and 49.1 (C-6a and C-7), 38.1 (C-4), 25.3 (C-3); MS (EI, 70 eV) m/z 354 (5, M⁺-18), 340 (1), 311 (2), 293 (1), 274 (10), 272 (19), 257 (70), 244 (68), 230 (17), 229 (43), 216 (18), 213 (52), 202 (21), 188 (23), 173 (24), 172 (39), 161 (21), 158 (50), 146 (43), 145 (87), 144 (67), 130 (30), 128 (65), 120 (20), 119 (41), 116 (83), 104 (47), 102 (54), 98 (43), 92 (20), 89 (27), 88 (47), 85 (55), 76 (43), 59 (80), 54 (100), 53 (45), 48 (21), 47 (25), 45 (29), 43 (47%).

(6aRS,7SR,8RS,10aSR,10bRS)-8-(2-Nitrophenyl)-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-a]isoindole-7-carboxylic acid (3Ah) and (6aRS,7SR,8RS,10aSR,10bSR)-8-(2-nitrophenyl)-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-a]isoindole-7-carboxylic acid (3Bh). The synthesis was carried out in accordance with the general procedure described above, but CHCl₃ was used as the reaction solvent because the starting 5-arylfurfural has a low solubility in CH₂Cl₂ and Me₂CO. Ratio of isomers **3Ah/3Bh** ~ 92/8, yellow powder (14.55 g, 39 %), m.p. 173–174 °C (decomp.); [Found: C, 58.29; H, 4.19; N, 7.28. $C_{18}H_{16}N_2O_7$ requires C, 58.06; H, 4.33; N, 7.52%]; ν_{max} (KBr) 3509, 1722, 1649, 1531, 1348, 1050 cm^{-1} ; δ_H (400 MHz, DMSO- d_6) (**3Ah**) 12.04 (1 H, br.s, CO₂H), 8.10 (1 H, d, $^3J_{3',4'}$ 7.6 Hz, H-3'), 7.76–7.72 (2 H, m, H-5' and H-6'), 7.66–7.59 (1 H, m, H-4'), 6.85 and 6.67 (1 H and 1 H, two d, $^3J_{9,10}$ 5.3 Hz, H-9 and H-10), 5.31 (1 H, s, H-10b), 4.17 (1 H, br.dd, $^2J_{2,2}$ 11.4, $^3J_{2e,3a}$ 4.4 Hz, H-2^{eq}), 4.00–3.93 (2 H, m, H-2^{ax} and H-4^{eq}), 3.26 and 3.07 (1 H and 1 H, two d, $^3J_{7,6a}$ 9.3 Hz, H-7 and H-6a), 3.16 (1 H, dt, $^2J_{4,4}$ ~ $^3J_{4a,3a}$ 13.4, $^3J_{4a,3e}$ 3.8 Hz, H-4^{ax}), 1.73–1.61 (1 H, m, H-3^{ax}),

1.55–1.52 (1 H, m, H-3^{eq}); **(3Bh)** 12.04 (1 H, br.s, CO₂H), 8.07 (1 H, dd, ⁴J_{3,5} 1.2, ³J_{3,4} 7.6 Hz, H-3'), 7.78–7.72 (2 H, m, H-5' and H-6'), 7.66–7.60 (1 H, m, H-4'), 6.87 and 6.61 (1 H and 1 H, two d, ³J_{9,10} 5.3 Hz, H-9 and H-10), 5.49 (1 H, s, H-10b), 4.19–4.15 (1 H, m, H-2^{eq}), 4.00–3.93 (2 H, m, H-2^{ax} and H-4^{eq}), 3.26 and 3.07 (1 H and 1 H, two d, ³J_{7,6a} 9.3 Hz, H-7 and H-6a), 3.18–3.14 (1 H, m, H-4^{ax}), 1.73–1.61 (1 H, m, H-3^{ax}), 1.55–1.52 (1 H, m, H-3^{eq}); δ_C (100.6 MHz, DMSO-*d*₆) **(3Ah)** 170.5 and 170.3 (CO₂H and C-6), 146.7 (C-2'), 138.8 and 134.9 (C-9 and C-10), 133.6, 129.6, 129.5 (C-4', C-5', C-6'), 130.9 (C-1'), 124.9 (C-3'), 92.7 and 88.1 (C-8 and C-10a), 85.1 (C-10b), 66.8 (C-2), 52.0 and 47.8 (C-6a and C-7), 38.1 (C-4), 24.9 (C-3); **(3Bh)** 170.5 and 167.5 (CO₂H and C-6), 146.7 (C-2'), 139.0 and 136.2 (C-9 and C-10), 135.5, 131.7, 130.0, 129.2 (C-4', C-5', C-6', C-1'), 124.8 (C-3'), 87.9, 83.2, 79.1 (C-8, C-10a, C-10b), 66.4 (C-2), 53.2 and 48.1 (C-6a and C-7), 37.6 (C-4), 23.2 (C-3); MS (EI, 70 eV) *m/z* 372 (6, M⁺), 328 (3), 284 (5), 276 (3), 274 (27), 244 (58), 231 (28), 230 (100), 217 (64), 216 (59), 202 (83), 183 (20), 172 (14), 156 (15), 128 (25), 115 (69), 89 (16), 76 (23), 63 (14), 59 (34), 54 (78), 43 (34%).

General procedure for preparation of epoxy[1,3]oxazino[2,3-*a*]isoindoles (4a–c). Acryloyl chloride (7.21 mL, 0.09 mol) was added dropwise to a stirred and water cooled (+5 °C) solution of the tautomeric mixture **1**⇌**2** obtained above (0.064 mol) and NEt₃ (16.6 mL, 0.12 mol) in PhH (80 mL). The reaction mixture was heated under reflux for 2 h (TLC control), then cooled and poured into cold water (250 mL). The organic layer was separated and the aqueous layer was extracted with EtOAc (2 × 100 mL). The combined organic phases were dried over MgSO₄. Solvents were removed under reduced pressure to give brown oil, which was purified by silica-gel column chromatography (3 × 10 cm) with Et₂O and then EtOAc/hexane, 1/1 as eluent. Adducts **4a–c** were obtained as colorless crystals.

(6aRS,8SR,10aSR,10bRS)-3,4,7,8-Tetrahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-*a*]isoindol-6(6aH,10bH)-one (4a). Fine colorless prisms (2.37 g, 18 %), m.p. 136–138 °C; [Found: C, 63.56; H, 6.42; N, 6.55. C₁₁H₁₃NO₃ requires C, 63.76; H, 6.32; N, 6.76%]; R_f (25% EtOAc/hexane) 0.35; ν_{max} (KBr) 2854, 1679 (br), 1433, 1266, 1045 cm⁻¹; δ_H (400 MHz, CDCl₃) 6.45 (1 H, d, ³J_{10,9} 6.0 Hz, H-10), 6.39 (1 H, dd, ³J_{9,10} 6.0, ³J_{9,8} 1.8 Hz, H-9), 5.40 (1 H, s, H-10b), 5.12 (1 H, dd, ³J_{8,7exo} 4.6, ³J_{8,9} 1.8 Hz, H-8), 4.23–4.16 (2 H, m, H-2^{eq} and H-4^{eq}), 3.73 (1 H, dt, ³J_{2a,3a} ~ ²J_{2,2} 12.0, ³J_{2a,3e} 1.8 Hz, H-2^{ax}), 3.00 (1 H, dddd, ²J_{4,4} 13.6, ³J_{4a,3a} 11.4, ³J_{4a,3e} 3.6, ⁵J_{4a,6} 1.6 Hz, H-4^{ax}), 2.39 (1 H, ddd, ⁵J_{4,6a} 1.6, ³J_{6a,7exo} 4.0, ³J_{6a,7endo} 8.7 Hz, H-6a), 2.23 (1 H, dt, ²J_{7,7} 11.7, ³J_{7exo,8} ~ ³J_{7exo,6a} 4.0 Hz, H-7^{exo}), 1.96–1.84 (1 H, m, H-3^{ax}), 1.60–1.54 (1 H, m, H-3^{eq}), 1.55 (1 H, dd, ²J_{7,7} 11.7, ³J_{7endo,6a} 8.7 Hz, H-7^{endo}); δ_C (100.6 MHz, CDCl₃) 173.9 (C-6), 135.9 (C-10), 132.0 (C-9), 90.1 (C-10a), 86.7 (C-10b), 79.8 (C-8), 67.6 (C-2), 46.3 (C-6a), 38.8 (C-4), 27.6 (C-7), 25.3 (C-3). GC-MS (EI, 70 eV) *m/z* 207 (6, M⁺), 179 (57), 178 (19), 152 (17), 151 (11), 150 (11), 138 (11), 137 (22), 124 (16), 123 (12), 122 (19), 96 (31), 95 (65), 94 (53), 86 (100), 84 (28), 81 (12), 77 (11), 66 (27), 65 (13), 56 (31), 55 (67), 41 (23), 39 (18), 29 (15), 28 (27), 27 (29%).

(6aRS,8SR,10aSR,10bRS)-8-Methyl-3,4,7,8-tetrahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-*a*]isoindol-6(6aH,10bH)-one (4b). Fine white prisms (2.68 g, 19 %), m.p. 132–133 °C; [Found: C, 65.19; H, 6.88; N, 6.00. C₁₂H₁₅NO₃ requires C, 65.14; H, 6.83; N, 6.33%]; R_f (25% EtOAc/hexane) 0.36; ν_{max} (KBr) 1698 cm⁻¹; δ_H (400 MHz, CDCl₃) 6.57 and 6.20 (1 H and 1 H, two d, ³J_{9,10} 5.6 Hz, H-10 and H-9), 5.00 (1 H, s, H-10b), 4.24–4.19 (2 H, m, H-2^{eq} and H-4^{eq}), 3.87 (1 H, dt, ³J_{2a,3a} ~ ²J_{2,2} 12.5, ³J_{2a,3e} 2.5 Hz, H-2^{ax}), 3.09 (1 H, dt, ³J_{4a,3a} ~ ²J_{4,4} 12.5, ³J_{4a,3e} 3.6 Hz, H-4^{ax}), 2.60 (1

H, dd, ³J_{6aendo,7endo} 8.7, ³J_{6a,7exo} 3.7 Hz, H-6a^{endo}), 1.88 (1 H, dd, ²J_{7,7} 11.8, ³J_{7exo,6a} 3.7 Hz, H-7^{exo}), 1.96–1.84 (1 H, m, H-3^{ax}), 1.71 (1 H, dd, ²J_{7,7} 11.8, ³J_{7endo,6a} 8.7 Hz, H-7^{endo}), 1.64 (3 H, s, Me-8), 1.48–1.52 (1 H, m, 3-H^{eq}); δ_C (100.6 MHz, CDCl₃) 174.1 (C-6), 139.3 and 132.5 (C-9 and C-10), 89.8 and 88.2 (C-8 and C-10a), 86.9 (C-10b), 67.7 (C-2), 49.6 (C-6a), 38.9 (C-4), 33.9 (C-7), 25.4 (C-3), 18.7 (Me-8). GC-MS (EI, 70 eV) *m/z* 221 (26, M⁺), 193 (47), 178 (60), 166 (25), 152 (16), 151 (49), 150 (22), 139 (12), 138 (20), 137 (14), 136 (34), 124 (25), 123 (12), 122 (23), 111 (16), 110 (39), 109 (92), 108 (75), 107 (12), 98 (11), 95 (15), 94 (11), 86 (100), 80 (38), 79 (14), 56 (17), 55 (51), 53 (10), 43 (20), 41 (11), 27 (14%).

(6aRS,8RS,10aSR,10bRS)-8-Bromo-3,4,7,8-tetrahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-*a*]isoindol-6(6aH,10bH)-one (4Ac) and (6aRS,8RS,10aSR,10bSR)-8-bromo-3,4,7,8-tetrahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-*a*]isoindol-6(6aH,10bH)-one (4Bc). Ratio of isomers **4Ac/4Bc** ~ 64/36, fine white crystals (3.86 g, 21 %), m.p. 113–114 °C; [Found: C, 46.21; H, 4.31; N, 5.12; Br, 28.38. C₁₁H₁₂BrNO₃ requires C, 46.18; H, 4.23; N, 4.90; Br, 27.93%]; R_f (25% EtOAc/hexane) 0.40; ν_{max} (KBr) 1690, 1045 cm⁻¹; δ_H (600 MHz, CDCl₃) **(4Ac)** 6.60 and 6.41 (1 H and 1 H, two d, ³J_{9,10} 5.8 Hz, H-10 and H-9), 5.04 (1 H, s, H-10b), 4.23–4.18 (2 H, m, H-2^{eq} and H-4^{eq}), 3.88 (1 H, dt, ²J_{2,2} ~ ³J_{2a,3a} 12.7, ³J_{2a,3e} 2.4 Hz, H-2^{ax}), 3.10 (1 H, dt, ²J_{4,4} ~ ³J_{4a,3a} 12.7, ³J_{4a,3e} 3.4 Hz, H-4^{ax}), 2.67 (1 H, dd, ³J_{6aendo,7endo} 8.9, ³J_{6a,7exo} 4.1 Hz, H-6a^{endo}), 2.47 (1 H, dd, ²J_{7,7} 11.9, ³J_{7exo,6a} 4.1 Hz, H-7^{exo}), 2.25 (1 H, dd, ²J_{7,7} 11.9, ³J_{7endo,6a} 8.9 Hz, H-7^{endo}), 1.93–1.86 (1 H, m, H-3^{ax}), 1.55–1.53 (1 H, m, H-3^{eq}); **(4Bc)** 6.68 and 6.37 (1 H and 1H, two d, ³J_{9,10} 5.8 Hz, H-10 and H-9), 5.04 (1 H, s, H-10b), 4.23–4.18 (2 H, m, H-2^{eq} and H-4^{eq}), 3.88 (1 H, dt, ²J_{2,2} ~ ³J_{2a,3a} 12.7, ³J_{2a,3e} 2.4 Hz, H-2^{ax}), 3.10 (1 H, dt, ²J_{4,4} ~ ³J_{4a,3a} 12.7, ³J_{4a,3e} 3.4 Hz, H-4^{ax}), 2.69 (1 H, dd, ³J_{6aendo,7endo} 8.9, ³J_{6a,7exo} 4.1 Hz, H-6a^{endo}), 2.37 (1 H, dd, ²J_{7,7} 11.9, ³J_{7exo,6a} 4.1 Hz, H-7^{exo}), 2.19 (1 H, dd, ²J_{7,7} 11.9, ³J_{7endo,6a} 8.9 Hz, H-7^{endo}), 1.93–1.86 (1 H, m, H-3^{ax}), 1.55–1.53 (1 H, m, H-3^{eq}); δ_C (100.6 MHz, CDCl₃) **(4Ac)** 172.1 (C-6), 139.9 (C-10), 133.0 (C-9), 99.4 (C-8), 89.1 (C-10a), 85.8 (C-10b), 67.7 (C-2), 49.1 (C-6a), 38.9 (C-7), 37.1 (C-4), 25.2 (C-3); **(4Bc)** 172.2 (C-6), 138.5 (C-10), 133.3 (C-9), 99.4 (C-8), 88.1 (C-10a), 86.0 (C-10b), 67.7 (C-2), 49.2 (C-6a), 38.8 (C-7), 37.1 (C-4), 25.2 (C-3). GC-MS (EI, 70 eV) *m/z* 287 (2, M⁺, for Br⁸¹), 286 (1), 285 (2), 284 (1), 260 (2), 259 (15), 258 (3), 257 (15), 218 (2), 217 (6), 216 (2), 215 (6), 207 (10), 206 (66), 178 (12), 175 (15), 174 (20), 173 (14), 172 (17), 152 (37), 146 (16), 144 (16), 121 (10), 93 (10), 86 (100), 85 (10), 65 (28), 56 (20), 55 (44), 41 (10), 39 (16), 27 (10%).

Multigram synthesis of 4-amino-4-methylpentan-2-ol.

A modified procedure²⁴ was used for the preparation of 4-amino-4-methylpentan-2-ol. A moderate stream of ammonia gas was bubbled until saturation (4–6 h) through a stirred solution of 4-methylpent-3-en-2-one (117 g, 1.20 mol) in MeOH (350 mL). The mixture was stirred at 26 °C for another 2 h. Then NaBH₄ (44.4 g, 1.80 mol) was added to this solution in small portions (during a ~ 1.5 h period). After addition was complete, the mixture was heated under reflux for another 2 h. The mixture was then cooled, poured into water (1400 mL) and extracted with Et₂O (4 × 250 mL). The organic phases were collected and dried over MgSO₄. Ether was removed under reduced pressure to give a pale-yellow oil. The residue was purified by distillation under reduced pressure to afford aminoalcohol as a colorless oil in 67% yield (86.4 g), b.p. 62–64 °C/21 mm Hg; [Found: C, 61.32; H, 12.81; N, 12.05. C₆H₁₅NO requires C, 61.49; H, 12.90; N, 11.95%]; n_D²² 1.3450; ν_{max} (liquid film) 3359 (br.) cm⁻¹; δ_H (400 MHz, CDCl₃) 6.70 (1 H, br.s, OH), 3.97 (1 H, ddd, ³J_{2,3B} 8.0,

$^3J_{\text{Me},2}$ 6.1, $^3J_{2,3A}$ 5.5 Hz, H-2), 1.31–1.26 (2 H, m, H-3), 1.09 (3 H, s, Me-4), 1.08 (3 H, s, Me-5), 1.02 (3 H, d, $^3J_{\text{Me},2}$ 6.1 Hz, Me-1); δ_{C} (100.6 MHz, CDCl_3) 65.1 (C-2), 50.3 (C-4), 49.2 (C-3), 35.8 (C-1), 26.8 and 23.9 (C-5 and Me-4).

2e-(Furan-2-yl)-4e,4a,6e-trimethyl-1,3-oxazinane (5). A mixture of 4-amino-4-methylpentan-2-ol (7.50 g, 65.0 mmol) and furfural (5.37 g, 65.0 mmol) was heated under reflux (3 h) in PhH (60 mL) with azeotropic removal of water using a Dean-Stark apparatus. After the theoretical amount of water (~ 1.2 mL) was collected, the mixture was cooled and PhH was removed under reduced pressure to afford a brown residue. The residue was purified by distillation under reduced pressure to give **5** as a viscous yellow oil (8.43 g, 66 %), b.p. 156–159 °C/ 7 mm Hg; [Found: C, 67.46; H, 8.59; N, 7.50. $\text{C}_{11}\text{H}_{17}\text{NO}_2$ requires C, 67.66; H, 8.78; N, 7.17%]; ν_{max} (liquid film) 3330 cm^{-1} ; δ_{H} (400 MHz, CDCl_3) 7.55 (1 H, dd, $^3J_{5',3'}$ 0.9, $^3J_{5',4'}$ 1.8 Hz, H-5'), 6.39 (1 H, dd, $^3J_{4',5'}$ 1.8, $^3J_{3',4'}$ 3.2 Hz, H-4), 6.36 (1 H, d, $^4J_{5',3'}$ 0.9, $^3J_{3',4'}$ 3.2 Hz, H-3'), 5.25 (1 H, d, $^3J_{2,\text{NH}}$ 12.0 Hz, H-2), 3.87 (1 H, ddq, $^3J_{6,5a}$ 13.0, $^3J_{6,\text{Me}}$ 6.1, $^3J_{6,5e}$ 2.2 Hz, H-6), 2.16 (1 H, d, $^3J_{\text{NH},2}$ 12.2 Hz, NH), 1.41 (1 H, dd, $^2J_{5,5}$ 13.0, $^3J_{5e,6}$ 2.2 Hz, H-5^{eq}), 1.10 (1 H, t, $^2J_{5,5} \sim ^3J_{6,5a}$ 13.0 Hz, H-5^{ax}), 1.14 (3 H, s, Me-4A), 1.09 (3 H, s, Me-4B), 1.08 (3 H, d, $^3J_{\text{Me},6}$ 6.1 Hz, Me-6); δ_{C} (100.6 MHz, CDCl_3) 152.8 (C-2'), 141.7 (C-5'), 109.8 and 106.2 (C-3' and C-4'), 78.7 (C-2), 68.9 (C-6), 48.9 (C-4), 45.1 (C-5), 32.4 (Me-6), 23.4 and 22.1 (Me-4 × 2). GC-MS (EI, 70 eV) m/z 195 (13, M⁺), 152 (27), 181 (3), 180 (14), 180 (24), 167 (12), 166 (11), 153 (3), 152 (27), 151 (67), 142 (3), 138 (5), 137 (24), 136 (53), 121 (5), 112 (11), 97 (28), 96 (100), 95 (95), 94 (38), 84 (44), 81 (11), 68 (8), 58 (8), 45 (7), 43 (13), 42 (35), 41 (32), 39 (24%).

(2RS,6aSR,7RS,8SR,10aRS,10bSR)-2,4,4-Trimethyl-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-a]isoindole-7(10bH)-carboxylic acid (6A) and (2RS,6aRS,7SR,8RS,10aSR,10bSR)-2,4,4-trimethyl-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-a]isoindole-7(10bH)-carboxylic acid (6B). A solution of 2-furyloxazine **5** (2.35 g, 12.0 mmol) in Et₂O (20 mL) was added to a solution of maleic anhydride (1.27 g, 13.0 mmol) in Et₂O (20 mL). The mixture was stirred at room temperature for 8 h. The solvent was then decanted from a yellow oil. Precipitate formed upon trituration of the residue with Me₂CO (20 mL) was separated by filtration, washed with Me₂CO (2 × 15 mL) and dried in air to give product **6** (1.0 g, 28 %) as a pale-yellow powder, ratio of isomers **6A/6B** ~ 75/25. M.p. 165–166 °C (for the mixture of isomers); [Found: C, 61.37; H, 6.94; N, 4.28. $\text{C}_{15}\text{H}_{19}\text{NO}_5$ requires C, 61.42; H, 6.53; N, 4.78%]; R_f (25% EtOAc/hexane) 0.35; ν_{max} (KBr) 3430, 1726, 1641 cm^{-1} ; δ_{H} (400 MHz, DMSO-*d*₆) (**6A**) 12.06 (1 H, br.s, CO₂H), 6.54 (1 H, d, $^3J_{10,9}$ 5.6 Hz, H-10), 6.43 (1 H, dd, $^3J_{9,10}$ 5.6, $^3J_{9,8}$ 1.0 Hz, H-9), 5.17 (1 H, s, H-10b), 4.97 (1 H, d, $^3J_{8,9}$ 1.0 Hz, H-8), 4.11 (1 H, ddq, $^3J_{2a,3a}$ 12.4, $^3J_{2,\text{Me}}$ 6.2, $^3J_{2a,3e}$ 2.4 Hz, H-2), 2.71 (1 H, d, $^3J_{7,6a}$ 9.1 Hz, H-7), 2.40 (1 H, br.d, $^3J_{6a,7}$ 9.1 Hz, H-6a), 1.55 (3 H, s, Me-4A), 1.53 (1 H, dd, $^2J_{3,3}$ 13.3, $^3J_{3e,2a}$ 2.4 Hz, H-3^{eq}), 1.49 (1 H, dd, $^2J_{3,3}$ 13.3, $^3J_{2a,3a}$ 12.4 Hz, H-3^{ax}), 1.29 (3 H, s, Me-4B), 1.17 (3 H, d, $^3J_{\text{Me},2}$ 6.2 Hz, Me-2); (**6B**) 12.06 (1 H, br.s, CO₂H), 6.56 (1 H, d, $^3J_{10,9}$ 5.6 Hz, H-10), 6.40 (1 H, dd, $^3J_{9,10}$ 5.6, $^3J_{9,8}$ 1.0 Hz, H-9), 5.44 (1 H, s, H-10b), 4.96 (1 H, d, $^3J_{8,9}$ 1.0 Hz, H-8), 3.95–3.91 (1 H, m, H-2), 2.62 (1 H, d, $^3J_{7,6a}$ 9.1 Hz, H-7), 2.41 (1 H, d, $^3J_{6a,7}$ 9.1 Hz, H-6a), 1.51 (3 H, s, Me-4A), 1.47–1.33 (2 H, m, H-3), 1.26 (3 H, s, Me-4B), 1.15 (3 H, d, $^3J_{\text{Me},2}$ 6.1 Hz, Me-2); δ_{C} (100.6 MHz, DMSO-*d*₆) (**6A**) 172.9 and 169.5 (CO₂H and C-6), 136.8 and 133.3 (C-9 and C-10), 88.3 (C-10a), 83.0 and 82.0 (C-8 and C-10b), 69.9 (C-2), 54.0 (C-4), 46.2 (C-3), 49.7 and 44.7 (C-6a and C-7), 28.7 and 24.5 (Me-4 × 2), 21.3 (Me-2). MS

(EI, 70 eV) m/z 293 (23, M⁺), 278 (74), 275 (2), 249 (8), 220 (17), 204 (3), 194 (30), 182 (51), 180 (30), 165 (8), 162 (15), 152 (17), 138 (29), 136 (47), 121 (42), 110 (14), 99 (69), 95 (49), 84 (100), 70 (13), 69 (20), 65 (43), 58 (43), 55 (31), 43 (35), 42 (65), 41 (59), 40 (60), 29 (21), 27 (33%).

The individual isomer **6A** was obtained by crystallization of the isomer mixture from hexane/EtOAc as a colorless powder, m.p. 149–153 °C (decomp.).

Synthesis of azomethines 7.

3-[[1-(2-Furyl)ethylidene]amino]propan-1-ol (7a). A mixture of 2-acetylfurane (5.49 g, 0.05 mol) and 3-aminopropan-1-ol (3.80 mL, 0.05 mol) in PhH (60 mL) was heated under reflux for 2 h with azeotropic removal of water using a Dean-Stark apparatus until the theoretical amount of water (~ 0.9 mL) was collected. The mixture was cooled and activated charcoal (3.0 g) was added to it. The mixture was then heated under reflux for 5 min and filtered. Benzene was removed under reduced pressure. A yellow oil was obtained (7.38 g, 78 %), which contained more than 80% of the target compound **7a** (according to ¹H NMR data, the compound was mainly contaminated with aminopropanol). The spectral data of the crude product are provided below. ν_{max} (KBr) 3398, 1647 cm^{-1} ; δ_{H} (400 MHz, CDCl_3) 7.45 (1 H, br.d, $^3J_{5',4'}$ 1.8 Hz, H-5'), 6.73 (1 H, br.d, $^3J_{3',4'}$ 3.7 Hz, H-3'), 6.41 (1 H, dd, $^3J_{3',4'}$ 3.7, $^3J_{5',4'}$ 1.8 Hz, H-4'), 3.86–3.90 (2 H, m, H-1), 3.63 (2 H, br.t, $^3J_{2,3}$ 6.0 Hz, H-3), 2.15 (3 H, s, Me), 1.94–1.97 (2 H, m, H-2); δ_{C} (100.6 MHz, CDCl_3) 156.7 and 153.6 (C-1 and C-2'), 143.9 (C-5'), 111.2 and 111.0 (C-3' and C-4'), 62.3 (C-1), 50.0 (C-3), 32.4 (C-2), 14.3 (Me). GC-MS (EI, 70 eV) m/z 167 (1, M⁺), 166 (2), 152 (12), 137 (17), 123 (79), 122 (45), 109 (10), 108 (10), 95 (26), 94 (100), 93 (21), 81 (84), 66 (26), 65 (31), 53 (15), 42 (27), 39 (57%).

3-[[1-(5-Methyl-2-furyl)ethylidene]amino]propan-1-ol (7b) was obtained in a similar way.

Attempted synthesis of 10b-methyl-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-a]isoindole-7(10bH)- and 8,10b-dimethyl-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-a]isoindole-7(10bH)-carboxylic acids (see Scheme 3).

Maleic anhydride (4.31 g, 44.0 mmol) was added with stirring and cooling (+10 °C) to a solution of the obtained above azomethine **7a** (7.38 g, 44.0 mmol) in CH₂Cl₂ (50 mL). The solution grew turbid and viscous brown oil formed almost right away. The reaction mixture was stirred at room temperature for 24 h. CH₂Cl₂ was decanted off and the obtained oil was washed with CH₂Cl₂ (2 × 15 mL). Our attempts to induce crystallization of the obtained mixture of products were unsuccessful. Use of PhH (reflux, 2 or 10 h) and Me₂CO as the reaction solvent lead to similar results.

Crystalline products of reaction of **7b** with maleic anhydride in the same conditions could not be isolated either.

2-[[1-(5-Methyl-2-furyl)ethylidene]amino]ethanol (8Ba). A solution of 5-methylacetylfuran (11.7 mL, 0.10 mol) in MeOH (30 mL) was added to a solution of ethanolamine (6.0 mL, 0.10 mol) in MeOH (30 mL) and the cherry red mixture was stirred at room temperature for 24 h. MeOH was evaporated under reduced pressure, the residue was dissolved in CH₂Cl₂ (30 mL) and purified by column chromatography (3 × 5 cm) on Al₂O₃ using CH₂Cl₂. After evaporation of the eluent, the viscous brown oil was obtained, which slowly crystallizes at +4 °C. Sticky crystals (7.89 g) containing more than 90% of the target compound (according to ¹H NMR) were obtained by crystallization from a petroleum ether/EtOAc/EtOH mixture. Repeated crystallization from petroleum ether/EtOAc gives rise to azomethine **8Ba** (4.51

g, 27 %) as light-brown amorphous crystals, m.p. 61.8–66.4 °C; [Found: C, 64.44; H, 7.94; N, 8.60. C₉H₁₃NO₂ requires C, 64.65; H, 7.84; N, 8.38%]; ν_{\max} (KBr) 3137, 1618, 1530 cm⁻¹; δ_{H} (400 MHz, CDCl₃) 6.66 (1 H, d, ³J_{3',4'} 3.2 Hz, H-3'), 6.03 (1 H, dq, ³J_{3',4'} 3.2, ⁴J_{Me,4'} 0.9 Hz, H-4'), 3.92 (2 H, t, ³J_{1,2} 5.5 Hz, H-1), 3.56 (2 H, t, ³J_{1,2} 5.5 Hz, H-2), 2.78 (1 H, br.s, OH), 2.34 (3 H, br.s, Me-5'), 2.13 (3 H, s, Me-C=N); δ_{C} (100.6 MHz, CDCl₃) 158.1 (C=N), 154.8 and 152.4 (C-2' and C-5'), 113.2 and 107.9 (C-3' and C-4'), 62.5 (O-CH₂), 53.6 (N-CH₂), 15.2 and 14.0 (Me-5' and C(Me)=N).

2-[(3*a*RS,6*RS*,7*a*SR)-6-Methyl-3-methylene-1-oxo-1,6,7,7a-tetrahydro-3*a*,6-epoxyisoindol-2(3*H*)-yl]ethyl acrylate (11). A solution of imine (**8Ba**) (0.50 g, 3.0 mmol), acryloyl chloride (0.36 mL, 4.50 mmol) and NEt₃ (0.83 mL, 6.0 mmol) in PhMe (50 mL) was heated under reflux for 4 h. The reaction mixture was cooled and poured into water (100 mL). The organic layer was separated and the water layer was extracted with EtOAc (3 × 20 mL). The organic phases were combined and dried (MgSO₄). Pale brown oil was obtained after evaporation of the solvent. ¹H NMR revealed at least four products in the mixture with about 20 % of the target compound **11**. The mixture was separated by column chromatography (1.8 × 12 cm) on Al₂O₃ using hexane and then EtOAc/hexane (1/20 → 1/10) mixtures as eluent. First the product of crotonic condensation of 5-methyl-2-acetylfuran and 1,3-bis(5-methyl-2-furyl)but-2-en-1-one was separated (colourless oil, 50 mg, 7%), then epoxyisoindolone **11** (0.12 g, 15 %) was isolated as a vitreous pale oil. [Found: C, 65.37; H, 6.16; N, 5.31. C₁₅H₁₇NO₄ requires C, 65.44; H, 6.22; N, 5.09%]; ν_{\max} (liquid film) 2974, 2943, 1720, 1656, 1364, 1182, 1063, 990 cm⁻¹; δ_{H} (400 MHz, CDCl₃) 6.53 (1 H, d, ³J_{5,4} 6.0 Hz, H-5), 6.41 (1 H, dd, ³J_{3'',trans,2''} 17.1, ²J_{3'',3''} 1.4 Hz, H-3'',^{trans}), 6.31 (1 H, d, ³J_{5,4} 6.0 Hz, H-4), 6.10 (1 H, d, ³J_{3'',trans,2''} 17.1, ³J_{2'',3''cis} 10.3 Hz, H-2''), 5.85 (1 H, dd, ³J_{2'',3''cis} 10.3, ²J_{3'',3''} 1.4 Hz, H-3'',^{cis}), 4.75 (1 H, d, ²J 2.3 Hz, C=CH₂A), 4.72 (1 H, d, ²J 2.3 Hz, C=CH₂B), 4.38–4.29 (2 H, m, N-CH₂-CH₂-O), 3.95 (1 H, dt, ²J 14.7, ³J ~ ³J 5.0 Hz, N-CH₂A-CH₂-O), 3.71 (1 H, dt, ²J 14.7, ³J ~ ³J 5.0 Hz, N-CH₂B-CH₂-O), 2.64 (1 H, dd, ³J_{7a,7endo} 9.0, ³J_{7exo,7a} 3.9 Hz, H-7a^{endo}), 1.98 (1 H, dd, ²J_{7,7} 11.7, ³J_{7exo,7a} 3.9 Hz, H-7^{exo}), 1.72 (1 H, dd, ²J_{7,7} 11.7, ³J_{7a,7endo} 9.0 Hz, H-7^{endo}), 1.64 (3 H, s, Me-6); δ_{C} (100.6 MHz, CDCl₃) 174.3 (C-1), 165.8 (O-CO-CH=CH₂), 143.2 (C-3), 141.3 (C-4), 132.6 (C-5), 131.2 (O-CO-CH=CH₂), 128.0 (O-CO-CH=CH₂), 90.0 (C₃=CH₂), 89.8 and 88.5 (C-3a and C-6), 60.6 (O-CH₂), 50.7 (C-7a), 39.2 (N-CH₂), 34.1 (C-7), 18.8 (Me-6). GC-MS (EI, 70 eV) *m/z* 220 (2, M⁺-55), 202 (2), 188 (4), 162 (7), 148 (4), 107 (18), 99 (19), 95 (7), 77 (11), 65 (5), 55 (100), 43 (14%).

Synthesis of compounds 12a, 12Ab/12Bb, 12c, some of their spectroscopic data and description of attempted synthesis of the isoindoles 13a–c.

2-[(2-Furylmethylene)amino]ethanol (12a) was obtained following the general synthetic procedure for compounds **1a–h** (**2a–h**). After MgSO₄ and CH₂Cl₂ were removed from a solution of furfural (0.10 mol) and 2-aminoethanol (0.10 mol), a pale yellow oil (~13 g), which contained ~ 90 % of the target compound, was isolated. The spectral data of the crude product are provided below. ν_{\max} (liquid film) 3390, 2889, 1647 cm⁻¹; δ_{H} (400 MHz, CDCl₃) 8.07 (1 H, s, CH=N), 7.48 (1 H, br.d, ³J_{5',4'} 1.8 Hz, H-5'), 6.72 (1 H, br.d, ³J_{3',4'} 3.2 Hz, H-3'), 6.44 (1 H, dd, ³J_{3',4'} 3.2, ³J_{5',4'} 1.8 Hz, H-4'), 3.88 (2 H, t, ³J_{1,2} 5.3 Hz, H-1), 3.68 (2 H, dt, ³J_{1,2} 5.3, *J* 0.9 Hz, H-2), 2.79 (br.s, 1 H, OH); δ_{C} (100.6 MHz, CDCl₃) 151.6 (C=N), 151.3 (C-2'), 144.9 (C-5'), 114.4 (C-3'), 111.7 (C-4'), 63.6 (O-CH₂), 62.1 (N-CH₂); GC-MS (EI, 70

eV) *m/z* 139 (8, M⁺), 108 (100), 94 (8), 81 (71), 53 (18), 39 (11%).

2-(2-Furyl)-4,4-dimethyl-1,3-oxazolidine (12Ab) and 2-[(2-furylmethylene)amino]-2-methylpropan-1-ol (12Bb). A solution of furfural (4.63 mL, 56.0 mmol) and 2-amino-2-methylpropan-1-ol (5.40 mL, 56.0 mmol) in PhMe (60 mL) was heated under reflux for 2 h. After PhMe removing a brown quickly crystallizing oil was obtained. Recrystallization from hexane affords a pale brown crystalline compound (6.39 g, 69 %). Mixture of tautomers **12Ab/12Bb** in ratio ~ 38/62. [Found: C, 64.64; H, 8.03; N, 8.42. C₉H₁₃NO₂ requires C, 64.65; H, 7.84; N, 8.38%]; δ_{H} (600 MHz, CDCl₃) (**12Ab**) 7.39 (1 H, br.d, ³J_{5',4'} 1.4 Hz, H-5'), 6.39 (1 H, br.d, ³J_{3',4'} 3.4 Hz, H-3'), 6.33 (1 H, dd, ³J_{3',4'} 3.4, ³J_{5',4'} 1.4 Hz, H-4'), 5.53 (1 H, s, H-2), 3.63 (1 H, d, ²J_{5,5} 6.9 Hz, H-5A), 3.50 (1 H, d, ²J_{5,5} 6.9 Hz, H-5B), 1.33 (3 H, s, Me-4A), 1.25 (3 H, s, Me-4B); (**12Bb**) 8.10 (1 H, s, CH=N), 7.50 (1 H, br.d, ³J_{5',4'} 1.4 Hz, H-5'), 6.73 (1 H, dd, ³J_{3',4'} 3.4, ⁴J_{3',5'} 0.7 Hz, H-3'), 6.46 (1 H, dd, ³J_{3',4'} 3.4, ³J_{5',4'} 1.4 Hz, H-4'), 3.54 (2 H, s, CH₂-OH), 2.36 (1 H, br.s, OH), 1.23 (6 H, s, C(Me)₂); δ_{C} (100.6 MHz, CDCl₃) (**12Ab**) 152.2 (C-2'), 147.0 (C-5'), 111.6 (C-3'), 108.2 (C-4'), 85.9 (C-2), 77.2 (C-5), 59.7 (C-4), 26.2 (Me-4A), 25.8 (Me-4B); (**12Bb**) 151.8 (C-2'), 144.6 (C-5'), 142.7 (C=N), 114.1 (C-3'), 110.3 (C-4'), 71.4 (CH₂-OH), 61.2 (CMe₂), 23.8 (2 C, CMe₂).

2-[(2-Furylmethylene)amino]phenol (12c). A solution of 2-aminophenol (10.0 g, 92.0 mmol) and furfural (7.61 mL, 92.0 mmol) in PhH (50 mL) was heated under reflux for 1.5 h with azeotropic removal of water using a Dean-Stark apparatus till the theoretical amount of water (~ 1.8 mL) was isolated. The solvent was evaporated under reduced pressure and the residue – a viscous brown oil – was used in the next step without further purification. The crude product contains ~ 92 % of the target compound according to ¹H NMR. The spectral data are given for this mixture. ν_{\max} (liquid film) 3394, 1628 cm⁻¹; δ_{H} (400 MHz, CDCl₃) 8.45 (1 H, s, CH=N), 7.60 (1 H, s, OH), 7.25–7.15 (3 H, m, H-3, H-5, H-6), 7.00–6.98 (2 H, m, H-3' and H-5'), 6.87 (1 H, br.t, ³J_{3,4} ~ ³J_{5,4} 7.3 Hz, H-4), 6.56 (1 H, dd, ³J_{3',4'} 3.7, ³J_{5',4'} 1.8 Hz, H-4'); δ_{C} (100.6 MHz, CDCl₃) 152.4 (C=N), 146.0 (2C) and 144.8 (C-1, C-2', C-5'), 135.7 (C-2), 129.0 (C-5), 120.2 (C-4), 116.3, 115.8, 115.3 (C-3, C-3', C-6), 112.6 (C-4').

Attempted synthesis of **3,3-dimethyl-5-oxo-2,3,5,5a,6,7-hexahydro-7,9a-epoxy[1,3]oxazol[2,3-*a*]isoindole-6-carboxylic acid (13b)**. Treatment of **12b** obtained above with an equimolar amount of maleic anhydride at room temperature in Me₂CO or CH₂Cl₂ (45 mL), or heating under reflux (2 h) in PhMe (50 mL) gives rise to (2*Z*)-4-[(2-hydroxy-1,1-dimethylethyl)amino]-4-oxobut-2-enoic acid (yields 17–38 %). According to ¹H NMR spectra, the reaction mixtures contain the target adduct **13b**, but it could not be isolated.

Attempted synthesis of **11-oxo-1,2,11,11a-tetrahydro-2,4a-epoxyisoindolo[1,2-*b*][1,3]benzoxazole-1-carboxylic acid (13c)**. Treatment of the imine **12c** obtained in a similar way with an equimolar amount of maleic anhydride at room temperature in Me₂CO or CH₂Cl₂ affords (2*Z*)-4-[(2-hydroxyphenyl)amino]-4-oxobut-2-enoic acid (**14**) as the main product (yield 52–63 %).

2,9b-Epoxy[1,3]oxazino[2,3-*a*]oxireno[*g*]isoindole-3-carboxylic acids (15). General experimental procedure. Formic acid (4.12 mL, 100 mmol) followed by 30% H₂O₂ (4.30 mL, 150 mmol) were added to a solution of acid **3Aa** or **3Ab** (~ 3.0 g, 10 mmol) in CHCl₃ (40 mL). The clear two-phase mixture was heated under reflux with intensive stirring for 12 h. The crystals formed upon cooling (~ +4 °C) were collected by filtration, washed with H₂O (2 × 30 mL), Et₂O (3 × 7 mL) and

dried in air. Diepoxides **15a,b** were obtained as well-formed transparent crystals. In some cases, the diepoxide **15** samples contained 2–3 % of the starting acids **3**. The latter can be easily removed by crystallization from an EtOH/DMF mixture.

(1aRS,2RS,3aSR,9bSR,9cRS)-4-Oxo-octahydro-6H-2,9b-epoxy[1,3]oxazino[2,3-a]xireno[g]isoindole-3-carboxylic acid (15a). Colourless prisms or white powder (1.25 g, 47 %), m.p. 261.0–262.7 °C (decomp.); [Found: C, 54.08; H, 4.72; N, 5.15. C₁₂H₁₃NO₆ requires C, 53.93; H, 4.90; N, 5.24%]; R_f (50% EtOH/DMF) 0.57; ν_{max} (KBr) 1745, 1672 cm⁻¹; δ_H (600 MHz, DMSO-*d*₆) 5.08 (1 H, s, H-9a), 4.63 (1 H, s, H-2), 4.09 (1 H, br.dd, ²J_{8,8} 11.7, ³J_{8,7a} 4.0 Hz, H-8^{eq}), 3.90–3.84 (2 H, m, H-8^{ax} and H-6^{eq}), 3.62 and 3.56 (1 H and 1 H, two d, ³J_{9c,1a} 3.5 Hz, H-9c and H-1a), 3.09 (1 H, d, ³J_{3,3a} 9.5 Hz, H-3), 3.05 (1 H, ddd, ²J_{6,6} 13.4, ³J_{6a,7a} 12.1, ³J_{6a,7c} 3.8 Hz, H-6^{ax}), 2.81 (1 H, d, ³J_{3a,3} 9.5 Hz, H-3a), 1.66–1.55 (1 H, m, H-7^{ax}), 1.51–1.47 (1 H, m, H-7^{eq}); δ_C (100.6 MHz, DMSO-*d*₆) 171.1 and 169.6 (CO₂H and C-4), 85.9 (C-9b), 84.1 and 78.6 (C-2 and C-9a), 66.5 (C-8), 50.7, 48.5, 47.0, 46.7 (C-1a, C-3, C-3a, C-9c), 38.1 (C-6), 24.8 (C-7). MS (EI, 70 eV) *m/z* 267 (50, M⁺), 260 (1), 252 (2), 250 (3), 239 (3), 238 (12), 224 (30), 223 (46), 208 (18), 194 (76), 180 (36), 167 (21), 166 (34), 164 (41), 152 (55), 138 (48), 137 (56), 125 (30), 123 (48), 122 (56), 111 (46), 110 (80), 99 (73), 87 (26), 86 (58), 85 (77), 84 (87), 71 (26), 69 (41), 66 (45), 57 (37), 56 (94), 55 (100), 45 (26), 43 (76%).

(1aRS,2SR,3SR,3aRS,9bRS,9cSR)-2-Methyl-4-oxo-octahydro-6H-2,9b-epoxy[1,3]oxazino[2,3-a]xireno[g]isoindole-3-carboxylic acid (15b). Thick colourless plates (1.31 g, 47 %), m.p. 252.1–253.6 °C (decomp.); [Found: C, 55.44; H, 5.29; N, 4.91. C₁₃H₁₅NO₆ requires C, 55.51; H, 5.38; N, 4.98%]; R_f (50% EtOH/DMF) 0.73; ν_{max} (KBr) 3533, 1732, 1683 cm⁻¹; δ_H (400 MHz, DMSO-*d*₆) 12.33 (1 H, br.s, CO₂H), 5.05 (1 H, s, H-9a), 4.09 (1 H, br.dd, ²J_{8,8} 11.4, ³J_{8,7a} 4.4 Hz, H-8^{eq}), 3.91–3.85 (2 H, m, H-8^{ax} and H-6^{eq}), 3.67 and 3.51 (1 H and 1 H, two d, ³J_{9c,1a} 3.5 Hz, H-9c and H-1a), 3.05 and 2.80 (1 H and 1 H, two d, ³J_{3,3a} 9.5 Hz, H-3 and H-3a), 3.07 (1 H, br.dt, ²J_{6,6} ~ ³J_{6a,7a} ~ 13.4, ³J_{6a,7c} 3.8 Hz, H-6^{ax}), 1.60–1.49 (1 H, m, H-7^{ax}), 1.43–1.41 (1 H, m, ²J_{7,7} 13.2 Hz, H-7^{eq}), 1.32 (3 H, br.s, Me-2); ¹³C NMR (D₂O/NaOD (5%), 100.6 MHz) δ 173.6 and 171.7 (CO₂H and C-4), 83.3 (C-9a), 84.7 and 83.7 (C-2 and C-9b), 65.7 (C-8), 51.6, 50.9, 50.0, 47.7 (C-1a, C-3, C-3a, C-9c), 36.9 (C-6), 22.5 (C-7), 11.2 (Me-2). δ_C (100.6 MHz, DMSO-*d*₆) 170.2 and 169.9 (CO₂H and C-4), 85.7 and 85.6 (C-2 and C-9b), 84.4 (C-9a), 66.6 (C-8), 52.1, 51.7, 50.4, 48.8 (C-1a, C-3, C-3a, C-9c), 38.1 (C-6), 24.9 (C-7), 13.6 (Me-2). MS (EI, 70 eV) *m/z* 281 (12, M⁺), 280 (9), 265 (1), 263 (6), 252 (9), 246 (34), 238 (41), 235 (11), 234 (14), 221 (24), 220 (56), 210 (22), 208 (52), 207 (17), 206 (19), 195 (29), 194 (41), 192 (44), 182 (13), 181 (54), 180 (70), 168 (37), 151 (67), 150 (59), 140 (57), 138 (36), 136 (35), 135 (17), 125 (44), 124 (66), 123 (76), 113 (10), 111 (23), 110 (22), 109 (41), 108 (49), 101 (13), 99 (46), 95 (54), 87 (13), 86 (77), 79 (41), 71 (13), 70 (18), 69 (41), 59 (54), 58 (100), 56 (91), 55 (86), 53 (62), 45 (34), 44 (51), 43 (54), 41 (56%).

6-Oxo-3,4,6,10b-tetrahydro-2H-[1,3]oxazino[2,3-a]isoindole-7-carboxylic acid (16). A solution of oxazino[2,3-a]isoindole carboxylic acid **3Aa** (1.01 g, 3.98 mmol) in 10% NaOH (15 mL) was heated under reflux for 2 h. After cooling, HCl (conc.) was added to the solution until it was slightly acidic. Crystals formed were collected by filtration, washed with water (2 × 20 mL) and Et₂O (2 × 10 mL) and dried in air until constant weight. The title acid **16** was obtained as a beige powder (0.12 g, 18 %), m.p. 169.2–172.2 °C; [Found: C, 61.68; H, 4.55; N, 5.97. C₁₂H₁₁NO₄ requires C, 61.80; H, 4.75; N, 6.01%]; ν_{max} (KBr) 3518, 1716,

1622 cm⁻¹; δ_H (600 MHz, DMSO-*d*₆) 8.09 (1 H, d, ³J_{8,9} 7.6 Hz, H-8), 7.84 (1 H, d, ³J_{10,9} 7.6 Hz, H-10), 7.79 (1 H, br.t, ³J_{8,9} ~ ³J_{9,10} 7.6 Hz, H-9), 5.82 (1 H, s, H-10b), 4.24 (1 H, br.dd, ²J_{2,2} 12.7, ³J_{2e,3a} 4.2 Hz, H-2^{eq}), 4.13 (1 H, br.dd, ²J_{4,4} 11.7, ³J_{4e,3a} 2.8 Hz, H-4^{eq}), 4.00 (1 H, dt, ²J_{4,4} ~ ³J_{4a,3a} 11.7, ³J_{4a,3e} 2.8 Hz, H-4^{ax}), 3.44 (1 H, dt, ²J_{2,2} ~ ³J_{2a,3a} 12.7, ³J_{2a,3e} 4.8 Hz, H-2^{ax}), 1.72–1.68 (2 H, m, H-3); δ_C (100.6 MHz, DMSO-*d*₆) 165.7 and 164.9 (CO₂H and C-6), 142.3 (C-10a), 132.8, 132.6, 127.4 (C-8, C-9, C-10), 129.1 (C-6a), 121.0 (C-7), 84.6 (C-10b), 66.4 (C-2), 38.1 (C-4), 24.0 (C-3). MS (EI, 70 eV) *m/z* 233 (8, M⁺), 232 (41), 216 (2), 214 (11), 204 (32), 203 (43), 190 (48), 189 (100), 175 (76), 160 (52), 157 (56), 149 (18), 130 (46), 105 (57), 104 (96), 103 (74), 77 (63), 76 (69), 75 (71), 63 (31), 59 (94), 53 (30), 43 (71%).

Esters of 8,10a-epoxy[1,3]oxazino[2,3-a]isoindole-7-carboxylic acids (17a–e). General experimental procedure. A solution of the appropriate acid **3Aa–d** (0.05 mol) and a catalytic amount of sulfuric acid (ca. 0.5 mL) in MeOH or abs. EtOH (150 mL) was heated under reflux for 5–25 h (the acid dissolves completely). The solvent was then evaporated under reduced pressure and the residue was purified by aluminum oxide column chromatography (with Et₂O and then EtOAc as eluent). Esters **17a–e** were obtained as colorless or pale yellow crystals after crystallization from MeOH or EtOH.

Methyl (6aRS,7SR,8RS,10aSR,10bRS)-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-a]isoindole-7-carboxylate (17a). Colorless rhombic crystals (6.89 g, 52 %), m.p. 169–170 °C (MeOH); [Found: C, 58.63; H, 5.57; N, 5.16. C₁₃H₁₅NO₅ requires C, 58.86; H, 5.70; N, 5.28%]; R_f (EtOAc) 0.62; ν_{max} (KBr) 1742, 1699 cm⁻¹; δ_H (400 MHz, DMSO-*d*₆) 6.62 (1 H, d, ³J_{10,9} 5.8 Hz, H-10), 6.48 (1 H, dd, ³J_{9,10} 5.8, ³J_{9,8} 1.7 Hz, H-9), 5.14 (1 H, s, H-10b), 5.12 (1 H, d, ³J_{8,9} 1.7 Hz, H-8), 4.12 (1 H, br.dd, ²J_{2,2} 11.4, ³J_{2e,3e} 4.4 Hz, H-2^{eq}), 3.94–3.87 (2 H, m, H-2^{ax} and H-4^{eq}), 3.57 (3 H, s, OMe), 3.10 (1 H, dt, ²J_{4,4} ~ ³J_{4a,3a} 12.7, ³J_{4a,3e} 3.6 Hz, H-4^{ax}), 2.82 (1 H, br.d, ³J_{7,6a} 9.1 Hz, H-7), 2.67 (1 H, d, ³J_{6a,7} 9.1 Hz, H-6a), 1.69–1.58 (1 H, m, H-3^{ax}), 1.52–1.48 (1 H, m, H-3^{eq}); δ_C (100.6 MHz, DMSO-*d*₆) 171.6 (CO₂Me), 170.4 (C-6), 136.6 (C-10), 133.6 (C-9), 89.4 (C-10a), 84.9 (C-10b), 81.8 (C-8), 66.7 (C-2), 51.3 (C-6a), 49.3 (CO₂Me), 43.7 (C-7), 38.1 (C-4), 25.0 (C-3). MS (EI, 70 eV) *m/z* 265 (12, M⁺), 250 (1), 237 (3), 234 (6), 206 (23), 153 (9), 152 (100), 138 (8), 124 (19), 121 (27), 113 (19), 95 (22), 86 (30), 85 (9), 65 (6), 59 (5), 56 (5%).

Methyl (6aRS,7SR,8RS,10aSR,10bRS)-8-methyl-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-a]isoindole-7-carboxylate (17b). Colorless prisms (6.42 g, 46 %), m.p. 177–179 °C (MeOH); [Found: C, 60.31; H, 6.07; N, 5.28. C₁₄H₁₇NO₅ requires C, 60.21; H, 6.14; N, 5.02%]; R_f (EtOAc) 0.67; ν_{max} (KBr) 1744, 1697 cm⁻¹; δ_H (400 MHz, CDCl₃) 6.70 (1 H, br.d, ³J_{9,10} 5.4 Hz, H-9), 6.22 (1 H, d, ³J_{10,9} 5.4 Hz, H-10), 5.15 (1 H, s, H-10b), 4.24–4.21 (2 H, m, H-2^{eq} and H-4^{eq}), 3.87 (1 H, br.t, ²J_{2,2} ~ ³J_{2a,3a} 12.1 Hz, H-2^{ax}), 3.75 (3 H, s, OMe), 3.11 (1 H, dt, ²J_{4,4} ~ ³J_{4a,3a} 12.1, ³J_{4a,3e} 2.8 Hz, H-4^{ax}), 2.85 (1 H, d, ³J_{7,6a} 8.9 Hz, H-7), 2.78 (1 H, d, ³J_{6a,7} 8.9 Hz, H-6a), 1.95–1.85 (1 H, m, H-3^{ax}), 1.62 (3 H, s, Me-8), 1.51–1.49 (1 H, m, H-3^{eq}); δ_C (100.6 MHz, DMSO-*d*₆) 170.5 and 170.4 (CO₂Me and C-6), 139.5 and 134.5 (C-9 and C-10), 89.6 and 89.0 (C-8 and C-10a), 85.1 (C-10b), 66.7 (C-2), 52.5, 51.1, 47.2 (CO₂Me, C-6a, C-7), 38.1 (C-4), 24.9 (C-3), 15.4 (Me-8). MS (EI, 70 eV) *m/z* 279 (54, M⁺), 261 (8), 251 (7), 249 (8), 248 (40), 247 (16), 236 (9), 220 (35), 219 (38), 204 (26), 194 (8), 190 (10), 176 (21), 167 (29), 166 (79), 150 (10), 139 (24), 138 (84), 137 (13), 136 (36), 135 (77), 124 (24), 123 (15), 122 (30), 114 (42), 113 (42), 110 (45), 109 (38), 108 (100), 107 (35), 101 (12), 99 (13), 95 (26), 94 (16),

87 (25), 86 (85), 85 (62), 81 (23), 80 (34), 67 (13), 59 (77), 57 (29), 56 (76), 55 (41), 54 (23), 53 (48), 51 (17), 44 (21), 43 (35), 42 (33), 41 (22%).

Methyl (6aRS,7RS,8SR,10aSR,10bRS)-8-bromo-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-a]isoindole-7(10bH)-carboxylate (17c). Fine yellow powder (7.88 g, 46 %), m.p. 201–202 °C (decomp., from MeOH); [Found: C, 45.39; H, 4.13; N, 4.04. C₁₃H₁₄BrNO₅ requires C, 45.37; H, 4.10; N, 4.07%]; R_f (65% EtOAc/hexane) 0.52; ν_{max} (KBr) 1754, 1706 cm⁻¹; δ_H (400 MHz, CDCl₃) 6.75 (1 H, d, ³J_{9,10} 5.5 Hz, H-9), 6.44 (1 H, d, ³J_{10,9} 5.5 Hz, H-10), 5.17 (1 H, s, H-10b), 4.22 (1 H, ddd, ²J_{2,2} 13.1, ³J_{2e,3a} 5.0, ³J_{2e,3e} 1.2 Hz, H-2^{eq}), 4.22 (1 H, ddd, ²J_{4,4} 13.0, ³J_{4e,3a} 5.0, ³J_{4e,3e} 1.2 Hz, H-4^{eq}), 3.88 (1 H, dt, ²J_{2,2} ~ ³J_{2a,3a} 13.1, ³J_{2a,3e} 2.7 Hz, H-2^{ax}), 3.80 (3 H, s, OMe), 3.19 (1 H, d, ³J_{7,6a} 8.7 Hz, H-7), 3.13 (1 H, ddd, ³J_{4a,3a} 14.3, ²J_{4,4} 13.0, ³J_{4a,3e} 4.1 Hz, H-4^{ax}), 2.92 (1 H, d, ³J_{6a,7} 8.7 Hz, H-6a), 1.93–1.85 (1 H, m, H-3^{ax}), 1.54–1.52 (1 H, m, H-3^{eq}); δ_C (150.9 MHz, CDCl₃) 170.0 and 168.9 (CO₂Me and C-6), 140.0 and 135.8 (C-9 and C-10), 90.1 and 88.5 (C-8 and C-10a), 85.4 (C-10b), 67.9 (C-2), 52.6, 52.5, 51.5 (CO₂Me, C-6a, C-7), 39.1 (C-4), 25.2 (C-3). GC-MS (EI, 70 eV) *m/z* 345 (3, M⁺, for Br⁸¹), 343 (4), 317 (4), 312 (5), 284 (19), 264 (24), 232 (16), 230 (36), 202 (29), 198 (34), 199 (35), 176 (22), 175 (28), 173 (21), 151 (71), 145 (23), 119 (20), 113 (66), 86 (100), 85 (56), 65 (44), 63 (49), 59 (52), 56 (68), 51 (16), 39 (43%).

Methyl (6aRS,7RS,8SR,10aSR,10bRS)-8-iodo-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-a]isoindole-7(10bH)-carboxylate (17d). Yellow powder (9.80 g, 50 %), m.p. 179–181 °C (decomp., from MeOH); [Found: C, 39.82; H, 3.57; N, 3.83. C₁₃H₁₄INO₅ requires C, 39.92; H, 3.61; N, 3.58%]; R_f (65% EtOAc/hexane) 0.67; ν_{max} (KBr) 1749, 1684 cm⁻¹; δ_H (400 MHz, DMSO-*d*₆) 6.57 and 6.51 (1 H and 1 H, two d, ³J_{9,10} 5.5 Hz, H-9 and H-10), 5.14 (1 H, s, H-10b), 4.23–4.16 (2 H, m, H-2^{eq} and H-4^{eq}), 3.86 (1 H, dt, ²J_{2,2} ~ ³J_{2a,3a} 12.4, ³J_{2a,3e} 2.3 Hz, H-2^{ax}), 3.79 (3 H, s, OMe), 3.12 (1 H, dd, *J* 0.9, ³J_{7,6a} 8.7 Hz, H-7), 3.10 (1 H, br.d, ²J_{4,4} ~ ³J_{4a,3a} 12.8, ³J_{2a,3e} 3.7 Hz, H-4^{ax}), 2.86 (1 H, d, ³J_{6a,7} 8.7 Hz, H-6a), 1.92–1.80 (1 H, m, H-3^{ax}), 1.51 (1 H, br.d, ³J_{3,3} 14.7 Hz, H-3^{eq}); δ_C (100.6 MHz, DMSO-*d*₆) 169.8 and 169.3 (CO₂Me and C-6), 143.0 and 135.0 (C-9 and C-10), 89.3 (C-10a), 85.0 (C-10b), 67.7 (C-2), 64.6 (C-8), 53.3, 52.2, 51.6 (C-6a, C-7, CO₂Me), 38.9 (C-4), 25.1 (C-3); MS (EI, 70 eV) *m/z* 391 (14, M⁺), 390 (2), 359 (3), 333 (75), 332 (20), 331 (6), 278 (32), 277 (51), 250 (16), 247 (37), 220 (17), 151 (24), 127 (27), 113 (30), 92 (19), 86 (59), 85 (50), 63 (46), 59 (68), 56 (100), 55 (22), 54 (15%).

Ethyl (6aRS,7SR,8RS,10aSR,10bRS)-6-oxo-3,4,6,6a,7,8-hexahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-a]isoindole-7-carboxylate (17e). Pale yellow powder (14.1 g, 72 %), m.p. 129–130 °C (from EtOH); [Found: C, 60.14; H, 6.32; N, 5.27. C₁₄H₁₇NO₅ requires C, 60.21; H, 6.14; N, 5.02%]; R_f (EtOAc) 0.72; ν_{max} (KBr) 1733, 1680 cm⁻¹; δ_H (400 MHz, CDCl₃) 6.70 (1 H, d, ³J_{10,9} 5.8 Hz, H-10), 6.43 (1 H, dd, ³J_{9,10} 5.8, ³J_{9,8} 1.6 Hz, H-9), 5.20 (1 H, d, ³J_{8,9} 1.6 Hz, H-8), 5.15 (1 H, s, H-10b), 4.26–4.16 (2 H, m, H-2^{eq} and H-4^{eq}), 4.22 (2 H, q, ³J_{CH₂Me} 7.1 Hz, CH₂CH₃), 3.88 (1 H, dt, ²J_{2,2} ~ ³J_{2a,3a} 12.6, ³J_{2a,3e} 2.1 Hz, H-2^{ax}), 3.10 (1 H, dt, ²J_{4,4} ~ ³J_{4a,3a} 12.6, ³J_{4a,3e} 3.5 Hz, H-4^{ax}), 2.82 and 2.75 (1 H and 1 H, two d, ³J_{7,6a} 9.1 Hz, H-6a and H-7), 1.95–1.87 (1 H, m, H-3^{ax}), 1.55–1.51 (1 H, m, H-3^{eq}), 1.31 (3 H, t, ³J_{CH₂Me} 7.1 Hz, CH₂CH₃); δ_C (100.6 MHz, CDCl₃) 171.2 and 170.8 (CO₂Me and C-6), 135.6 and 134.2 (C-10 and C-9), 89.6 (C-10a), 85.8 (C-10b), 82.4 (C-8), 67.5 (C-2), 60.9 (OCH₂CH₃), 49.8 (C-6a), 44.2 (C-7), 38.8 (C-4), 25.1 (C-3), 14.0 (OCH₂CH₃); MS (EI, 70 eV) *m/z* 279 (9, M⁺), 234 (7), 206 (26), 202 (3), 166 (13), 153

(6), 152 (100), 138 (27), 124 (15), 121 (35), 110 (6), 100 (5), 99 (34), 96 (11), 95 (36), 94 (9), 86 (40), 85 (5), 65 (8), 56 (8), 44 (13), 39 (11), 29 (17), 27 (16), 26 (14%).

Methyl (6aRS,7SR,8SR,9RS,10RS,10aSR,10bRS)-9,10-dibromo-6-oxooctahydro-2H-8,10a-epoxy[1,3]oxazino[2,3-a]isoindole-7-carboxylate (18). A solution of methyl ester **17a** (0.51 g, 2.00 mmol) and Me₂N⁺HCOMe·Br₃·Me₂NCOMe (0.80 g, 2.00 mmol) in CHCl₃ (10 mL) was heated under reflux for 12 h. The residue obtained after evaporation of the solvent was purified by silica gel column chromatography (1.2 × 10 cm, eluent: EtOAc/hexane, 1/2). The target dibromide **18** was isolated as a white powder (0.45 g, 56 %). Analytical sample was obtained by crystallization from a hexane/EtOAc mixture as fine transparent needles (elongated prisms), m.p. 181.1–182.0 °C; [Found: C, 36.52; H, 3.28; N, 3.45; Hal, 37.91. C₁₃H₁₅Br₂NO₅ requires C, 36.73; H, 3.56; N, 3.30; Br 37.60%]; R_f (25% EtOAc/hexane) 0.73; ν_{max} (KBr) 1733 (br.) cm⁻¹; δ_H (600 MHz, CDCl₃) 5.00 (1 H, s, H-10b), 4.81 (1 H, d, ³J_{10,9} 5.4 Hz, H-10), 4.44 (1 H, dd, ³J_{9,10} 5.4, ³J_{9,8} 2.2 Hz, H-9), 4.14 (1 H, d, ³J_{8,9} 2.2 Hz, H-8), 4.14–4.10 (2 H, m, H-2^{eq} and H-4^{eq}), 3.82 (1 H, d, ³J_{7,6a} 9.6 Hz, H-6a), 3.77 (1 H, ddd, ²J_{2,2} 13.1, ³J_{2a,3a} 12.5, ³J_{2a,3e} 2.3 Hz, H-2^{ax}), 3.67 (3 H, s, CO₂Me), 3.09 (1 H, d, ³J_{6a,7} 9.6 Hz, H-7), 3.04 (1 H, ddd, ²J_{4,4} 13.3, ³J_{4a,3a} 12.5, ³J_{4a,3e} 3.8 Hz, H-4^{ax}), 1.81–1.73 (1 H, m, H-3^{ax}), 1.43–1.41 (1 H, m, H-3^{eq}); δ_C (100.6 MHz, CDCl₃) 170.4 and 170.2 (CO₂Me and C-6), 90.2 (C-10a), 86.0 and 83.4 (C-8 and C-10b), 67.6 (C-2), 53.0 and 52.4 (C-9 and C-10), 52.7 (CO₂Me), 50.6 (C-7), 46.1 (C-6a), 39.3 (C-4), 25.0 (C-3); GC-MS (EI, 70 eV) *m/z* 427 (1, M⁺ for Br⁸¹), 425 (2), 423 (1), 396 (1), 394 (2), 392 (1), 346 (18), 344 (18), 244 (2), 242 (3), 121 (3), 113 (2), 95 (2), 86 (3), 85 (5), 84 (4), 65 (6), 59 (100), 56 (14), 55 (6), 54 (3), 42 (4), 41 (9), 39 (5%).

Methyl (3RS,3aSR,6RS,7SR,7aRS)-3-(acetyloxy)-2-[3-(acetyloxy)propyl]-1-oxo-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole-7-carboxylate (19). BF₃·OEt₂ (1.42 mL, 11.3 mmol) was added to a cooled (-5 °C) solution of methyl ester **17a** (1.00 g, 3.80 mmol) in Ac₂O (10 mL). The reaction mixture was stirred at room temperature for 24 h (TLC monitoring), poured into water (100 mL). A saturated sodium carbonate solution was added to the mixture until it was slightly basic. The mixture was extracted with CHCl₃ (3 × 50 mL) and the combined organic phases were dried (MgSO₄). The residue obtained after evaporation of the solvent was purified by silica gel column chromatography (3 × 10 cm, eluent: EtOAc/hexane, 1/2). The target product **19** was isolated as colorless rhombus-shaped crystals (0.17 g, 12 %), m.p. 74–76 °C; [Found: C, 55.35; H, 5.82; N, 3.77. C₁₇H₂₁NO₈ requires C, 55.58; H, 5.76; N, 3.81%]; R_f (EtOAc) 0.85; ν_{max} (KBr) 1724, 1707 cm⁻¹; δ_H (600 MHz, CDCl₃) 6.48 (1 H, d, ³J_{4,5} 5.9 Hz, H-4), 6.43 (1 H, dd, ³J_{5,4} 5.9, ³J_{5,6} 1.7 Hz, H-5), 6.39 (1 H, s, H-3), 5.19 (1 H, d, ³J_{6,5} 1.7 Hz, H-6), 4.04 (2 H, t, ³J_{2,3} 6.4 Hz, H-3'), 3.73 (3 H, s, CO₂Me), 3.54 (1 H, dt, ²J_{1,1'} 14.2, ³J_{1A',2'} 7.2 Hz, H-1'A), 3.29 (1 H, dt, ²J_{1,1'} 14.2, ³J_{1B',2'} 7.2 Hz, H-1'B), 2.89 (1 H, d, ³J_{7,7a} 9.1 Hz, H-7), 2.73 (1 H, d, ³J_{7a,7} 9.1 Hz, H-7a), 2.17 (3 H, s, OCOMe), 2.03 (3 H, s, OCOMe), 1.94–1.81 (2 H, m, H-2'); δ_C (100.6 MHz, CDCl₃) 172.3, 171.6, 170.9, 169.9 (OCOMe × 2, CO₂Me, C-1), 136.5 and 133.4 (C-4 and C-5), 90.1 (C-3a), 82.4 and 81.6 (C-3 and C-6), 61.4 (C-3'), 52.1 (CO₂Me), 48.6 and 44.9 (C-7a and C-7), 39.0 (C-1'), 26.8 (C-2'), 20.8 (OCOMe × 2); MS (EI, 70 eV) *m/z* 367 (8, M⁺), 350 (1), 325 (3), 309 (6), 308 (14), 307 (19), 281 (5), 265 (15), 248 (14), 232 (7), 230 (12), 212 (38), 211 (46), 198 (15), 197 (17), 196 (99), 170 (61), 169 (70), 154 (10), 152 (44), 139 (44), 135 (57), 134 (73), 124 (27), 122 (38), 114 (43), 113

(82), 101 (94), 97 (100), 86 (14), 85 (19), 82 (29), 81 (37), 73 (25), 66 (17), 65 (26), 59 (40), 56 (54), 45 (43), 43 (85%).

6b,9-Epoxyisindolo[2,1-*a*][3,1]benzoxazine-10-carboxylic acids (20a–c). General experimental procedure. Method A (thermal). A mixture of (2-aminophenyl)methanol (10.0 g, 80.0 mmol) and a suitable furfural (80.0 mmol) was heated under reflux in PhH (60 mL) with azeotropic removal of water using a Dean-Stark apparatus (1–2 h). After the theoretical amount of water (~ 1.4 mL) was collected, the mixture was cooled and crude 2-furanyl-1,4-dihydro-2*H*-3,1-benzoxazine was used in the next step without further purification, assuming quantitative yield. According to ¹H NMR, in the case of **2-(furan-2-yl)-2,4-dihydro-1*H*-benzo[d][1,3]oxazine**, the ratio of the ring/chain tautomeric forms (formed as viscous brown oil after solvent evaporation) in the mixture was ~ 78/22.

A solution of maleic anhydride (8.82 g, 0.09 mol) in PhH (50 mL) was added to a solution of the freshly prepared benzoxazine (0.08 mol) in PhH (~ 50 mL). The mixture was heated under reflux for 2 h and then cooled. Benzene was decanted from the viscous brown oil. The precipitate formed upon trituration of the residue with Me₂CO (40 mL) was collected by filtration, washed with acetone (2 × 30 mL), dried in air and further purified if necessary by recrystallization from *i*-PrOH/DMF mixtures. A white powder (6.45 g, 27 %) was obtained in the case of the synthesis of the acid **20a**. The **20Aa/20Ba** isomeric ratio was ~ 96/4.

Method B (ambient temperature) presented for the synthesis of the acid 20a, as an example (gives slightly lower yields of adducts 20, but higher diastereoselectivity). Anhydrous powdered MgSO₄ (12.0 g, 100 mmol) was added to a solution of (2-aminophenyl)methanol (5.0 g, 41 mmol) and furfural (3.4 mL, 41 mmol) in CH₂Cl₂ (80 mL). The mixture was stirred at room temperature for 24 h. MgSO₄ was then filtered off and washed with CH₂Cl₂ (2 × 40 mL). The organic phases were combined and concentrated under reduced pressure to give **2-(furan-2-yl)-2,4-dihydro-1*H*-benzo[d][1,3]oxazine** as a yellow oil. The oxazinane was used in the next step without further purification, assuming quantitative yield.

Maleic anhydride (4.47 g, 45.0 mmol) was added to a solution of the 2-furyloxazine (41 mmol) in Me₂CO (60 mL). The mixture was stirred at 24 °C for 2 d. The yellowish precipitate formed was collected by filtration, washed with Me₂CO (2 × 15 mL), Et₂O (20 mL) and dried in air to give the acid **20Aa** as a light yellow powder (2.8 g, 23 %).

Other acids (**20b,c**) were obtained following *Method A*.

(6aRS,6bSR,9RS,10SR,10aRS)-11-Oxo-9,10,10a,11-tetrahydro-5*H*-6b,9-epoxyisindolo[2,1-*a*][3,1]benzoxazine-10(6a*H*)-carboxylic acid (20Aa) and (6aRS,6bRS,9SR,10RS,10aSR)-11-oxo-9,10,10a,11-tetrahydro-5*H*-6b,9-epoxyisindolo[2,1-*a*][3,1]benzoxazine-10(6a*H*)-carboxylic acid (20Ba). The adduct yields and the ratio of the isomers in the samples obtained following methods A and B are given above. The single isomer **20Aa** was isolated by crystallization of the isomer mixture from *i*-PrOH/DMF, m.p. 197–202 °C (decomp.); [Found: C, 64.49; H, 4.29; N, 4.31. C₁₆H₁₃NO₅ requires C, 64.21; H, 4.38; N, 4.68%]; R_f (50% EtOH/DMF) 0.46; ν_{max} (KBr) 1710 cm⁻¹; δ_H (400 MHz, DMSO-*d*₆) (**20Aa**) 8.36 (1 H, dd, ³J_{1,2} 7.5, ⁴J_{1,3} 1.0 Hz, H-1), 7.25 (1 H, dt, ³J_{1,2} ~ ³J_{2,3} 7.5, ⁴J_{2,4} 1.0 Hz, H-2), 7.17 (1 H, br.d, ³J_{4,3} 7.5 Hz, H-4), 7.08 (1 H, dt, ³J_{3,2} ~ ³J_{3,4} 7.5, ⁴J_{3,1} 1.0 Hz, H-3), 6.64 (1 H, d, ³J_{7,8} 5.7 Hz, H-7), 6.51 (1 H, dd, ³J_{8,7} 5.7, ³J_{8,9} 1.7 Hz, H-8), 5.93 (1 H, s, H-6a), 5.11 (1 H, d, ²J_{5,5} 15.2 Hz, H-5A), 5.08 (1 H, d, ³J_{9,8} 1.7 Hz, H-9), 4.96 (1 H, d, ²J_{5,5} 15.2 Hz, H-5B), 3.13 (1 H,

d, ³J_{10a,10} 9.1 Hz, H-10a), 2.56 (1 H, d, ³J_{10,10a} 9.1 Hz, H-10); (**20Ba**) 7.68 (1 H, dd, ³J_{1,2} 7.5, ⁴J_{1,3} 1.0 Hz, H-1), 7.25 (1 H, dt, ³J_{1,2} ~ ³J_{2,3} 7.5, ⁴J_{2,4} 1.0 Hz, H-2), 7.17 (1 H, br.d, ³J_{4,3} 7.5 Hz, H-4), 7.08 (1 H, dt, ³J_{3,2} ~ ³J_{3,4} 7.5, ⁴J_{3,1} 1.0 Hz, H-3), 6.74 (1 H, d, ³J_{7,8} 5.7 Hz, H-7), 6.55 (1 H, dd, ³J_{8,7} 5.7, ³J_{8,9} 1.7 Hz, H-8), 5.47 (1 H, s, H-6a), 5.23 (1 H, d, ²J_{5,5} 15.1 Hz, H-5A), 5.19 (1 H, d, ³J_{9,8} 1.7 Hz, H-9), 5.06 (1 H, d, ²J_{5,5} 15.1 Hz, H-5B), 3.05 (1 H, d, ³J_{10a,10} 9.1 Hz, H-10a), 2.64 (1 H, d, ³J_{10,10a} 9.1 Hz, H-10); δ_C (150.9 MHz, CDCl₃) (**20Aa**) 172.6 and 168.4 (CO₂H and C-11), 138.0 (C-7), 134.7 (C-12a), 134.3 (C-8), 128.0, 125.4, 123.9 (C-2, C-3, C-4), 123.5 (C-4a), 117.9 (C-1), 89.2 (C-6b), 83.6 (C-6a), 81.7 (C-9), 68.0 (C-5), 52.0 (C-10a), 45.3 (C-10); MS (EI, 70 eV) *m/z* 299 (38, M⁺), 281 (2), 255 (3), 237 (6), 201 (47), 200 (100), 172 (16), 159 (30), 158 (14), 131 (15), 132 (50), 130 (16), 117 (10), 106 (14), 105 (34), 104 (40), 95 (18), 91 (23), 78 (30), 77 (32), 54 (13), 51 (14), 44 (19), 39 (16), 28 (26), 26 (15%).

(6aRS,6bSR,9RS,10SR,10aRS)-9-Methyl-11-oxo-9,10,10a,11-tetrahydro-5*H*-6b,9-epoxyisindolo[2,1-*a*][3,1]benzoxazine-10(6a*H*)-carboxylic acid (20Ab) and (6aRS,6bRS,9SR,10RS,10aSR)-9-methyl-11-oxo-9,10,10a,11-tetrahydro-5*H*-6b,9-epoxyisindolo[2,1-*a*][3,1]benzoxazine-10(6a*H*)-carboxylic acid (20Bb). Ratio of isomers **20Ab/20Bb** ~ 57/43, yellowish powder (5.76 g, 23 %), m.p. 167–168 °C (decomp.); [Found: C, 65.42; H, 4.57; N, 4.72. C₁₇H₁₅NO₅ requires C, 65.17; H, 4.83; N, 4.47%]; R_f (50% EtOH/DMF) 0.68; ν_{max} (KBr) 3534, 1725, 1679 cm⁻¹; δ_H (400 MHz, DMSO-*d*₆) (**20Ab**) 12.40 (1 H, br.s, CO₂H), 8.42 (1 H, d, ³J_{1,2} 8.2 Hz, H-1), 7.31–7.22 (3 H, m, H-2, H-3, H-4), 6.67 (1 H, d, ³J_{8,7} 5.6 Hz, H-8), 6.33 (1 H, d, ³J_{7,8} 5.6 Hz, H-7), 5.85 (1 H, s, H-6a), 5.10 (1 H, d, ²J_{5,5} 15.3 Hz, H-5A), 4.95 (1 H, d, ²J_{5,5} 15.3 Hz, H-5B), 3.14 (1 H, d, ³J_{10a,10} 8.9 Hz, H-10a), 2.59 (1 H, d, ³J_{10,10a} 8.9 Hz, H-10), 1.54 (3 H, s, Me-9); (**20Bb**) 12.40 (1 H, br.s, CO₂H), 7.66 (1 H, d, ³J_{1,2} 8.2 Hz, H-1), 7.31–7.22 (3 H, m, H-2, H-3, H-4), 6.77 (1 H, d, ³J_{8,7} 5.6 Hz, H-8), 6.39 (1 H, d, ³J_{7,8} 5.6 Hz, H-7), 5.45 (1 H, s, H-6a), 5.21 (1 H, d, ²J_{5,5} 15.3 Hz, H-5A), 5.06 (1 H, d, ²J_{5,5} 15.3 Hz, H-5B), 3.04 (1 H, d, ³J_{10a,10} 8.9 Hz, H-10a), 2.67 (1 H, d, ³J_{10,10a} 8.9 Hz, H-10), 1.56 (3 H, s, Me-9); δ_C (100.6 MHz, DMSO-*d*₆) (**20Ab**) 172.0 and 168.6 (CO₂H and C-11), 140.7 (C-8), 135.6 (C-7), 135.1 (C-12a), 127.9, 125.4, 123.8 (C-2, C-3, C-4), 123.4 (C-4a), 117.6 (C-1), 89.4 and 88.2 (C-6b and C-9), 83.9 (C-6a), 68.1 (C-5), 54.7 (C-10a), 48.6 (C-10b), 16.1 (Me-9); (**20Bb**) 171.8 (CO₂H), 170.9 (C-11), 140.3 (C-8), 134.9 (C-7), 134.0 (C-12a), 127.4, 125.4, 125.1 (C-2, C-3, C-4), 125.7 (C-4a), 121.4 (C-1), 90.4 and 88.9 (C-6b and C-9), 84.9 (C-6a), 67.7 (C-5), 53.2 (C-10a), 48.5 (C-10), 16.1 (Me-9); MS (EI, 70 eV) *m/z* 313 (36, M⁺), 295 (5), 268 (2), 251 (17), 215 (35), 214 (100), 213 (17), 186 (17), 183 (13), 172 (22), 159 (30), 158 (24), 152 (45), 135 (34), 134 (87), 133 (26), 132 (72), 130 (30), 110 (35), 109 (43), 106 (31), 105 (36), 104 (53), 99 (30), 95 (63), 93 (22), 91 (22), 82 (12), 79 (19), 78 (58), 77 (82), 65 (20), 54 (41), 53 (48), 52 (24), 51 (48), 50 (18), 45 (15), 43 (51), 39 (35), 38 (16%).

(6aRS,6bSR,9SR,10RS,10aRS)-9-Bromo-11-oxo-9,10,10a,11-tetrahydro-5*H*-6b,9-epoxyisindolo[2,1-*a*][3,1]benzoxazine-10(6a*H*)-carboxylic acid (20Ac) and (6aRS,6bRS,9RS,10SR,10aSR)-9-bromo-11-oxo-9,10,10a,11-tetrahydro-5*H*-6b,9-epoxyisindolo[2,1-*a*][3,1]benzoxazine-10(6a*H*)-carboxylic acid (20Bc). Ratio of isomers **20Ac/20Bc** ~ 93/7, yellowish powder (5.15 g, 17 %), m.p. > 250 °C (decomp.); [Found: C, 50.80; H, 3.34; N, 3.58; Br, 21.48. C₁₆H₁₂BrNO₅ requires C, 50.82; H, 3.20; N, 3.70; Br, 21.13%]; ν_{max} (KBr) 3098, 1751, 1665, 525 cm⁻¹; δ_H (400 MHz, DMSO-*d*₆) (**20Ac**) 12.33 (1 H, br.s, CO₂H), 8.41 (1 H, d, ³J_{1,2} 8.1 Hz, H-1), 7.26 (1 H, ddd, ³J_{2,1} 8.1, ³J_{2,3} 6.9, ⁴J_{2,4} 0.7 Hz, H-2), 7.20 (1 H, dd, ³J_{4,3}

Tetrahedron

6.9, $^4J_{4,2}$ 0.7 Hz, H-4), 7.12 (1 H, dt, $^3J_{3,4} \sim ^3J_{3,2}$ 6.9, $^4J_{3,1}$ 0.7 Hz, H-3), 6.85 (1 H, d, $^3J_{8,7}$ 5.5 Hz, H-8), 6.60 (1 H, d, $^2J_{7,8}$ 5.5 Hz, H-7), 5.93 (1 H, s, H-6a), 5.13 (1 H, d, $^2J_{5,5}$ 15.4 Hz, H-5A), 5.00 (1 H, d, $^2J_{5,5}$ 15.4 Hz, H-5B), 3.32 (1 H, d, $^3J_{10a,10}$ 8.8 Hz, H-10a), 3.09 (1 H, d, $^3J_{10,10a}$ 8.8 Hz, H-10); (**20Bc**) 12.33 (1 H, br.s, CO₂H), 7.68 (1 H, d, $^3J_{1,2}$ 8.1 Hz, H-1), 7.44 (1 H, dd, $^3J_{4,3}$ 7.0, $^4J_{2,4}$ 1.2 Hz, H-4), 7.39 (1 H, br.dd, $^3J_{2,3}$ 7.0, $^3J_{1,2}$ 8.1 Hz, H-2), 7.31–7.29 (1 H, m, H-3), 6.93 (1 H, d, $^3J_{8,7}$ 5.7 Hz, H-7), 6.67 (1 H, d, $^3J_{7,8}$ 5.7 Hz, H-8), 5.57 (1 H, s, H-6a), 5.25 (1 H, d, $^2J_{5,5}$ 15.3 Hz, H-5A), 5.10 (1 H, d, $^2J_{5,5}$ 15.3 Hz, H-5B), ~ 3.30 (1 H, d, $^3J_{10a,10}$ 8.3 Hz, H-10a), 3.14 (1 H, d, $^3J_{10,10a}$ 8.3 Hz, H-10); δ_C (100.6 MHz, DMSO-*d*₆) (**20Ac**) 169.5 (CO₂H), 166.8 (C-11), 140.6 (C-8), 136.2 (C-7), 134.3 (C-12a), 127.4 (C-2), 124.9 (C-4), 123.6 (C-3), 122.9 (C-4a), 117.2 (C-1), 90.7 (C-9), 87.1 (C-6b), 82.9 (C-6a), 67.6 (C-5), 53.6 (C-10a), 51.4 (C-10); (**20Bc**) 169.1 (CO₂H), 166.7 (C-11), 140.3 (C-8), 135.4 (C-7), 133.1 (C-12a), 129.9, 128.6, 127.0 (C-2, C-3, C-4), 125.1 (C-4a), 120.9 (C-1), 90.7 (C-9), 87.5 (C-6b), 83.5 (C-6a), 67.3 (C-5), 52.1 (C-10a), 51.2 (C-10). MS (EI, 70 eV) *m/z* 379 (5, M⁺ for Br⁸¹), 377 (5), 333 (2), 315 (2), 313 (3), 298 (2), 280 (26), 278 (31), 270 (2), 252 (4), 224 (5), 214 (14), 198 (12), 185 (10), 174 (11), 173 (10), 170 (22), 159 (47), 158 (24), 134 (71), 132 (84), 121 (18), 104 (67), 99 (40), 91 (21), 77 (100), 65 (31), 51 (67), 44 (49), 39 (62%).

Methyl (6aRS,6bSR,9RS,10SR,10aRS)-11-oxo-9,10,10a,11-tetrahydro-5H-6b,9-epoxyisoindolo[2,1-a][3,1]benzoxazine-10(6aH)-carboxylate (21). A solution of the acid **20Aa** (15.65 g, 0.05 mol) and a catalytic amount of sulfuric acid (ca. 0.5 mL) in MeOH (160 mL) was heated under reflux for 8 h. The acid dissolved completely by the end of the reaction. The solvent was then evaporated under reduced pressure and the residue, a yellow oil, was purified by aluminum oxide column chromatography (2 × 10 cm, eluent: EtOAc). Ester **21** was obtained as colorless prisms (12.67 g, 82 %), m.p. 183–184 °C; [Found: C, 65.14; H, 4.74; N, 4.58. C₁₇H₁₅NO₅ requires C, 65.17; H, 4.83; N, 4.47%]; R_f (65% EtOAc/hexane) 0.34; ν_{\max} (KBr) 1703, 1600 cm⁻¹; δ_H (400 MHz, CDCl₃) 8.37 (1 H, dd, $^3J_{1,2}$ 8.3, $^4J_{1,3}$ 1.1 Hz, H-1), 7.20 (1 H, ddd, $^3J_{1,2}$ 8.3, $^3J_{2,3}$ 7.6, $^4J_{2,4}$ 1.7 Hz, H-2), 7.03 (1 H, dt, $^3J_{2,3} \sim ^3J_{4,3}$ 7.6, $^4J_{3,1}$ 1.1 Hz, H-3), 6.98 (1 H, dd, $^3J_{3,4}$ 7.6, $^4J_{2,4}$ 1.7 Hz, H-4), 6.58 (1 H, d, $^3J_{7,8}$ 5.8 Hz, H-7), 6.49 (1 H, dd, $^3J_{7,8}$ 5.8, $^3J_{9,8}$ 1.8 Hz, H-8), 5.70 (1 H, s, H-6a), 5.23 (1 H, d, $^3J_{8,9}$ 1.8 Hz, H-9), 5.10 (1 H, d, $^2J_{5,5}$ 15.0 Hz, H-5A), 4.98 (1 H, d, $^2J_{5,5}$ 15.0 Hz, H-5B), 3.72 (3 H, s, CO₂Me), 2.97 (1 H, d, $^3J_{10,10a}$ 9.0 Hz, H-10a), 2.74 (1 H, d, $^3J_{10,10a}$ 9.0 Hz, H-10); δ_C (100.6 MHz, CDCl₃) 171.5 and 167.1 (two s, CO₂Me and C-11), 137.7 (d, *J* 178.2 Hz, C-7), 134.0 (s, C-12a), 133.3 (d, *J* 179.5 Hz, C-8), 127.7 (d, *J* 162.0 Hz, C-2), 124.1 (d, *J* 158.0 Hz, C-4), 123.8 (d, *J* 163.0 Hz, C-3), 122.4 (s, C-4a), 118.5 (d, *J* 167.3 Hz, C-1), 88.6 (s, C-6b), 83.1 (d, *J* 161.2 Hz, C-6a), 81.6 (d, *J* 168.5 Hz, C-9), 68.3 (t, *J* 147.0 Hz, C-5), 52.1 (q, *J* 147.3 Hz, CO₂Me), 51.1 (d, *J* 140.0 Hz, C-10a), 45.3 (d, *J* 139.0 Hz, C-10). 1D NOE ¹H NMR, %: $\eta_{H-1}\{H-6a\}$ 2.4 %; $\eta_{H-6a}\{H_A-5\}$ 8.7 %; $\eta_{H-6a}\{H-10a\}$ 3.1 %; $\eta_{H-7}\{H-6a\}$ 5.1 %; $\eta_{H-7}\{H-10a\}$ 2.4 %; $\eta_{H-8}\{H-10\}$ 2.9 %; $\eta_{H-9}\{H-10\}$ 5.6 %; $\eta_{H-10}\{H-10a\}$ 10.0 %. MS (EI, 70 eV) *m/z* 313 (35, M⁺), 295 (1), 282 (2), 254 (2), 236 (2), 217 (4), 202 (19), 201 (23), 200 (100), 186 (22), 185 (11), 174 (19), 157 (9), 134 (10), 132 (36), 113 (45), 104 (12), 95 (10), 77 (17), 65 (7), 59 (10), 51 (7), 39 (7), 28 (4%).

2,4a-Epoxyisoindolo[1,2-b][1,3]benzoxazine-1(4bH)-carboxylic acids (22). **General experimental procedure.** A mixture of 2-(aminomethyl)phenol^[27] (1.23 g, 10.0 mmol) and furfural (or 5-methylfurfural) (~1 mL, 10.0 mmol) in PhMe (50 mL) was heated under reflux with azeotropic removal of water

using a Dean-Stark apparatus for 0.5–1 h. About 0.2 mL of water was collected. The solvent was removed under reduced pressure and a yellow-brown oil was obtained. The ratio of the ring/chain tautomeric forms (according to ¹H NMR) in the case of 2-(furan-2-yl)-3,4-dihydro-2H-1,3-benzoxazine was found ~ 39/61. The oil was then dissolved in CH₂Cl₂ (30 mL) and maleic anhydride (0.98 g, 10.0 mmol) was added. The solution was stored at room temperature for 24 h. The solvent was removed and the residue, a viscous brown oil, was triturated with Et₂O (5 × 15 mL). A pale brown powder formed was collected by filtration, air-dried until constant weight and analyzed by NMR. Analytical samples of adducts **22A** were obtained by crystallization from an EtOAc/MeOH mixture.

(1RS,2SR,4aRS,4bSR,12aSR)-12-Oxo-1,2,12,12a-tetrahydro-10H-2,4a-epoxyisoindolo[1,2-b][1,3]benzoxazine-1(4bH)-carboxylic acid (22Aa). Cream-colored powder (1.02 g, 34 %), m.p. 144.8–145.3 °C (decomp. from EtOAc/MeOH); [Found: C, 64.17; H, 4.33; N, 4.53. C₁₆H₁₃NO₅ requires C, 64.21; H, 4.38; N, 4.68%]; ν_{\max} (KBr) 3468, 1739, 1676 cm⁻¹; δ_H (400 MHz, CDCl₃) 9.45 (1 H, br.s, CO₂H), 7.17 (1 H, dd, $^3J_{6,7}$ 8.2, $^3J_{8,7}$ 7.5 Hz, H-7), 7.08 (1 H, br.d, $^3J_{8,9}$ 7.5 Hz, H-9), 7.00 (1 H, br.t, $^3J_{8,9} \sim ^3J_{8,7}$ 7.5 Hz, H-8), 6.95 (1 H, br.d, $^3J_{6,7}$ 8.2 Hz, H-6), 6.87 (1 H, d, $^3J_{3,4}$ 5.8 Hz, H-4), 6.49 (1 H, br.d, $^3J_{3,4}$ 5.8 Hz, H-3), 5.55 (1 H, s, H-4b), 5.30 (1 H, br.s, H-2), 4.96 (1 H, d, $^2J_{10,10}$ 16.8 Hz, H-10A), 4.36 (1 H, d, $^2J_{10,10}$ 16.8 Hz, H-10B), 2.93 (1 H, d, $^3J_{12a,1}$ 9.0 Hz, H-12a), 2.84 (1 H, d, $^3J_{1,12a}$ 9.0 Hz, H-1); δ_C (100.6 MHz, CDCl₃) 174.2 (CO₂H), 172.1 (C₁₂), 152.5 (C_{5a}), 136.1 (C₃), 134.1 (C₄), 128.3 (C₇), 127.2 (C₉), 122.7 (C₈), 119.7 (C_{9a}), 117.9 (C₆), 89.9 (C_{4a}), 83.3 (C₂), 82.9 (C_{4b}), 49.9 (C_{12a}), 44.6 (C₁), 40.0 (C₁₀). MS (EI, 70 eV) *m/z* 299 (39, M⁺), 281 (37), 202 (9), 201 (66), 200 (100), 184 (14), 172 (17), 108 (9), 107 (73), 99 (17), 81 (37), 78 (48), 77 (45), 26 (9%).

(1RS,2SR,4aRS,4bSR,12aSR)-2-Methyl-12-oxo-1,2,12,12a-tetrahydro-10H-2,4a-epoxyisoindolo[1,2-b][1,3]benzoxazine-1(4bH)-carboxylic acid (22Ab) and (1RS,2SR,4aRS,4bRS,12aSR)-2-methyl-12-oxo-1,2,12,12a-tetrahydro-10H-2,4a-epoxyisoindolo[1,2-b][1,3]benzoxazine-1(4bH)-carboxylic acid (22Bb). A pale-brown powder (1.11 g, 35 %) was obtained by trituration with ether, ratio of isomers **22Ab/22Bb** ~ 86/14. δ_H (400 MHz, DMSO-*d*₆, **22Bb** in mixture **22Ab/22Bb** ~ 86/14) 7.31 (1 H, dd, $^4J_{9,7}$ 1.3, $^3J_{8,9}$ 7.7 Hz, H-9), 7.23–6.70 (4 H, these signals are overlapping with the signals of *major* isomer **22Ab**, H-9, H-8, H-6 and H-4), 6.31 (1 H, d, $^3J_{3,4}$ 5.5 Hz, H-3), 5.84 (1 H, s, H-4b), 5.55 (1 H, d, $^2J_{10,10}$ 16.9 Hz, H-10A), 4.31 (1 H, d, $^2J_{10,10}$ 16.9 Hz, H-10B), 2.93 (1 H, d, $^3J_{12a,1}$ 8.7 Hz, H-12a), 2.54 (1 H, d, $^3J_{1,12a}$ 8.7 Hz, H-1), 1.52 (3 H, s, Me-2). Single isomer **22Ab** was obtained by crystallization from EtOAc/MeOH as a white powder, m.p. 176.3–177.1 °C (decomp.); [Found: C, 64.91; H, 4.75; N, 4.49. C₁₇H₁₅NO₅ requires C, 65.17; H, 4.83; N, 4.47%]; ν_{\max} (KBr) 3441, 3182, 1743, 1696, 1439, 1189 cm⁻¹; δ_H (400 MHz, CDCl₃) (**22Ab**) 7.19 (1 H, br.dt, $^3J_{6,7} \sim ^3J_{8,7}$ 7.7, $^4J_{9,7}$ 1.4 Hz, H-7), 7.10 (1 H, dd, $^3J_{8,9}$ 7.7, $^4J_{9,7}$ 1.4 Hz, H-9), 7.02 (1 H, dt, $^3J_{8,9} \sim ^3J_{8,7}$ 7.7, $^4J_{8,6}$ 1.4 Hz, H-8), 6.96 (1 H, dd, $^3J_{6,7}$ 7.7, $^4J_{6,8}$ 1.4 Hz, H-6), 6.92 (1 H, d, $^3J_{3,4}$ 5.5 Hz, H-4), 6.31 (1 H, d, $^3J_{3,4}$ 5.5 Hz, H-3), 5.59 (1 H, s, H-4b), 5.04 (1 H, d, $^2J_{10,10}$ 16.7 Hz, H-10A), 4.41 (1 H, d, $^2J_{10,10}$ 16.7 Hz, H-10B), 3.00 (1 H, d, $^3J_{12a,1}$ 8.7 Hz, H-12a), 2.88 (1 H, d, $^3J_{1,12a}$ 8.7 Hz, H-1), 1.74 (3 H, s, Me-2); δ_C (100.6 MHz, CDCl₃) 173.2 (CO₂H), 172.7 (C-12), 152.6 (C-5a), 139.4 (C-3), 135.0 (C-4), 128.3 (C-7), 127.2 (C-9), 122.9 (C-8), 119.7 (C-9a), 118.0 (C-6), 91.1 (C-4a), 89.5 (C-2), 83.1 (C-4b), 53.2 and 48.2 (C-12a and C-1), 40.0 (C-10), 16.0 (Me-2). MALDI-TOF HR: MNa⁺, found 336.0853. C₁₇H₁₅NNaO₅ requires 336.0842.

(2RS,4aRS,4bSR,12aSR)-1,12a-Dihydro-10H-2,4a-epoxyisoindolo[1,2-b][1,3]benzoxazin-12(2H,4bH)-one (23).

The condensation adduct (20 mmol), obtained as described above from 2-hydroxybenzylamine and furfural, was heated under reflux with NEt₃ (4.16 mL, 30.0 mmol) and acryloyl chloride (1.92 mL, 24.0 mmol) in PhMe (50 mL) for 4 h. The mixture was cooled, poured into water (250 mL), acidified with hydrochloric acid and extracted with EtOAc (4 × 60 mL). The combined organic phases were washed with a 2% HCl solution (100 mL), dried (MgSO₄), and concentrated. The residue was purified by silica gel column chromatography (2 × 25 cm, eluent: EtOAc/hexane, 1/3). The isolated vitreous pale yellow oil (1.28 g, 25 %) slowly crystallized on standing to give elongated thin colorless needles, m.p. 106.1–110.5 °C; [Found: C, 70.36; H, 5.15; N, 5.54. C₁₅H₁₃NO₃ requires C, 70.58; H, 5.13; N, 5.49%]; ν_{\max} (KBr) 1708, 1432, 1215 cm⁻¹; δ_{H} (400 MHz, CDCl₃) 7.19 (1 H, ddd, ³J_{6,7} 8.3, ³J_{8,7} 7.5, ⁴J_{9,7} 1.2 Hz, H-7), 7.09 (1 H, br.d, ³J_{8,9} 7.5 Hz, H-9), 7.00 (1 H, dt, ³J_{8,7} ~ ³J_{8,9} 7.5, ⁴J_{8,6} 1.2 Hz, H-8), 6.97 (1 H, dd, ³J_{6,7} 8.3, ³J_{8,6} 1.2 Hz, H-6), 6.78 (1 H, d, ³J_{3,4} 5.6 Hz, H-4), 6.43 (1 H, dd, ³J_{3,4} 5.6, ³J_{3,2} 1.5 Hz, H-3), 5.47 (1 H, s, H-4b), 5.18 (1 H, dd, ³J_{2,1exo} 4.4, ³J_{3,2} 1.5 Hz, H-2), 4.99 (1 H, d, ²J_{10,10} 16.8 Hz, H-10A), 4.36 (1 H, d, ²J_{10,10} 16.8 Hz, H-10B), 2.57 (1 H, dd, ³J_{12a,1exo} 3.7, ³J_{12a,1endo} 9.1 Hz, H-12a^{endo}), 2.22 (1 H, ddd, ²J_{1,1} 11.8, ³J_{2,1exo} 4.4, ³J_{12a,1exo} 3.7 Hz, H-1^{exo}), 1.68 (1 H, dd, ²J_{1,1} 11.8, ³J_{12a,1endo} 9.1 Hz, H-1^{endo}); δ_{C} (100.6 MHz, CDCl₃) 174.0 (C-12), 152.7 (C-5a), 136.1 (C-3), 131.8 (C-4), 128.1 (C-7), 127.0 (C-9), 122.3 (C-8), 119.8 (C-9a), 117.8 (C-6), 89.9 (C-4a), 83.3 (C-2), 80.0 (C-4b), 45.8 (C-12a), 39.7 (C-10), 27.5 (C-1). GC-MS (EI, 70 eV) *m/z* 255 (28, M⁺), 226 (4), 201 (31), 200 (63), 187 (7), 172 (5), 149 (7), 132 (11), 107 (28), 94 (8), 81 (17), 78 (42), 77 (31), 65 (10), 55 (100), 39 (24%).

7,9a-Epoxy[1,3]thiazolo[2,3-a]isoindole-6(9bH)-carboxylic acids (24). *Method A (two-step).* Freshly distilled furfural (10.9 mL, 0.13 mol) was added in one portion to a stirred solution of 2-aminoethanethiol hydrochloride (15.0 g, 0.13 mol) and anhydrous Na₂CO₃ powder (27.6 g, 0.26 mol) in CHCl₃ (250 mL) at room temperature. The mixture was stirred at room temperature for 24 h. The precipitate of inorganic salts was filtered off, washed with CHCl₃ (2 × 50 mL) and the solvent was then evaporated under reduced pressure. The residue was purified by column chromatography (silica gel, hexane/EtOAc, 1/1) to provide **2-(2-furyl)-1,3-thiazolidine** as a yellow oil, which crystallized upon cooling to give a yellow powder (17.8 g, 87 %); [Found: C, 54.20; H, 5.82; N, 9.04. C₇H₉NOS requires C, 54.17; H, 5.84; N, 9.02%]; ν_{\max} (KBr) 3188, 1484, 930, 733 cm⁻¹; δ_{H} (400 MHz, CDCl₃) 7.38 (1 H, dd, ³J_{4,5'} 1.6, ⁴J_{3,5'} 0.6 Hz, H-5'), 6.34 (1 H, dd, ³J_{3,4'} 3.1, ⁴J_{3,5'} 0.6 Hz, H-3'), 6.31 (1 H, dd, ³J_{3,4'} 3.1, ³J_{4,5'} 1.6 Hz, H-4'), 5.59 (1 H, s, H-2), 3.54–3.52 (1 H, m, H-5A), 3.19–3.04 (3 H, m, H-4, H-5B), 2.16 (1 H, br.s, NH); δ_{C} (100.6 MHz, CDCl₃) 152.7 (C-2'), 142.5 (C-5'), 110.2 and 107.5 (C-3' and C-4'), 65.4 (C-2), 52.4 (C-4), 36.0 (C-5). GC-MS (EI, 70 eV) *m/z* 155 (82, M⁺), 154 (9), 122 (11), 109 (78), 108 (26), 96 (51), 95 (51), 94 (100), 81 (73), 80 (74), 67 (22), 53 (23), 52 (37), 45 (36), 39 (70%).

2-[2-(5-Methylfuryl)-1,3-thiazolidine was obtained in a similar way.

A solution of maleic anhydride (5.59 g, 57.0 mmol) in PhH (100 mL) was added to a solution of (2-furyl)-1,3-thiazolidine (8.81 g, 57.0 mmol) in PhH (100 mL) and the mixture was stirred overnight at room temperature. The formed precipitate was collected by filtration, washed first with PhH (50 mL) and then with Et₂O (2 × 25 mL), and dried in air affording acids **24a** as

white powders (7.71 g, 56 %) with the **24Aa/24Ba** ratio of ~ 17/83.

This reaction can be carried out in a *one-pot* procedure (the yields of **24a** and the isomers ratio are comparable).

Method B (one pot). Freshly distilled furfural (1.78 mL, 21.7 mmol) was added in one portion at 0 °C to a stirred solution of 2-aminoethanethiol hydrochloride (2.47 g, 21.7 mmol) and NEt₃ (3.01 mL, 21.7 mmol) in CHCl₃ (15 mL). The mixture was stirred for 30 min at room temperature, then cooled to 0 °C and a solution of maleic anhydride (2.13 g, 21.7 mmol) in CHCl₃ (10 mL) was added at this temperature. The mixture was warmed to room temperature and stirred overnight. The formed precipitate was collected by filtration and dried affording **24a** (2.70 g, 49 %) as a white powder (ratio **24Aa/24Ba** is 15/85), m.p. 157–158 °C (EtOH/DMF, decomp.).

Generally, the title compound obtained by *Method B* was contaminated with 5–10 % NEt₃·HCl.

The individual isomer **24Ba** was obtained after recrystallization from EtOH/DMF as transparent tiny rhombus-shaped crystals.

(5aRS,6SR,7RS,9aSR,9bSR)-5-Oxo-2,3,5,5a,6,7-hexahydro-7,9a-epoxy[1,3]thiazolo[2,3-a]isoindole-6(9bH)-carboxylic acid (24Ba). M.p. 155–156 °C (decomp.); [Found: C, 52.13; H, 4.57; N, 5.42. C₁₁H₁₁NO₄S requires C, 52.16; H, 4.38; N, 5.53%]; ν_{\max} (KBr) 3184, 1743, 1679, 1402, 1168 cm⁻¹; δ_{H} (400 MHz, DMSO-*d*₆) 12.06 (1 H, br.s, CO₂H), 6.57 (1 H, d, ³J_{8,9} 5.6 Hz, H-9), 6.48 (1 H, dd, ³J_{8,9} 5.6, ³J_{7,8} 1.8 Hz, H-8), 5.66 (1 H, s, H-9b), 4.99 (1 H, d, ³J_{7,8} 1.8 Hz, H-7), 4.07 (1 H, ddd, ²J_{3,3} 11.2, ³J_{3a,2B} 5.6, ³J_{3a,2A} 2.5 Hz, H-3A), 3.18 (1 H, d, ³J_{5a,6} 8.7 Hz, H-6), 3.09–2.92 (2 H, m, H-2A and H-3B), 2.75–2.68 (1 H, m, H-2B), 2.49 (1 H, d, ³J_{5a,6} 8.7 Hz, H-5a); δ_{C} (100.6 MHz, DMSO-*d*₆) 172.6 and 170.3 (C-5 and CO₂H), 137.7 (C-9), 133.9 (C-8), 92.1 (C-9a), 80.5 (C-7), 63.7 (C-9b), 52.6 and 45.8 (C-5a and C-6), 44.9 (C-3), 31.9 (C-2). MS (EI, 70 eV) *m/z* 253 (10, M⁺), 209 (6), 156 (9), 155 (51), 154 (62), 127 (13), 122 (14), 111 (23), 108 (94), 99 (24), 96 (41), 88 (10), 85 (44), 80 (35), 71 (11), 68 (17), 61 (17), 60 (46), 56 (20), 55 (100), 45 (48), 43 (67%).

(5aRS,6SR,7RS,9aSR,9bRS)-5-Oxo-2,3,5,5a,6,7-hexahydro-7,9a-epoxy[1,3]thiazolo[2,3-a]isoindole-6(9bH)-carboxylic acid (24Aa) (in the mixture of **24Aa/24Ba** in ratio ~ 15/85). δ_{H} (400 MHz, DMSO-*d*₆) 12.18 (1 H, br.s, CO₂H), 6.61 (1 H, d, ³J_{8,9} 5.6 Hz, H-9), 6.52 (1 H, dd, ³J_{8,9} 5.6, ³J_{7,8} 1.4 Hz, H-8), 5.18 (1 H, s, H-9b), 5.16 (1 H, d, ³J_{7,8} 1.4 Hz, H-7), 4.24–4.18 (1 H, m, H-3A), 3.06–3.02 and 2.98–2.92 (1 H and 1 H, two m, H-2A and H-3B), 2.70 (1 H, br.dt, ³J_{2B,3} 6.4, ²J_{2,2} ~ ³J_{2B,3} 9.6 Hz, H-2B), 2.76 and 2.63 (1 H and 1 H, two d, ³J_{5a,6} 9.2 Hz, H-6 and H-5a); δ_{C} (100.6 MHz, DMSO-*d*₆) 174.8 and 172.1 (C-5 and CO₂H), 137.4 (C-9), 135.6 (C-8), 90.0 (C-9a), 82.5 (C-7), 65.6 (C-9b), 49.7 and 44.4 (C-5a and C-6), 45.6 (C-3), 33.0 (C-2).

Acids **24b** were obtained according to *Method A*, ratio of **24Ab/24Bb** ~ 67/33, yield 48 %. The individual isomer **24Ab** was obtained after three-fold recrystallization from EtOH as crystalline aggregates of thick colorless needles.

(5aRS,6SR,7RS,9aSR,9bSR)-7-Methyl-5-oxo-2,3,5,5a,6,7-hexahydro-7,9a-epoxy[1,3]thiazolo[2,3-a]isoindole-6(9bH)-carboxylic acid (24Ab). M.p. > 160 °C (decomp.); [Found: C, 53.82; H, 5.14; N, 5.58. C₁₂H₁₃NO₄S requires C, 53.92; H, 4.90; N, 5.24%]; ν_{\max} (KBr) 1717, 1697, 1666, 1220 cm⁻¹; δ_{H} (400 MHz, DMSO-*d*₆) 12.34 (1 H, br.s, CO₂H), 6.61 (1 H, d, ³J_{8,9} 5.5 Hz, H-9), 6.36 (1 H, d, ³J_{8,9} 5.5 Hz, H-8), 5.16 (1 H, s, H-9b), 4.24–4.16 (1 H, m, H-3A), 3.22–3.12 (3 H, m, H-2 and H-3B), 2.81 (1 H, d, ³J_{5a,6} 8.9 Hz, H-5a), 2.65 (1 H, ³J_{5a,6} 8.9 Hz, H-6), 1.53 (3 H, s, Me-7); δ_{C} (100.6 MHz, DMSO-*d*₆) 174.9 and 171.0 (C-5 and CO₂H), 140.3 and 136.3 (C-8 and C-9), 89.6 and 89.2

Tetrahedron

(C-7 and C-9a), 65.8 (C-9b), 52.7 and 48.0 (C-5a and C-6), 45.4 (C-3), 32.7 (C-2), 15.7 (Me-7). MS (EI, 70 eV) m/z 267 (M^+ , 17), 249 (20), 222 (4), 207 (2), 194 (5), 180 (5), 175 (4), 170 (27), 169 (100), 168 (87), 154 (36), 136 (45), 123 (50), 122 (96), 113 (13), 110 (42), 109 (73), 108 (42), 98 (72), 95 (47), 94 (38), 85 (68), 80 (37), 59 (40), 54 (84), 53 (95), 45 (37), 43 (94%).

(5aRS,6SR,7RS,9aSR,9bRS)-7-Methyl-5-oxo-2,3,5,6,7-hexahydro-7,9a-epoxy[1,3]thiazolo[2,3-a]isoindole-6(9bH)-carboxylic acid (24Bb) (in the mixture of **24Ab/24Bb** in ratio ~ 10/90). White powder. δ_H (400 MHz, DMSO- d_6) 12.18 (1 H, br.s, CO₂H), 6.62 (1 H, d, $^3J_{8,9}$ 5.7 Hz, H-9), 6.27 (1 H, d, $^3J_{8,9}$ 5.7 Hz, H-8), 5.60 (1 H, s, H-9b), 4.03 (1 H, ddd, $^2J_{3,3}$ 11.4, $^3J_{3,2}$ 6.4, $^3J_{3,2}$ 3.2 Hz, H-3A), 3.20 (1 H, dd, J 1.3, $^3J_{5a,6}$ 8.7 Hz, H-5a), 3.16–2.94 and 2.83–2.77 (2 H and 1 H, m and m, H-2 and H-3B), 2.52 (1 H, d, $^3J_{5a,6}$ 8.7 Hz, H-6), 1.55 (3 H, s, Me-7); δ_C (100.6 MHz, DMSO- d_6) 171.3 and 169.8 (C-5 and CO₂H), 140.2 and 135.4 (C-8 and C-9), 90.8 and 87.9 (C-7 and C-9a), 64.0 (C-9b), 56.3 and 48.3 (C-5a and C-6), 44.6 (C-3), 32.3 (C-2), 15.7 (Me-7).

7,9a-Epoxy[1,3]thiazolo[2,3-a]isoindol-5(5aH,9bH)-ones (25).

General experimental procedure. Freshly distilled furfural (8.0 mL, 96 mmol) was added in one portion at room temperature to a stirred solution of 2-aminoethanethiol hydrochloride (11.0 g, 96.0 mmol) and NEt₃ (13.3 mL, 96.0 mmol) in CHCl₃ (100 mL). The mixture was stirred for 30 min then cooled to 0 °C and a solution of acryloyl chloride (7.69 mL, 96.0 mmol) in CHCl₃ (100 mL) was added drop-wise at this temperature. The mixture was then warmed to room temperature and stirred overnight. The mixture was washed with water (100 mL) and brine (100 mL), dried over Na₂SO₄. The brown oil obtained after solvent evaporation was purified by silica gel column chromatography (hexane/EtOAc, 1/1). **3-Acryloyl-2-(2-furyl)-1,3-thiazolidine** obtained this way was used for thermal IMDAF reaction (see below). Yellow powder (19.0 g, 95 %); [Found: C, 57.50; H, 5.22; N, 6.74. C₁₀H₁₁NO₂S requires C, 57.39; H, 5.30; N, 6.69%]; ν_{max} (KBr) 1644, 1601 cm⁻¹. NMR spectra of this compound are difficult for interpretation due to strong widening of the signals even under heating up to 90 °C (DMSO- d_6). δ_H (600 MHz, CDCl₃) 7.37 (1 H, br.d, $^3J_{4',5'}$ 1.6 Hz, H-5'), 6.45 (1 H, dd, $^3J_{2'',3''}$ cis 10.0, $^2J_{3'',3''}$ 1.2 Hz, H-3'' cis), 6.38 (1 H, dd, $^3J_{2'',3''}$ trans 15.6, $^2J_{3'',3''}$ 1.2 Hz, H-3'' trans), 6.12–6.30 (3 H, m, H-3', H-4', H-2''), 5.71 (1 H, br.s, H-2), 4.23 (1 H, m, H-5A), 3.95 (1 H, m, H-4A), 3.17–3.09 (2 H, m, H-4B, H-5B); δ_C (100.6 MHz, CDCl₃) 164.4, 153.1, 142.9, 142.3, 129.4, 128.9, 128.2, 110.4, 107.3, 106.9, 58.29, 57.64, 49.13, 31.04, 29.10 some signals are double due to amidic rotation. GC-MS (EI, 70 eV) m/z 209 (40, M⁺), 182 (14), 181 (26), 155 (13), 154 (20), 148 (21), 126 (10), 122 (28), 109 (16), 108 (71), 96 (21), 95 (26), 88 (20), 80 (26), 55 (100), 45 (19), 43 (51%).

Intermediate 1-[2-(5-methylfuran-2-yl)thiazolidin-3-yl]prop-2-en-1-one (pale yellow oil, yield 73 %) was obtained in a similar way.

(5aRS,7SR,9aSR,9bSR)-2,3,6,7-Tetrahydro-7,9a-epoxy[1,3]thiazolo[2,3-a]isoindol-5(5aH,9bH)-one (25a). 3-Acryloyl-2-(2-furyl)-1,3-thiazolidine (10.6 g, 51.0 mmol) obtained in the previous step was heated under reflux in PhMe (100 mL) for 40 h. The precipitate formed upon cooling was collected by filtration and dried in air. Compound **25a** was obtained as a white powder (7.13 g, 67 %); m.p. 127–129 °C; [Found: C, 57.52; H, 5.24; N, 6.60. C₁₀H₁₁NO₂S requires C, 57.39; H, 5.30; N, 6.69%]; R_f (50% EtOAc/hexane) 0.45; ν_{max} (KBr) 1689 cm⁻¹; δ_H (600 MHz, CDCl₃) 6.42 (1 H, dd, $^3J_{8,9}$ 5.5, $^3J_{7,8}$ 1.8 Hz, H-8), 6.37 (1 H, d, $^3J_{8,9}$ 5.5 Hz, H-9), 5.56 (1 H, s, H-9b), 5.06 (1 H, dd, $^3J_{6exo,7}$ 3.7, $^3J_{7,8}$ 1.8 Hz, H-7), 4.38 (1 H, ddd,

$^2J_{3,3}$ 11.9, $^3J_{3A,2B}$ 6.4, $^3J_{3A,2A}$ 1.8 Hz, H-3A), 2.99 (1 H, dt, $^2J_{3,3}$ 11.9, $^3J_{3B,2A} \sim ^3J_{3B,2B}$ 6.4 Hz, H-3B), 2.93 (1 H, ddd, $^2J_{2,2}$ 11.0, $^3J_{3B,2A}$ 6.4, $^3J_{3A,2A}$ 1.8 Hz, H-2A), 2.85 (1 H, dt, $^2J_{2,2}$ 11.0, $^3J_{2B,3A} \sim ^3J_{2B,3B}$ 6.4 Hz, H-2B), 2.74 (1 H, dd, $^3J_{5a,6endo}$ 8.3, $^3J_{5a,6exo}$ 3.7 Hz, H-5a^{endo}), 2.26 (1 H, br.dt, $^2J_{6,6}$ 11.9, $^3J_{6exo,7} \sim ^3J_{5a,6exo}$ 3.7 Hz, H-6^{exo}), 1.52 (1 H, dd, $^2J_{6,6}$ 11.9, $^3J_{5a,6endo}$ 8.3 Hz, H-6^{endo}); δ_C (100.6 MHz, CDCl₃) 174.2 (C-5), 138.0 and 131.7 (C-8 and C-9), 92.9 (C-9a), 78.7 (C-7), 65.3 (C-9b), 50.5 (C-5a) 45.5 (C-3), 32.3 (C-2), 28.6 (C-6). GC-MS (EI, 70 eV) m/z 209 (63, M⁺), 181 (36), 164 (5), 155 (19), 154 (37), 148 (24), 126 (12), 109 (24), 108 (40), 96 (32), 94 (78), 88 (78), 80 (32) 77 (15), 70 (21), 66 (19), 65 (50), 61 (63), 56 (24), 55 (100), 45 (32%).

(5aRS,7SR,9aSR,9bSR)-7-Methyl-2,3,6,7-tetrahydro-7,9a-epoxy[1,3]thiazolo[2,3-a]isoindol-5(5aH,9bH)-one (25b). 1-[2-(5-Methyl-2-furyl)-1,3-thiazolidin-3-yl]prop-2-en-1-one (5.0 g, 22.4 mmol) obtained following the procedure above was heated under reflux in PhMe (100 mL) for 25 h. Evaporation of toluene under reduced pressure afforded a brown oil which solidified on cooling. The solid substance was purified by recrystallization (with activated carbon) from a hexane/EtOAc mixture. Compound **25b** was obtained as colorless, long needles (hedgehog-like crystalline aggregates) (2.85 g, 57 %); m.p. 161–162 °C; [Found: C, 59.06; H, 5.91; N, 6.53. C₁₁H₁₃NO₂S requires C, 59.17; H, 5.87; N, 6.27%]; R_f (50% EtOAc/hexane) 0.42; ν_{max} (KBr) 2942, 1682, 1396, 705 cm⁻¹; δ_H (400 MHz, CDCl₃) 6.40 (1 H, d, $^3J_{8,9}$ 5.9 Hz, H-8), 6.27 (1 H, d, $^3J_{8,9}$ 5.9 Hz, H-9), 5.53 (1 H, s, H-9b), 4.40 (1 H, ddd, $^2J_{3,3}$ 11.5, $^3J_{3A,2B}$ 5.9, $^3J_{3A,2A}$ 2.2 Hz, H-3A), 3.07–2.89 (3 H, m, H-3B, H-2), 2.85 (1 H, ddd, $^3J_{5a,6endo}$ 8.7, $^3J_{5a,6exo}$ 3.3, 5J 1.2 Hz, H-5a^{endo}), 2.03 (1 H, dd, $^2J_{6,6}$ 11.8, $^3J_{6exo,5a}$ 3.3 Hz, H-6^{exo}), 1.66 (3 H, s, Me-7), 1.64 (1 H, dd, $^2J_{6,6}$ 11.8, $^3J_{6endo,5a}$ 8.7 Hz, H-6^{endo}); δ_C (100.6 MHz, CDCl₃) 174.2 (C-5), 141.0 (C-8), 132.3 (C-9), 92.5 (C-9a), 86.8 (C-7), 65.4 (C-9b), 53.6 (C-5a), 45.2 (C-3), 34.6 and 32.3 (C-6 and C-2), 18.7 (Me-7). GC-MS (EI, 70 eV) m/z 223 (18, M⁺), 208 (8), 195 (9), 180 (39), 168 (9), 162 (15), 152 (17), 136 (10), 122 (31), 113 (7), 109 (14), 108 (28), 95 (26), 88 (8), 79 (9), 55 (100), 53 (12), 43 (22%).

Methyl esters of 7,9a-epoxy[1,3]thiazolo[2,3-a]isoindole-6(9bH)carboxylic acids (26).

Methyl (5aRS,6SR,7RS,9aSR,9bRS)-5-oxo-2,3,5,6,7-hexahydro-7,9a-epoxy[1,3]thiazolo[2,3-a]isoindole-6(9bH)-carboxylate (26Aa) and methyl (5aRS,6SR,7RS,9aSR,9bSR)-5-oxo-2,3,5,6,7-hexahydro-7,9a-epoxy[1,3]thiazolo[2,3-a]isoindole-6(9bH)-carboxylate (26Ba). The acid **24Ba** (1.0 g, 3.91 mmol) was dissolved in MeOH (50 mL) and one drop of H₂SO₄ (conc.) was added. The mixture was refluxed for 4 h. EtOAc (200 mL) was then added. The mixture was washed with saturated sodium bicarbonate solution (50 mL), then with water (50 mL) and dried over Na₂SO₄. Evaporation of the solvent under reduced pressure yielded the desired product **26a** (0.74 g, 73 %), as a mixture of isomers in ratio **26Aa/26Ba** ~ 29/71, white powder, m.p. 122.0–122.8 °C (EtOAc). δ_H (600 MHz, CDCl₃) (**26Aa**) 6.61 (1 H, dd, $^3J_{8,9}$ 6.0, $^3J_{7,8}$ 1.9 Hz, H-8), 6.43 (1 H, d, $^3J_{8,9}$ 6.0 Hz, H-9), 5.22 (1 H, d, $^3J_{7,8}$ 1.9 Hz, H-7), 5.20 (1 H, s, H-9b), 4.45 (1 H, ddd, $^2J_{3,3}$ 11.7, $^3J_{3A,2B}$ 6.7, $^3J_{3A,2A}$ 2.1 Hz, H-3A), 3.73 (3 H, s, CO₂Me), 3.16–3.13 (1 H, m, H-3B), 3.05–2.93 (2 H, m, H-2), 2.81 and 2.77 (1 H and 1 H, two d, $^3J_{5a,6}$ 8.9 Hz, H-6 and H-5a); δ_C (100.6 MHz, CDCl₃) 174.7 and 171.2 (C-2 and CO₂Me), 136.4 and 136.1 (C-9 and C-8), 90.4 (C-9a), 82.6 (C-7), 65.9 (C-9b), 52.2, 50.2 and 44.9 (C-5a, C-6 and CO₂Me), 45.9 (C-3), 33.4 (C-2). After recrystallization of the isomer mixture from EtOAc/heptane the isomer **26Ba** was obtained (0.40 g, 40 %) as white needles, m.p. 131.8–133.0 °C; [Found: C, 53.81; H,

4.83; N, 5.36. C₁₂H₁₃NO₄S requires C, 53.92; H, 4.90; N, 5.24%; R_f (EtOAc) 0.43; ν_{max} (KBr) 2948, 1727, 1688, 1387, 1270 cm⁻¹; δ_H (400 MHz, CDCl₃) 6.53 (1 H, dd, ³J_{8,9} 5.8, ³J_{7,8} 1.2 Hz, H-8), 6.49 (1 H, d, ³J_{8,9} 5.8 Hz, H-9), 5.54 (1 H, s, H-9b), 5.22 (1 H, d, ³J_{7,8} 1.2 Hz, H-7), 4.43 (1 H, ddd, ²J_{3,3} 11.2, ³J_{3A,2B} 4.4, ³J_{3A,2A} 2.5 Hz, H-3A), 3.77 (3 H, s, CO₂Me), 3.11 (1 H, br.d, ³J_{5a,6} 9.1 Hz, H-6), 3.04–2.92 (3 H, m, H-2 and H-3B), 2.72 (1 H, d, ³J_{5a,6} 9.1 Hz, H-5a); δ_C (100.6 MHz, CDCl₃) 172.0 and 170.8 (C-2 and CO₂Me), 138.1 (C-9), 133.6 (C-8), 92.7 (C-9a), 80.8 (C-7), 64.2 (C-9b), 53.2, 52.1 and 46.1 (C-5a, C-6 and CO₂Me), 45.9 (C-3), 32.3 (C-2). GC-MS (EI, 70 eV) *m/z* 267 (8, M⁺), 235 (9), 208 (2), 180 (4), 156 (7), 155 (11), 154 (100), 153 (16), 152 (5), 122 (8), 113 (33), 108 (24), 96 (7), 94 (8), 85 (26), 81 (19), 80 (8), 60 (5), 59 (23), 53 (6), 39 (7%).

Isomeric mixture of methyl (5*aRS*,6*SR*,7*RS*,9*aSR*,9*bRS*)-7-methyl-5-oxo-2,3,5,5*a*,6,7-hexahydro-7,9*a*-

epoxy[1,3]thiazolo[2,3-*a*]isoindole-6(9*bH*)-carboxylate (26*Ab*) and methyl (5*aRS*,6*SR*,7*RS*,9*aSR*,9*bSR*)-7-methyl-5-oxo-2,3,5,5*a*,6,7-hexahydro-7,9*a*-epoxy[1,3]thiazolo[2,3-

a]isoindole-6(9*bH*)-carboxylate (26*Bb*) (0.63 g, 63 %) is obtained in a similar way from acid 24*Ab*, 26*Ab*/26*Bb* ~ 67/33, white powder, m.p. 104.8–105.8 °C; [Found: C, 55.31; H, 5.38; N, 5.20. C₁₃H₁₅NO₄S requires C, 55.50; H, 5.37; N, 4.98%]; R_f (EtOAc) 0.74; ν_{max} (KBr) 1720, 1687 (br.), 1030 cm⁻¹; δ_H (600 MHz, CDCl₃) (26*Bb*) 6.52 and 6.23 (1 H and 1 H, two d, ³J_{8,9} 5.5 Hz, H-9 and H-8), 5.47 (1 H, s, H-9b), 4.38 (1 H, ddd, ²J_{3,3} 11.2, ³J_{3A,2B} 4.1, ³J_{3A,2A} 3.2 Hz, H-3A), 3.72 (3 H, s, CO₂Me), 3.16–2.98 (3 H, m, H-3B and H-2), 3.14 and 2.74 (1 H and 1 H, br.d, ³J_{5a,6} 9.0 Hz, H-5a and H-6), 1.68 (3 H, s, Me-7); (26*Ab*) 6.62 and 6.25 (1 H and 1 H, two d, ³J_{8,9} 5.5 Hz, H-9 and H-8), 5.23 (1 H, s, H-9b), 4.50 (1 H, ddd, ²J_{3,3} 11.7, ³J_{3A,2B} 4.1, ³J_{3A,2A} 2.2 Hz, H-3A), 3.75 (3H, s, CO₂Me), 3.16–2.98 (3 H, m, H-3B, H-2), 2.85 and 2.82 (1 H and 1 H, two d, ³J_{5a,6} 9.0 Hz, H-5a and H-6), 1.62 (3 H, s, Me-7); δ_C (100.6 MHz, DMSO-*d*₆) (mixture of 26*Ab* and 26*Bb*) 174.7, 170.6, 170.2, 170.0 (CO₂Me and C-5), 140.3, 140.2, 136.3, 135.4 (C-8 and C-9), 91.1, 89.7, 89.3, 87.7 (C-7 and C-9a), 65.7, 64.0 (C-9b), 56.5, 52.9, 51.3, 51.0, 48.0, 47.9 (C-5a, C-6, CO₂Me), 45.4, 44.7 (C-3), 32.8, 32.3 (C-2), 15.59, 15.56 (Me-1); GC-MS (EI, 70 eV) *m/z* 281 (5, M⁺), 250 (4), 249 (5), 248 (6), 222 (3), 194 (5), 169 (12), 168 (100), 136 (7), 135 (14), 122 (15), 114 (10), 113 (70), 108 (17), 95 (20), 85 (18), 59 (20), 53 (11), 43 (16%). All of the presented data was obtained for the mixture of isomers.

(3*RS*,3*aSR*,6*SR*,7*aRS*)-2-[2-(Acetylthio)ethyl]-1-oxo-

1,2,3,6,7*a*-hexahydro-3*a*,6-epoxyisoindol-3-yl acetate (27). A catalytic amount of BF₃·Et₂O (~ 0.2 mL) was added to a stirred solution of thiazolo[2,3-*a*]isoindol-5-one 25*a* (1.0 g, 4.8 mmol) in Ac₂O (10 mL). The reaction mixture was stirred at room temperature for 24 h, then poured into water (100 mL) and 1 M KOH solution was added to the cooled mixture till pH ~ 8. The mixture was extracted with CHCl₃ (4 × 60 mL) and the combined organic phases were dried over Na₂SO₄. A viscous brown residue obtained after solvent evaporation was purified by column chromatography (silica gel, hexane/EtOAc, 1/1) affording the compound 27 (0.39 g, 25 %) as a white powder. M.p. 102.7–104.3 °C; [Found: C, 54.04; H, 5.47; N, 4.72. C₁₄H₁₇NO₅S requires C, 54.01; H, 5.50; N, 4.50%]; R_f (65% EtOAc/hexane) 0.43; ν_{max} (KBr) 2946, 1758, 1712, 1705, 1225, 956, 623 cm⁻¹; δ_H (400 MHz, CDCl₃) 6.44 (1 H, s, H-3), 6.40 (1 H, dd, ³J_{5,4} 6.2, ³J_{5,6} 1.3 Hz, H-5), 6.38 (1 H, d, ³J_{5,4} 6.2 Hz, H-4), 5.11 (1 H, dd, ³J_{5,6} 1.3, ³J_{6,7*exo*} 4.6 Hz, H-6), 3.64–3.57 (1 H, m, NCH₂A), 3.48–3.41 (1 H, m, NCH₂B), 3.11–3.07 (2 H, m, SCH₂), 2.56 (1 H, dd, ³J_{7*endo*,7*a*} 8.7, ³J_{7*exo*,7*a*} 3.1 Hz, H-7a), 2.33 (3 H, s, OAc), 2.21 (3 H,

s, SAc), 2.17 (1 H, ddd, ²J_{7,7} 11.8, ³J_{6,7*exo*} 4.6, ³J_{7*exo*,7*a*} 3.1 Hz, H-7*exo*), 1.61 (1 H, dd, ²J_{7,7} 11.8, ³J_{7*endo*,7*a*} 8.7 Hz, H-7*endo*); δ_C (100.6 MHz, CDCl₃) 194.9 (SCOME), 175.8 (C-1), 170.1 (OCOME), 136.7 (C-5), 131.4 (C-4), 90.6 (C-3a), 82.7 and 80.2 (C-3 and C-6), 45.0 (C-7a), 41.6 (NCH₂), 30.6 (SCOME), 28.1 (C-7), 27.2 (SCH₂), 21.0 (OCOME); MS (EI, 70 eV) *m/z* 311 (2, M⁺), 252 (13), 236 (86), 222 (15), 210 (36), 209 (88), 180 (5), 154 (10), 150 (16), 139 (24), 126 (9), 122 (70), 108 (88), 98 (12), 97 (75), 81 (16), 66 (16), 55 (45), 43 (100%).

8,10*a*-Epoxy[1,3]thiazino[2,3-*a*]isoindole-7(10*bH*)-carboxylic acids (31). General experimental procedure. A suspension of 3-aminopropane-1-thiol (0.91 g, 10.0 mmol), corresponding furfural (~ 0.9 mL, 10.0 mmol) and anhydrous powdered MgSO₄ (2.42 g, 20 mmol) in CH₂Cl₂ (30 mL) was stirred at room temperature for 2 h. MgSO₄ was filtered off and washed with CH₂Cl₂ (2 × 10 mL). To the obtained solution of 2-furanyl-1,3-thiazinane, maleic anhydride (1.08 g, 11.0 mmol) was added (some blurring and warming of the reaction mixture was observed). The mixture was stirred at room temperature for 24 h. Viscous yellow oil was formed. The solvent was removed under reduced pressure and the residue, a slowly crystallizing yellow oil was purified by crystallization from MeOH. The title acids 31 were obtained as colorless needle-shaped crystals.

Intermediate 2-(furan-2-yl)-1,3-thiazinane was isolated and characterized during preparation of acid 31*a*. δ_H (400 MHz, CDCl₃) 7.35 (1 H, dd, ³J_{5,4} 1.9, ⁴J_{5,3} 0.8 Hz, H-5'), 6.31 (1 H, dd, ³J_{4,3} 3.2, ³J_{5,4} 1.9, Hz H-4'), 6.29 (1 H, br.d, ³J_{4,3} 3.2 Hz, H-3'), 5.29 (1 H, s, H-2), 3.33 (1H, ddd, ²J_{4,4} 14.5, ³J_{4e,5a} 3.5, ³J_{4e,5e} 1.2 Hz, H-4^{eq}), 3.14 (1H, ddd, ²J_{6,6} 13.7, ³J_{5a,6a} 11.2, ³J_{6a,5e} 3.5 Hz, H-6^{ax}), 2.93 (1H, ddd, ²J_{4,4} 14.5, ³J_{5a,4a} 11.8, ³J_{4a,5e} 3.5 Hz, H-4^{ax}), 2.90–2.85 (1 H, m, H-6^{eq}), 1.93 (1 H, br.s, NH), 1.79–1.63 (2 H, m, H-5); δ_C (100.6 MHz, CDCl₃) 153.1 (C-2'), 141.7 (C-5'), 110.0 and 106.0 (C-3' and C-4'), 58.5 (C-2), 46.7 (C-6), 29.0 (C-4), 25.6 (C-5). GC-MS (EI, 70 eV) *m/z* 169 (61, M⁺), 136 (12), 122 (100), 109 (59), 108 (35), 95 (82), 94 (74), 81 (61), 80 (54), 67 (24), 52 (25), 45 (24), 41 (33), 39 (57%).

(6*aRS*,7*SR*,8*RS*,10*aSR*,10*bRS*)-6-Oxo-3,4,6,6*a*,7,8-hexahydro-2*H*-8,10*a*-epoxy[1,3]thiazino[2,3-*a*]isoindole-7(10*bH*)-carboxylic acid (31*a*). Thick colorless needles (1.29 g, 48 %), m.p. 183.5–189 °C (decomp., from MeOH); [Found: C, 53.98; H, 5.01; N, 5.41. C₁₂H₁₃NO₄S requires C, 53.92; H, 4.90; N, 5.24%]; ν_{max} (KBr) 3006, 1735, 1658, 1444, 1172 cm⁻¹; δ_H (400 MHz, DMSO-*d*₆) 12.20 (1 H, br.s, CO₂H), 6.51 (1 H, dd, ³J_{9,10} 5.7, ³J_{9,8} 1.3 Hz, H-9), 6.49 (1 H, d, ³J_{10,9} 5.7 Hz, H-10), 5.26 (1 H, s, H-10*b*), 5.07 (1 H, d, ³J_{8,9} 1.3 Hz, H-8), 3.99 (1 H, ddd, ²J_{4,4} 13.4, ³J_{4e,3a} 3.6, ³J_{4e,3e} 1.9 Hz, H-4^{eq}), 3.17 (1 H, dt, ³J_{2a,3a} ~ ²J_{2,2} 13.4, ³J_{2e,2a} 2.5 Hz, H-2^{ax}), 2.92 (1 H, dt, ²J_{4,4} ~ ³J_{4a,3a} 13.4, ³J_{4a,3e} 3.1 Hz, H-4^{ax}), 2.92–2.87 (1 H, m, H-2^{eq}), 2.75 (1 H, d, ³J_{6a,7} 9.1 Hz, H-6*a*), 2.56 (1 H, d, ³J_{7,6a} 9.1 Hz, H-7), 1.87–1.80 (1 H, m, H-3^{eq}), 1.53–1.40 (1 H, m, H-3^{ax}); δ_C (100.6 MHz, DMSO-*d*₆) 172.4 (CO₂H), 168.9 (C-6), 137.6 (C-9), 133.0 (C-10), 89.8 (C-10*a*), 81.8 (C-8), 59.0 (C-10*b*), 49.3 (C-6*a*), 44.1 (C-7), 39.7 (C-4), 27.5 (C-2), 24.9 (C-3). MS (EI, 70 eV) *m/z* 267 (13, M⁺), 221 (7), 169 (12), 168 (100), 167 (13), 166 (8), 122 (11), 121 (8), 102 (11), 99 (30), 81 (12), 46 (11), 45 (45), 44 (7), 42 (6), 41 (24), 39 (16), 29 (14), 28 (16), 27 (17%).

(6*aRS*,7*SR*,8*RS*,10*aSR*,10*bRS*)-8-Methyl-6-oxo-3,4,6,6*a*,7,8-hexahydro-2*H*-8,10*a*-epoxy[1,3]thiazino[2,3-*a*]isoindole-7(10*bH*)-carboxylic acid (31*b*). Colorless needles (1.29 g, 46 %), m.p. 184.2–185.2 °C (MeOH); [Found: C, 55.54; H, 5.09; N, 5.34. C₁₃H₁₅NO₄S requires C, 55.50; H, 5.37; N, 4.98%]; ν_{max} (KBr) 1732, 1653, 1430, 1170, 1131, 871 cm⁻¹; δ_H (400 MHz, DMSO-*d*₆) 12.22 (1 H, br.s, CO₂H), 6.53 (1 H, d, ³J_{9,10} 5.7 Hz, H-

Tetrahedron

9), 6.35 (1 H, d, $^3J_{10,9}$ 5.7 Hz, H-10), 5.25 (1 H, s, H-10b), 4.01–3.98 (1 H, m, $^2J_{4,4} \sim 14.0$ Hz, H-4^{eq}), 3.16 (1 H, dt, $^3J_{2a,3a} \sim ^2J_{2,2}$ 13.5, $^3J_{2e,2a}$ 1.9 Hz, H-2^{ax}), 2.95–2.87 (2 H, m, H-4^{ax} and H-2^{eq}), 2.79 (1 H, d, $^3J_{6a,7}$ 8.9 Hz, H-6a), 2.58 (1 H, d, $^3J_{7,6a}$ 8.9 Hz, H-7), 1.85–1.80 (1 H, m, H-3^{eq}), 1.52 (3 H, s, Me-8), 1.55–1.42 (1 H, m, H-3^{ax}); δ_C (100.6 MHz, DMSO-*d*₆) 171.3 (CO₂H), 169.2 (C-6), 140.4 (C-9), 134.0 (C-10), 89.2 (2C, C-10a and C-8), 59.3 (C-10b), 52.5 (C-6a), 47.5 (C-7), 39.7 (C-4), 27.4 (C-2), 24.8 (C-3), 15.5 (Me-8). MS (EI, 70 eV) *m/z* 281 (16, M⁺), 236 (7), 235 (19), 220 (13), 183 (16), 182 (100), 162 (7), 152 (8), 136 (19), 135 (11), 125 (10), 110 (9), 109 (8), 102 (18), 99 (8), 95 (10), 73 (10), 45 (8), 43 (16), 41 (11%).

(6aRS,8SR,10aSR,10bRS)-3,4,7,8-Tetrahydro-2H-8,10a-epoxy[1,3]thiazino[2,3-*a*]isoindol-6(6aH,10bH)-one (32).

Furfural (0.65 mL, 7.90 mmol) and anhydrous powdered MgSO₄ (1.89 g, 16.0 mmol) was added to a solution of 3-aminopropanethiol (0.72 g, 7.90 mmol) in CH₂Cl₂ (30 mL). The reaction mixture was stirred at room temperature for 2 h. MgSO₄ was filtered off, washed with CH₂Cl₂ (2 × 10 mL), and the solvent was evaporated under reduced pressure. Obtained 2-(2-furyl)-1,3-thiazinane (~ 7.9 mmol) was dissolved in PhMe (50 mL) and then acryloyl chloride (0.96 mL, 12.0 mmol) and NEt₃ (2.22 mL, 16.0 mmol) were added to the solution. The reaction mixture was heated under reflux for 3 h, then cooled and poured into water (50 mL). The organic layer was separated and the water layer was extracted with EtOAc (3 × 20 mL). The organic phases were combined and dried over MgSO₄. The brown oil obtained after solvent evaporation was crystallized in Et₂O (10 mL). After recrystallization of the precipitate from an EtOAc/hexane mixture, thiazino[2,3-*a*]isoindol **32** was isolated (0.46 g, 26 %) as fine colorless needles, m.p. 140–141 °C (EtOAc/hexane); [Found: C, 59.04; H, 5.60; N, 6.53. C₁₁H₁₃NO₂S requires C, 59.17; H, 5.87; N, 6.27%]; ν_{\max} (KBr) 1676, 1419, 1253, 956 cm⁻¹; δ_H (400 MHz, CDCl₃) 6.43 (1 H, d, $^3J_{10,9}$ 5.8 Hz, H-10), 6.37 (1 H, dd, $^3J_{9,10}$ 5.8, $^3J_{9,8}$ 1.5 Hz, H-9), 5.07 (1 H, dd, $^3J_{8,7\text{exo}}$ 4.4, $^3J_{8,9}$ 1.5 Hz, H-8), 5.04 (1 H, s, H-10b), 4.29 (1 H, dd, $^2J_{4,4}$ 13.7, $^3J_{4e,3a}$ 2.5, $^3J_{4e,3e}$ 1.9 Hz, H-4^{eq}), 3.09 (1 H, ddd, $^2J_{2,2}$ 13.7, $^3J_{2a,3a}$ 12.5, $^3J_{2a,3e}$ 3.1 Hz, H-2^{ax}), 2.93–2.81 (2 H, m, H-2^{eq} and H-4^{ax}), 2.52 (1 H, dd, $^3J_{6a,7\text{endo}}$ 8.7, $^3J_{6a,7\text{exo}}$ 3.7 Hz, H-6a), 2.15 (1 H, ddd, $^2J_{7,7}$ 11.5, $^3J_{7\text{exo},8}$ 4.4, $^3J_{7\text{exo},6a}$ 3.7 Hz, H-7^{exo}), 1.89–1.82 (1 H, m, H-3^{eq}), 1.80–1.72 (1 H, m, H-3^{ax}), 1.60 (1 H, dd, $^2J_{7,7}$ 11.5, $^3J_{7\text{endo},6a}$ 8.7 Hz, H-7^{endo}); δ_C (100.6 MHz, CDCl₃) 172.4 (C-6), 136.7 (C-9), 131.6 (C-10), 90.6 (C-10a), 79.5 (C-8), 61.0 (C-10b), 46.4 (C-6a), 40.5 (C-4), 28.6 and 27.8 (C-2 and C-7), 25.1 (C-3). GC-MS (EI, 70 eV) *m/z* 223 (50, M⁺), 196 (4), 195 (22), 168 (100), 148 (11), 134 (10), 122 (18), 111 (20), 108 (27), 102 (28), 94 (35), 81 (34), 65 (36), 56 (31), 55 (85), 45 (37), 41 (50), 39 (62%).

2,4a-Epoxyisoindolo[1,2-*b*][1,3]benzothiazole-1(4bH)-carboxylic acids (33). General experimental procedure.

Anhydrous powdered MgSO₄ (7.21 g, 60 mmol) and then 2-aminothiophenol (3.30 mL, 30 mmol) were added to a solution of the corresponding furaldehyde (30 mmol) in CH₂Cl₂ (50 mL). The reaction mixture was stirred at room temperature for 3–4 h. MgSO₄ was filtered off and washed with CH₂Cl₂ (2 × 25 mL). The organic phases were combined and concentrated under reduced pressure. The residue, a yellow-brown oil, was dissolved in Me₂CO (30 mL) and a solution of maleic anhydride (3.09 g, 31.5 mmol) in Me₂CO (20 mL) was added in one portion with stirring. The reaction mixture was then stirred at room temperature for 12 h. The precipitate formed was collected by filtration, washed with Me₂CO (3 × 20 mL) and air-dried till

constant weight. Isoindolo[1,2-*b*][1,3]benzothiazole acids **33a–c** were obtained as white easy-electrifiable powders.

(1RS,2SR,4aRS,4bRS,11aSR)-11-Oxo-1,2,11,11a-tetrahydro-2,4a-epoxyisoindolo[1,2-*b*][1,3]benzothiazole-1(4bH)-carboxylic acid (33a).

White powder (5.38 g, 60 %), m.p. 176–176.7 °C (decomp.); [Found: C, 59.63; H, 3.52; N, 4.78. C₁₅H₁₁NO₄S requires C, 59.79; H, 3.68; N, 4.65%]; ν_{\max} (KBr) 3540, 1719, 1707, 1470, 1362, 759 cm⁻¹; δ_H (600 MHz, DMSO-*d*₆) 12.32 (1 H, br.s, CO₂H), 7.42 (1 H, dd, $^3J_{8,9}$ 8.0, $^4J_{7,9}$ 1.4 Hz, H-9), 7.28 (1 H, br.d, $^3J_{6,7}$ 7.6 Hz, H-6), 7.08 (1 H, dt, $^3J_{6,7} \sim ^3J_{7,8}$ 7.6, $^4J_{7,9}$ 1.4 Hz, H-7), 7.03 (1 H, ddd, $^3J_{8,9}$ 8.0, $^3J_{8,7}$ 7.6, $^4J_{6,8}$ 1.4 Hz, H-8), 6.68 (1 H, s, H-4b), 6.60 (1 H, d, $^3J_{3,4}$ 5.7 Hz, H-4), 6.52 (1 H, dd, $^3J_{3,4}$ 5.7, $^3J_{3,2}$ 1.6 Hz, H-3), 5.08 (1 H, d, $^3J_{2,3}$ 1.6 Hz, H-2), 3.40 (1 H, d, $^3J_{1,11a}$ 8.9 Hz, H-1), 2.59 (1 H, d, $^3J_{1,11a}$ 8.9 Hz, H-11a); δ_C (150.9 MHz, DMSO-*d*₆) 173.2 and 169.9 (CO₂H and C-11), 138.7, 135.4, 133.8, 132.4 (C-3, C-4, C-5a, C-9a), 125.8, 125.7, 123.2 (C-6, C-7, C-8), 116.4 (C-9), 91.7 (C-4a), 82.0 (C-2), 67.3 (C-4b), 54.8 and 46.5 (C-1 and C-11a). MS (EI, 70 eV) *m/z* 301 (66, M⁺), 285 (2), 258 (4), 228 (10), 205 (25), 204 (47), 203 (72), 202 (100), 186 (20), 175 (13), 174 (71), 173 (60), 172 (16), 170 (43), 162 (10), 149 (26), 136 (86), 135 (30), 117 (24), 110 (33), 109 (35), 101 (14), 99 (45), 83 (18), 77 (15), 69 (35), 65 (55), 59 (27), 55 (26), 54 (80), 51 (25), 45 (38), 43 (55), 41 (18%).

(1RS,2SR,4aRS,4bRS,11aSR)-2-Methyl-11-oxo-1,2,11,11a-tetrahydro-2,4a-epoxyisoindolo[1,2-*b*][1,3]benzothiazole-1(4bH)-carboxylic acid (33b).

White powder (5.10 g, 54 %) (33 % after recrystallization from *i*-PrOH/DMF), m.p. 129.1–129.6 °C (decomp.); [Found: C, 60.99; H, 4.39; N, 4.25. C₁₆H₁₃NO₄S requires C, 60.94; H, 4.16; N, 4.44%]; ν_{\max} (KBr) 3437, 1746, 1691, 1469, 1367, 1367, 1183, 754 cm⁻¹; δ_H (600 MHz, DMSO-*d*₆) 12.34 (1 H, br.s, CO₂H), 7.46 (1 H, br.d, $^3J_{8,9}$ 7.7 Hz, H-9), 7.28 (1 H, br.d, $^3J_{6,7}$ 7.7 Hz, H-6), 7.08 (1 H, br.t, $^3J_{6,7} \sim ^3J_{7,8}$ 7.7 Hz, H-7), 7.03 (1 H, br.t, $^3J_{8,9} \sim ^3J_{8,7}$ 7.7 Hz, H-8), 6.64 (1 H, d, $^3J_{3,4}$ 5.8 Hz, H-4), 6.63 (1 H, s, H-4b), 6.34 (1 H, d, $^3J_{3,4}$ 5.8 Hz, H-3), 3.41 (1 H, d, $^3J_{1,11a}$ 9.1 Hz, H-1), 2.63 (1 H, d, $^3J_{1,11a}$ 9.1 Hz, H-11a), 1.55 (3 H, s, Me-2); δ_C (100.6 MHz, DMSO-*d*₆) 171.2 and 169.0 (CO₂H and C-11), 140.7 and 134.6 (C-3 and C-4), 135.0 and 132.0 (C-5a and C-9a), 125.2 (2 C) and 122.7 (C-6, C-7, C-8), 115.5 (C-9), 90.0 and 88.9 (C-2 and C-4a), 67.1 (C-4b), 57.9 and 48.9 (C-1 and C-11a), 15.6 (Me-2). MS (EI, 70 eV) *m/z* (%): 315 (13 M⁺), 271 (1), 254 (3), 242 (6), 223 (9), 218 (20), 217 (85), 216 (100), 215 (30), 210 (8), 202 (40), 187 (8), 186 (10), 177 (26), 174 (89), 170 (10), 157 (9), 136 (78), 125 (12), 110 (20), 109 (38), 98 (33), 95 (47), 81 (22), 76 (14), 69 (24), 65 (30), 60 (14), 55 (14), 54 (39), 53 (35), 51 (10), 45 (32), 43 (25), 42 (10%).

(1RS,2SR,4aSR,4bSR,11aRS)-2-Bromo-11-oxo-1,2,11,11a-tetrahydro-2,4a-epoxyisoindolo[1,2-*b*][1,3]benzothiazole-1(4bH)-carboxylic acid (33c)

was obtained following the procedure above. After addition of maleic anhydride, a dark purple reaction mixture was formed with a little precipitate present. The mixture was stirred at room temperature for 4 h. The precipitate was collected by filtration, washed with boiling Me₂CO (4 × 15 mL), and finally recrystallized from an *i*-PrOH/DMF mixture. A pale pink powder was obtained (0.68 g, 6 %), m.p. 145.4–147.5 °C (decomp.); [Found: C, 47.16; H, 2.68; N, 3.84; Br, 21.02%]; ν_{\max} (KBr) 3413, 1752, 1691, 1554, 1469, 1370, 1237, 1178 cm⁻¹; δ_H (400 MHz, DMSO-*d*₆) 12.62 (1 H, br.s, CO₂H), 7.50 (1 H, dd, $^3J_{8,9}$ 7.6, $^4J_{7,9}$ 1.2 Hz, H-9), 7.34 (1 H, dd, $^3J_{6,7}$ 7.6, $^4J_{6,8}$ 1.2 Hz, H-6), 7.14 (1 H, dt, $^3J_{6,7} \sim ^3J_{7,8}$ 7.6 Hz, $^4J_{7,9}$ 1.2 Hz, H-7), 7.08 (1 H, dt, $^3J_{8,9} \sim ^3J_{8,7}$ 7.6, $^4J_{6,8}$ 1.2 Hz, H-8),

6.84 (1 H, d, $^3J_{3,4}$ 5.5 Hz, H-4), 6.71 (1 H, s, H-4b), 6.62 (1 H, d, $^3J_{3,4}$ 5.5 Hz, H-3), 3.62 (1 H, d, $^3J_{1,11a}$ 8.9 Hz, H-11a), 3.14 (1 H, d, $^3J_{1,11a}$ 8.9 Hz, H-1); δ_C (100.6 MHz, DMSO- d_6) 169.3 and 167.9 (CO₂H and C-11), 140.7 and 136.0 (C-3 and C-4), 134.7 and 131.7 (C-5a and C-9a), 125.40, 125.34, 122.8 (C-6, C-7, C-8), 115.4 (C-9), 90.5 and 89.5 (C-2 and C-4a), 66.5 (C-4b), 57.3 and 52.1 (C-1 and C-11a). HRMS (DART): MH⁺, found 379.9569 (for Br⁷⁹) and 381.9585 (for Br⁸¹). C₁₅H₁₁BrNO₄S requires 379.9592 (for Br⁷⁹).

Synthesis of **isoindolo[1,2-*b*][1,3]benzothiazol-11-one (34) and N-acryloyl derivative (34*)**. A suspension of 2-aminobenzenethiol (3.30 mL, 30 mmol), furfural (2.52 mL, 30 mmol) and anhydrous powdered MgSO₄ (3.60 g, 30 mmol) in CH₂Cl₂ (50 mL) was stirred at room temperature for 3 h. MgSO₄ was filtered off, the solvent was evaporated and the residue, a yellow oil, was dissolved in PhMe (50 mL). NEt₃ (6.24 mL, 45 mmol) was added and the mixture was cooled to 0 °C. Acryloyl chloride (2.40 mL, 30.0 mmol) was then added with intensive stirring. The red-brown reaction mixture was heated under reflux for 4 h, then cooled and poured into a saturated solution of Na₂CO₃ (100 mL). The organic layer was separated and the water layer was extracted with EtOAc (2 × 70 mL). The organic phases were combined and dried over MgSO₄. After filtration and solvent evaporation, the residue, a brown oil, was separated by silica gel column chromatography (2.5 × 20 cm, eluent: EtOAc/hexane, 1/5) affording intermediate 3-acryloyl-2-(2-furyl)-2,3-dihydro-1,3-benzothiazole (**34***) 1.15 g (15 %). Then 2,4a-epoxyisoindolo[1,2-*b*][1,3]benzothiazol-11-one (**34**) 1.54 g (20 %) was isolated using a more polar eluent mixture (EtOAc/hexane, 1/1). Increase of the reaction time to 22 h raises the yield of the target adduct **34** to 2.15 g (28 %, after column chromatography).

3-Acryloyl-2-(2-furyl)-2,3-dihydro-1,3-benzothiazole (34*). Beige plates, m.p. 87.8–88.7 °C (from EtOAc/hexane); [Found: C, 65.64; H, 4.52; N, 5.08. C₁₄H₁₁NO₂S requires C, 65.35; H, 4.31; N, 5.44%]; R_f (65% EtOAc/hexane) 0.70; v_{max} (KBr) 1650, 1611, 1463, 1407, 1229, 750 cm⁻¹; δ_H (400 MHz, CDCl₃) 7.65 (1 H, br.s, H-4), 7.34–7.32 (1 H, m, H-5'), 7.21 (1 H, dd, $^4J_{7,5}$ 1.0, $^3J_{7,6}$ 7.5 Hz, H-7), 7.13 (1 H, dt, $^3J_{6,7} \sim ^3J_{6,5}$ 7.5, $^4J_{6,4}$ 1.0 Hz, H-6), 7.07 (1 H, dt, $^3J_{5,6} \sim ^3J_{5,4}$ 7.5, $^4J_{5,7}$ 1.0 Hz, H-5), 6.86 (1 H, br.s, H-2), 6.67 (1 H, dd, $^3J_{2'',3''trans}$ 16.8, $^3J_{2'',3''cis}$ 10.3 Hz, H-2''), 6.52 (1 H, dd, $^3J_{3''trans,2''}$ 16.8, $^2J_{3'',3''}$ 1.6 Hz, H-3''^{trans}), 6.26–6.24 (2 H, m, H-3' and H-4'), 5.85 (1 H, dd, $^3J_{3'',2''cis}$ 10.3, $^2J_{3'',3''}$ 1.6 Hz, H-3''^{cis}); δ_C (100.6 MHz, CDCl₃) 164.1 (C-1''), 152.0 (C-2''), 142.9 (C-5'), 137.1 (C-3a), 130.3 (C-3''), 128.1, 125.4 and 125.1 (C-5, C-6 and C-7), 122.9 and 119.0 (br.s, 2 C) (C-4, C-2'' and C-7a), 110.4 (C-3'), 107.4 (C-4'), 61.0 (C-2). GC-MS (EI, 70 eV) *m/z* 259 (5, M⁺+2 for S³⁴), 257 (44, M⁺), 255 (2), 228 (5), 204 (8), 203 (38), 202 (43), 201 (10), 174 (40), 173 (58), 172 (12), 147 (13), 136 (14), 135 (15), 109 (38), 108 (18), 94 (30), 82 (12), 69 (39), 65 (48), 55 (100), 51 (16), 45 (15), 39 (35%).

(2RS,4aRS,4bRS,11aSR)-1,11a-Dihydro-2,4a-epoxyisoindolo[1,2-*b*][1,3]benzothiazol-11(2H,4bH)-one (34). White powder, m.p. 167.8–169.0 °C (from EtOAc/hexane); [Found: C, 65.35; H, 4.41; N, 5.14. C₁₄H₁₁NO₂S requires C, 65.35; H, 4.31; N, 5.44%]; R_f (50% EtOAc/hexane) 0.78; v_{max} (KBr) 1719, 1699, 1465, 1356, 1179, 753 cm⁻¹; δ_H (400 MHz, CDCl₃) 7.61 (1 H, d, $^3J_{8,9}$ 7.5 Hz, H-9), 7.14 (1 H, d, $^3J_{6,7}$ 7.5 Hz, H-6), 7.08 (1 H, br.t, $^3J_{6,7} \sim ^3J_{8,7}$ 7.5 Hz, H-7), 7.00 (1 H, br.t, $^3J_{8,7} \sim ^3J_{8,9}$ 7.5 Hz, H-8), 6.52 (1 H, s, H-4b), 6.49 (1 H, dd, $^3J_{4,3}$ 5.6, $^3J_{2,3}$ 1.2 Hz, H-3), 6.44 (1 H, d, $^3J_{4,3}$ 5.6 Hz, H-4), 5.18 (1 H, dd, $^3J_{2,3}$ 1.2, $^3J_{2,1exo}$ 4.9 Hz, H-2), 2.89 (1 H, dd, $^3J_{1endo,11a}$ 8.7, $^3J_{1exo,11a}$ 3.7 Hz, H-11a), 2.39 (1 H, ddd, $^2J_{1,1}$ 11.8, $^3J_{2,1exo}$ 4.9, $^3J_{1exo,11a}$ 3.7

Hz, H-1^{exo}), 1.65 (1 H, dd, $^2J_{1,1}$ 11.8, $^3J_{1endo,11a}$ 8.7 Hz, H-1^{endo}); δ_C (100.6 MHz, CDCl₃) 172.3 (C-11), 138.3 (C-4), 135.1 and 131.8 (C-5a and C-9a), 131.3, 125.4 (2 C), 122.5, 116.8 (C-3, C-6, C-7, C-8, C-9), 91.6 (C-4a), 79.5 (C-2), 68.4 (C-4b), 52.2 (C-11a), 29.0 (C-1). GC-MS (EI, 70 eV) *m/z* 259 (4, M⁺+2 for S³⁴), 257 (26, M⁺), 256 (18), 255 (2), 228 (4), 203 (20), 202 (40), 201 (39), 174 (27), 173 (39), 172 (36), 147 (12), 135 (14), 130 (12), 109 (37), 94 (30), 82 (10), 69 (35), 65 (47), 55 (100), 51 (17), 45 (11), 39 (36%).

Methyl (1RS,2SR,4aRS,4bRS,11aSR)-11-oxo-1,2,11,11a-tetrahydro-2,4a-epoxyisoindolo[1,2-*b*][1,3]benzothiazole-1(4bH)-carboxylate (35). Carbonic acid **33a** (1.0 g, 3.30 mmol) was heated under reflux in MeOH (40 mL) with conc. H₂SO₄ (0.25 mL) for 2 h. White needle-shaped crystals of the target ester are formed on cooling of the yellow solution to +4 °C. The precipitate was collected by filtration, washed with Et₂O (2 × 20 mL), recrystallized from MeOH. The ester **35** was obtained as colorless needle-shaped crystals (0.75 g, 72 %), m.p. 180–180.6 °C; [Found: C, 60.86; H, 4.29; N, 4.51. C₁₆H₁₃NO₄S requires C, 60.94; H, 4.16; N, 4.44%]; R_f (EtOAc) 0.73; v_{max} (KBr) 1727, 1720, 1470, 1361, 1228, 1184, 761 cm⁻¹; δ_H (600 MHz, DMSO- d_6) 7.40 (1 H, dd, $^3J_{8,9}$ 7.7, $^4J_{7,9}$ 1.3 Hz, H-9), 7.28 (1 H, dd, $^3J_{6,7}$ 7.7, $^4J_{6,8}$ 1.3 Hz, H-6), 7.08 (1 H, dt, $^3J_{6,7} \sim ^3J_{8,7}$ 7.7, $^4J_{9,7}$ 1.3 Hz, H-7), 7.04 (1 H, dt, $^3J_{8,7} \sim ^3J_{8,9}$ 7.7, $^4J_{6,8}$ 1.3 Hz, H-8), 6.69 (1 H, s, H-4b), 6.62 (1 H, d, $^3J_{4,3}$ 5.8 Hz, H-4), 6.53 (1 H, dd, $^3J_{4,3}$ 5.8, $^3J_{2,3}$ 1.7 Hz, H-3), 5.13 (1 H, d, $^3J_{2,3}$ 1.7 Hz, H-2), 3.56 (3 H, s, CO₂Me), 3.46 (1 H, d, $^3J_{1,11a}$ 9.1 Hz, H-1), 2.75 (1 H, d, $^3J_{1,11a}$ 9.1 Hz, H-11a); δ_C (150.9 MHz, DMSO- d_6) 172.4 and 170.0 (CO₂Me and C-11), 138.7 and 133.9 (C-3 and C-4), 135.3 and 132.3 (C-5a and C-9a), 125.93, 125.70, 123.2 (C-6, C-7, C-8), 116.6 (C-9), 91.9 (C-4a), 81.6 (C-2), 67.3 (C-4b), 55.0 and 46.3 (C-1 and C-11a), 52.0 (CO₂Me). GC-MS (EI, 70 eV) *m/z* 315 (11, M⁺), 272 (2), 228 (1), 203 (33), 202 (100), 174 (26), 172 (24), 147 (5), 121 (7), 114 (10), 113 (95), 109 (24), 85 (14), 69 (15), 65 (26), 59 (21), 45 (7), 39 (27%).

Synthesis of epoxides 36. General experimental procedure. Compound **4a**, **17a** or **17b** (24 mmol) was added to a solution of 85% *m*-CPBA (9.74 g, 48.0 mmol) in CHCl₃ (90 mL) at 0 °C. The mixture was stirred at 0 °C for 30 min and then for 4–14 h at room temperature. The reaction mixture was then poured into a saturated Na₂CO₃ solution (150 mL). The organic layer was separated and the water layer was extracted with CHCl₃ (2 × 80 mL). Combined organic extracts were washed with a saturated sodium bicarbonate solution (3 × 80 mL) and dried over MgSO₄. Then MgSO₄ was then filtered off. Crystals obtained by solvent evaporation were recrystallized from a hexane/EtOAc mixture using activated carbon. Diperoxides **36a–c** were obtained as colorless crystalline compounds.

Methyl (1aRS,2RS,3RS,3aSR,9aSR,9bSR,9cRS)-4-oxooctahydro-6H-2,9b-epoxy[1,3]oxazino[2,3-*a*]oxireno[*g*]isoindole-3(9aH)-carboxylate (36a). Colorless prisms (5.33 g, 79 %), m.p. 231–233 °C; [Found: C, 55.63; H, 5.48; N, 4.93. C₁₃H₁₅NO₆ requires C, 55.51; H, 5.38; N, 4.98%]; R_f (EtOAc) 0.50; v_{max} (KBr) 1753, 1704, 1436, 1211, 1173, 1071, 1039 cm⁻¹; δ_H (600 MHz, CDCl₃) 5.09 (1 H, s, H-9a), 4.75 (1 H, s, H-2), 4.17 (1 H, ddd, $^2J_{8,8}$ 12.6, $^3J_{8e,7a}$ 5.0, $^3J_{8e,7e}$ 2.2 Hz, H-8^{eq}), 4.12 (1 H, ddd, $^2J_{6,6}$ 13.2, $^3J_{6e,7a}$ 5.0, $^3J_{6e,7e}$ 1.7 Hz, H-6^{eq}), 3.83 (1 H, dt, $^2J_{8,8} \sim ^3J_{8a,7a}$ 12.6, $^3J_{8a,7e}$ 2.2 Hz, H-8^{ax}), 3.69 (3 H, s, CO₂Me), 3.63 (1 H, d, $^3J_{1a,9c}$ 3.3 Hz, H-1a), 3.41 (1 H, d, $^3J_{9c,1a}$ 3.3 Hz, H-9c), 3.06 (1 H, ddd, $^2J_{6,6}$ 13.2, $^3J_{6a,7a}$ 12.6, $^3J_{6a,7e}$ 3.8 Hz, H-6^{ax}), 2.98 and 2.93 (1 H and 1 H, two d, $^3J_{3,3a}$ 9.5, H-3 and H-3a), 1.86–1.78 (1 H, m, H-7^{ax}), 1.50–1.47 (1 H, m, H-7^{eq}); δ_C (100.6 MHz, CDCl₃) 170.3 and 169.6 (CO₂Me and C-4), 86.0 (C-

9b), 84.1 (C-9a), 78.2 (C-2), 66.6 (C-8), 51.4 (CO₂Me), 51.0, 48.5, 46.7, 46.6 (C-1a, C-3, C-3a, C-9c), 38.2 (C-6), 24.9 (C-7). MS (EI, 70 eV) *m/z* 281 (15, M⁺), 280 (8), 250 (14), 238 (2), 232 (1), 224 (2), 222 (4), 220 (4), 209 (3), 194 (9), 192 (13), 180 (10), 167 (11), 164 (11), 152 (13), 151 (17), 139 (30), 138 (80), 137 (18), 136 (10), 123 (11), 113 (10), 109 (16), 98 (7), 95 (10), 86 (46), 85 (26), 84 (25), 81 (100), 79 (17), 69 (4), 59 (21), 58 (11), 56 (38), 55 (10), 53 (15), 41 (21), 29 (19), 28 (22), 27 (12%).

Methyl (1aRS,2SR,3SR,3aRS,9aRS,9bRS,9cSR)-2-methyl-4-oxooctahydro-6H-2,9b-epoxy[1,3]oxazino[2,3-a]oxireno[g]isoindole-3(9aH)-carboxylate (36b). Colorless prisms (4.10 g, 58 %), m.p. 190–193 °C; [Found: C, 56.59; H, 5.35; N, 5.03. C₁₄H₁₇NO₆ requires C, 56.94; H, 5.80; N, 4.74%]; R_f (EtOAc) 0.47; ν_{max} (KBr) 1747, 1691, 1436, 1203, 1064, 1029 cm⁻¹; δ_H (400 MHz, CDCl₃) 4.97 (1 H, s, H-9a), 4.00–4.08 (2 H, m, H-8^{eq} and H-6^{eq}), 3.73 (1 H, br.d, ²J_{8,8} ~ ³J_{8a,7a} 12.5, ³J_{8a,7c} 1.9 Hz, 8-H^{ax}), 3.58 (3 H, s, CO₂Me), 3.56 (1 H, d, ³J_{1a,9c} 3.1 Hz, H-1a), 3.18 (1 H, d, ³J_{9c,1a} 3.1 Hz, H-9c), 2.97 (1 H, br.d, ²J_{6,6} ~ ³J_{6a,7a} 13.1, ³J_{6a,7c} 3.7 Hz, 6-H^{ax}), 2.84 and 2.79 (1 H and 1 H, two d, ³J_{3,3a} 9.4 Hz, H-3 and H-3a), 1.76–1.65 (1 H, m, H-7^{ax}), 1.39 (3 H, s, Me-2), 1.39–1.36 (1 H, m, H-7^{eq}); δ_C (100.6 MHz, CDCl₃) 170.0 and 169.1 (CO₂Me and C-4), 86.4, 85.9, 85.1 (C-2, C-9a, C-9b), 67.5 (C-8), 52.8, 51.9, 51.8, 50.8, 49.1 (CO₂Me, C-1a, C-3, C-3a, C-9c), 38.9 (C-6), 25.0 (C-7), 13.7 (Me-2). MS (EI, 70 eV) *m/z* 295 (3, M⁺), 279 (2), 266 (30), 264 (43), 252 (53), 246 (38), 220 (40), 206 (24), 192 (33), 180 (100), 179 (32), 166 (24), 164 (28), 152 (50), 151 (69), 139 (26), 136 (23), 123 (40), 95 (37), 86 (33), 56 (39), 43 (39%).

(1aRS,2RS,3aSR,9aSR,9bSR,9cRS)-Hexahydro-6H-2,9b-epoxy[1,3]oxazino[2,3-a]oxireno[g]isoindol-4(2H,9aH)-one (36c). Colorless prisms (3.84 g, 71 %), m.p. 198–199.2 °C; [Found: C, 59.19; H, 5.87; N, 6.27. C₁₁H₁₃NO₄ requires C, 59.43; H, 5.76; N, 6.09%]; R_f (80% EtOAc/EtOH) 0.73; ν_{max} (KBr) 1694, 1435, 1263, 1064, 744 cm⁻¹; δ_H (400 MHz, DMSO-*d*₆) 5.06 (1 H, s, H-9a), 4.58 (1 H, d, ²J_{2,3exo} 4.5 Hz, H-2), 4.12 (1 H, br.dd, ³J_{8c,7a} 4.5, ²J_{8,8} 11.5 Hz, H-8^{eq}), 3.93–3.87 (2 H, m, H-8^{ax} and H-6^{eq}), 3.60 and 3.54 (1 H and 1 H, two d, ³J_{1a,9c} 3.5 Hz, H-1a and H-9c), 3.09 (1 H, dt, ²J_{6,6} ~ ³J_{6a,7a} 12.7, ³J_{6a,7c} 3.8 Hz, H-6^{ax}), 2.73 (1 H, dd, ³J_{3endo,3a} 8.9, ³J_{3exo,3a} 5.1 Hz, H-3a), 1.84–1.74 (2 H, m, H-3), 1.68–1.56 (1 H, m, H-7^{ax}), 1.53–1.47 (1 H, m, H-7^{eq}); δ_C (100.6 MHz, DMSO-*d*₆) 172.4 (C-4), 86.2 (C-9b), 84.7 (C-9a), 75.7 (C-2), 66.7 (C-8), 49.1, 47.0, 46.4 (C-1a, C-3a, C-9c), 38.2 (C-6), 30.5 (C-3), 25.0 (C-7). GC-MS (EI, 70 eV) *m/z* 223 (20, M⁺), 222 (15), 194 (10), 180 (12), 166 (14), 152 (22), 151 (35), 139 (34), 123 (24), 109 (30), 94 (37), 86 (94), 81 (86), 80 (26), 66 (44), 56 (93), 55 (100), 53 (72), 41 (74), 39 (84%).

(1aRS,2RS,3aSR,8aRS,8bSR,8cRS)-Hexahydro-2,8b-epoxyoxireno[g][1,3]thiazolo[2,3-a]isoindol-4(2H,8aH)-one 8,8-dioxide (38a). Formic acid (3.6 mL, 96.0 mmol) and then 35% H₂O₂ (8.2 mL, 96.0 mmol) were added to a solution of thiazoloisoindolone **25a** (2.0 g, 9.60 mmol) in CH₂Cl₂ (30 mL). The reaction mixture was intensively stirred at room temperature for 16 h (TLC monitoring) and then poured into water (150 mL). Aqueous ammonia was added to the mixture until pH ~ 8–9. The organic layer was separated and the water layer was extracted with CH₂Cl₂ (4 × 50 mL). The combined organic phases were dried over MgSO₄. After the solvent was evaporated, the residue was triturated with Et₂O (15 mL). The crystals formed were collected by filtration and recrystallized from a heptane/EtOAc mixture. The sulfone **38a** was obtained as a white powder (0.97 g, 40 %), m.p. 238–241 °C (decomp.); R_f (EtOAc) 0.80; ν_{max} (KBr) 1707, 1387, 1314, 1119, 736 cm⁻¹; δ_H (600 MHz, DMSO-*d*₆) 5.27 (1 H, s, H-8a), 4.60 (1 H, d, ³J_{2,3exo} 4.8 Hz, H-2), 4.16 (1

H, ddd, ²J_{6,6} 12.6, ³J_{6a,7B} 7.6, ³J_{6a,7A} 2.8 Hz, H-6A), 3.77 (1 H, d, ³J_{8c,1a} 3.4 Hz, H-8c), 3.53 (1 H, d, ³J_{1a,8c} 3.4 Hz, H-1a), 3.47 (1 H, ddd, ²J_{7,7} 12.6, ³J_{7A,6B} 5.8, ³J_{7A,6A} 2.8 Hz, H-7A), 3.34 (1 H, ddd, ²J_{6,6} 12.6, ³J_{6B,7B} 10.3, ³J_{6B,7A} 5.8 Hz, H-6B), 3.14 (1 H, dd, ³J_{3aendo,3endo} 9.2, ³J_{3aendo,3exo} 3.4 Hz, H-3a^{endo}), 3.00 (1 H, ddd, ²J_{7,7} 12.6, ³J_{7B,6B} 10.3, ³J_{7B,6A} 7.6 Hz, H-7B), 1.81 (1 H, ddd, ²J_{3,3} 12.4, ³J_{3exo,2} 4.8, ³J_{3exo,3aendo} 3.4 Hz, H-3^{exo}), 1.67 (1 H, dd, ²J_{3,3} 12.4, ³J_{3endo,3aendo} 9.2 Hz, H-3^{endo}); δ_C (100.6 MHz, DMSO-*d*₆) 173.8 (C-4), 86.2 (C-8b), 75.6 (C-2), 71.8 (C-8a), 52.6 (C-3a), 49.6 (C-7), 49.1 and 47.1 (C-1a and C-8c), 38.5 (C-6), 29.4 (C-3). GC-MS (EI, 70 eV) *m/z* 207 (3, M⁺-64), 194 (5), 193 127 (1), 121 (2), 97 (3), 93 (3), 77 (5), 73 (53), 72 (6), 45 (8), 44 (100), 43 (9), 42 (40%). HRMS (DART): MH⁺, found 258.0422. C₁₀H₁₂NO₅S requires 258.0436.

(1aRS,2SR,3aRS,8aSR,8bRS,8cSR)-2-Methylhexahydro-2,8b-epoxyoxireno[g][1,3]thiazolo[2,3-a]isoindol-4(2H,8aH)-one 8,8-dioxide (38b). A solution of *m*-CPBA (3.87 g, 22.4 mmol) and thiazoloisoindolone **25b** (1.0 g, 4.50 mmol) in CH₂Cl₂ (25 mL) was stirred for 7 h. The reaction mixture was then poured into a saturated Na₂CO₃ solution (100 mL). The organic layer was separated and the water layer was extracted with CH₂Cl₂ (3 × 50 mL). The organic phases were combined, washed with saturated Na₂CO₃ solution (2 × 60 mL) and dried over MgSO₄. The residue obtained after the filtration and the solvent evaporation was triturated with Et₂O (20 mL). The crystalline precipitate formed was collected by filtration and crystallized from a hexane/EtOAc mixture. The target diepoxide **38b** (3.94 g, 65 %) was obtained as a white powder, m.p. 239.4–241.2 °C; R_f (50% EtOAc/EtOH) 0.51; ν_{max} (KBr) 2949, 1711, 1367, 1338, 1310, 1256, 1117, 902 cm⁻¹; δ_H (600 MHz, DMSO-*d*₆) 5.23 (1 H, s, H-8a), 4.15 (1 H, ddd, ²J_{6,6} 12.6, ³J_{6a,7B} 7.7, ³J_{6a,7A} 3.3 Hz, H-6A), 3.82 (1 H, d, ³J_{8c,1a} 3.5 Hz, H-8c), 3.46 (1 H, ddd, ²J_{7,7} 12.6, ³J_{7A,6B} 6.0, ³J_{7A,6A} 3.3 Hz, H-7A), 3.43 (1 H, d, ³J_{1a,8c} 3.5 Hz, H-1a), 3.34 (1 H, ddd, ²J_{6,6} 12.6, ³J_{6B,7B} 9.3, ³J_{6B,7A} 6.0 Hz, H-6B), 3.16 (1 H, dd, ³J_{3aendo,3endo} 9.1, ³J_{3aendo,3exo} 3.5 Hz, H-3a^{endo}), 3.00 (1 H, ddd, ²J_{7,7} 12.6, ³J_{7B,6B} 9.3, ³J_{7B,6A} 7.7 Hz, H-7B), 1.77 (1 H, dd, ²J_{3,3} 12.2, ³J_{3endo,3aendo} 9.1 Hz, H-3^{endo}), 1.55 (1 H, dd, ²J_{3,3} 12.2, ³J_{3exo,3aendo} 3.5 Hz, H-3^{exo}), 1.38 (3 H, s, Me-2); δ_C (100.6 MHz, DMSO-*d*₆) 174.0 (C-4), 86.2 (C-8b), 84.0 (C-2), 72.1 (C-8a), 54.1 (C-3a), 51.7 and 49.0 (C-1a and C-8c), 49.7 (C-7), 38.6 (C-6), 35.3 (C-3), 16.4 (Me-2). MS (EI, 70 eV) *m/z* 207 (63, M⁺-64), 206 (11), 192 (12), 178 (16), 165 (32), 164 (91), 153 (12), 138 (13), 137 (32), 136 (52), 122 (33), 111 (57), 108 (48), 95 (50), 83 (31), 82 (64), 67 (63), 59 (37), 56 (36), 55 (100), 54 (56), 53 (59), 43 (67%). HRMS (DART): MH⁺, found 272.0584. C₁₁H₁₄NO₅S requires 272.0593.

Methyl (6aRS,7SR,8SR,9RS,9aRS,10RS,10aRS)-9,10-bis(acetyloxy)-6-oxodecahydro-2H-8,10-epoxycyclopenta[4,5]pyrido[2,1-b][1,3]oxazine-7-carboxylate (37a). Boron trifluoride etherate (BF₃·OEt₂, 1.52 mL, 11.4 mmol) was added in one portion to an intensively stirred and cooled (0 °C) suspension of the ester **36a** (1.0 g, 3.79 mmol) in Ac₂O (15 mL). The pale yellow transparent reaction mixture was stirred at room temperature for 1 h, and then poured into water (150 mL). Saturated Na₂CO₃ was added till the mixture was basic. The mixture was extracted with CHCl₃ (3 × 50 mL). The organic phases were combined, washed with saturated Na₂CO₃ solution (100 mL) and dried over MgSO₄. MgSO₄ was filtered off and the solvent was evaporated. The residue was recrystallized twice from a hexane/EtOAc mixture. The compound **37a** was obtained as colorless prism-shaped crystals (0.36 g, 25 %), m.p. 186–187 °C; [Found: C, 53.42; H, 5.37; N, 3.52. C₁₇H₂₁NO₉ requires C, 53.26; H, 5.52; N, 3.65%]; R_f (EtOAc) 0.45; ν_{max} (KBr) 3475,

1743, 1648, 1367, 1250, 1226, 1063 cm^{-1} ; δ_{H} (400 MHz, CDCl_3) 5.34 (1 H, s, H-10a), 4.75 (1 H, br.d, $^3J_{9,9a}$ 1.7 Hz, H-9), 4.73 (1 H, t, $^3J_{8,7} \sim ^3J_{8,9}$ 1.0 Hz, H-8), 4.56 (1 H, ddt, $^2J_{4,4}$ 13.2, $^3J_{4e,3a}$ 4.9, $^3J_{4e,3e} \sim ^4J_{4e,2e}$ 1.7 Hz, H-4^{eq}), 4.03 (1 H, ddt, $^2J_{2,2}$ 12.7, $^3J_{2e,3a}$ 5.1, $^3J_{2e,3e} \sim ^4J_{2e,4e}$ 1.7 Hz, H-2^{eq}), 3.62 (1 H, ddd, $^2J_{2,2}$ 12.7, $^3J_{2a,3a}$ 11.4, $^3J_{2a,3e}$ 2.6 Hz, H-2^{ax}), 3.54 (3 H, s, CO_2Me), 3.17 (1 H, dd, $^3J_{6a,9a}$ 4.5, $^3J_{9,9a}$ 1.7 Hz, H-9a), 3.10 (1 H, dd, $^3J_{6a,7}$ 11.5, $^3J_{6a,9a}$ 4.5 Hz, H-6a), 3.09 (1 H, dd, $^3J_{6a,7}$ 11.5, $^3J_{7,8}$ 1.0 Hz, H-7), 2.70 (1 H, dt, $^2J_{4,4} \sim ^3J_{4a,3a}$ 13.2, $^3J_{4a,3e}$ 3.3 Hz, H-4^{ax}), 1.99 (3 H, s, OCOMe), 1.94 (3 H, s, OCOMe), 1.87–1.75 (1 H, m, H-3^{ax}), 1.45–1.41 (1 H, m, $^2J_{3,3}$ 13.6 Hz, H-3^{eq}). The ^1H NMR spectrum was recorded in deuterobenzene for unequivocal assignment of signals. In this case traces of pentadeuteriobenzene ($\text{C}_6\text{D}_5\text{H}$, δ 7.15 ppm) were used as the internal standard. δ_{H} (400 MHz, C_6D_6) 5.73 (1 H, s, H-10a), 4.69 (1 H, ddt, $^2J_{4,4}$ 13.2, $^3J_{4e,3a}$ 4.9, $^3J_{4e,3e} \sim ^4J_{4e,2e}$ 1.7 Hz, H-4^{eq}), 4.54 (1 H, t, $^3J_{8,7} \sim ^3J_{8,9}$ 1.0 Hz, H-8), 4.29 (1 H, br.d, $^3J_{9,9a}$ 1.7 Hz, H-9), 3.71 (1 H, ddt, $^2J_{2,2}$ 11.4, $^3J_{2e,3a}$ 5.1, $^3J_{2e,3e} \sim ^4J_{2e,4e}$ 1.7 Hz, H-2^{eq}), 3.30 (1 H, ddd, $^2J_{2,2}$ 12.7, $^3J_{2a,3a}$ 11.4, $^3J_{2a,3e}$ 2.6 Hz, H-2^{ax}), 3.29 (3 H, s, CO_2Me), 3.21 (1 H, dd, $^3J_{6a,9a}$ 4.5, $^3J_{9,9a}$ 1.7 Hz, H-9a), 2.89 (1 H, dd, $^3J_{6a,7}$ 11.5, $^3J_{6a,9a}$ 4.5 Hz, H-6a), 2.57 (1 H, dd, $^3J_{6a,7}$ 11.5, $^3J_{7,8}$ 1.0 Hz, H-7), 2.43 (1 H, dt, $^2J_{4,4} \sim ^3J_{4a,3a}$ 13.2, $^3J_{4a,3e}$ 3.3 Hz, H-4^{ax}), 1.70 (3 H, s, OCOMe), 1.63 (3 H, s, OCOMe), 1.63–1.56 (1 H, m, H-3^{ax}), 0.68–0.64 (1 H, m, H-3^{eq}); δ_{C} (100.6 MHz, CDCl_3) 169.7 (s, C(9)-OC=O), 168.0 (s, C(10)-OC=O), 167.4 (s, CO_2Me), 164.7 (s, C-6), 102.2 (s, C-10), 85.2 (d, J 165.7 Hz, C-10a), 81.6 (d, J 175.8 Hz, C-8), 76.2 (d, J 159.0 Hz, C-9), 68.4 (t, J 144.5 Hz, C-2), 51.9 (q, J 147.5 Hz, CO_2Me), 45.2 (d, J 135.0 Hz, C-7), 44.0 (d, J 157.2 Hz, C-9a), 41.2 (t, J 141.5 Hz, C-4), 37.9 (d, J 144.5 Hz, C-6a), 24.8 (t, J 129.5 Hz, C-3), 21.3 (q, J 129.8 Hz, OCOMe), 20.4 (q, J 130.0 Hz, OCOMe). 1D NOE ^1H NMR (CDCl_3), %: $\eta_{\text{H-10a}}\{2\text{-H}_a\}$ 12.6 %; $\eta_{\text{H-10a}}\{4\text{-H}_a\}$ 9.5 %; NOE 1D (C_6D_6), %: $\eta_{\text{H-9}}\{H-9_a\}$ 5.9 %; $\eta_{\text{H-6a}}\{H-9_a\}$ 6.8 %; $\eta_{\text{H-2}}\{H-10_a\}$ 8.0 %; $\eta_{\text{H-4}}\{H-10_a\}$ 6.3 %; $\eta_{\text{H-7}}\{H-8\}$ 7.3 %; $\eta_{\text{H-8}}\{H-9\}$ 6.8 %; $\eta_{\text{H-6a}}\{H-9\}$ 13.0 %; $\eta_{\text{H-7}}\{H-9\}$ 11.3 %; $\eta_{\text{H-9a}}\{H-9\}$ 3.9 %. GC-MS (EI, 70 eV) m/z 383 (4, M^+), 352 (2), 341 (35), 340 (45), 324 (11), 310 (7), 299 (4), 281 (5), 264 (22), 255 (36), 236 (4), 213 (5), 166 (7), 151 (6), 124 (7), 113 (10), 86 (100), 81 (4), 58 (5), 43 (51%).

(6aRS,8SR,9RS,9aRS,10RS,10aRS)-6-Oxoocctahydro-2H-8,10-epoxycyclopenta[4,5]pyrido[2,1-b][1,3]oxazine-9,10(10aH)-diyl diacetate (37b) was obtained similar to the preparation of the polycyclic compound **37a** from diepoxide **36b** (0.45 g, 2.02 mmol), $\text{BF}_3\cdot\text{OEt}_2$ (0.89 mL, 7.06 mmol) and Ac_2O (6 mL). About 0.5 g of dark brown oil was isolated, which was purified by Al_2O_3 column chromatography (3 \times 20 cm, eluent: hexane/EtOAc, 4/1 \rightarrow 1/1). After recrystallization from EtOAc with a little EtOH added, the compound **37b** was isolated as a white powder (0.20 g, 30 %), m.p. 166 $^\circ\text{C}$; [Found: C, 55.45; H, 5.81; N, 4.47. $\text{C}_{15}\text{H}_{19}\text{NO}_7$ requires C, 55.38; H, 5.89; N, 4.31%]; ν_{max} (KBr) 1738, 1666, 1256, 1232, 1080, 1059, 904 cm^{-1} ; δ_{H} (400 MHz, CDCl_3) 5.59 (1 H, s, H-10a), 4.74 (1 H, s, H-9), 4.64 (1 H, ddd, $^2J_{4,4}$ 13.1, $^3J_{4e,3a}$ 5.0, $^3J_{4e,3e}$ 1.9 Hz, H-4^{eq}), 4.59 (1 H, s, H-8), 4.13 (1 H, ddd, $^2J_{2,2}$ 12.5, $^3J_{2e,3a}$ 5.0, $^3J_{2e,3e} \sim 1.0$ Hz, H-2^{eq}), 3.75 (1 H, dt, $^2J_{2,2} \sim ^3J_{2a,3a}$ 12.5, $^3J_{2a,3e}$ 2.5 Hz, H-2^{ax}), 3.20 (1 H, br.d, $^3J_{6a,9a}$ 3.1 Hz, H-9a), 2.89 (1 H, dt, $^2J_{6a,7\text{exo}}$ 12.1, $^3J_{6a,9a} \sim ^3J_{6a,7\text{endo}}$ 3.1 Hz, H-6a), 2.76 (1 H, dt, $^2J_{4,4} \sim ^3J_{4a,3a}$ 13.1, $^3J_{4a,3e}$ 3.1 Hz, H-4^{ax}), 2.15 (1 H, dd, $^2J_{7,7}$ 13.7, $^3J_{6a,7\text{exo}}$ 12.1 Hz, H-7^{endo}), 2.07 (3 H, s, OCOMe-9), 2.02 (3 H, s, OCOMe-10), 1.88 (1 H, m, H-3^{ax}), 1.60 (1 H, dd, $^2J_{7,7}$ 13.7, $^3J_{6a,7\text{endo}}$ 3.1 Hz, H-7^{endo}), 1.48–1.44 (1 H, m, H-3^{eq}); δ_{C} (100.6 MHz, CDCl_3) 170.2 (C(9)-OC=O), 169.2 (C-6), 168.7 (C(10)-OC=O), 102.4 (C-10), 85.3 (C-10a), 80.7 (C-8), 78.0 (C-9), 69.0 (C-2), 43.5 (C-9a), 42.0 (C-4), 35.8 (C-6a), 33.4 (C-7), 25.7 (C-3), 21.9 (C(10)-OCOMe), 20.8 (C(9)-

OCOMe). GC-MS (EI, 70 eV) m/z 325 (2, M^+), 284 (4), 282 (30), 281 (46), 266 (13), 265 (22), 264 (13), 224 (9), 223 (12), 222 (8), 206 (23), 205 (62), 166 (13), 138 (5), 128 (5), 97 (6), 93 (7), 86 (69), 83 (19), 66 (14), 55 (11), 43 (100%).

Synthesis of 7,9-epoxycyclopenta[*d*][1,3]thiazolo[3,2-*a*]pyridines (39). General experimental procedure. $\text{BF}_3\cdot\text{OEt}_2$ (1.33 mL, 10.5 mmol) was added to a cooled (0 $^\circ\text{C}$) suspension of diepoxide **38a** (**38b**) (~0.54 g, 2.1 mmol) in Ac_2O (6 mL) and the mixture was cooled at this temperature for 2 h (TLC monitoring). The reaction mixture was then poured into a saturated Na_2CO_3 solution (70 mL) and extracted with CHCl_3 (3 \times 50 mL). The combined organic phases were washed with saturated Na_2CO_3 solution (100 mL) and dried with MgSO_4 , which was then removed by filtration. The solvent was removed under reduced pressure and the dark brown oil obtained was purified by column chromatography (Al_2O_3 , 2 \times 20 cm, eluent: hexane/EtOAc, 4/1 \rightarrow 1/1). The polycycles **39** were obtained as white or pale yellow crystalline compounds.

(5aRS,7SR,8RS,8aRS,9RS,9aSR)-1,1-Dioxido-5-oxoocctahydro-7,9-epoxycyclopenta[*d*][1,3]thiazolo[3,2-*a*]pyridine-8,9(9aH)-diyl diacetate (39a). White powder (0.50 g, 46 %), m.p. 253.7–254.8 $^\circ\text{C}$ (decomp., from EtOAc); R_f (EtOAc) 0.46; ν_{max} (KBr) 1746, 1677, 1256 cm^{-1} ; δ_{H} (400 MHz, CDCl_3) 5.07 (1 H, s, H-9a), 4.83 (1 H, br.s, H-7), 4.82 (1 H, d, $^3J_{8,8a}$ 1.8 Hz, H-8), 4.59 (1 H, ddd, $^2J_{3,3}$ 12.6, $^3J_{3A,2A}$ 8.2, $^3J_{3A,2B}$ 3.7 Hz, H-3A), 3.99 (1 H, ddd, $^3J_{8a,5a}$ 4.6, $^3J_{8,8a}$ 1.8, $^4J_{7,8a}$ 0.9 Hz, H-8a), 3.47 (1 H, ddd, $^2J_{3,3}$ 12.6, $^3J_{3B,2A}$ 8.7, $^3J_{3B,2B}$ 7.3 Hz, H-3B), 3.29–3.15 (2 H, m, H-2), 3.03 (1 H, ddd, $^3J_{5a,6\text{endo}}$ 11.5, $^3J_{8a,5a}$ 4.6, $^3J_{5a,6\text{exo}}$ 3.5 Hz, H-5a), 2.31 (1 H, ddd, $^2J_{6,6}$ 13.3, $^3J_{5a,6\text{endo}}$ 11.5, $^3J_{7,6\text{endo}}$ 0.9 Hz, H-6^{endo}), 2.17 (3 H, s, OAc), 2.08 (3 H, s, OAc), 1.73 (1 H, ddd, $^2J_{6,6}$ 13.3, $^3J_{5a,6\text{exo}}$ 3.5, $^3J_{7,6\text{exo}}$ 1.4 Hz, H-6^{exo}); δ_{C} (100.6 MHz, $\text{DMSO-}d_6$) 169.5, 169.0, 168.7 (2 \times COMe and C-5), 103.6 (C-9), 80.1, 75.6, 70.0 (C-7, C-8, C-9a), 47.3 (C-2), 43.7 (C-8a), 38.7 (C-3), 36.0 (C-5a), 33.8 (C-6), 21.1 and 20.3 (2 \times COMe). GC-MS (EI, 70 eV) m/z 341 (1, M^+ -18), 323 (1), 295 (6, M^+ -64), 281 (3), 266 (4), 253 (14), 235 (5), 207 (5), 193 (6), 164 (3), 138 (3), 111 (2), 96 (3), 82 (6), 81 (2), 66 (26), 65 (7), 44 (13), 43 (100%). HRMS (DART): MH^+ , found 360.3580. $\text{C}_{14}\text{H}_{18}\text{NO}_8\text{S}$ requires 360.3596.

(5aRS,7SR,8RS,8aRS,9RS,9aSR)-7-Methyl-1,1-dioxido-5-oxoocctahydro-7,9-epoxycyclopenta[*d*][1,3]thiazolo[3,2-*a*]pyridine-8,9(9aH)-diyl diacetate (39b). Pale yellow powder (0.52 g, 67 %), m.p. 225.8–226.4 $^\circ\text{C}$ (decomp., from EtOH/DMF); R_f (EtOAc) 0.61; ν_{max} (KBr) 1742, 1666, 1327, 1261, 1248, 1225, 1140 cm^{-1} ; δ_{H} (600 MHz, CDCl_3) 5.03 (1 H, s, H-9a), 4.86 (1 H, d, $^3J_{8,8a}$ 1.4 Hz, H-8), 4.55 (1 H, ddd, $^2J_{3,3}$ 13.1, $^3J_{3A,2A}$ 8.9, $^3J_{3A,2B}$ 4.1 Hz, H-3A), 3.94 (1 H, dd, $^3J_{8a,5a}$ 3.8, $^3J_{8,8a}$ 1.4 Hz, H-8a), 3.47 (1 H, br.dt, $^2J_{3,3}$ 13.1, $^3J_{3B,2A} \sim ^3J_{3B,2B}$ 8.3 Hz, H-3B), 3.27–3.16 (2 H, m, H-2), 3.00 (1 H, br.dt, $^3J_{5a,6\text{endo}}$ 11.7, $^3J_{8a,5a} \sim ^3J_{5a,6\text{exo}}$ 3.8 Hz, H-5a), 2.24 (1 H, dd, $^2J_{6,6}$ 13.7, $^3J_{5a,6\text{endo}}$ 11.7 Hz, H-6^{endo}), 2.15 (3 H, s, OAc), 2.09 (3 H, s, OAc), 1.69 (1 H, dd, $^2J_{6,6}$ 13.7, $^3J_{5a,6\text{exo}}$ 3.8 Hz, H-6^{exo}), 1.45 (3 H, s, Me-7); δ_{C} (100.6 MHz, $\text{DMSO-}d_6$) 169.5, 169.1, 168.8 (2 \times COMe and C-5), 103.8 (C-9), 87.8 (C-7), 76.0 (C-8), 70.2 (C-9a), 47.3 (C-2), 45.0 (C-8a), 38.9 and 38.7 (C-3 and C-6), 36.0 (C-5a), 21.2 and 20.3 (2 \times COMe), 14.5 (Me-7). The C₃ and C₆ signals in a ^{13}C NMR spectrum of **39b** in DMSO were overlapped by solvent peaks, therefore, a spectrum in CDCl_3 was recorded. δ_{C} (100.6 MHz, CDCl_3) 170.1, 169.7, 168.9 (2 \times COMe and C-5), 103.9 (C-9), 88.7 (C-7), 76.6 (C-8), 71.3 (C-9a), 48.7 (C-2), 45.4 (C-8a), 39.9 and 38.9 (C-2 and C-6), 36.7 (C-5a), 21.7 and 20.7 (2 \times COMe), 15.0 (Me-7). GC-MS (EI, 70 eV) m/z 309 (3, M^+ -64), 272 (3), 271 (15), 270 (5), 250 (3), 243 (2), 207 (5), 202 (6), 179 (4), 150 (3), 138 (8), 124 (7), 109 (6), 96 (14), 80 (13), 69 (7), 55

(7), 44 (8), 43 (100%). HRMS (DART): MH^+ , found 374.0867. $C_{15}H_{20}NO_8S$ requires 374.0910.

Synthesis of 7b,10-epoxyisoindolo[2,1-a]perimidines (41).
General experimental procedure. A solution of naphthalene-1,8-diamine (0.79 g, 5.0 mmol) and furfural (5-methylfurfural) (~0.5 mL, 5.0 mmol) in EtOH (10 mL) was stirred at room temperature for 10 min. The solvent was removed under reduced pressure affording intermediate 2-(2-furyl)-2,3-dihydro-1H-perimidines (**40a,b**) as brown, quickly crystallizing oils, which were used for the next step without further purification and assuming quantitative yield. No spectral data on perimidines (**40**) were found in the literature, therefore, we obtained analytically pure samples by recrystallization and characterized them by NMR spectra.

2-(2-Furyl)-2,3-dihydro-1H-perimidine (40a), colorless needles (yield 85 %), m.p. 101.2–102.0 °C (hexane–EtOAc), [Lit.:^[36a] m.p. 100–101 °C]; ν_{max} (KBr) 3346, 3307, 1597, 1409, 749 cm^{-1} ; δ_H (400 MHz, $CDCl_3$) 7.42 (1 H, br.d, $^3J_{5',4'}$ 1.6 Hz, H-5'), 7.28–7.21 (4 H, m, H-Ar), 6.57 (2 H, dd, $^3J_{4(9),5(8)}$ 7.2, $^4J_{4(9),6(7)}$ 1.6 Hz, H-4 and H-9), 6.40 (1 H, br.d, $^3J_{3',4'}$ 3.3 Hz, H-3'), 6.35 (1 H, dd, $^3J_{3',4'}$ 3.3, $^3J_{5',4'}$ 1.6 Hz, H-4'), 5.63 (1 H, s, H-2), 4.45 (2 H, br.s, NH); δ_C (100.6 MHz, $CDCl_3$) 153.5 (C-2'), 142.7 (2 C, C-3a and C-9a), 140.8 (C-5'), 134.8 (C-6a), 127.0 (2 C, C-5 and C-8), 118.3 (2 C, C-6 and C-7), 114.0 (C-9b), 110.6 and 107.8 (2 C, C-3' and C-4'), 106.7 (2 C, C-4 and C-9), 61.6 (C-2). GC-MS (EI, 70 eV) m/z 236 (100, M^+), 235 (87), 219 (14), 207 (18), 206 (20), 205 (22), 182 (9), 169 (53), 168 (50), 140 (25), 127 (11), 115 (41), 103 (12), 39 (20%).

2-[2-(5-Methylfuryl)]-2,3-dihydro-1H-perimidine (40b), aggregates of tiny yellow needles (yield 57 %), m.p. 124.7–126.5 °C (hexane–EtOAc), [Lit.:^[36a] m.p. 123 °C]; ν_{max} (KBr) 3332, 3272, 1600, 1411, 821, 758 cm^{-1} ; δ_H (400 MHz, $CDCl_3$) 7.27–7.20 (4 H, m, H-Ar), 6.56 (2 H, dd, $^3J_{4(9),5(8)}$ 6.9, $^4J_{4(9),6(7)}$ 1.5 Hz, H-4 and H-9), 6.30 (1 H, d, $^3J_{3',4'}$ 3.0 Hz, H-3'), 5.94 (1 H, dq, $^3J_{3',4'}$ 3.0, $^4J_{Me-5',4'}$ 1.1 Hz, H-4'), 5.55 (1 H, s, H-2), 4.65 (2 H, br.s, NH), 2.32 (3 H, br.s, Me-5'); δ_C (100.6 MHz, $CDCl_3$) 152.7 (C-2'), 151.3 (C-5'), 141.1 (2 C, C-3a and C-9a), 134.9 (C-6a), 126.9 (2 C, C-5 and C-8), 118.3 (2 C, C-6 and C-7), 114.0 (C-9b), 108.9 and 106.5 (2 C, C-3' and C-4'), 106.7 (2 C, C-4 and C-9), 61.8 (C-2), 13.7 (Me-5'). GC-MS (EI, 70 eV) m/z 250 (2, M^+), 248 (100), 219 (16), 207 (34), 205 (49), 166 (7), 140 (31), 113 (10), 53 (21), 44 (19%).

Crude perimidines **40** (~ 5 mmol) were dissolved in the appropriate solvent (CH_2Cl_2 , Me_2CO or PhMe, 10 mL) and maleic anhydride (0.49 g, 5.0 mmol) was added with intensive stirring. The orange-red color of the reaction mixture disappeared in 2–3 min, and a plentiful precipitation formed. The mixture was stored at room temperature for 1 d. The precipitate was collected by filtration, washed with CH_2Cl_2 (2 × 5 mL), dried in air till constant weight and its isomeric composition was analyzed by 1H NMR.

(7aRS,7bRS,10SR,11RS,11aSR)-12-Oxo-7,7a,10,11,11a,12-hexahydro-7b,10-epoxyisoindolo[2,1-a]perimidine-11-carboxylic acid (41Aa) and **(7aRS,7bSR,10RS,11SR,11aRS)-12-oxo-7,7a,10,11,11a,12-hexahydro-7b,10-epoxyisoindolo[2,1-a]perimidine-11-carboxylic acid (41Ba)**. Colorless powder. Reaction in CH_2Cl_2 gives rise to a mixture of isomers in ratio **41Aa/41Ba** ~ 60/40 (1.52 g, 91 %). The ratio of **41Aa/41Ba** ~ 89/11, (1.08 g, 65 %) was obtained in Me_2CO . A similar synthesis in toluene under reflux (Δ , 10 min) affords the following mixture of isomers: **41Aa/41Ba** ~ 54/46 (1.58 g, 95 %). M.p. 202–206 °C (decomp.); [Found: C, 68.17; H, 4.08; N, 8.48. $C_{19}H_{14}N_2O_4$ requires C, 68.26; H, 4.22; N, 8.38%]; ν_{max}

(KBr) 3298, 1725, 1688, 1610, 1421, 1210 cm^{-1} ; δ_H (400 MHz, $DMSO-d_6$) (**41Aa**) 12.38 (1 H, br.s, CO_2H), 7.62 (1 H, dd, $^3J_{3,2}$ 7.7, $^4J_{1,3}$ 1.6 Hz, H-3), 7.49 (1 H, dd, $^3J_{1,2}$ 7.1, $^4J_{1,3}$ 1.6 Hz, H-1), 7.46 (1 H, dd, $^3J_{2,3}$ 7.7, $^3J_{1,2}$ 7.1 Hz, H-2), 7.38 (1 H, dd, $^3J_{5,4}$ 7.7, $^3J_{5,6}$ 7.2 Hz, H-5), 7.35 (1 H, s, NH), 7.32 (1 H, dd, $^3J_{4,5}$ 7.7, $^4J_{4,6}$ 0.9 Hz, H-4), 7.01 (1 H, d, $^3J_{9,8}$ 5.8 Hz, H-8), 6.89 (1 H, dd, $^3J_{5,6}$ 7.2, $^4J_{6,4}$ 0.9 Hz, H-6), 6.61 (1 H, dd, $^3J_{9,8}$ 5.8, $^3J_{9,10}$ 1.6 Hz, H-9), 5.21 (1 H, d, $^3J_{9,10}$ 1.6 Hz, H-10), 5.20 (1 H, s, H-7a), 3.09 (1 H, d, $^3J_{11,11a}$ 9.1 Hz, H-11a), 2.69 (1 H, d, $^3J_{11,11a}$ 9.1 Hz, H-11); (**41Ba**) 12.36 (1 H, br.s, CO_2H), 8.21 (1 H, dd, $^3J_{1,2}$ 7.6, $^4J_{1,3}$ 0.8 Hz, H-1), 7.53 (1 H, dd, $^3J_{3,2}$ 7.6, $^4J_{1,3}$ 0.8 Hz, H-3), 7.42 (1 H, t, $^3J_{1,2}$ ~ $^3J_{2,3}$ 7.6 Hz, H-2), 7.32 (1 H, t, $^3J_{5,4}$ ~ $^3J_{5,6}$ 7.5 Hz, H-5), 7.23 (1 H, dd, $^3J_{4,5}$ 7.5, $^4J_{4,6}$ 0.7 Hz, H-4), 7.09 (1 H, d, $^3J_{NH,7a}$ 1.3 Hz, NH), 6.81 (1 H, dd, $^3J_{5,6}$ 7.5, $^4J_{6,4}$ 0.7 Hz, H-6), 6.73 (1 H, d, $^3J_{9,8}$ 5.7 Hz, H-8), 6.57 (1 H, dd, $^3J_{9,8}$ 5.7, $^3J_{9,10}$ 1.7 Hz, H-9), 5.64 (1 H, d, $^3J_{NH,7a}$ 1.3 Hz, H-7a), 5.16 (1 H, d, $^3J_{9,10}$ 1.7 Hz, H-10), 3.21 (1 H, d, $^3J_{11,11a}$ 9.1 Hz, H-11a), 2.66 (1 H, d, $^3J_{11,11a}$ 9.1 Hz, H-11); δ_C (100.6 MHz, $DMSO-d_6$) (**41Aa**) 172.5 (CO_2H), 169.4 (C-12), 141.5 (C-6a), 136.6 (C-9), 133.9 (2 C, C-3a and C-8), 131.2 (C-13a), 127.0 (C-5), 125.8 (C-2), 123.6 (C-3), 117.6 (C-4), 115.6 (C-13b), 114.7 (C-1), 108.5 (C-6), 89.2 (C-7b), 81.9 (C-10), 67.4 (C-7a), 50.0 (C-11a), 44.5 (C-11); (**41Ba**) 172.6 (CO_2H), 168.5 (C-12), 140.7 (C-6a), 137.2 (C-9), 134.5 (C-8), 133.9 (C-3a), 132.3 (C-13a), 127.0 (C-5), 125.9 (C-2), 122.5 (C-3), 116.8 (C-4), 113.5 (C-13b), 110.9 (C-1), 107.8 (C-6), 88.4 (C-7b), 81.3 (C-10), 65.3 (C-7a), 51.0 (C-11a), 45.0 (C-11). MS (EI, 70 eV) m/z for isomer **41Aa** 334 (19, M^+), 316 (10), 300 (2), 290 (5), 272 (7), 262 (4), 243 (4), 237 (41), 236 (70), 235 (100), 234 (73), 219 (8), 205 (41), 200 (15), 184 (27), 183 (26), 169 (46), 168 (50), 154 (11), 143 (26), 140 (36), 127 (16), 118 (14), 115 (34), 106 (23), 98 (32), 91 (24), 81 (25), 73 (28), 65 (17), 54 (51), 43 (50%).

The single isomer **41Aa** was isolated by fractional crystallization of the isomer mixtures from *i*-PrOH/DMF as a grey powder, m.p. 205.5–207 °C (decomp.).

(7aRS,7bRS,10SR,11RS,11aSR)-10-Methyl-12-oxo-7,7a,10,11,11a,12-hexahydro-7b,10-epoxyisoindolo[2,1-a]perimidine-11-carboxylic acid (41Ab) and **(7aRS,7bSR,10RS,11SR,11aRS)-10-methyl-12-oxo-7,7a,10,11,11a,12-hexahydro-7b,10-epoxyisoindolo[2,1-a]perimidine-11-carboxylic acid (41Bb)**. The mixture of isomers **41Ab/41Bb** ~ 54/46 was obtained when the reaction was carried out in CH_2Cl_2 (1.63 g, 94 %), beige powder, m.p. 168.3–169.4 °C (decomp.); [Found: C, 69.12; H, 4.60; N, 8.25. $C_{20}H_{16}N_2O_4$ requires C, 68.96; H, 4.63; N, 8.04%]; ν_{max} (KBr) 3444, 1728, 1666 cm^{-1} ; δ_H (400 MHz, $DMSO-d_6$) (**41Ab**) 12.43 (1 H, br.s, CO_2H), 7.60 (1 H, dd, $^3J_{5,4}$ 7.5, $^3J_{5,6}$ 6.5 Hz, H-5), 7.48–7.45 (2 H, m, H-4 and H-6), 7.37 (1 H, dd, $^3J_{2,3}$ 7.6, $^3J_{2,1}$ 6.4 Hz, H-2), 7.32 (1 H, dd, $^3J_{3,2}$ 7.6, $^4J_{1,3}$ 0.8 Hz, H-3), 7.31 (1 H, br.s, NH), 7.02 (1 H, d, $^3J_{8,9}$ 5.7 Hz, H-8), 6.87 (1 H, dd, $^3J_{2,1}$ 6.4, $^4J_{1,3}$ 0.8 Hz, H-1), 6.43 (1 H, d, $^3J_{8,9}$ 5.7 Hz, H-9), 5.18 (1 H, s, H-7a), 3.10 (1 H, d, $^3J_{11,11a}$ 8.9 Hz, H-11a), 2.71 (1 H, d, $^3J_{11,11a}$ 8.9 Hz, H-11), 1.61 (3 H, s, Me-10); (**41Bb**) 12.38 (1 H, br.s, CO_2H), 8.29 (1 H, d, $^3J_{2,1}$ 7.6 Hz, H-1), 7.53 (1 H, br.d, $^3J_{3,2}$ 7.6 Hz, H-3), 7.42 (1 H, t, $^3J_{2,1}$ ~ $^3J_{2,3}$ 7.6 Hz, H-2), 7.31 (1 H, t, $^3J_{5,6}$ ~ $^3J_{5,4}$ 7.6 Hz, H-5), 7.23 (1 H, br.d, $^3J_{5,4}$ 7.6 Hz, H-4), 7.08 (1 H, br.s, NH), 6.82 (1 H, dd, $^3J_{5,6}$ 7.6, $^4J_{4,6}$ 1.3 Hz, H-6), 6.74 (1 H, d, $^3J_{8,9}$ 5.1 Hz, H-8), 6.37 (1 H, d, $^3J_{8,9}$ 5.1 Hz, H-9), 5.55 (1 H, s, H-7a), 3.21 (1 H, d, $^3J_{11,11a}$ 8.9 Hz, H-11), 2.70 (1 H, d, $^3J_{11,11a}$ 8.9 Hz, H-11a), 1.62 (3 H, s, Me-10); δ_C (100.6 MHz, $DMSO-d_6$) (**41Ab**) 171.4 (CO_2H), 169.7 (C-12), 141.5 (C-6a), 139.5 (C-9), 134.9 (C-8), 133.9 (C-13a), 131.2 (C-3a), 127.0 (C-2), 125.9 (C-6), 123.6 (C-5), 117.6 (C-3), 115.7 (C-13b), 115.0 (C-4), 108.5 (C-

1), 89.3 (C-10), 88.8 (C-7b), 67.8 (C-7a), 53.3 (C-11a), 48.0 (C-11), 15.6 (Me-10); (**41Bb**) 171.4 (CO₂H), 168.9 (C-12), 140.8 (C-6a), 139.9 (C-9), 135.8 (C-8), 133.9 (C-13a), 132.6 (C-3a), 127.1 (C-2), 125.9 (C-6), 122.6 (C-5), 116.8 (C-3), 113.5 (C-13b), 110.8 (C-4), 107.8 (C-1), 88.8 (C-10), 87.8 (C-7b), 65.7 (C-7a), 54.3 (C-11a), 48.2 (C-11), 15.7 (Me-10). MS (EI, 70 eV) *m/z* 348 (4, M⁺), 330 (2), 273 (3), 252 (23), 251 (64), 250 (100), 249 (47), 236 (6), 219 (8), 206 (27), 195 (4), 183 (5), 169 (43), 168 (66), 140 (14), 127 (10), 115 (14), 106 (7), 97 (8), 54 (27), 43 (38%).

(7aRS,7bRS,10RS,11aSR)-7,7a,11,11a-Tetrahydro-7b,10-epoxyisoindolo[2,1-a]perimidin-12(10H)-one (42A) and (7aRS,7bSR,10SR,11aRS)-7,7a,11,11a-tetrahydro-7b,10-epoxyisoindolo[2,1-a]perimidin-12(10H)-one (42B). A mixture of 2-(2-furyl)-2,3-dihydro-1H-perimidine (**40a**) (0.46 g, 1.90 mmol), acryloyl chloride (0.16 mL, 2.0 mmol) and NEt₃ (0.32 mL, 2.3 mmol) in PhMe (30 mL) was heated under reflux for 2 h, then cooled and poured into water (50 mL). The organic layer was separated and the water layer was extracted with EtOAc (3 × 20 mL). The organic phases were combined and dried over MgSO₄, which was then filtered off. After the solvents were evaporated under reduced pressure, dark-brown oil was obtained, which was triturated with EtOAc (4 mL). Brown crystals obtained were collected by filtration and recrystallized from a hexane/EtOAc mixture affording a mixture of **42A/42B** in the ratio of ~ 48/52 (0.15 g, 27 %). The mother liquors were combined and purified by silica gel column chromatography (1.8 × 11.5 cm, eluent: EtOAc/hexane 1/10→1/1). Additional 70 mg (9%) of the individual isomer **42B** (70 mg, 9 %) were isolated.

Compound 42B, thick colourless plates, m.p. 199–200 °C (hexane/EtOAc); [Found: C, 74.53; H, 4.87; N, 9.74. C₁₈H₁₄N₂O₂ requires C, 74.47; H, 4.86; N, 9.65%]; *v*_{max} (KBr) 3292, 1685, 1596, 1423, 817, 765 cm⁻¹; δ_H (400 MHz, CDCl₃) (**42B**) 8.33 (1 H, dd, ³J_{1,2} 7.3, ⁴J_{1,3} 0.9 Hz, H-1), 7.58 (1 H, dd, ³J_{3,2} 7.3, ⁴J_{1,3} 0.9 Hz, H-3), 7.47 (1 H, t, ³J_{1,2} ~ ³J_{2,3} 7.3 Hz, H-2), 7.45 (1 H, dd, ³J_{4,5} 8.0, ⁴J_{4,6} 0.9 Hz, H-4), 7.36 (1 H, dd, ³J_{5,4} 8.0, ³J_{5,6} 7.3 Hz, H-5), 6.92 (1 H, dd, ³J_{5,6} 7.3, ⁴J_{6,4} 0.9 Hz, H-6), 6.59 (1 H, d, ³J_{9,8} 6.0 Hz, H-8), 6.53 (1 H, dd, ³J_{9,8} 6.0, ³J_{9,10} 1.6 Hz, H-9), 5.56 (1 H, s, H-7a), 5.21 (1 H, dd, ³J_{11exo,10} 4.6, ³J_{9,10} 1.6 Hz, H-10), 2.77 (1 H, dd, ³J_{11a,11exo} 3.7, ³J_{11endo,11a} 8.7 Hz, H-11a), 2.39 (1 H, ddd, ³J_{11exo,10} 4.6, ²J_{11,11} 11.9, ³J_{11a,11exo} 3.7 Hz, H-11^{exo}), 1.74 (1 H, dd, ²J_{11,11} 11.9, ³J_{11endo,11a} 8.7 Hz, H-11^{endo}); δ_C (100.6 MHz, CDCl₃) (**42B**) 171.2 (C-12), 138.1 and 132.2 (C-9 and C-8), 137.9 (C-6a), 134.4 (C-3a), 131.8 (C-13a), 126.7 and 126.6 (C-5 and C-2), 123.6 and 121.6 (C-3 and C-4), 116.6 (C-13b), 113.9 and 113.5 (C-1 and C-6), 89.2 (C-7b), 79.5 (C-10), 67.2 (C-7a), 48.5 (C-11a), 28.7 (C-11). MALDI-TOF HR: MNa⁺, found 313.1015. C₁₈H₁₄N₂NaO₂ requires 313.0953. δ_H (400 MHz, CDCl₃) (**42A** in mixture **42A/42B** ~ 13/87) 7.76 (1 H, dd, ³J_{1,2} 7.5, ⁴J_{1,3} 1.2 Hz, H-1), 7.57 (1 H, br.d, ³J_{3,2} 7.5 Hz, H-3), 7.47 (4 H, three m overlapping with signals of **42B**, H-2, H-4, H-5), 6.77 (1 H, dd, ³J_{6,5} 7.5, ⁴J_{6,4} 1.2 Hz, H-6), 6.65 (1 H, d, ³J_{9,8} 6.2 Hz, H-8), 6.46 (1 H, dd, ³J_{9,8} 6.2, ³J_{9,10} 1.8 Hz, H-9), 5.24 (1 H, s, H-7a), 5.19 (1 H, dd, ³J_{11exo,10} 4.5, ³J_{9,10} 1.8 Hz, H-10), 2.70 (1 H, dd, ³J_{11endo,11a} 8.7, ³J_{11a,11exo} 3.7 Hz, H-11a), 2.36 (1 H, ddd, ²J_{11,11} 11.8, ³J_{11exo,10} 4.5, ³J_{11a,11exo} 3.7 Hz, H-11^{exo}), 1.70 (1 H, dd, ²J_{11,11} 11.8, ³J_{11endo,11a} 8.7 Hz, H-11^{endo}); δ_C (100.6 MHz, CDCl₃) (**42A**) 171.1 (C-12), 140.4 (C-6a), 137.4 and 131.1 (C-9 and C-8), 134.4 (C-3a), 131.8 (C-13a), 126.6 and 126.5 (C-5 and C-2), 124.2 and 119.8 (C-3 and C-4), 115.8 (C-13b), 113.5 and 113.3 (C-1 and C-6), 90.0 (C-7b), 79.9 (C-10), 69.1 (C-7a), 47.3 (C-11a), 28.3 (C-11).

Synthesis of 2,4a-epoxyisoindolo[1,2-b]quinazolin-12-ones (44). **General experimental procedure.** A mixture of 2-

(aminomethyl)aniline (1.22 g, 10.0 mmol), furfural (0.89 mL, 10.5 mmol) and anhydrous powdered MgSO₄ (2.40 g, 20.0 mmol) in CH₂Cl₂ (20 mL) was stirred at room temperature for 2 h. MgSO₄ was filtered off and washed with CH₂Cl₂ (2 × 10 mL). The obtained solution was used in the next step with maleic anhydride assuming quantitative yield of quinazoline **43a**. According to ¹H NMR, the mixture contains ~ 93% of the target **2-(furan-2-yl)-1,2,3,4-tetrahydroquinazoline (43a)** (the chain tautomeric form was not observed). Some spectral data of **43a** are presented. White needle-shaped crystals. δ_H (400 MHz, CDCl₃) 7.40 (1 H, br.d, ³J_{5,4} 1.6 Hz, H-5'), 7.04 (1 H, br.dd, ³J_{7,8} 8.1, ³J_{6,7} 7.5 Hz, H-7), 6.91 (1 H, br.d, ³J_{5,6} 7.5 Hz, H-5), 6.72 (1 H, dt, ³J_{6,5} ~ ³J_{6,7} 7.5, ⁴J_{6,8} 1.2 Hz, H-6), 6.59 (1 H, br.d, ³J_{7,8} 8.1 Hz, H-8), 6.38 (1 H, br.d, ³J_{3,4} 3.1 Hz, H-3'), 6.35 (1 H, dd, ³J_{3,4} 3.1, ³J_{5,4} 1.6 Hz, H-4'), 5.35 (1 H, s, H-2), 4.17 (1 H, d, ²J_{4,4} 16.8 Hz, H-4A), 3.96 (1 H, d, ²J_{4,4} 16.8 Hz, H-4B); δ_C (100.6 MHz, CDCl₃) 154.0 (C-2'), 142.8 (C-8a), 142.4 (C-5'), 127.5 and 126.3 (C-5 and C-7), 121.4 (C-4a), 118.6 (C-6), 115.5 (C-8), 110.4 and 106.8 (C-3' and C-4'), 63.9 (C-2), 45.6 (C-4).

Maleic anhydride (1.03 g, 10.5 mmol) was added to a solution of quinazoline **43a** (~ 10 mmol) obtained above in CH₂Cl₂ (~ 35 mL). The brown-red transparent reaction mixture was stirred for 1 h and then stored at room temperature for 24 h. The crystals formed were collected by filtration, washed with Me₂CO (3 × 6 mL), Et₂O (2 × 10 mL) and air-dried till constant weight. The mixture of isomers **44a** was obtained as pale pink powder (2.34 g, 78 %), isomer ratio **44Aa/44Ba** ~ 82/18; m.p. 134.3–136 °C (decomp.).

A transparent solution is formed when this mixture (1.0 g) was brought to reflux in MeOH/DMF (10 mL/7 mL). The solution was cooled and Me₂CO (5 mL) was added to it. The solution was stored at -4 °C for 24 h. The precipitate formed was collected by filtration, washed with Me₂CO (2 × 3 mL) and air-dried till constant weight. The *minor* isomer **44Ba** (95 mg) was obtained as a white powder. The mother liquor was stored open at 26 °C for a week. The crystals formed were collected by filtration, washed with acetone (2 × 5 mL) and dried in air. The isomer **44Aa** (0.3 g) was obtained as elongated pale-yellow needles.

When Me₂CO (20 mL) was used as the solvent in the second step with the same load and the mixture was then stored for 2 d at room temperature, the title acids **44Aa/44Ba** (1.45 g, 48 %) were obtained in the ratio of 82/18 (small needles).

When PhMe (20 mL) was used as the solvent in the second step with the same load and heated under reflux for 10 min, the title acids **44Aa/44Ba** (1.0 g, 33 %) were obtained in the ratio of 50/50. In this case, some resinification occurred and the products were obtained by multiple trituration of the brown oil with Me₂CO.

(1RS,2SR,4aRS,4bRS,12aSR)-12-Oxo-1,2,5,10,12,12a-hexahydro-4bH-2,4a-epoxyisoindolo[1,2-b]quinazoline-1-carboxylic acid (44Aa). *Major* isomer, transparent needles, m.p. 123.1–125 °C (decomp., from MeOH/DMF); [Found: 64.45; H, 4.84; N, 9.17. C₁₆H₁₄N₂O₄ requires C, 64.42; H, 4.73; N, 9.39%]; *v*_{max} (KBr) 3611, 3293, 1728, 1674, 1636, 1492, 1060 cm⁻¹; δ_H (400 MHz, DMSO-*d*₆) 12.20 (1 H, br.s, CO₂H), 7.00 (1 H, br.t, ³J_{7,8} ~ ³J_{6,7} 7.3 Hz, H-7), 6.99 (1 H, d, ³J_{8,9} 7.3 Hz, H-9), 6.83 (1 H, d, ³J_{4,3} 6.0 Hz, H-4), 6.71 (1 H, br.d, ³J_{6,7} 7.3 Hz, H-6), 6.68 (1 H, br.t, ³J_{8,9} ~ ³J_{7,8} 7.3 Hz, H-8), 6.51 (1 H, br.s, NH), 6.48 (1 H, dd, ³J_{3,4} 6.0, ³J_{2,3} 0.9 Hz, H-3), 5.08 (1 H, d, ³J_{2,3} 0.9 Hz, H-2), 4.99 (1 H, s, H-4b), 4.72 (1 H, d, ²J_{10,10} 16.9 Hz, H-10A), 4.22 (1 H, d, ²J_{10,10} 16.9 Hz, H-10B), 2.74 (1 H, d, ³J_{1,12a} 9.2 Hz, H-12a), 2.52 (1 H, d, ³J_{1,12a} 9.2 Hz, H-1); δ_C (100.6 MHz, DMSO-*d*₆) 172.2 (CO₂H), 170.3 (C-12), 143.0 (C-5a), 136.2 (C-3), 134.0

(C-4), 127.0 and 126.5 (C-7 and C-9), 118.51 and 118.46 (C-8 and C-9a), 116.2 (C-6), 89.8 (C-4a), 81.8 (C-2), 65.7 (C-4b), 48.8 (C-12a), 44.0 (C-1), 40.0 (C-10). MS (EI, 70 eV) m/z 298 (4, M^+), 235 (2), 220 (4), 201 (11), 200 (82), 199 (49), 184 (41), 183 (67), 170 (11), 154 (12), 133 (12), 131 (29), 107 (14), 106 (100), 104 (30), 91 (19), 81 (28), 78 (33), 77 (48), 73 (29), 54 (82), 43 (32%). (**1RS,2SR,4aRS,4bSR,12aSR**)-12-Oxo-1,2,5,10,12,12a-hexahydro-4bH-2,4a-epoxyisoindolo[1,2-*b*]quinazoline-1-carboxylic acid (**44Ba**). *Minor* isomer, white powder, m.p. 166.5–167 °C (decomp., from MeOH/DMF); [Found: C, 64.38; H, 4.90; N, 9.24. $C_{16}H_{14}N_2O_4$ requires C, 64.42; H, 4.73; N, 9.39%]; ν_{\max} (KBr) 3345, 1729, 1670, 1503, 1181 cm^{-1} ; δ_H (400 MHz, DMSO- d_6) 12.15 (1 H, br.s, CO₂H), 7.04 (1 H, dd, $^3J_{8,9}$ 7.5, $^4J_{7,9}$ 1.3 Hz, H-9), 7.00 (1 H, br.d, $^3J_{7,8} \sim ^3J_{6,7}$ 7.5, $^4J_{7,9}$ 1.3 Hz, H-7), 6.76 (1 H, dd, $^3J_{6,7}$ 7.5, $^4J_{6,8}$ 1.0 Hz, H-6), 6.67 (1 H, d, $^3J_{4,3}$ 5.7 Hz, H-4), 6.66 (1 H, br.d, $^3J_{8,9} \sim ^3J_{7,8}$ 7.5, $^4J_{8,6}$ 1.0 Hz, H-8), 6.50 (1 H, dd, $^3J_{3,4}$ 5.7, $^3J_{2,3}$ 1.7 Hz, H-3), 6.17 (1 H, d, $^3J_{NH,4b}$ 2.0 Hz, NH), 5.33 (1 H, d, $^3J_{NH,4b}$ 2.0 Hz, H-4b), 5.06 (1 H, d, $^3J_{2,3}$ 1.7 Hz, H-2), 4.53 (1 H, d, $^2J_{10,10}$ 16.9 Hz, H-10A), 4.21 (1 H, d, $^2J_{10,10}$ 16.9 Hz, H-10B), 2.90 (1 H, d, $^3J_{1,12a}$ 8.9 Hz, H-12a), 2.53 (1 H, d, $^3J_{1,12a}$ 8.9 Hz, H-1); δ_C (100.6 MHz, DMSO- d_6) 172.7 (CO₂H), 168.6 (C₁₂), 142.8 (C_{5a}), 136.9 (C₃), 135.0 (C₄), 127.1 (C₉), 126.9 (C₇), 117.8 (C₈), 116.9 (C_{9a}), 116.0 (C₆), 89.7 (C_{4a}), 81.1 (C₂), 63.8 (C_{4b}), 50.6 (C_{12a}), 44.4 (C₁), 40.2 (C₁₀). MS (EI, 70 eV) m/z 298 (9, M^+), 280 (7), 263 (3), 254 (4), 235 (4), 225 (4), 220 (4), 200 (99), 199 (100), 184 (39), 183 (97), 169 (27), 154 (12), 133 (18), 132 (19), 131 (39), 107 (40), 106 (94), 104 (61), 98 (20), 91 (19), 81 (22), 79 (25), 78 (50), 77 (77), 69 (10), 65 (18), 54 (93), 51 (33), 43 (39%).

(**1RS,2SR,4aRS,4bRS,12aSR**)-2-Methyl-12-oxo-1,2,5,10,12,12a-hexahydro-4bH-2,4a-epoxyisoindolo[1,2-*b*]quinazoline-1-carboxylic acid (**44Ab**). Similarly to the procedure for preparation of **44a**, 2-(aminomethyl)aniline (1.22 g, 10.0 mmol), 5-methylfurfural (1.05 mL, 10.5 mmol), anhydrous powdered MgSO₄ (2.40 g, 20.0 mmol) and maleic anhydride (1.03 g, 10.5 mmol) in CH₂Cl₂ (30 mL) were used to afford **44Ab** (1.21 g, 39 %) as white powder, m.p. 115.6–116.9 °C (decomp., from *i*-PrOH/DMF); [Found: C, 65.31; H, 5.04; N, 9.14. $C_{17}H_{16}N_2O_4$ requires C, 65.38; H, 5.16; N, 8.97%]; ν_{\max} (KBr) 3515, 3381, 1727, 1649, 741 cm^{-1} ; δ_H (400 MHz, DMSO- d_6) 12.24 (1 H, br.s, CO₂H), 7.05–7.02 (2 H, m, H-7 and H-9), 6.90 (1 H, d, $^3J_{3,4}$ 5.7 Hz, H-3), 6.75 (1 H, br.d, $^3J_{7,6}$ 7.7 Hz, H-6), 6.73 (1 H, t, $^3J_{7,8} \sim ^3J_{9,8}$ 7.7 Hz, H-8), 6.48 (1 H, br.s, NH), 6.35 (1 H, d, $^3J_{3,4}$ 5.7 Hz, H-4), 5.01 (1 H, s, H-4b), 4.78 (1 H, d, $^2J_{10,10}$ 16.5 Hz, H-10A), 4.24 (1 H, d, $^2J_{10,10}$ 16.5 Hz, H-10B), 2.81 (1 H, d, $^3J_{1,12a}$ 8.9 Hz, H-12a), 2.60 (1 H, d, $^3J_{1,12a}$ 8.9 Hz, H-1), 1.55 (3 H, s, Me-2); δ_C (100.6 MHz, DMSO- d_6) 180.9 (CO₂H), 180.2 (C-12), 152.7 (C-5a), 148.8 (C-3), 144.5 (C-4), 136.6 (C-7), 136.1 (C-9), 127.97 (C-6), 127.93 (C-9a), 125.7 (C-8), 98.8 (C-2), 98.6 (C-4a), 75.2 (C-4b), 61.6 (C-1), 57.0 (C-12a), 49.4 (C-10), 25.0 (Me-2). MS (EI, 70 eV) m/z 294 (3, M^+ -18), 263 (3), 257 (4), 215 (59), 214 (78), 213 (67), 199 (46), 198 (69), 197 (90), 186 (18), 184 (27), 171 (38), 169 (31), 156 (28), 154 (31), 144 (13), 133 (30), 131 (36), 121 (39), 110 (42), 108 (86), 107 (81), 106 (63), 98 (73), 94 (60), 92 (62), 91 (100), 81 (32), 79 (42), 77 (71), 73 (23), 65 (53), 60 (29), 54 (68), 53 (90), 51 (64), 43 (56%).

(**1RS,2SR,4aSR,4bSR,12aSR**)-2-Bromo-12-oxo-1,2,5,10,12,12a-hexahydro-4bH-2,4a-epoxyisoindolo[1,2-*b*]quinazoline-1-carboxylic acid (**44Ac**) and (**1RS,2SR,4aSR,4bRS,12aRS**)-2-bromo-12-oxo-1,2,5,10,12,12a-hexahydro-4bH-2,4a-epoxyisoindolo[1,2-*b*]quinazoline-1-carboxylic acid (**44Bc**). Similarly to the preparation procedure presented for **44a**, 2-(aminomethyl)aniline

(0.61 g, 5.0 mmol), 5-bromofurfural (0.88 g, 5.0 mmol), anhydrous powdered MgSO₄ (1.20 g, 10.0 mmol) and maleic anhydride (0.49 g, 5.0 mmol) in CH₂Cl₂ (30 mL) were used to afford **44c** (0.46 g, 26 %) as a yellow powder, isomer ratio **44Ac/44Bc** ~ 76/24. The *minor* isomer **44Bc** (0.08 g) was obtained as a pale yellow powder by recrystallization of the mixture from EtOH/DMF, m.p. > 210.3 °C (decomp.); [Found: C, 50.79; H, 3.30; N, 7.46. $C_{16}H_{13}BrN_2O_4$ requires C, 50.95; H, 3.47; N, 7.43; Br, 21.18%]; ν_{\max} (KBr) 3514, 3338, 1740, 1667, 1185, 744 cm^{-1} ; δ_H (400 MHz, DMSO- d_6) (**44Bc**) 12.51 (1 H, br.s, CO₂H), 7.05 (1 H, br.d, $^3J_{9,8}$ 7.4 Hz, H-9), 7.05 (1 H, dd, $^3J_{7,6}$ 8.0, $^3J_{7,8}$ 7.4 Hz, H-7), 6.86 (1 H, d, $^3J_{3,4}$ 5.4 Hz, H-4), 6.76 (1 H, br.d, $^3J_{7,6}$ 8.0 Hz, H-6), 6.68 (1 H, br.t, $^3J_{7,8} \sim ^3J_{9,8}$ 7.4 Hz, H-8), 6.57 (1 H, d, $^3J_{3,4}$ 5.4 Hz, H-3), 6.40 (1 H, br.s, NH), 5.34 (1 H, s, H-4b), 4.53 (1 H, d, $^2J_{10,10}$ 16.5 Hz, H-10A), 4.24 (1 H, d, $^2J_{10,10}$ 16.5 Hz, H-10B), 3.10 (1 H, d, $^3J_{1,12a}$ 8.3 Hz, H-12a), 3.01 (1 H, d, $^3J_{1,12a}$ 8.3 Hz, H-1); δ_C (100.6 MHz, DMSO- d_6) (**44Bc**) 169.5 (CO₂H), 167.6 (C-12), 142.6 (C-5a), 139.9 (C-3), 137.3 (C-4), 127.2 (C-7), 126.9 (C-9), 117.8 (C-8), 116.3 (C-9a), 115.6 (C-6), 90.7 (C-2), 88.3 (C-4a), 63.8 (C-4b), 53.3 (C-12a), 50.9 (C-1), 40.4 (C-10); δ_H (400 MHz, DMSO- d_6) (**44Ac** in mixture with **44Bc**, ratio **44Ac/44Bc** ~ 76/24) 12.60 (1 H, br.s, CO₂H), 7.06–7.00 (2 H, m, H-9 and H-7), 6.74 (1 H, d, $^3J_{3,4}$ 5.7 Hz, H-4), 6.77–6.71 (2 H, m, H-6 and H-8), 6.62 (1 H, d, $^3J_{3,4}$ 5.7 Hz, H-3), 6.54 (1 H, br.s, NH), 5.12 (1 H, s, H-4b), 4.78 (1 H, d, $^2J_{10,10}$ 16.7 Hz, H-10A), 4.28 (1 H, d, $^2J_{10,10}$ 16.7 Hz, H-10B), 3.05–3.01 (2 H, m, H-12a and H-1); δ_C (100.6 MHz, DMSO- d_6) (**44Ac** in mixture with **44Bc**, ratio **44Ac/44Bc** ~ 76/24) 169.6 and 169.5 (CO₂H and C-12), 142.9 (C-5a), 139.7 (C-3), 136.0 (C-4), 127.2 (C-7), 126.6 (C-9), 118.7 (C-8), 118.3 (C-9a), 116.3 (C-6), 90.5 (C-2), 88.4 (C-4a), 65.1 (C-4b), 51.5 (C-12a), 50.8 (C-1), 40.0 (C-10). MS (EI, 70 eV) m/z 378 (6, M^+ for ⁸¹Br), 376 (5), 357 (9), 329 (1), 280 (91), 278 (100), 263 (56), 261 (28), 250 (8), 199 (70), 197 (17), 202 (14), 199 (70), 184 (33), 182 (35), 174 (18), 169 (32), 133 (37), 121 (42), 107 (73), 106 (76), 98 (89), 91 (71), 85 (78), 78 (62), 77 (77), 72 (38), 65 (32), 61 (34), 54 (100), 45 (76), 43 (78%).

Synthesis of 2,4a-epoxyisoindolo[1,2-*b*]quinazolin-12-ones (45, 46). Furfural (0.42 mL, 5.10 mmol) and anhydrous powdered MgSO₄ (1.20 g, 10.0 mmol) were added to a solution of 2-aminobenzylamine (0.61 g, 5.0 mmol) in CH₂Cl₂ (20 mL). The reaction mixture was stirred at room temperature for 1 h. MgSO₄ was filtered off and washed with CH₂Cl₂ (2 × 10 mL), the solvent was evaporated under reduced pressure. A solution of the obtained quinazoline **43a** (5 mmol), acryloyl chloride (0.44 mL, 5.50 mmol) and NEt₃ (0.97 mL, 7.0 mmol) in PhMe (30 mL) was heated under reflux for 3 h. The mixture was cooled and poured into water (50 mL). The organic layer was separated and the water layer was extracted with EtOAc (3 × 20 mL). The organic phases were combined and dried over MgSO₄. The dark-brown oil obtained by evaporation of the solvent, was crystallized in EtOAc to afford a brown crystalline compound (0.23 g, 18 %) - the mixture of isomers **45A/45B** in the ratio of ~ 70/30. The mother liquor was separated by silica gel column chromatography (1.7 × 17 cm) using EtOAc/hexane (1/10→1/1) mixtures. Isoindoloquinazoline **45A** (70 mg) is obtained first, followed by isoindoloquinazoline **45B** (120 mg, ~ 92 % pure). The latter fraction was recrystallized from a hexane/EtOAc mixture to obtain an analytical sample of the isomer **45B**. Then the compound **46** (60 mg) was eluted. The ratio of the isomers and the yields of the isolated products are the following: **45A/45B/46** ~ 50 (18 %)/ 39 (14 %)/ 11 (4 %).

(2RS,4aRS,4bRS,12aSR)-1,5,10,12a-Tetrahydro-4bH-2,4a-epoxyisoindolo[1,2-b]quinazolin-12(2H)-one (45A). Fine colorless needles (hedgehog-like crystalline aggregates), m.p. 212.5–214.5 °C (decomp., from EtOAc); [Found: C, 70.71; H, 5.63; N, 11.21. C₁₅H₁₄N₂O₂ requires C, 70.85; H, 5.55; N, 11.02%]; ν_{\max} (KBr) 3315, 1676, 1610, 1493, 1418, 1257, 1054, 757, 709 cm⁻¹; δ_{H} (400 MHz, CDCl₃) 7.08 (1 H, ddd, ³J_{7,6} 8.1, ³J_{7,8} 7.5, ⁴J_{7,9} 1.2 Hz, H-7), 7.03 (1 H, dd, ³J_{9,8} 7.5, ⁴J_{7,9} 1.2 Hz, H-9), 6.85 (1 H, dt, ³J_{8,9} ~ ³J_{7,8} 7.5, ⁴J_{6,8} 1.2 Hz, H-8), 6.73 (1 H, br.d, ³J_{6,7} 8.1 Hz, H-6), 6.61 (1 H, d, ³J_{4,3} 6.0 Hz, H-4), 6.44 (1 H, dd, ³J_{3,4} 6.0, ³J_{2,3} 1.8 Hz, H-3), 5.15 (1 H, dd, ³J_{1,2} 4.4, ³J_{2,3} 1.8 Hz, H-2), 5.06 (1 H, s, H-4b), 5.01 (1 H, d, ²J_{10,10} 16.8 Hz, H-10A), 4.29 (1 H, d, ²J_{10,10} 16.8 Hz, H-10B), 2.55 (1 H, dd, ³J_{1endo,12a} 9.3, ³J_{1exo,12a} 4.4 Hz, H-12a), 2.20 (1 H, dt, ²J_{1,1} 11.8, ³J_{1exo,12a} ~ ³J_{1exo,2} 4.4 Hz, H-1^{exo}), 1.63 (1 H, dd, ²J_{1,1} 11.8, ³J_{1endo,12a} 9.3 Hz, H-1^{endo}); δ_{C} (100.6 MHz, CDCl₃) 173.7 (C-12), 142.3 (C-5a), 137.2 (C-3), 131.3 (C-4), 127.7 and 127.2 (C-7 and C-9), 120.6 (C-8), 119.8 (C-9a), 117.1 (C-6), 90.7 (C-4a), 79.8 (C-2), 67.3 (C-4b), 46.2 (C-12a), 40.9 (C-10), 27.7 (C-1). MALDI-TOF HR: MNa⁺, found 277.0962. C₁₅H₁₄N₂NaO₂ requires 277.0947.

(2RS,4aRS,4bSR,12aSR)-1,5,10,12a-Tetrahydro-4bH-2,4a-epoxyisoindolo[1,2-b]quinazolin-12(2H)-one (45B). Colorless plates, m.p. 192.2–192.5 °C (hexane/EtOAc); [Found: C, 70.75; H, 5.58; N, 11.17. C₁₅H₁₄N₂O₂ requires C, 70.85; H, 5.55; N, 11.02%]; ν_{\max} (KBr) 3298, 1660, 1495, 1260, 966, 780, 707 cm⁻¹; δ_{H} (400 MHz, CDCl₃) 7.11 (1 H, dd, ³J_{7,6} 8.2, ³J_{7,8} 7.5 Hz, H-7), 7.08 (1 H, br.d, ³J_{9,8} 7.5 Hz, H-9), 6.92 (1 H, br.t, ³J_{8,9} ~ ³J_{7,8} 7.5 Hz, H-8), 6.84 (1 H, br.d, ³J_{6,7} 8.2 Hz, H-6), 6.53 (1 H, d, ³J_{4,3} 5.7 Hz, H-4), 6.45 (1 H, dd, ³J_{3,4} 5.7, ³J_{2,3} 1.5 Hz, H-3), 5.28 (1 H, br.s, H-4b), 5.14 (1 H, dd, ³J_{1,2} 4.4, ³J_{2,3} 1.5 Hz, H-2), 4.84 (1 H, d, ²J_{10,10} 17.0 Hz, H-10A), 4.37 (1 H, d, ²J_{10,10} 17.0 Hz, H-10B), 4.24 (1 H, br.s, NH), 2.56 (1 H, dd, ³J_{1endo,12a} 9.0, ³J_{1exo,12a} 3.3 Hz, H-12a), 2.27 (1 H, ddd, ²J_{1,1} 12.0, ³J_{1exo,2} 4.4, ³J_{1exo,12a} 3.3 Hz, H-1^{exo}), 1.63 (1 H, dd, ²J_{1,1} 12.0, ³J_{1endo,12a} 9.0 Hz, H-1^{endo}); δ_{C} (100.6 MHz, CDCl₃) 172.0 (C-12), 141.1 (C-5a), 137.6 (C-3), 132.6 (C-4), 127.7 and 127.3 (C-7 and C-9), 121.8 (C-8), 120.9 (C-9a), 120.2 (C-6), 90.3 (C-4a), 79.2 (C-2), 65.6 (C-4b), 48.0 (C-12a), 40.9 (C-10), 28.2 (C-1). MS (EI, 70 eV) *m/z* 254 (72, M⁺), 237 (7), 225 (4), 207 (6), 199 (27), 183 (100), 181 (14), 132 (14), 131 (43), 106 (34), 104 (18), 78 (27), 77 (32), 59 (32), 55 (51), 43 (49%).

(2RS,4aRS,4bRS,12aSR)-5-Acryloyl-1,5,10,12a-tetrahydro-4bH-2,4a-epoxyisoindolo[1,2-b]quinazolin-12(2H)-one (46). Colorless needles, m.p. 209.5–210 °C (decomp., from EtOH); [Found: C, 70.18; H, 5.39; N, 9.09. C₁₈H₁₆N₂O₃ requires C, 70.12; H, 5.23; N, 9.09%]; ν_{\max} (KBr) 1685, 1648, 1615, 1409, 1328, 1251 cm⁻¹; δ_{H} (400 MHz, CDCl₃) 7.25–7.22 (2 H, m, H-7 and H-9), 7.17 (1 H, dt, ³J_{8,9} ~ ³J_{7,8} 7.5, ⁴J_{6,8} 1.2 Hz, H-8), 7.07 (1 H, br.d, ³J_{7,6} 8.4 Hz, H-6), 6.75 (1 H, d, ³J_{4,3} 6.2 Hz, H-4), 6.61 (1 H, s, H-4b), 6.50 (1 H, dd, ³J_{3^{trans,2}} 16.8, ²J_{3^{trans,2}} 3.1 Hz, H-3^{trans}), 6.44 (1 H, dd, ³J_{3^{trans,2}} 16.8, ³J_{3^{cis,2}} 9.3 Hz, H-2'), 6.30 (1 H, dd, ³J_{3,4} 6.2, ³J_{2,3} 1.9 Hz, H-3), 5.71 (1 H, dd, ³J_{3^{cis,2}} 9.3, ²J_{3^{trans,2}} 3.1 Hz, H-3^{cis}), 4.95 (1 H, d, ²J_{10,10} 14.7 Hz, H-10A), 4.85 (1 H, dd, ³J_{1exo,2} 4.6, ³J_{2,3} 1.9 Hz, H-2), 3.86 (1 H, d, ²J_{10,10} 14.7 Hz, H-10B), 2.64 (1 H, dd, ³J_{1endo,12a} 8.7, ³J_{1exo,12a} 3.1 Hz, H-12a), 2.07 (1 H, ddd, ²J_{1,1} 11.8, ³J_{1exo,2} 4.6, ³J_{1exo,12a} 3.1 Hz, H-1^{exo}), 1.49 (1 H, dd, ²J_{1,1} 11.8, ³J_{1endo,12a} 8.7 Hz, H-1^{endo}); δ_{C} (100.6 MHz, CDCl₃) 172.9 (C-12), 165.6 (COCH=CH₂), 136.3 (C-5a), 135.9 (C-3), 133.7 (C-4), 131.3 (C-9a), 129.5 (COCH=CH₂), 128.9 (COCH=CH₂), 128.1 (C-7), 126.4 (C-9), 125.9 (C-8), 125.8 (C-6), 92.4 (C-4a), 78.8 (C-2), 69.4 (C-4b), 48.9 (C-12a), 40.3 (C-10), 28.2 (C-1). GC-MS (EI, 70 eV) *m/z* 308 (2, M⁺), 291 (1),

280 (5), 264 (3), 253 (9), 237 (11), 207 (4), 199 (23), 183 (10), 160 (4), 132 (20), 131 (14), 130 (9), 104 (6), 77 (13), 55 (100%). **Preparation of compounds 48–50 and attempted synthesis of 8,10a-epoxyisindolo[2,1-a]isoindole-7-carboxylic acid (51).** A suspension of propane-1,3-diamine (8.33 mL, 0.10 mol), furfural (8.27 mL, 0.10 mol) and anhydrous powdered MgSO₄ (24.0 g, 0.20 mol) in CH₂Cl₂ (100 mL) was stirred at room temperature for 1 h. MgSO₄ was filtered off and washed with CH₂Cl₂ (2 × 30 mL), the solvent was removed under reduced pressure. The residue, a brown mobile oil, was analyzed by NMR. The mixture contained three major products (~ 95 % overall): **2-(2-furyl)hexahydropyrimidine (48)**, **N-(2-furylmethylene)propane-1,3-diamine (49)** and **N,N'-bis(2-furylmethylene)propane-1,3-diamine (50)** in ratio **48/49/50** ~ 58/28/14. δ_{H} (400 MHz, CDCl₃) (**48**) 7.31 (1 H, dd, ³J_{5',4'} 1.8, ⁴J_{5',3'} 0.8 Hz, H-5'), 6.28 (1 H, dd, ³J_{3',4'} 3.1, ³J_{5',4'} 1.8 Hz, H-4'), 6.25 (1 H, dd, ³J_{3',4'} 3.1, ⁴J_{5',3'} 0.8 Hz, H-3'), 4.67 (1 H, s, H-2), 3.23 (2 H, ddd, ²J_{4(6),4(6)} 13.7, ³J_{4e(6e),5a} 4.4, ³J_{4e(6e),5e} 2.5 Hz, H-4^{eq} and H-6^{eq}), 2.95 (2 H, dddd, ²J_{4(6),4(6)} 13.7, ³J_{4a(6a),5a} 11.8, ³J_{4a(6a),5e} 3.1, *J* 1.2 Hz, H-4^{ax} and H-6^{ax}), 1.66–1.46 (2 H, m, H-5); (**49**) 8.07 (1 H, s, N=CH), 7.47 (1 H, d, ³J_{5',4'} 1.8 Hz, H-5'), 6.70 (1 H, d, ³J_{3',4'} 3.3 Hz, H-3'), 6.44 (1 H, dd, ³J_{3',4'} 3.3, ³J_{5',4'} 1.8 Hz, H-4'), 3.61 (2 H, dt, *J* 1.2, *J* 6.9 Hz, CH=N-CH₂-CH₂-CH₂-NH₂), 2.76 (2 H, t, ³J_{6,9} 6.9 Hz, CH=N-CH₂-CH₂-CH₂-NH₂), 1.83 (2 H, p, ³J_{6,9} 6.9 Hz, CH=N-CH₂-CH₂-CH₂-NH₂); (**50**) 8.07 (2 H, s, N=CH), 7.47 (2 H, d, ³J_{5',4'} 1.8 Hz, H-5'), 6.70 (2 H, d, ³J_{3',4'} 3.3 Hz, H-3'), 6.44 (2 H, dd, ³J_{3',4'} 3.3, ³J_{5',4'} 1.8 Hz, H-4'), 3.64 (4 H, dt, *J* 1.2, *J* 6.9 Hz, CH=N-CH₂-CH₂-CH₂-N=CH), 2.11 (2 H, p, ³J_{6,9} 6.9 Hz, CH=N-CH₂-CH₂-CH₂-N=CH); δ_{C} (100.6 MHz, CDCl₃) (**48**) 151.7 (C-2'), 141.8 (C-5'), 110.1 (C-4'), 105.3 (C-3'), 68.7 (C-2), 45.7 (2 C, C-3 and C-5), 27.5 (C-4); (**49**) 155.0 (C-2'), 149.8 (CH=N), 144.7 (C-5'), 113.8 (C-3'), 111.6 (C-4'), 59.5 (CH=N-CH₂-CH₂-CH₂-NH₂), 40.2 (CH=N-CH₂-CH₂-CH₂-NH₂), 34.8 (CH=N-CH₂-CH₂-CH₂-NH₂); (**50**) 155.0 (2 C, C-2'), 150.1 (2 C, CH=N), 144.7 (2 C, C-5'), 113.8 (2 C, C-3'), 111.6 (2 C, C-4'), 59.4 (2 C, CH=N-CH₂-CH₂-CH₂-N=CH), 31.9 (CH=N-CH₂-CH₂-CH₂-N=CH).

The obtained mixture of products **48–50** was divided into 5 portions and introduced into a reaction with equimolar amount of maleic anhydride (3.92 g, 0.04 mol) in CH₂Cl₂ (50 mL), or Me₂CO (50 mL) at room temperature or at -10 °C, or stirred under reflux in PhMe (50 mL) for 1 h. In all of the five cases, a viscous brown oil was obtained after the solvent was removed. According to ¹H NMR, the mixtures contained mainly polymeric products.

A procedure for the synthesis of 8-aminonaphthalene-1-thiol from readily available potassium 8-aminonaphthalene-1-sulfonate is reported^[39] and is well-reproducible (Scheme 19), whereas the methods of preparation of 8-aminonaphthalene-1-ol from the same starting compound were described in relatively old and hard to access sources.^[40] We could not find any spectral data on this compound. Therefore, we describe its preparation here.

8-Aminonaphthalene-1-ol. A fine mixture of potassium 8-aminonaphthalene-1-sulfonate (26.1 g, 0.10 mol) and KOH (84.2 g, 1.50 mol) was melted in a steel bowl with an untight cover and then heated at 220–225 °C for 1.5 h with periodical stirring. After cooling, the melt was dissolved in water (300 mL), filtered through coarse Al₂O₃ (3 × 6 cm) and Al₂O₃, washed with water (2 × 50 mL). HCl (18%) was added at 15–20 °C to the brown solution until it was strongly acidic (pH ~ 1–2). The mixture was filtered through Al₂O₃ (3 × 6 cm) again and washed with water (50 mL). NH₄OH (25 %) was carefully added to the obtained solution at stirring until the precipitation formation ceased (pH ~ 7). The grey solid was filtered off and dried in the air to a

constant weight. The obtained product (3.7–4.0 g, 23–25%) was rather pure for most purposes and stable in the air at +4 °C (unlike its analogue, 8-aminonaphthalene-1-thiol, which quickly turns orange and decomposes at this temperature). Attempted recrystallization from hexane/ethyl acetate mixtures lead to resinification of the product. Analytically pure sample may be obtained by slow vaporization of the ethereal solution. M.p. > 82 °C (decomp.); δ_{H} (400 MHz, CDCl_3) 7.42 (1 H, d, $^3J_{5,6}$ 7.9 Hz, H-5), 7.29–7.20 (3 H, m, H-3, H-4, H-6), 6.79 (1 H, d, $^3J_{6,7}$ 7.5 Hz, H-7), 6.76 (1 H, d, $^3J_{2,3}$ 6.9 Hz, H-2), 6.30 (3 H, br.s, NH_2 and OH); δ_{C} (100.6 MHz, CDCl_3) 155.2 (C-1), 139.9 (C-8), 136.8 (C-4a), 126.9 and 125.9 (C-3 and C-6), 123.0 (C-4), 119.5 (C-2), 118.3 (C-8a), 117.7 (C-5), 109.6 (C-7).

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Supplementary data

Copies of ^1H , ^{13}C and DEPT-135 NMR spectra for all new compounds, X-ray description of compounds **17a**, **37a** and **39b** are available free of charge via the Internet at <http://>

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Supporting Information**General Synthetic Approach towards Annelated 3a,6-Epoxyisoindoles by Tandem Acylation/IMDAF Reaction of Furylazaheterocycles. Scope and Limitations.**

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X-Ray description of compounds 17a, 37a and 39b

X-ray structure determination. The crystal of **17a** ($C_{13}H_{15}NO_5$, $M = 265.26$) is orthorhombic, space group $P2_12_12_1$, at $T = 293$ K: $a = 9.327(2)$ Å, $b = 10.719(2)$ Å, $c = 12.261(2)$ Å, $V = 1225.8(4)$ Å³, $Z = 4$, $d_{\text{calc}} = 1.437$ g/cm³, $F(000) = 560$, $\mu = 0.111$ mm⁻¹. 2058 total reflections (2035 unique reflections, $R_{\text{int}} = 0.009$) were measured on a four-circle Enraf Nonius CAD-4 diffractometer ($\lambda(\text{MoK}\alpha)$ -radiation, graphite monochromator, $\omega/2\theta$ scan mode, $2\theta_{\text{max}} = 60^\circ$). The structure was determined by direct methods and refined by full-matrix least squares technique on F^2 with anisotropic displacement parameters for non-hydrogen atoms. The hydrogen atoms were placed in calculated positions and refined within the riding model with fixed isotropic displacement parameters [$U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for the CH_3 -groups and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for the other groups]. The final divergence factors were $R_1 = 0.051$ for 1683 independent reflections with $I > 2\sigma(I)$ and $wR_2 = 0.143$ for all independent reflections, $S = 0.998$. All calculations were carried out using the SHELXTL program.¹

The crystal of **37a** ($C_{19.5}H_{26.5}NO_{9.5}$, $M = 426.92$) is monoclinic, space group $P2_1/c$, at $T = 100$ K: $a = 9.7028(4)$ Å, $b = 10.9965(5)$ Å, $c = 19.1443(9)$ Å, $\beta = 98.299(1)^\circ$, $V = 2021.25(16)$ Å³, $Z = 4$, $d_{\text{calc}} = 1.403$ g/cm³, $F(000) = 906$, $\mu = 0.113$ mm⁻¹. 29463 total reflections (4854 unique reflections, $R_{\text{int}} = 0.029$) were measured on a three-circle diffractometer ($\lambda(\text{MoK}\alpha)$ -radiation, graphite monochromator, φ and ω scan mode, $2\theta_{\text{max}} = 56^\circ$). The structure was determined by direct methods and refined by full-matrix least squares technique on F^2 with anisotropic displacement parameters for non-hydrogen atoms. There was a region in the asymmetric unit of **37a** that appeared to be occupied by solvent molecules. It looked like this region contained hexane and ethyl acetate molecules, which were strongly disordered around the inversion center. Attempts to model this region were unsatisfactory. The contribution to the scattering by the solvate molecules was removed by the use of the SQUEEZE utility in PLATON98.² The hydrogen atoms were placed in calculated positions and refined within the

riding model with fixed isotropic displacement parameters [$U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for the CH_3 -groups and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for the other groups]. The final divergence factors were $R_1 = 0.038$ for 4246 independent reflections with $I > 2\sigma(I)$ and $wR_2 = 0.098$ for all independent reflections, $S = 1.002$. All calculations were carried out using the SHELXTL program.¹

The crystal of **39b** ($\text{C}_{15}\text{H}_{19}\text{NO}_8\text{S}$, $M = 373.37$) is orthorhombic, space group $Pbca$, at $T = 100$ K: $a = 9.3166(14)$ Å, $b = 15.249(2)$ Å, $c = 23.198(3)$ Å, $V = 3295.7(8)$ Å³, $Z = 8$, $d_{\text{calc}} = 1.505$ g/cm³, $F(000) = 1568$, $\mu = 0.242$ mm⁻¹. 29586 total reflections (3261 unique reflections, $R_{\text{int}} = 0.049$) were measured on a three-circle diffractometer ($\lambda(\text{MoK}\alpha)$ -radiation, graphite monochromator, φ and ω scan mode, $2\theta_{\text{max}} = 52^\circ$). The structure was determined by direct methods and refined by full-matrix least squares technique on F^2 with anisotropic displacement parameters for non-hydrogen atoms. The hydrogen atoms were placed in calculated positions and refined within the riding model with fixed isotropic displacement parameters [$U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for the CH_3 -groups and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for the other groups]. The final divergence factors were $R_1 = 0.039$ for 2342 independent reflections with $I > 2\sigma(I)$ and $wR_2 = 0.096$ for all independent reflections, $S = 1.001$. All calculations were carried out using the SHELXTL program.¹

Crystallographic data for the investigated compounds have been deposited with the Cambridge Crystallographic Data Center, CCDC 824681 (**17a**), CCDC 824682 (**37a**) and CCDC 824683 (**39b**). Copies of this information may be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk or www.ccdc.cam.ac.uk).

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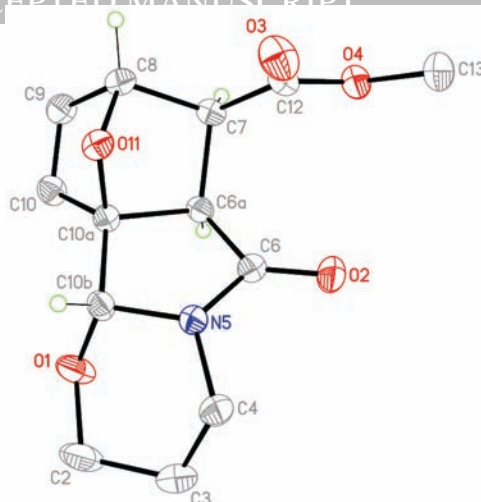


Figure S1 Molecular structure of methyl (6a*R**,7*S**,8*R**,10a*S**,10b*R**)-6-oxo-3,4,6,6a,7,8-hexahydro-2*H*-8,10a-epoxy[1,3]oxazino[2,3-*a*]isoindole-7-carboxylate **17a**. Displacement ellipsoids are depicted at the 40% probability level. Only hydrogen atoms at the asymmetric centers are presented.

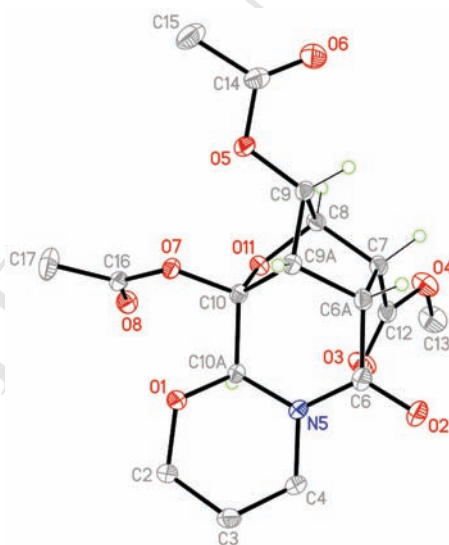


Figure S2 Molecular structure of methyl (6a*RS*,7*SR*,8*SR*,9*RS*,9a*RS*,10*RS*,10a*RS*)-9,10-bis(acetyloxy)-6-oxodecahydro-2*H*-8,10-epoxycyclopenta[4,5]pyrido[2,1-*b*][1,3]oxazine-7-carboxylate **37a**. Displacement ellipsoids are depicted at the 50% probability level. Only hydrogen atoms at the asymmetric centers are presented.

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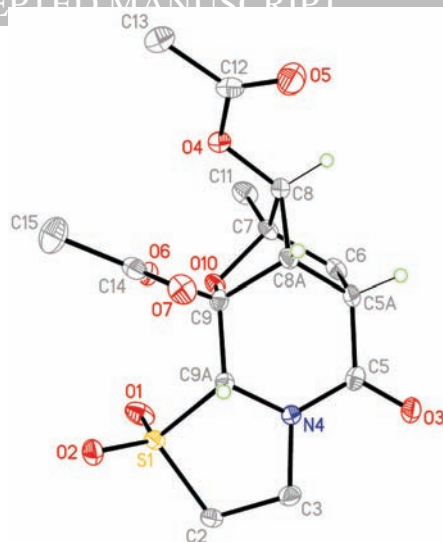


Figure S3 Molecular structure of (5*aRS*,7*SR*,8*RS*,8*aRS*,9*RS*,9*aSR*)-7-methyl-1,1-dioxido-5-oxooctahydro-7,9-epoxycyclopenta[*d*][1,3]thiazolo[3,2-*a*]pyridine-8,9-diyl diacetate **39b**. Displacement ellipsoids are depicted at the 50% probability level. Only hydrogen atoms at the asymmetric centers are presented.

According to the X-ray data, the molecules **17a**, **37a** and **39b** are fused tetracyclic systems containing: **17a** – three five-membered (two tetrahydrofurans and one pyrrolidinone) and one six-membered (oxazinane), **37a** – two five-membered (cyclopentane and tetrahydrofuran) and two six-membered (tetrahydropyridinone and oxazinane), and **39b**: three five-membered (cyclopentane, tetrahydrofuran and thiazolidine) and one six-membered (tetrahydropyridinone) rings. All the five-membered rings have the regular *envelope* conformation, and the oxazole rings have the usual *chair* conformation. The conformation of the six-membered tetrahydropyridinone ring in **37a** is a flattened *boat*, whereas, in **39b**, this ring adopts a distorted *chair* conformation. The nitrogen atoms in all of the compounds have a slightly pyramidalized configuration. The two *O*-carboxylate substituents in **37a** and **39b** occupying the same positions in the 2-oxabicyclo[2.2.1]heptane fragment (C9 and C10 in **37a**, and C8 and C9 in **39b**) are in the sterically unfavorable *syn*-periplanar configuration relative to the tetrahydrofuran ring. Such a disposition is determined by the direction of the Wagner-Meerwein rearrangement.

References

X-Ray

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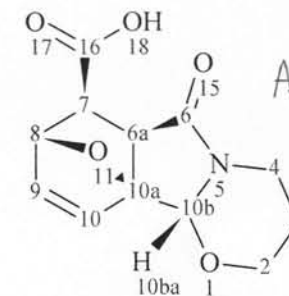
Copies of ^1H , ^{13}C and ^{13}C DEPT-135 spectra of the compounds reported and characterized in the main article

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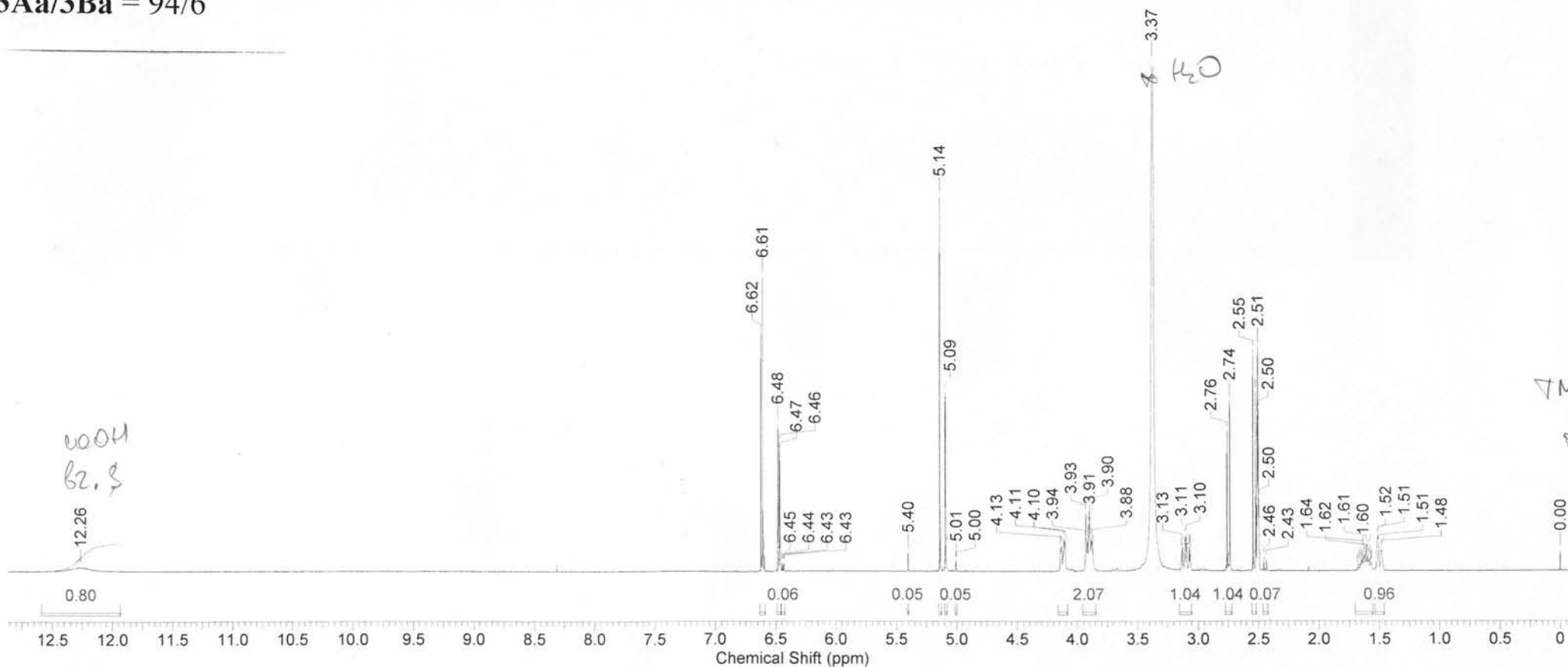
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Compounds 3Aa/3Ba



A/B ~
94/6

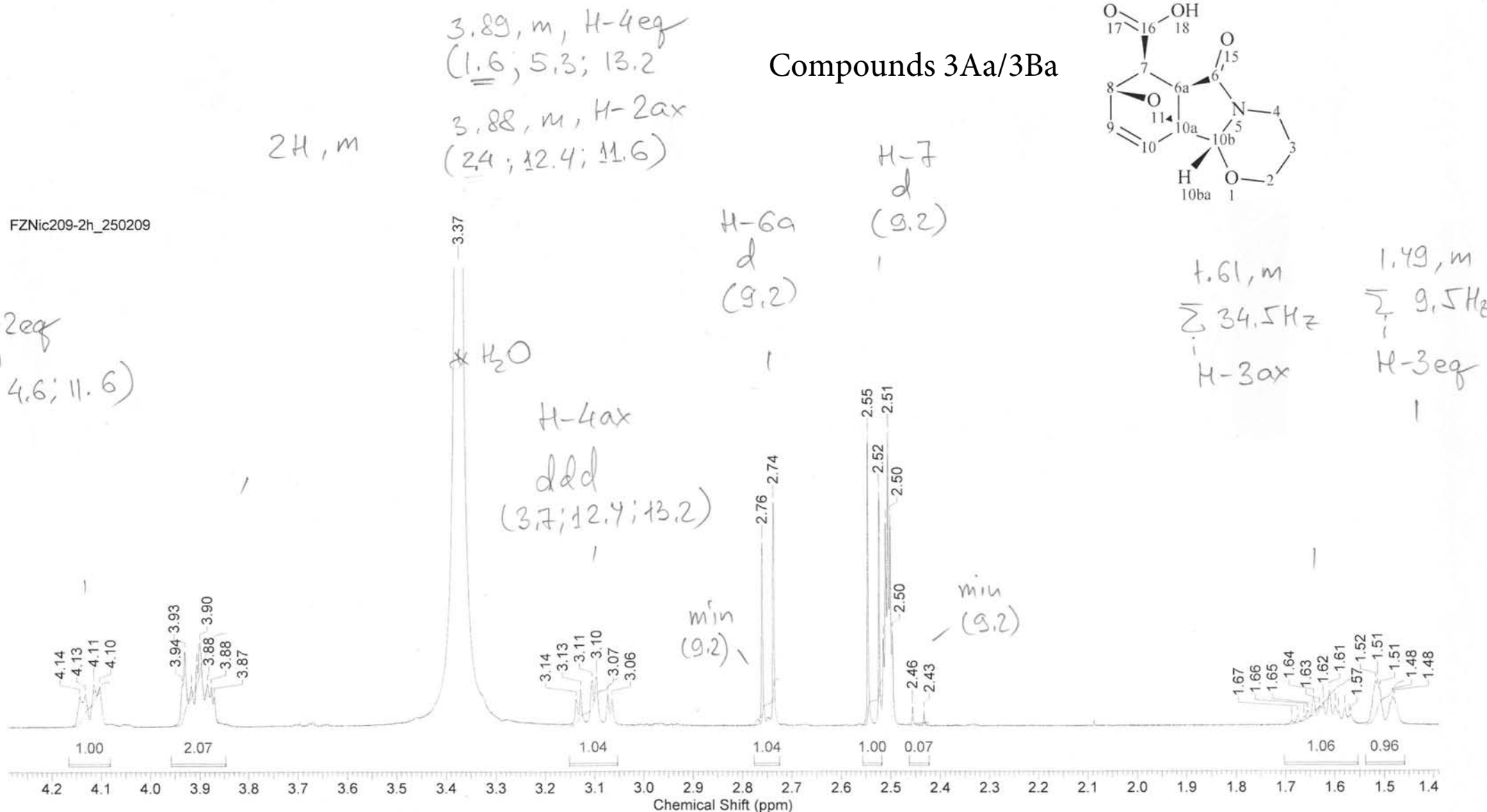
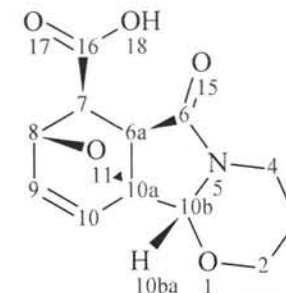
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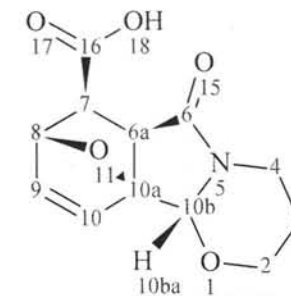
Compounds 3Aa/3Ba



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Compounds 3Aa/3Ba



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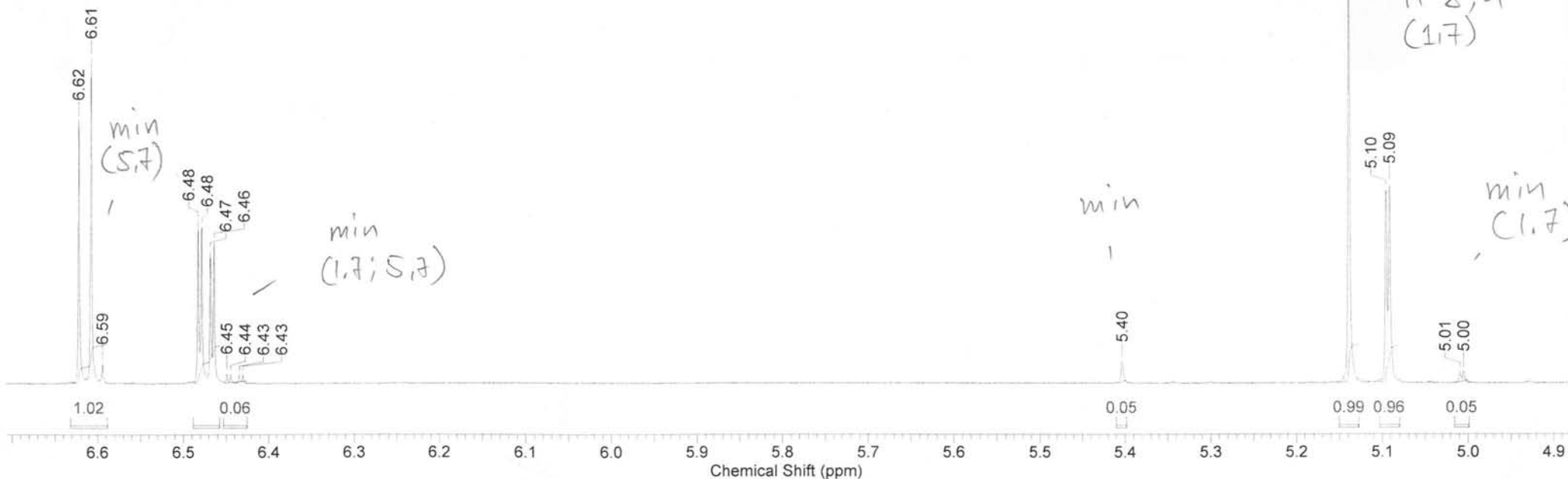
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H-10b

s

H-8, d
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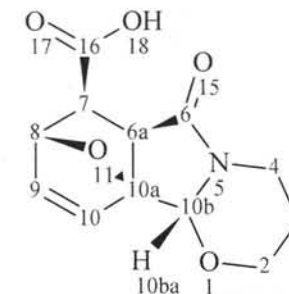
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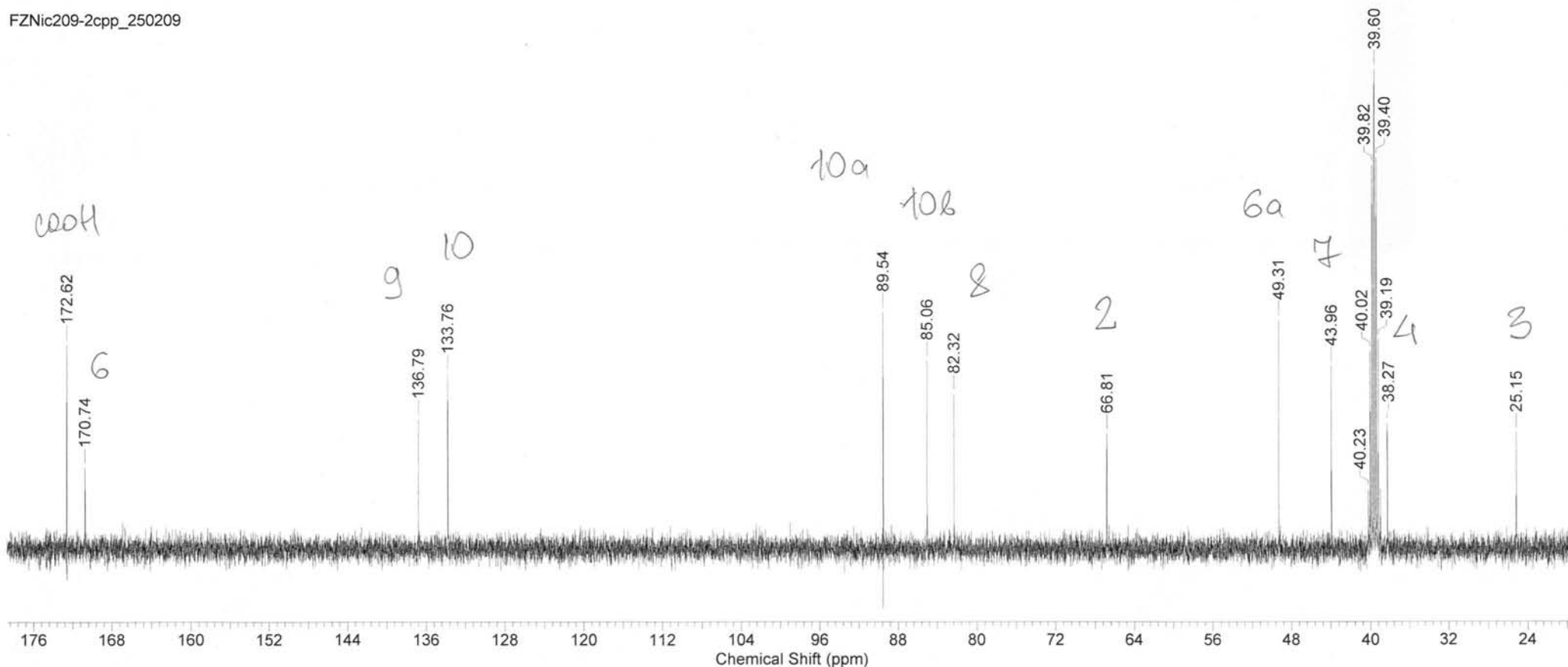
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Compounds 3Aa/3Ba

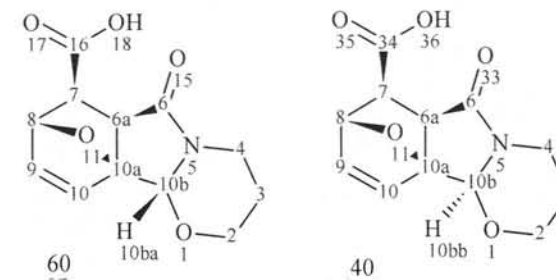


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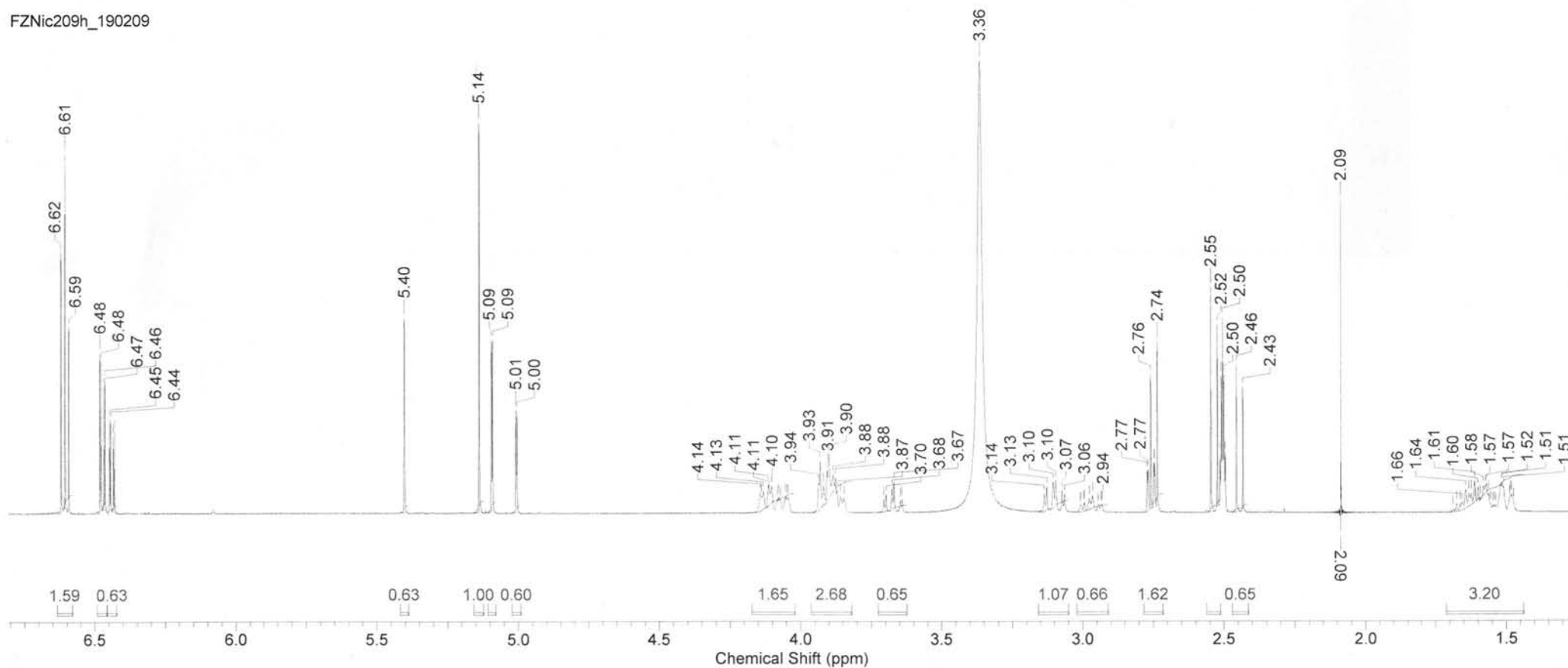


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Points Count 65536	Pulse Sequence s2pul	Receiver Gain 40.00	Solvent DMSO-d6
Spectrum Offset (Hz) 3519.4019	Sweep Width (Hz) 8000.00	Temperature (degree C) 70.000	

Compounds 3Aa/3Ba

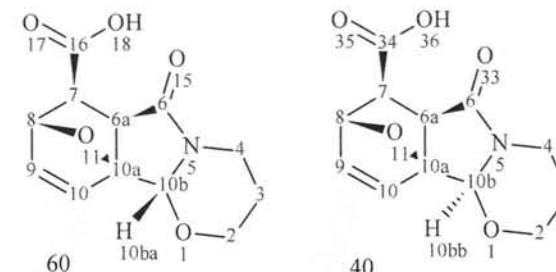


FZNic209h_190209

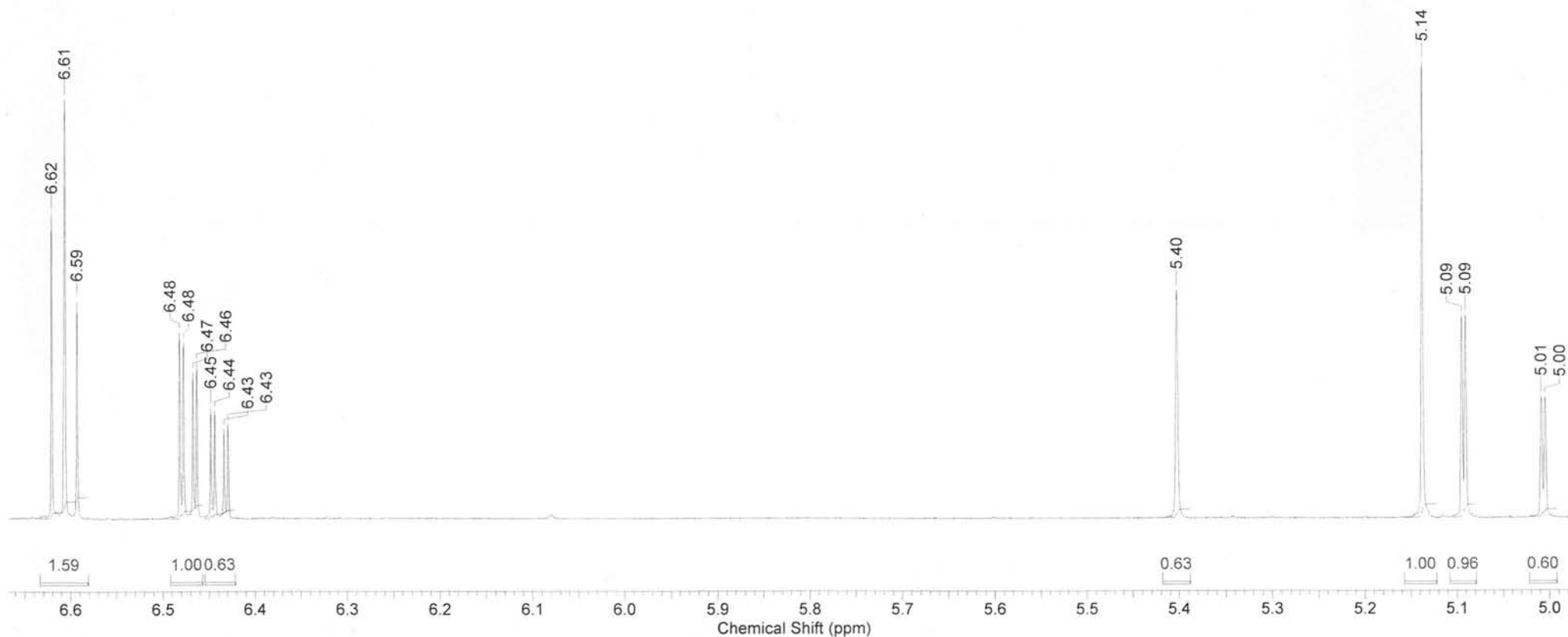


Formula C ₂₄ H ₂₆ N ₂ O ₁₀ ?		FW 502.4706+? (251.2353+251.2353+???)					
Acquisition Time (sec)	4.9999	Comment	STANDARD 1H OBSERVE		Date	Feb 19 2009	
Date Stamp	Feb 19 2009	File Name	D:\NMR\IC_13\ТУРЧИН зима 2009\Nic 209 = FZ 506 (оксазол, Турчин)\FZNic209h_190209				
Frequency (MHz)	399.96	Nucleus	1H	Number of Transients	64	Original Points Count	39999
Points Count	65536	Pulse Sequence	s2pul	Receiver Gain	40.00	Solvent	DMSO-d6
Spectrum Offset (Hz)	3519.4019	Sweep Width (Hz)	8000.00	Temperature (degree C)	70.000		

Compounds 3Aa/3Ba

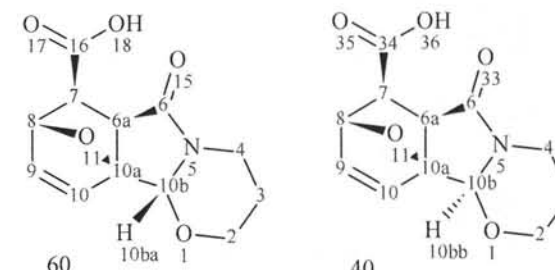


FZNic209h_190209

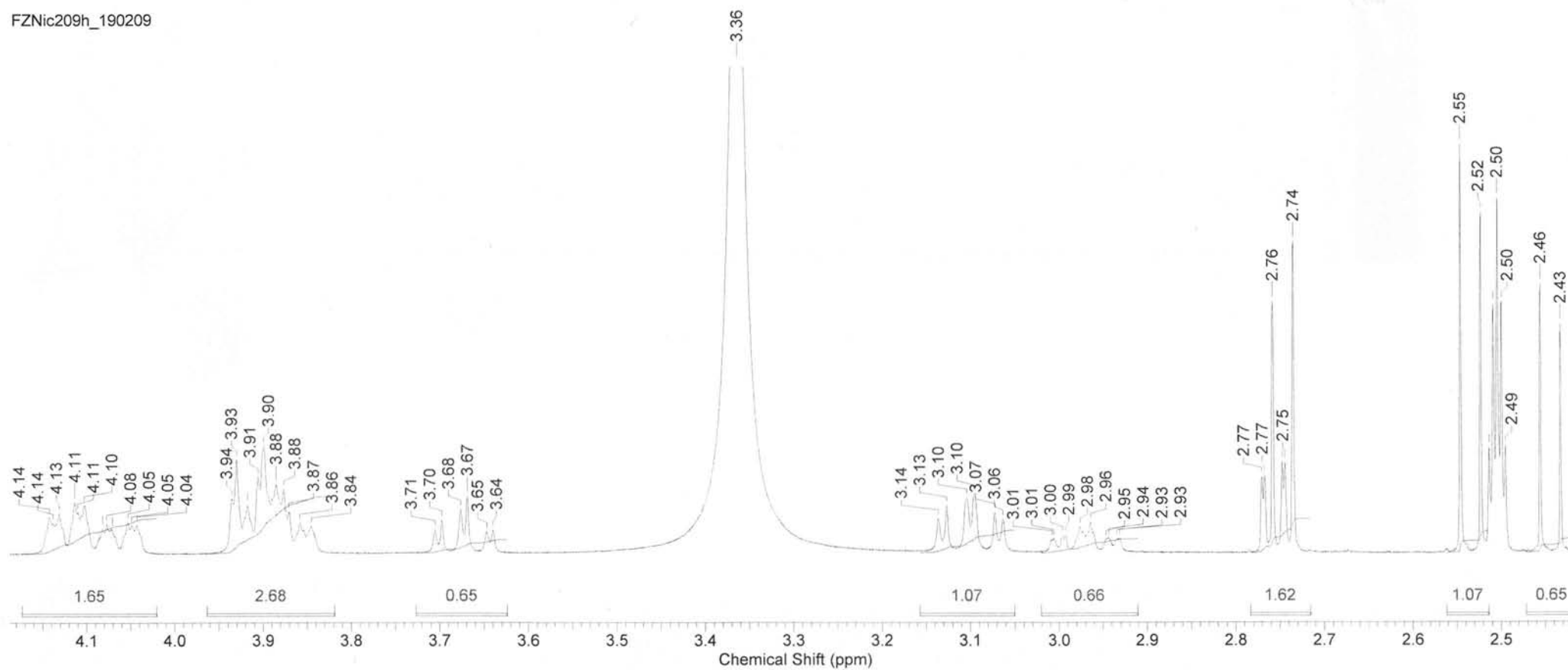


Formula C ₂₄ H ₂₆ N ₂ O ₁₀ ?		FW 502.4706+? (251.2353+251.2353+???)	
Acquisition Time (sec) 4.9999	Comment STANDARD 1H OBSERVE		Date Feb 19 2009
Date Stamp Feb 19 2009	File Name D:\NMR\IC_13\ТУРЧИН зима 2009\Nic 209 = FZ 506 (оксазол, Турчин)\FZNic209h_190209		
Frequency (MHz) 399.96	Nucleus 1H	Number of Transients 64	Original Points Count 39999
Points Count 65536	Pulse Sequence s2pul	Receiver Gain 40.00	Solvent DMSO-d6
Spectrum Offset (Hz) 3519.4019	Sweep Width (Hz) 8000.00	Temperature (degree C) 70.000	

Compounds 3Aa/3Ba

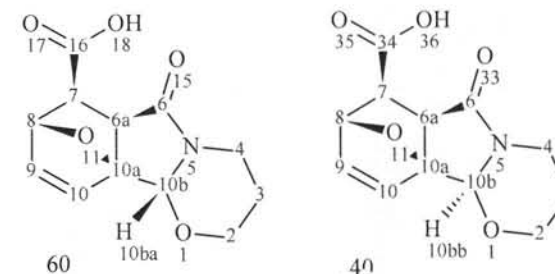


FZNic209h_190209

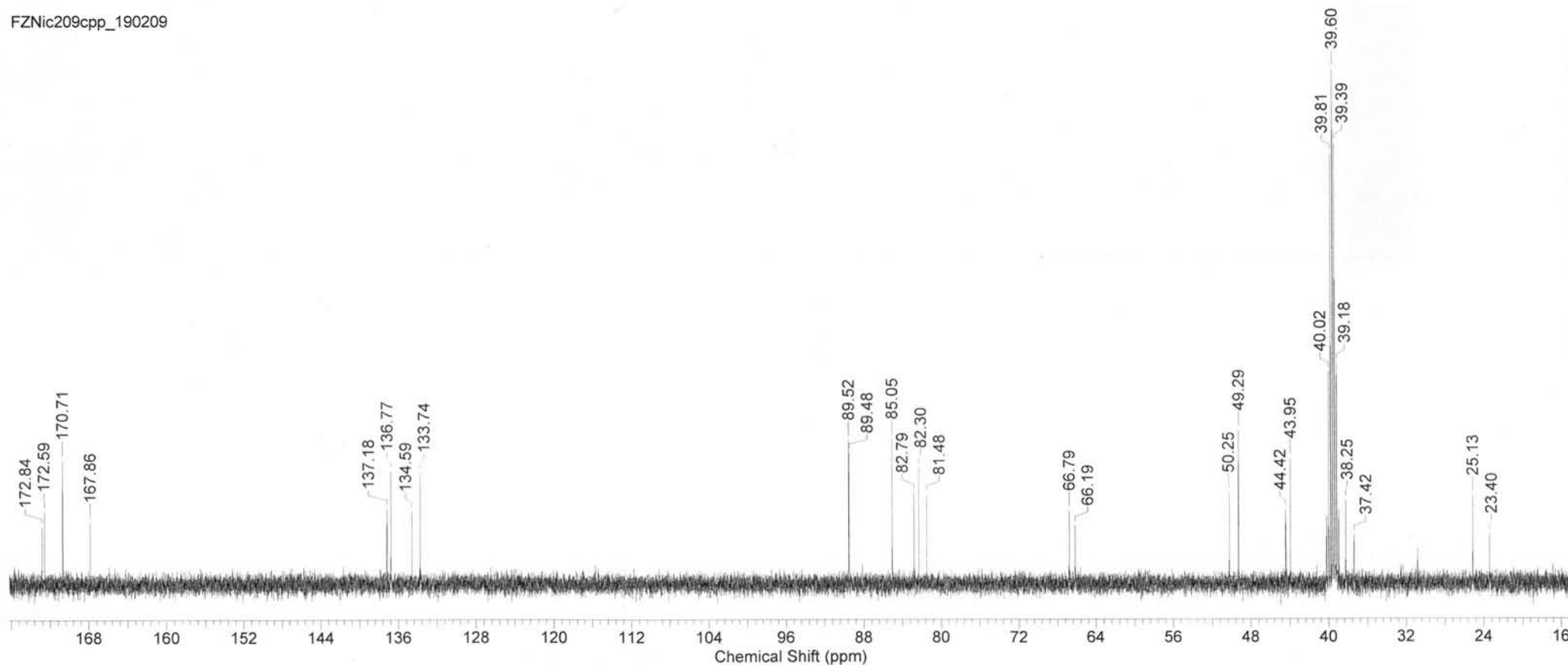


Formula C ₂₄ H ₂₆ N ₂ O ₁₀ ?		FW 502.4706+? (251.2353+251.2353+?+?)	
Acquisition Time (sec) 1.5000	Comment ILTP8qq4absurd ser.20070601	Date Feb 19 2009	
Date Stamp Feb 19 2009	File Name D:\NMR\13\ТУРЧИН зима 2009\Nic 209 = FZ 506 (оксазол, Турчин)\FZNic209cpp_190209		
Frequency (MHz) 100.58	Nucleus 13C	Number of Transients 54000	Original Points Count 37500
Points Count 65536	Pulse Sequence s2pul	Receiver Gain 56.00	Solvent DMSO-d6
Spectrum Offset (Hz) 9462.2764	Sweep Width (Hz) 25000.00	Temperature (degree C) 29.000	

Compounds 3Aa/3Ba

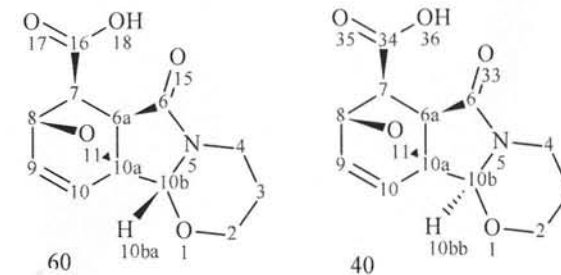


FZNic209cpp_190209

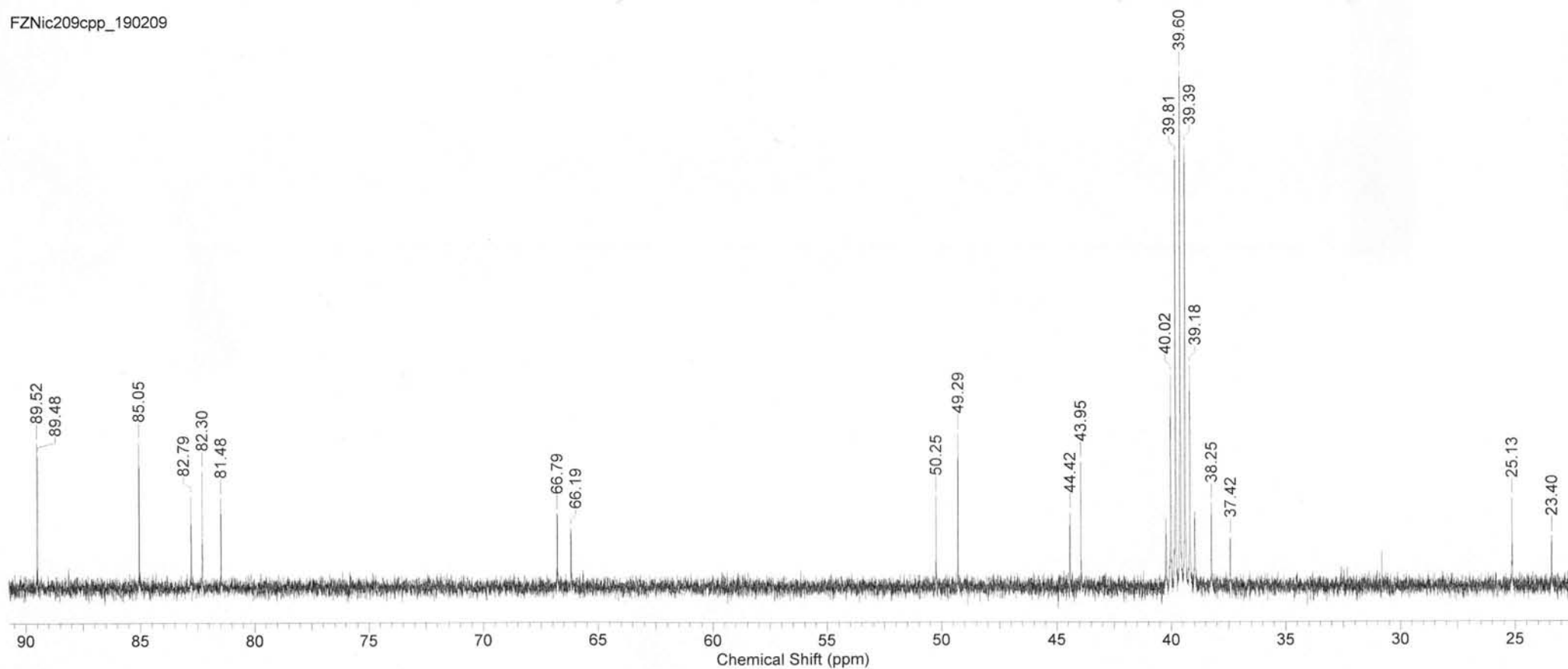


Formula C ₂₄ H ₂₆ N ₂ O ₁₀ ?		FW 502.4706+? (251.2353+251.2353+?+?)					
Acquisition Time (sec)	1.5000	Comment	ILTP8qq4absurd ser.20070601		Date	Feb 19 2009	
Date Stamp	Feb 19 2009	File Name	D:\NMR\13\ТУРЧИН зима 2009\Nic 209 = FZ 506 (оксазол, Турчин)\FZNic209cpp_190209				
Frequency (MHz)	100.58	Nucleus	13C	Number of Transients	54000	Original Points Count	37500
Points Count	65536	Pulse Sequence	s2pul	Receiver Gain	56.00	Solvent	DMSO-d6
Spectrum Offset (Hz)	9462.2764	Sweep Width (Hz)	25000.00	Temperature (degree C)	29.000		

Compounds 3Aa/3Ba



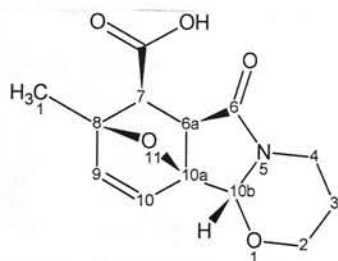
FZNic209cpp_190209



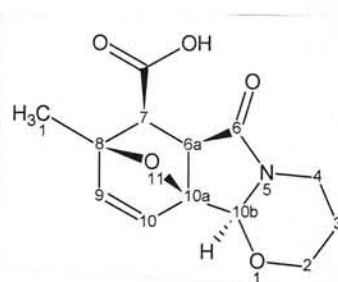
Formula	C ₁₃ H ₁₅ NO ₅	FW	265.2619
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Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	21 Jun 2012 17:18:56
Date Stamp	21 Jun 2012 17:18:56				
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-3Bb\rudn-250512-3Bb_001000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	16	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zg
SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542
Temperature (degree C)	32.000			Sweep Width (Hz)	10416.03

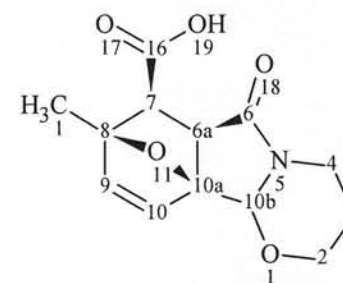
3Ab/3Bb = 95/5



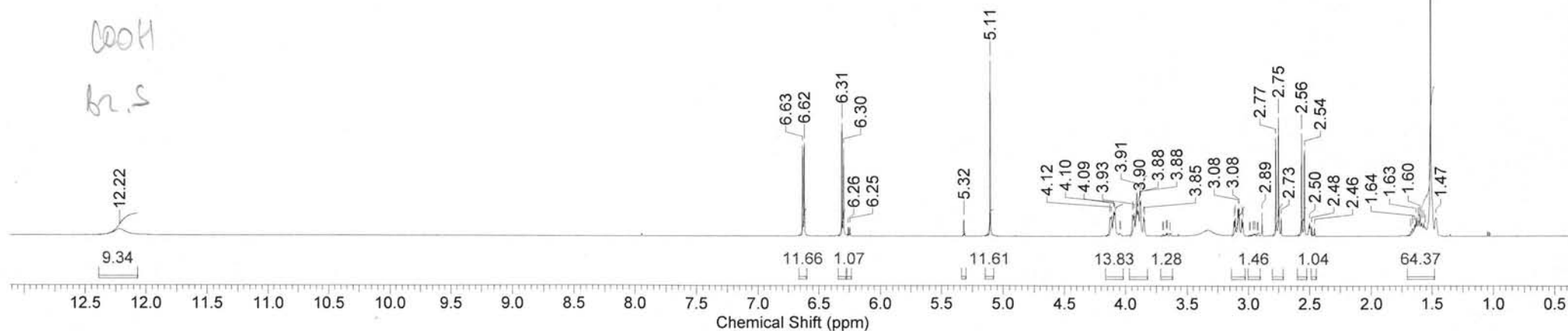
maj



min

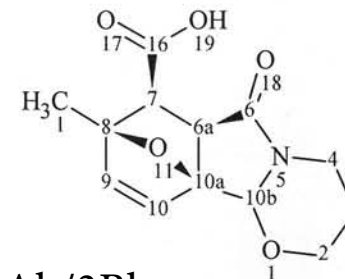


Compounds 3Ab/3Bb



Formula	C ₁₃ H ₁₅ NO ₅	FW	265.2619
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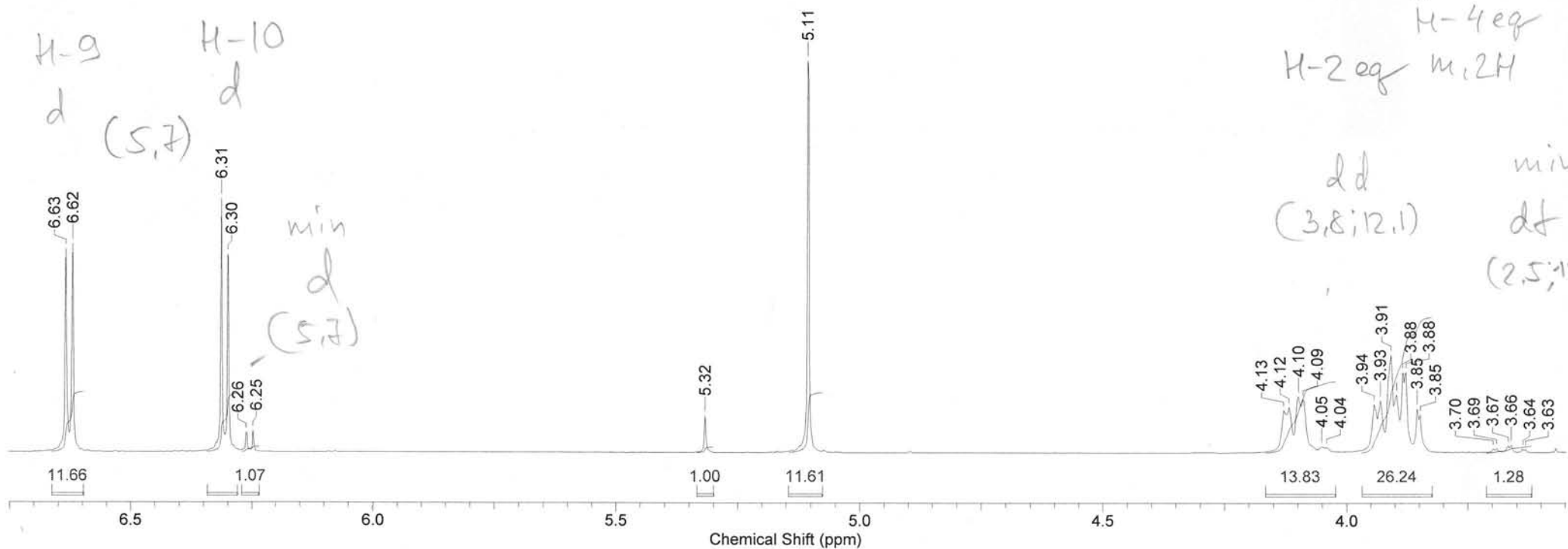
Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	21 Jun 2012 17:18:56
Date Stamp	21 Jun 2012 17:18:56				
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-3Bb\rudn-250512-3Bb_001000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	16	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zg
SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542
Temperature (degree C)	32.000			Sweep Width (Hz)	10416.03



H-10b
S

Compounds 3Ab/3Bb

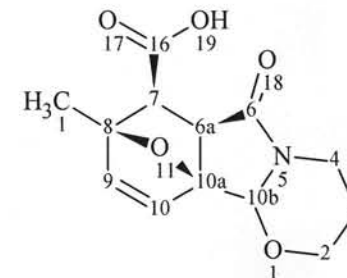
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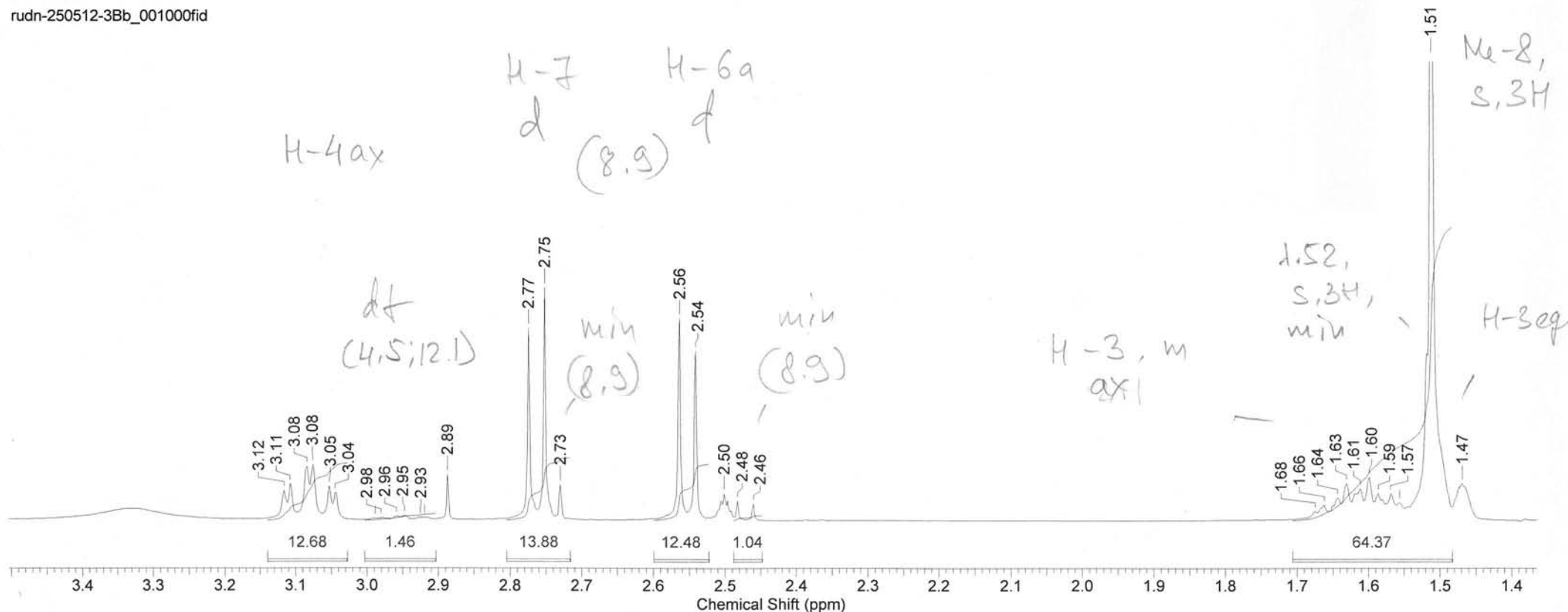
Formula	C ₁₃ H ₁₅ NO ₅	FW	265.2619
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Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	21 Jun 2012 17:18:56
Date Stamp	21 Jun 2012 17:18:56				
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-3Bb\rudn-250512-3Bb_001000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	16	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zg
SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542
Temperature (degree C)	32.000			Sweep Width (Hz)	10416.03

Compounds 3Ab/3Bb



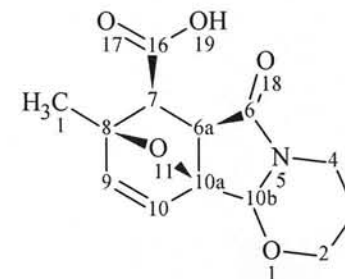
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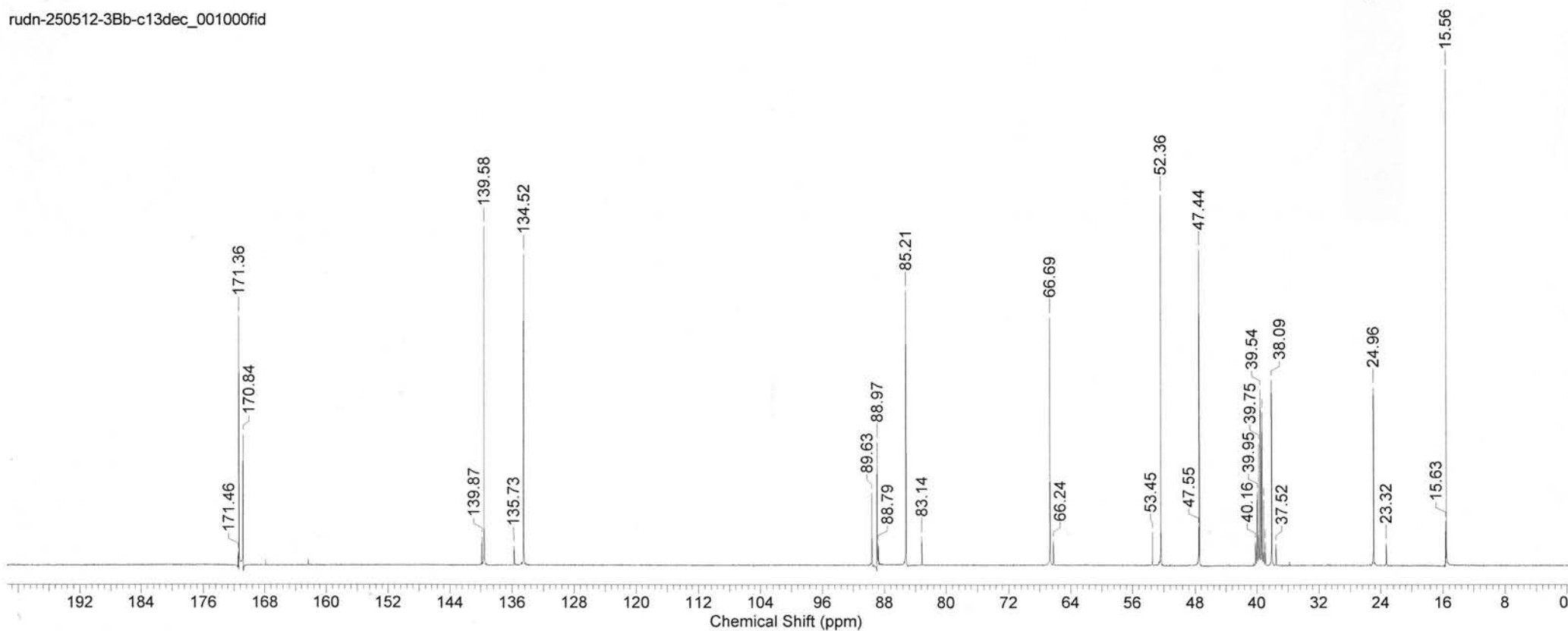
Formula C ₁₃ H ₁₅ NO ₅	FW 265.2619
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Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 21 Jun 2012 22:09:04	
Date Stamp 21 Jun 2012 22:09:04			
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-3Bb-c13dec\rudn-250512-3Bb-c13dec_001000fid			
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 31322	Origin spect
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10554.8018
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000		

Compounds 3Ab/3Bb

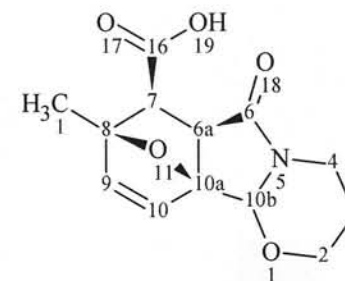


rudn-250512-3Bb-c13dec_001000fid

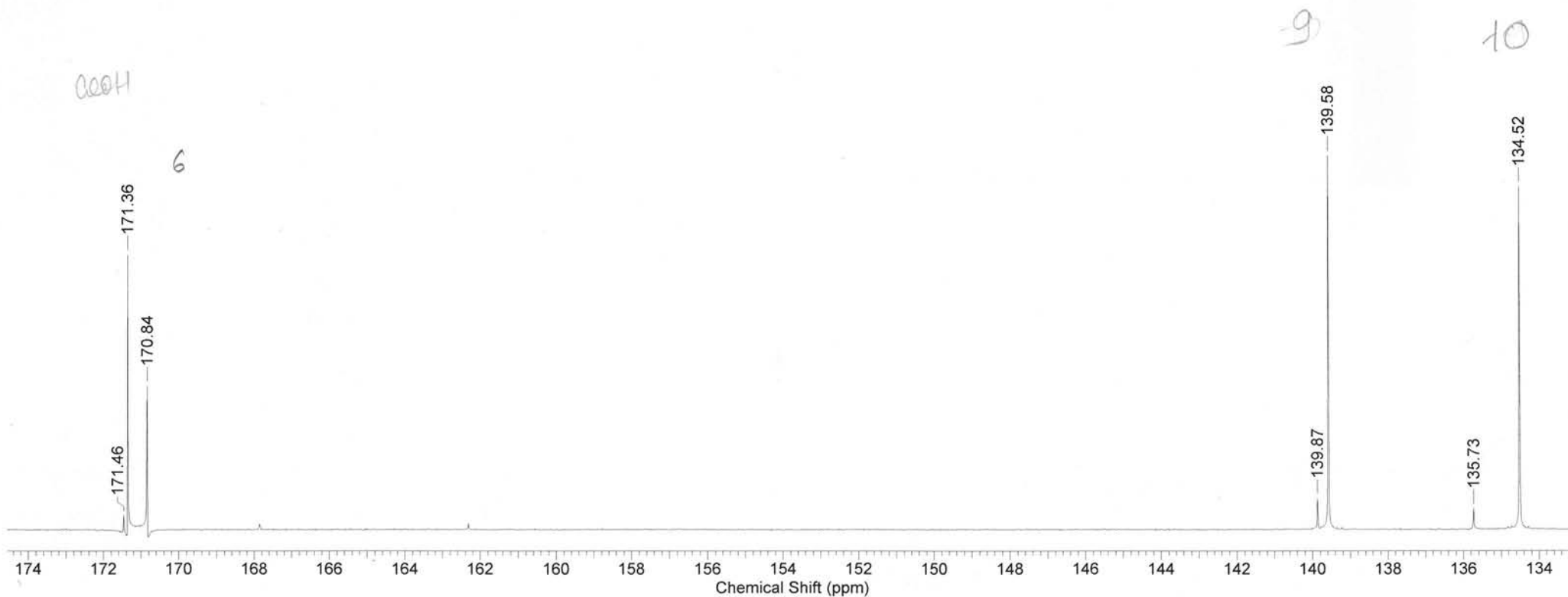


Formula C ₁₃ H ₁₅ NO ₅	FW 265.2619			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 21 Jun 2012 22:09:04		
Date Stamp 21 Jun 2012 22:09:04				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-3Bb-c13dec\rudn-250512-3Bb-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 31322	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10554.8018	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compounds 3Ab/3Bb

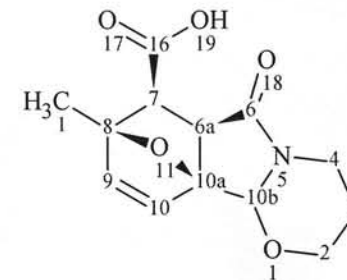


rudn-250512-3Bb-c13dec_001000fid

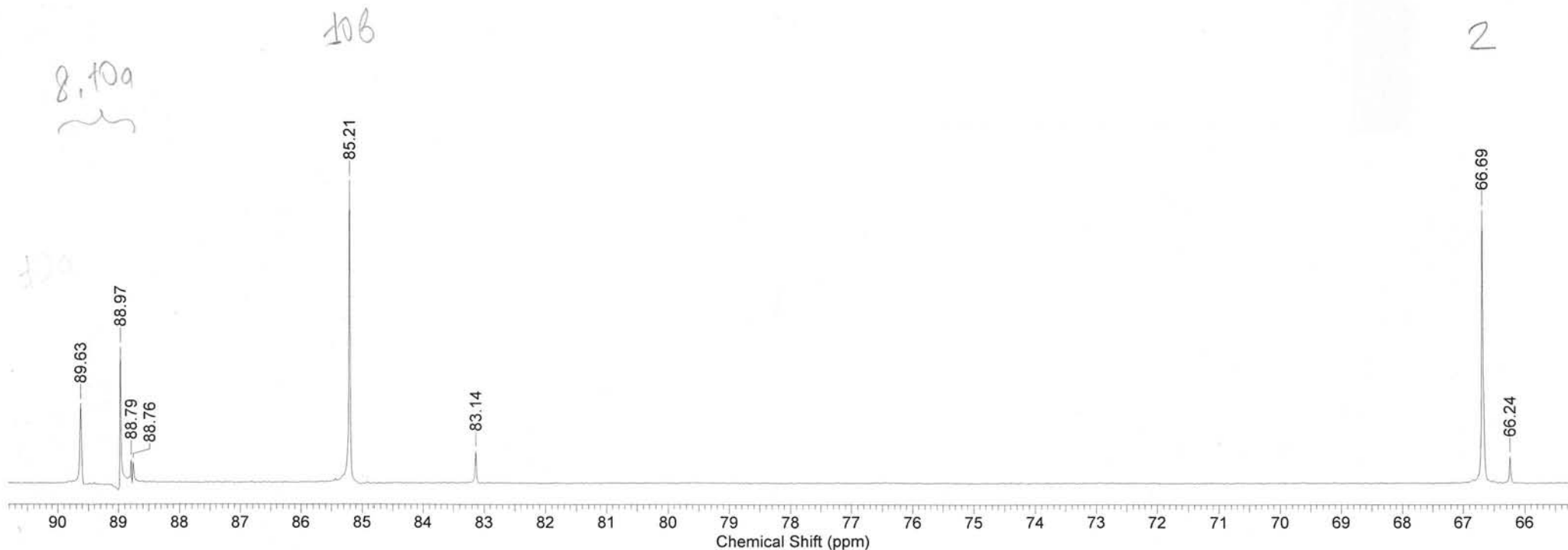


Formula C ₁₃ H ₁₅ NO ₅	FW 265.2619			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 21 Jun 2012 22:09:04		
Date Stamp 21 Jun 2012 22:09:04				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-3Bb-c13dec\rudn-250512-3Bb-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 31322	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpgg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10554.8018	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compounds 3Ab/3Bb

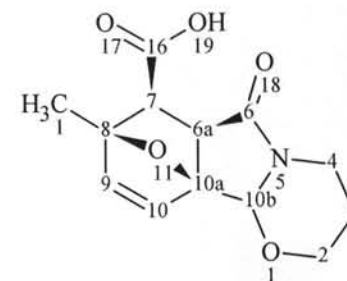


rudn-250512-3Bb-c13dec_001000fid

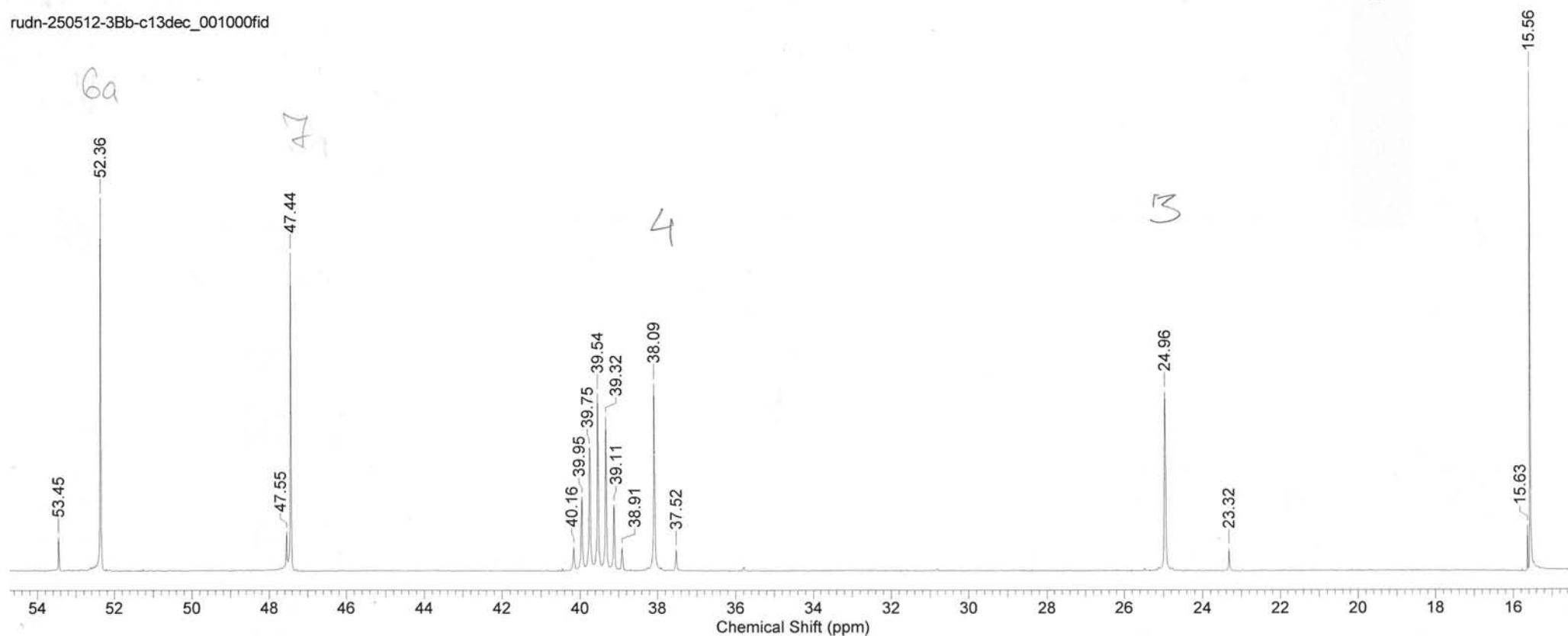


Formula C ₁₃ H ₁₅ NO ₅	FW 265.2619			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 21 Jun 2012 22:09:04		
Date Stamp 21 Jun 2012 22:09:04				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-3Bb-c13dec\rudn-250512-3Bb-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 31322	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10554.8018	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compounds 3Ab/3Bb

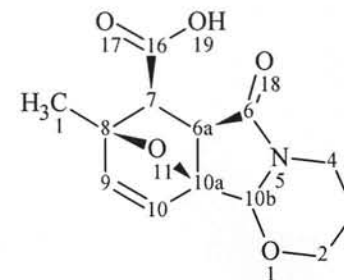


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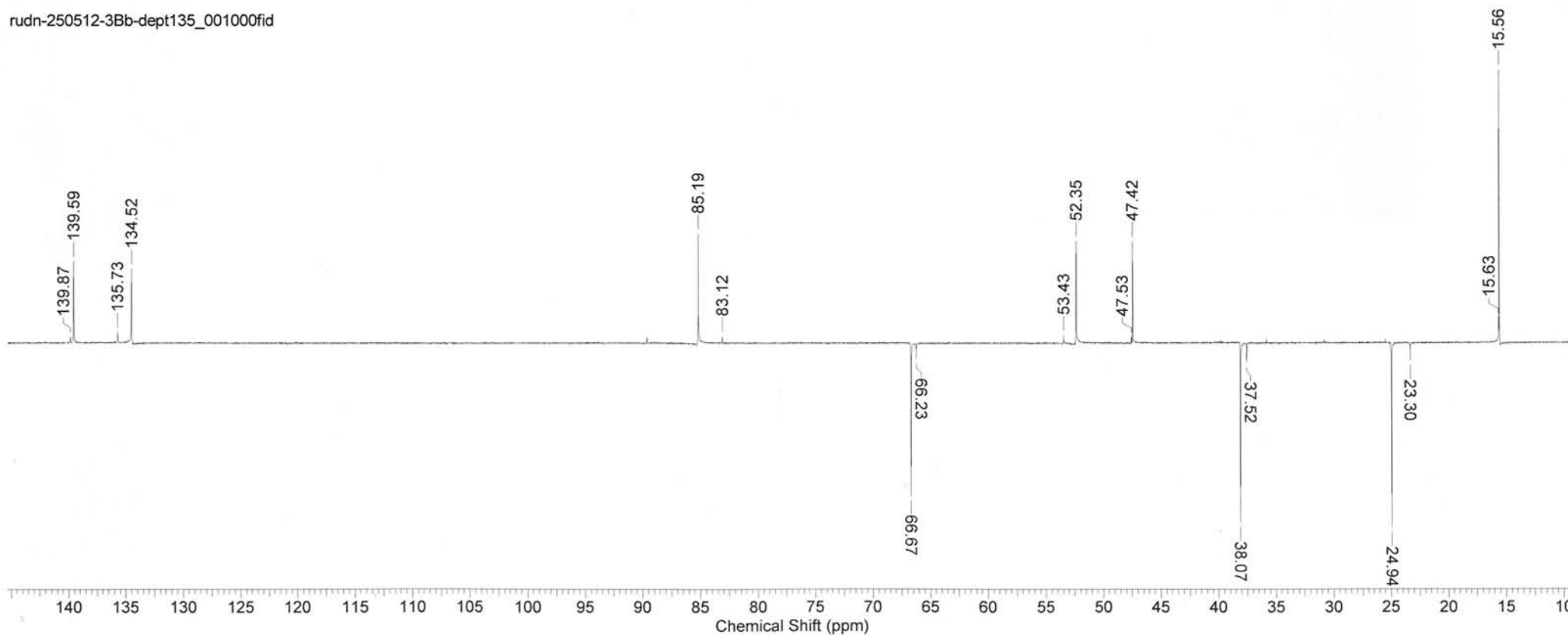


Formula C ₁₃ H ₁₅ NO ₅	FW 265.2619			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 21 Jun 2012 17:21:04		
Date Stamp 21 Jun 2012 17:21:04				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-3Bb-dept135\rudn-250512-3Bb-dept135_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 10000	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence dept135	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 9104.3936	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compounds 3Ab/3Bb

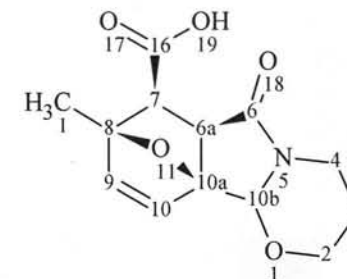


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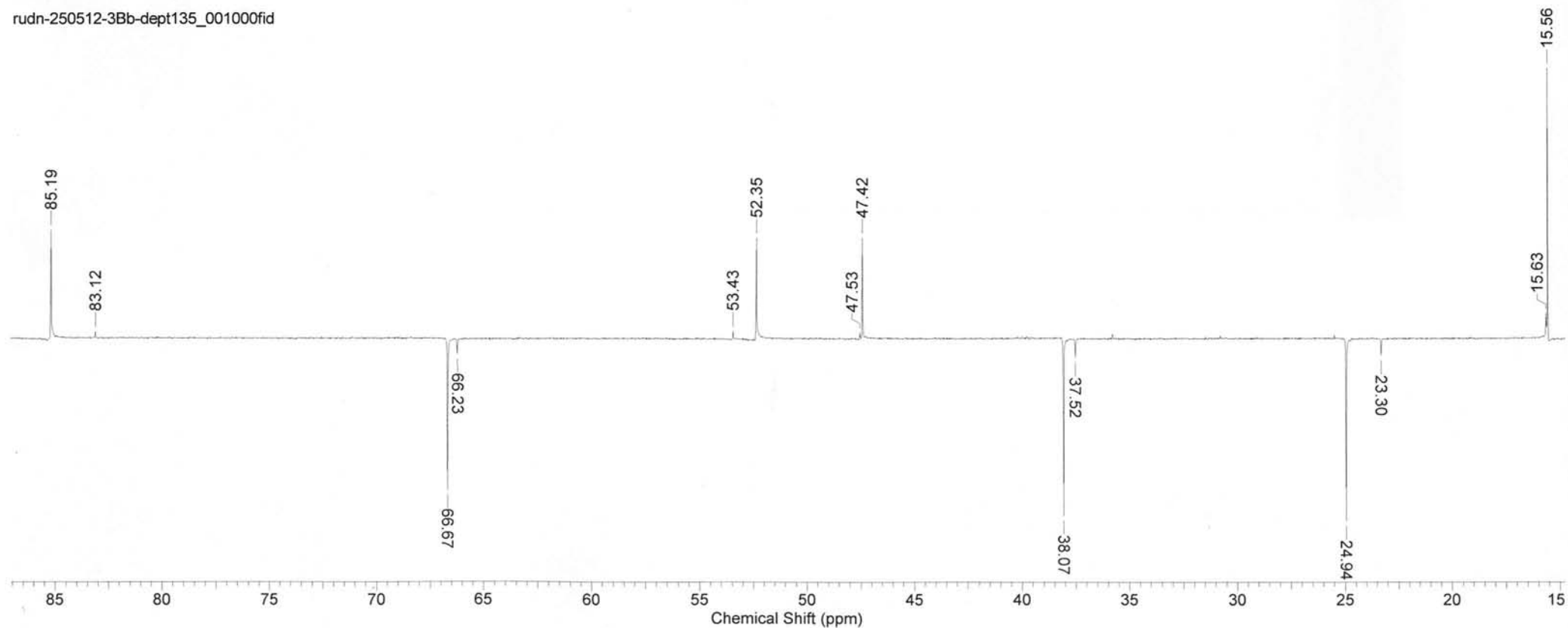


Formula C ₁₃ H ₁₅ NO ₅	FW 265.2619			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 21 Jun 2012 17:21:04		
Date Stamp 21 Jun 2012 17:21:04				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-3Bb-dept135\rudn-250512-3Bb-dept135_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 10000	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence dept135	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 9104.3936	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compounds 3Ab/3Bb



rudn-250512-3Bb-dept135_001000fid

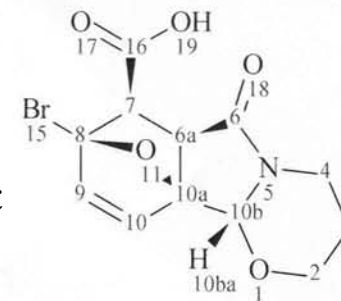


Formula C₁₂H₁₂BrNO₅ FW 330.1314

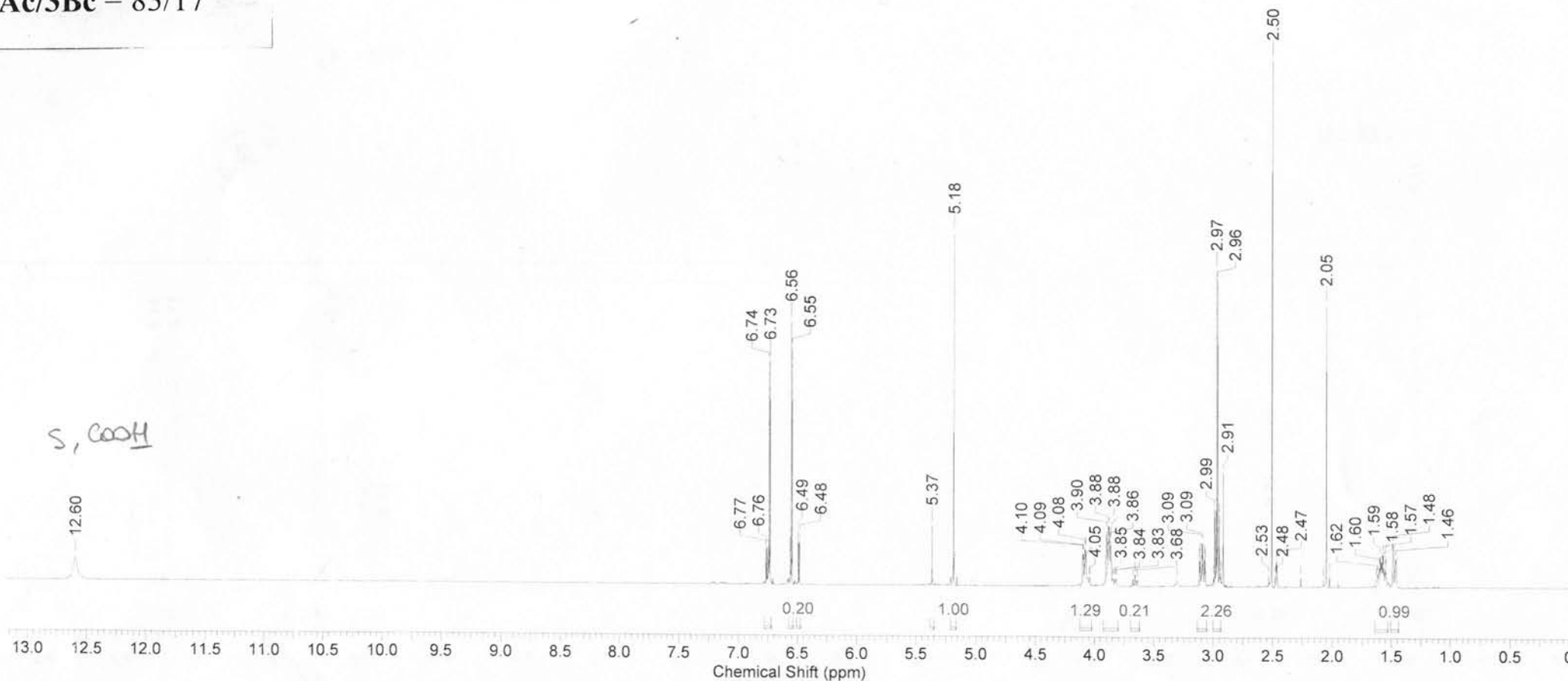
Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	09 Apr 2010 13:35:52	Date Stamp	09 Apr 2010 13:34:40
File Name	D:\NMR\6.04.10\FZ1138-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	32.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3000.8616	Sweep Width (Hz)	11261.26
						Temperature (degree C)	21.200

isomers mixture

Compounds 3Ac/3Bc



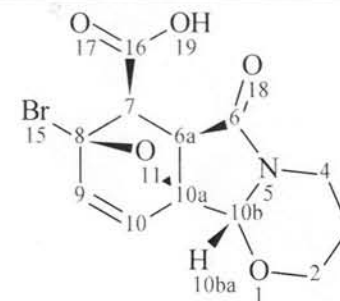
3Ac/3Bc = 83/17



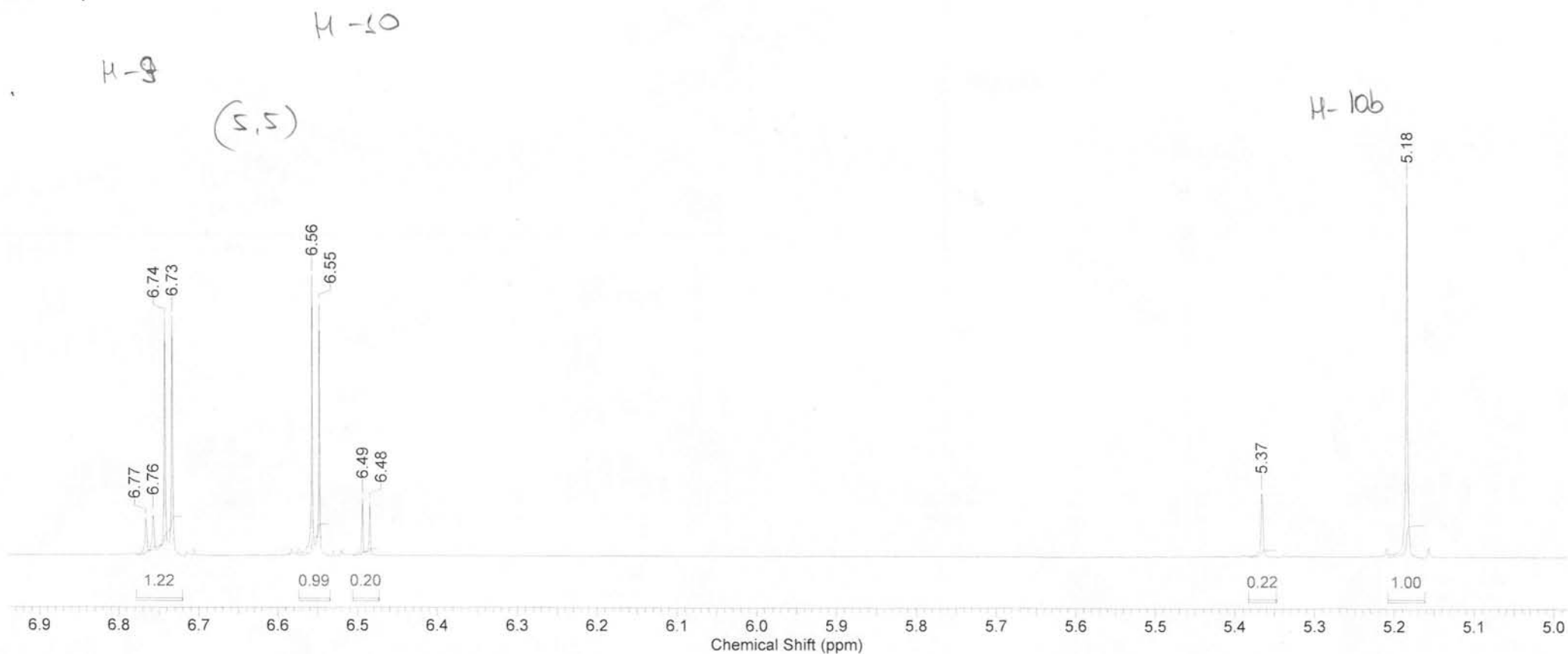
Formula C₁₂H₁₂BrNO₅ FW 330.1314

Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	09 Apr 2010 13:35:52	Date Stamp	09 Apr 2010 13:34:40
File Name	D:\NMR\6.04.10\FZ1138-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	32.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3000.8616	Sweep Width (Hz)	11261.26
						Temperature (degree C)	21.200

Compounds 3Ac/3Bc



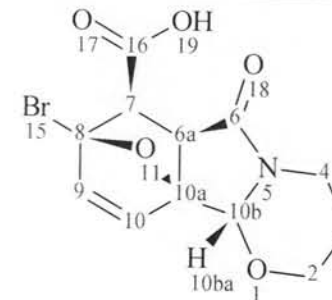
FZ1138-1.jdf



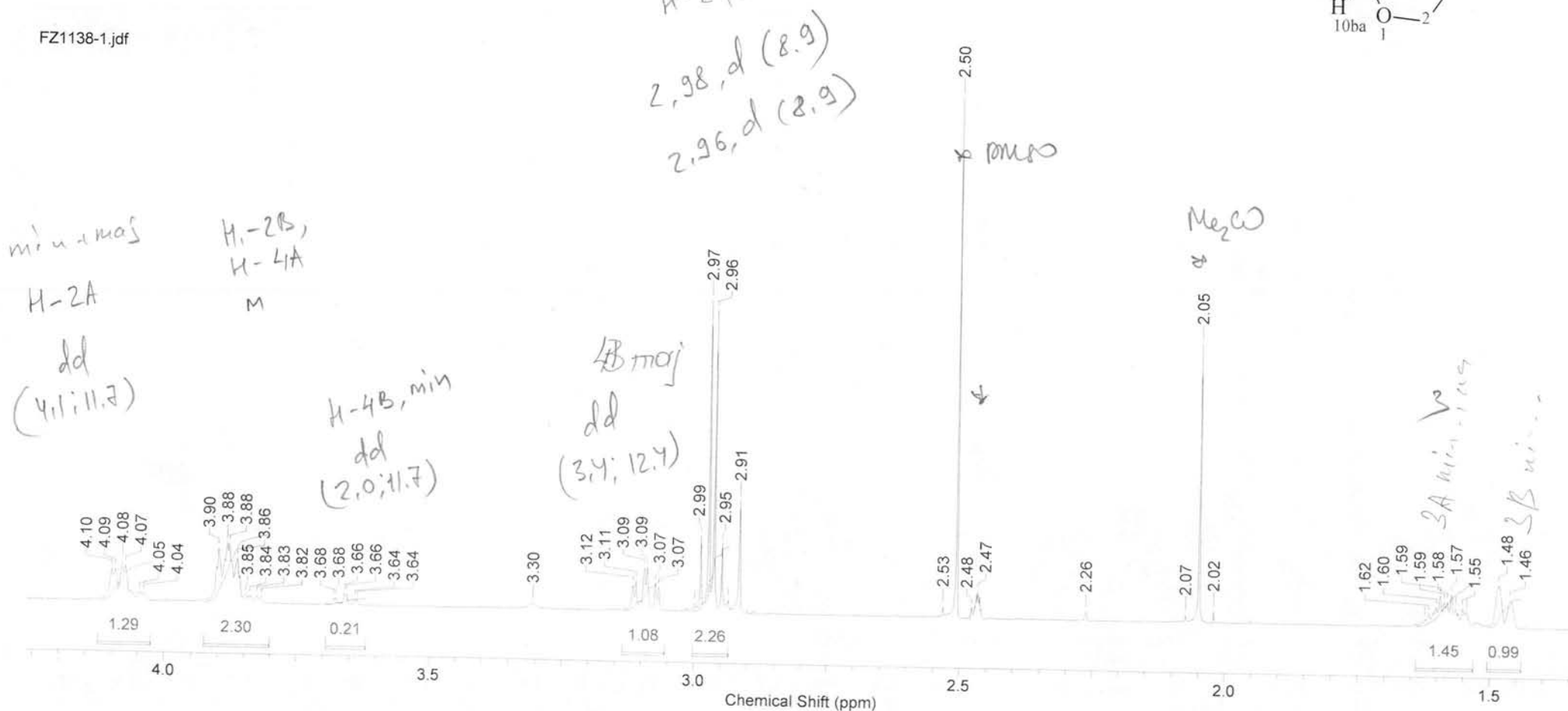
Formula $C_{12}H_{12}BrNO_5$ FW 330.1314

Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	09 Apr 2010 13:35:52		Date Stamp	09 Apr 2010 13:34:40	
File Name	D:\NMR\6.04.10\FZ1138-1.jdf			Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384	Pulse Sequence	single_pulse.ex2
Receiver Gain	32.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3000.8616	Sweep Width (Hz)	11261.26	Temperature (degree C)	21.200

Compounds 3Ac/3Bc



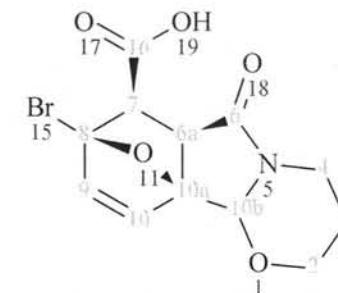
FZ1138-1.jdf



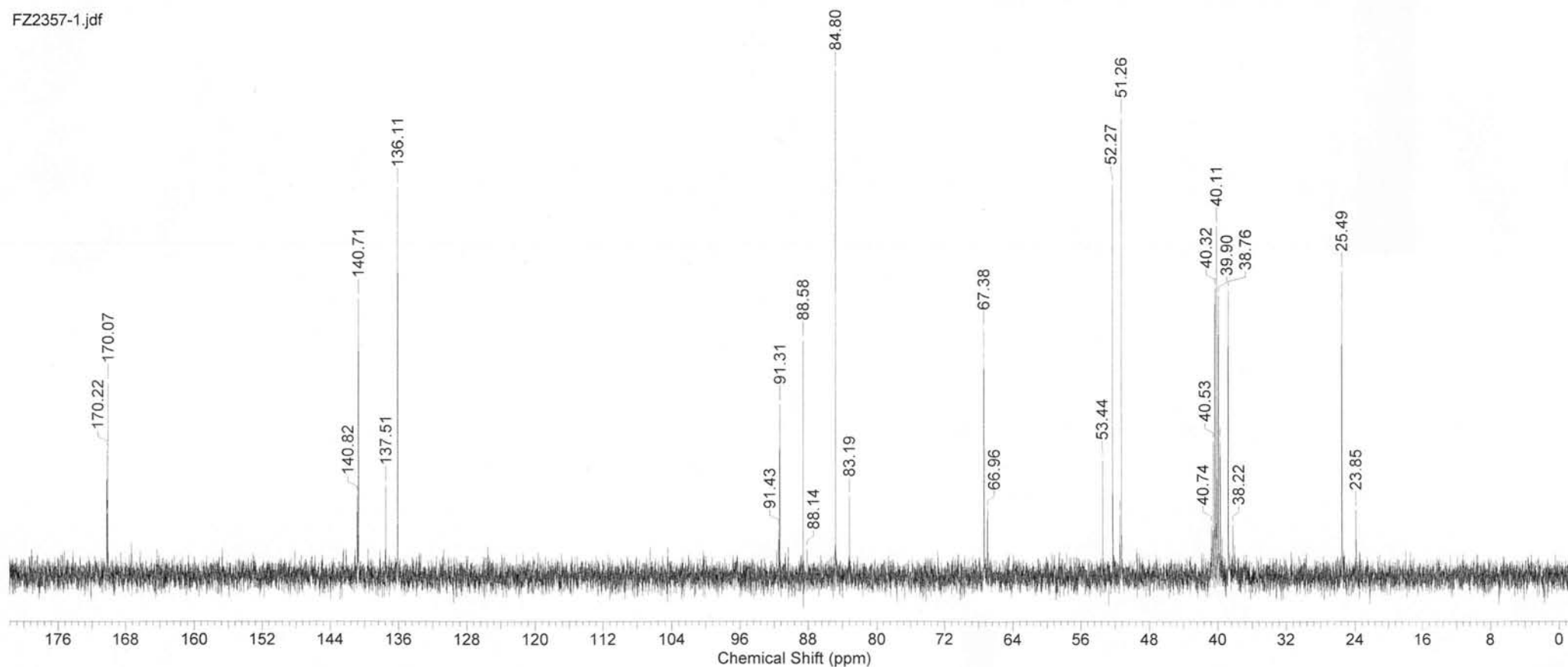
Formula C₁₂H₁₂BrNO₅ FW 330.1314

Acquisition Time (sec)	1.0433	Comment	single pulse decoupled gated NOE		Date	26 Apr 2012 13:23:04			
Date Stamp	26 Apr 2012 17:12:02	File Name	D:\NMR\20.04.12\FZ2357-1.jdf		Frequency (MHz)	100.53			
Nucleus	13C	Number of Transients	229	Origin	ECS 400	Original Points Count	32768		
Points Count	32768	Pulse Sequence	single_pulse_dec		Receiver Gain	60.00	Owner	delta	
Spectrum Offset (Hz)	10052.5303	Sweep Width (Hz)	31407.04	Temperature (degree C)	24.400			Solvent	DMSO-d6

Compounds 3Ac/3Bc

80/20
A/B

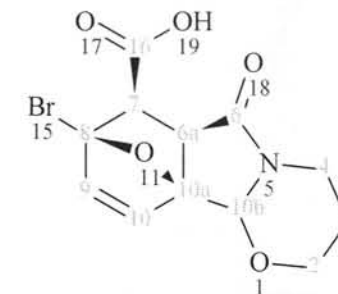
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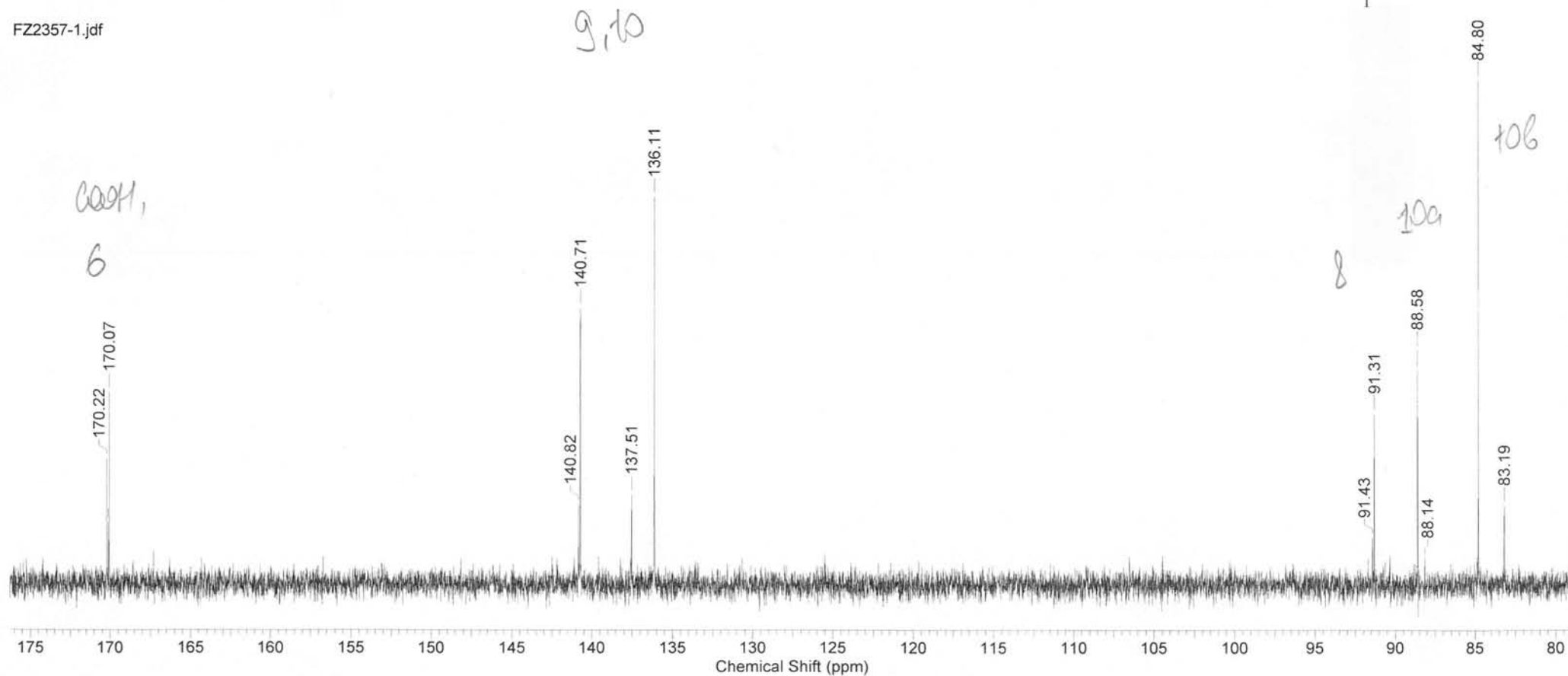
Formula C₁₂H₁₂BrNO₅ FW 330.1314

Acquisition Time (sec)	1.0433	Comment	single pulse decoupled gated NOE		Date	26 Apr 2012 13:23:04		
Date Stamp	26 Apr 2012 17:12:02	File Name	D:\NMR\20.04.12\FZ2357-1.jdf		Frequency (MHz)	100.53		
Nucleus	13C	Number of Transients	229	Origin	ECS 400	Original Points Count	32768	
Points Count	32768	Pulse Sequence	single_pulse_dec		Receiver Gain	60.00	Solvent	DMSO-d6
Spectrum Offset (Hz)	10052.5303	Sweep Width (Hz)	31407.04	Temperature (degree C)	24.400			

Compounds 3Ac/3Bc



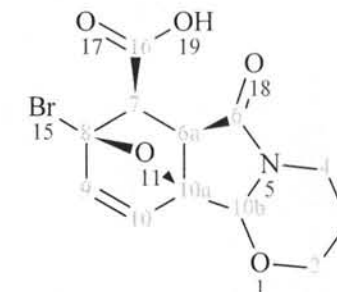
FZ2357-1.jdf



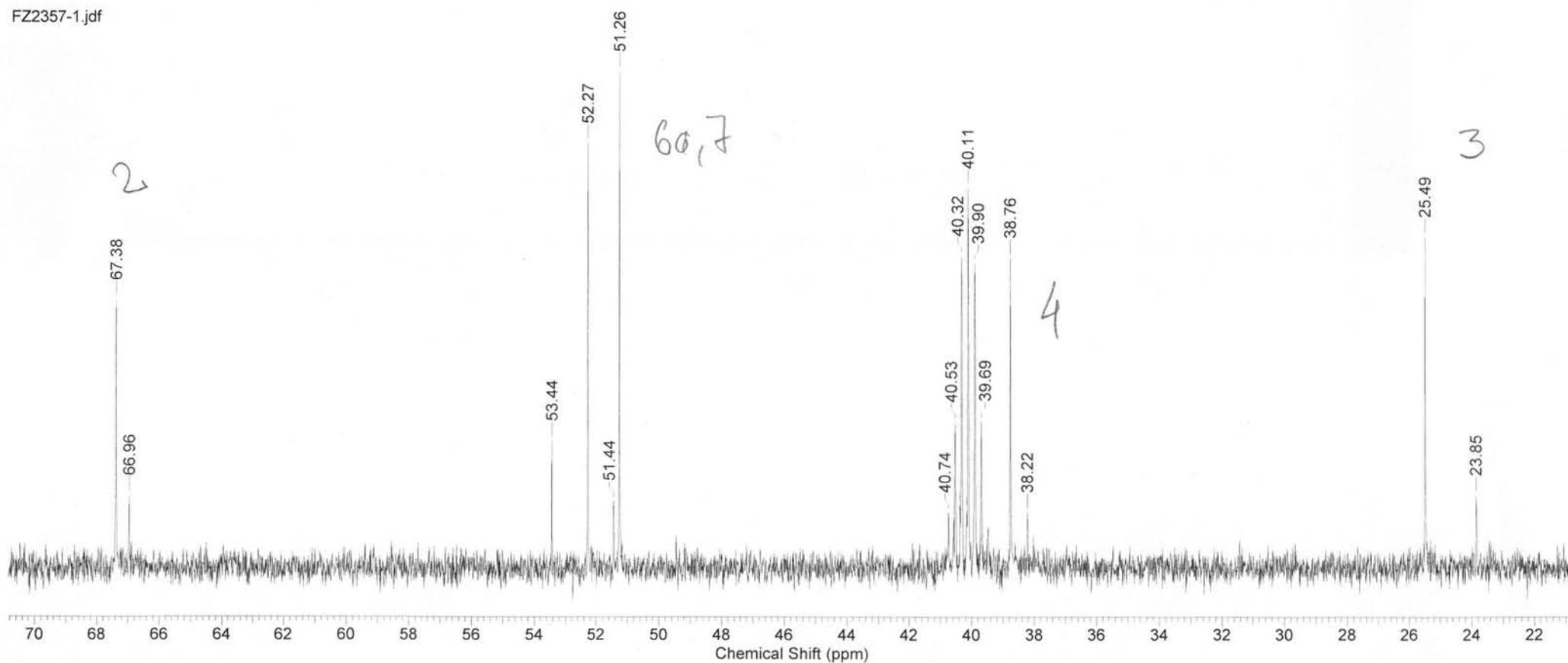
Formula C₁₂H₁₂BrNO₅ FW 330.1314

Acquisition Time (sec)	1.0433	Comment	single pulse decoupled gated NOE		Date	26 Apr 2012 13:23:04		
Date Stamp	26 Apr 2012 17:12:02	File Name	D:\NMR\20.04.12\FZ2357-1.jdf		Frequency (MHz)	100.53		
Nucleus	13C	Number of Transients	229	Origin	ECS 400	Original Points Count	32768	
Points Count	32768	Pulse Sequence	single_pulse_dec		Receiver Gain	60.00	Solvent	DMSO-d6
Spectrum Offset (Hz)	10052.5303	Sweep Width (Hz)	31407.04	Temperature (degree C)	24.400			

Compounds 3Ac/3Bc



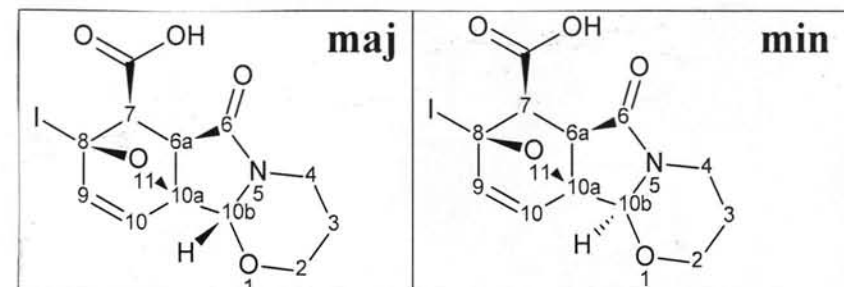
FZ2357-1.jdf



Formula	C ₁₂ H ₁₂ INO ₅	FW	377.1319
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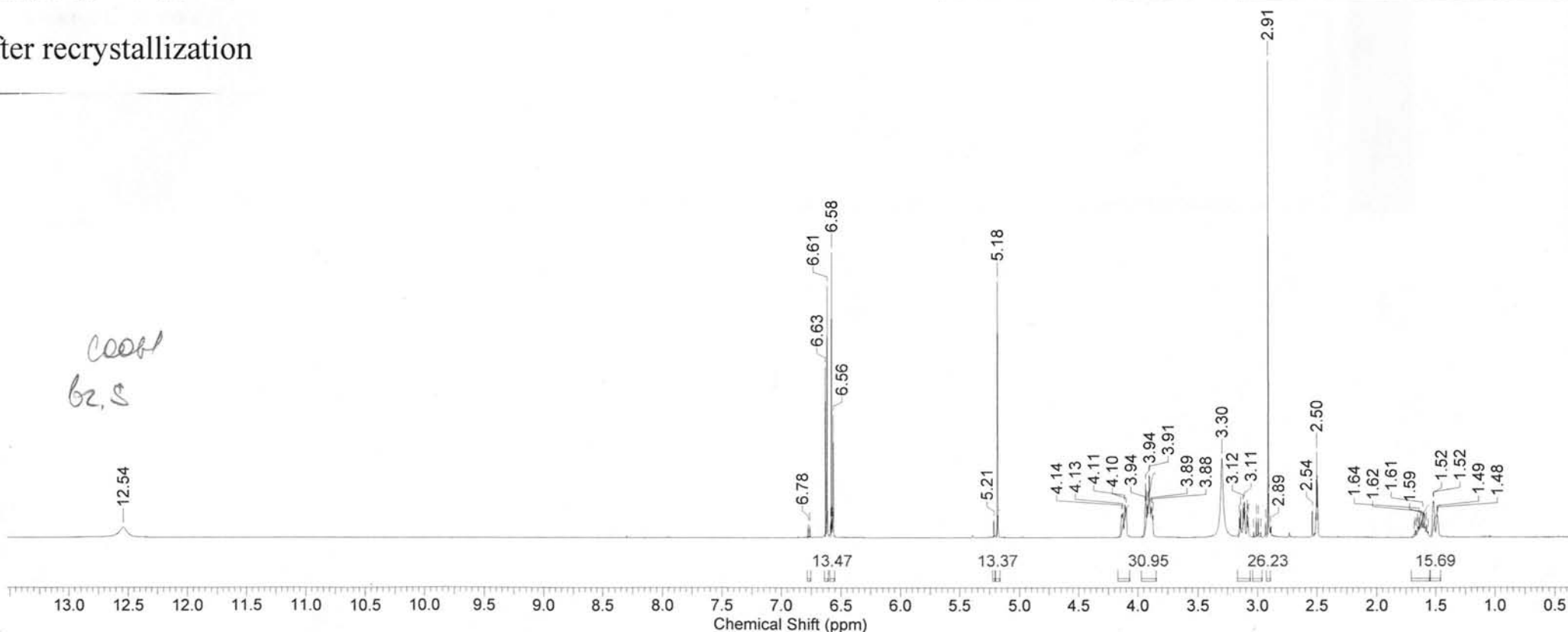
Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	08 Jun 2012 15:28:00
Date Stamp	08 Jun 2012 15:28:00				
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-3d\rudn-040612-3d_001000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	64	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zg
SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542
Temperature (degree C)	32.000			Sweep Width (Hz)	10416.03

Compounds 3Ad/3Bd



3Ad/3Bd = 94/6

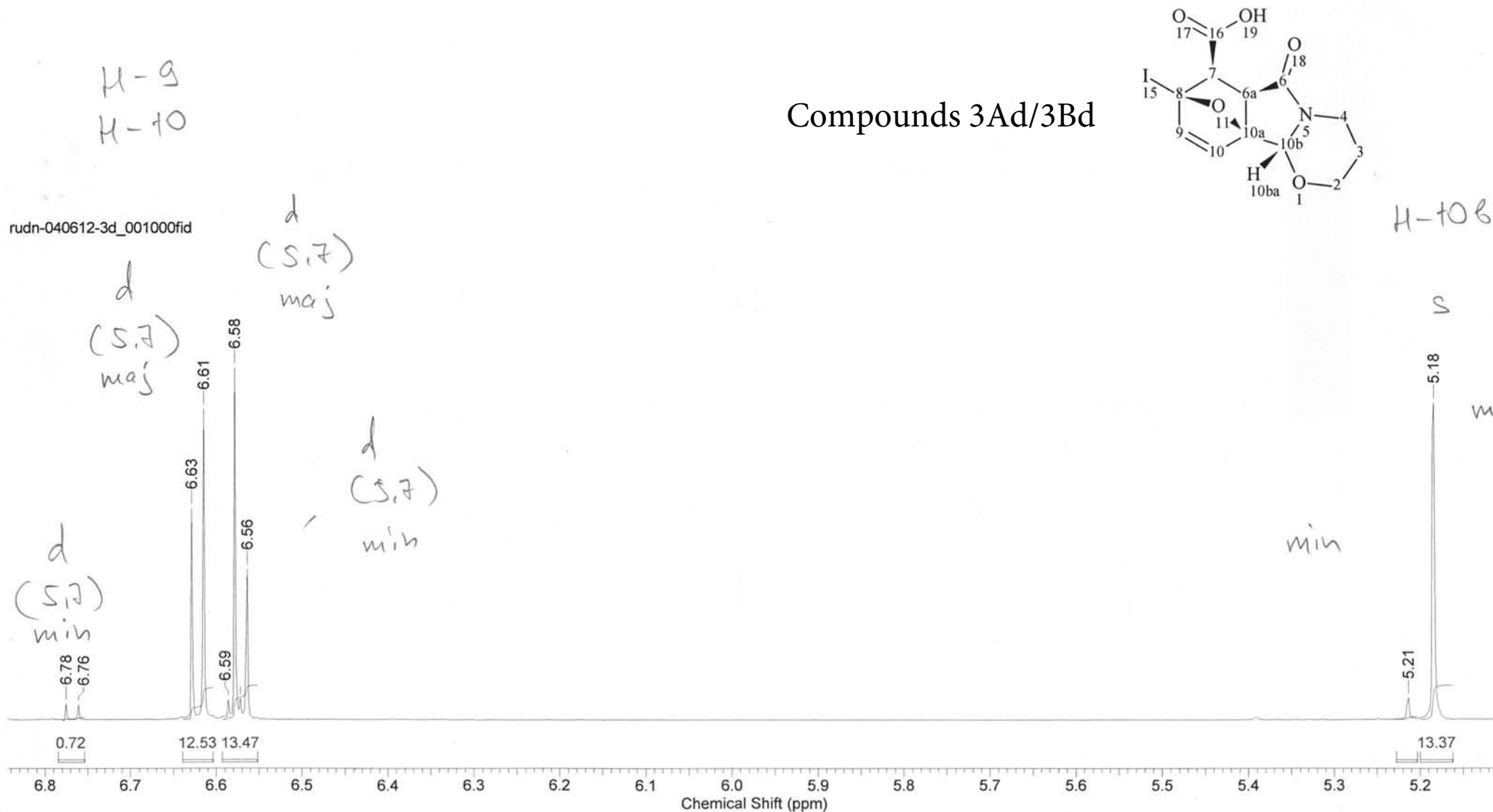
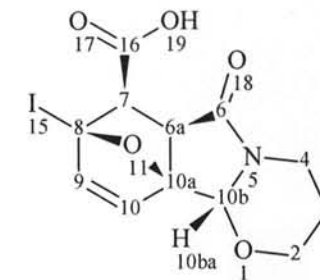
after recrystallization



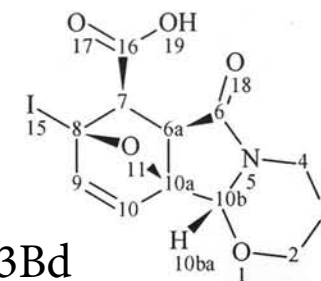
Formula	C ₁₂ H ₁₂ INO ₅	FW	377.1319
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Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	08 Jun 2012 15:28:00
Date Stamp	08 Jun 2012 15:28:00				
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-3d\rudn-040612-3d_001000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	64	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zg
SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542
Temperature (degree C)	32.000			Sweep Width (Hz)	10416.03

Compounds 3Ad/3Bd

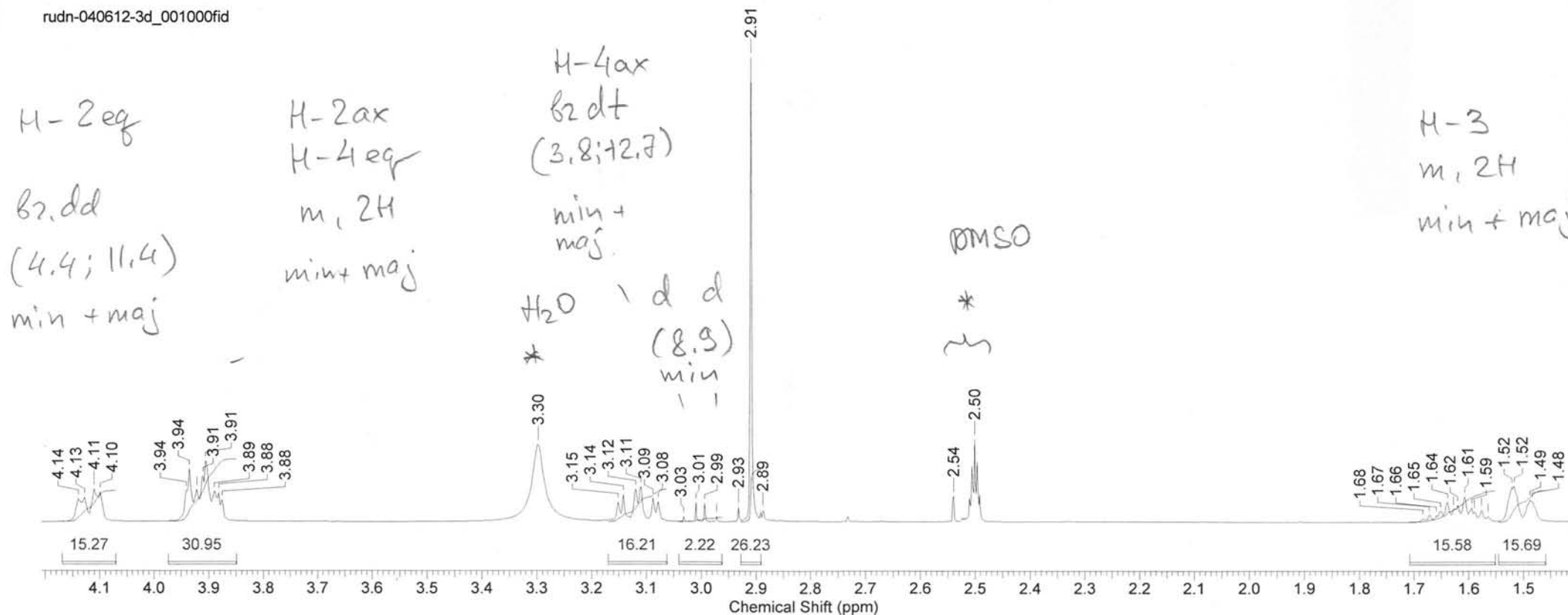


Formula C ₁₂ H ₁₂ INO ₅	FW 377.1319			
Acquisition Time (sec) 1.5729	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 08 Jun 2012 15:28:00		
Date Stamp 08 Jun 2012 15:28:00				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-3d\rudn-040612-3d_001000fid	Frequency (MHz) 400.14			
Nucleus 1H	Number of Transients 64	Origin spect	Original Points Count 16384	
Owner root	Points Count 16384	Pulse Sequence zg	Receiver Gain 128.00	
SW(cyclical) (Hz) 10416.67	Solvent DMSO-d6	Spectrum Offset (Hz) 2712.0542	Sweep Width (Hz) 10416.03	
Temperature (degree C) 32.000				



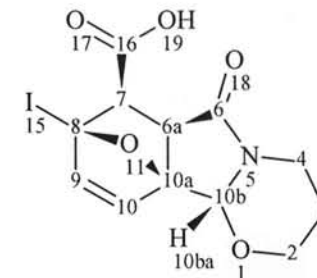
Compounds 3Ad/3Bd

rudn-040612-3d_001000fid

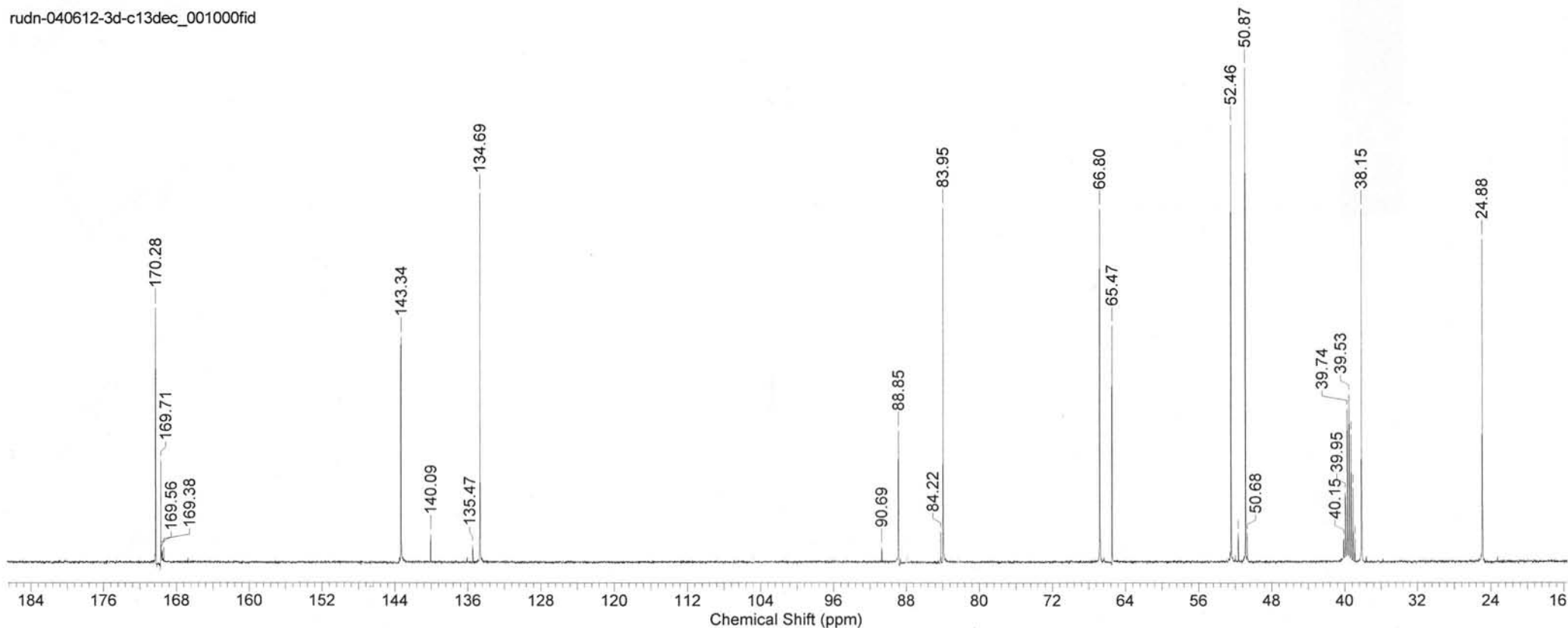


Formula C ₁₂ H ₁₂ INO ₅	FW 377.1319			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 09 Jun 2012 12:05:20		
Date Stamp 09 Jun 2012 12:05:20				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-3d-c13dec\rudn-040612-3d-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 3328	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10552.1055	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compounds 3Ad/3Bd

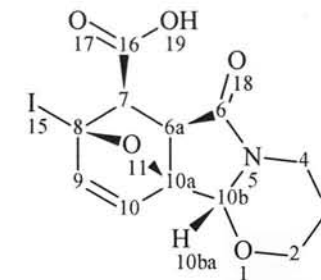


rudn-040612-3d-c13dec_001000fid

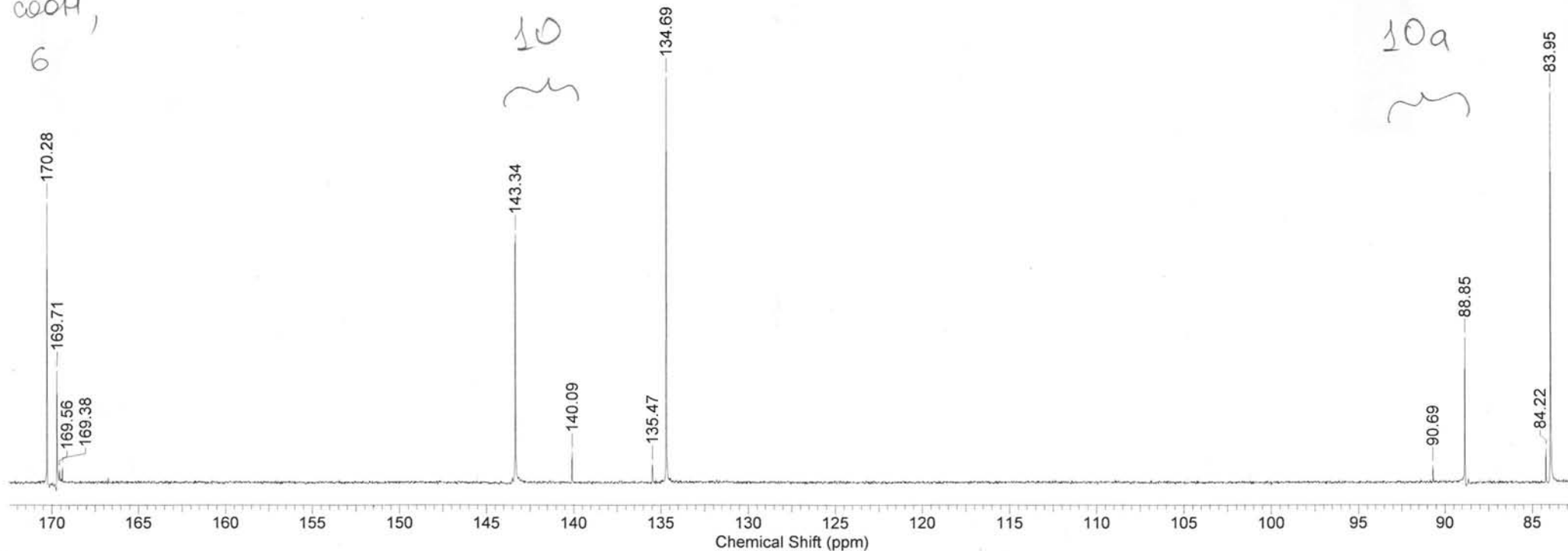


Formula	C ₁₂ H ₁₂ INO ₅	FW	377.1319
Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400
Date Stamp	09 Jun 2012 12:05:20	Date	09 Jun 2012 12:05:20
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-3d-c13dec\rudn-040612-3d-c13dec_001000fid		
Frequency (MHz)	100.62	Nucleus	13C
Original Points Count	16384	Number of Transients	3328
Receiver Gain	32768.00	Owner	root
Sweep Width (Hz)	29409.97	Points Count	16384
		SW(cyclical) (Hz)	29411.77
		Solvent	DMSO-d6
		Spectrum Offset (Hz)	10552.1055
		Temperature (degree C)	27.000

Compounds 3Ad/3Bd

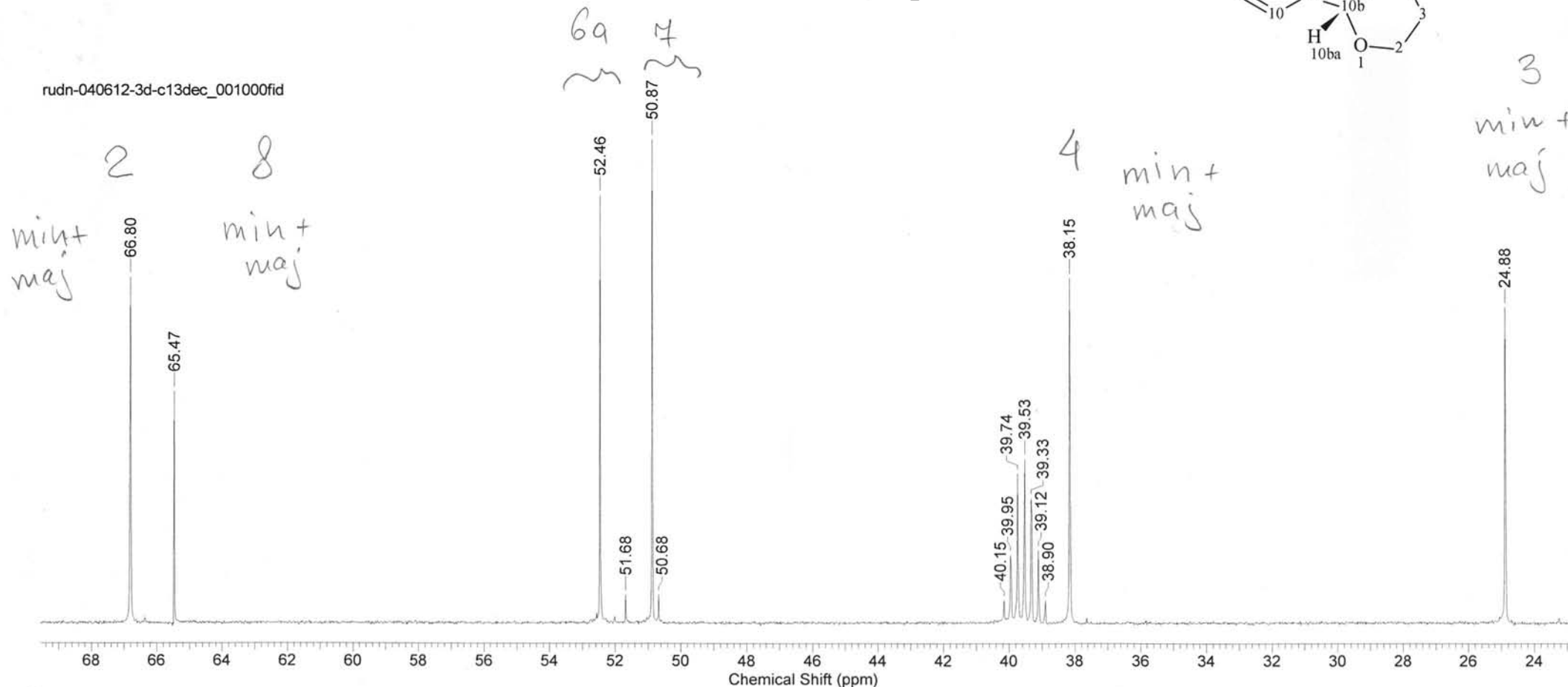
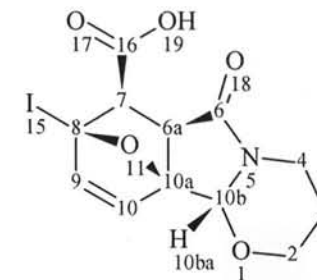


rudn-040612-3d-c13dec_001000fid

COOH,
6

Formula C ₁₂ H ₁₂ INO ₅	FW 377.1319			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 09 Jun 2012 12:05:20		
Date Stamp 09 Jun 2012 12:05:20				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-3d-c13dec\rudn-040612-3d-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 3328	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10552.1055	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

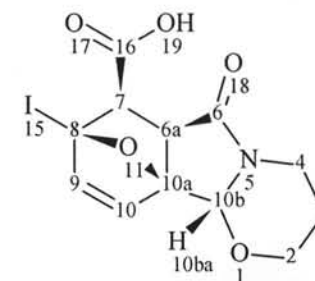
Compounds 3Ad/3Bd



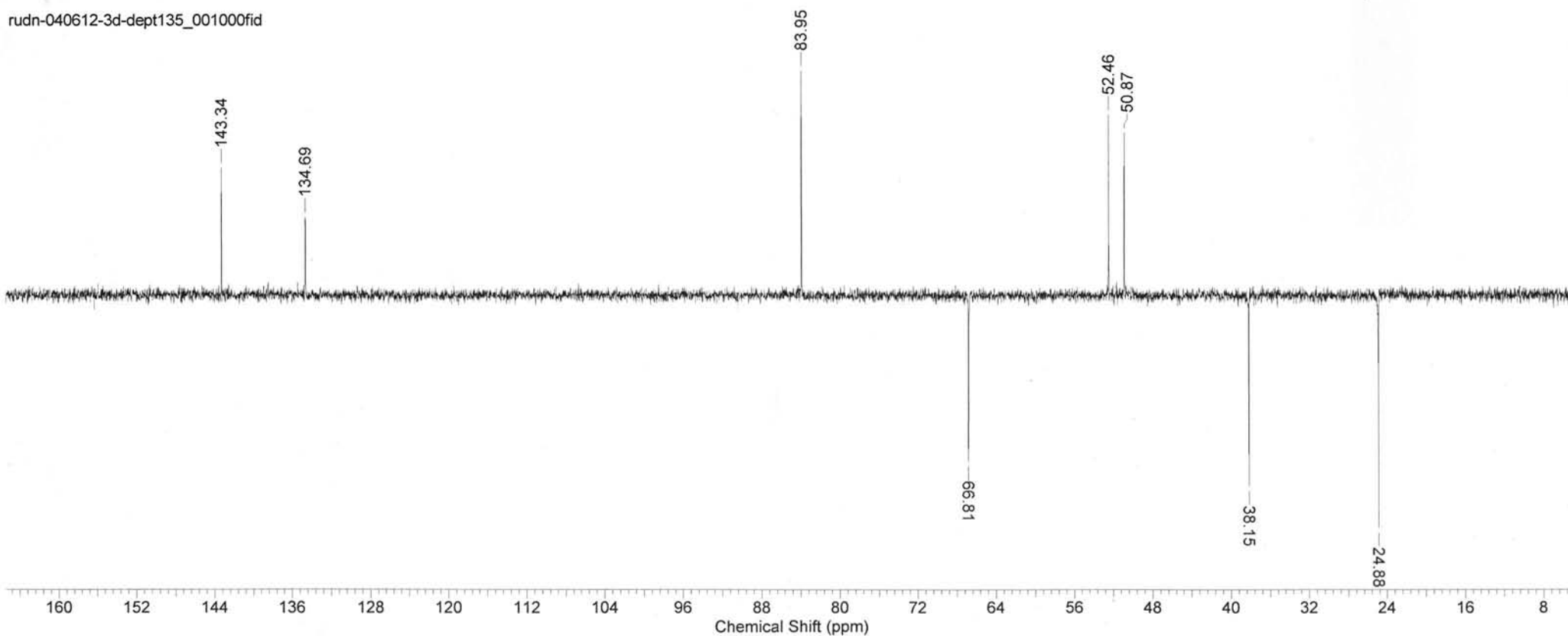
Formula	C ₁₂ H ₁₂ INO ₅	FW	377.1319
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	09 Jun 2012 13:11:28		
Date Stamp	09 Jun 2012 13:11:28						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-3d-dept135\rudn-040612-3d-dept135_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	129	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	dept135
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6	Spectrum Offset (Hz)	9101.6973
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				

Compounds 3Ad/3Bd



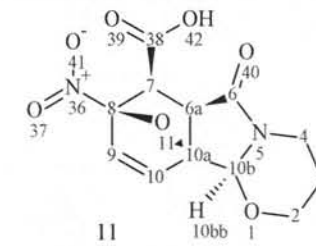
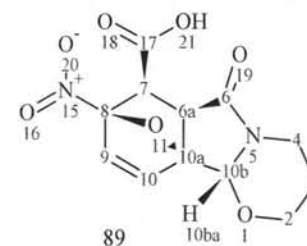
rudn-040612-3d-dept135_001000fid



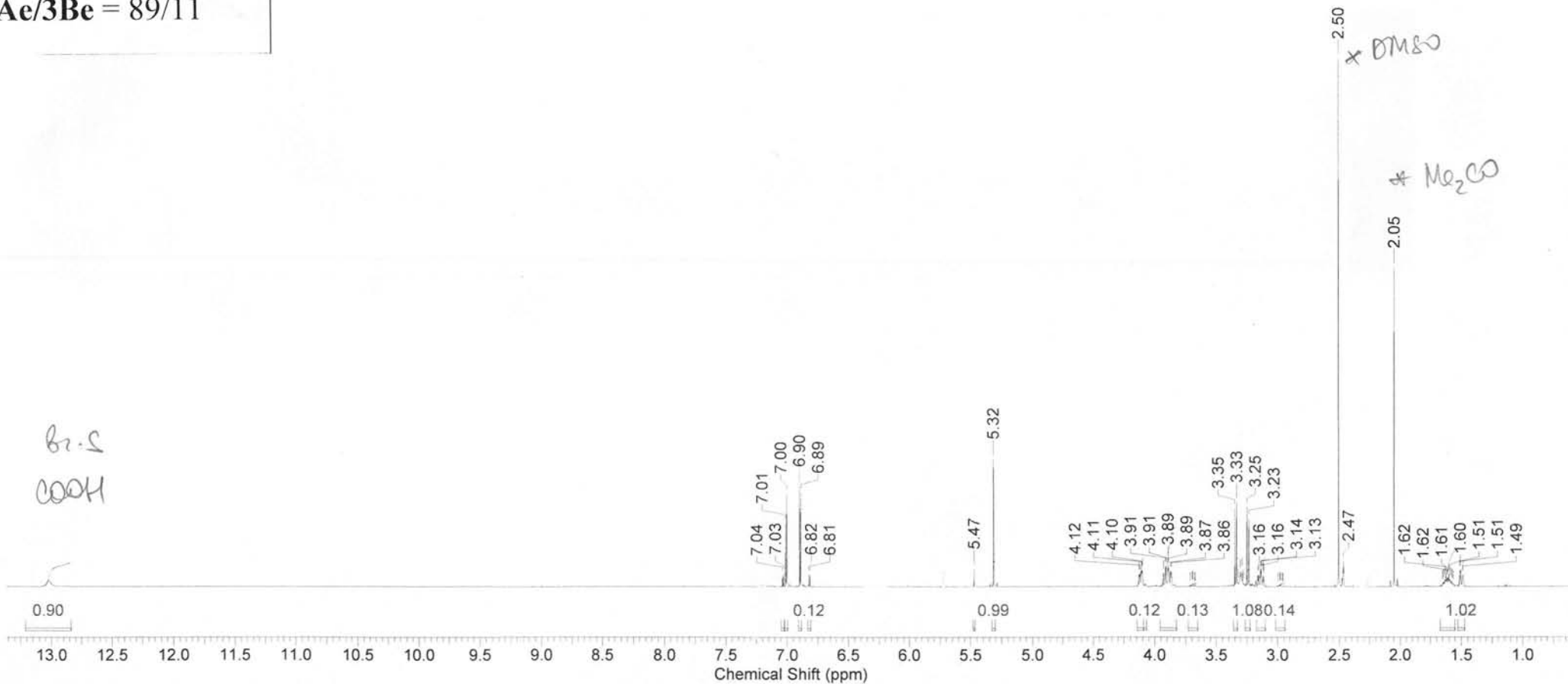
Formula C ₂₄ H ₂₄ N ₄ O ₁₄ ?		FW 592.4658+? (296.2329+296.2329+?+?)					
Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	09 Apr 2010 12:57:25	Date Stamp	09 Apr 2010 12:56:14
File Name	D:\NMR\06.04.10\FZ1136-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	42.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3000.8616	Sweep Width (Hz)	11261.26
						Temperature (degree C)	21.500

mixture

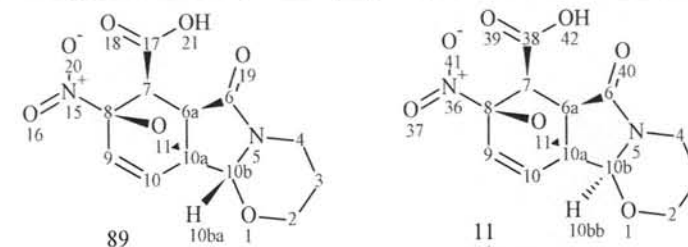
Compounds 3Ae/3Be



3Ae/3Be = 89/11

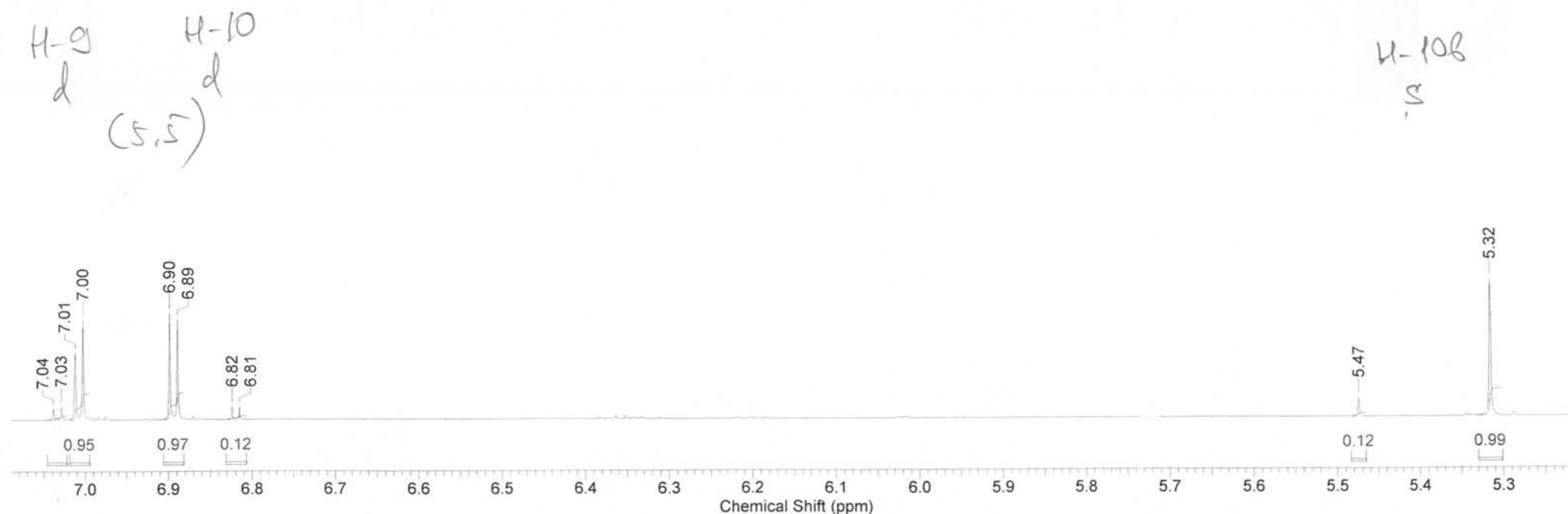


Formula C ₂₄ H ₂₄ N ₄ O ₁₄ ?		FW 592.4658+? (296.2329+296.2329+?+?)					
Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	09 Apr 2010 12:57:25	Date Stamp	09 Apr 2010 12:56:14
File Name	D:\NMR\06.04.10\FZ1136-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	42.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3000.8616	Sweep Width (Hz)	11261.26
						Pulse Sequence	single_pulse.ex2
						Temperature (degree C)	21.500



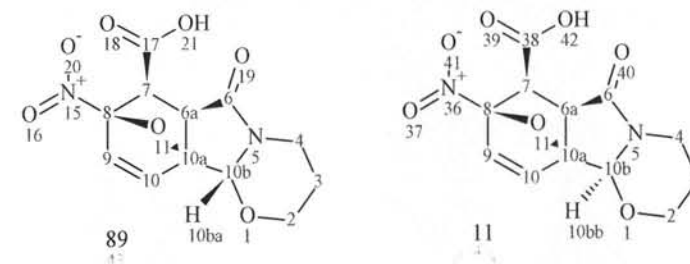
FZ1136-1.jdf

Compounds 3Ae/3Be

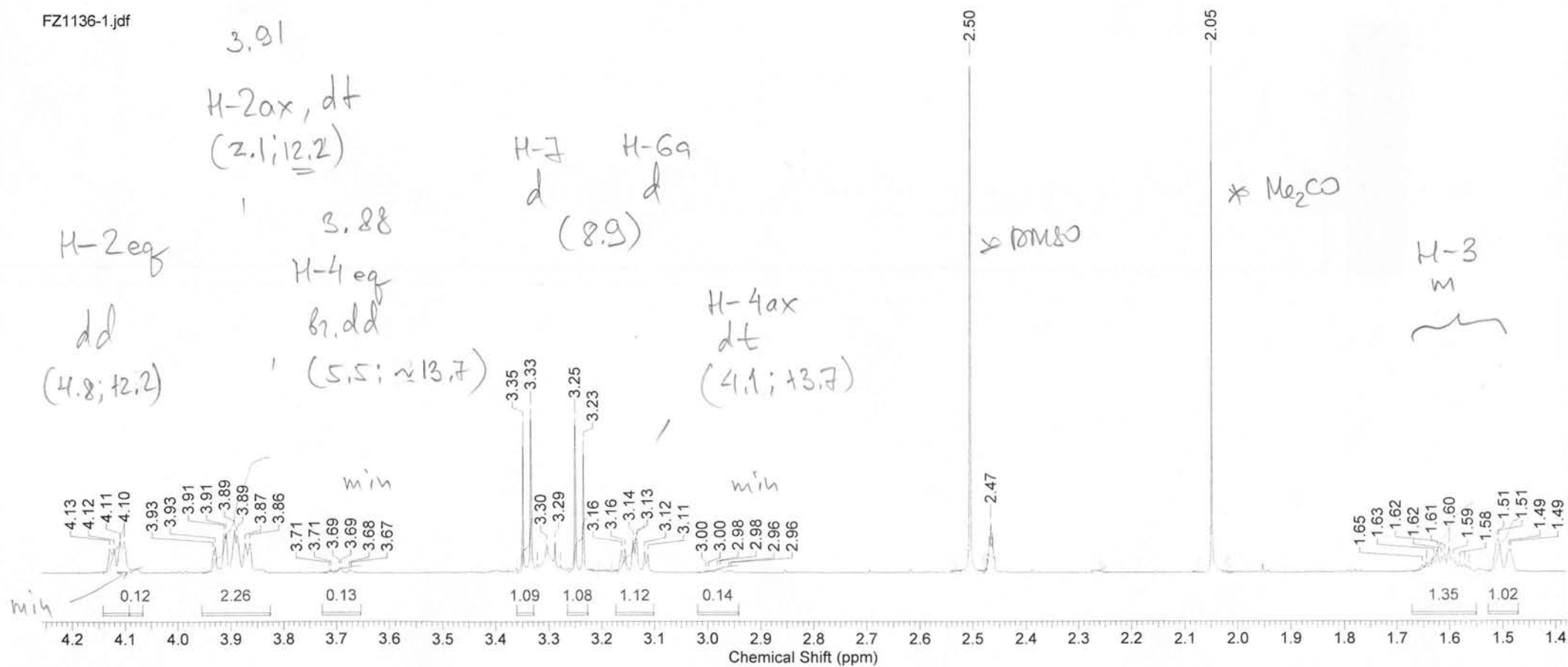


Formula C ₂₄ H ₂₄ N ₄ O ₁₄ ?	FW 592.4658+? (296.2329+296.2329+?+?)					
Acquisition Time (sec) 1.4549	Comment single_pulse	Date 09 Apr 2010 12:57:25	Date Stamp 09 Apr 2010 12:56:14			
File Name D:\NMR\06.04.10\FZ1136-1.jdf		Frequency (MHz) 600.17	Nucleus 1H	Number of Transients 8		
Origin ECA 600	Original Points Count 16384	Owner delta	Points Count 16384	Pulse Sequence single_pulse.ex2		
Receiver Gain 42.00	Solvent DMSO-d6	Spectrum Offset (Hz) 3000.8616	Sweep Width (Hz) 11261.26	Temperature (degree C) 21.500		

Compounds 3Ae/3Be



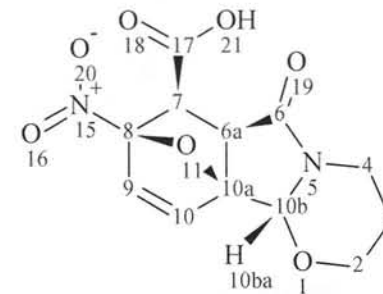
FZ1136-1.jdf



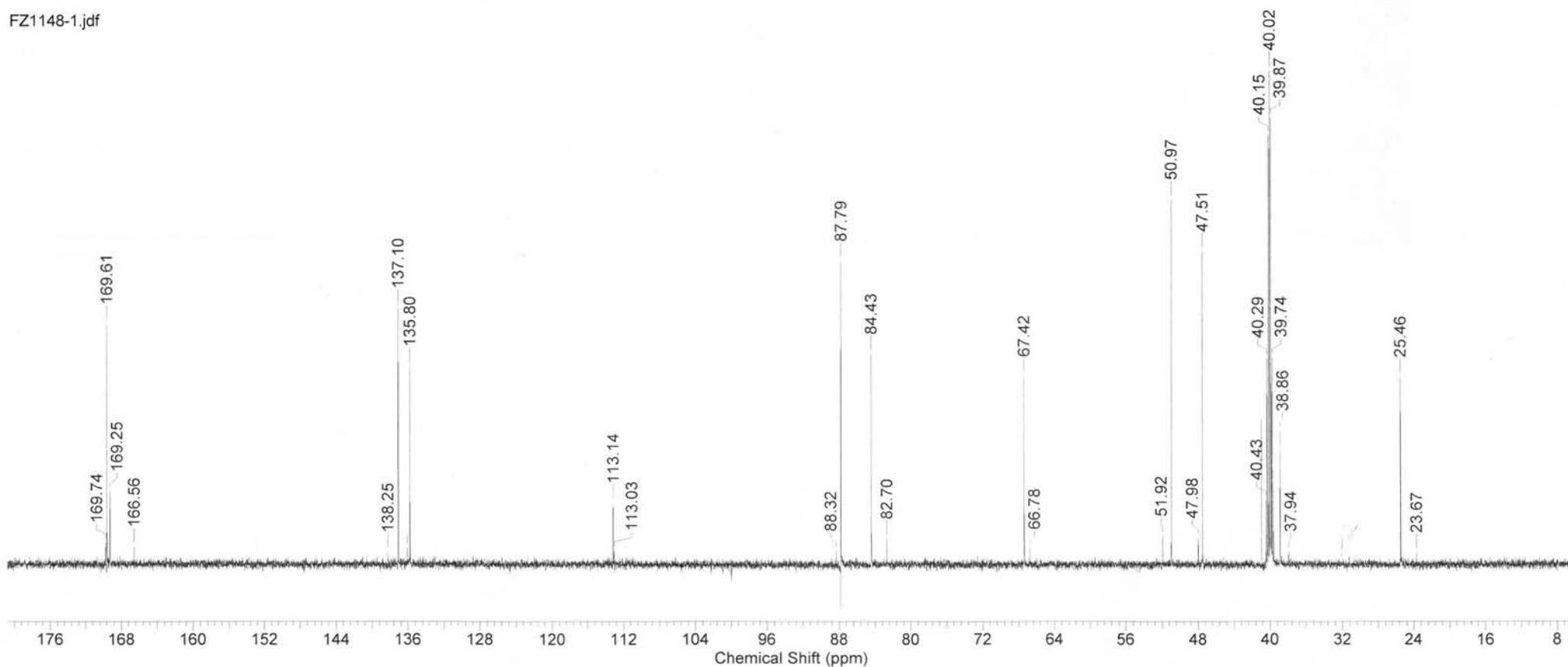
Formula	C ₁₂ H ₁₂ N ₂ O ₇	FW	296.2329
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Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	15 Apr 2010 14:03:50
Date Stamp	15 Apr 2010 14:02:46	File Name	D:\NMR\14.04.10\FZ1148-1.jdf	Frequency (MHz)	150.91
Nucleus	13C	Number of Transients	200	Origin	ECA 600
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49	Receiver Gain	50.00
		Temperature (degree C)	22.000	Owner	delta
				Solvent	DMSO-d6

Compounds 3Ae/3Be



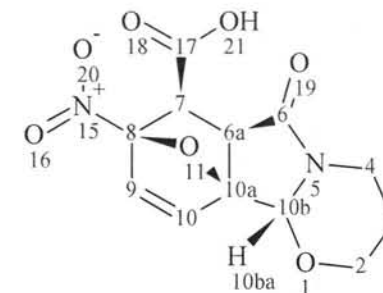
FZ1148-1.jdf



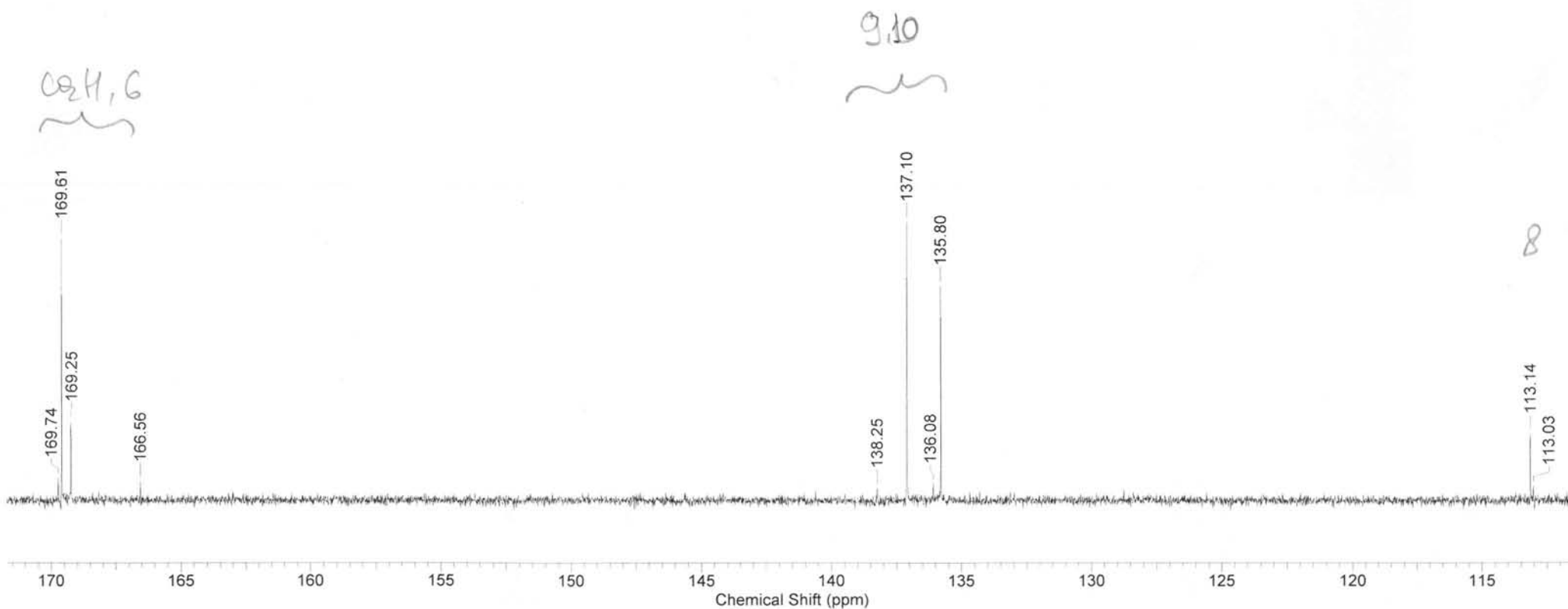
Formula C₁₂H₁₂N₂O₇ FW 296.2329

Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	15 Apr 2010 14:03:50			
Date Stamp	15 Apr 2010 14:02:46	File Name	D:\NMR\14.04.10\FZ1148-1.jdf		Frequency (MHz)	150.91			
Nucleus	13C	Number of Transients	200	Origin	ECA 600	Original Points Count	32768		
Points Count	32768	Pulse Sequence	single_pulse_dec		Receiver Gain	50.00	Owner	delta	
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49	Temperature (degree C)	22.000			Solvent	DMSO-d6

Compounds 3Ae/3Be



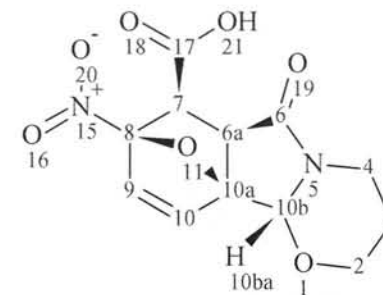
FZ1148-1.jdf



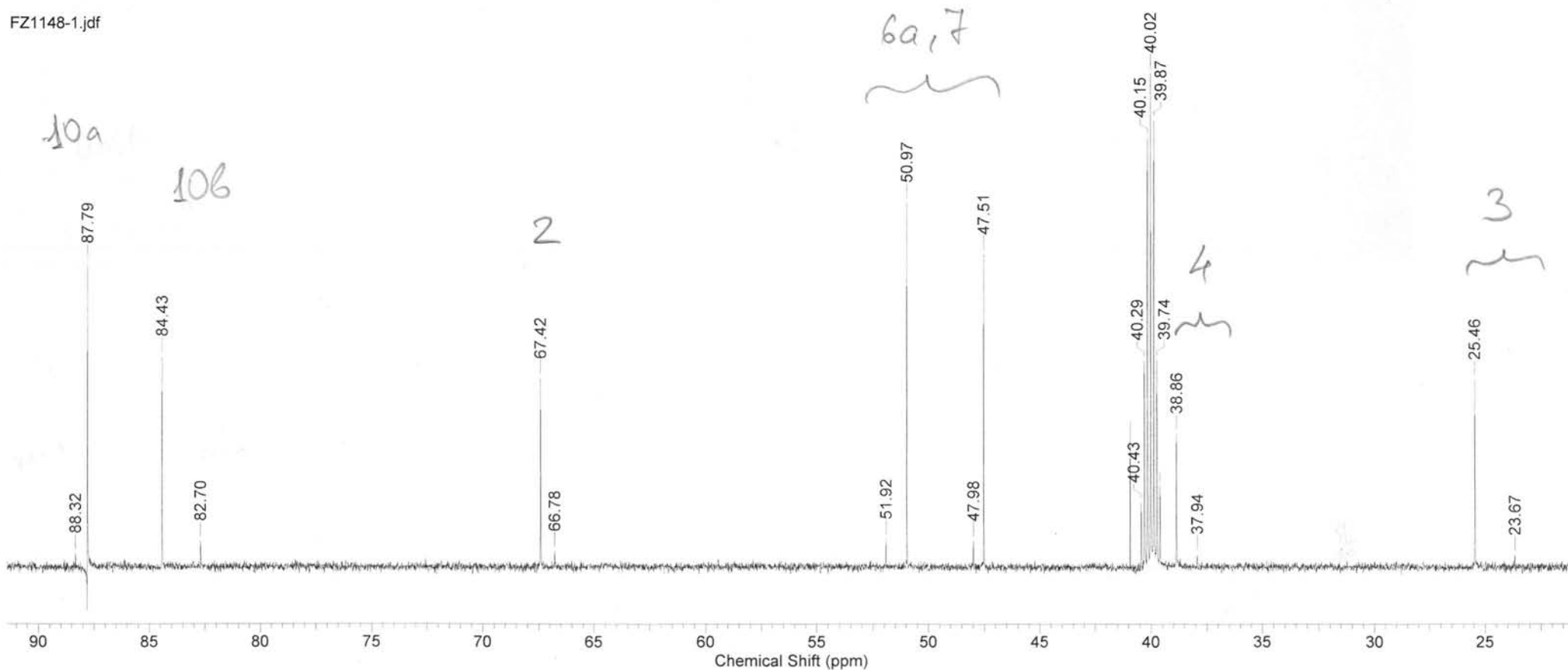
Formula $C_{12}H_{12}N_2O_7$ FW 296.2329

Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	15 Apr 2010 14:03:50
Date Stamp	15 Apr 2010 14:02:46	File Name	D:\NMR\14.04.10\FZ1148-1.jdf	Frequency (MHz)	150.91
Nucleus	13C	Number of Transients	200	Origin	ECA 600
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49	Receiver Gain	50.00
		Temperature (degree C)	22.000	Owner	delta
				Solvent	DMSO-d6

Compounds 3Ae/3Be



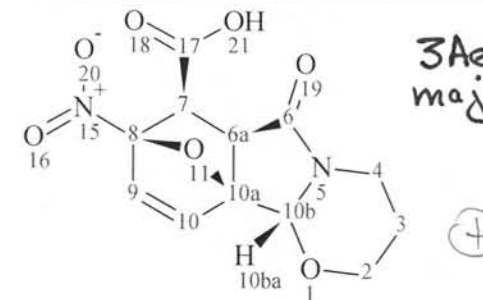
FZ1148-1.jdf



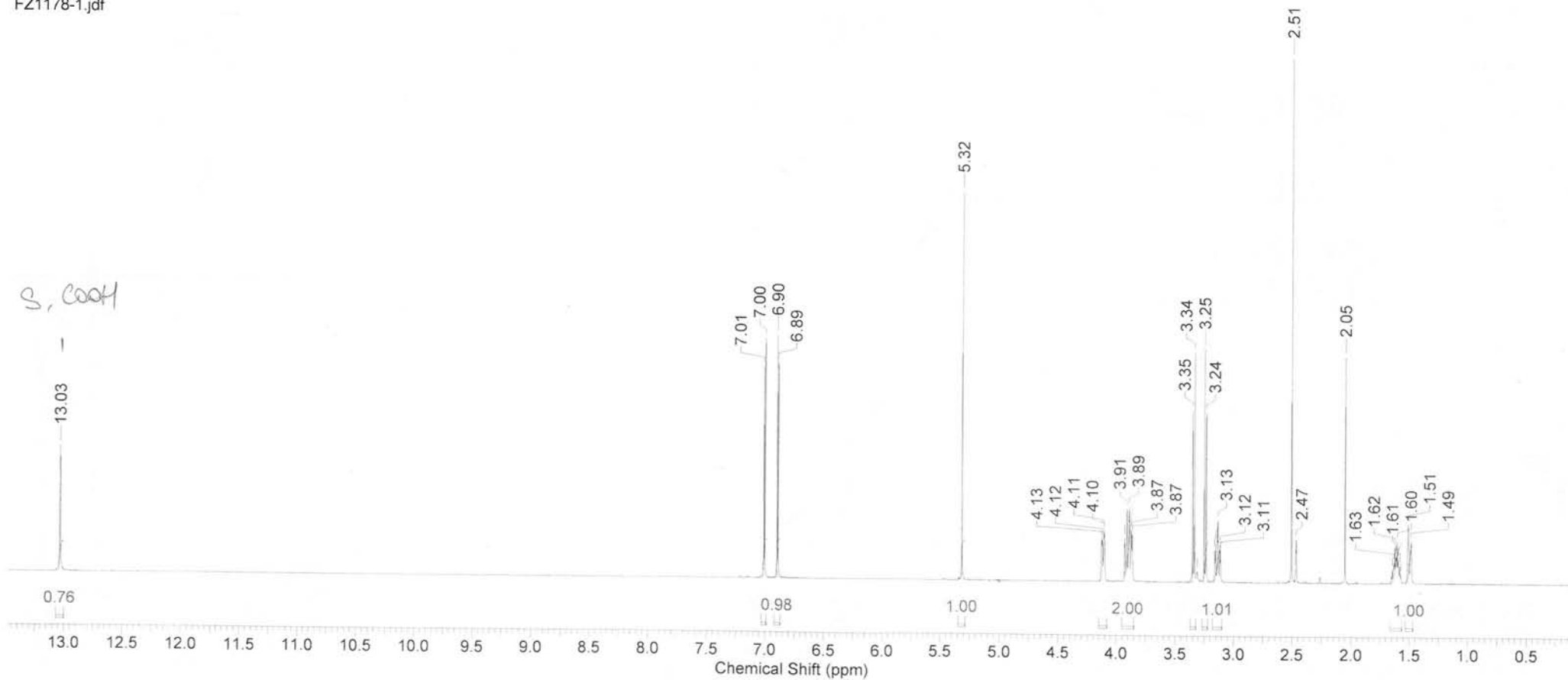
Formula $C_{12}H_{12}N_2O_7$ FW 296.2329

Acquisition Time (sec)	2.9098	Comment	single_pulse	Date	04 May 2010 10:35:03		Date Stamp	04 May 2010 10:33:49		
File Name	D:\NMR\22.04.10\FZ1178-1.jdf			Frequency (MHz)	600.17	Nucleus	1H			
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768			
Receiver Gain	26.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3000.8616	Sweep Width (Hz)	11261.26		Temperature (degree C)	20.500

Compounds 3Ae/3Be



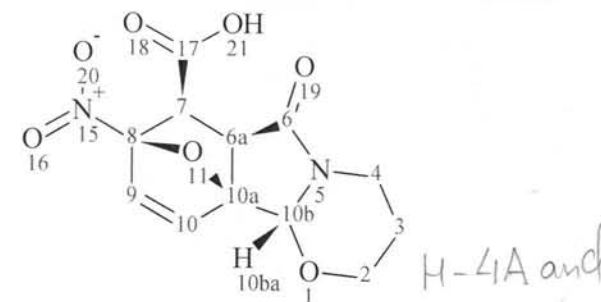
FZ1178-1.jdf



Formula $C_{12}H_{12}N_2O_7$ FW 296.2329

Acquisition Time (sec)	2.9098	Comment	single_pulse	Date	04 May 2010 10:35:03	Date Stamp	04 May 2010 10:33:49
File Name	D:\NMR\22.04.10\FZ1178-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	26.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3000.8616	Sweep Width (Hz)	11261.26
						Temperature (degree C)	20.500

Compounds 3Ae/3Be



FZ1178-1.jdf

H-9 and H-10

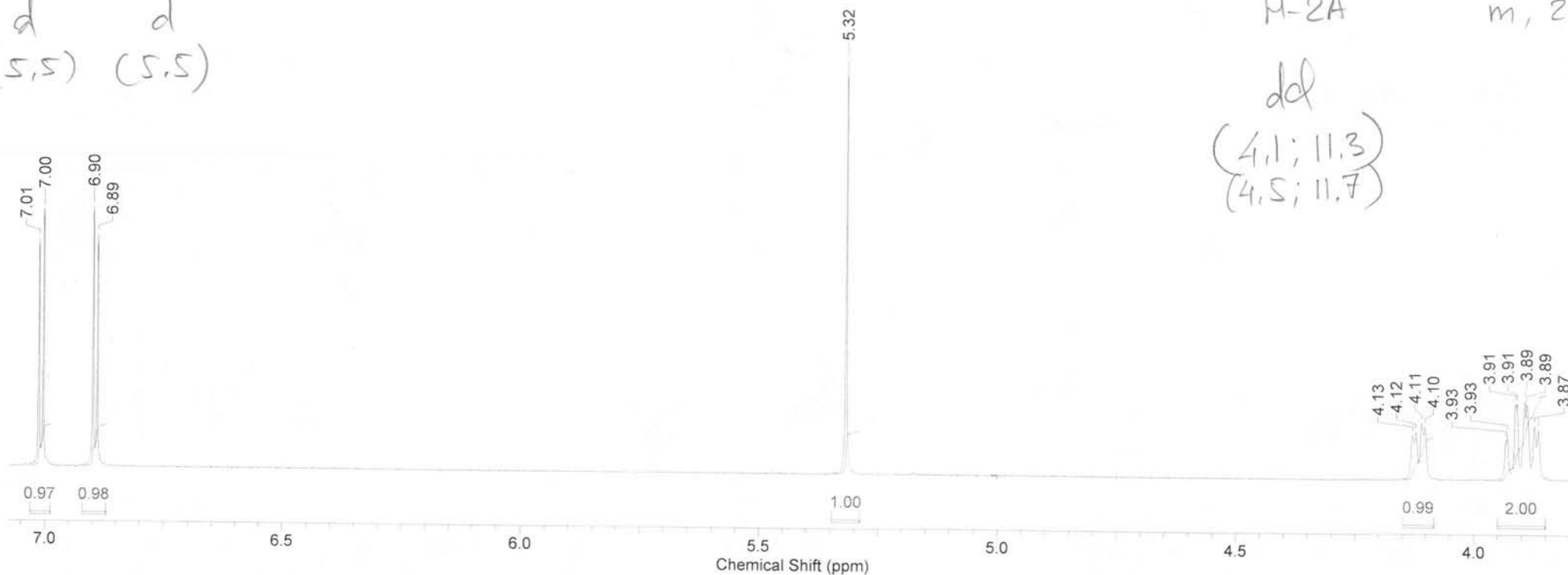
d d
(5,5) (5,5)

H-10b, f

H-4A and
H-2B and
3.93-3.87,
m, 2H

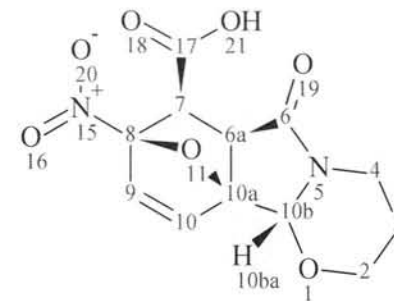
H-2A

dd
(4.1; 11.3)
(4.5; 11.7)

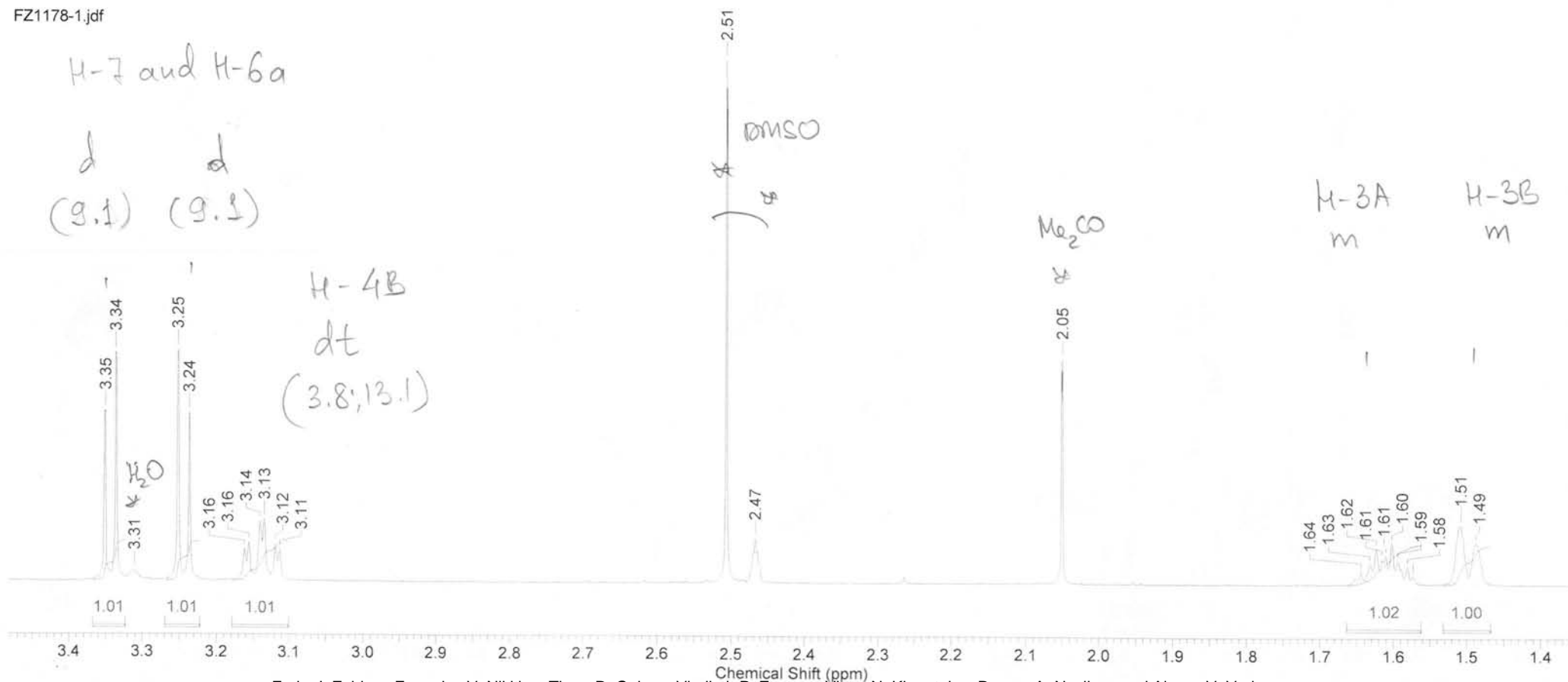


Formula	C ₁₂ H ₁₂ N ₂ O ₇	FW	296.2329						
Acquisition Time (sec)	2.9098	Comment	single_pulse	Date	04 May 2010 10:35:03	Date Stamp	04 May 2010 10:33:49		
File Name	D:\NMR\22.04.10\FZ1178-1.jdf			Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single_pulse.ex2
Receiver Gain	26.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3000.8616	Sweep Width (Hz)	11261.26	Temperature (degree C)	20.500

Compounds 3Ae/3Be



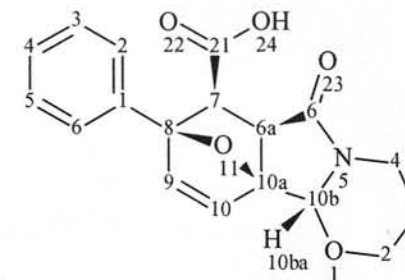
FZ1178-1.jdf



Formula	C ₁₈ H ₁₇ NO ₅	FW	327.3313
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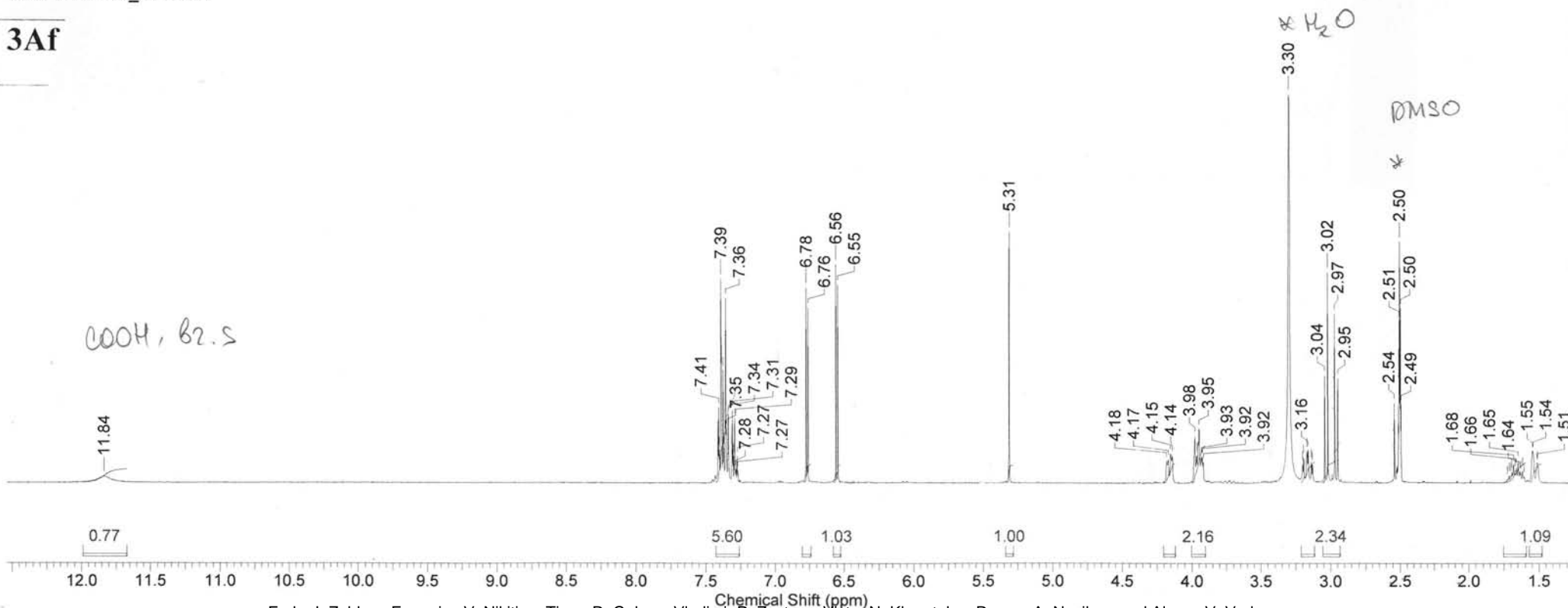
Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	08 Jun 2012 15:21:36
Date Stamp	08 Jun 2012 15:21:36				
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-3Af\rudn-040612-3Af_001000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	16	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zg
SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542
Temperature (degree C)	32.000			Sweep Width (Hz)	10416.03

Compound 3Af



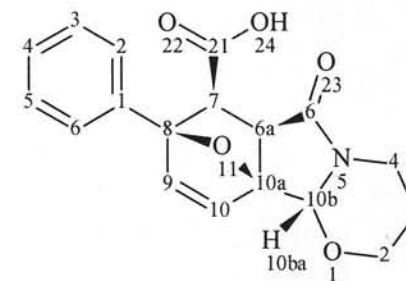
rudn-040612-3Af_001000fid

3Af



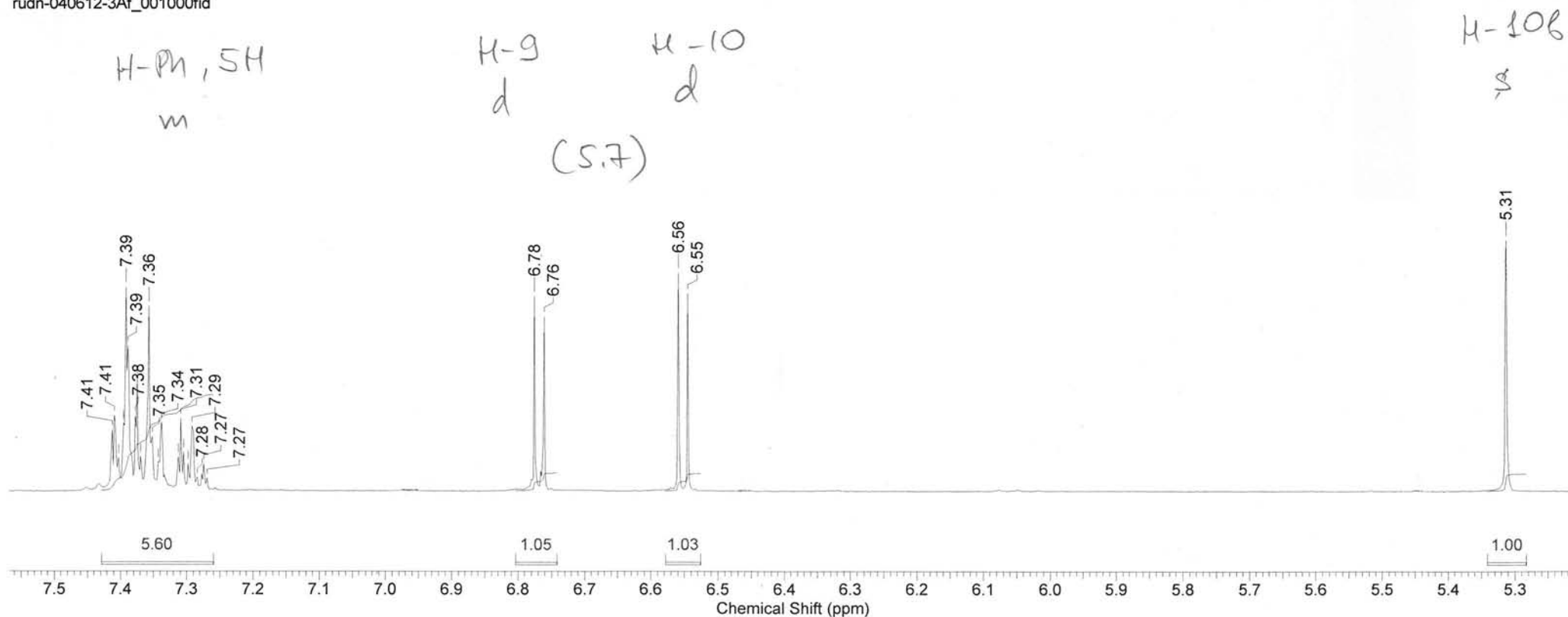
Formula $C_{18}H_{17}NO_5$ FW 327.3313

Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	08 Jun 2012 15:21:36
Date Stamp	08 Jun 2012 15:21:36				
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-3Af\rudn-040612-3Af_001000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	16	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zg
SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542
Temperature (degree C)	32.000			Sweep Width (Hz)	10416.03

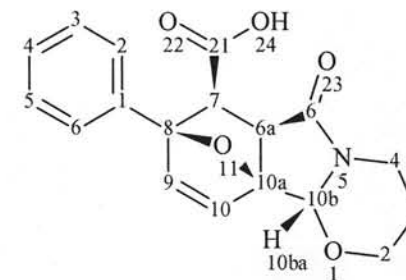


Compound 3Af

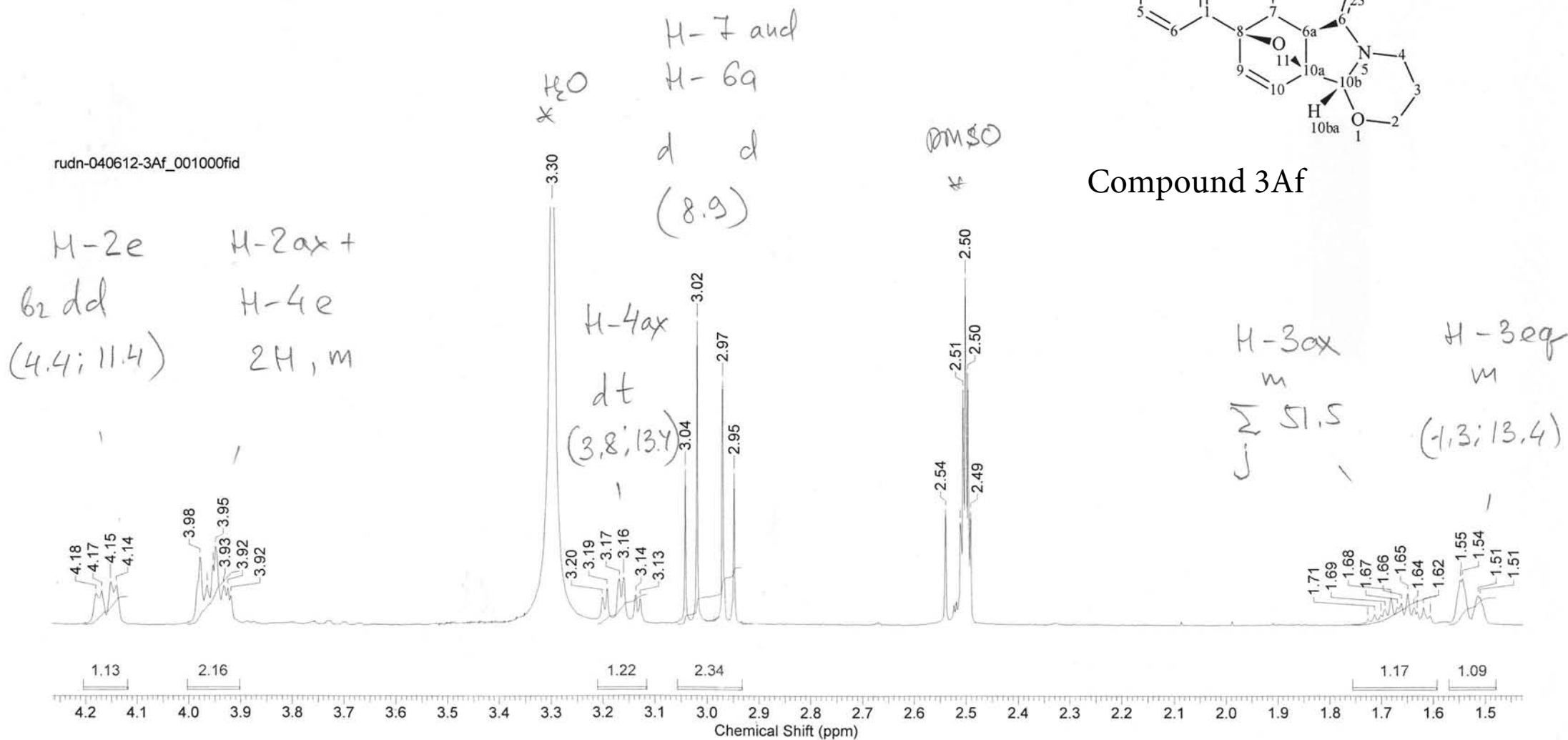
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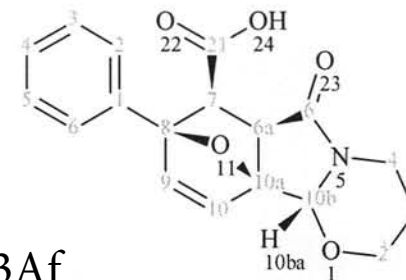
Formula C ₁₈ H ₁₇ NO ₅	FW 327.3313			
Acquisition Time (sec) 1.5729	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 08 Jun 2012 15:21:36		
Date Stamp 08 Jun 2012 15:21:36				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-3Af\rudn-040612-3Af_001000fid	Frequency (MHz) 400.14			
Nucleus 1H	Number of Transients 16	Origin spect	Original Points Count 16384	
Owner root	Points Count 16384	Pulse Sequence zg	Receiver Gain 128.00	
SW(cyclical) (Hz) 10416.67	Solvent DMSO-d6	Spectrum Offset (Hz) 2712.0542	Sweep Width (Hz) 10416.03	
Temperature (degree C) 32.000				



Compound 3Af

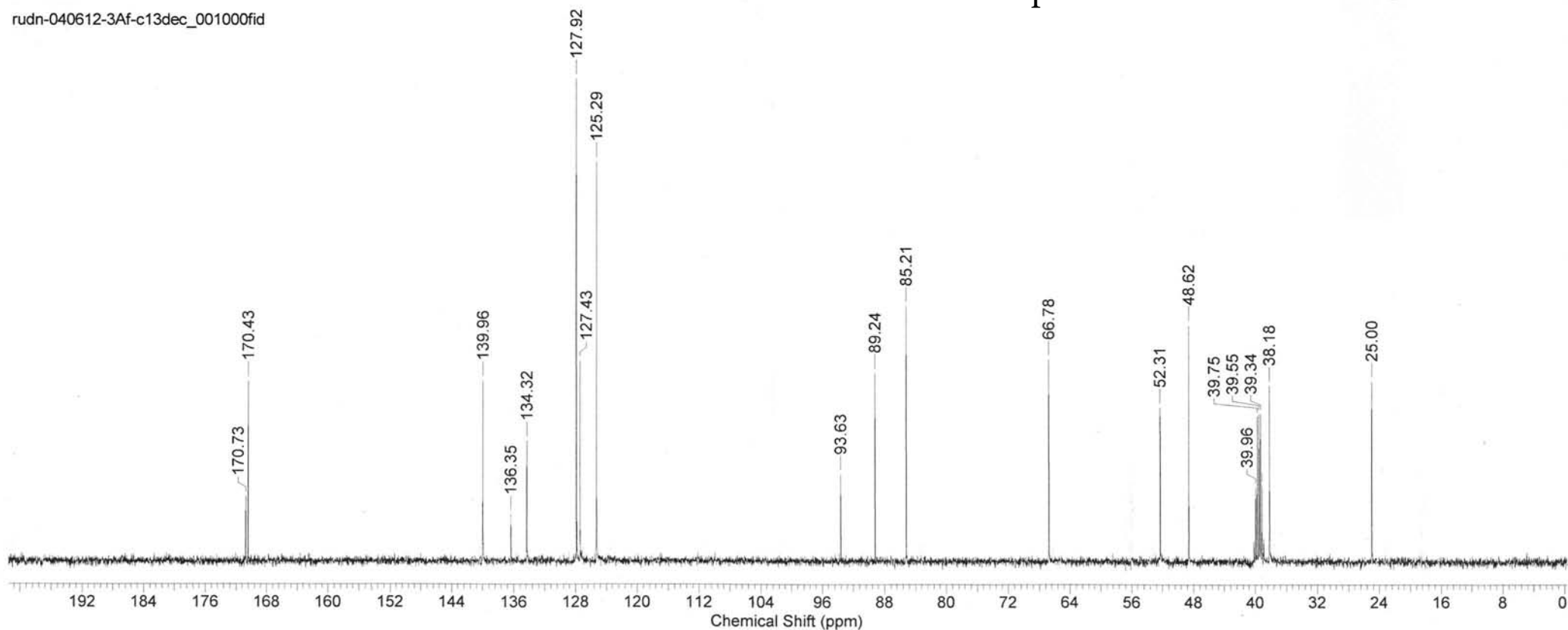


Formula C ₁₈ H ₁₇ NO ₅	FW 327.3313			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 08 Jun 2012 16:42:40		
Date Stamp 08 Jun 2012 16:42:40				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-3Af-c13dec\rudn-040612-3Af-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 386	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10554.8018	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			



Compound 3Af

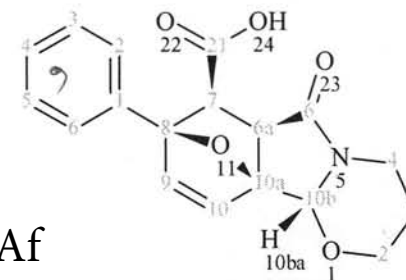
rudn-040612-3Af-c13dec_001000fid



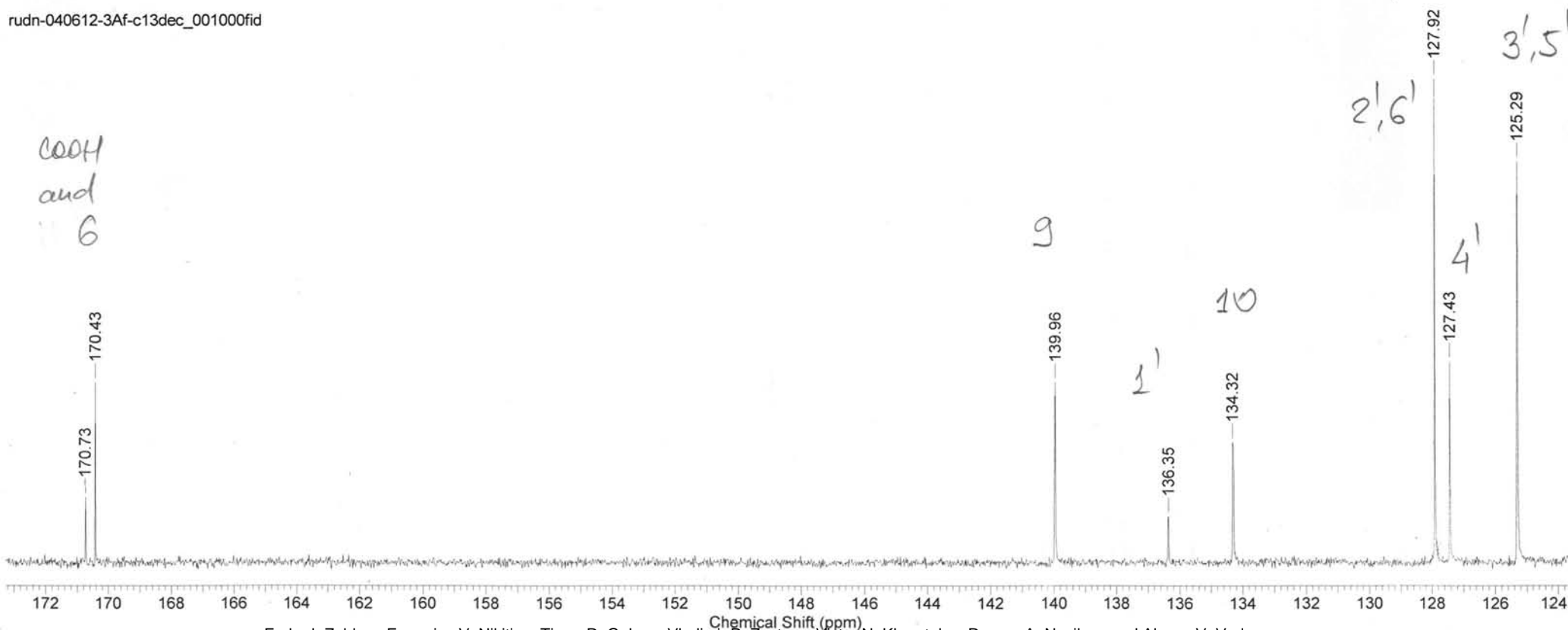
Formula	C ₁₈ H ₁₇ NO ₅	FW	327.3313
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	08 Jun 2012 16:42:40	
Date Stamp	08 Jun 2012 16:42:40						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-3Af-c13dec\rudn-040612-3Af-c13dec_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	386	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zgpg
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6	Spectrum Offset (Hz)	10554.8018
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				

Compound 3Af

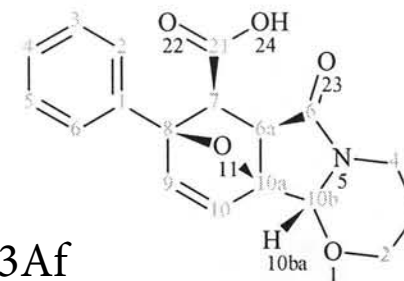


rudn-040612-3Af-c13dec_001000fid



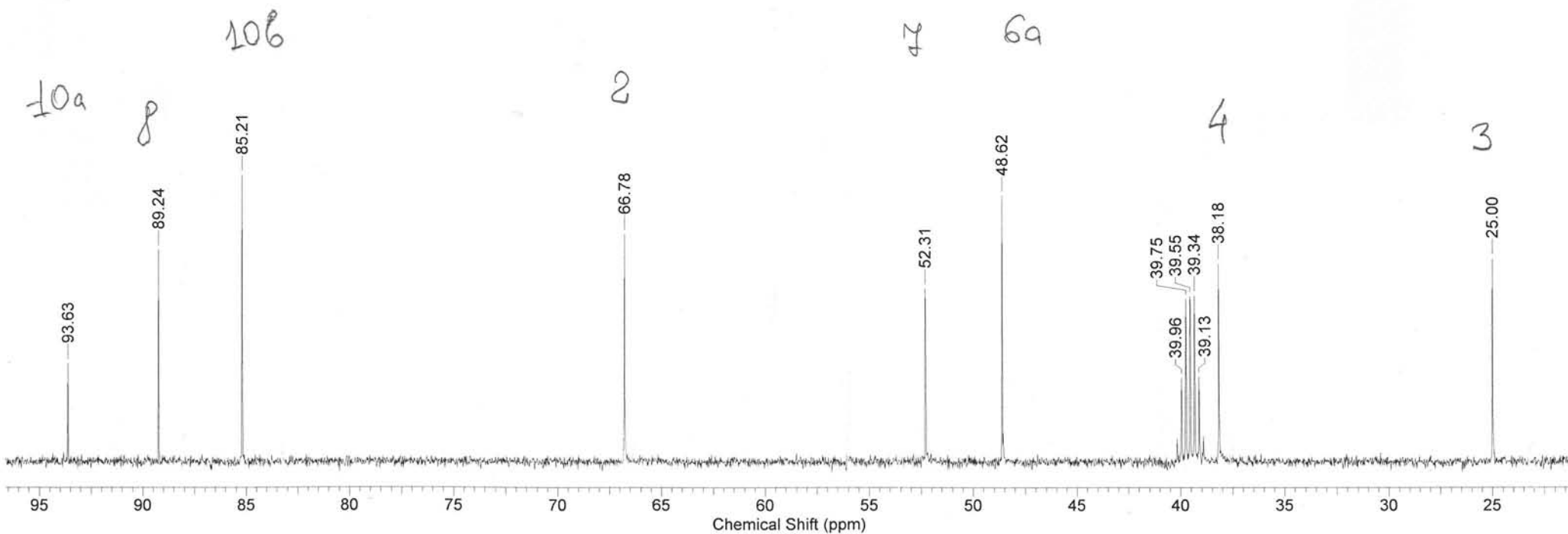
Formula	C ₁₈ H ₁₇ NO ₅	FW	327.3313
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	08 Jun 2012 16:42:40		
Date Stamp	08 Jun 2012 16:42:40						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-3Af-c13dec\rudn-040612-3Af-c13dec_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	386	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zgpg
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6	Spectrum Offset (Hz)	10554.8018
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				

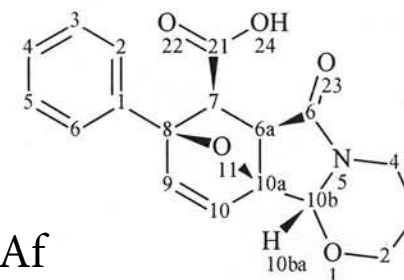


Compound 3Af

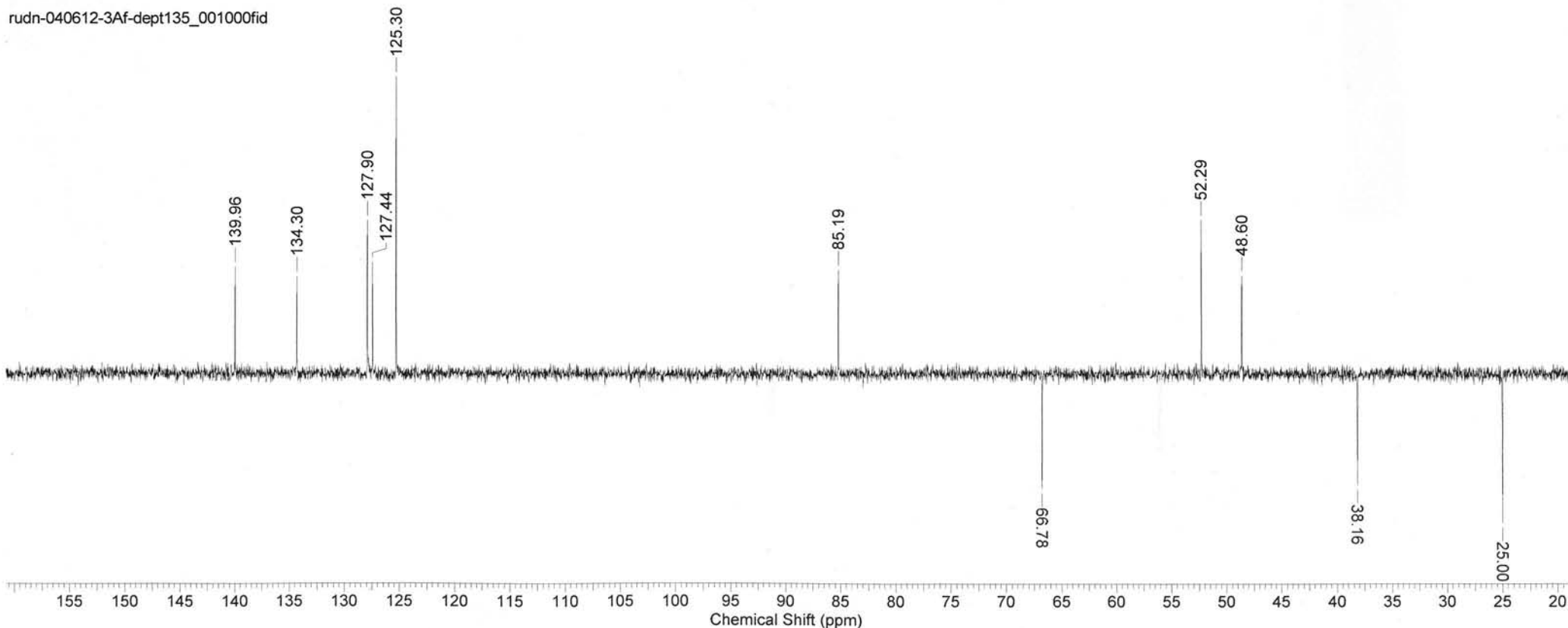
rudn-040612-3Af-c13dec_001000fid



Formula C ₁₈ H ₁₇ NO ₅	FW 327.3313			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 08 Jun 2012 16:51:12		
Date Stamp 08 Jun 2012 16:51:12				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-3Af-dept135\rudn-040612-3Af-dept135_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 166	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence dept135	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 9104.3936	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			



Compound 3Af

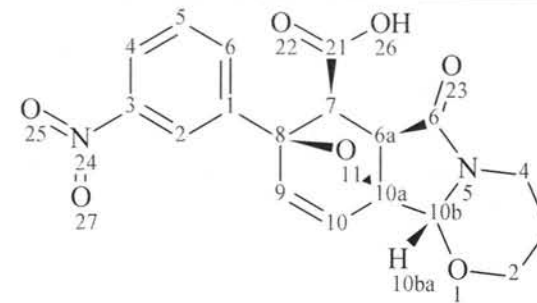


isomers mixture 10:1 A/B

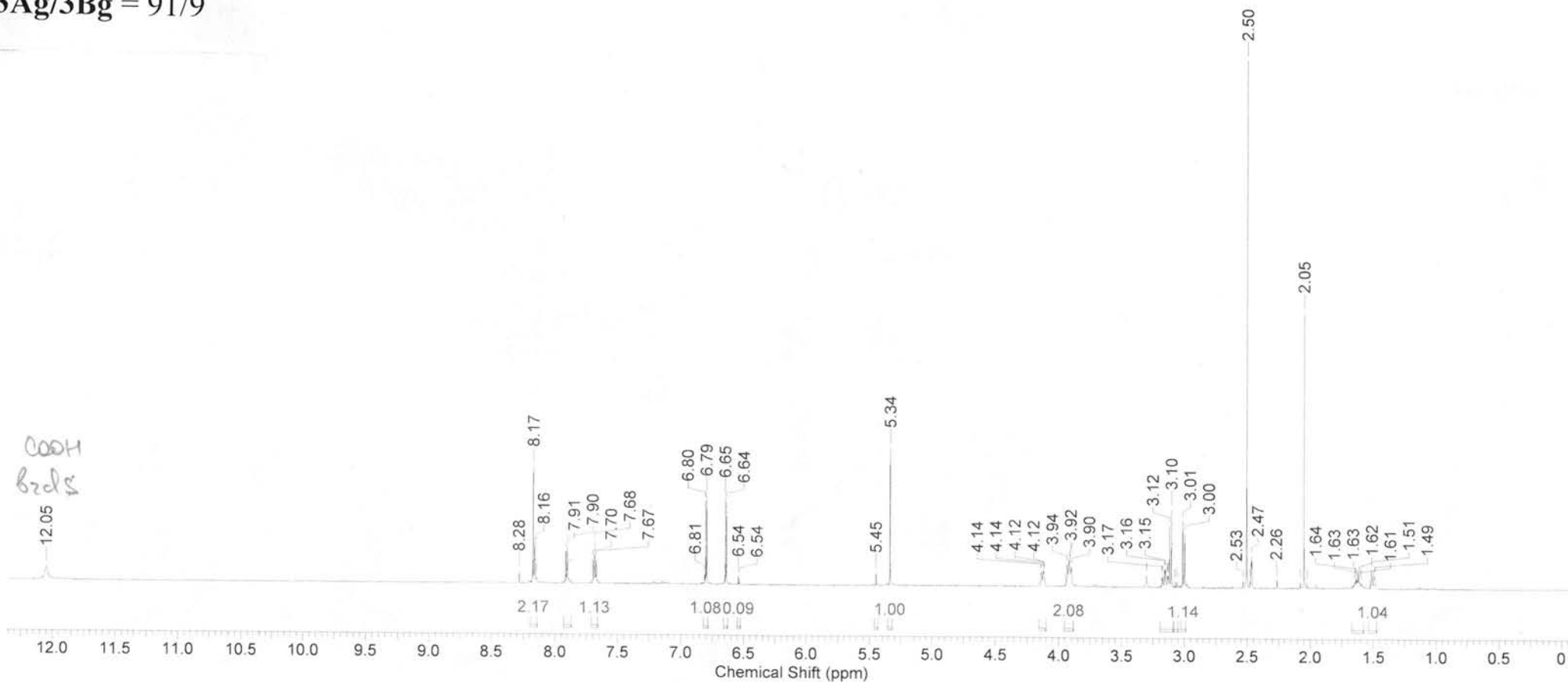
Formula C₁₈H₁₆N₂O₇ FW 372.3288

Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	09 Apr 2010 13:02:56	Date Stamp	09 Apr 2010 13:01:44
File Name	D:\NMR\6.04.10\FZ1139-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	32.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3000.8616	Sweep Width (Hz)	11261.26
						Temperature (degree C)	21.300

Compounds 3Ag/3Bg



3Ag/3Bg = 91/9



Formula $C_{18}H_{16}N_2O_7$ FW 372.3288

Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	09 Apr 2010 13:02:56	Date Stamp	09 Apr 2010 13:01:44
File Name	D:\NMR\6.04.10\FZ1139-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	32.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3000.8616	Sweep Width (Hz)	11261.26
						Temperature (degree C)	21.300

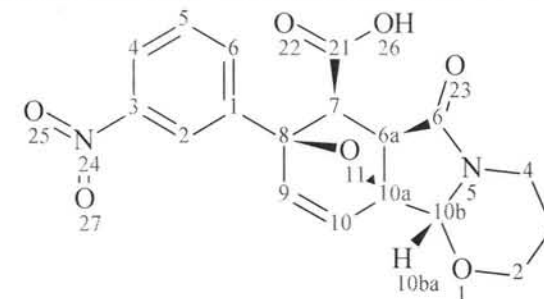
min + maj, H-4'
8.16, d (8.3)

maj
H-2'
8.17, s brd

FZ1139-1.jdf

6.81, min, d

Compounds 3Ag/3Bg



H-10b

min
H-2'
8.28, s

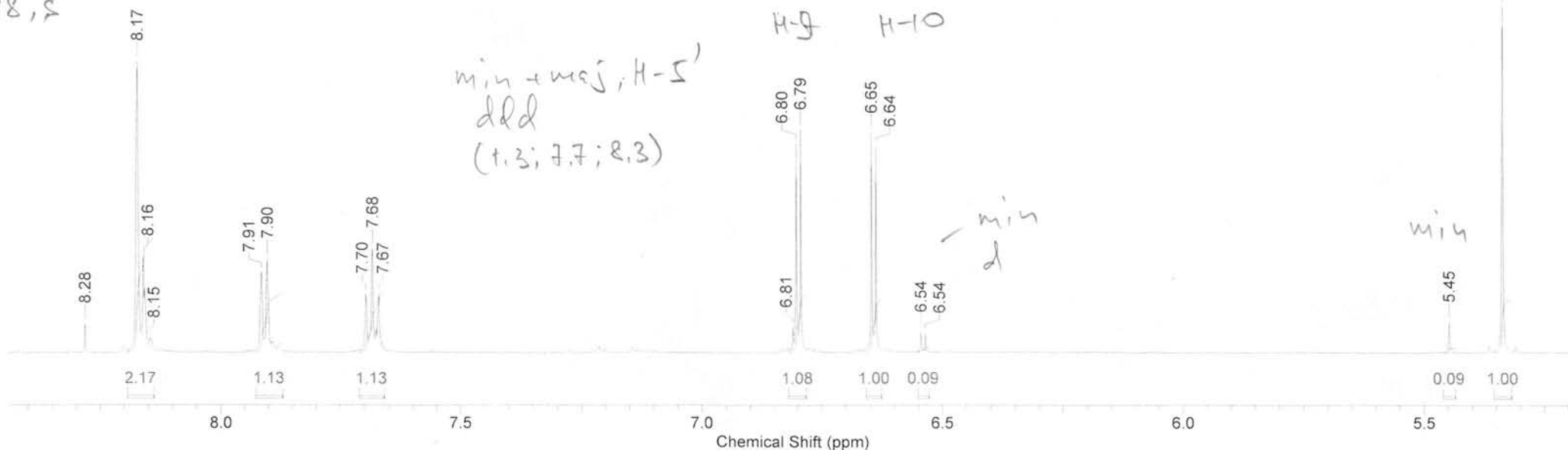
min + maj, H-6'
d (7.7)

(5.5)

maj

min + maj, H-5'
ddd
(1.3; 7.7; 8.3)

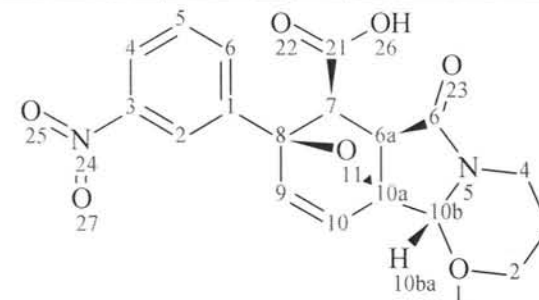
H-9 H-10



Formula $C_{18}H_{16}N_2O_7$ FW 372.3288

Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	09 Apr 2010 13:02:56	Date Stamp	09 Apr 2010 13:01:44
File Name	D:\NMR\6.04.10\FZ1139-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	32.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3000.8616	Sweep Width (Hz)	11261.26
						Temperature (degree C)	21.300

min+maj
3,5, dt, H-4B
(3.4; 3.1)



FZ1139-1.jdf

H-2A
dd
min+maj
(4.1; 3.7)

H-2B + H-4A
min+maj
m, 2H

min+maj
H-7
d
(8.9)

H-6a
maj
d
(8.9)

min
3.06
(8.9)

Me_2CO Compounds 3Ag/3Bg

2.05

H-3A H-3B
m m

4.14
4.14
4.12
4.12

1.10

3.94
3.92
3.90

2.08

3.30
3.18
3.17
3.16
3.15

3.12
3.10
3.07
3.06
3.01
3.00

2.15 1.14

DMSO

2.50

2.53

2.47

2.26

2.08

2.02

1.65

1.64

1.63

1.63

1.62

1.61

1.51

1.49

1.12

1.04

4.0

3.5

Chemical Shift (ppm)

2.5

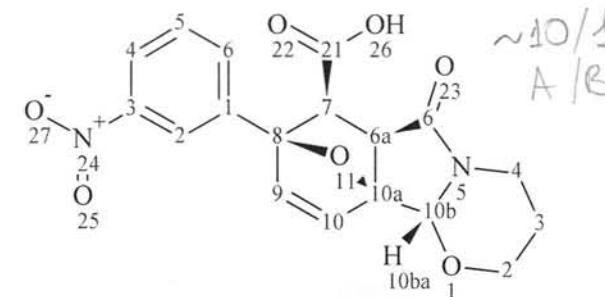
2.0

1.5

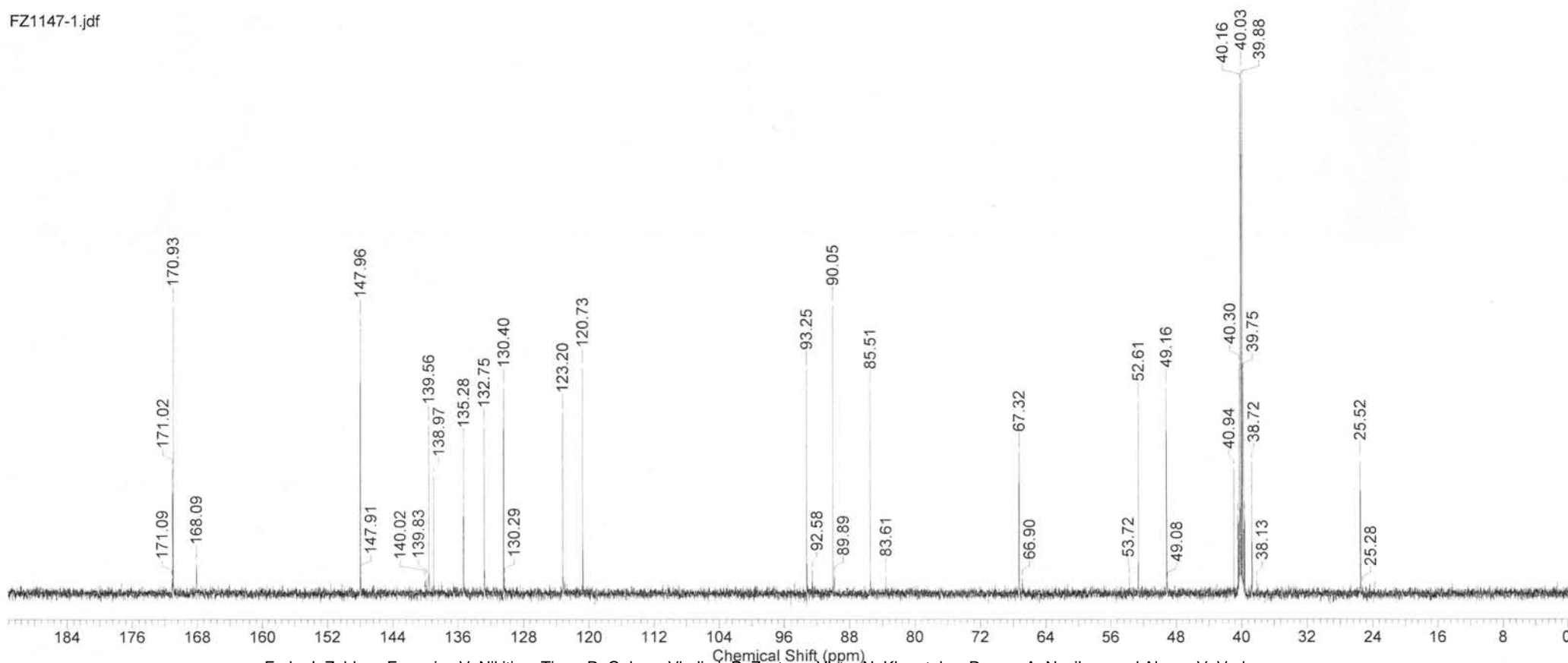
Formula C₁₈H₁₆N₂O₇ FW 372.3288

Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	15 Apr 2010 14:38:46
Date Stamp	15 Apr 2010 14:37:42	File Name	D:\NMR\14.04.10\FZ1147-1.jdf	Frequency (MHz)	150.91
Nucleus	13C	Number of Transients	200	Origin	ECA 600
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49	Receiver Gain	50.00
		Temperature (degree C)	21.300	Owner	delta
				Solvent	DMSO-d6

Compounds 3Ag/3Bg

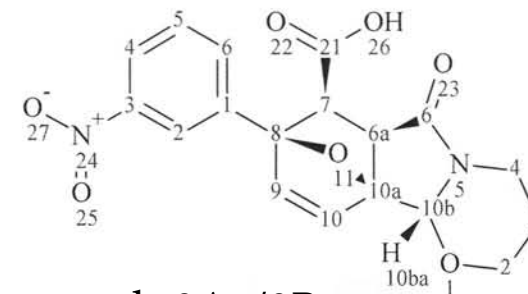


FZ1147-1.jdf



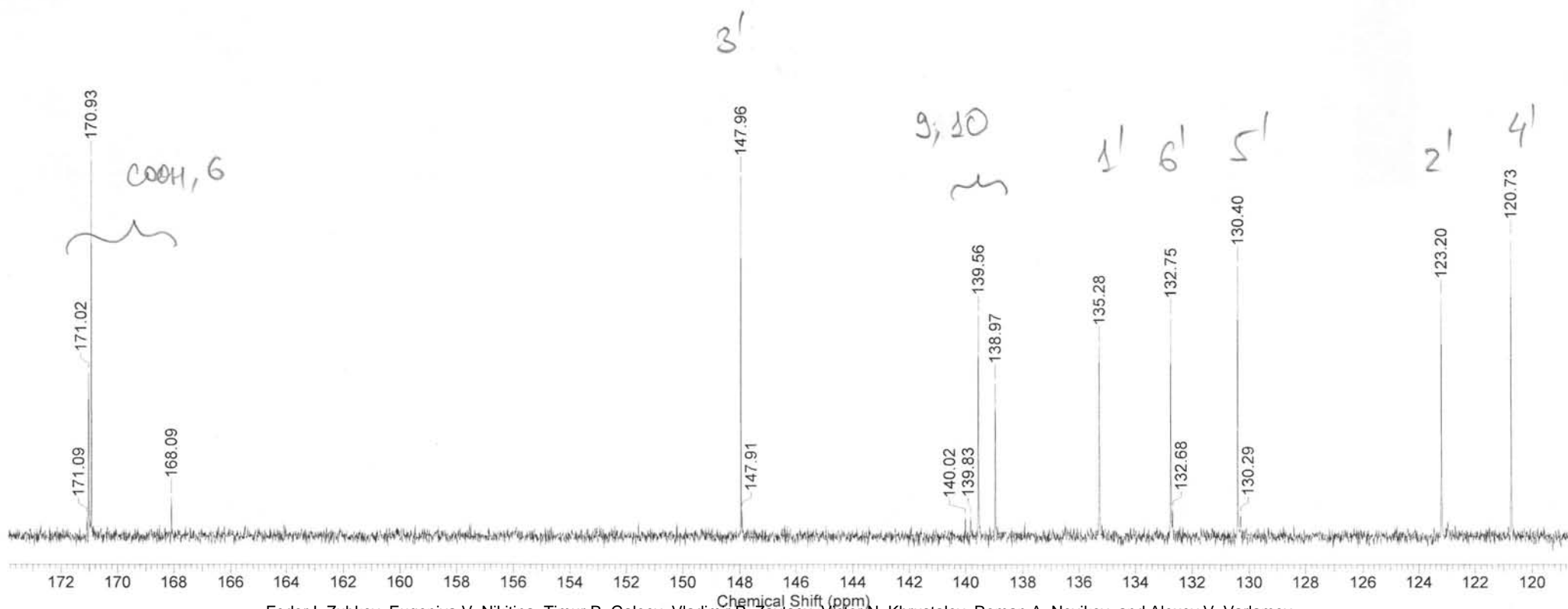
Formula $C_{18}H_{16}N_2O_7$ FW 372.3288

Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	15 Apr 2010 14:38:46
Date Stamp	15 Apr 2010 14:37:42	File Name	D:\NMR\14.04.10\FZ1147-1.jdf	Frequency (MHz)	150.91
Nucleus	^{13}C	Number of Transients	200	Origin	ECA 600
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49	Receiver Gain	50.00
		Temperature (degree C)	21.300	Owner	delta
				Solvent	DMSO-d6



Compounds 3Ag/3Bg

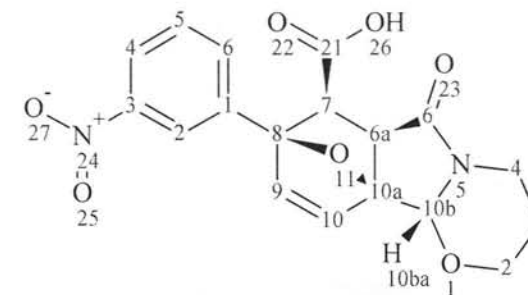
FZ1147-1.jdf



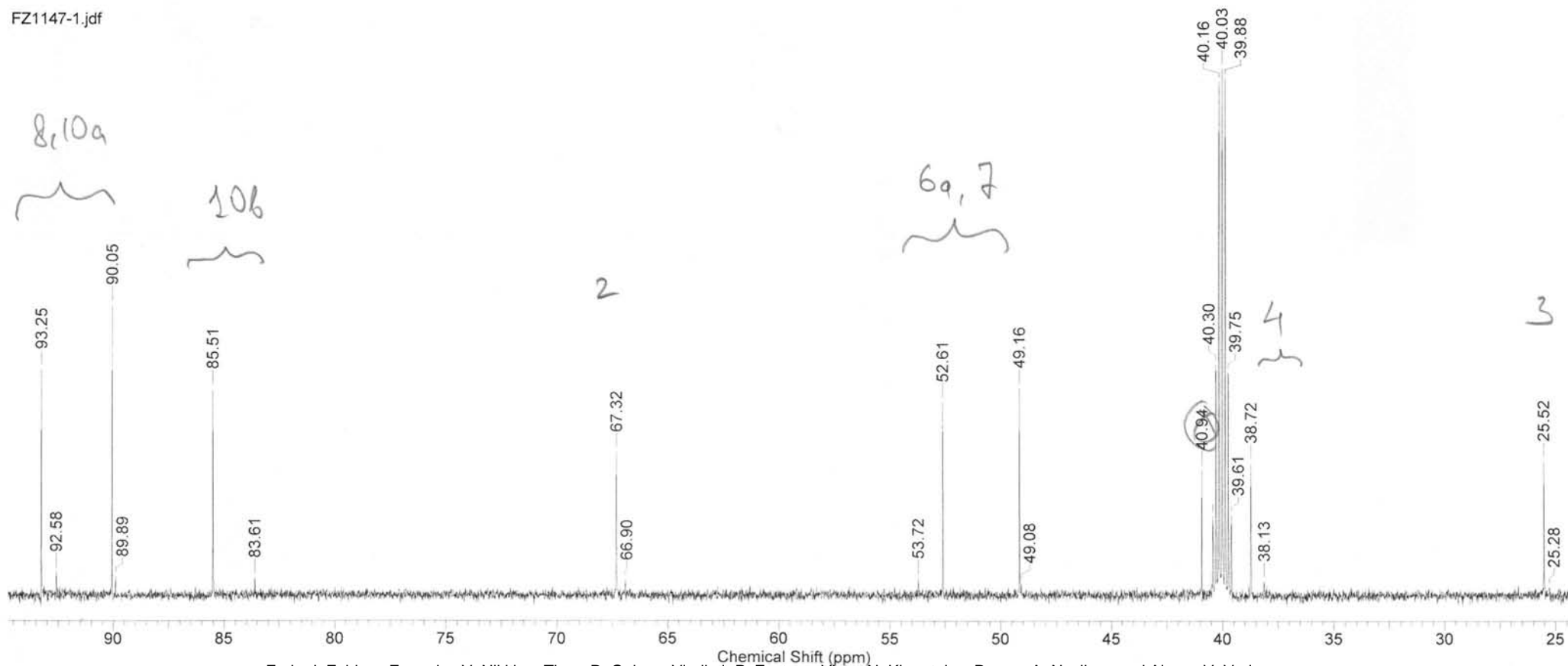
Formula $C_{18}H_{16}N_2O_7$ FW 372.3288

Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	15 Apr 2010 14:38:46
Date Stamp	15 Apr 2010 14:37:42	File Name	D:\NMR\14.04.10\FZ1147-1.jdf	Frequency (MHz)	150.91
Nucleus	^{13}C	Number of Transients	200	Origin	ECA 600
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49	Receiver Gain	50.00
		Temperature (degree C)	21.300	Owner	delta
				Solvent	DMSO-d6

Compounds 3Ag/3Bg

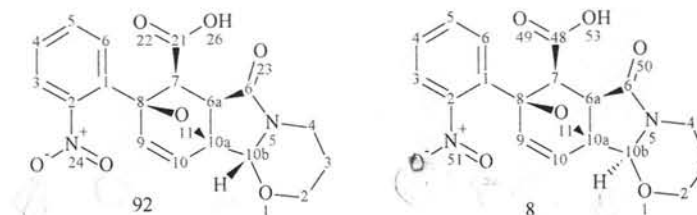


FZ1147-1.jdf

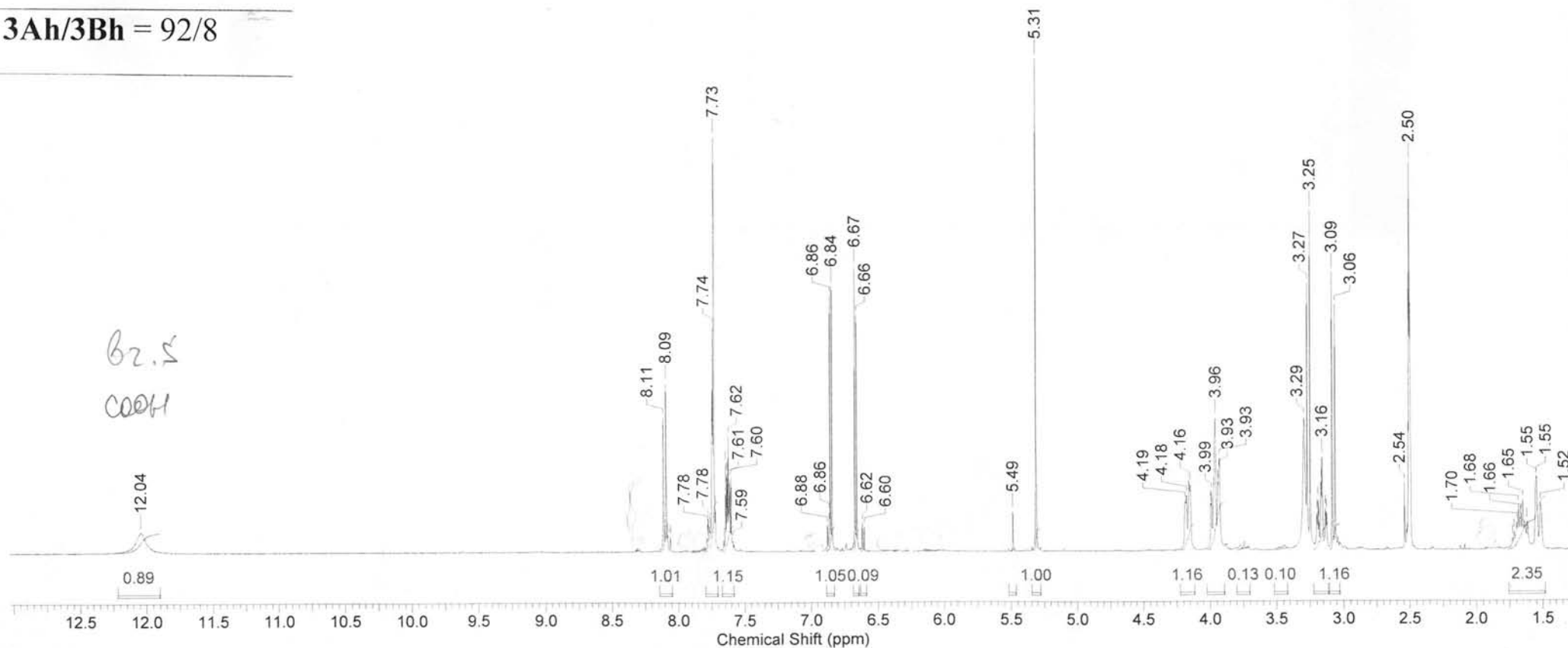


Formula C ₃₆ H ₃₂ N ₄ O ₁₄ ?	FW 744.6577+? (372.3288+372.3288+?+?)		
Acquisition Time (sec) 1.5729	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 08 Jun 2010 05:58:24	
Date Stamp 08 Jun 2010 05:58:24	File Name D:\NMR\IC_13\07.06.10 (Poma)\rudn_1_N6\rudn_1_N6_001000fid		
Frequency (MHz) 400.14	Nucleus 1H	Number of Transients 32	Origin spect
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zg
Receiver Gain 512.00	SW(cyclical) (Hz) 10416.67	Solvent DMSO-d6	Spectrum Offset (Hz) 2712.0542
Sweep Width (Hz) 10416.03	Temperature (degree C) 27.000		

Compounds 3Ah/3Bh



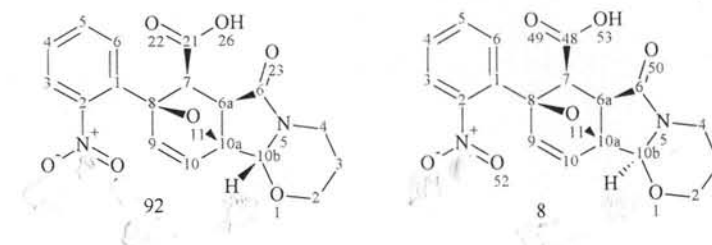
3Ah/3Bh = 92/8



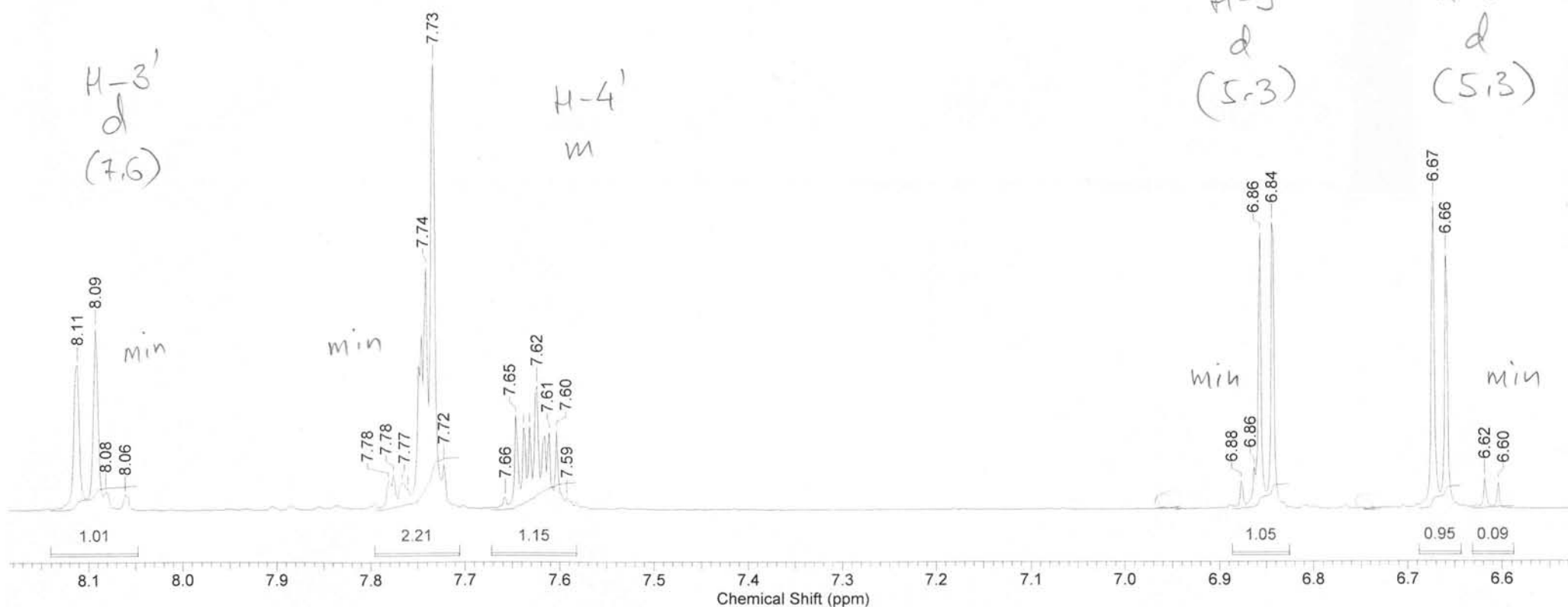
Formula C ₃₆ H ₃₂ N ₄ O ₁₄ ?	FW 744.6577+? (372.3288+372.3288+?+?)		
Acquisition Time (sec) 1.5729	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 08 Jun 2010 05:58:24	
Date Stamp 08 Jun 2010 05:58:24	File Name D:\NMR\IC_13\07.06.10 (Рома)\rudn_1_N6\rudn_1_N6_001000fid	Number of Transients 32	Origin spect
Frequency (MHz) 400.14	Nucleus 1H	Points Count 16384	Pulse Sequence zg
Original Points Count 16384	Owner root	Solvent DMSO-d6	Spectrum Offset (Hz) 2712.0542
Receiver Gain 512.00	SW(cyclical) (Hz) 10416.67		
Sweep Width (Hz) 10416.03	Temperature (degree C) 27.000		

H-5', H-6'
m, 2H

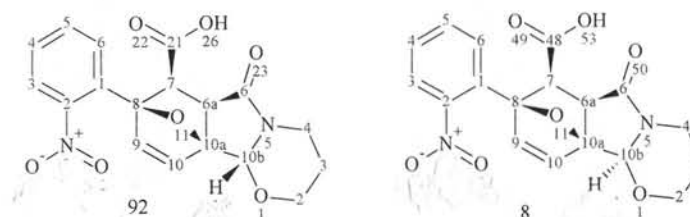
Compounds 3Ah/3Bh



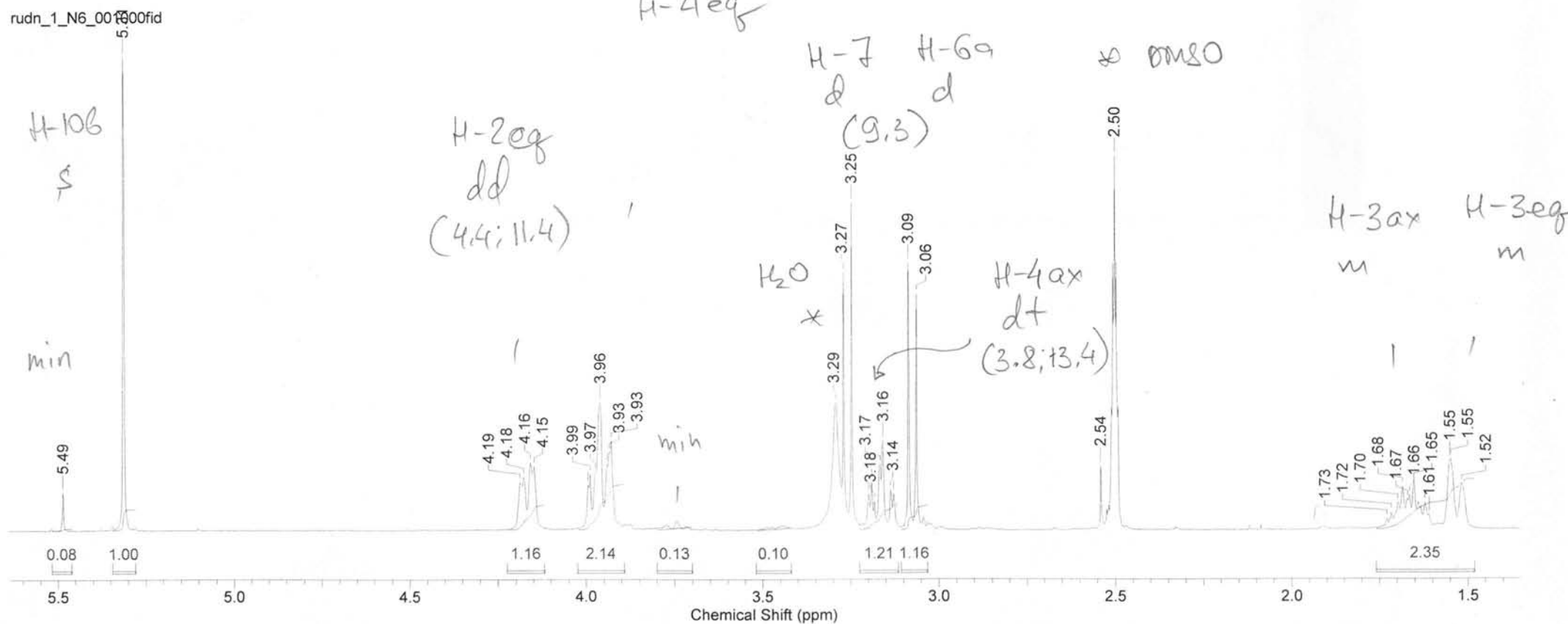
rudn_1_N6_001000fid



Formula	C ₃₆ H ₃₂ N ₄ O ₁₄ ?	FW	744.6577+? (372.3288+372.3288+?+?)
Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400
Date Stamp	08 Jun 2010 05:58:24	File Name	D:\NMR\13\07.06.10 (Poma)\rudn_1_N6\rudn_1_N6_001000fid
Frequency (MHz)	400.14	Nucleus	1H
Original Points Count	16384	Owner	root
Receiver Gain	512.00	SW(cyclical) (Hz)	10416.67
Sweep Width (Hz)	10416.03	Temperature (degree C)	27.000
		Number of Transients	32
		Points Count	16384
		Solvent	DMSO-d6
		Pulse Sequence	zg
		Spectrum Offset (Hz)	2712.0542

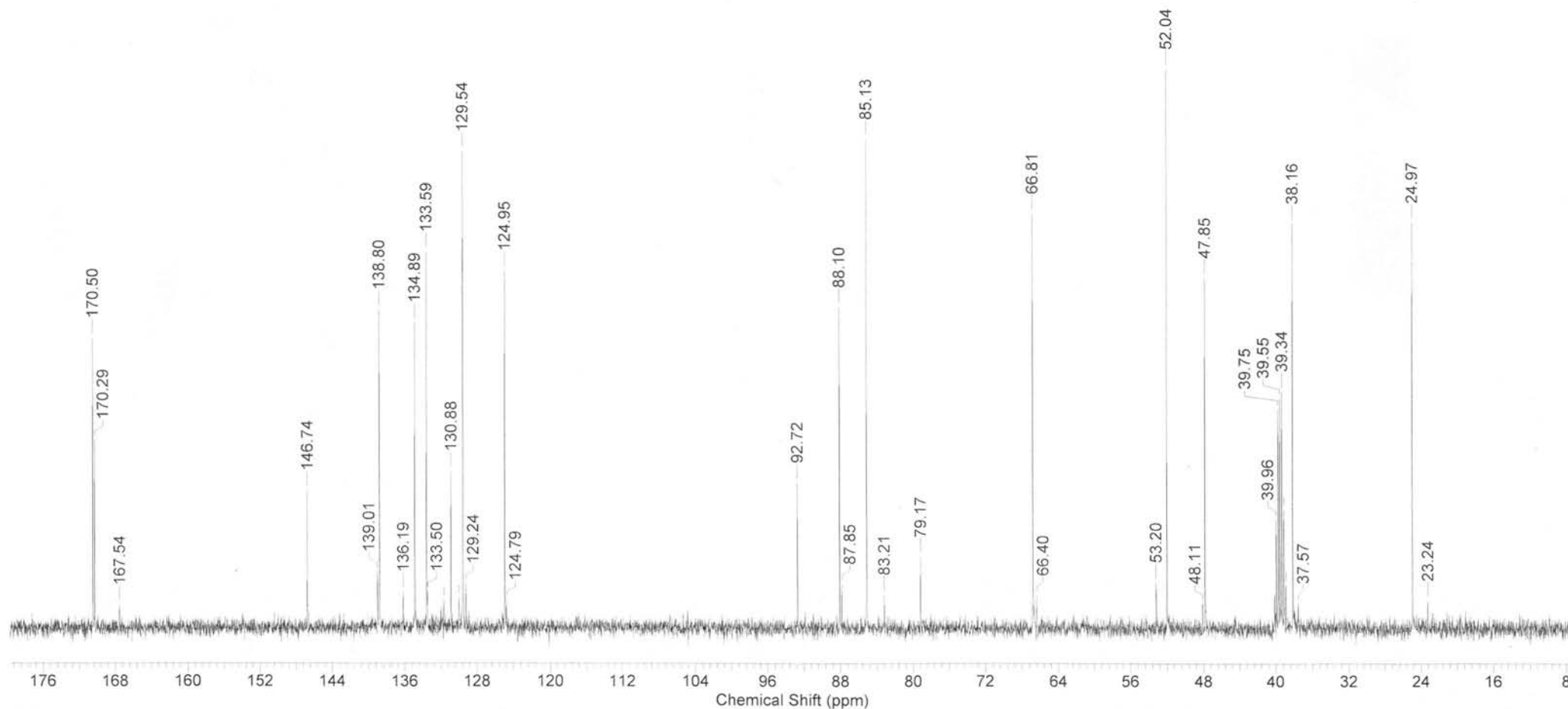
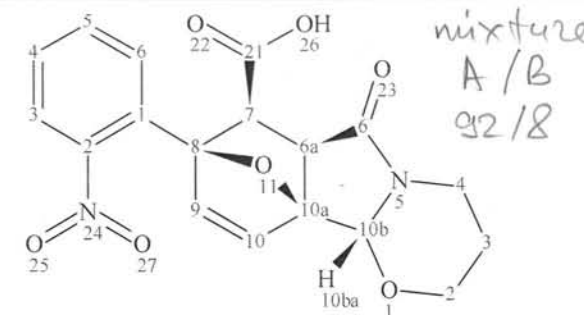


Compounds 3Ah/3Bh



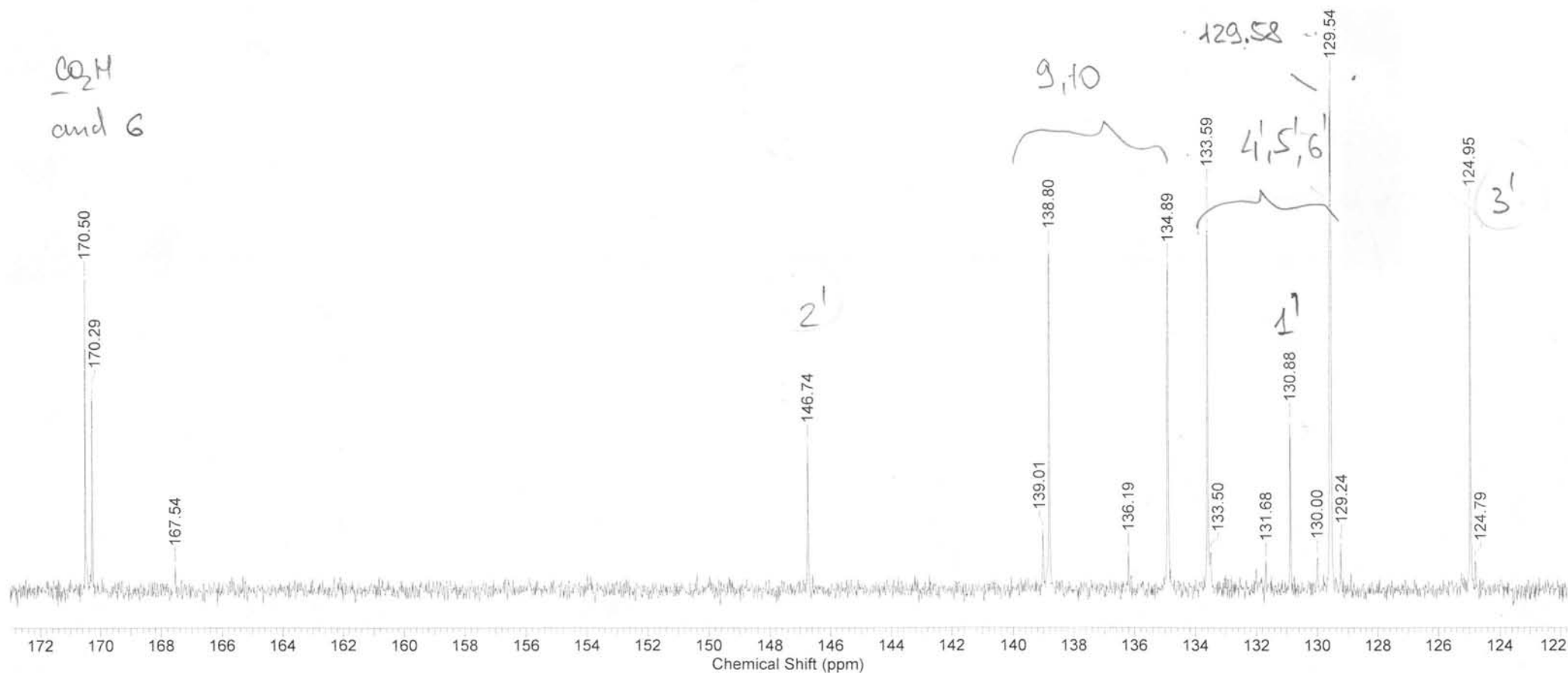
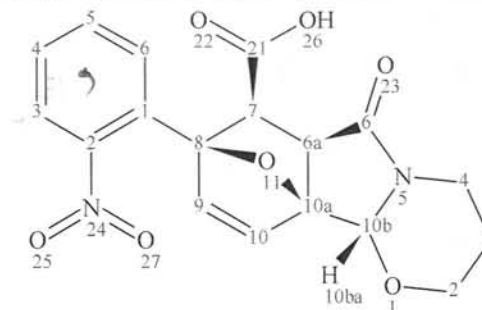
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File Name	C:\Users\Fedor\Desktop\07.06.10 (Poma)\rudn_1_N6c13dec\rudn_1_N6c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	306	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compounds 3Ah/3Bh



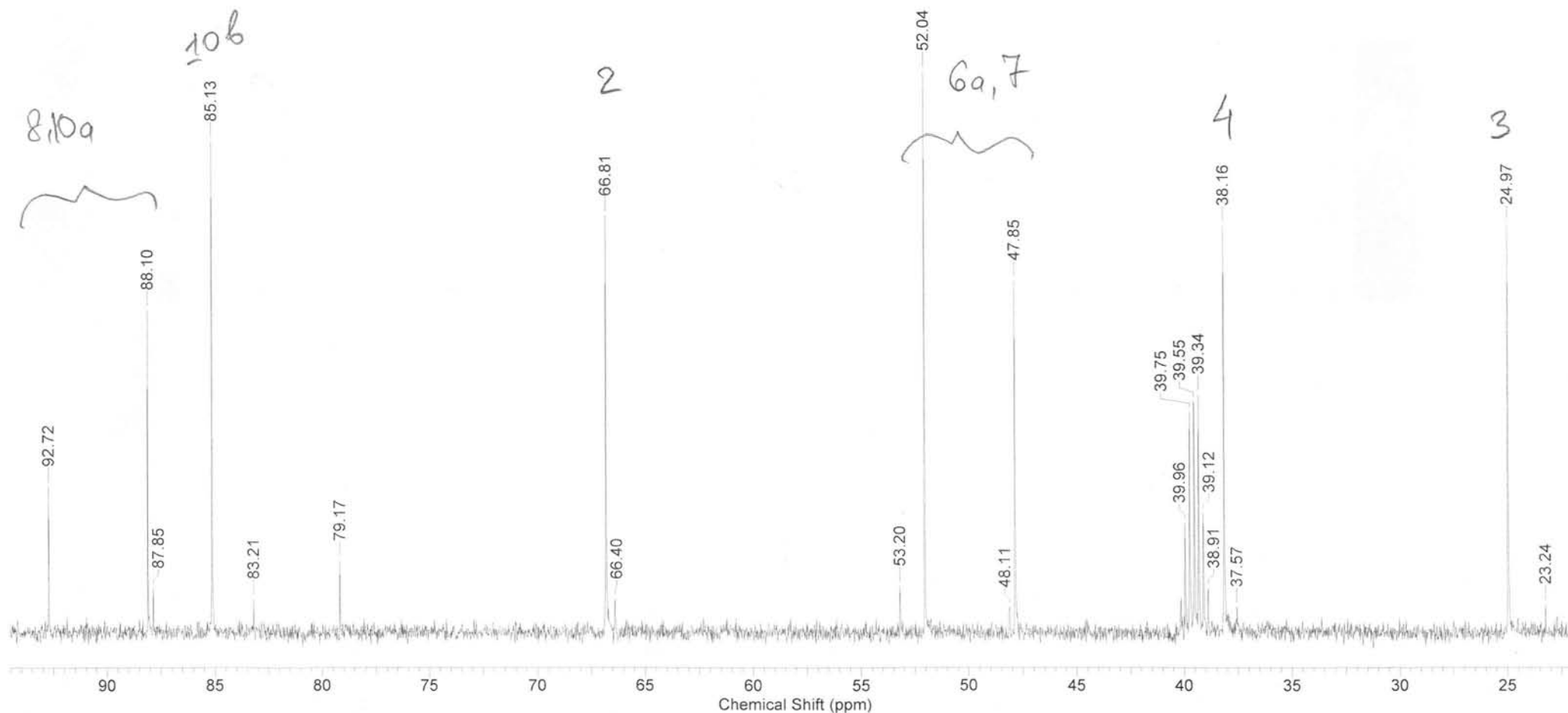
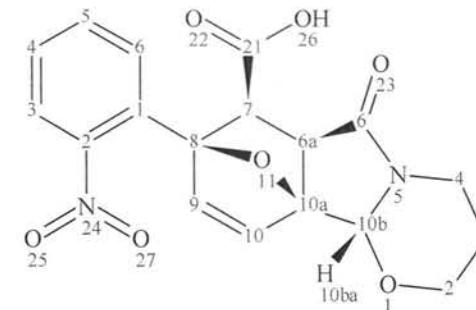
Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	08 Jun 2010 08:57:36	
File Name	C:\Users\Fedor\Desktop\07.06.10 (Poma)\rudn_1_N6c13dec\rudn_1_N6c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	306	Original Points Count	16384	Points Count	16384
Pulse Sequence	zpgg	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compounds 3Ah/3Bh



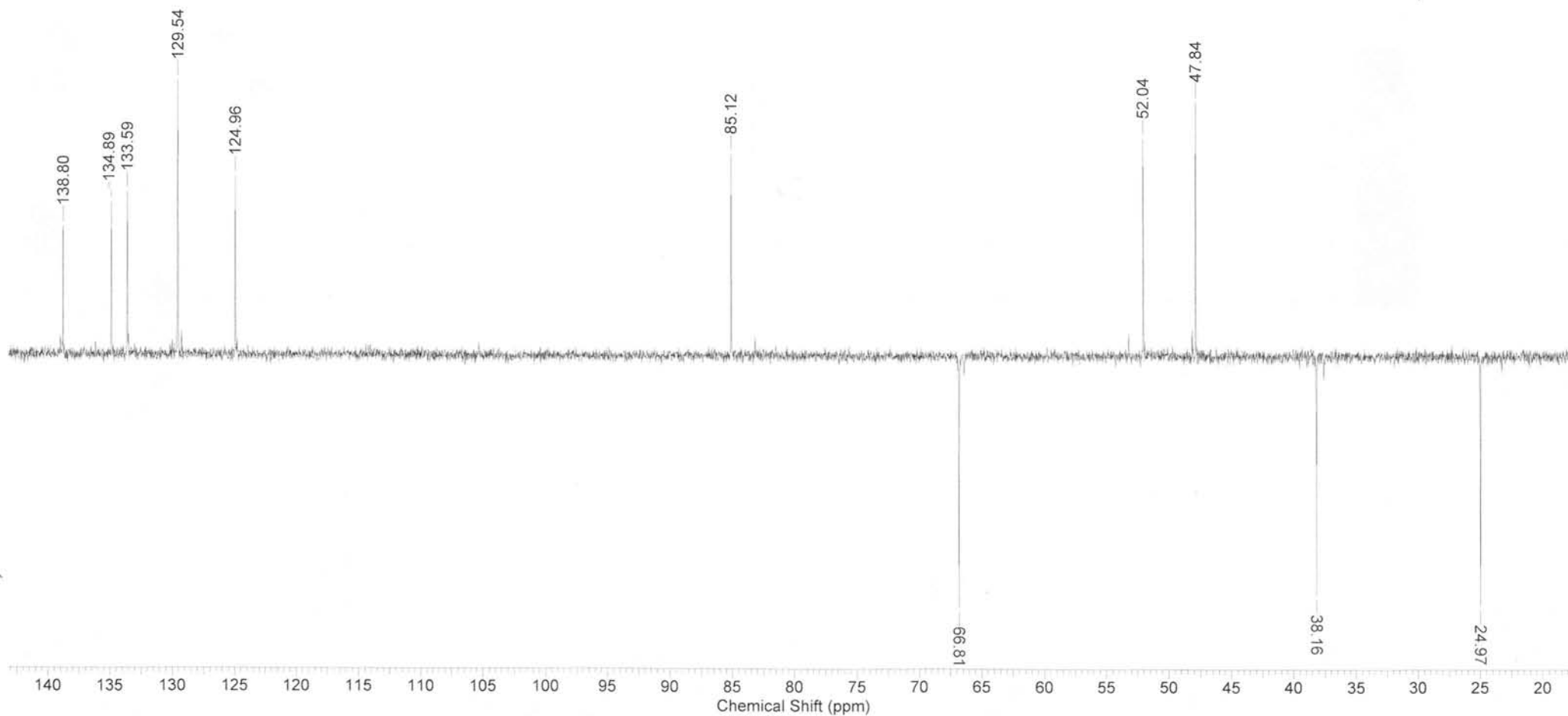
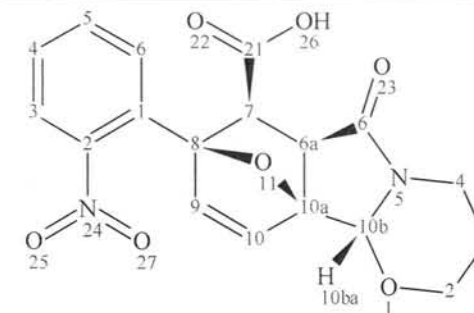
Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	08 Jun 2010 08:57:36	
File Name	C:\Users\Fedor\Desktop\07.06.10 (Poma)\rudn_1_N6c13dec\rudn_1_N6c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	306	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compounds 3Ah/3Bh



Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	08 Jun 2010 09:04:00	
File Name	C:\Users\Fedor\Desktop\07.06.10 (Роман)\rudn_1_N6dept135\rudn_1_N6dept135_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	148	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

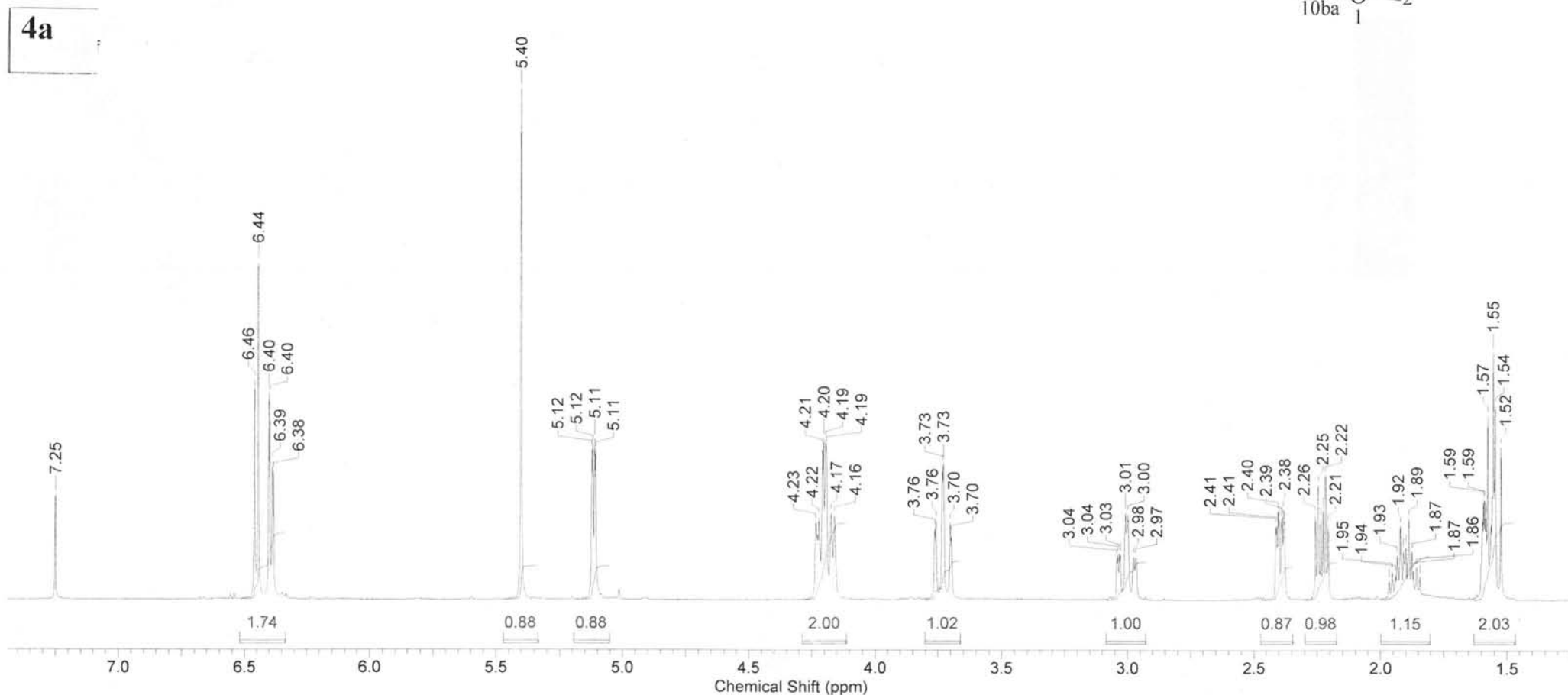
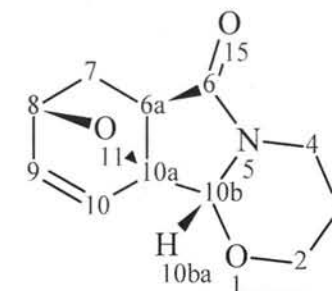
Compounds 3Ah/3Bh



Formula $C_{11}H_{13}NO_3$ FW 207.2258

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	26 Apr 2011 09:38:00	Date Stamp	26 Apr 2011 13:26:06
File Name	D:\NMR\19.04.11\FZ1784-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	18
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	30.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2398.6931	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	21.400					Sweep Width (Hz)	7503.00

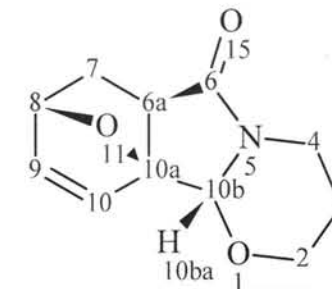
Compound 4a



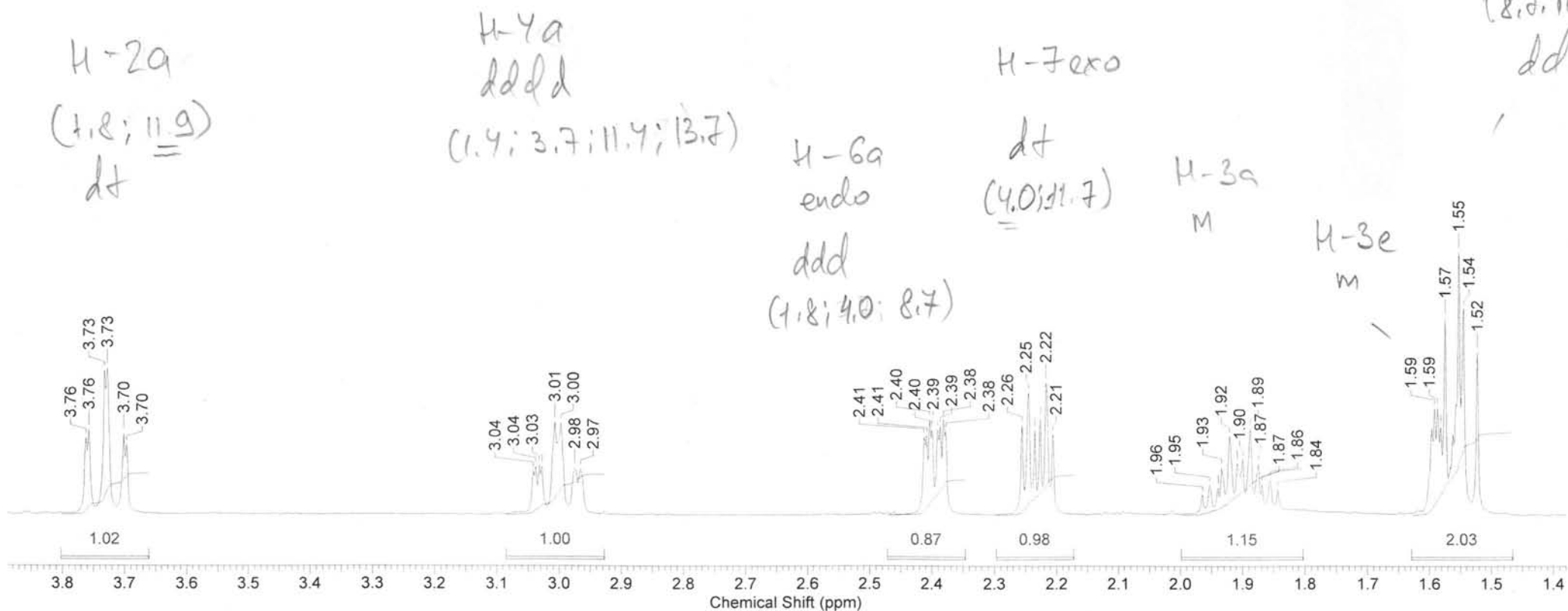
Formula C₁₁H₁₃NO₃ FW 207.2258

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	26 Apr 2011 09:38:00	Date Stamp	26 Apr 2011 13:26:06
File Name	D:\NMR\19.04.11\FZ1784-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	18
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	30.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2398.6931	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	21.400			Sweep Width (Hz)	7503.00		

Compound 4a

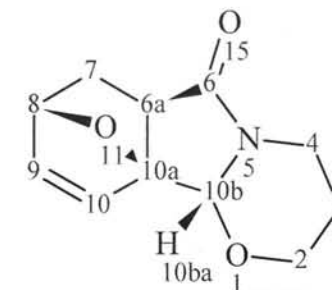


FZ1784-1.jdf

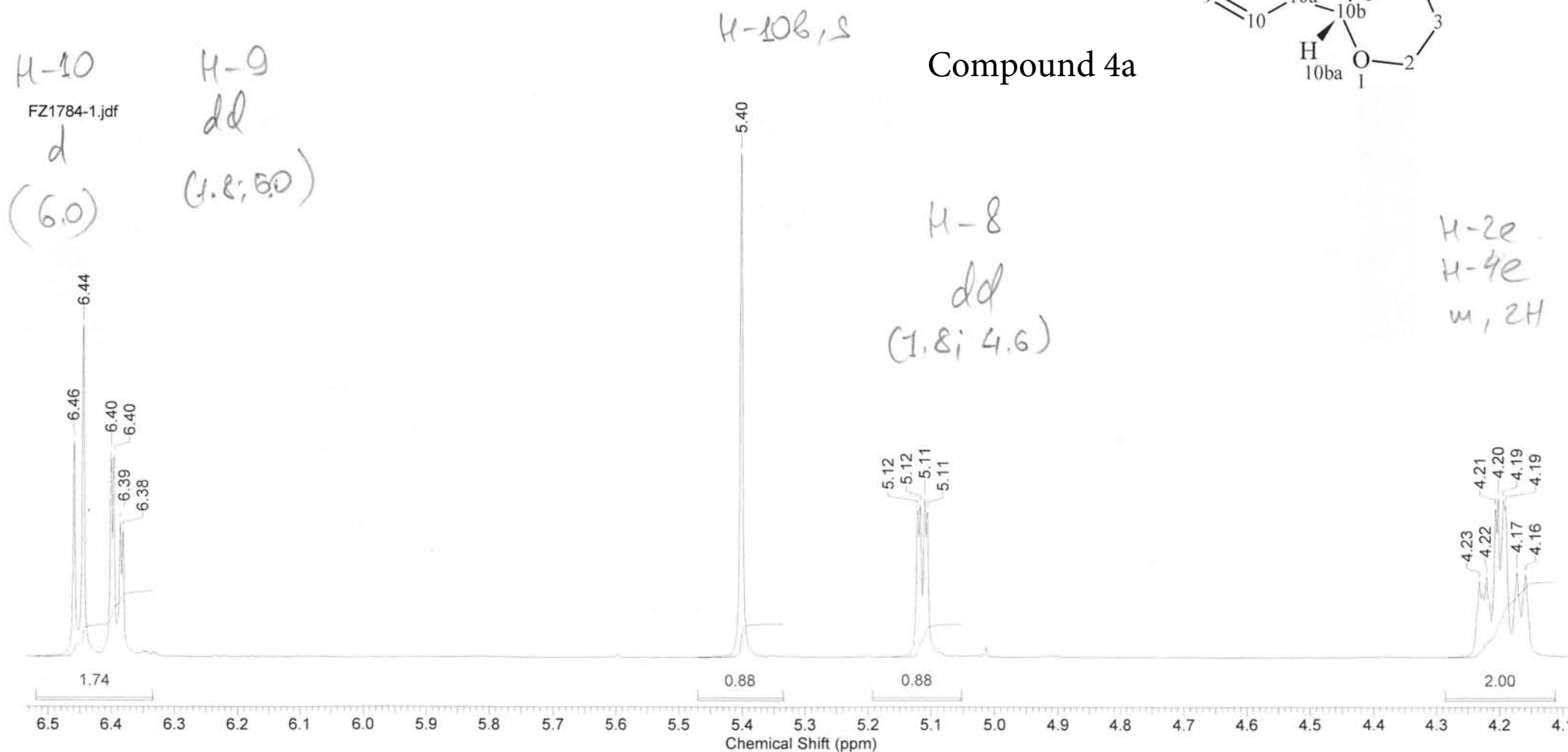


Formula C₁₁H₁₃NO₃ FW 207.2258

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	26 Apr 2011 09:38:00	Date Stamp	26 Apr 2011 13:26:06
File Name	D:\NMR\19.04.11\FZ1784-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	18
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	30.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2398.6931	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	21.400					Sweep Width (Hz)	7503.00

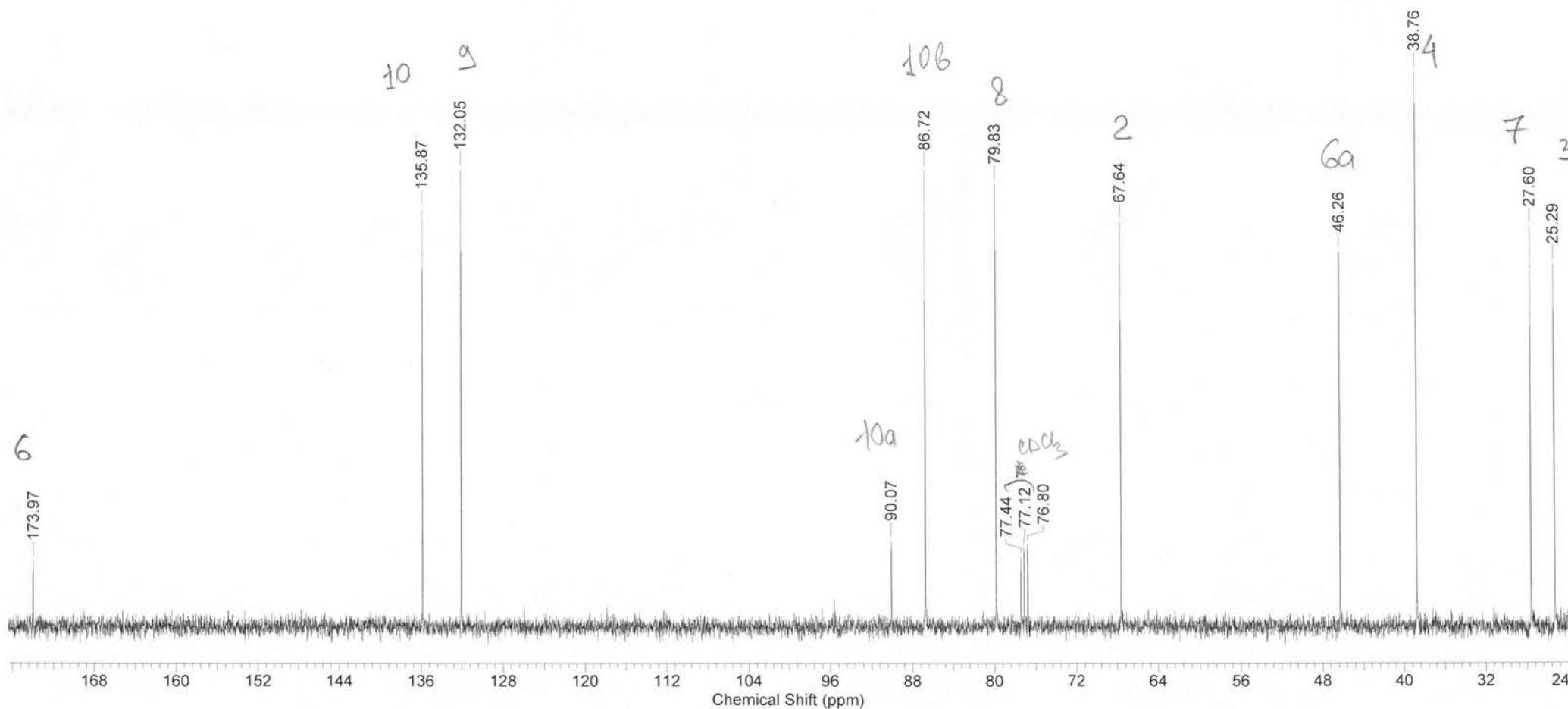
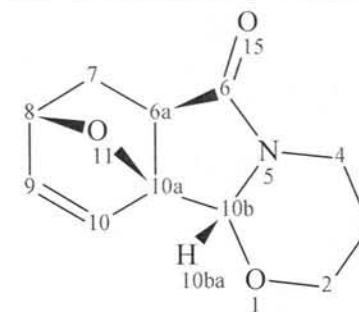


Compound 4a

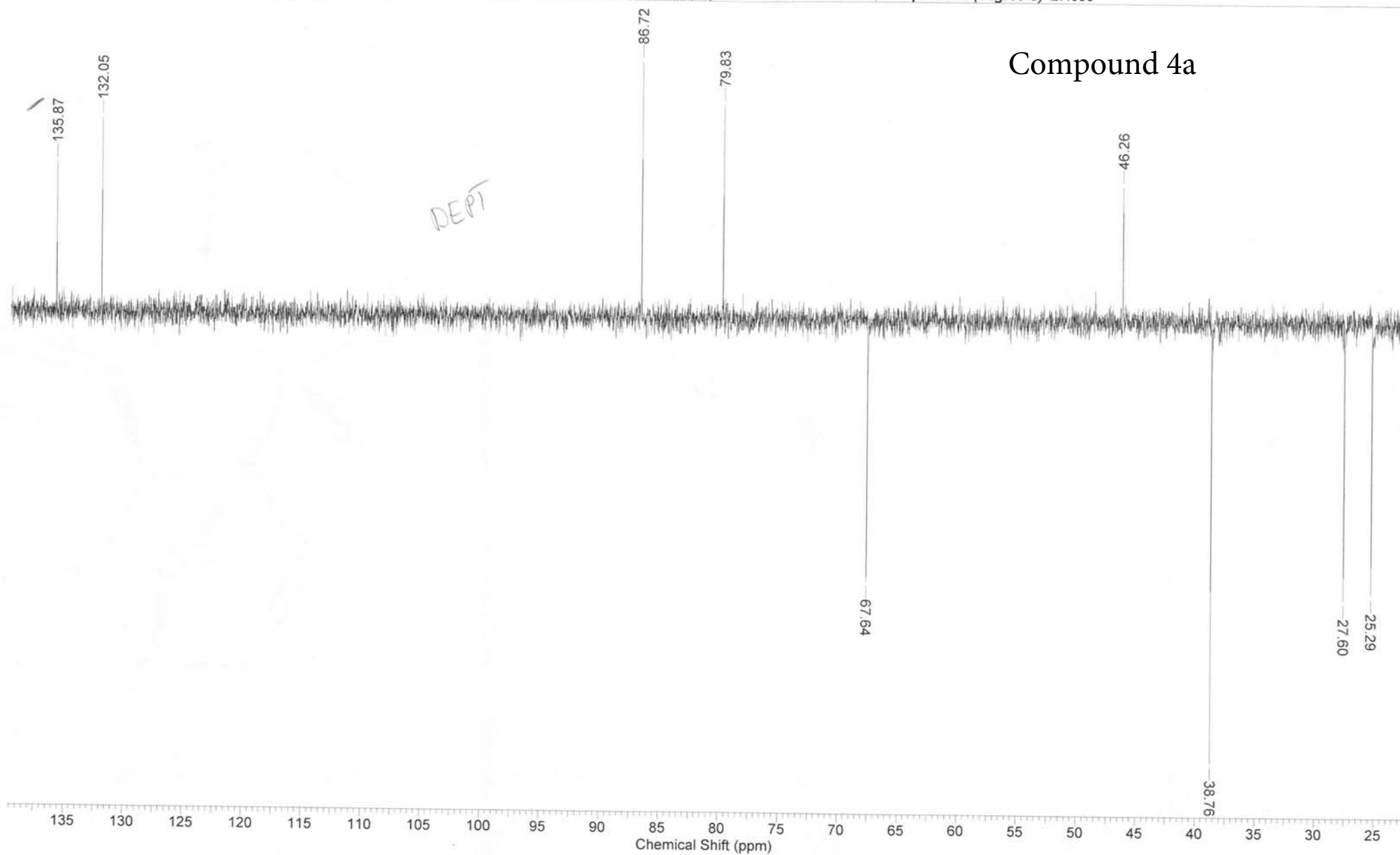


Acquisition Time (sec)	0.6226	Comment	Imported from UXNMR.		Date	30 Apr 2009 14:43:12	
File Name	D:\NMR\IC_13\30.04.09\5lazc13dec\5lazc13dec_001000fid	Frequency (MHz)	100.62	Nucleus	13C		
Number of Transients	89	Original Points Count	16384	Points Count	16384	Pulse Sequence	zgpg
Solvent	CHLOROFORM-D	Sweep Width (Hz)	26315.79	Temperature (degree C)	27.000		

Compound 4a

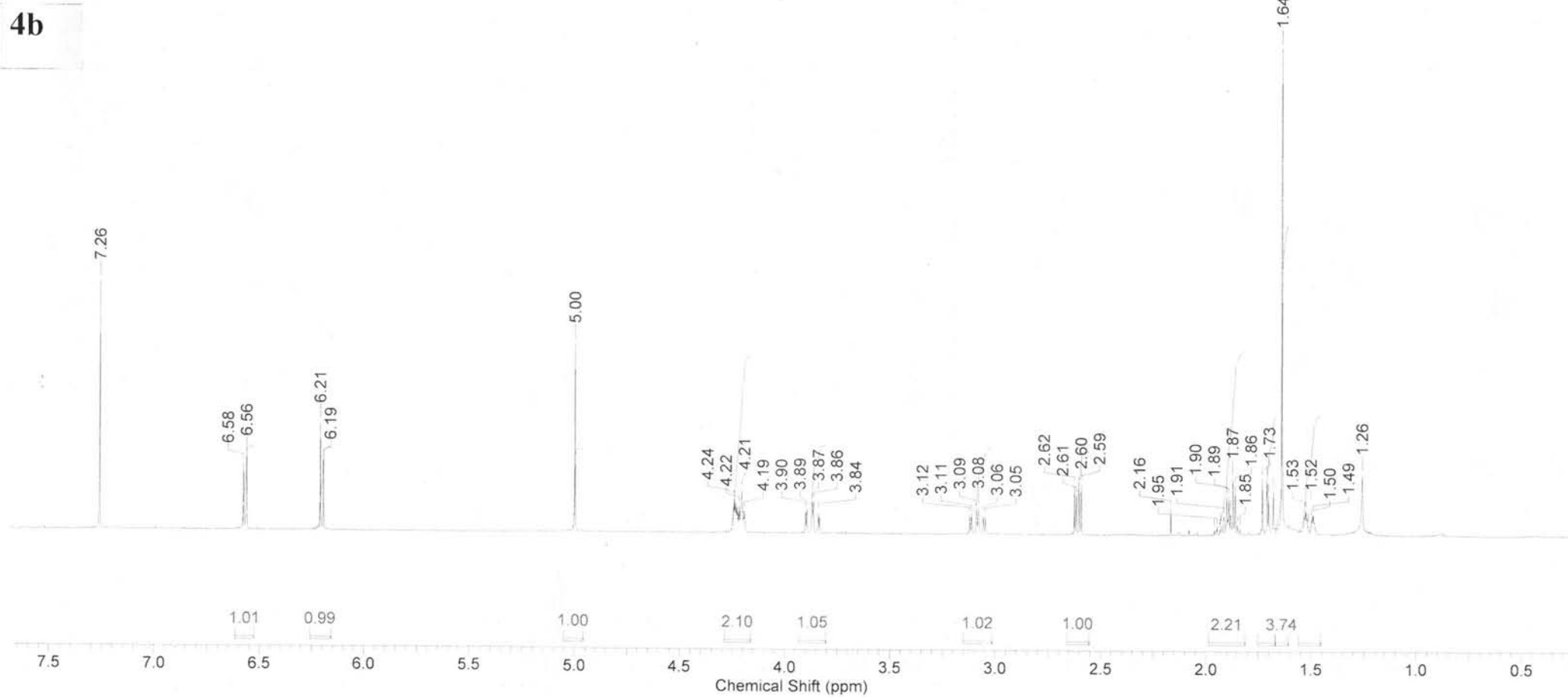
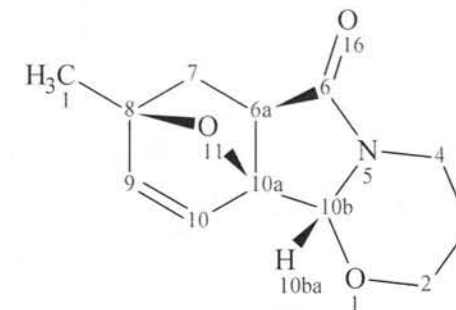


Acquisition Time (sec)	0.6226	Comment	Imported from UXNMR.		Date	30 Apr 2009 14:45:20	
File Name	D:\NMR\C_13\30.04.09\5lazdept135\5lazdept135_001000fid	Frequency (MHz)	100.62	Nucleus	13C		
Number of Transients	56	Original Points Count	16384	Points Count	16384	Pulse Sequence	dept135
Solvent	CHLOROFORM-D	Sweep Width (Hz)	26315.79	Temperature (degree C)	27.000		



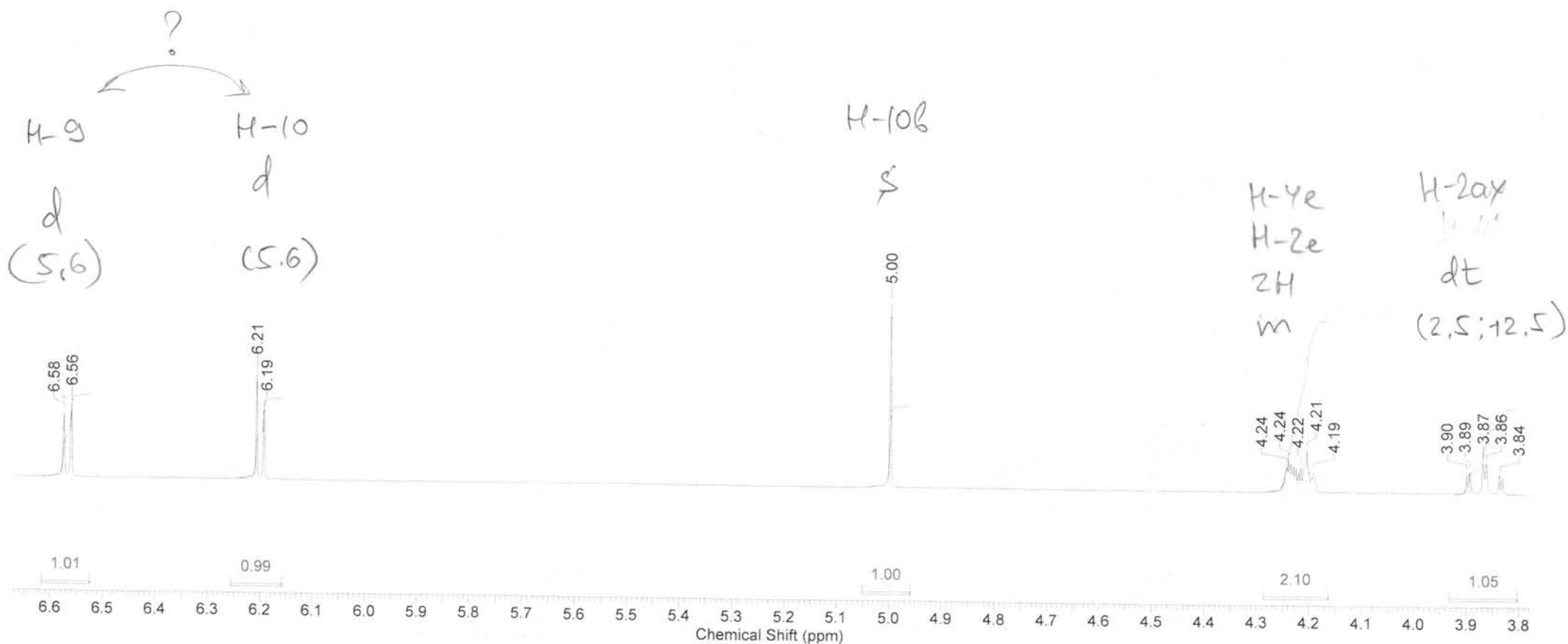
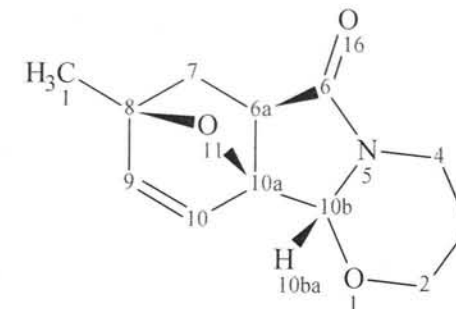
Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.		Date	30 Mar 2010 14:24:00		
File Name	D:\NMR\23 and 25.03.10\N846\N846_001000fid		Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	32
Original Points Count	16384	Points Count	16384	Pulse Sequence	zg	Solvent	CHLOROFORM-D	
Sweep Width (Hz)	10204.08	Temperature (degree C)	27.000					

Compound 4b



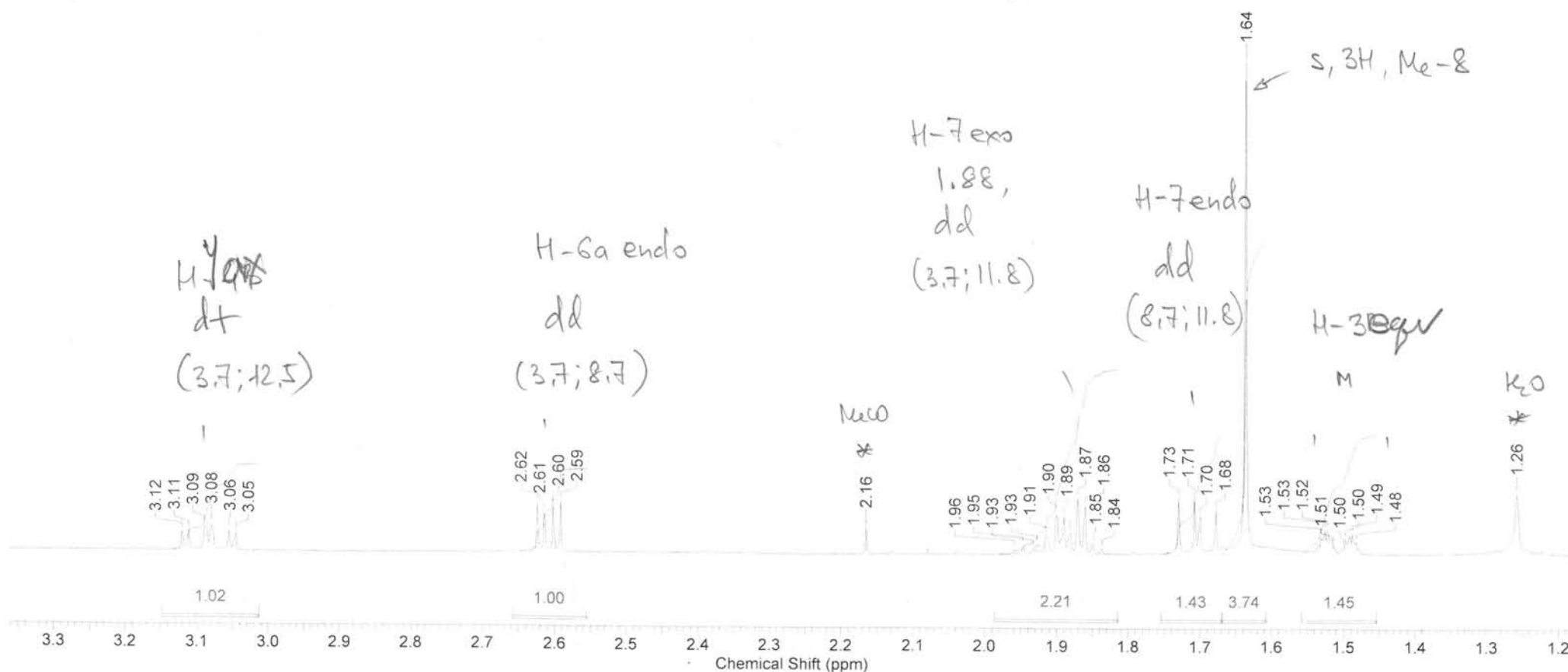
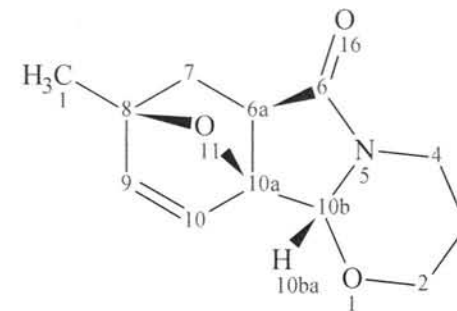
Acquisition Time (sec)	1.6056	Comment	Imported from UXNMR.		Date	30 Mar 2010 14:24:00	
File Name	D:\NMR\23 and 25.03.10\N846\N846_001000fid	Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	32
Original Points Count	16384	Points Count	16384	Pulse Sequence	zg	Solvent	CHLOROFORM-D
Sweep Width (Hz)	10204.08	Temperature (degree C)	27.000				

Compound 4b



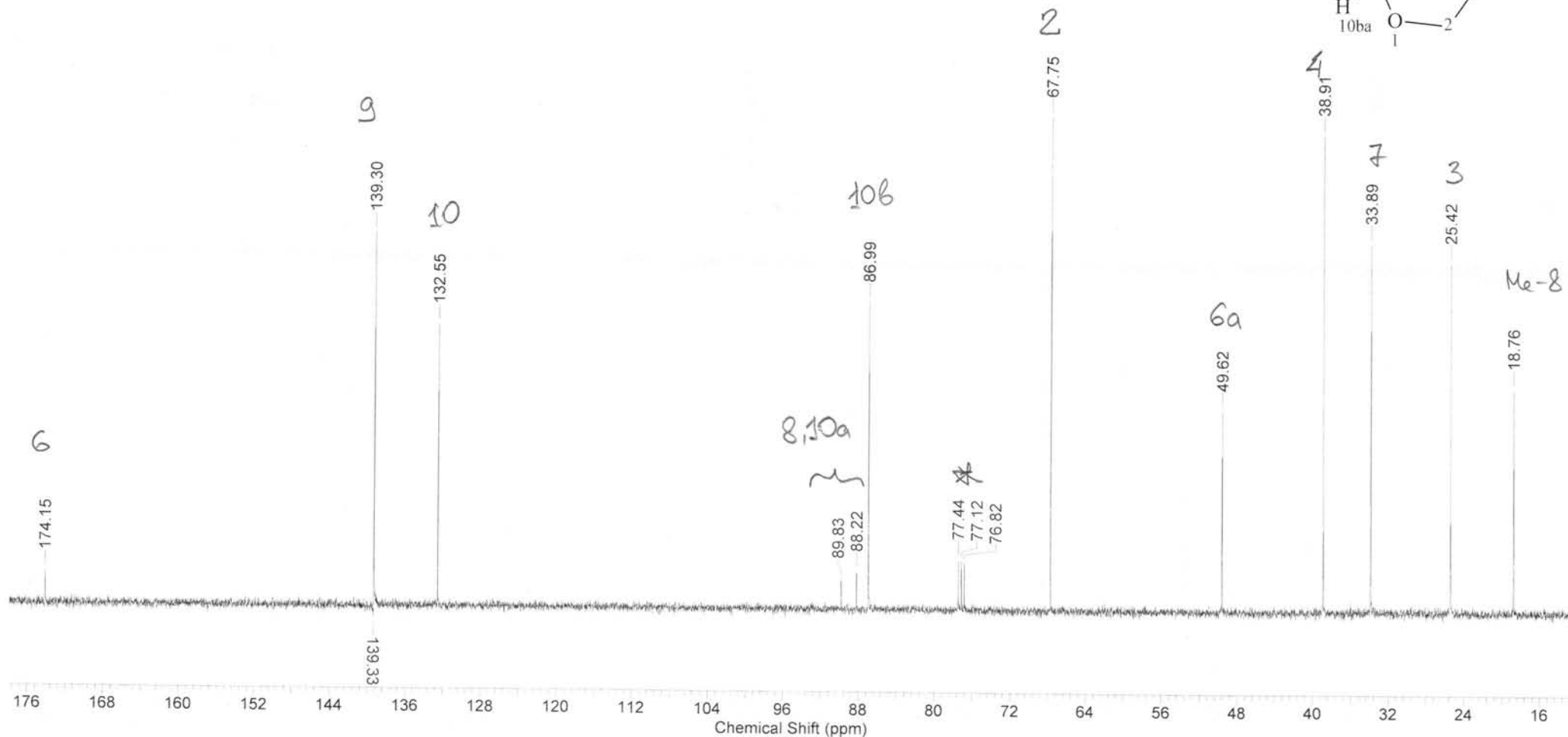
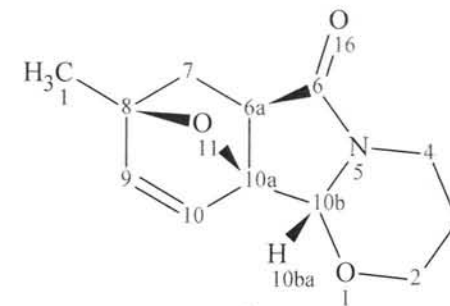
Acquisition Time (sec)	1.6056	Comment	Imported from UXNMR.		Date	30 Mar 2010 14:24:00	
File Name	D:\NMR\23 and 25.03.10\N846\N846_001000fid	Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	32
Original Points Count	16384	Points Count	16384	Pulse Sequence	zg	Solvent	CHLOROFORM-D
Sweep Width (Hz)	10204.08	Temperature (degree C)	27.000				

Compound 4b



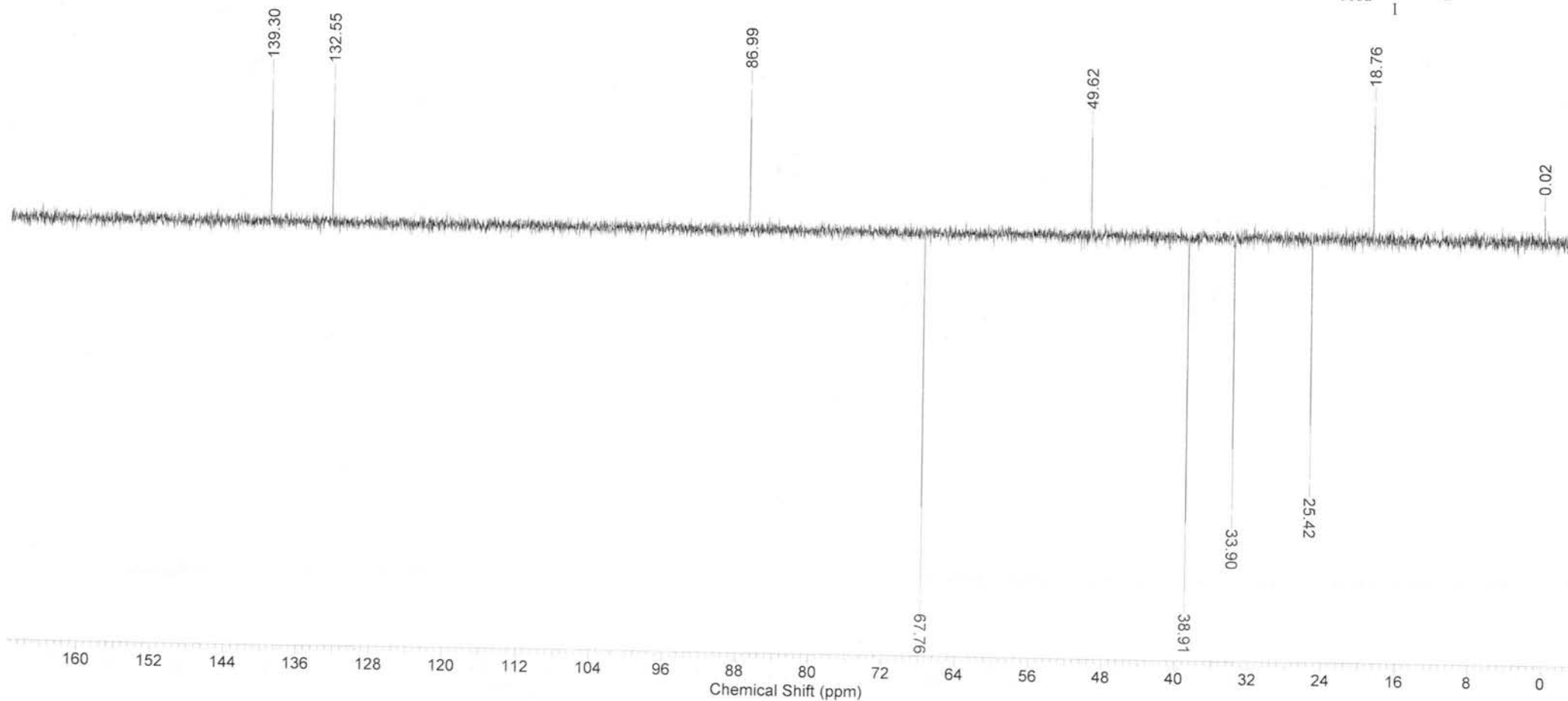
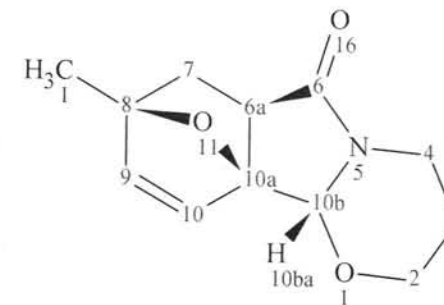
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File Name	D:\NMR\23 and 25.03.10\N846c13dec\N846c13dec_001000fid			Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	305	Original Points Count	16384	
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D		Points Count	16384
Temperature (degree C)	27.000				Sweep Width (Hz)	26315.79

Compound 4b



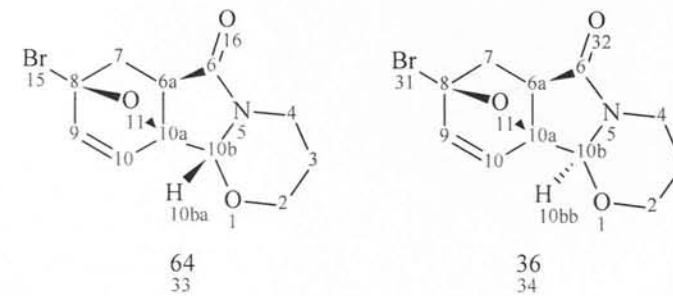
Acquisition Time (sec)	0.6226	Comment	Imported from UXMNR.	Date	30 Mar 2010 14:32:32
File Name	D:\NMR\23 and 25.03.10\N846dept135\N846dept135_001000fid	Number of Transients	185	Frequency (MHz)	100.62
Nucleus	13C	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	CHLOROFORM-D	Sweep Width (Hz)	26315.79
Temperature (degree C)	27.000				

Compound 4b

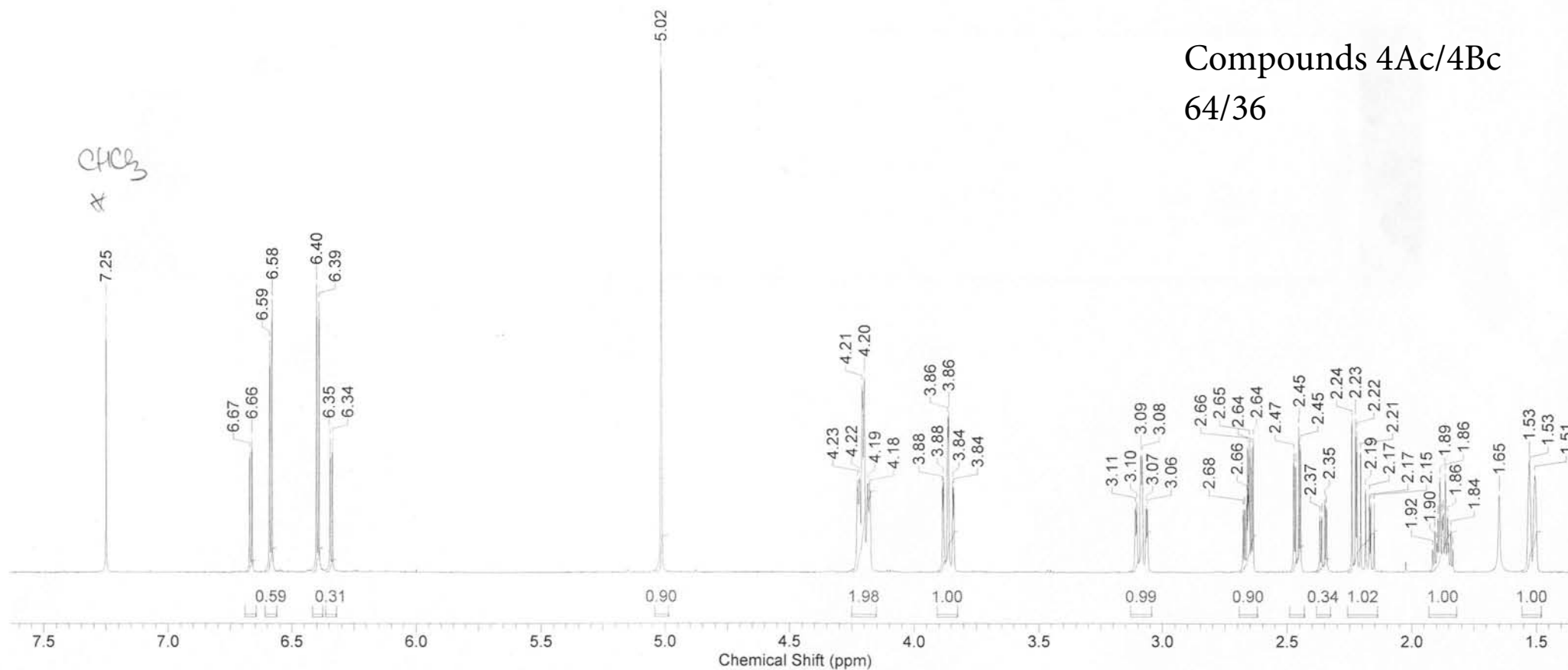


Formula $C_{22}H_{24}Br_2N_2O_6$? FW 572.2438+? (286.1219+286.1219+?+?)

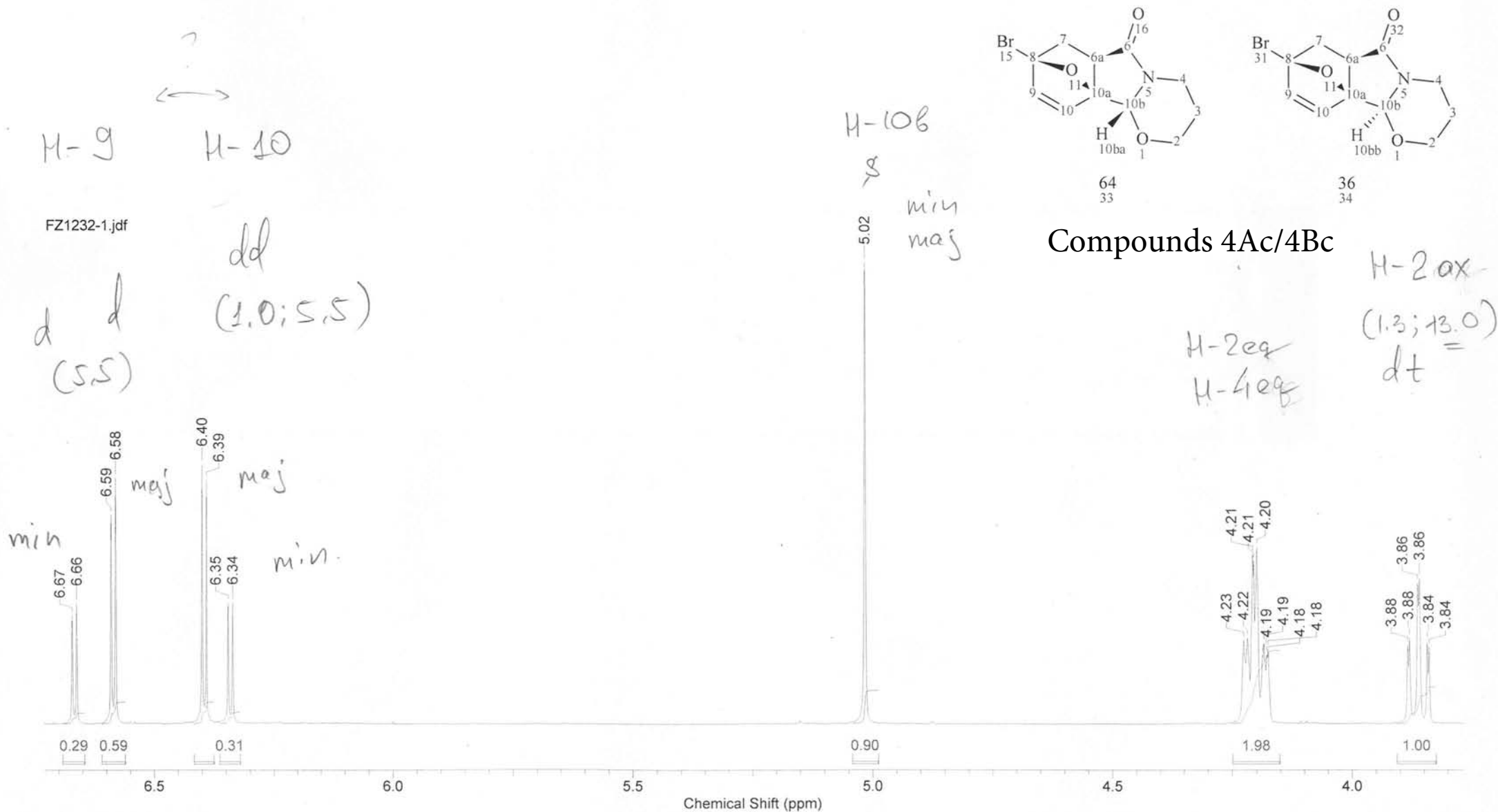
Acquisition Time (sec)	1.8193	Comment	single_pulse	Date	24 May 2010 11:59:32	Date Stamp	24 May 2010 11:58:13
File Name	D:\NMR\11.05.10\FZ1232-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	2
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3601.0339	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	25.000			Sweep Width (Hz)	9005.76		



Compounds 4Ac/4Bc
64/36

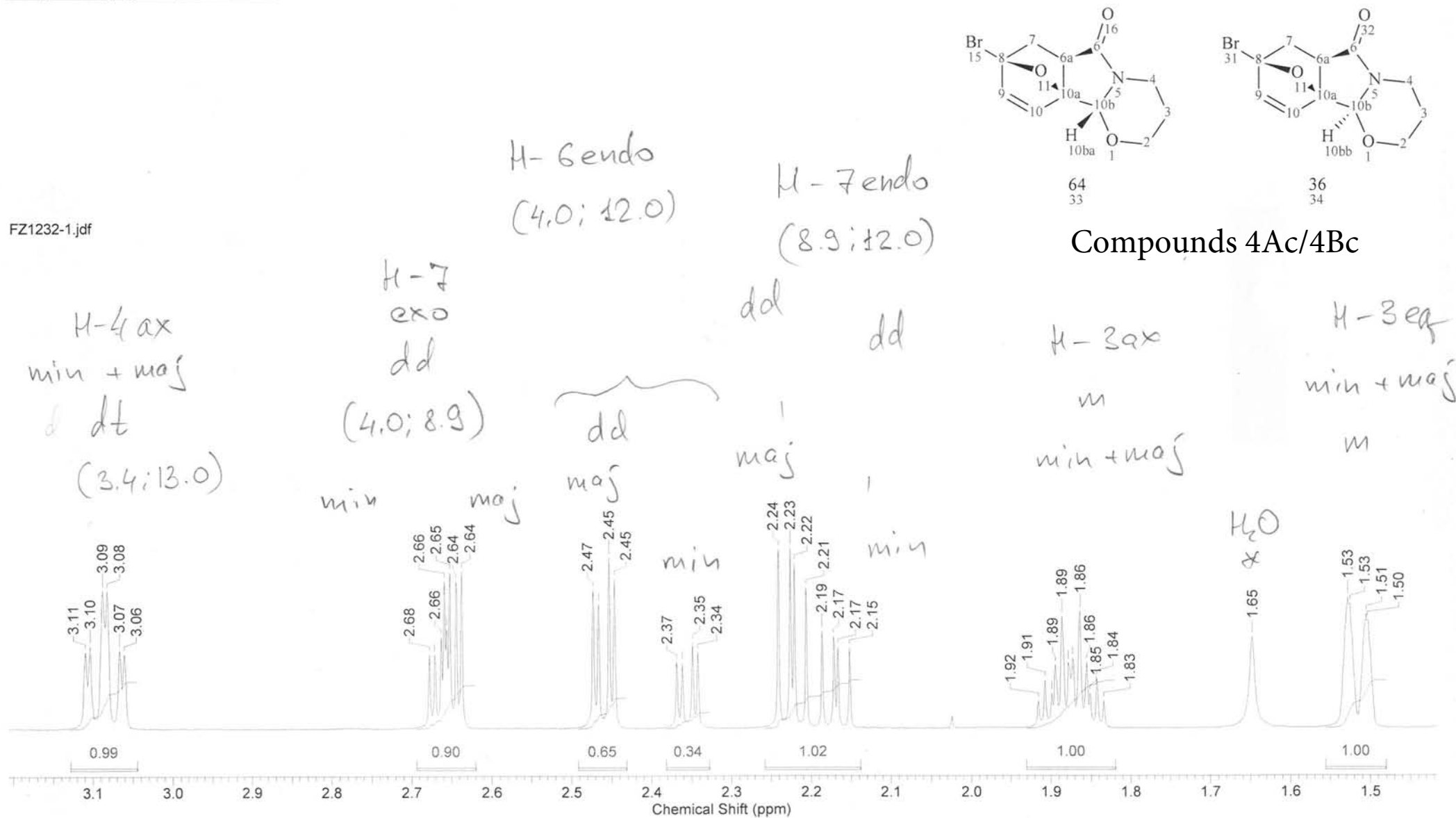


Formula C ₂₂ H ₂₄ Br ₂ N ₂ O ₆ ?		FW 572.2438+? (286.1219+286.1219+?+?)					
Acquisition Time (sec)	1.8193	Comment	single_pulse	Date	24 May 2010 11:59:32	Date Stamp	24 May 2010 11:58:13
File Name	D:\NMR\11.05.10\FZ1232-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	2
Origin	ECA 600	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3601.0339	Sweep Width (Hz)	9005.76
Temperature (degree C)	25.000						



Formula C ₂₂ H ₂₄ Br ₂ N ₂ O ₆ ?		FW 572.2438+? (286.1219+286.1219+?+?)					
Acquisition Time (sec)	1.8193	Comment	single_pulse	Date	24 May 2010 11:59:32	Date Stamp	24 May 2010 11:58:13
File Name	D:\NMR\11.05.10\FZ1232-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	2
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3601.0339	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	25.000					Sweep Width (Hz)	9005.76

FZ1232-1.jdf

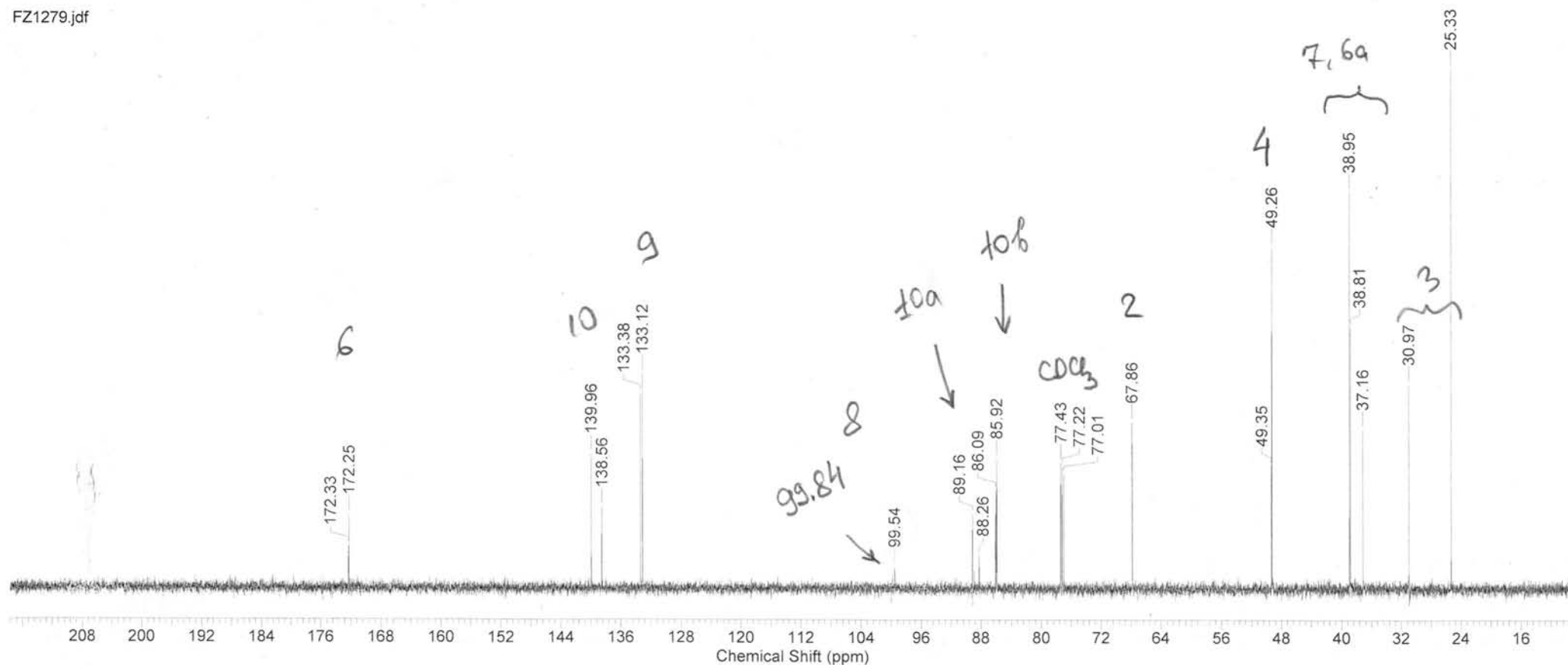
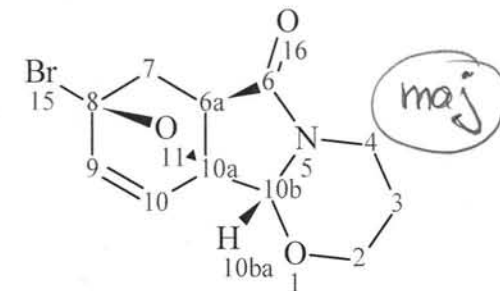


Formula	C ₁₁ H ₁₂ BrNO ₃	FW	286.1219						
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	23 Jun 2010 10:49:17				
Date Stamp	23 Jun 2010 10:47:50	File Name	D:\NMR\16.06.10\FZ1279.jdf	Frequency (MHz)	150.91				
Nucleus	13C	Number of Transients	200	Origin	ECA 600	Original Points Count	32768	Owner	delta
Points Count	32768	Pulse Sequence	single_pulse_dec	Receiver Gain	50.00				
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49	Temperature (degree C)	22.600		

N850/II

FZ1279.jdf

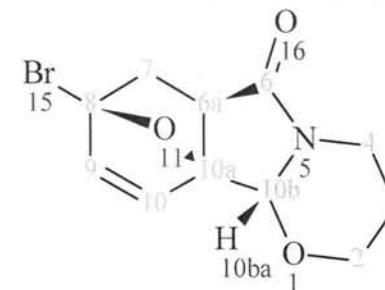
Compounds 4Ac/4Bc



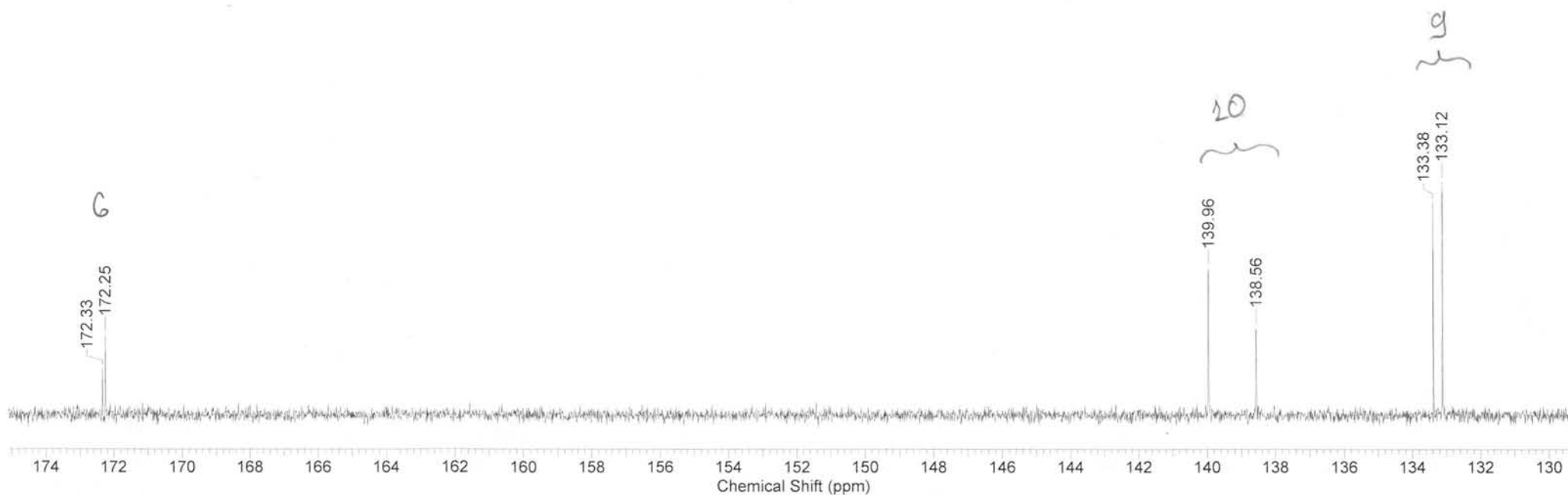
Formula C₁₁H₁₂BrNO₃ FW 286.1219

Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	23 Jun 2010 10:49:17
Date Stamp	23 Jun 2010 10:47:50	File Name	D:\NMR\16.06.10\FZ1279.jdf	Frequency (MHz)	150.91
Nucleus	13C	Number of Transients	200	Origin	ECA 600
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	15091.3428	Receiver Gain	50.00
		Sweep Width (Hz)	47348.49	Temperature (degree C)	22.600

Compounds 4Ac/4Bc



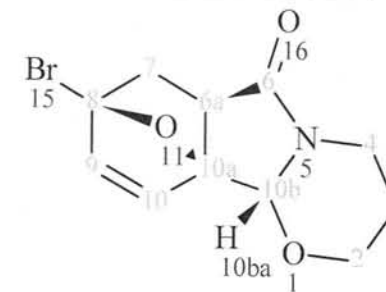
FZ1279.jdf



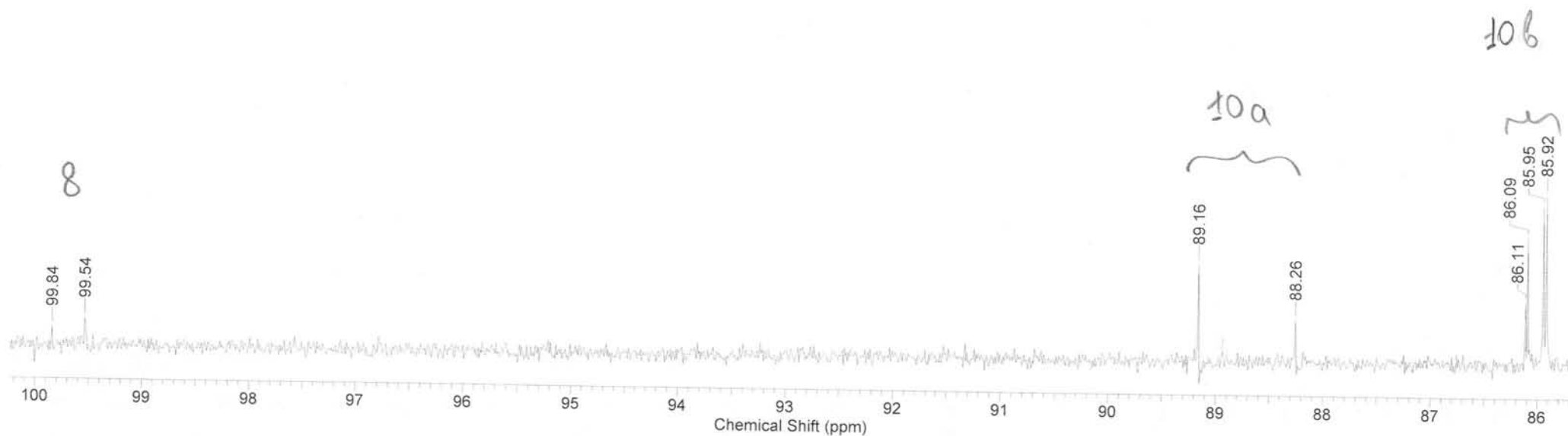
Formula	C ₁₁ H ₁₂ BrNO ₃	FW	286.1219
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Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	23 Jun 2010 10:49:17
Date Stamp	23 Jun 2010 10:47:50	File Name	D:\NMR\16.06.10\FZ1279.jdf	Frequency (MHz)	150.91
Nucleus	13C	Number of Transients	200	Origin	ECA 600
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Solvent	CHLOROFORM-d	Receiver Gain	50.00	Owner	delta
		Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49
				Temperature (degree C)	22.600

Compounds 4Ac/4Bc

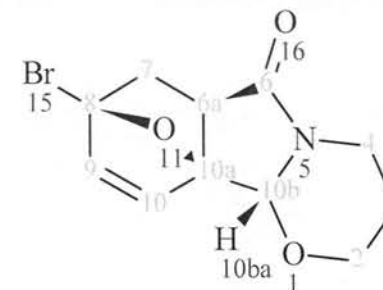


FZ1279.jdf

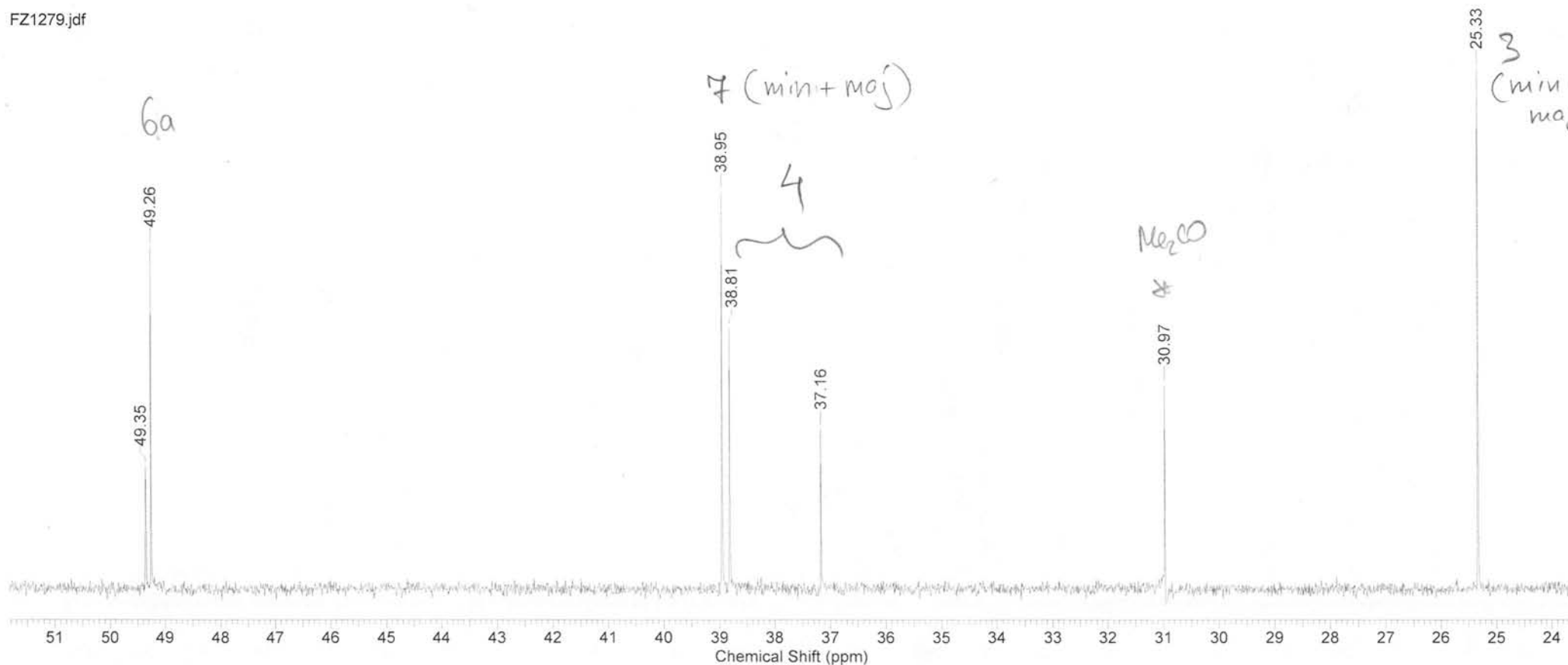


Formula	C ₁₁ H ₁₂ BrNO ₃	FW	286.1219						
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	23 Jun 2010 10:49:17				
Date Stamp	23 Jun 2010 10:47:50	File Name	D:\NMR\16.06.10\FZ1279.jdf	Frequency (MHz)	150.91				
Nucleus	13C	Number of Transients	200	Origin	ECA 600	Original Points Count	32768	Owner	delta
Points Count	32768	Pulse Sequence	single_pulse_dec	Receiver Gain	50.00				
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49	Temperature (degree C)	22.600		

Compounds 4Ac/4Bc

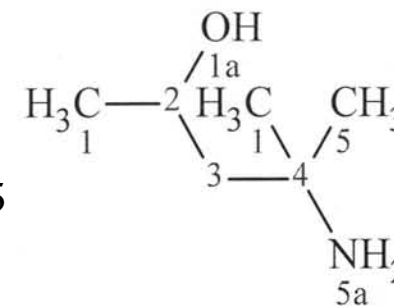


FZ1279.jdf

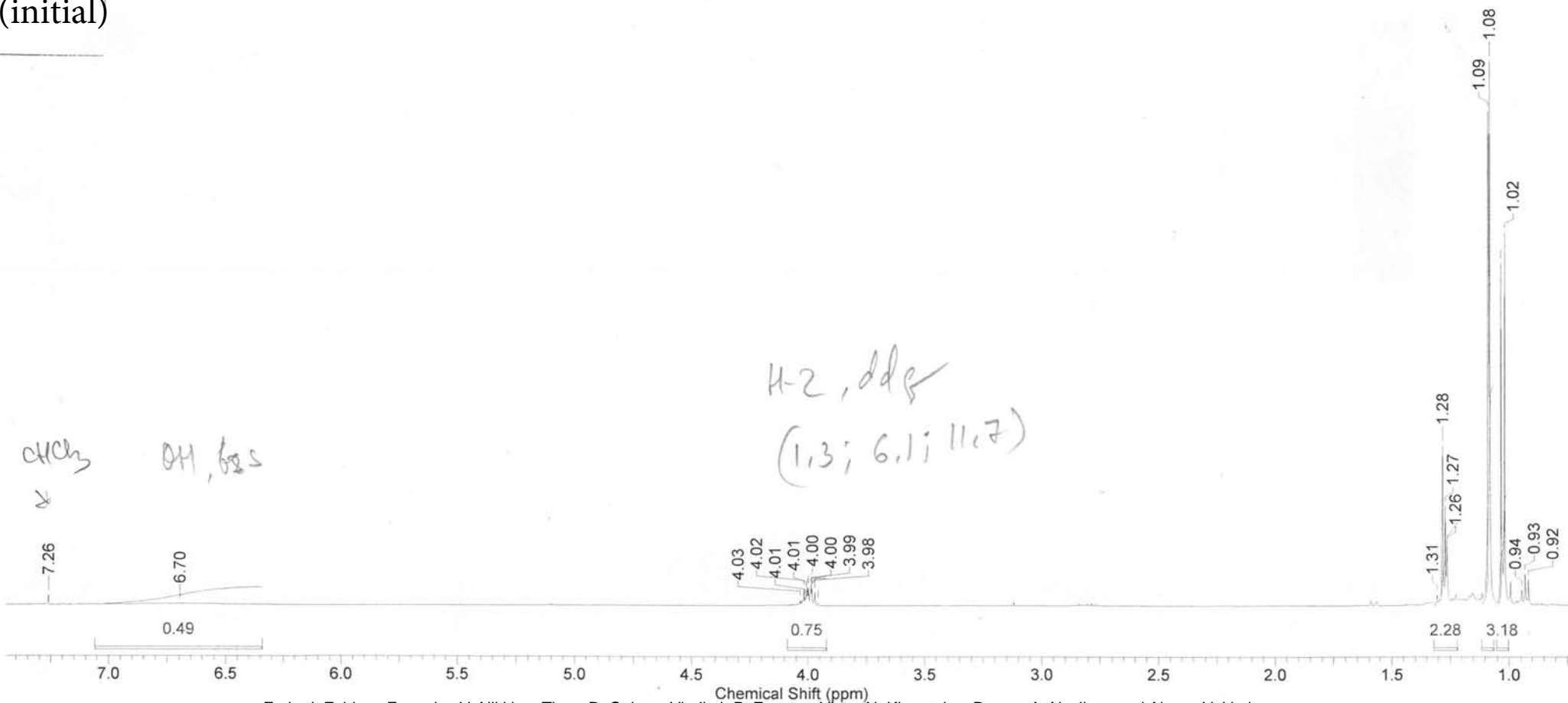


Formula C₆H₁₅NO FW 117.1894

Acquisition Time (sec)	1.4909	Comment	FZ.9	Date	22/06/2004 00:00:00	Date Stamp	22/06/2004 00:00:00		
File Name	D:\NMR\24.06.04\FZ.013		Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	16	
Original Points Count	8192	Points Count	8192	Spectrum Offset (Hz)	1605.9999	Sweep Width (Hz)	5494.51	Temperature (degree C)	24.000



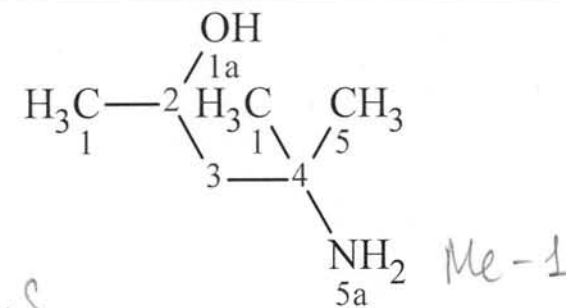
5 (initial)



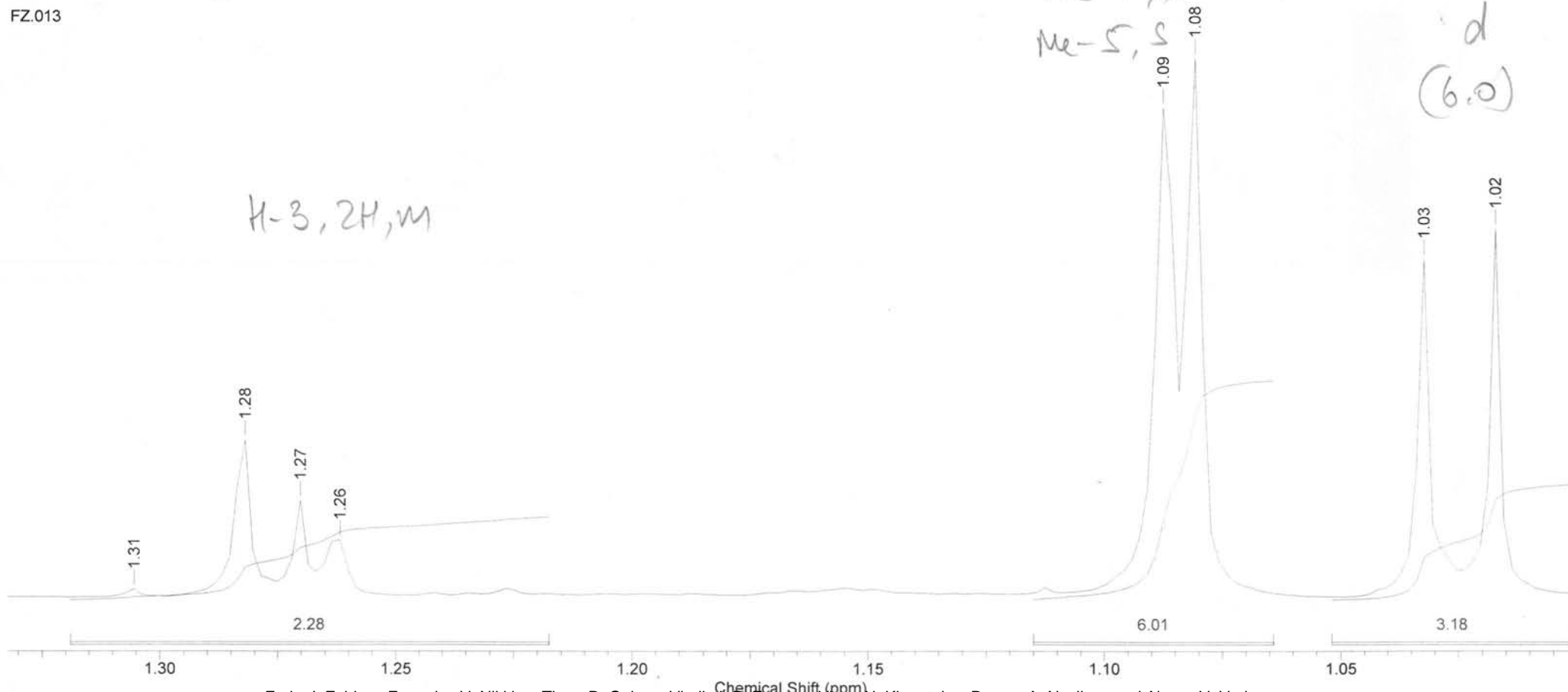
Formula	C ₆ H ₁₅ NO	FW	117.1894
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Acquisition Time (sec)	1.4909	Comment	FZ.9	Date	22/06/2004 00:00:00	Date Stamp	22/06/2004 00:00:00		
File Name	D:\NMR\24.06.04\FZ.013		Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	16	
Original Points Count	8192	Points Count	8192	Spectrum Offset (Hz)	1605.9999	Sweep Width (Hz)	5494.51	Temperature (degree C)	24.000

Initial for compound 5

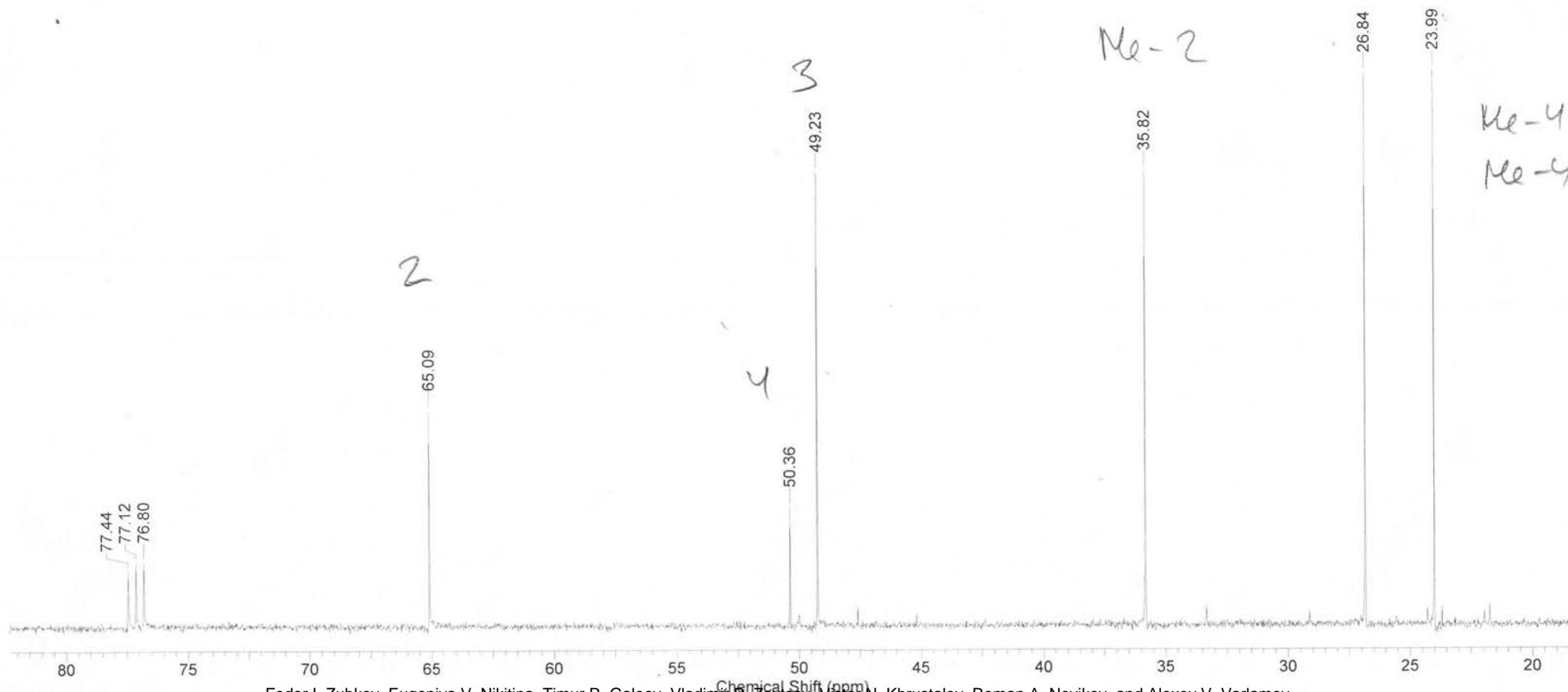
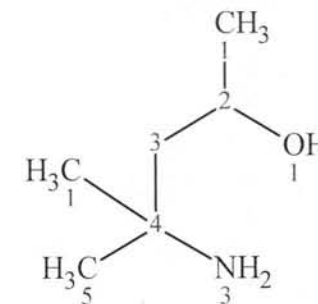


FZ.013



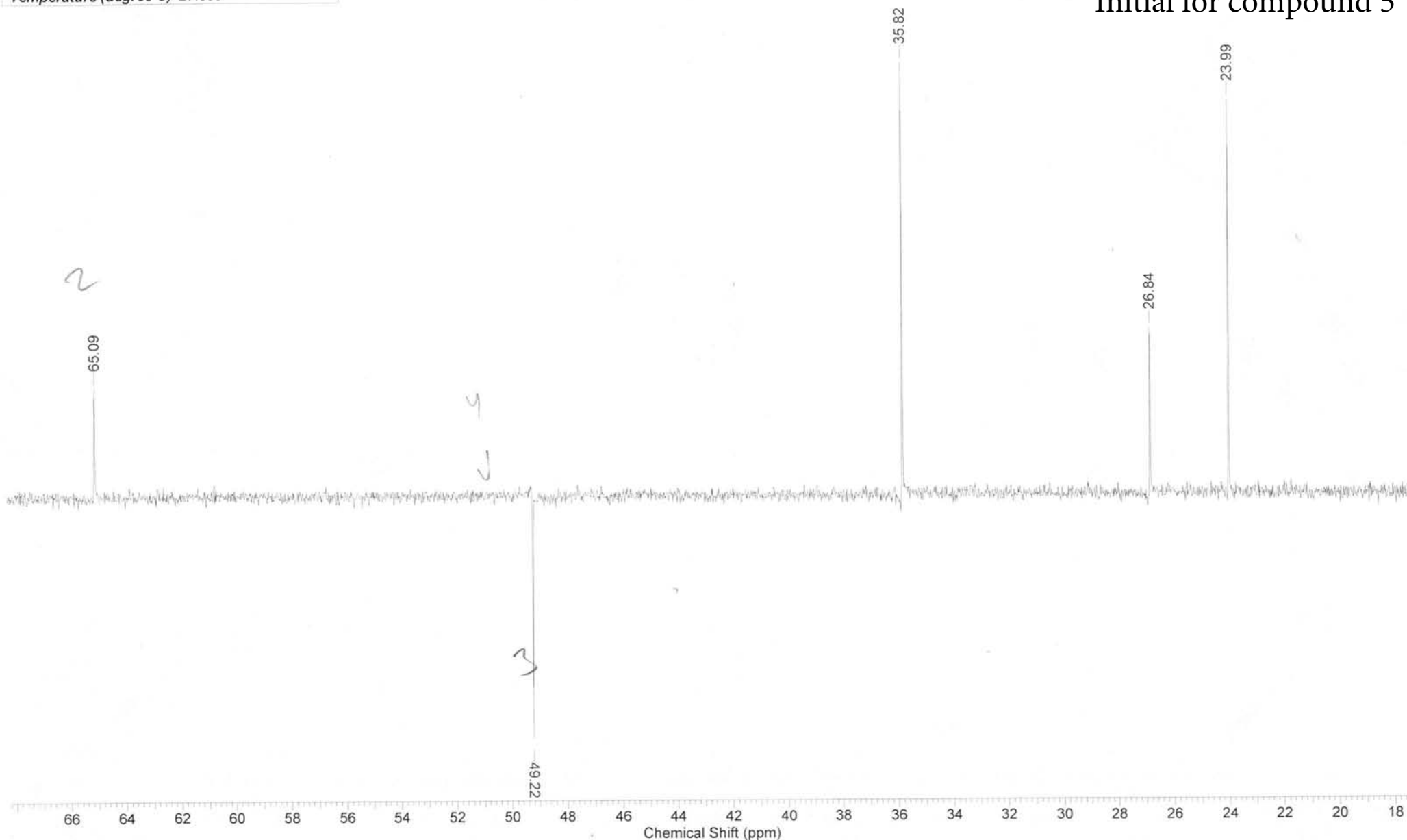
Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.	Date	31 May 2011 15:10:56		
File Name	C:\Users\Fedor\Desktop\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\rudn-300511-N5-c13dec\rudn-300511-N5-c13dec_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	227	Original Points Count	16384
Points Count	16384	Pulse Sequence	zgpg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	29411.77
Temperature (degree C)	27.000						

Initial for compound 5



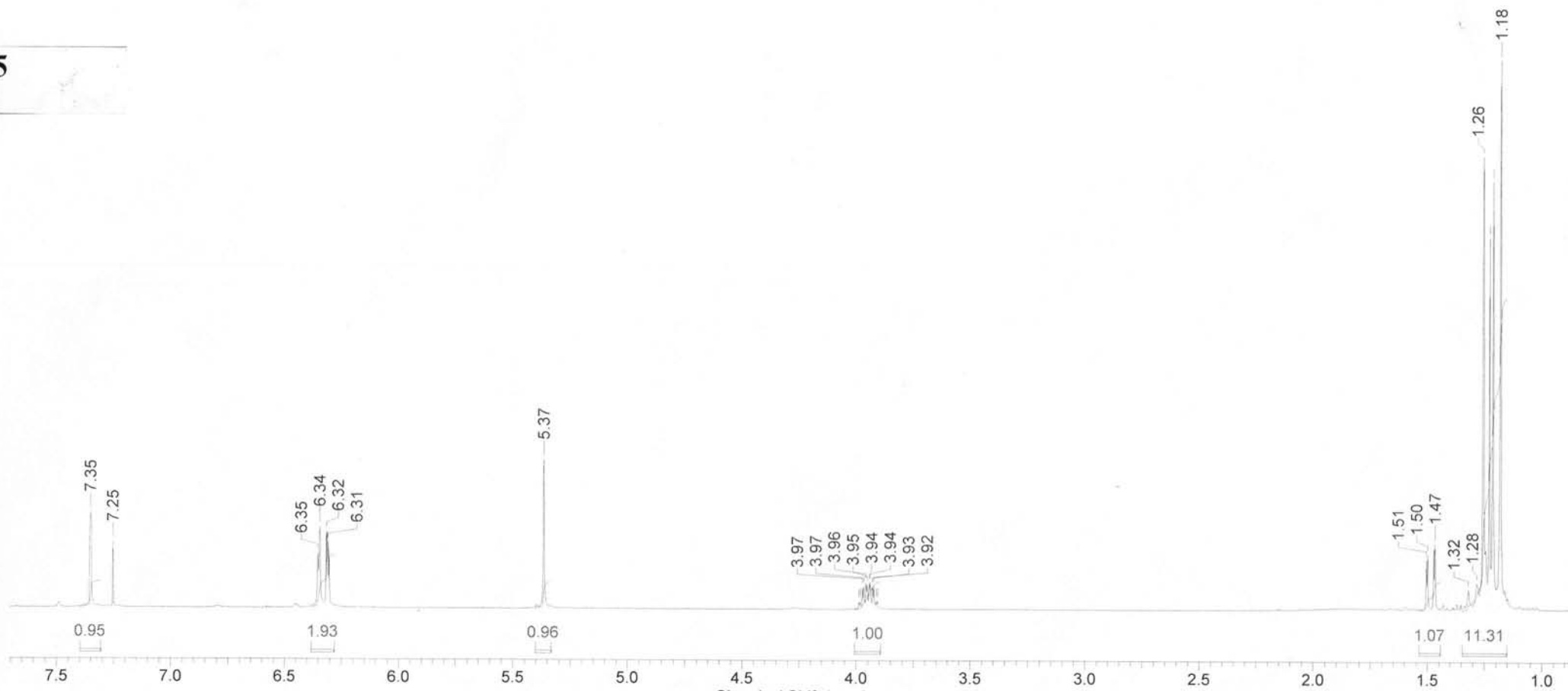
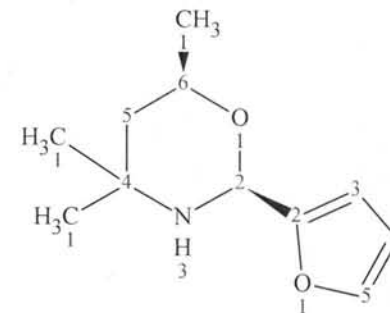
Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.	Date	31 May 2011 15:17:20		
File Name	C:\Users\Fedor\Desktop\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\rudn-300511-N5-dept135\rudn-300511-N5-dept135_001000fid						
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	152	Original Points Count	16384
Points Count	16384	Pulse Sequence	dept135	Solvent	CHLOROFORM-D	Sweep Width (Hz)	29411.77
Temperature (degree C)	27.000						

Initial for compound 5



Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.		Date	31 May 2011 14:11:12
File Name	C:\Users\Fedor\Desktop\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\rudn-300511-N4\rudn-300511-N4_001000fid			Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	8	Original Points Count	16384	
Pulse Sequence	zg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	10204.08	
				Temperature (degree C)	27.000	

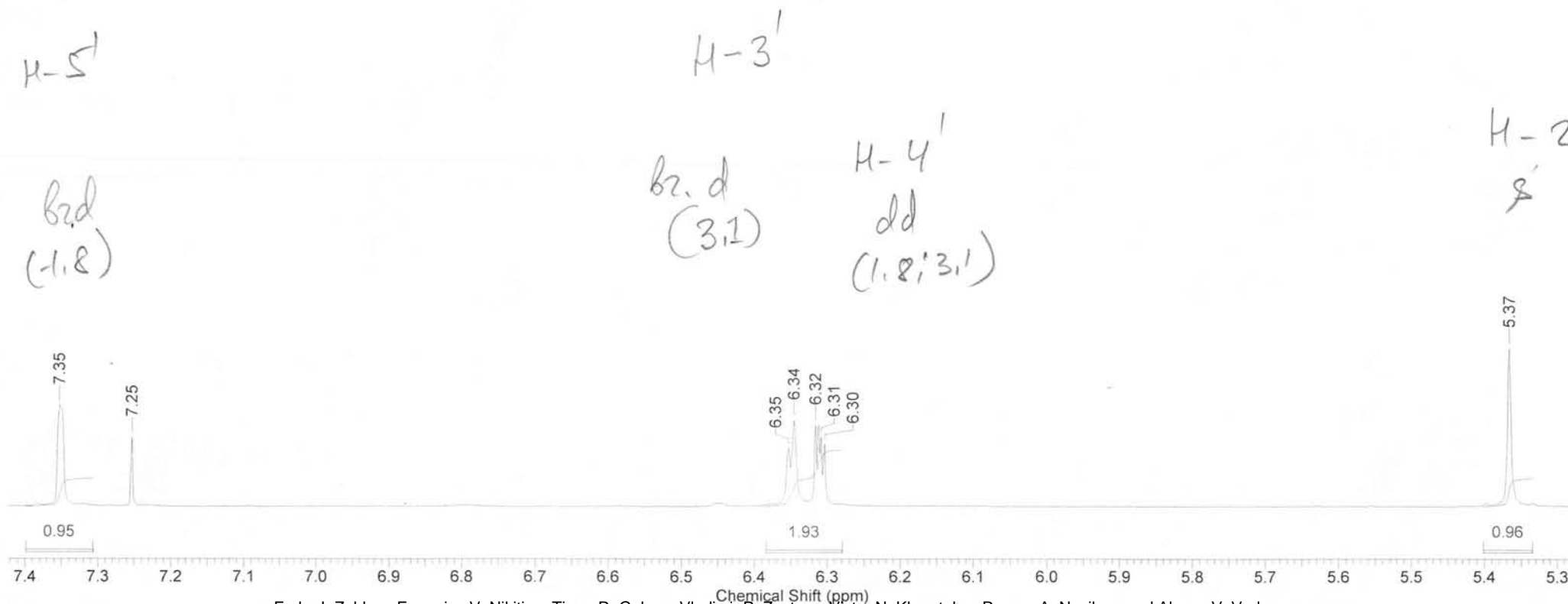
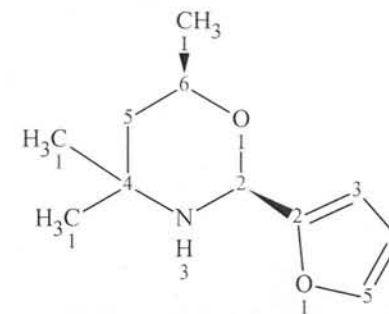
Compound 5



3 Jun 2011

Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.	Date	31 May 2011 14:11:12
File Name	C:\Users\Fedor\Desktop\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\rudn-300511-N4\rudn-300511-N4_001000fid			Frequency (MHz)	400.14
Nucleus	¹ H	Number of Transients	8	Original Points Count	16384
Pulse Sequence	zg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	10204.08
				Points Count	16384
				Temperature (degree C)	27.000

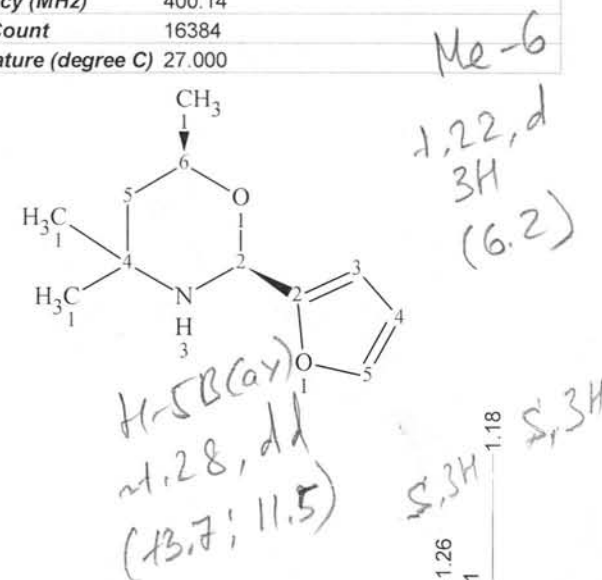
Compound 5



3 Jun 2011

Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.		Date	31 May 2011 14:11:12
File Name	C:\Users\Fedor\Desktop\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\rudn-300511-N4\rudn-300511-N4_001000fid			Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	8	Original Points Count	16384	
Pulse Sequence	zg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	10204.08	
				Points Count	16384	
				Temperature (degree C)	27.000	

Compound 5



H-6, ddq

(2.5; 6.2; 11.5)

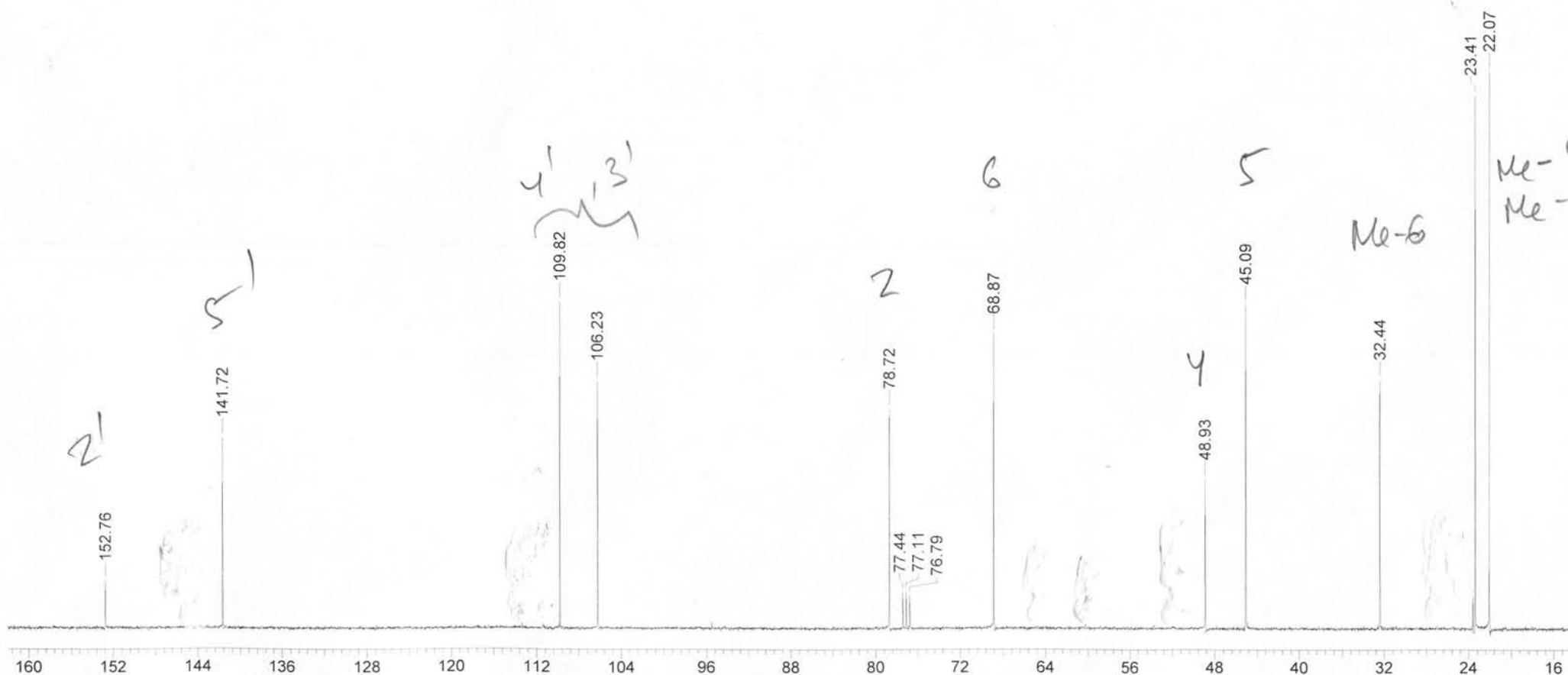
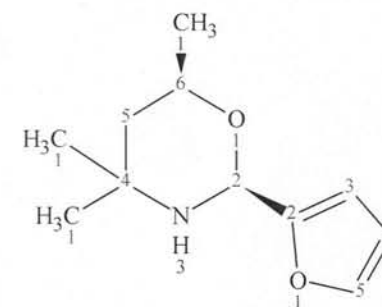
32.4 Hz

H-5A(eqv)
dd
(2.5; 13.7)S, 3H
1.18 S, 3H

3 Jun 2011

Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.	Date	31 May 2011 14:58:08		
File Name	C:\Users\Fedor\Desktop\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\rudn-300511-N4-c13dec\rudn-300511-N4-c13dec_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	258	Original Points Count	16384
Points Count	16384	Pulse Sequence	zgpg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	29411.77
Temperature (degree C)	27.000						

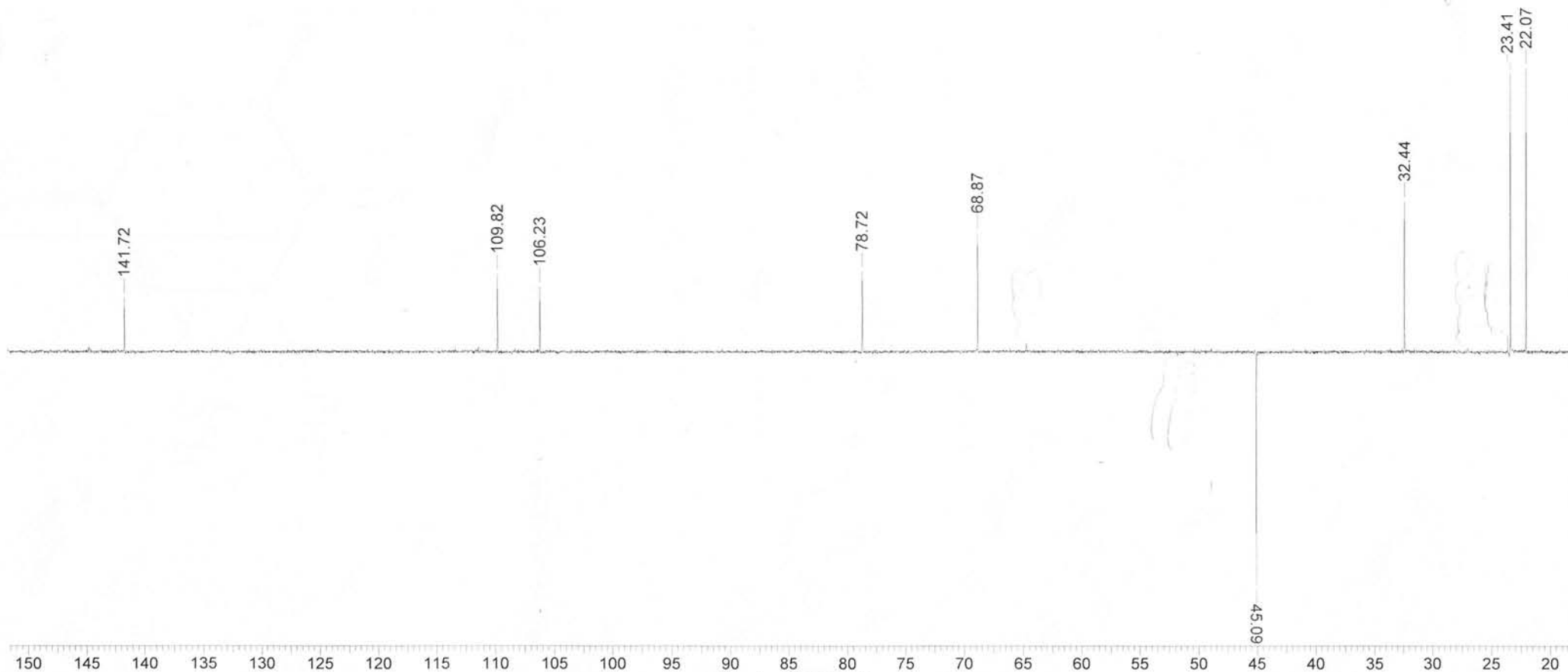
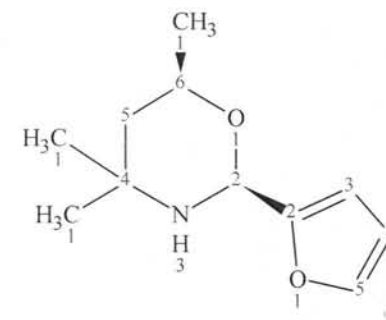
Compound 5



3 Jun 2011

Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.	Date	31 May 2011 15:04:32
File Name	C:\Users\Fedor\Desktop\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\rudn-300511-N4-dept135\rudn-300511-N4-dept135_001000fid				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	212
Points Count	16384	Pulse Sequence	dept135	Solvent	CHLOROFORM-D
Temperature (degree C)	27.000			Original Points Count	16384
				Sweep Width (Hz)	29411.77

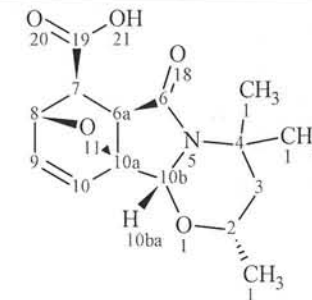
Compound 5



Formula	C ₁₅ H ₁₉ NO ₅	FW	293.3151
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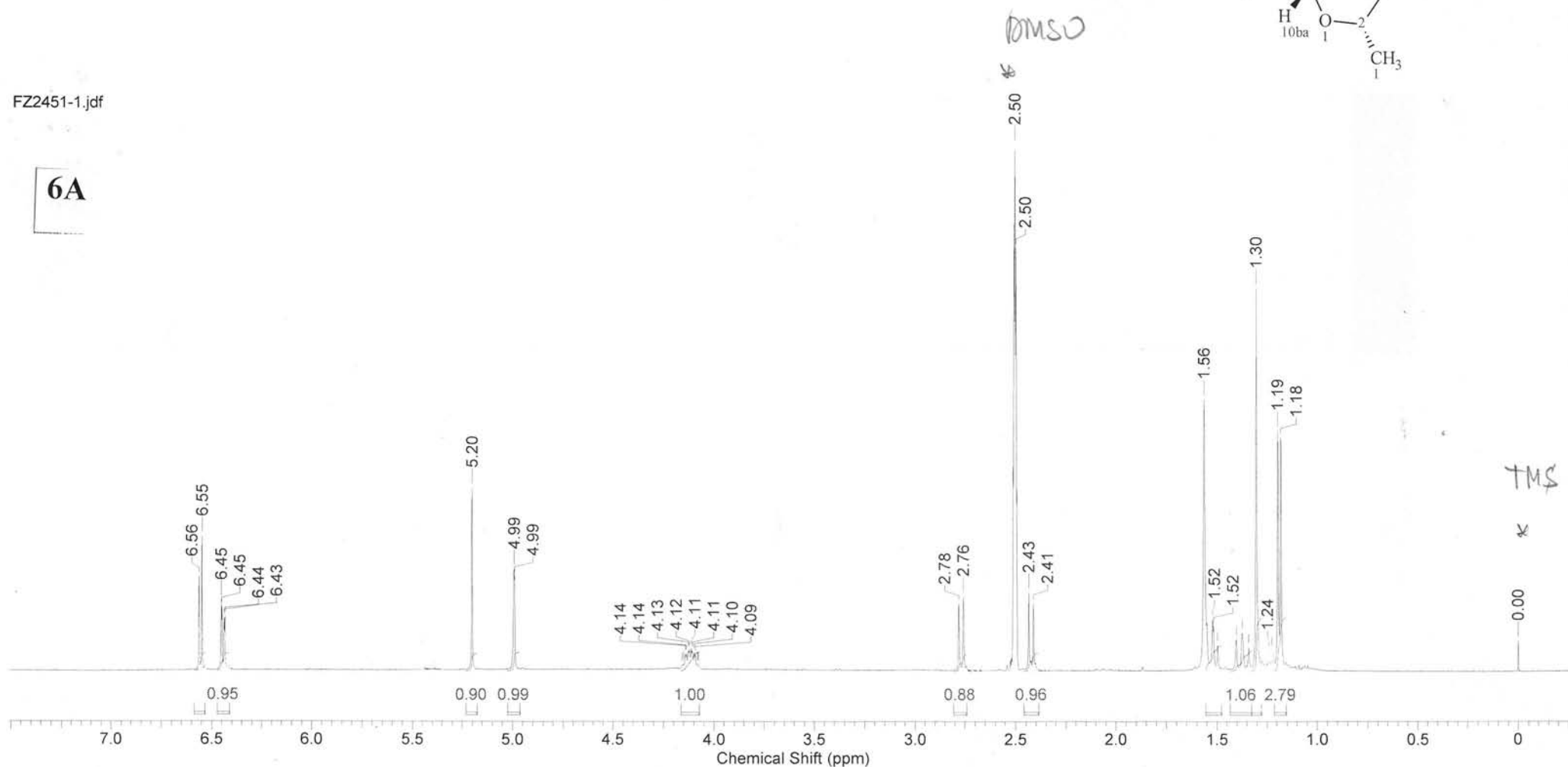
Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	06 Jun 2012 11:15:07	Date Stamp	06 Jun 2012 15:04:23
File Name	D:\NMR\04.06.12\FZ2451-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	25
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	38.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	2414.2141	Sweep Width (Hz)	7503.00
						Temperature (degree C)	23.300

Compound 6



FZ2451-1.jdf

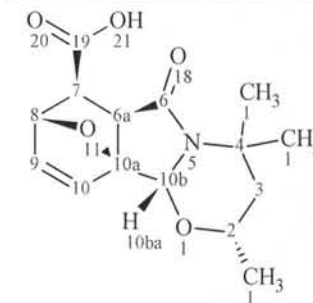
6A



Formula	C ₁₅ H ₁₉ NO ₅	FW	293.3151
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Acquisition Time (sec)	2.1837	Comment	single_pulse,	Date	06 Jun 2012 11:15:07	Date Stamp	06 Jun 2012 15:04:23
File Name	D:\NMR\04.06.12\FZ2451-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	25
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	38.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	2414.2141	Sweep Width (Hz)	7503.00
						Temperature (degree C)	23.300

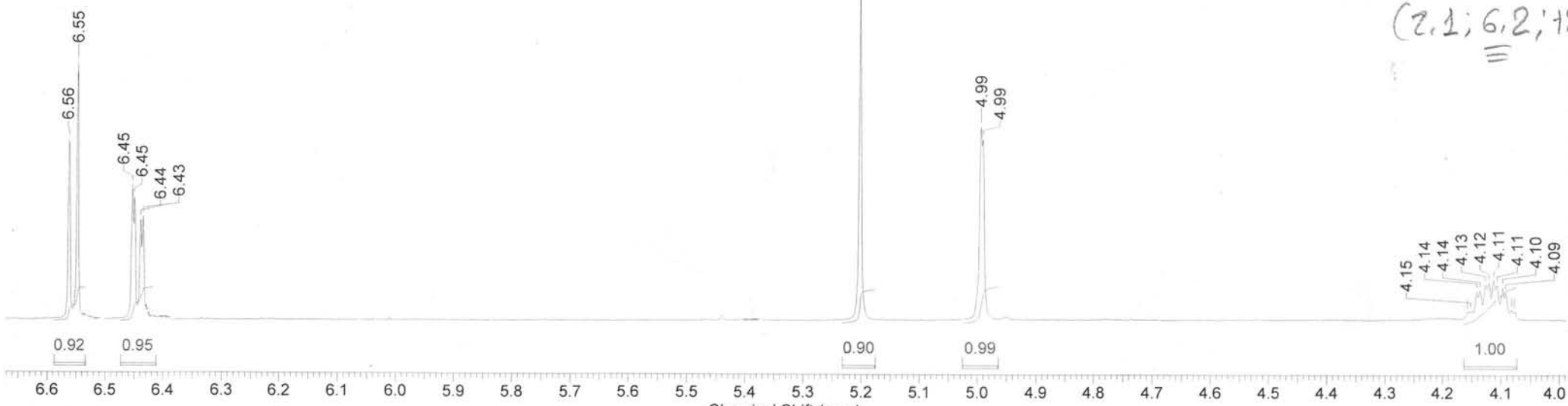
Compound 6



FZ2451-1.jdf

H-10
d
(6.0)

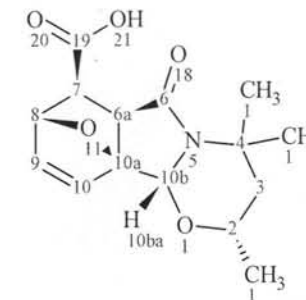
H-9
dd
(1.4; 6.0)



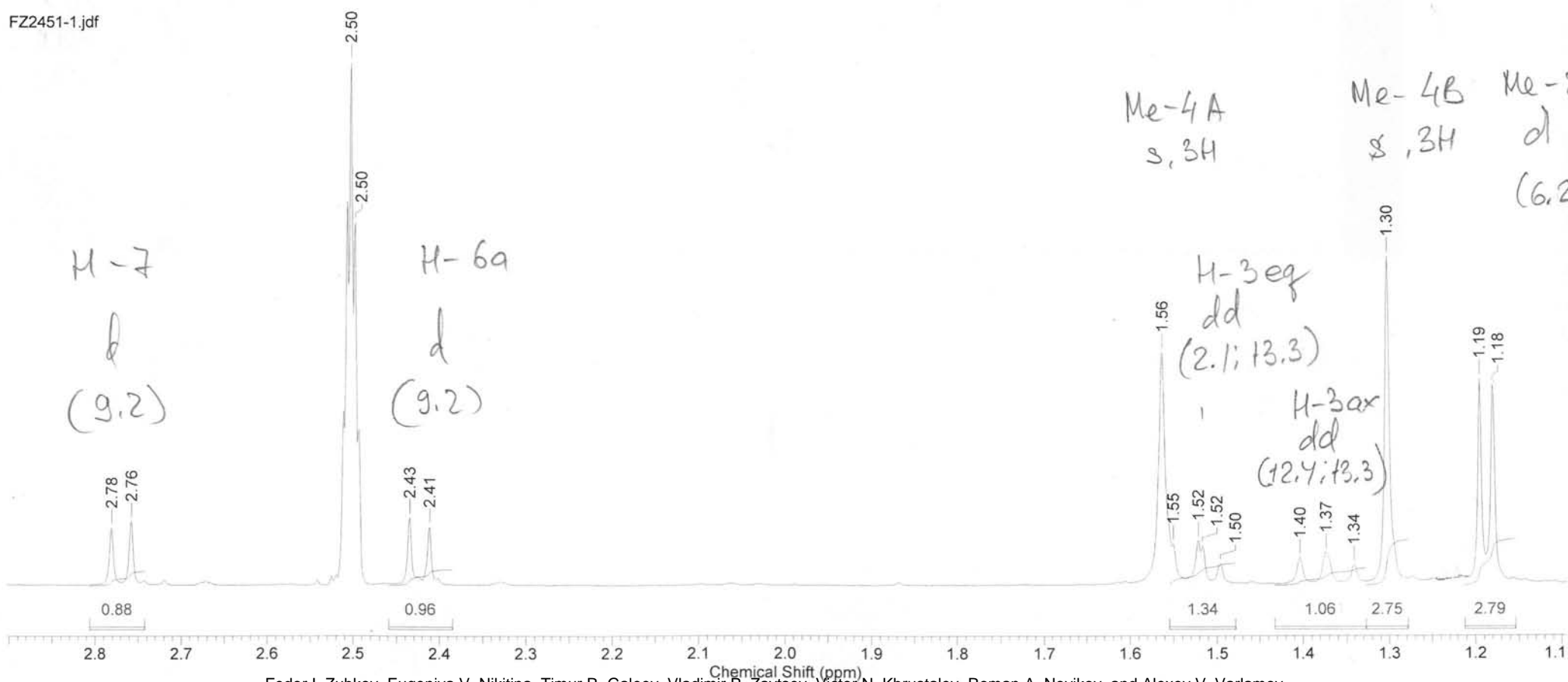
Formula	C ₁₅ H ₁₉ NO ₅	FW	293.3151
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Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	06 Jun 2012 11:15:07	Date Stamp	06 Jun 2012 15:04:23
File Name	D:\NMR\04.06.12\FZ2451-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	25
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	38.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	2414.2141	Sweep Width (Hz)	7503.00
						Temperature (degree C)	23.300

Compound 6

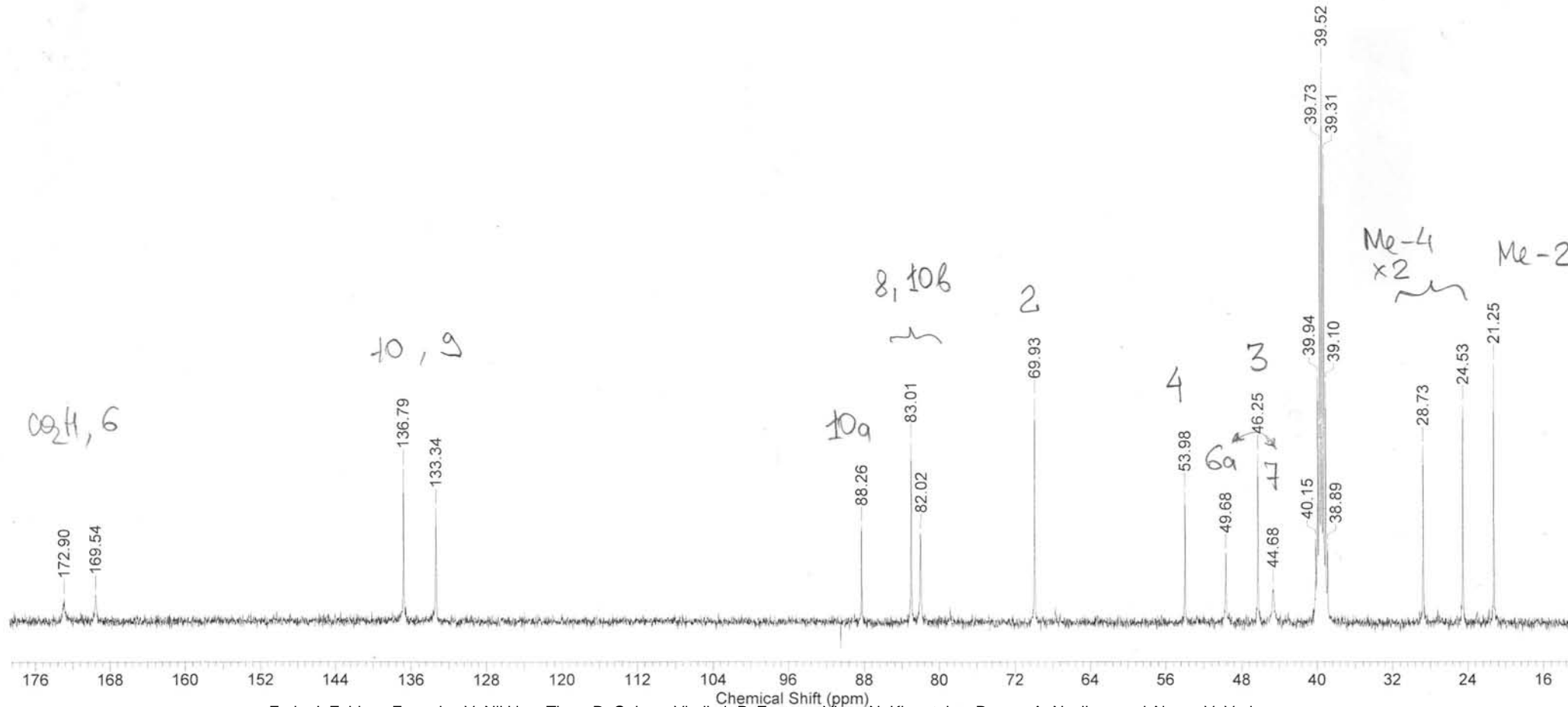
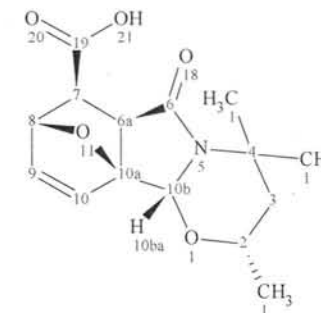


FZ2451-1.jdf



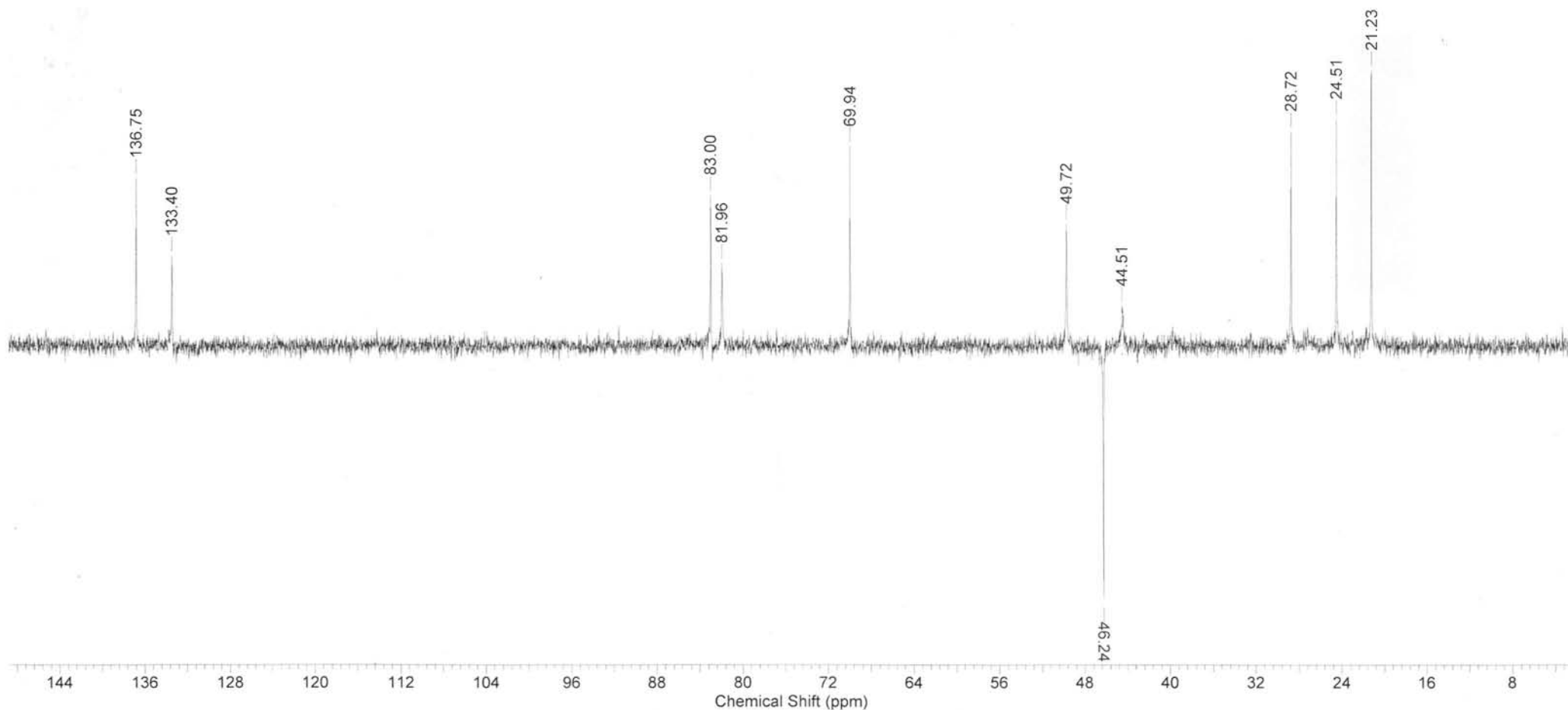
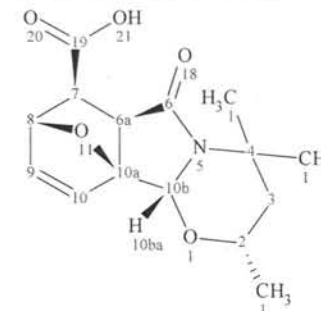
Acquisition Time (sec)	0.5243	Comment	Imported from UXMNR.		Date	23 Aug 2011 11:07:44	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-120811-N1-c13dec\rudn-120811-N1-c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	4000	Original Points Count	16384	Points Count	16384
Pulse Sequence	zpgp	Solvent	DMSO-D6	Sweep Width (Hz)	31250.00	Temperature (degree C)	27.000

Compound 6



Acquisition Time (sec)	0.5571	Comment	Imported from UXNMR.		Date	23 Aug 2011 14:02:40	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-120811-N1-dept135\rudn-120811-N1-dept135_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	4000	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

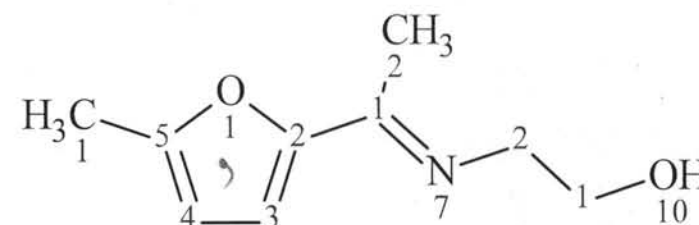
Compound 6



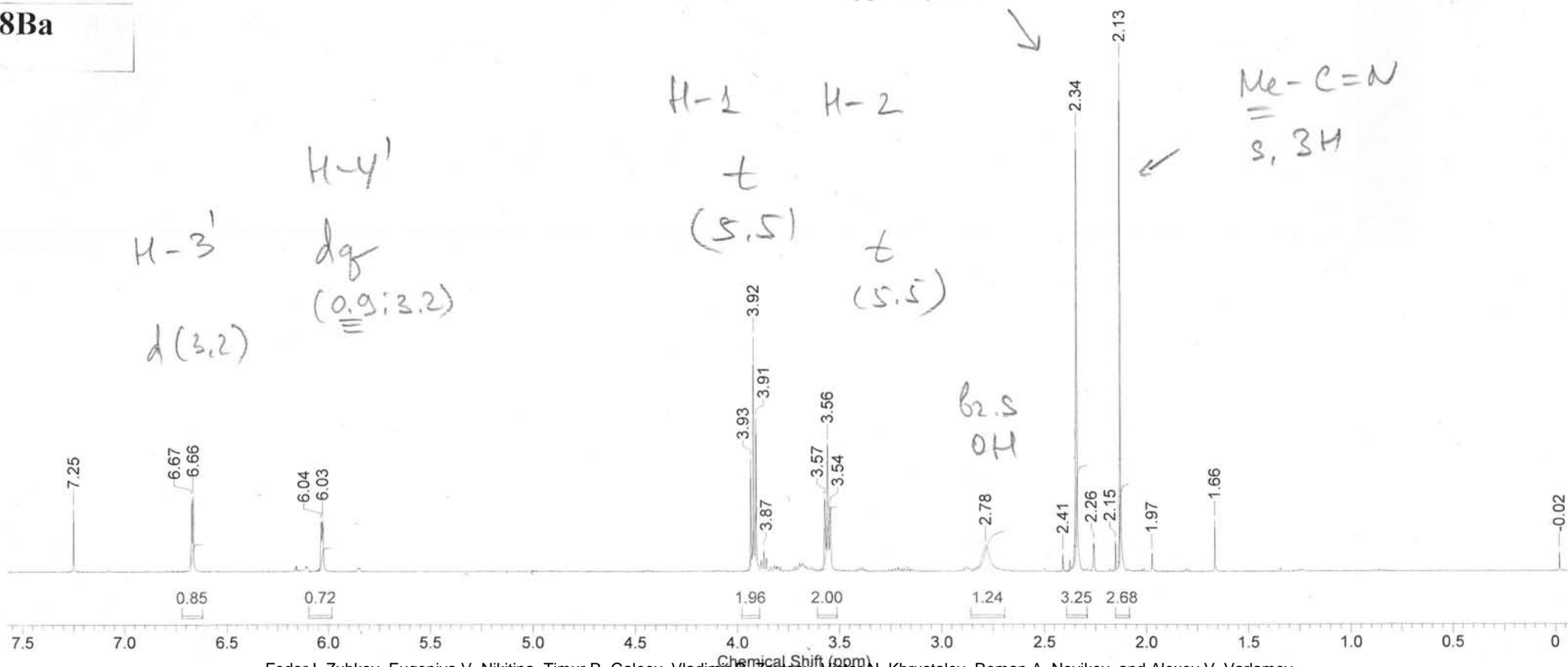
Formula $C_9H_{13}NO_2$ FW 167.2050

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	06 Mar 2012 09:17:10	Date Stamp	06 Mar 2012 13:51:58
File Name	D:\NMR\05.03.12\FZ2263-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	18.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	1998.9109	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	24.000			Sweep Width (Hz)			7503.00

Compound 8Ba



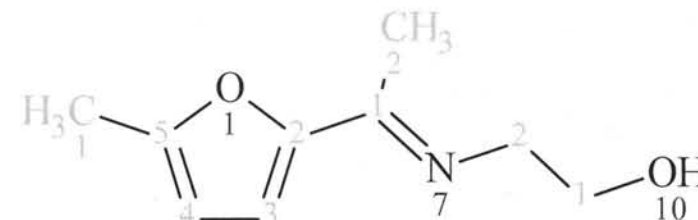
8Ba



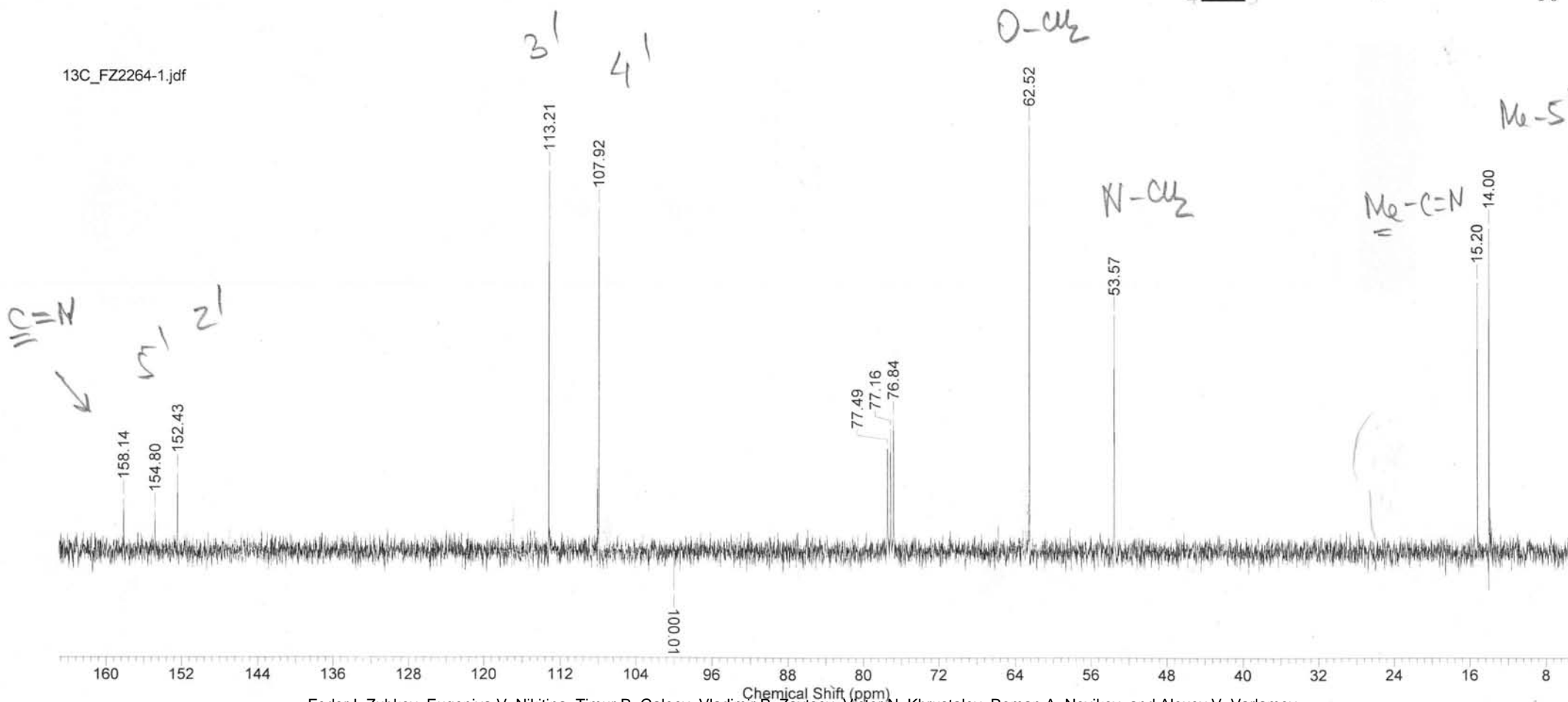
Formula C₉H₁₃NO₂ FW 167.2050

Acquisition Time (sec)	0.5217	Comment	single pulse decoupled gated NOE	Date	06 Mar 2012 09:58:23
Date Stamp	06 Mar 2012 14:33:11	File Name	D:\NMR\05.03.12\13C_FZ2264-1.jdf	Frequency (MHz)	100.53
Nucleus	13C	Number of Transients	89	Origin	ECS 400
Points Count	16384	Pulse Sequence	single_pulse_dec	Original Points Count	16384
Solvent	CHLOROFORM-d	Receiver Gain	54.00	Owner	delta
		Spectrum Offset (Hz)	10052.5303	Sweep Width (Hz)	31407.04
				Temperature (degree C)	24.400

Compound 8Ba



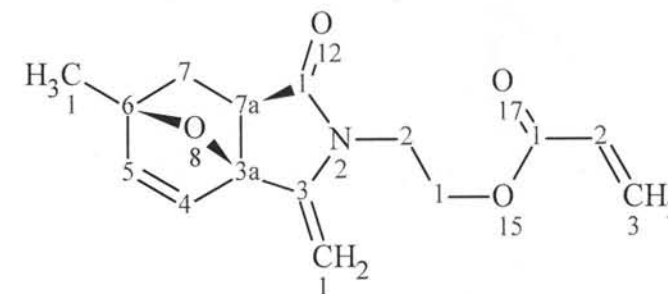
13C_FZ2264-1.jdf



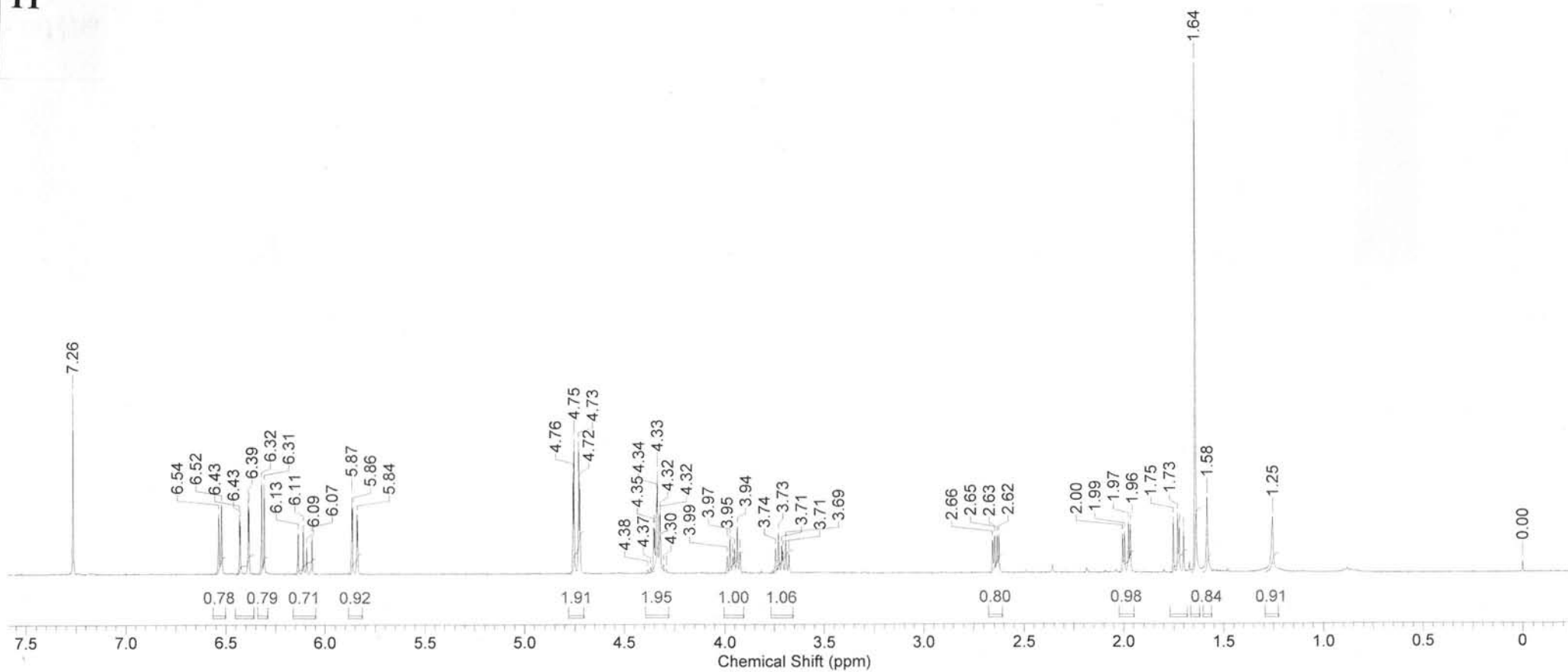
Formula C₁₅H₁₇NO₄ FW 275.2998

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	05 May 2012 09:04:34	Date Stamp	05 May 2012 12:53:53
File Name	D:\NMR\03.05.12\FZ2367-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	4
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	40.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	1992.4193	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	23.200	Sweep Width (Hz)					7503.00

Compound 11



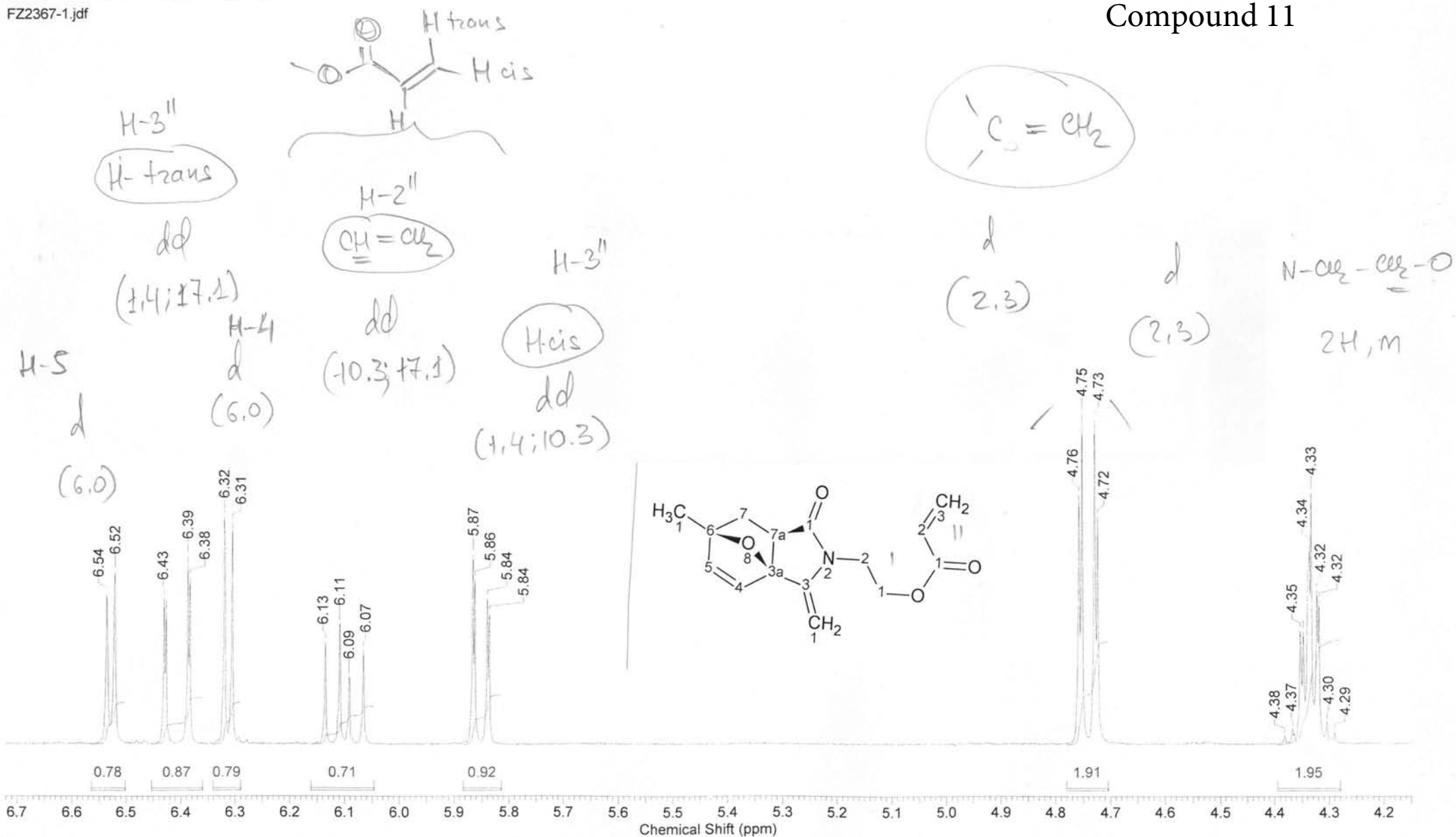
11



Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	05 May 2012 09:04:34	Date Stamp	05 May 2012 12:53:53
File Name	D:\NMR\03.05.12\FZ2367-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	4
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	40.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	1992.4193	Sweep Width (Hz)	7503.00
Temperature (degree C)	23.200						

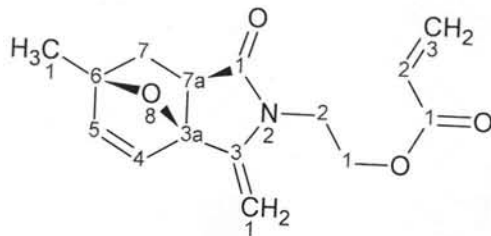
FZ2367-1.jdf

Compound 11

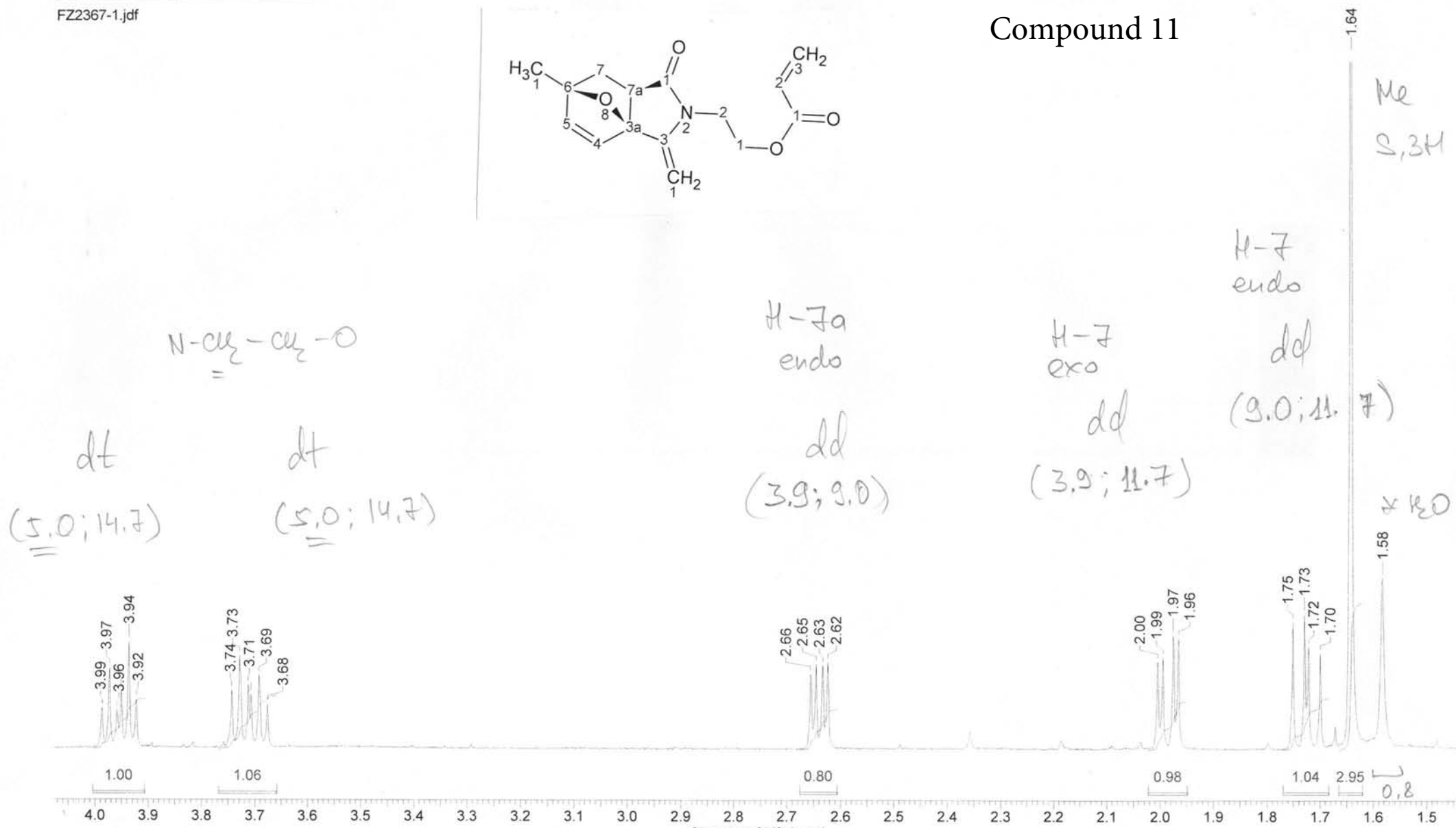


Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	05 May 2012 09:04:34	Date Stamp	05 May 2012 12:53:53
File Name	D:\NMR\03.05.12\FZ2367-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	4
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	40.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	1992.4193	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	23.200			Sweep Width (Hz)	7503.00		

FZ2367-1.jdf

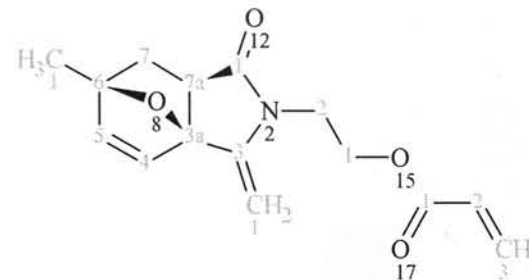


Compound 11

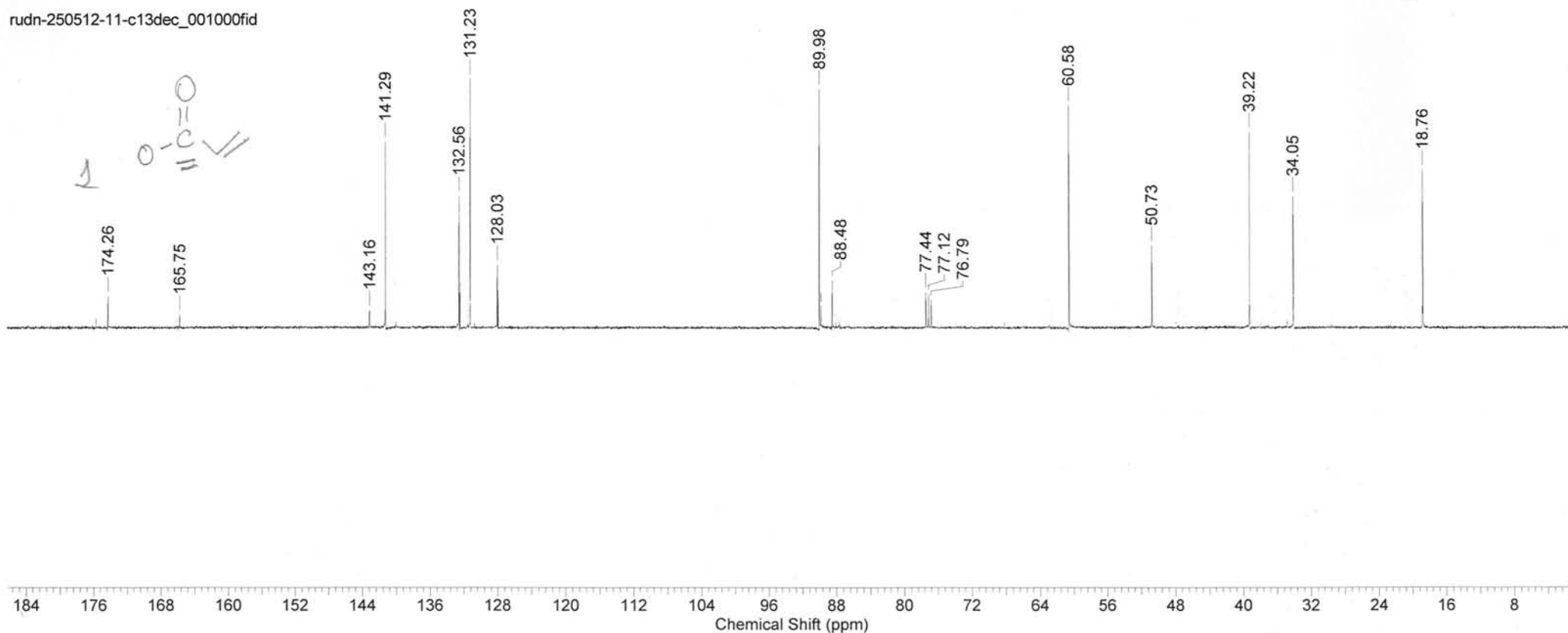


Formula C ₁₅ H ₁₇ NO ₄	FW 275.2998			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 28 May 2012 17:16:48		
Date Stamp 28 May 2012 17:16:48				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-11-c13dec\rudn-250512-11-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 445	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpgg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent CHLOROFORM-d	Spectrum Offset (Hz) 9627.5156	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compound 11

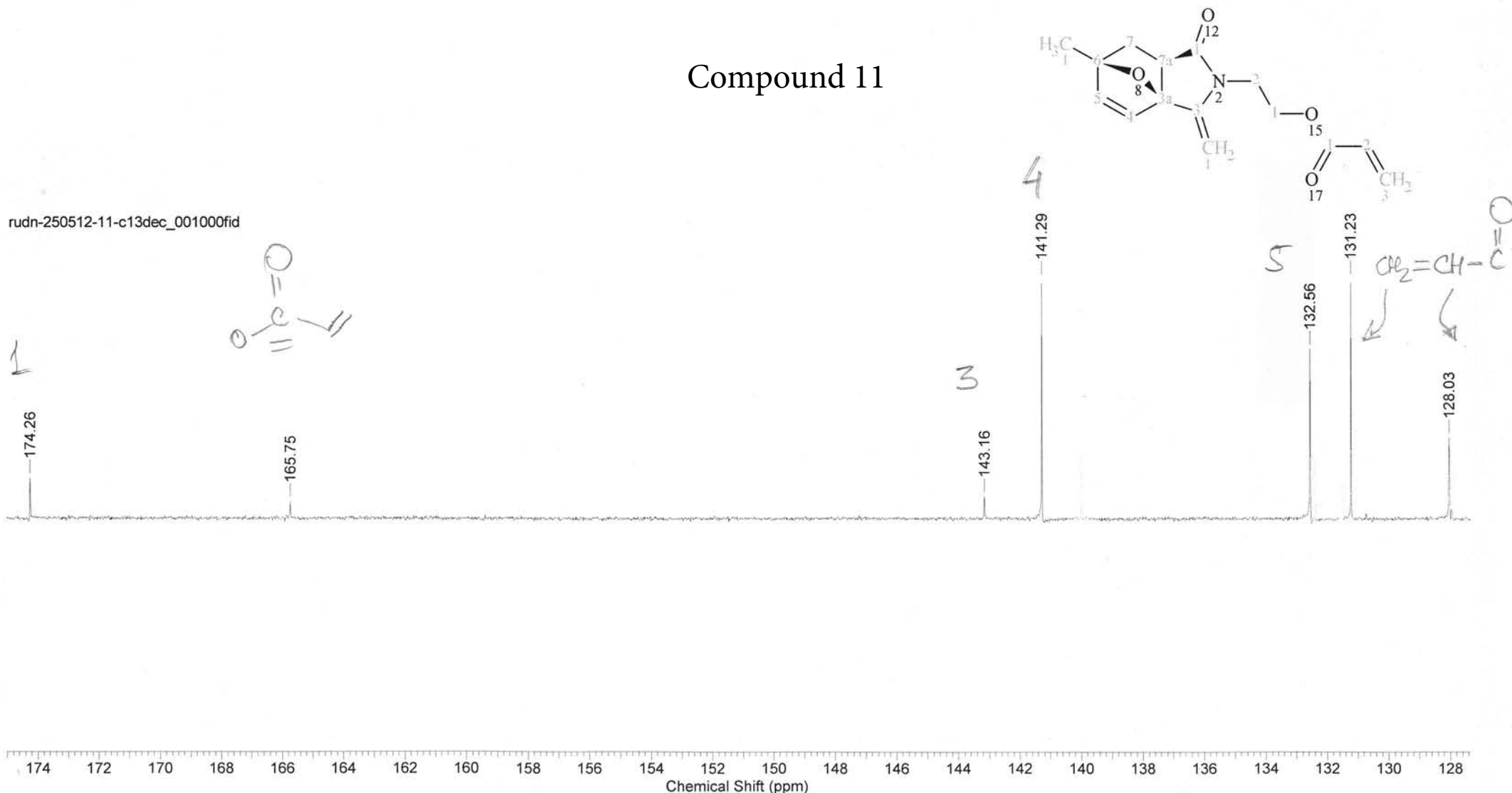


rudn-250512-11-c13dec_001000fid



Formula C ₁₅ H ₁₇ NO ₄	FW 275.2998			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 28 May 2012 17:16:48		
Date Stamp 28 May 2012 17:16:48				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-11-c13dec\rudn-250512-11-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 445	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent CHLOROFORM-d	Spectrum Offset (Hz) 9627.5156	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

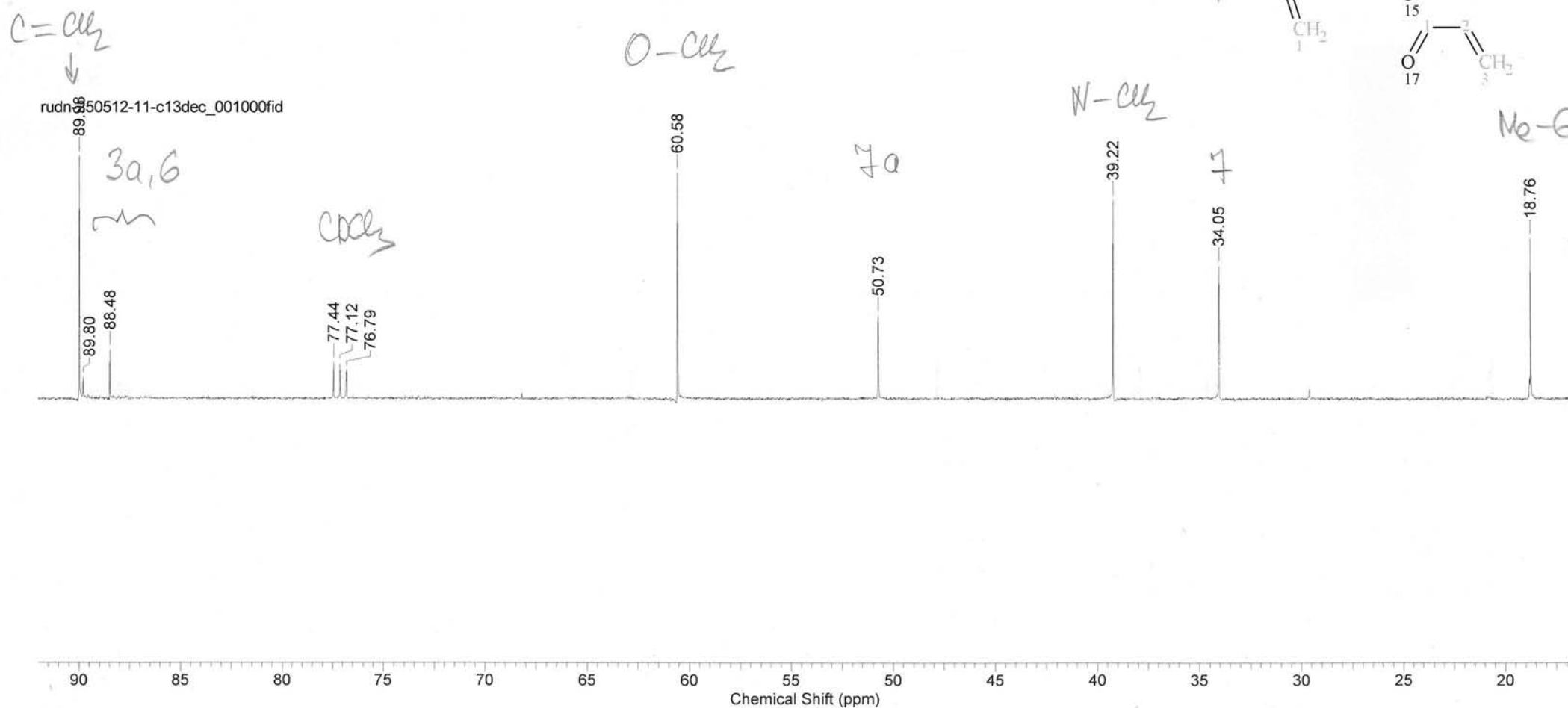
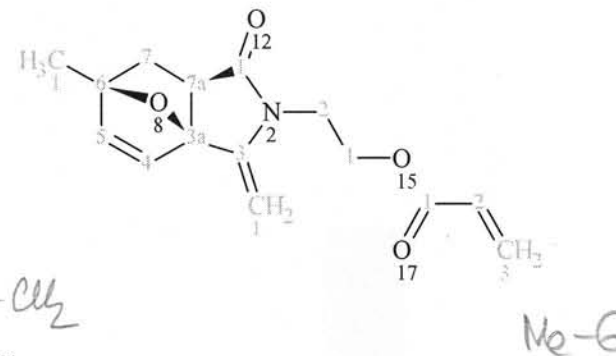
Compound 11



Formula	C ₁₅ H ₁₇ NO ₄	FW	275.2998
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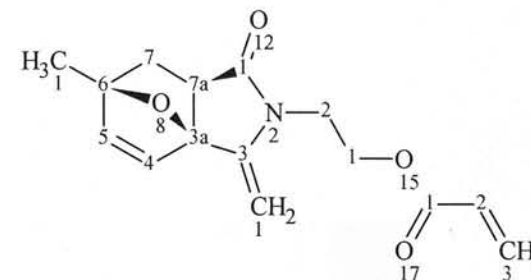
Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	28 May 2012 17:16:48
Date Stamp	28 May 2012 17:16:48				
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-11-c13dec\rudn-250512-11-c13dec_001000fid				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	445
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	CHLOROFORM-d
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000	Spectrum Offset (Hz)	9627.5156

Compound 11

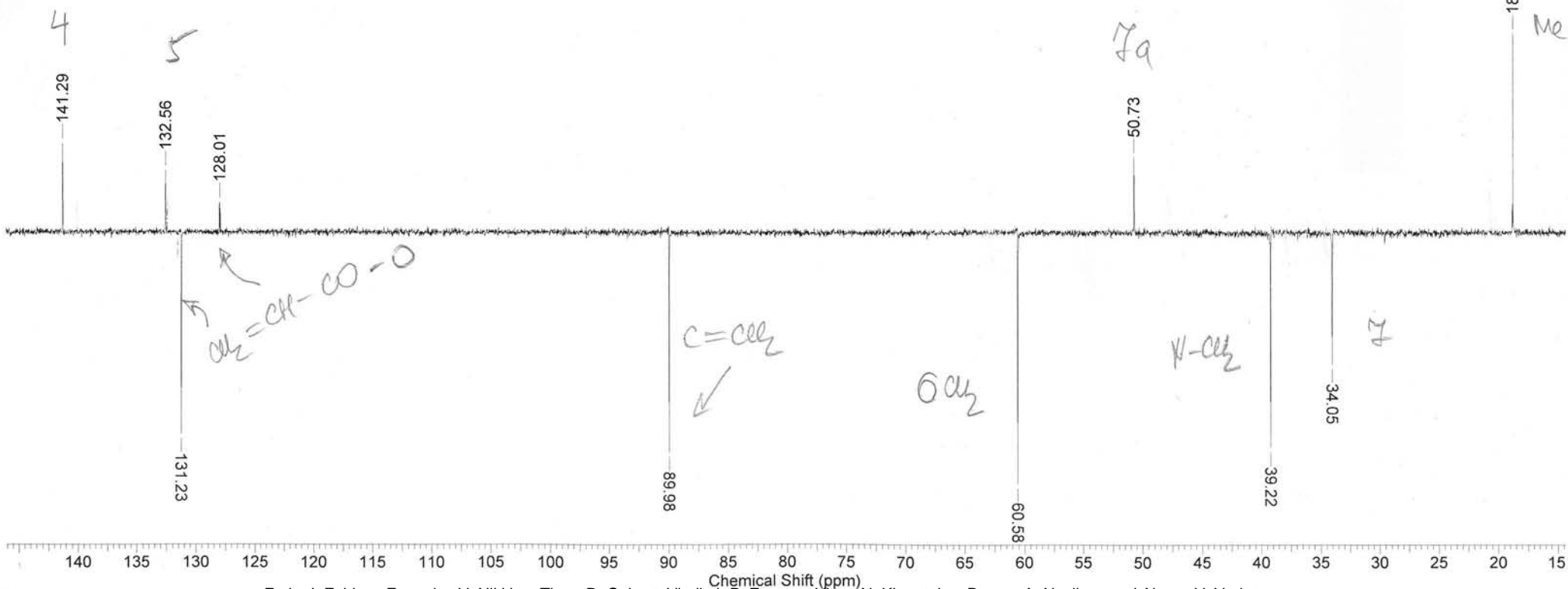


Formula C ₁₅ H ₁₇ NO ₄	FW 275.2998			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 28 May 2012 17:25:20		
Date Stamp 28 May 2012 17:25:20				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-11-dept135\rudn-250512-11-dept135_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 273	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence dept135	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent CHLOROFORM-d	Spectrum Offset (Hz) 9627.5049	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compound 11



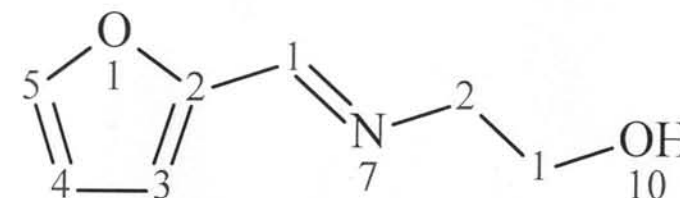
rudn-250512-11-dept135_001000fid



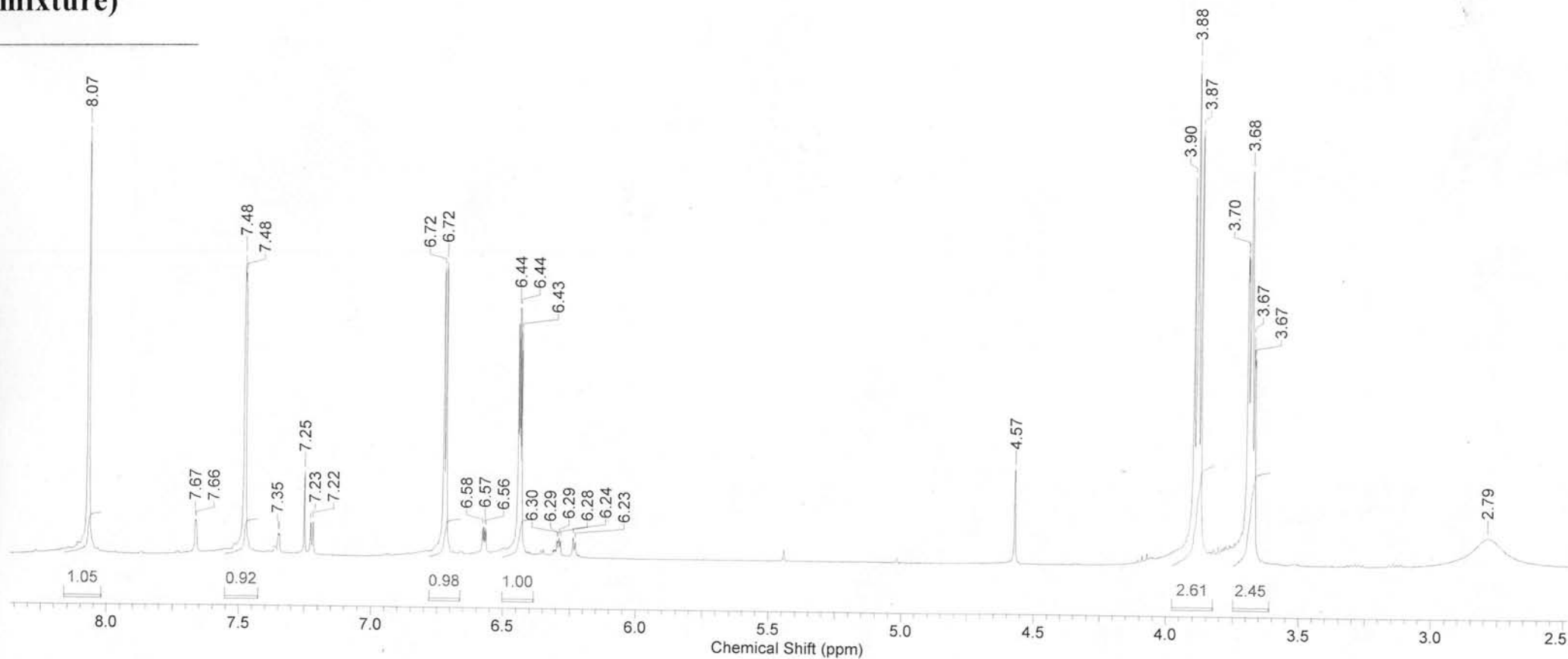
Formula	C ₇ H ₉ NO ₂	FW	139.1519
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Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	13 Jul 2011 08:58:11	Date Stamp	13 Jul 2011 12:46:56
File Name	D:\NMR\01.07.11\FZ1919-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	30.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	1998.9109	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	24.300					Sweep Width (Hz)	7503.00

Compound 12a
reaction mixture



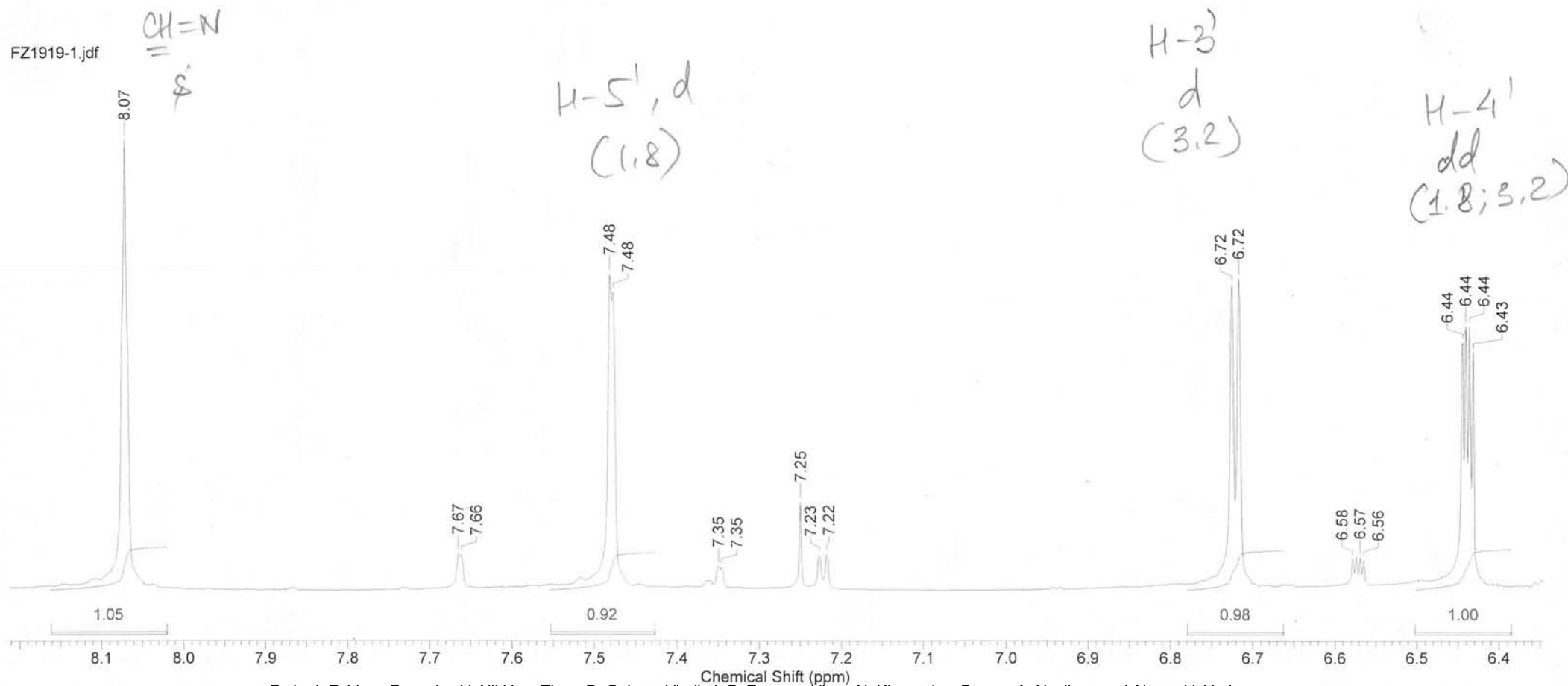
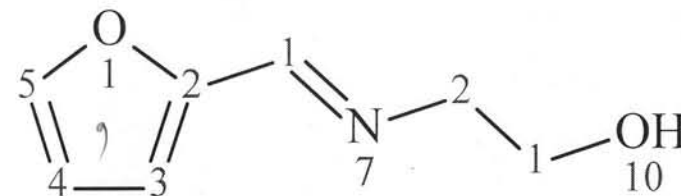
12a (reaction
mixture)



Formula C₇H₉NO₂ FW 139.1519

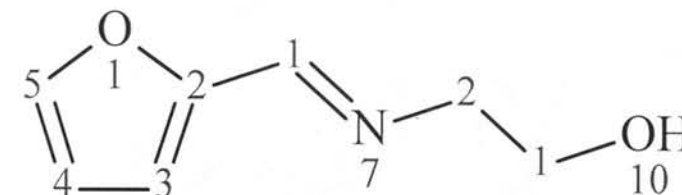
Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	13 Jul 2011 08:58:11	Date Stamp	13 Jul 2011 12:46:56
File Name	D:\NMR\01.07.11\FZ1919-1.jdf	Original Points Count	16384	Frequency (MHz)	399.78	Nucleus	1H
Origin	ECS 400	Solvent	CHLOROFORM-d	Owner	delta	Points Count	16384
Receiver Gain	30.00	Spectrum Offset (Hz)	1998.9109	Pulse Sequence	single_pulse.ex2	Sweep Width (Hz)	7503.00
Temperature (degree C)	24.300						

Compound 12a
reaction mixture



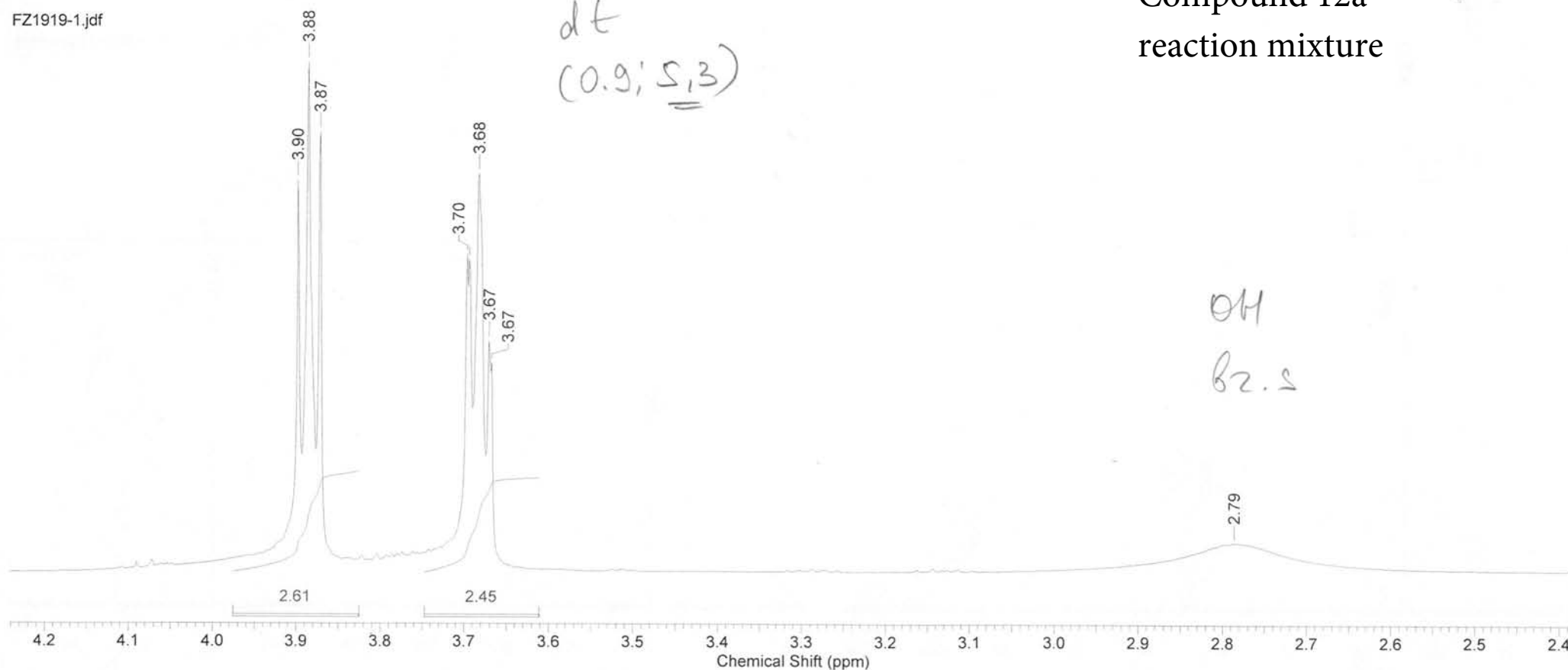
Formula C₇H₉NO₂ FW 139.1519

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	13 Jul 2011 08:58:11	Date Stamp	13 Jul 2011 12:46:56
File Name	D:\NMR\01.07.11\FZ1919-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8
Origin	ECS 400	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	30.00	Solvent	CHLOROFORM-d	Points Count	16384	Spectrum Offset (Hz)	1998.9109
Temperature (degree C)	24.300	Sweep Width (Hz)					7503.00



Compound 12a
reaction mixture

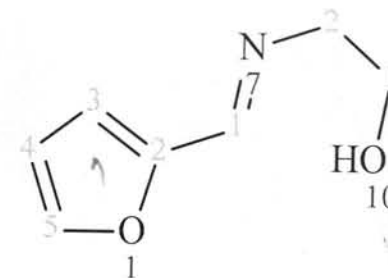
FZ1919-1.jdf



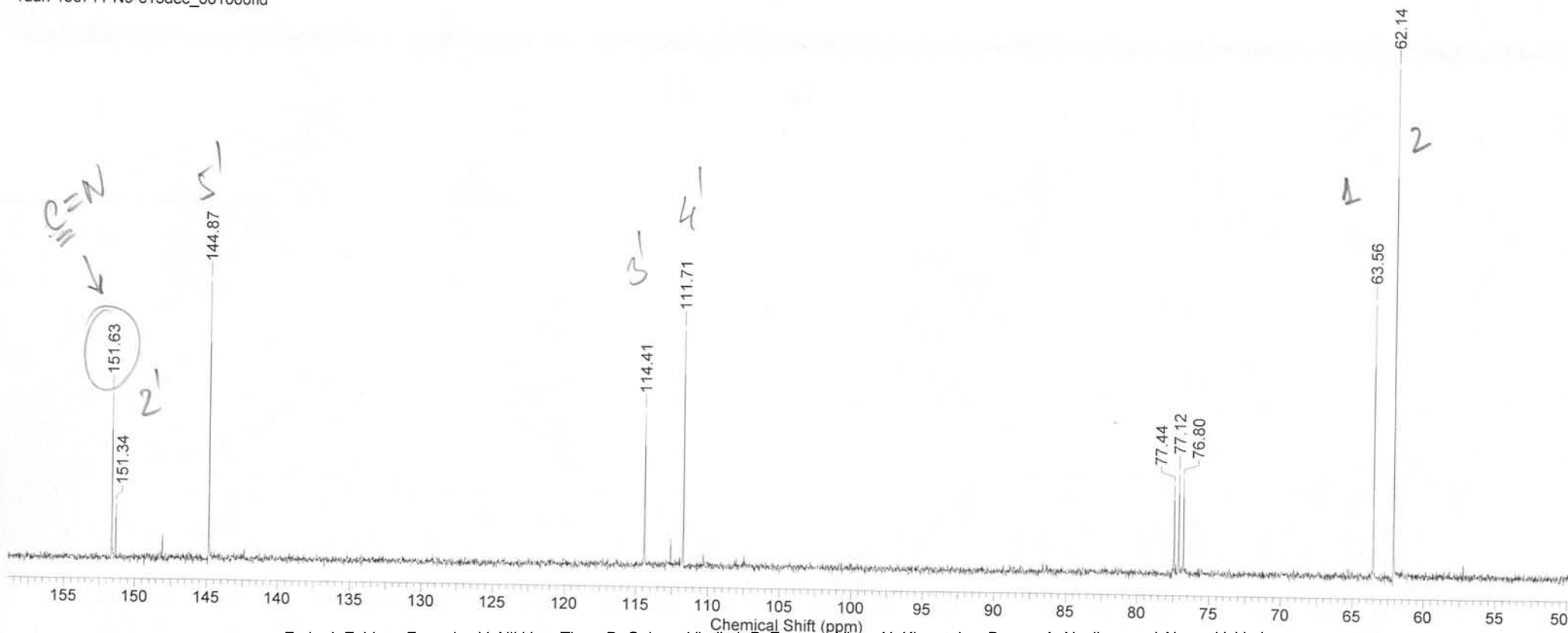
Formula $C_7H_9NO_2$ FW 139.1519

Acquisition Time (sec)	0.5898	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	22 Jul 2011 11:54:40
Date Stamp	22 Jul 2011 11:54:40	File Name	D:\NMR\19.07.11 (Poma)\rudn-190711-N9-c13dec\rudn-190711-N9-c13dec_001000fid	Number of Transients	636
Frequency (MHz)	100.62	Nucleus	13C	Points Count	16384
Original Points Count	16384	Owner	root	Solvent	CHLOROFORM-d
Receiver Gain	32768.00	SW(cyclical) (Hz)	27777.78	Temperature (degree C)	27.000
Spectrum Offset (Hz)	9634.7207	Sweep Width (Hz)	27776.08		

Compound 12a reaction mixture

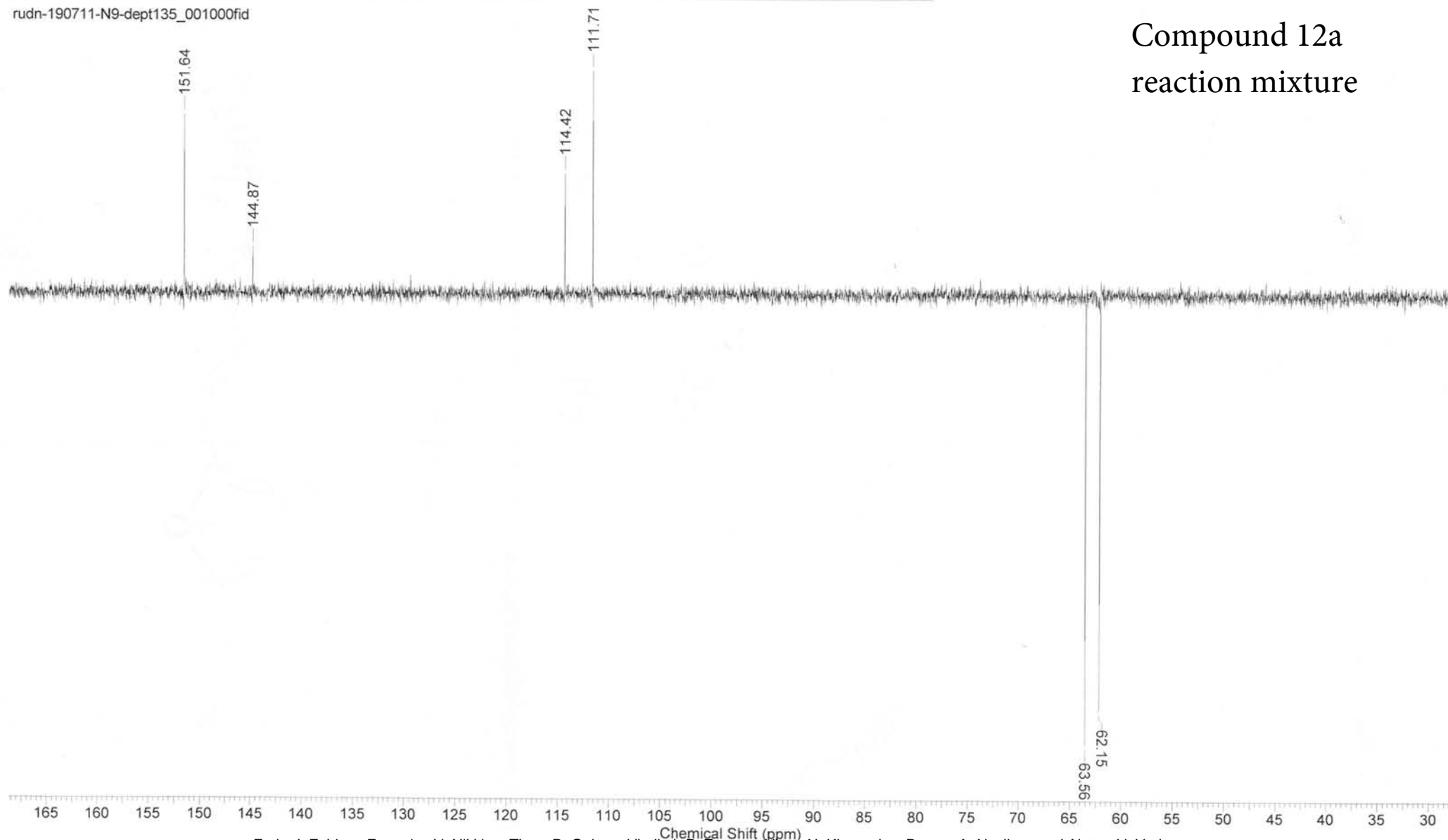


rudn-190711-N9-c13dec_001000fid



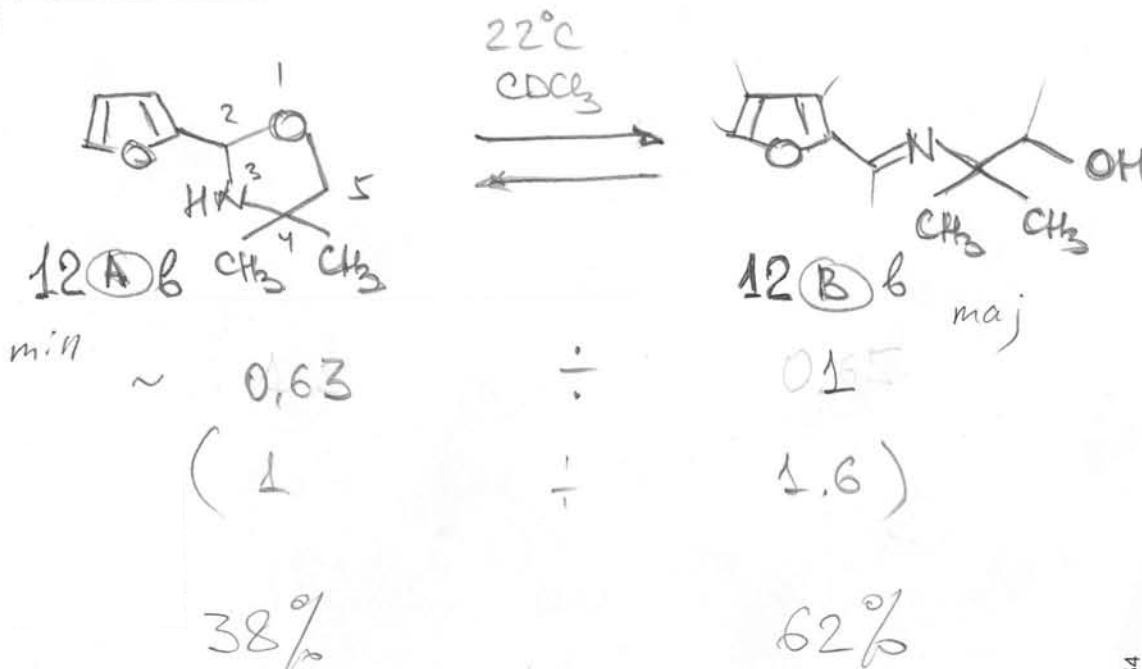
Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	22 Jul 2011 12:09:36
Date Stamp	22 Jul 2011 12:09:36	File Name	D:\NMR\19.07.11 (Poma)\rudn-190711-N9-dept135\rudn-190711-N9-dept135_001000fid		
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	659
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	9634.8008	Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000
				Origin	spect
				Pulse Sequence	dept135

rudn-190711-N9-dept135_001000fid



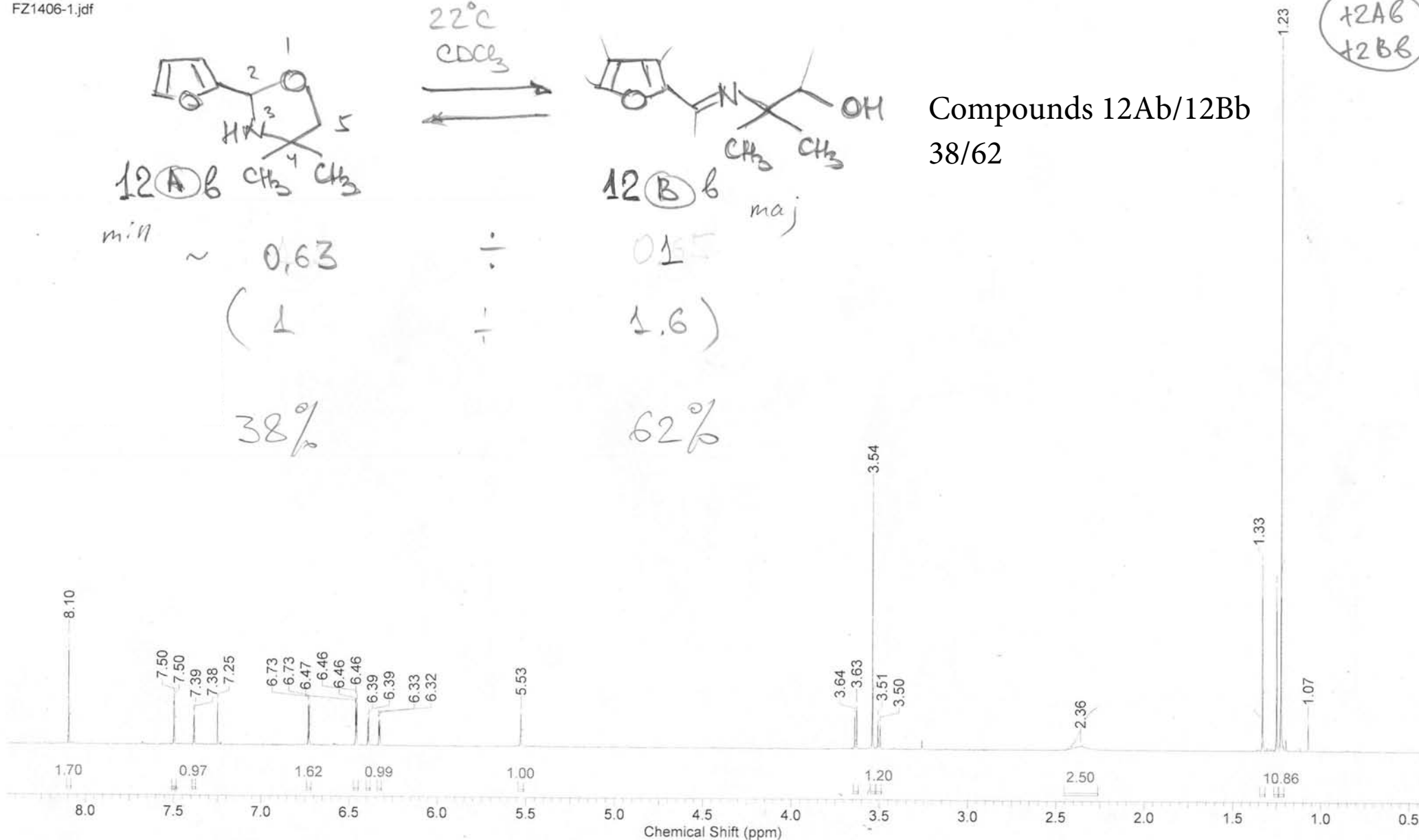
Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	26 Oct 2010 12:01:47	Date Stamp	26 Oct 2010 11:14:25
File Name	D:\NMR\22.10.10\FZ1406-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	32.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3000.8616	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	21.700					Sweep Width (Hz)	11261.26

FZ1406-1.jdf



Compounds 12Ab/12Bb
38/62

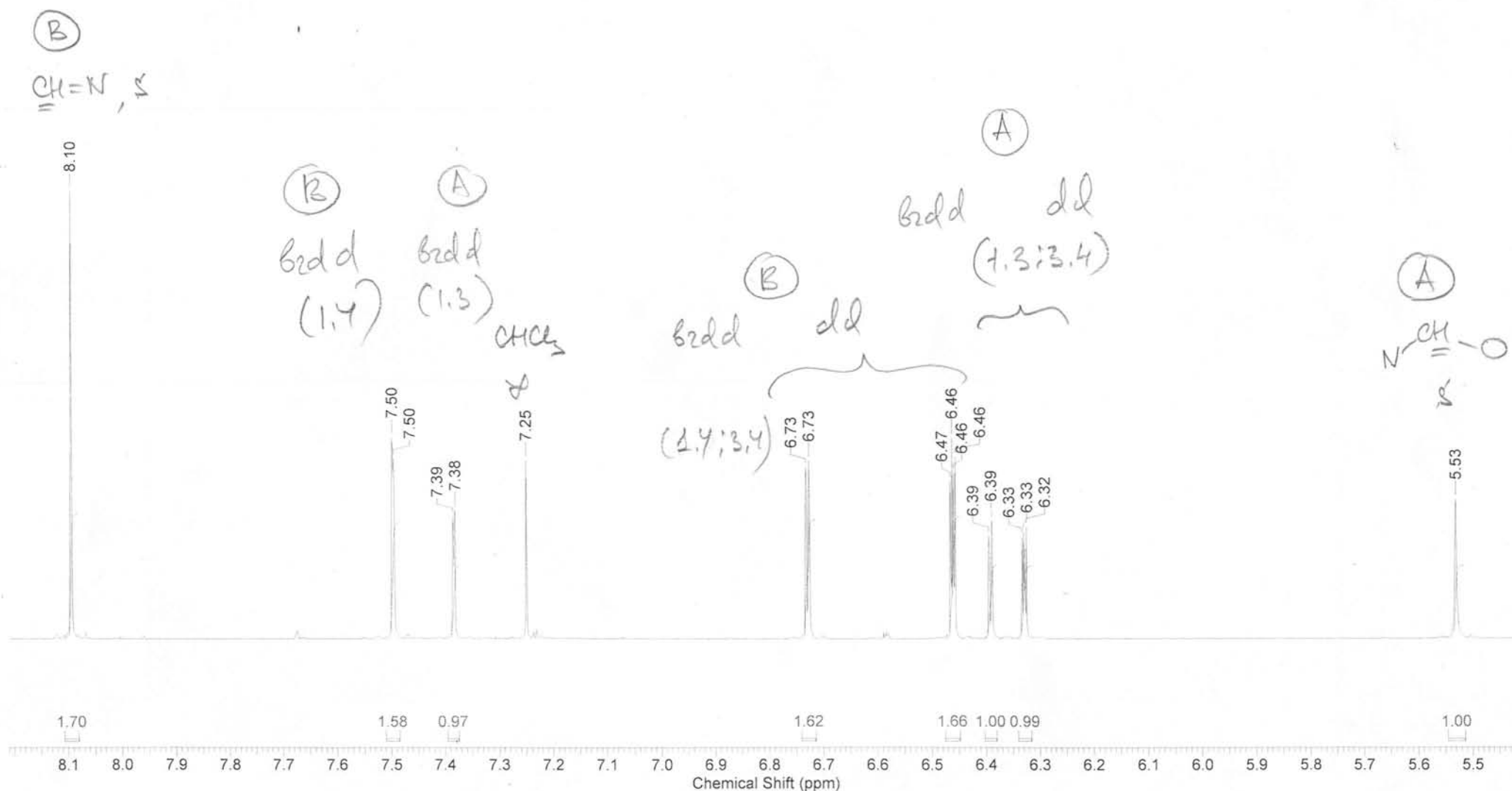
12Ab
12Bb



Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	26 Oct 2010 12:01:47	Date Stamp	26 Oct 2010 11:14:25
File Name	D:\NMR\22.10.10\FZ1406-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	32.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3000.8616	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	21.700					Sweep Width (Hz)	11261.26

FZ1406-1.jdf

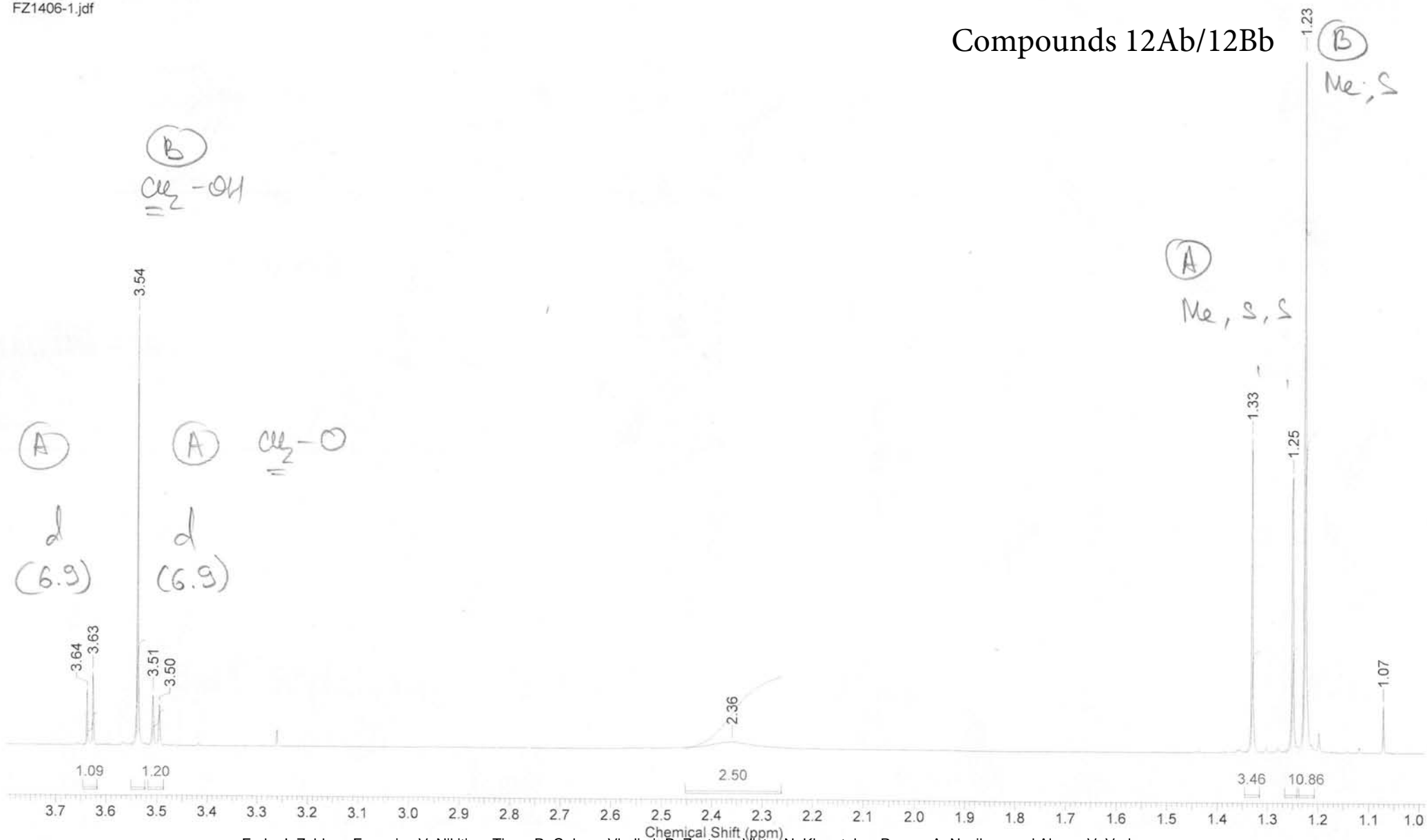
Compounds 12Ab/12Bb



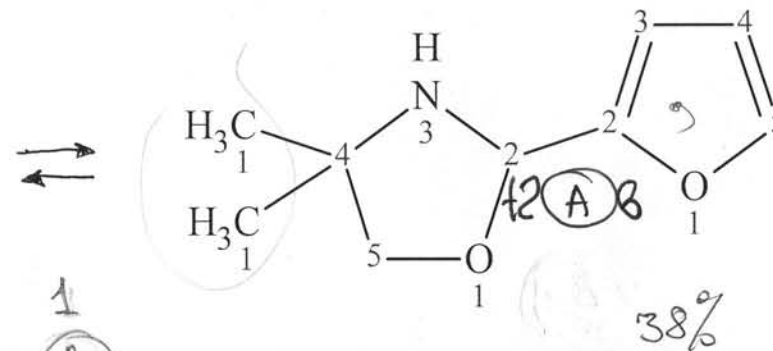
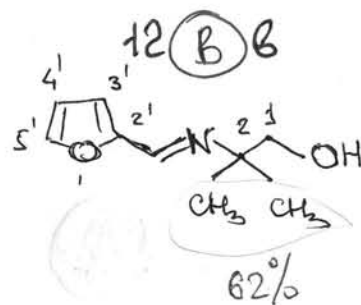
Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	26 Oct 2010 12:01:47	Date Stamp	26 Oct 2010 11:14:25
File Name	D:\NMR\22.10.10\FZ1406-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	32.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3000.8616	Sweep Width (Hz)	11261.26
Temperature (degree C)	21.700						

FZ1406-1.jdf

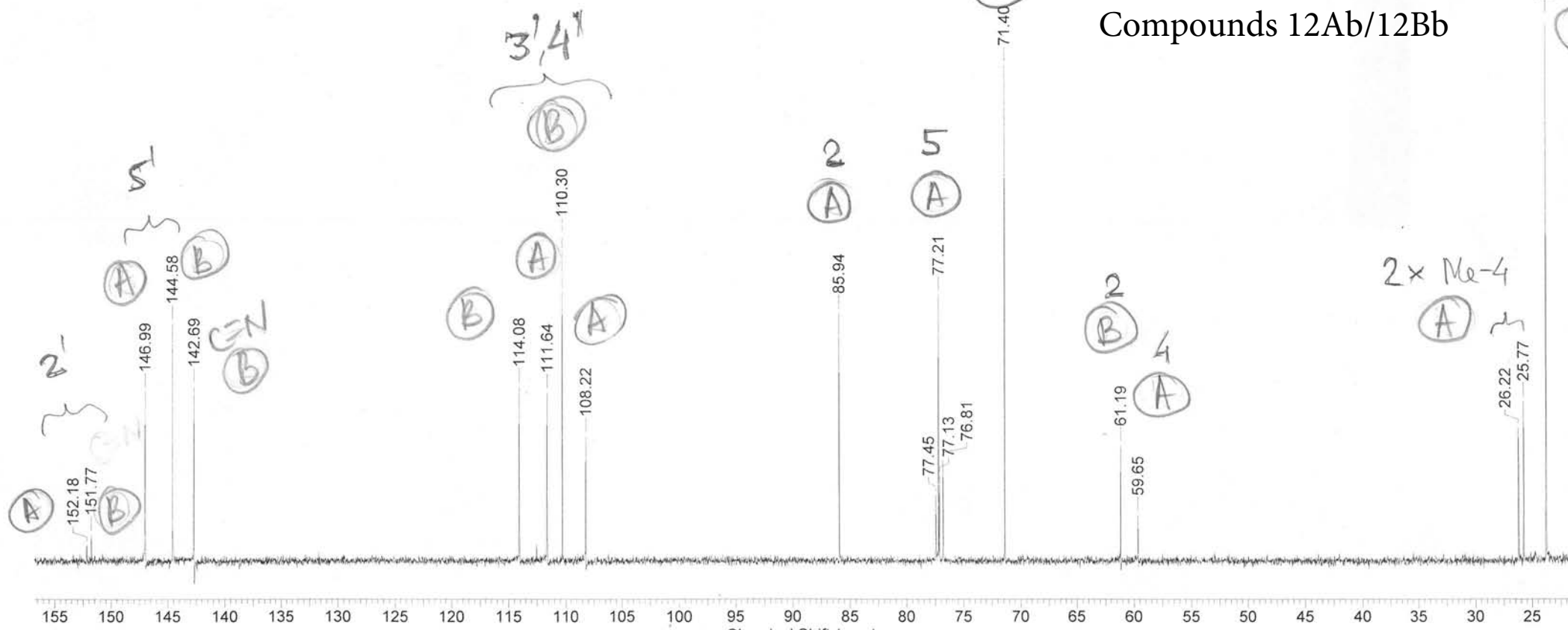
Compounds 12Ab/12Bb



Acquisition Time (sec)	0.5898	Comment	Imported from UXNMR.		Date	01 Sep 2011 09:53:04	
File Name	C:\Users\Fedor\Desktop\26.08.11\rudn-260811-N5-c13dec\rudn-260811-N5-c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	564	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	27777.78	Temperature (degree C)	27.000

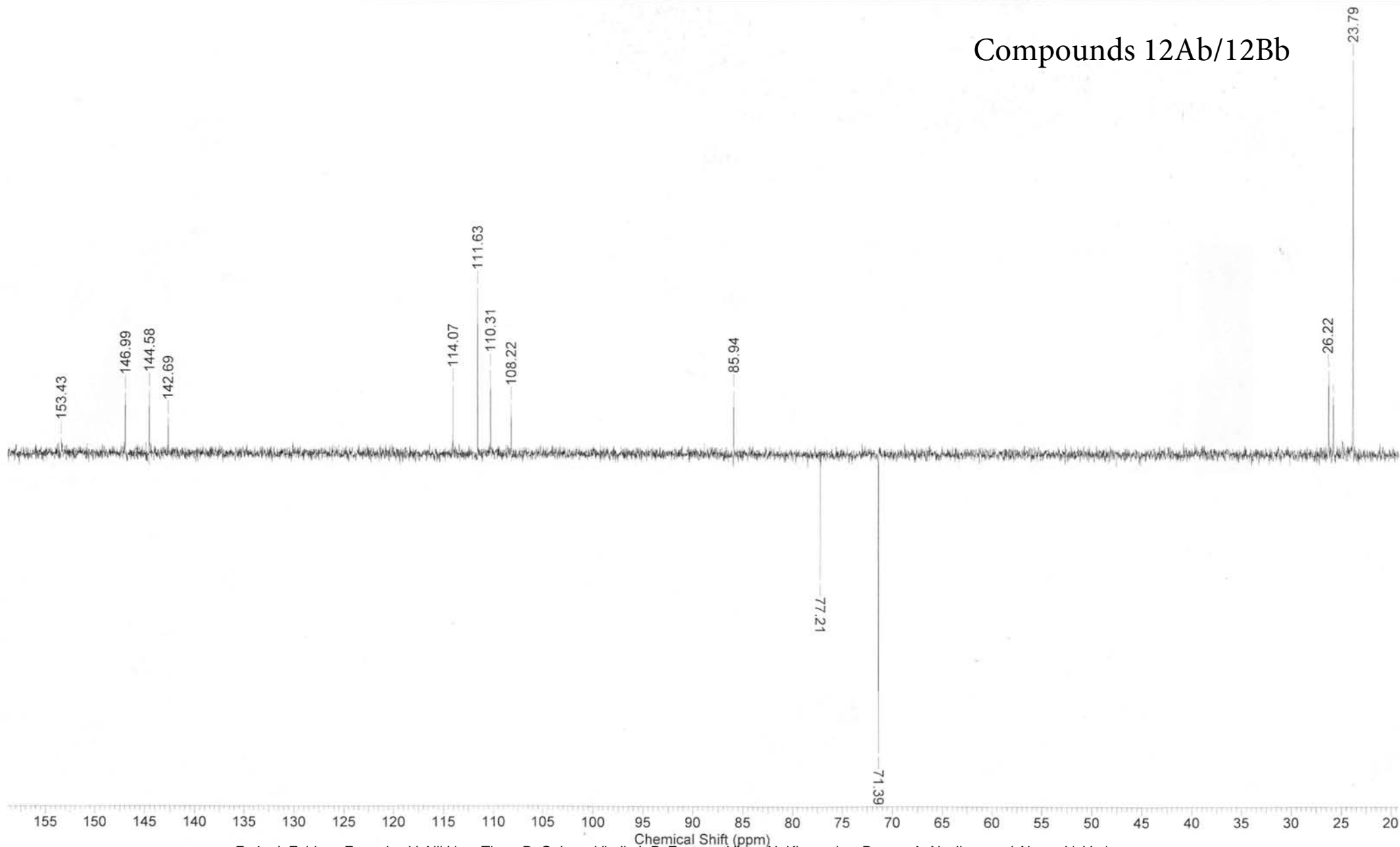


Compounds 12Ab/12Bb



Acquisition Time (sec)	0.5571	Comment	Imported from UXNMR.		Date	01 Sep 2011 10:10:08	
File Name	C:\Users\Fedor\Desktop\26.08.11\rudn-260811-N5-dept135\rudn-260811-N5-dept135_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	251	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	CHLOROFORM-D	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

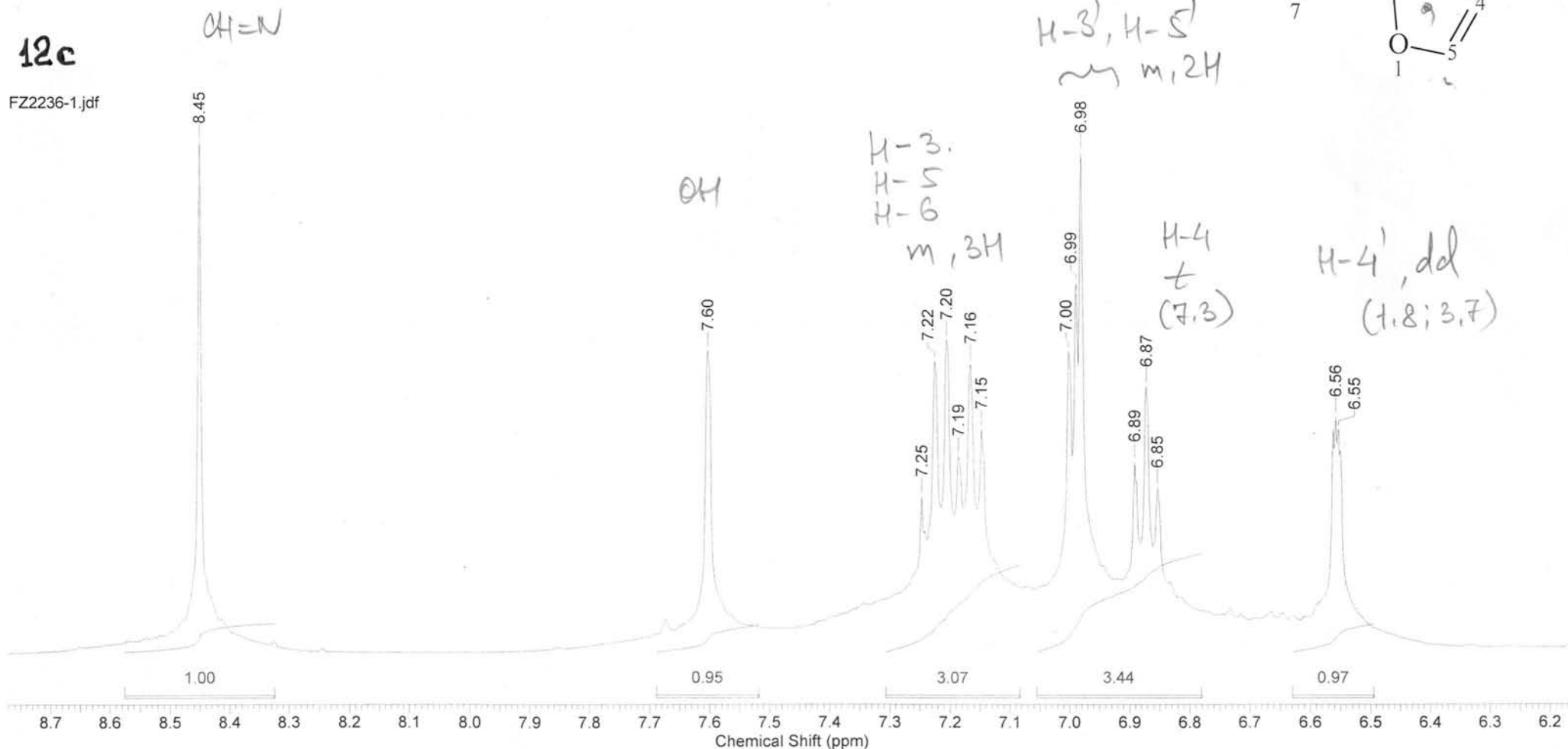
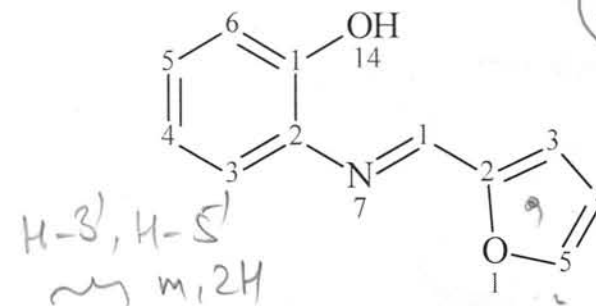
Compounds 12Ab/12Bb



Formula C₁₁H₉NO₂ FW 187.1947

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	28 Feb 2012 09:05:05	Date Stamp	28 Feb 2012 13:39:38
File Name	D:\NMR\21.02.12\FZ2236-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	4
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	32.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	1998.9109	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	24.100			Sweep Width (Hz)	7503.00		

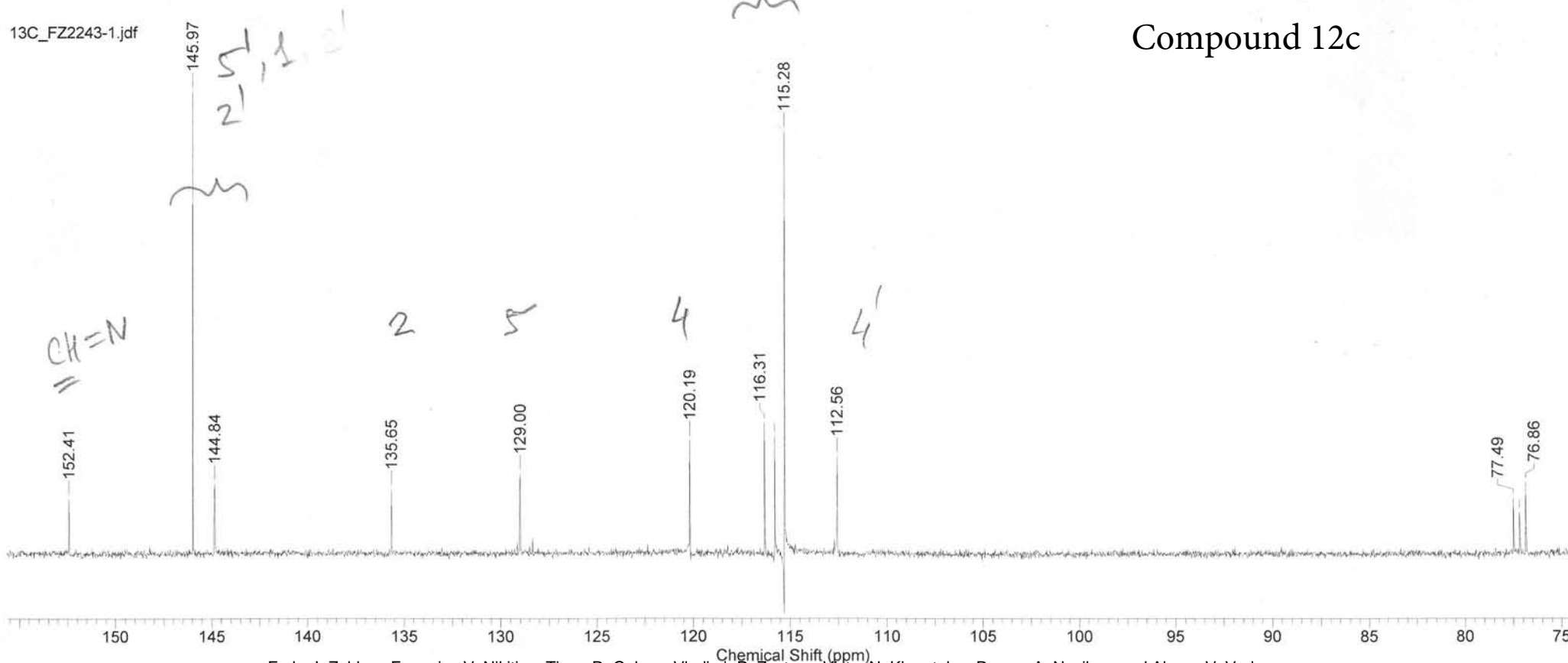
Compound 12c



Formula C₁₁H₉NO₂ FW 187.1947

Acquisition Time (sec)	0.5217	Comment	single pulse decoupled gated NOE	Date	06 Mar 2012 09:53:18
Date Stamp	06 Mar 2012 14:28:06	File Name	D:\NMR\05.03.12\13C_FZ2243-1.jdf	Origin	ECS 400
Frequency (MHz)	100.53	Nucleus	13C	Number of Transients	106
Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	54.00	Solvent	CHLOROFORM-d	Pulse Sequence	single_pulse_dec
Sweep Width (Hz)	31407.04	Temperature (degree C)	24.400	Spectrum Offset (Hz)	10052.5303

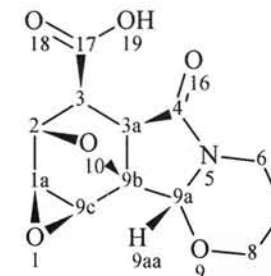
13C_FZ2243-1.jdf



Compound 12c

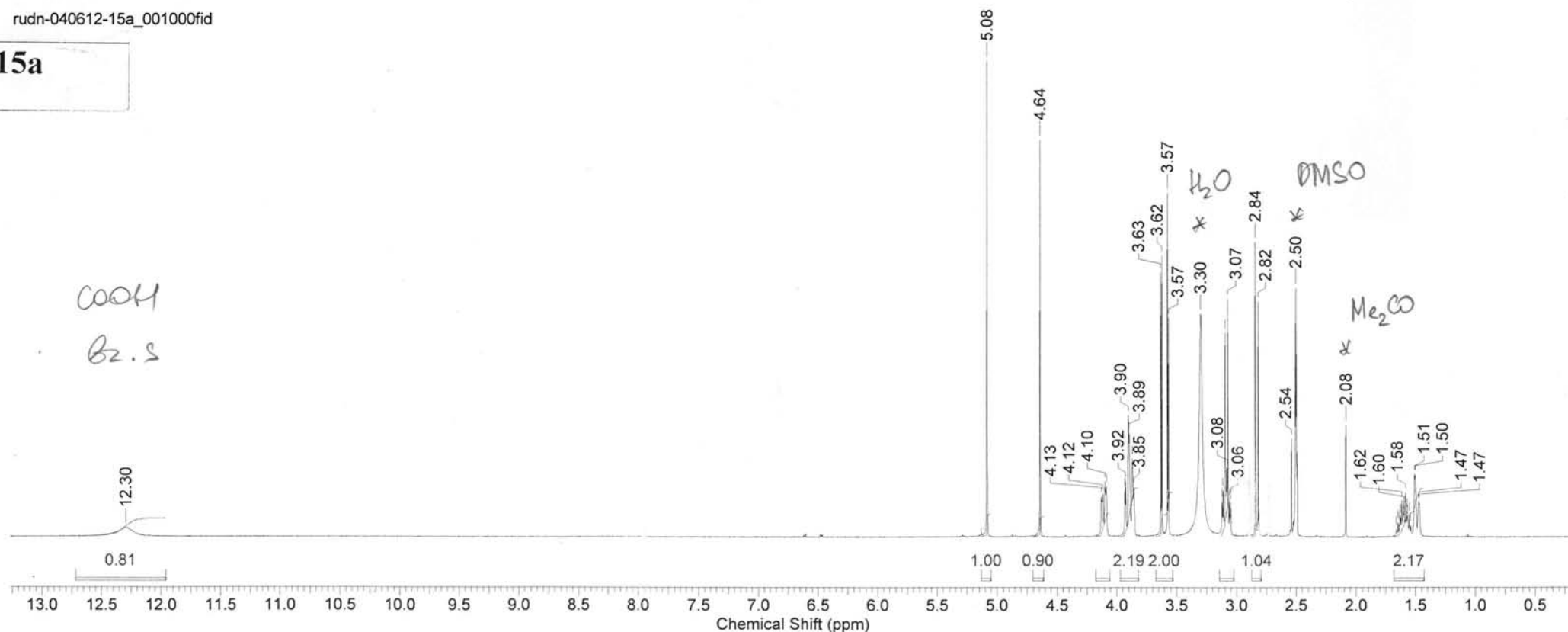
Formula C ₁₂ H ₁₃ NO ₆		FW 267.2347	
Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400
Date Stamp	08 Jun 2012 15:15:12		Date 08 Jun 2012 15:15:12
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-15a\rudn-040612-15a_001000fid		Frequency (MHz) 400.14
Nucleus	1H	Number of Transients	20
Owner	root	Points Count	16384
SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6
Temperature (degree C)	32.000	Spectrum Offset (Hz)	2712.0542
		Origin	spect
		Pulse Sequence	zg
		Original Points Count	16384
		Receiver Gain	128.00
		Sweep Width (Hz)	10416.03

Compound 15a



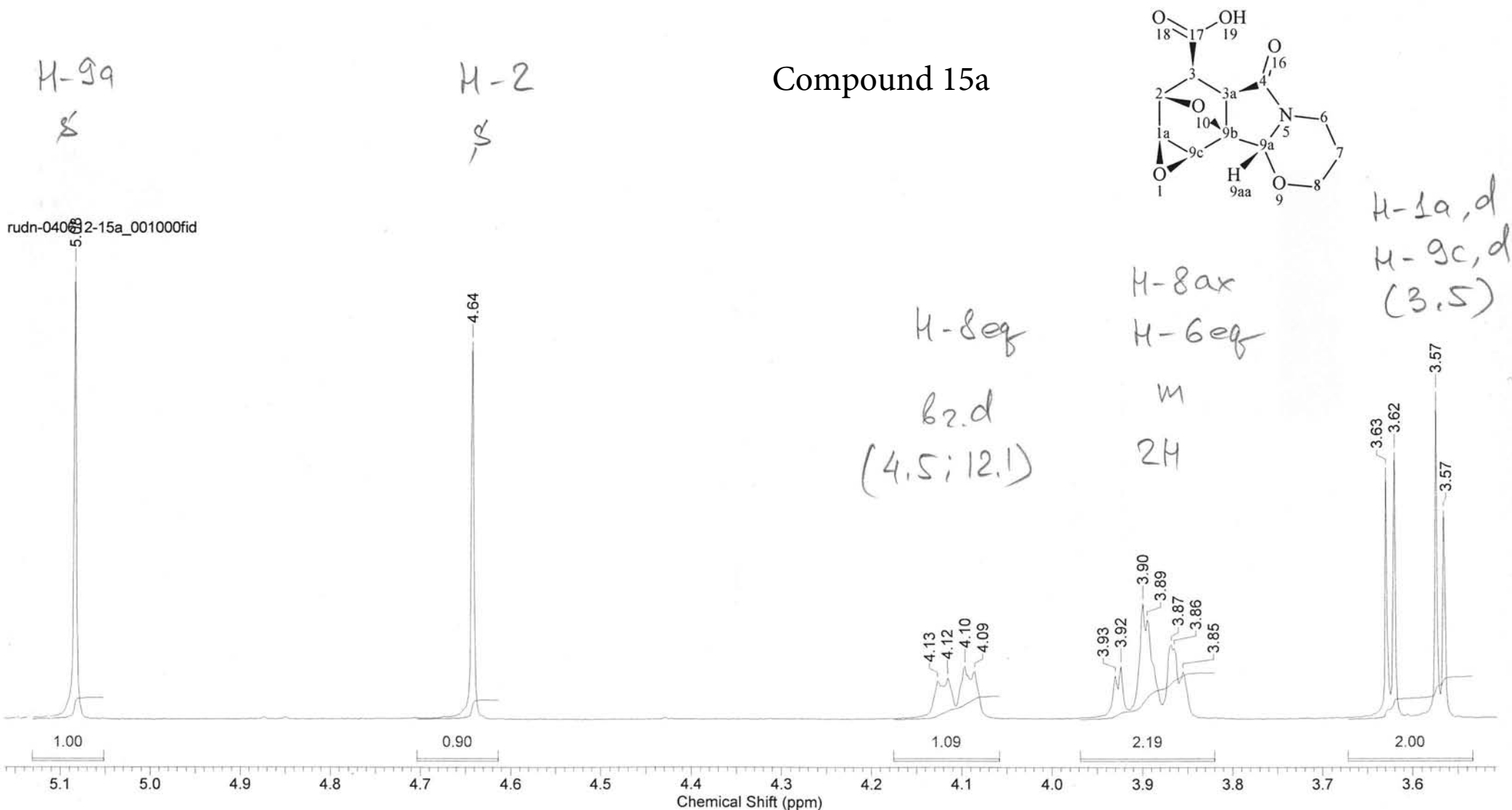
rudn-040612-15a_001000fid

15a



Formula C₁₂H₁₃NO₆ FW 267.2347

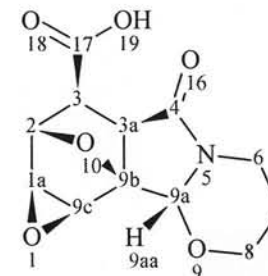
Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	08 Jun 2012 15:15:12
Date Stamp	08 Jun 2012 15:15:12				
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-15a\rudn-040612-15a_001000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	20	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zg
SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542
Temperature (degree C)	32.000			Sweep Width (Hz)	10416.03



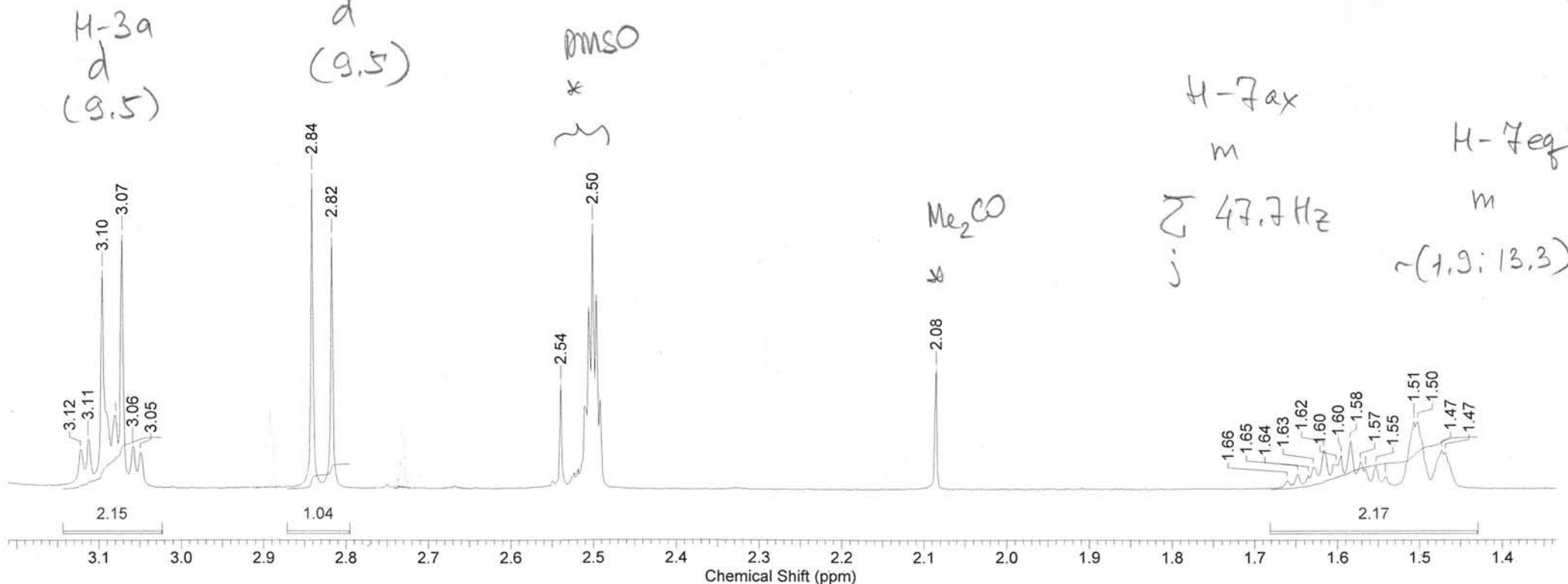
Formula C ₁₂ H ₁₃ NO ₆		FW 267.2347	
Acquisition Time (sec) 1.5729	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400		Date 08 Jun 2012 15:15:12
Date Stamp 08 Jun 2012 15:15:12			
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-15a\rudn-040612-15a_001000fid	Frequency (MHz) 400.14		Original Points Count 16384
Nucleus 1H	Number of Transients 20	Origin spect	Receiver Gain 128.00
Owner root	Points Count 16384	Pulse Sequence zg	Sweep Width (Hz) 10416.03
SW(cyclical) (Hz) 10416.67	Solvent DMSO-d6	Spectrum Offset (Hz) 2712.0542	
Temperature (degree C) 32.000			

H-6 ax
ddd
(3.8; 12.1; 13.4)

Compound 15a



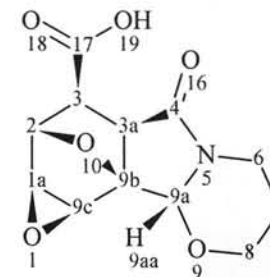
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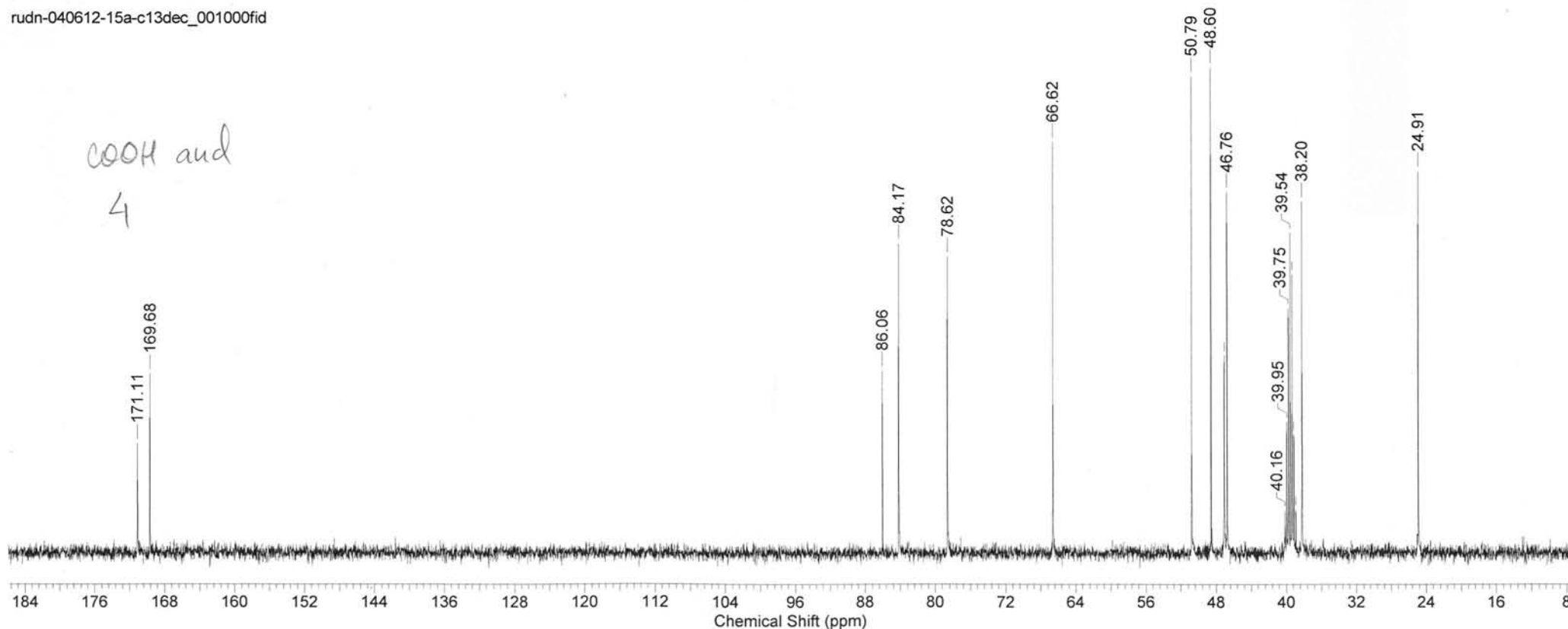
Formula	C ₁₂ H ₁₃ NO ₆	FW	267.2347
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	08 Jun 2012 13:39:12		
Date Stamp	08 Jun 2012 13:39:12						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-15a-c13dec\rudn-040612-15a-c13dec_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	427	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zgpg
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6	Spectrum Offset (Hz)	10554.7930
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				

Compound 15a



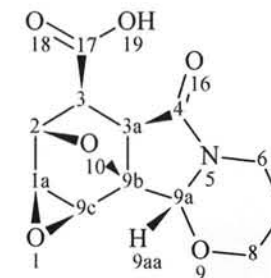
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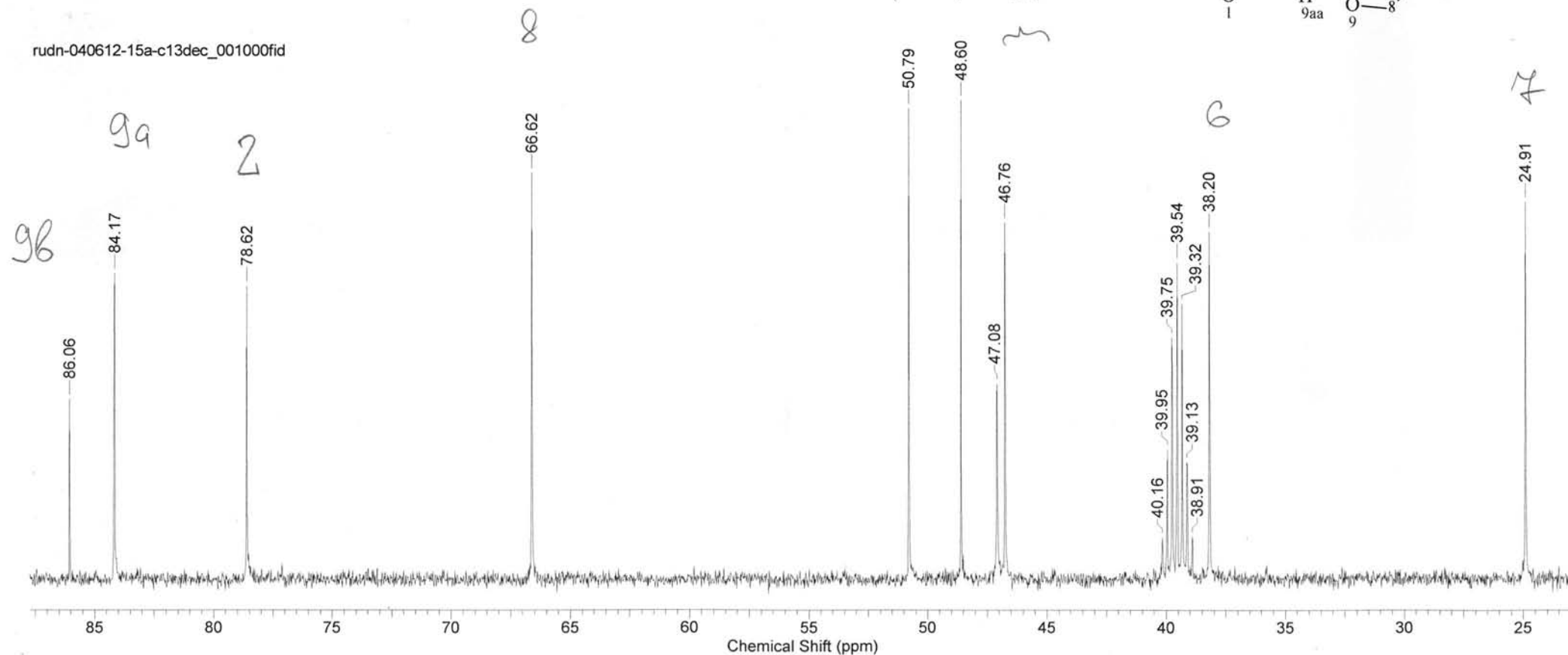
Formula	C ₁₂ H ₁₃ NO ₆	FW	267.2347
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	08 Jun 2012 13:39:12		
Date Stamp	08 Jun 2012 13:39:12						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-15a-c13dec\rudn-040612-15a-c13dec_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	427	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zgpg
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6	Spectrum Offset (Hz)	10554.7930
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				

Compound 15a

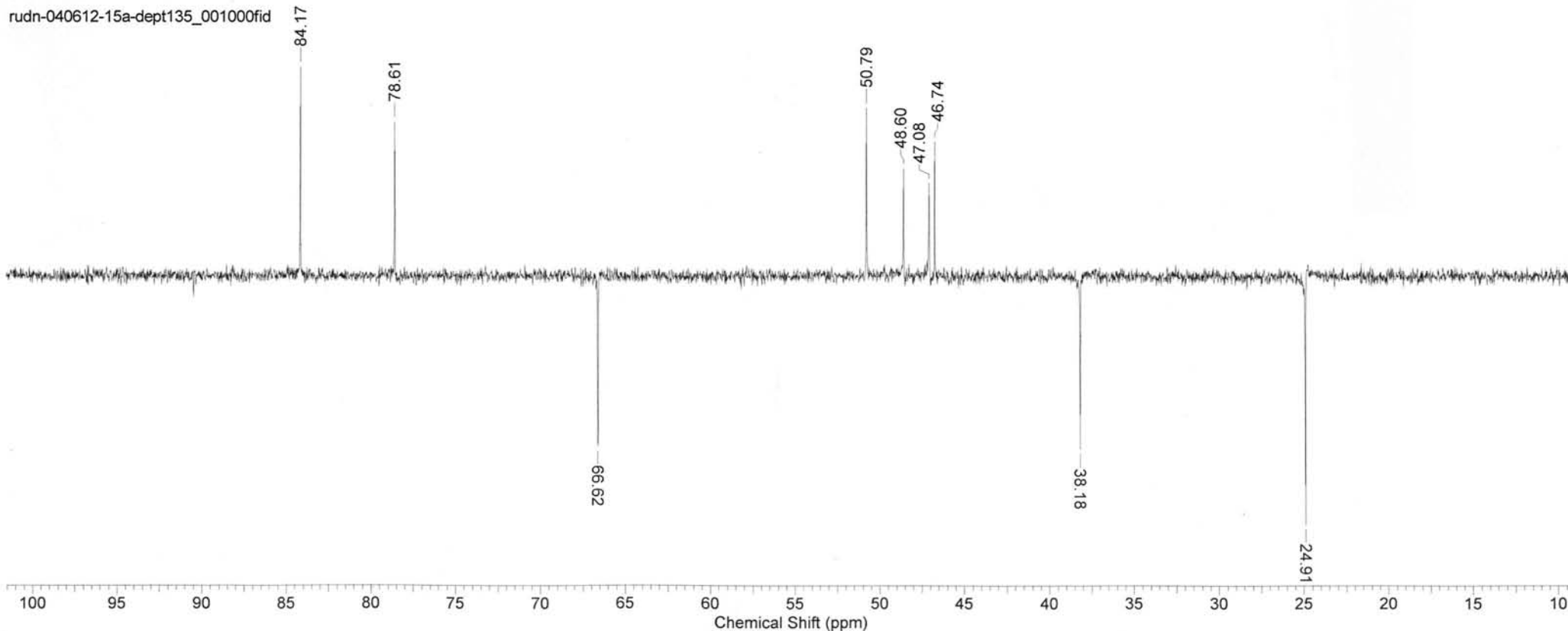
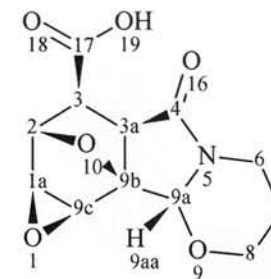


rudn-040612-15a-c13dec_001000fid



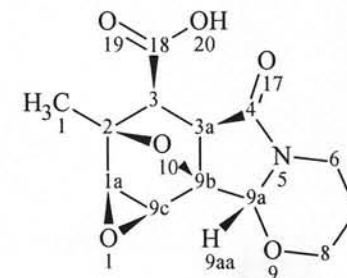
Formula C ₁₂ H ₁₃ NO ₆	FW 267.2347			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 08 Jun 2012 13:45:36		
Date Stamp 08 Jun 2012 13:45:36				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-15a-dept135\rudn-040612-15a-dept135_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 322	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence dept135	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 9104.3838	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compound 15a



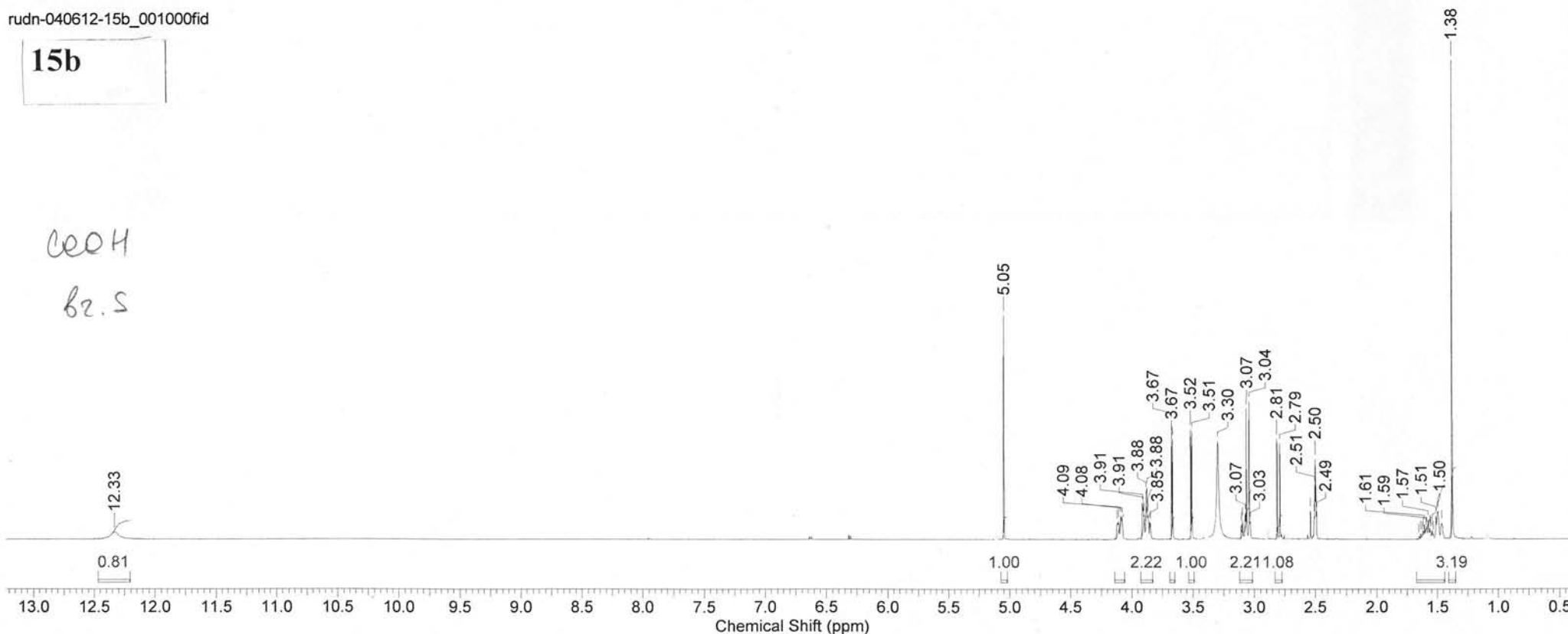
Formula C ₁₃ H ₁₅ NO ₆	FW 281.2613			
Acquisition Time (sec) 1.5729	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 08 Jun 2012 15:17:20		
Date Stamp 08 Jun 2012 15:17:20				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-15b\rudn-040612-15b_001000fid	Frequency (MHz) 400.14			
Nucleus 1H	Number of Transients 20	Origin spect	Original Points Count 16384	
Owner root	Points Count 16384	Pulse Sequence zg	Receiver Gain 128.00	
SW(cyclical) (Hz) 10416.67	Solvent DMSO-d6	Spectrum Offset (Hz) 2712.0542	Sweep Width (Hz) 10416.03	
Temperature (degree C) 32.000				

Compound 15b



rudn-040612-15b_001000fid

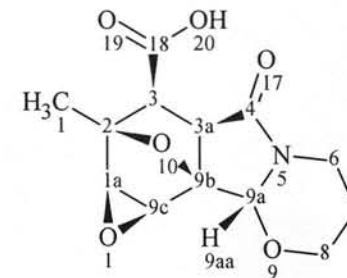
15b

ceOH
bz.s

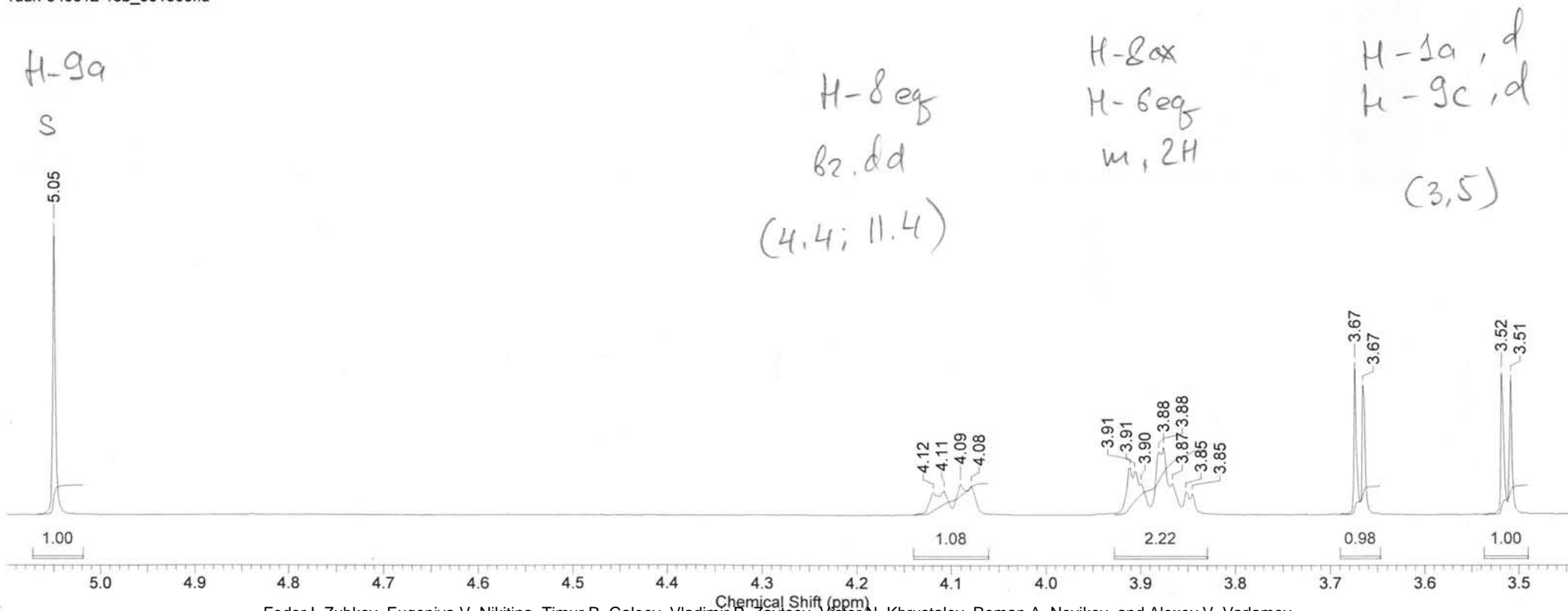
Formula	C ₁₃ H ₁₅ NO ₆	FW	281.2613
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Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	08 Jun 2012 15:17:20
Date Stamp	08 Jun 2012 15:17:20				
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-15b\rudn-040612-15b_001000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	20	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zg
SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542
Temperature (degree C)	32.000			Sweep Width (Hz)	10416.03

Compound 15b



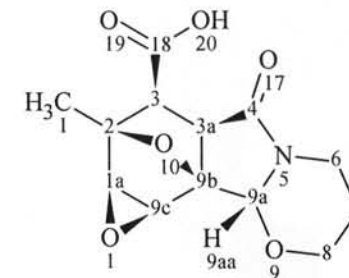
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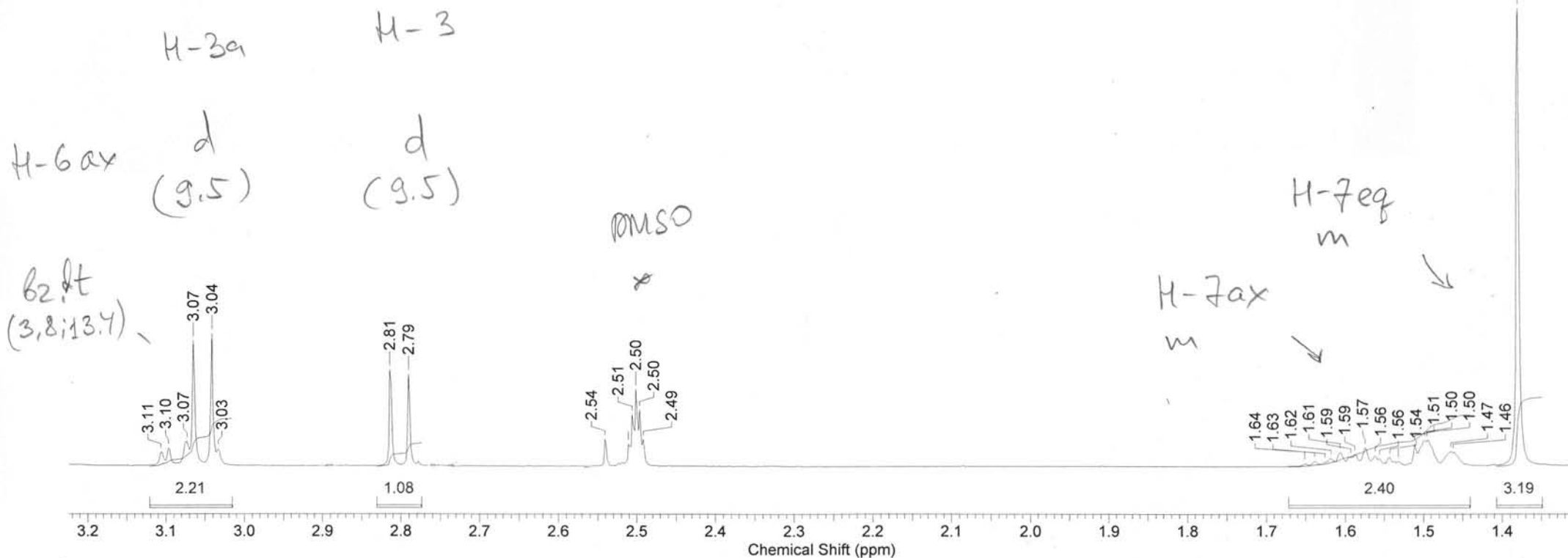
Formula $C_{13}H_{15}NO_6$ FW 281.2613

Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	08 Jun 2012 15:17:20
Date Stamp	08 Jun 2012 15:17:20				
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-15b\rudn-040612-15b_001000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	20	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zg
SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542
Temperature (degree C)	32.000			Sweep Width (Hz)	10416.03

Compound 15b

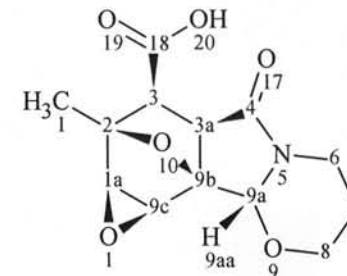


rudn-040612-15b_001000fid

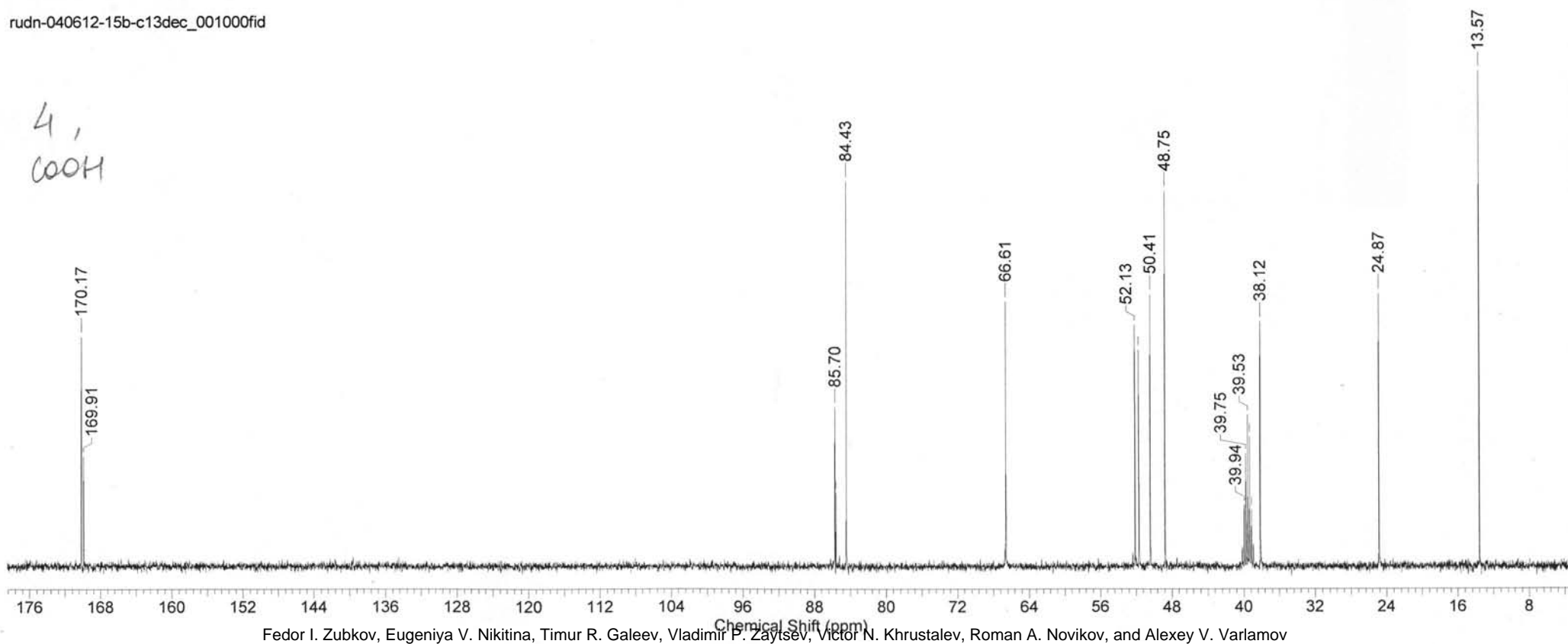


Formula C ₁₃ H ₁₅ NO ₆		FW 281.2613	
Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400
Date Stamp	08 Jun 2012 16:34:08		Date 08 Jun 2012 16:34:08
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-15b-c13dec\rudn-040612-15b-c13dec_001000fid		
Frequency (MHz)	100.62	Nucleus	13C
Original Points Count	16384	Owner	root
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000
		Number of Transients	227
		Points Count	16384
		Solvent	DMSO-d6
		Origin	spect
		Pulse Sequence	zgpg
		Spectrum Offset (Hz)	10556.1514

Compound 15b

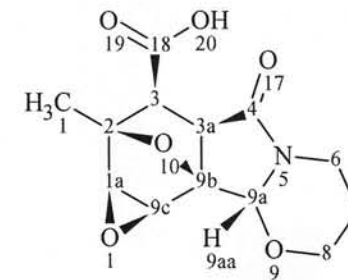


rudn-040612-15b-c13dec_001000fid

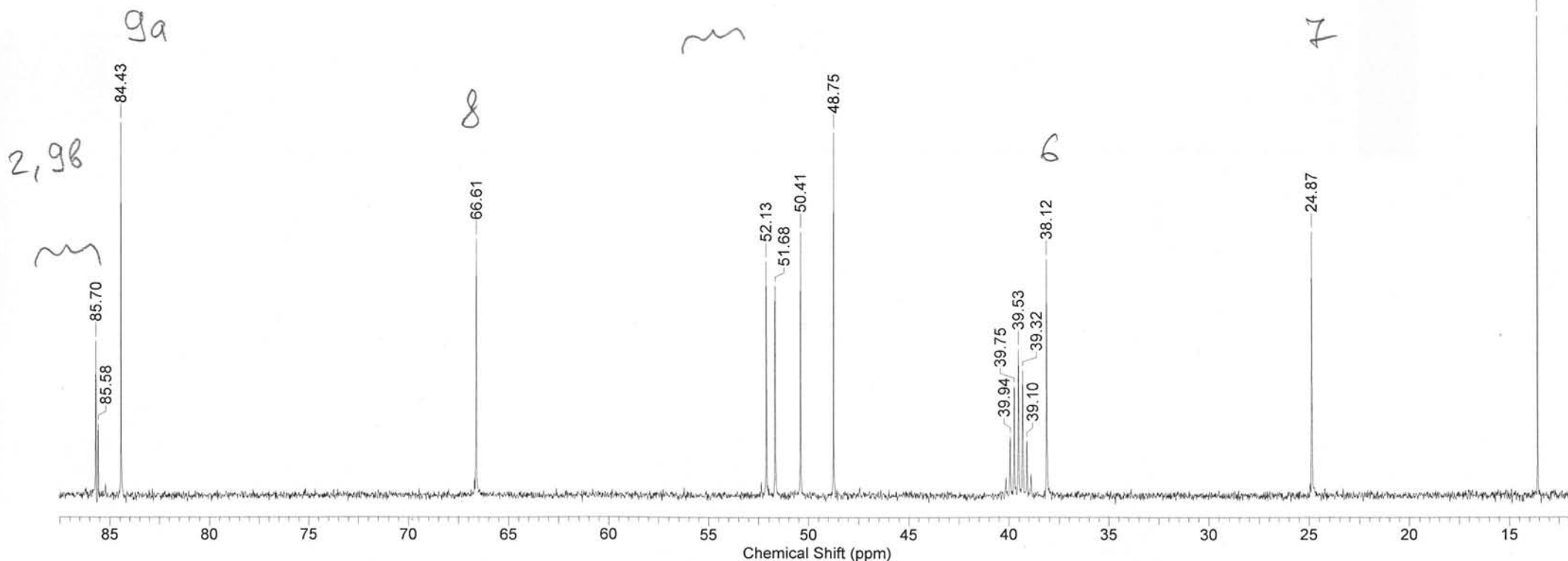


Formula C ₁₃ H ₁₅ NO ₆	FW 281.2613			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 08 Jun 2012 16:34:08		
Date Stamp 08 Jun 2012 16:34:08				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-15b-c13dec\rudn-040612-15b-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 227	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10556.1514	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compound 15b



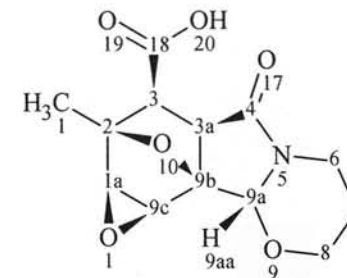
rudn-040612-15b-c13dec_001000fid



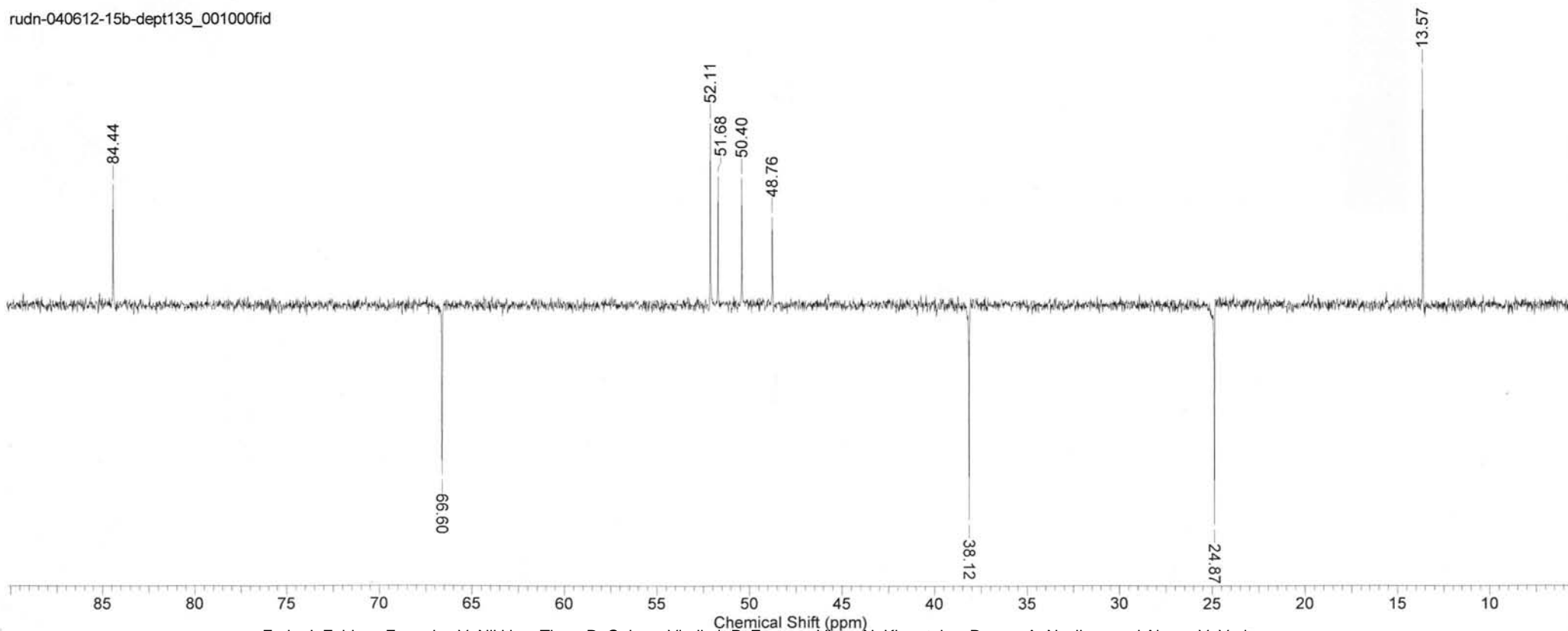
Formula	C ₁₃ H ₁₅ NO ₆	FW	281.2613
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	08 Jun 2012 16:40:32	
Date Stamp	08 Jun 2012 16:40:32						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-040612-15b-dept135\rudn-040612-15b-dept135_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	129	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	dept135
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6	Spectrum Offset (Hz)	9105.7412
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				

Compound 15b

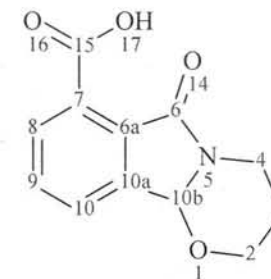


rudn-040612-15b-dept135_001000fid



Formula C ₁₂ H ₁₁ NO ₄		FW 233.2200	
Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400
Date Stamp	06 Jul 2011 16:25:36	Date	06 Jul 2011 16:25:36
File Name	C:\Users\Fedor\Desktop\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\rudn-0611-N38\rudn-0611-N38_001000fid		
Frequency (MHz)	400.14	Nucleus	1H
Original Points Count	16384	Number of Transients	16
Receiver Gain	256.00	Owner	root
Sweep Width (Hz)	10416.03	Points Count	16384
		Pulse Sequence	zg
		Solvent	DMSO-d6
		Spectrum Offset (Hz)	2712.0542
		SW(cyclical) (Hz)	10416.67
		Temperature (degree C)	32.000

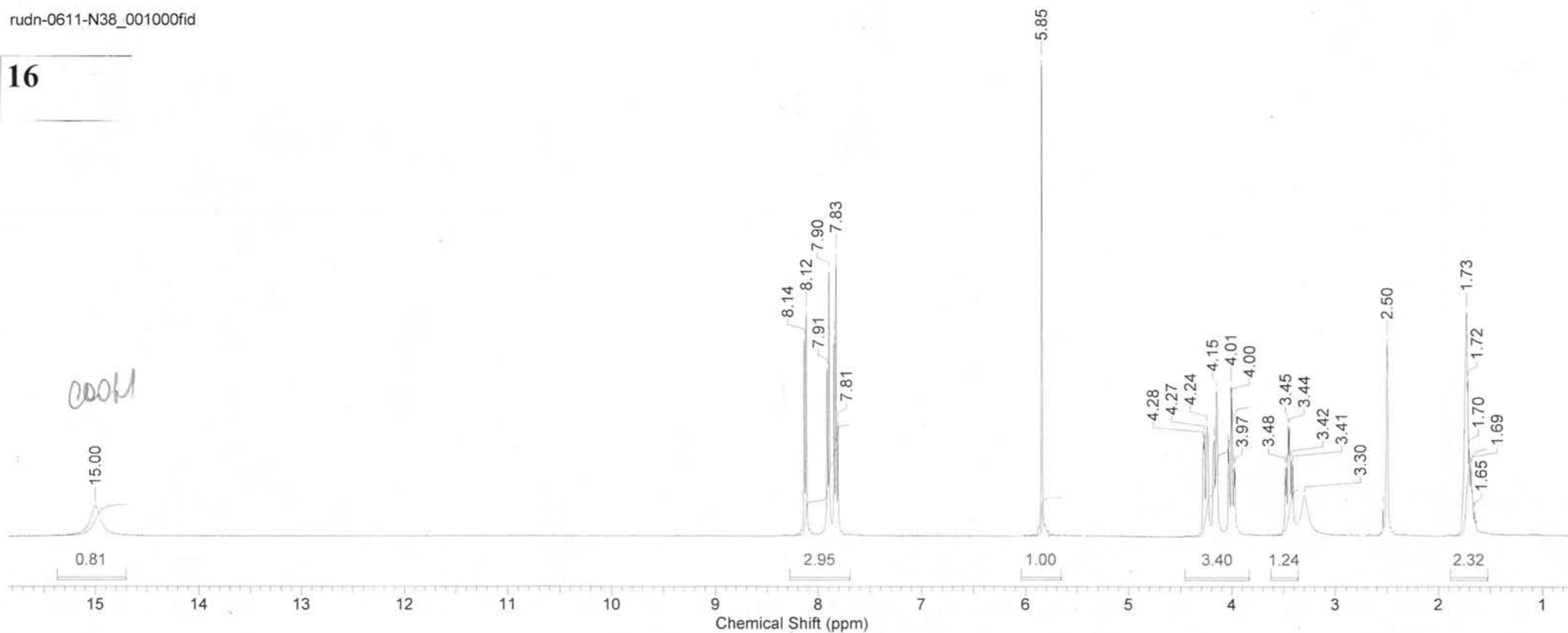
Compound 16



H-10b, s

rudn-0611-N38_001000fid

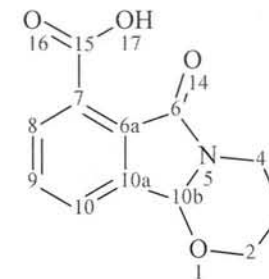
16



Formula C₁₂H₁₁NO₄ FW 233.2200

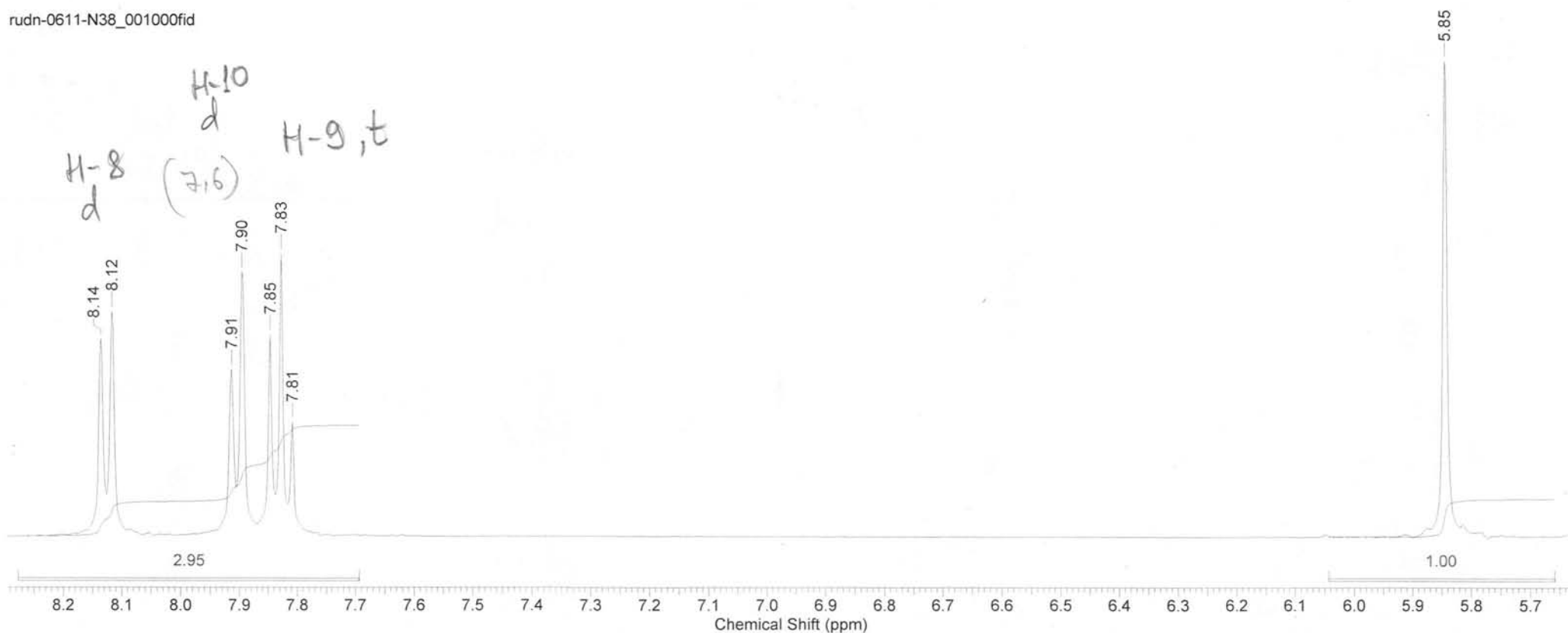
Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	06 Jul 2011 16:25:36	
Date Stamp	06 Jul 2011 16:25:36						
File Name	C:\Users\Fedor\Desktop\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\rudn-0611-N38\rudn-0611-N38_001000fid						
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	16	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zg
Receiver Gain	256.00	SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542
Sweep Width (Hz)	10416.03	Temperature (degree C)	32.000				

Compound 16



H-10b, s

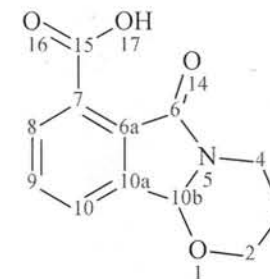
rudn-0611-N38_001000fid



Formula	C ₁₂ H ₁₁ NO ₄	FW	233.2200		
Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	06 Jul 2011 16:25:36
Date Stamp	06 Jul 2011 16:25:36				
File Name	C:\Users\Fedor\Desktop\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\rudn-0611-N38\rudn-0611-N38_001000fid				
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	16
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	256.00	SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6
Sweep Width (Hz)	10416.03	Temperature (degree C)	32.000	Spectrum Offset (Hz)	2712.0542

H-2eq
ddd
(1.8; 3.8; 11.4)

Compound 16



rudn-0611-N38_001000fid

H-4eq
ddd
(0.5; 4.5; 12.1)

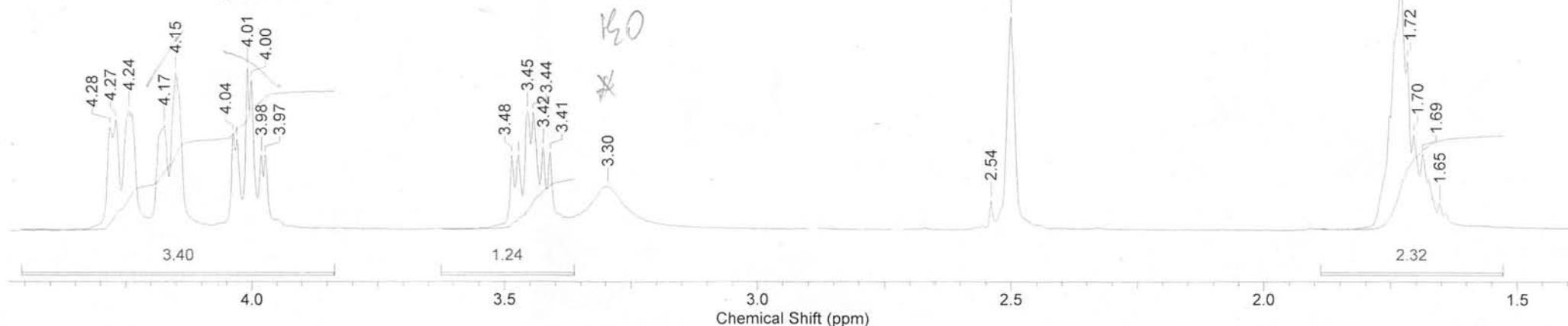
1.65-1.80

H-3, 2H

M

H-2ax
dt
(3.2; 11.4)

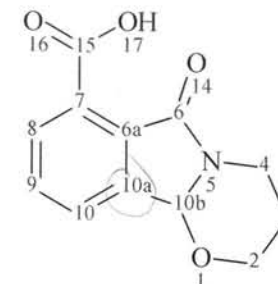
H-4ax
dt
(5.1; 12.1)



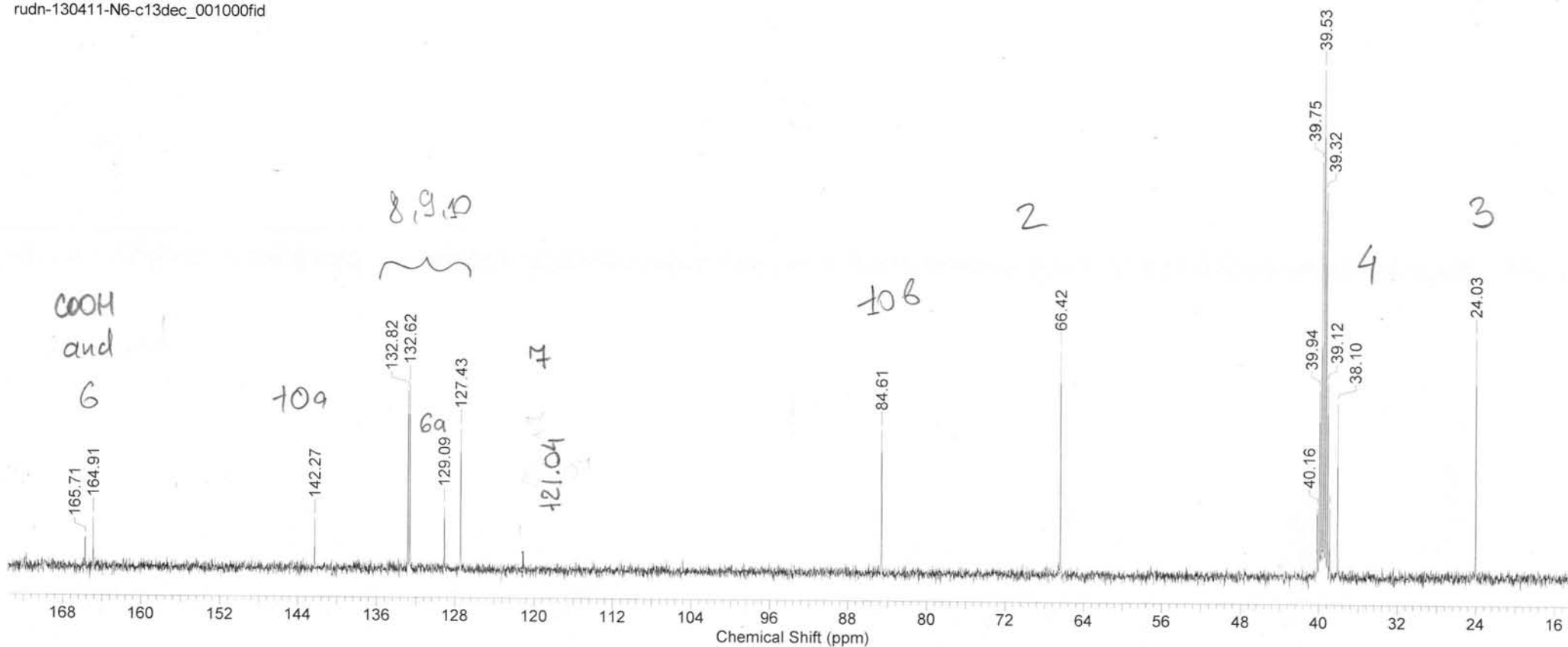
Formula C₁₂H₁₁NO₄ FW 233.2200

Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	14 Apr 2011 06:24:00
Date Stamp	14 Apr 2011 06:24:00	File Name	D:\NMR\13.04.2011 C-13\rudn-130411-N6-c13dec\rudn-130411-N6-c13dec_001000fid		
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	671
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6
Sweep Width (Hz)	29409.97	Temperature (degree C)	32.000	Pulse Sequence	zgpg
				Spectrum Offset (Hz)	10548.9658

Compound 16



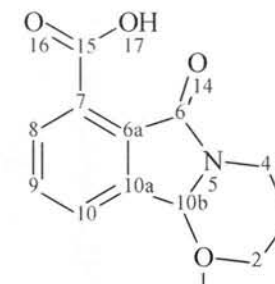
rudn-130411-N6-c13dec_001000fid



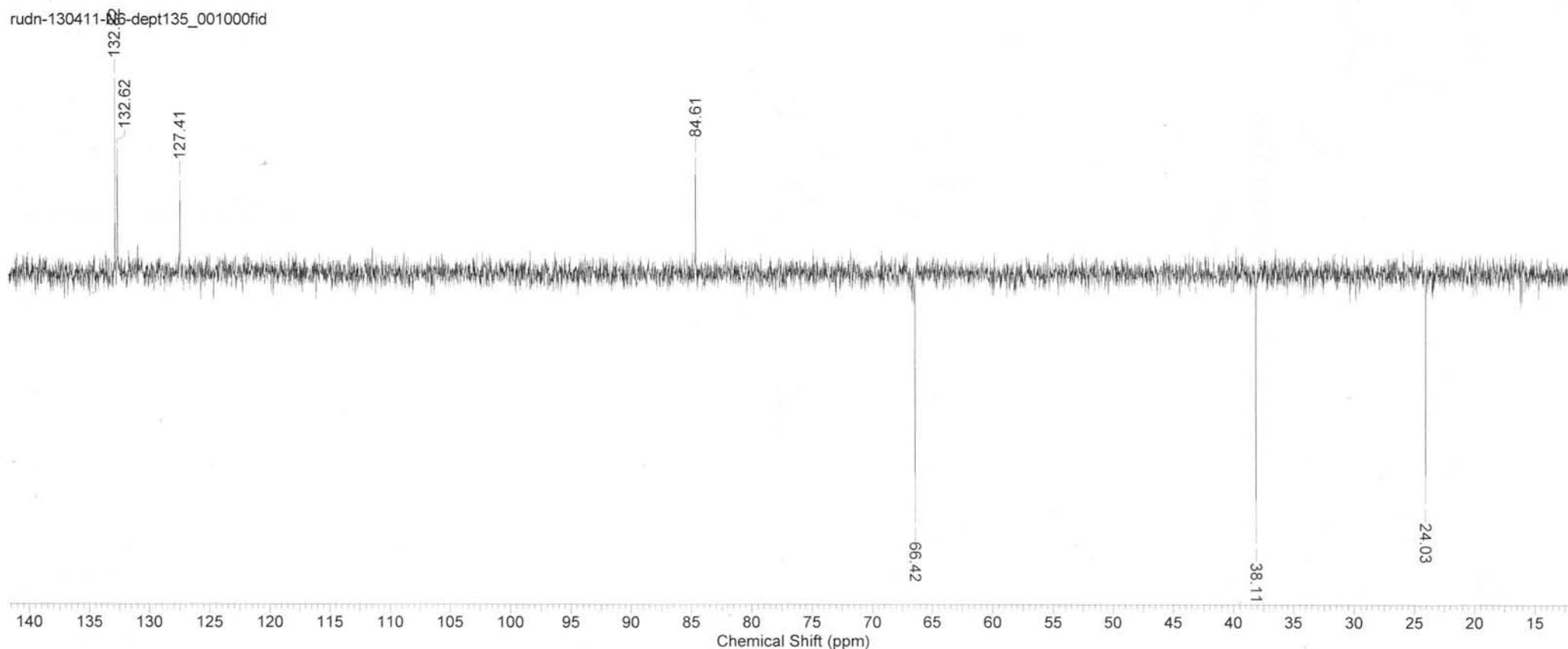
Formula C₁₂H₁₁NO₄ FW 233.2200

Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	14 Apr 2011 06:38:56
Date Stamp	14 Apr 2011 06:38:56	File Name	D:\NMR\13.04.2011 C-13\rudn-130411-N6-dept135\rudn-130411-N6-dept135_001000fid	Number of Transients	448
Frequency (MHz)	100.62	Nucleus	13C	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Pulse Sequence	dept135
Sweep Width (Hz)	29409.97	Temperature (degree C)	32.000	Solvent	DMSO-d6
				Spectrum Offset (Hz)	9098.5479

Compound 16

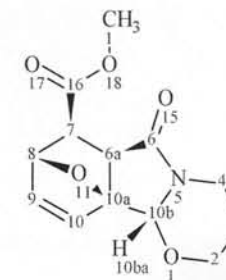


rudn-130411-N6-dept135_001000fid



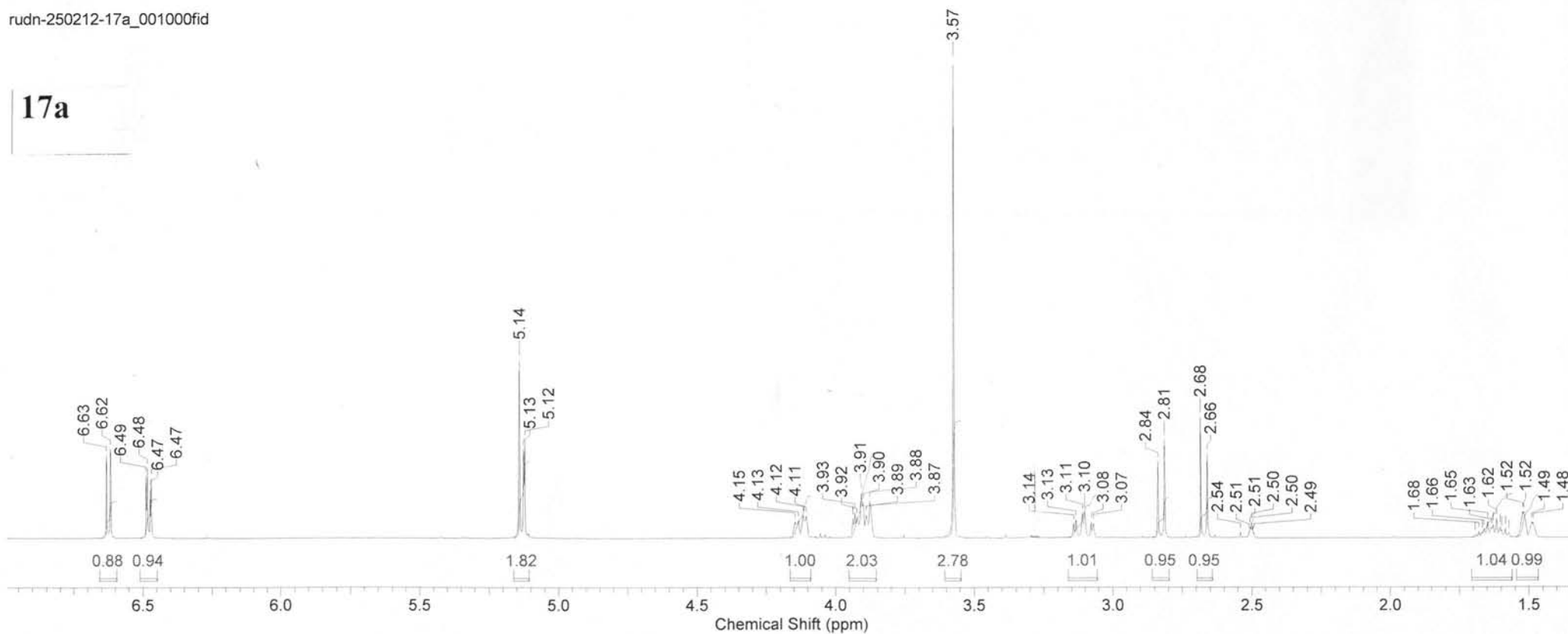
Formula C ₁₃ H ₁₅ NO ₅	FW 265.2619			
Acquisition Time (sec) 1.5729	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 28 May 2012 16:36:16		
Date Stamp 28 May 2012 16:36:16				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250212-17a\rudn-250212-17a_001000fid	Frequency (MHz) 400.14			
Nucleus 1H	Number of Transients 6	Origin spect	Original Points Count 16384	
Owner root	Points Count 16384	Pulse Sequence zg	Receiver Gain 128.00	
SW(cyclical) (Hz) 10416.67	Solvent DMSO-d6	Spectrum Offset (Hz) 2712.0542	Sweep Width (Hz) 10416.03	
Temperature (degree C) 32.000				

Compound 17a



rudn-250212-17a_001000fid

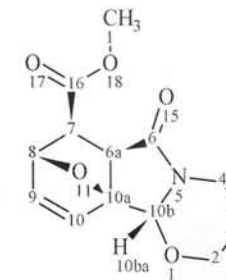
17a



Formula	C ₁₃ H ₁₅ NO ₅	FW	265.2619
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Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	28 May 2012 16:36:16
Date Stamp	28 May 2012 16:36:16				
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250212-17a\rudn-250212-17a_001000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	6	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zg
SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542
Temperature (degree C)	32.000			Sweep Width (Hz)	10416.03

Compound 17a



rudn-250212-17a_001000fid

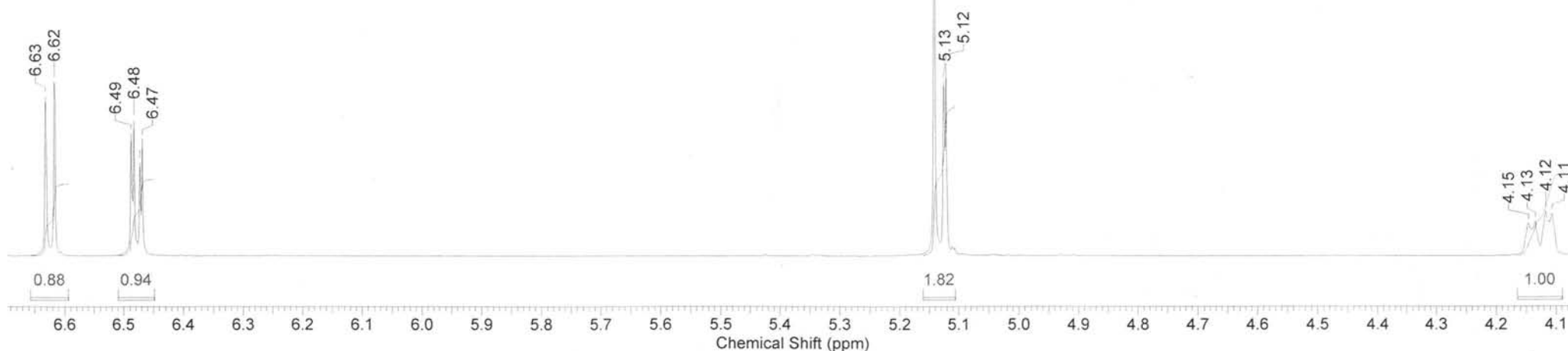
H-10
d
(5,7)

H-9
dd
(1.9; 5,7)

H-10b
s

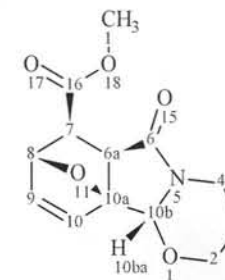
H-8
d
(1,9)

H-2 eq
br dd
(4,4; 11,4)



Formula C ₁₃ H ₁₅ NO ₅	FW 265.2619			
Acquisition Time (sec) 1.5729	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 28 May 2012 16:36:16		
Date Stamp 28 May 2012 16:36:16				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250212-17a\rudn-250212-17a_001000fid	Frequency (MHz) 400.14			
Nucleus 1H	Number of Transients 6	Origin spect	Original Points Count 16384	
Owner root	Points Count 16384	Pulse Sequence zg	Receiver Gain 128.00	
SW(cyclical) (Hz) 10416.67	Solvent DMSO-d6	Spectrum Offset (Hz) 2712.0542	Sweep Width (Hz) 10416.03	
Temperature (degree C) 32.000				

Compound 17a



rudn-250212-17a_001000fid

H-2ax and
H-4eq
m, 2H

s, 3H

CO₂Me

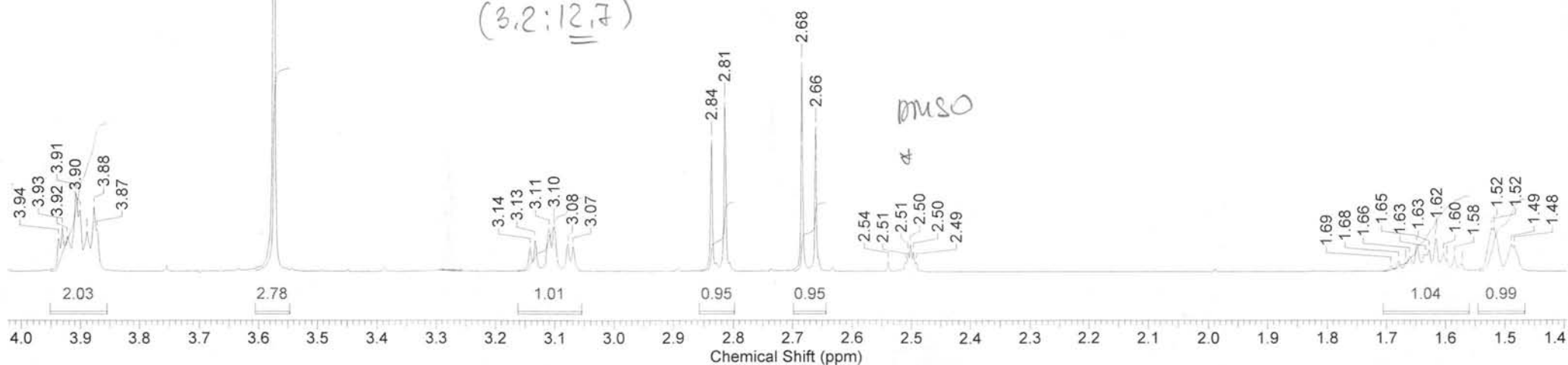
H-4ax
dt
(3.2:12.7)

H-6a
d
(9.1)

H-7
d
(9.1)

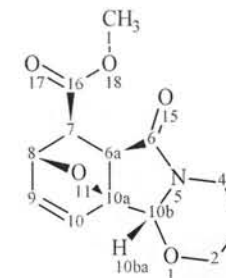
H-3ax
m

H-3eq
m

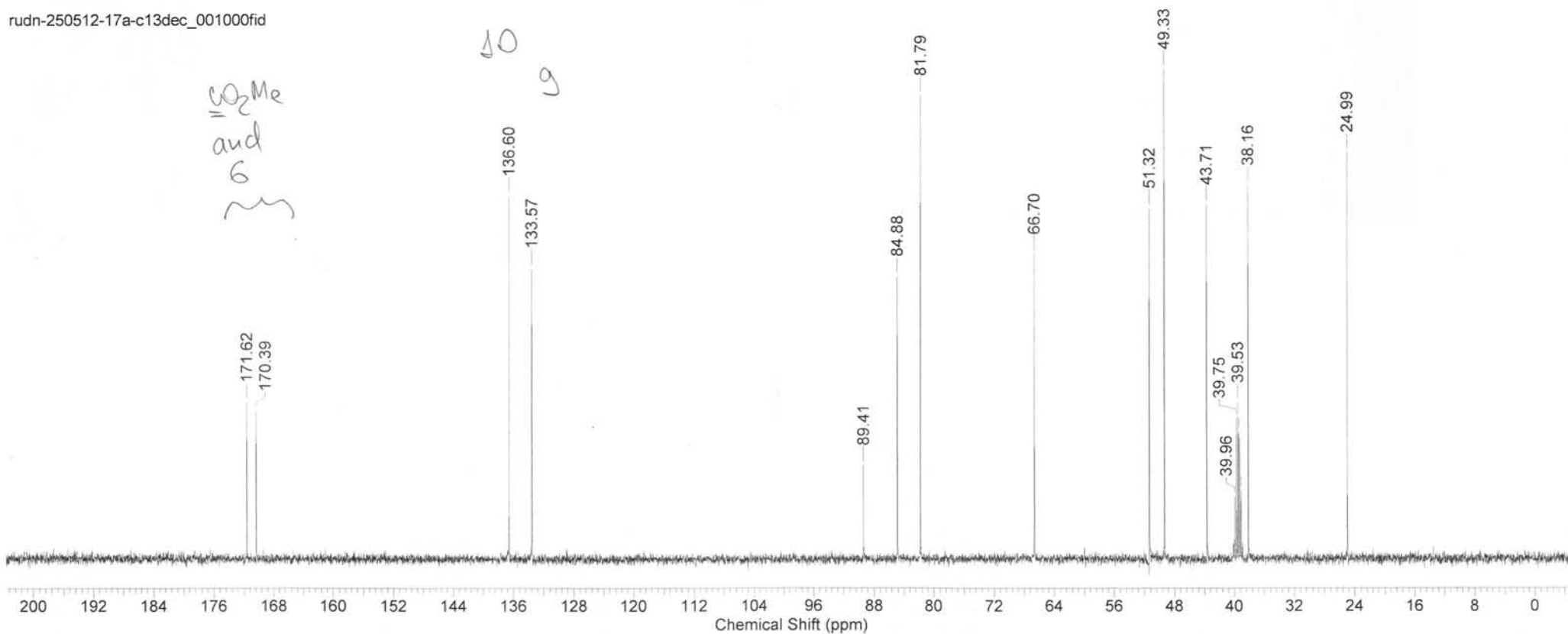


Formula C ₁₃ H ₁₅ NO ₅	FW 265.2619				
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400			Date 28 May 2012 16:36:16	
Date Stamp 28 May 2012 16:36:16					
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-17a-c13dec\rudn-250512-17a-c13dec_001000fid					
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 222	Origin spect		
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg		
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10548.9570		
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000				

Compound 17a

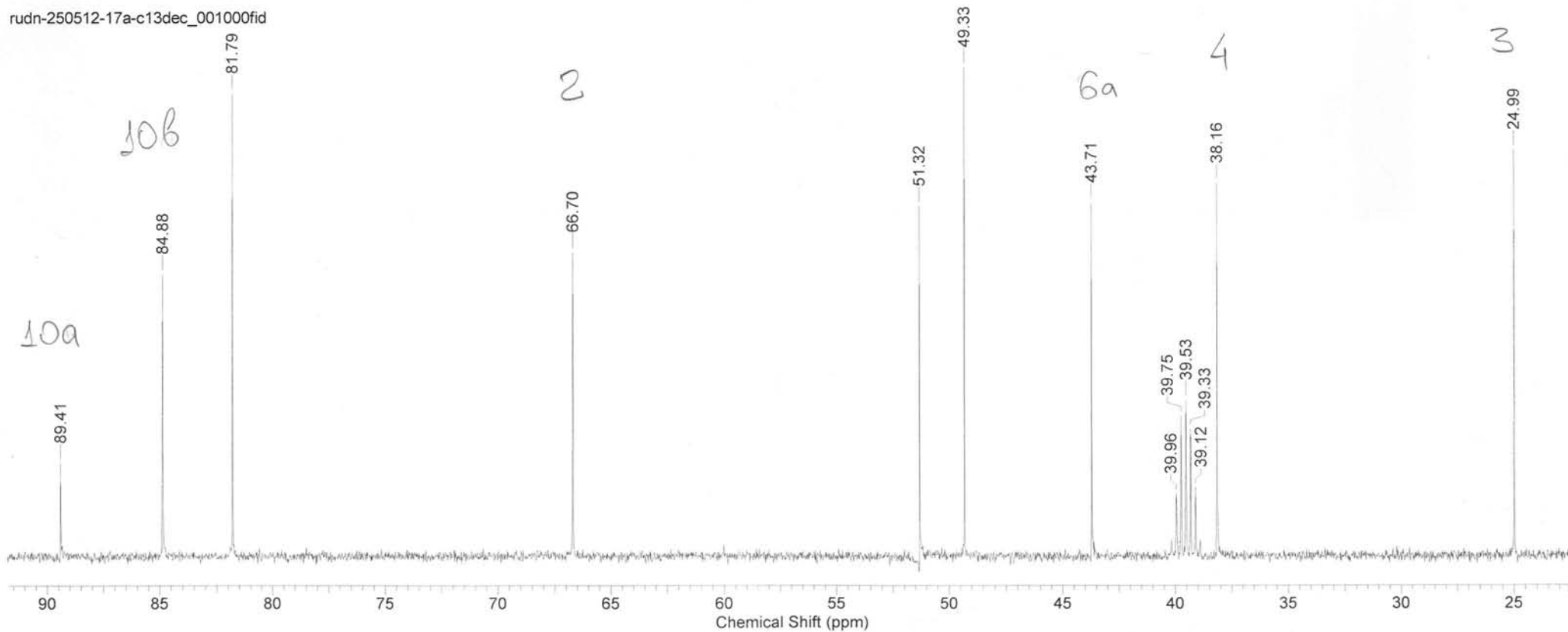
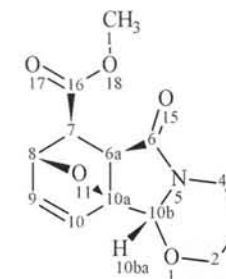


rudn-250512-17a-c13dec_001000fid



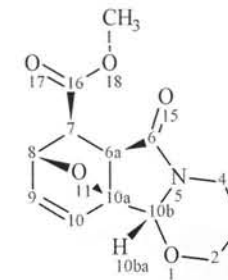
Formula C ₁₃ H ₁₅ NO ₅	FW 265.2619			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 28 May 2012 16:36:16		
Date Stamp 28 May 2012 16:36:16				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-17a-c13dec\rudn-250512-17a-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 222	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10548.9570	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compound 17a

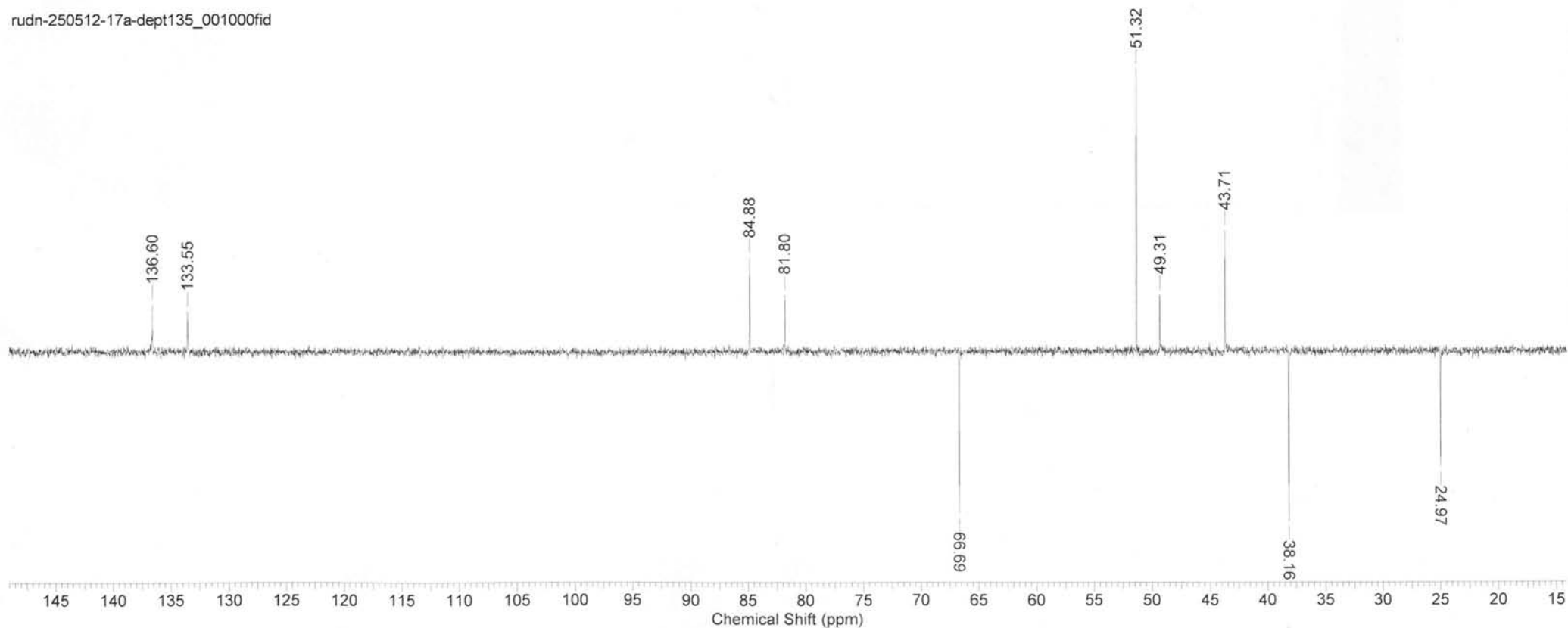


Formula C ₁₃ H ₁₅ NO ₅	FW 265.2619			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 28 May 2012 16:40:32		
Date Stamp 28 May 2012 16:40:32				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-17a-dept135\rudn-250512-17a-dept135_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 203	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence dept135	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 9098.5479	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compound 17a

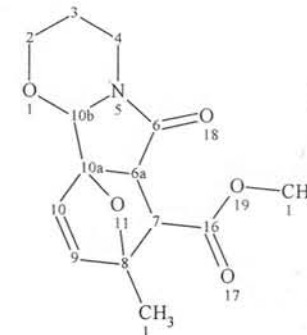


rudn-250512-17a-dept135_001000fid

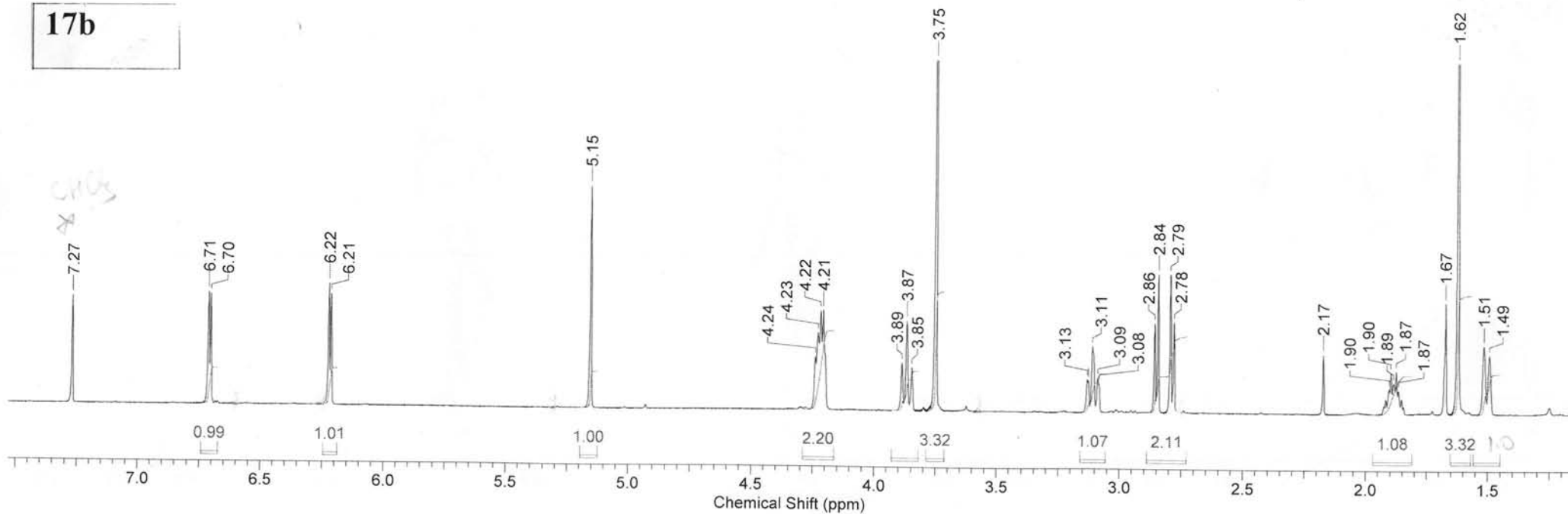


Acquisition Time (sec)	1.2386	Comment	HMBCGP	Date	28 Nov 2007 14:00:32				
File Name	D:\NMR\27.11.07\71\71_001000fid		Frequency (MHz)	600.22	Nucleus	1H	Number of Transients	4	
Original Points Count	16384	Points Count	32768	Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	13227.51
Temperature (degree C)	22.500								

Compound 17b

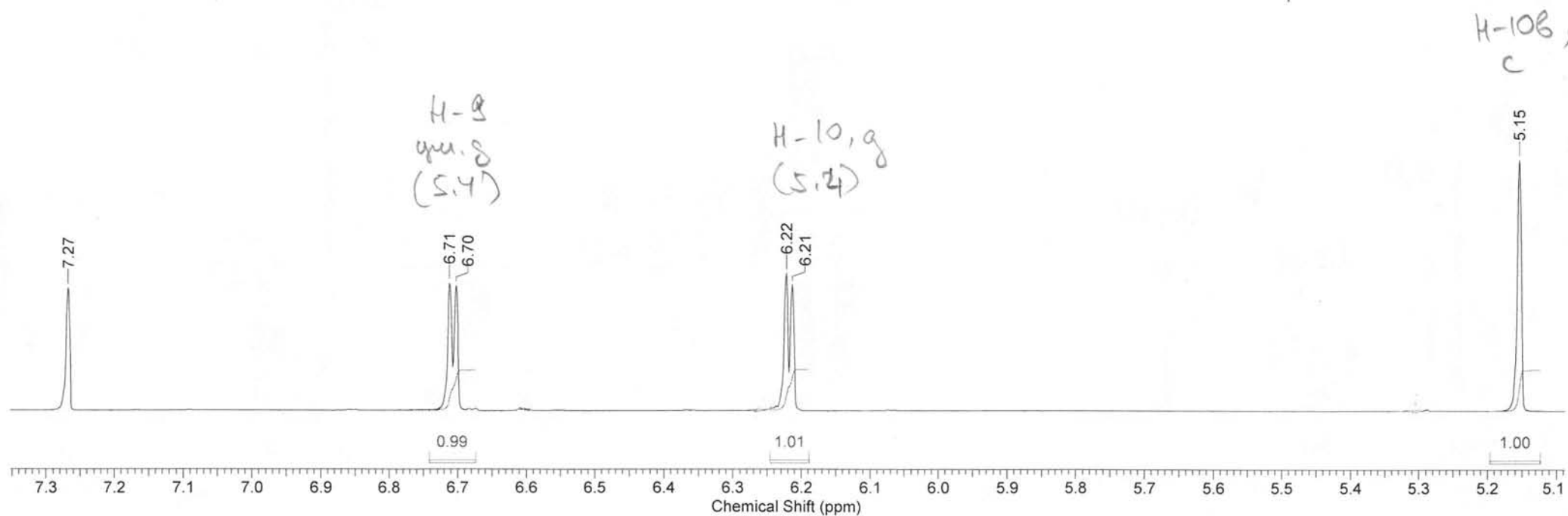
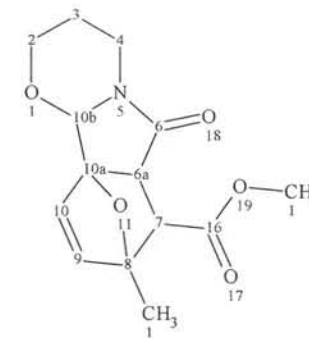


17b

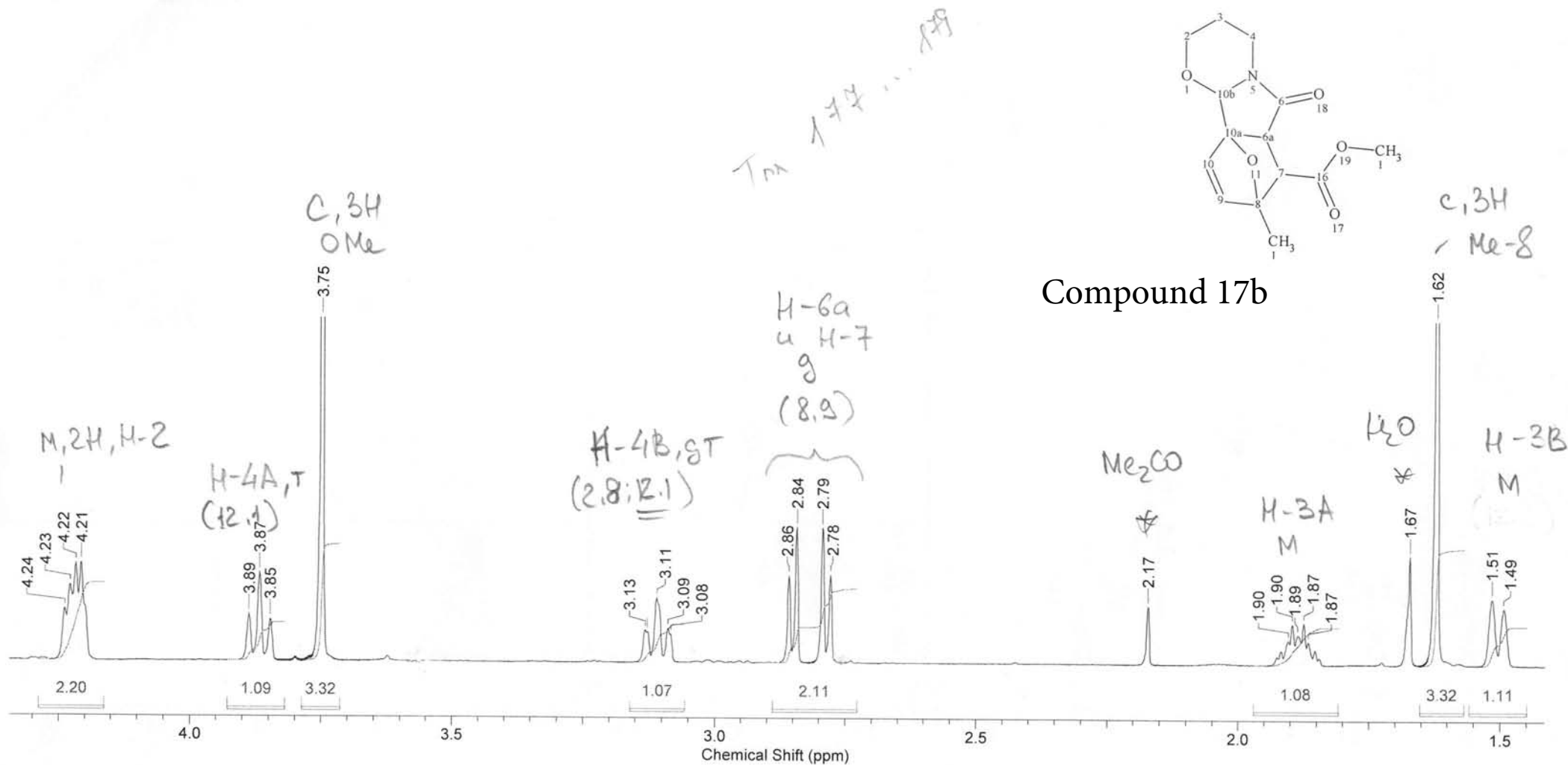


Acquisition Time (sec)	1.2386	Comment	HMBCGP	Date	28 Nov 2007 14:00:32		
File Name	D:\NMR\27.11.07\171_001000fid	Frequency (MHz)	600.22	Nucleus	1H	Number of Transients	4
Original Points Count	16384	Points Count	32768	Pulse Sequence	zg	Solvent	DMSO-D6
Temperature (degree C)	22.500	Sweep Width (Hz)	13227.51				

Compound 17b

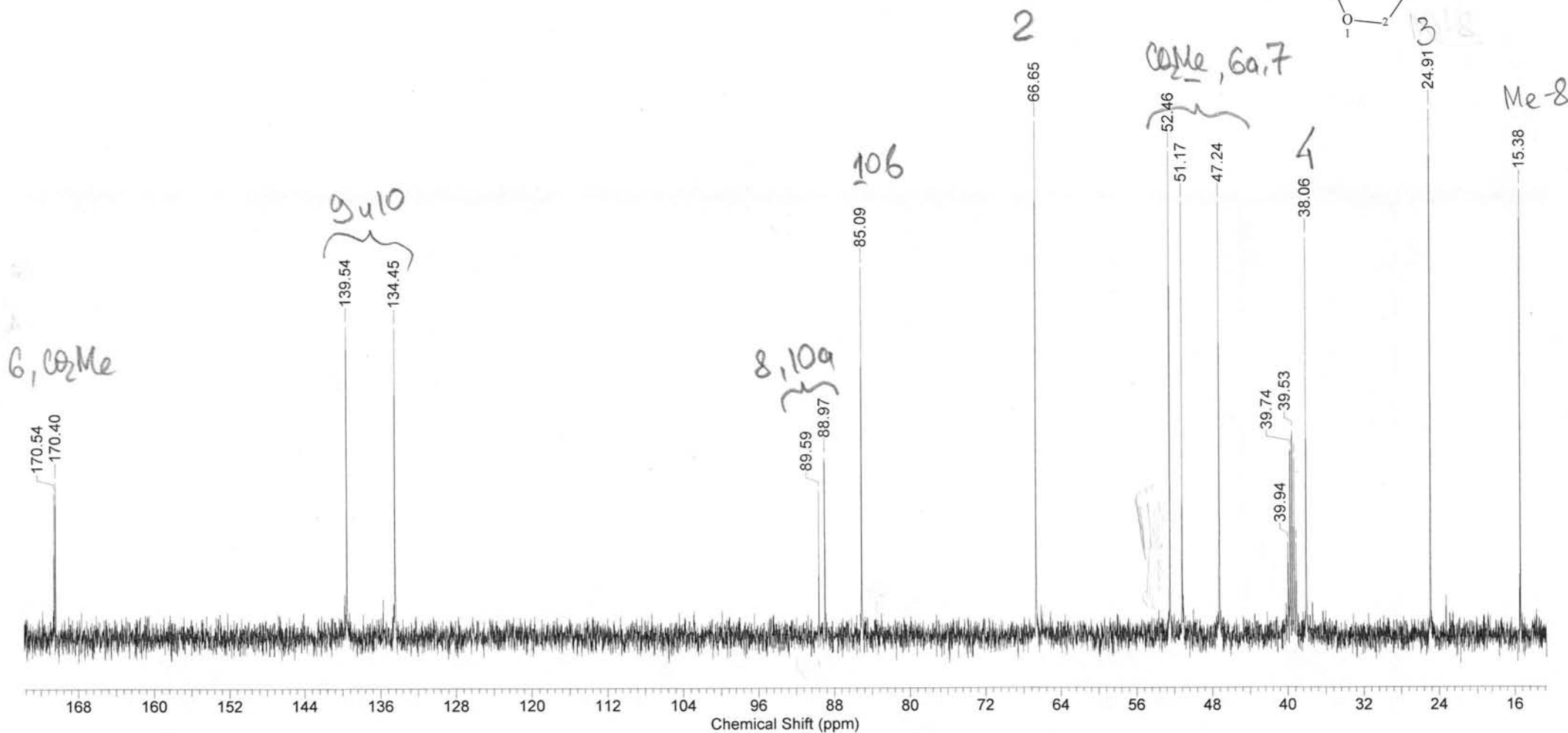
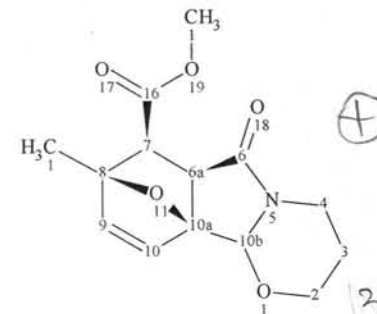


Acquisition Time (sec)	1.2386	Comment	HMBCGP	Date	28 Nov 2007 14:00:32				
File Name	D:\NMR\27.11.07\71\71_001000fid		Frequency (MHz)	600.22	Nucleus	1H	Number of Transients	4	
Original Points Count	16384	Points Count	32768	Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	13227.51
Temperature (degree C)	22.500								

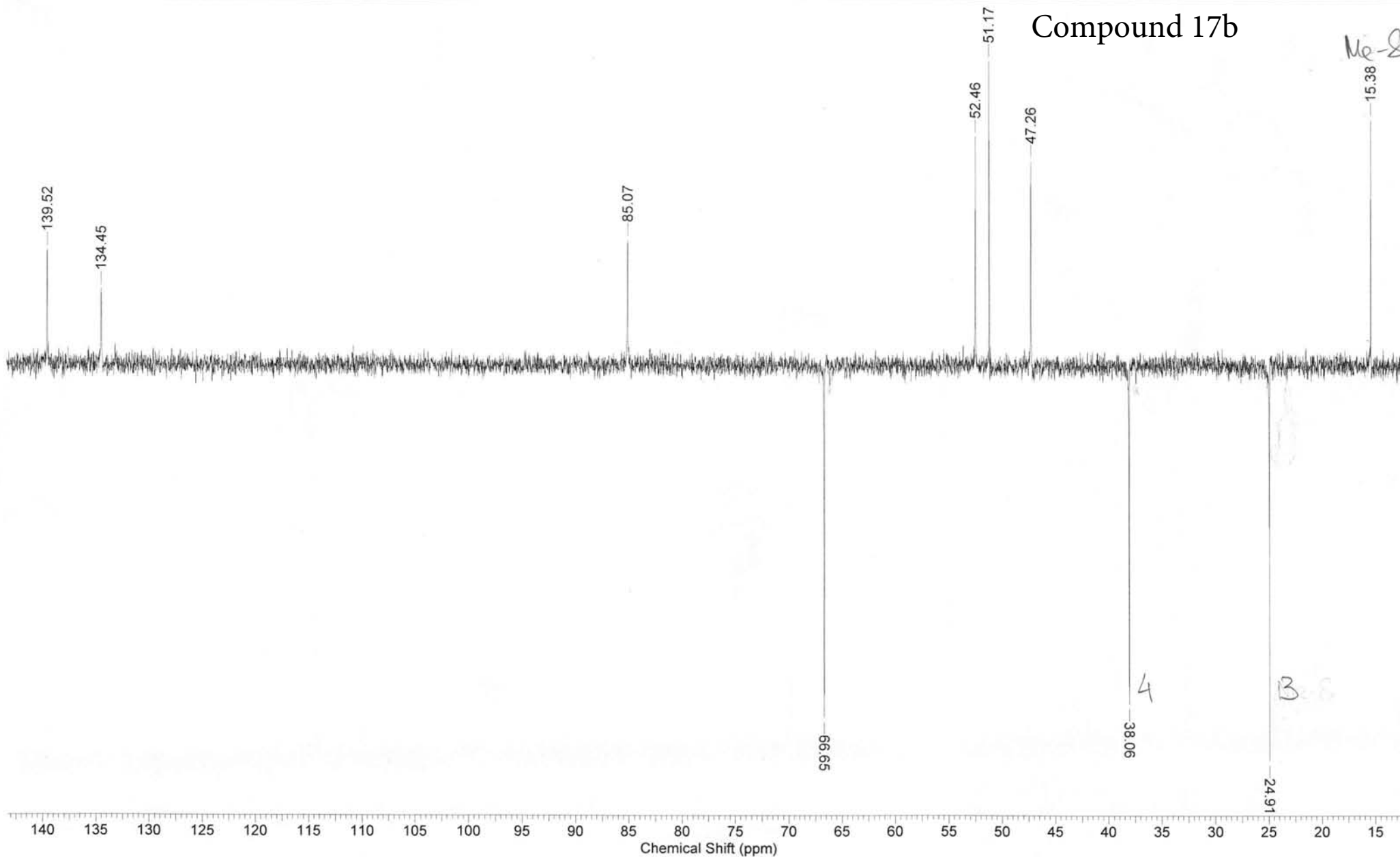


Acquisition Time (sec)	0.6226	Comment	Imported from UXNMR.		Date	29 Dec 2008 17:33:52	
File Name	D:\NMR\13\Женя и Инга (ЮС конец 2008)\10laz_c13dec\10laz_c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	86	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	26315.79	Temperature (degree C)	27.000

Compound 17b



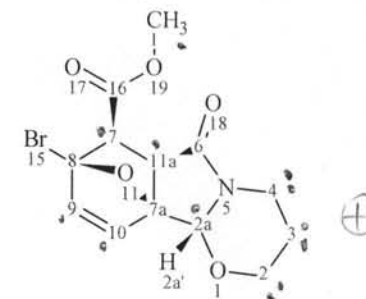
Acquisition Time (sec)	0.6226	Comment	Imported from UXMNR.		Date	29 Dec 2008 17:36:00	
File Name	D:\NMR\C_13\Женя и Инга (ЮС конец 2008)\10laz_dept135\10laz_dept135_001000fid			Frequency (MHz)	100.62		
Nucleus	13C	Number of Transients	107	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	DMSO-D6	Sweep Width (Hz)	26315.79	Temperature (degree C)	27.000



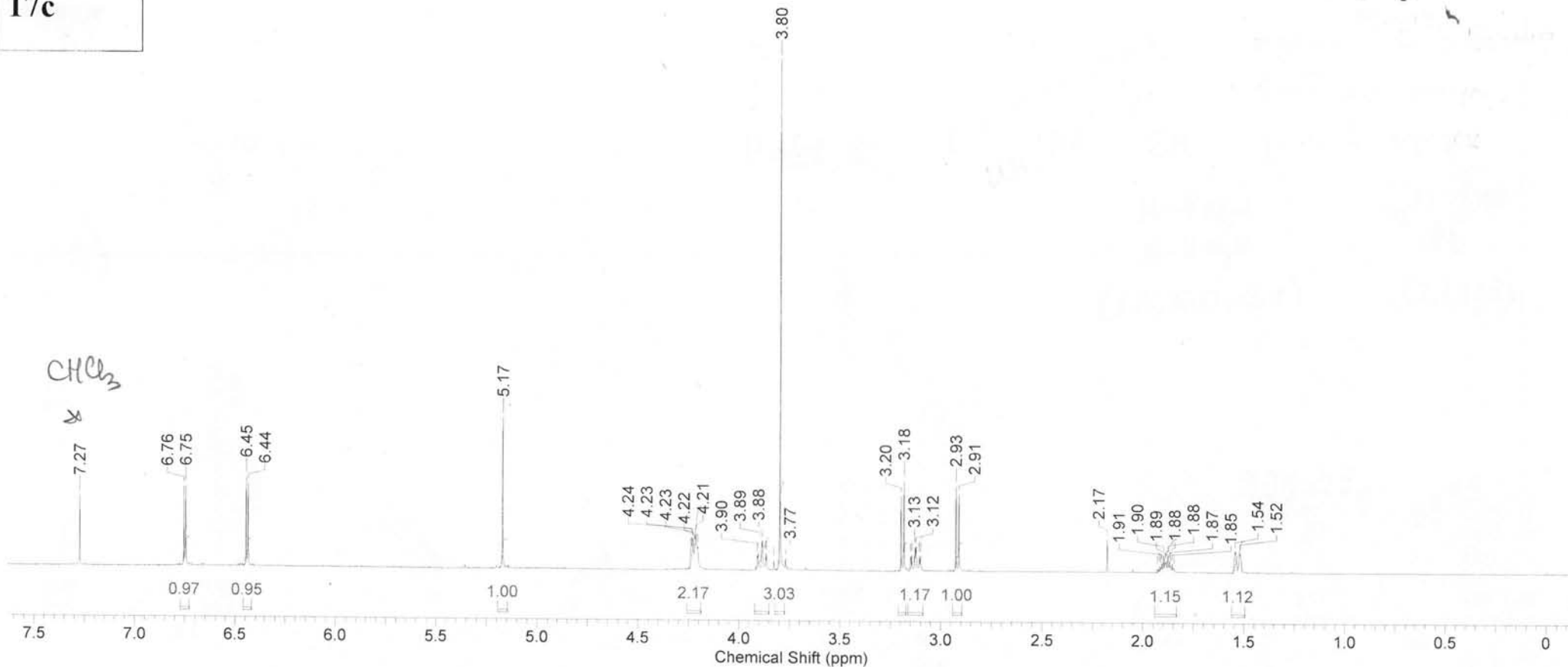
Formula $C_{13}H_{14}BrNO_5$ FW 344.1580

Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	09 Apr 2010 10:36:13	Date Stamp	09 Apr 2010 10:35:01
File Name	D:\NMR\6.04.10\FZ1128-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	26.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3014.4822	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	21.200					Sweep Width (Hz)	11261.26

Compound 17c



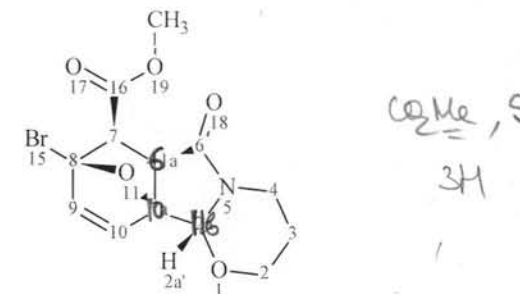
17c



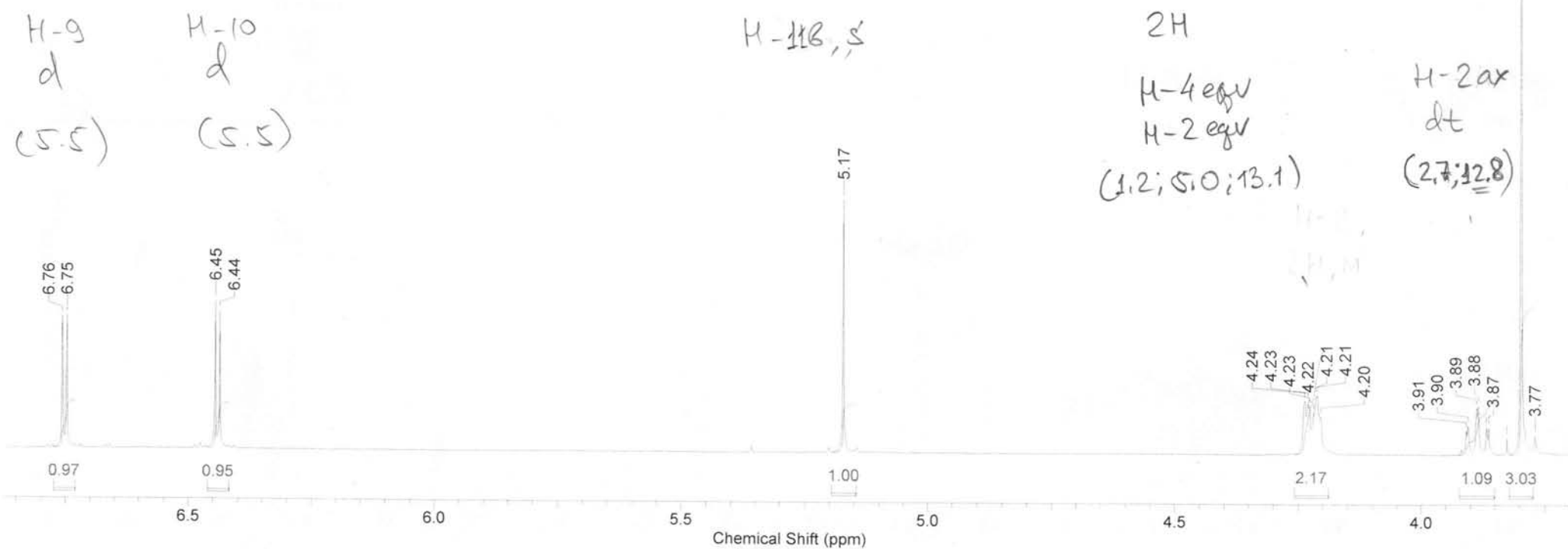
Formula C₁₃H₁₄BrNO₅ FW 344.1580

Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	09 Apr 2010 10:36:13	Date Stamp	09 Apr 2010 10:35:01
File Name	D:\NMR\6.04.10\FZ1128-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	26.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3014.4822	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	21.200			Sweep Width (Hz)	11261.26		

Compound 17c



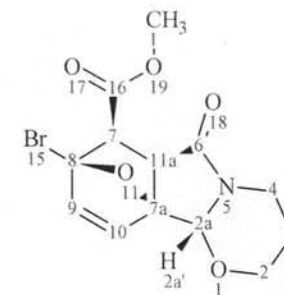
FZ1128-1.jdf



Formula C₁₃H₁₄BrNO₅ FW 344.1580

Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	09 Apr 2010 10:36:13	Date Stamp	09 Apr 2010 10:35:01
File Name	D:\NMR\6.04.10\FZ1128-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	26.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3014.4822	Sweep Width (Hz)	11261.26
Temperature (degree C)	21.200						

Compound 17c



H-4ax
3,12, dt
(4.1; 12.8)

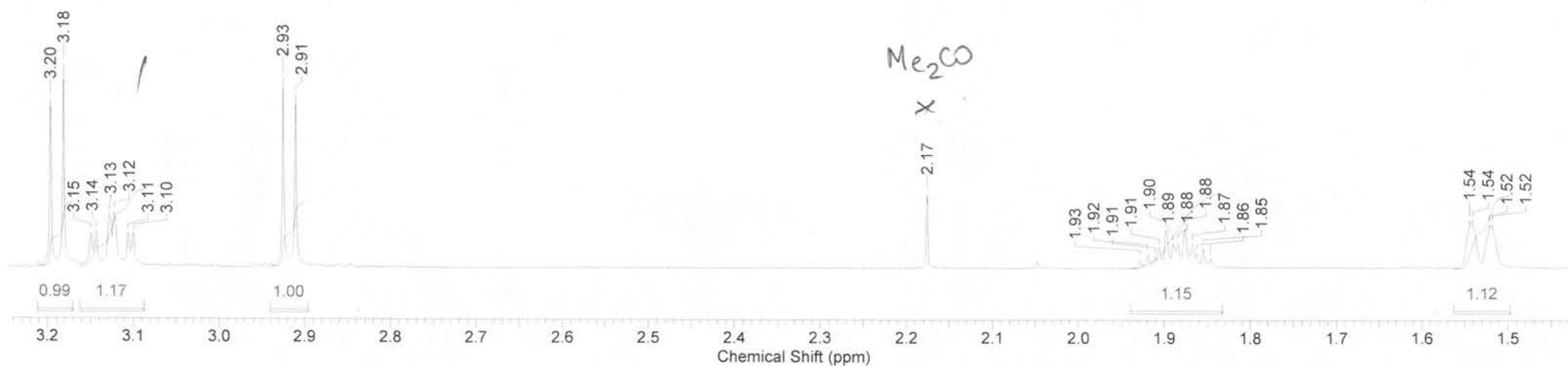
FZ1128-1.jdf

H-7
d
(8.9)

H-6s
d
(8.9)

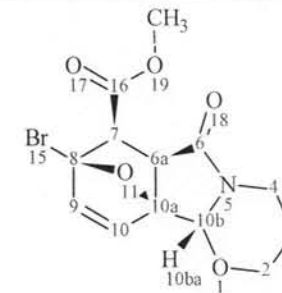
H-3ax
m

H-3eq
m

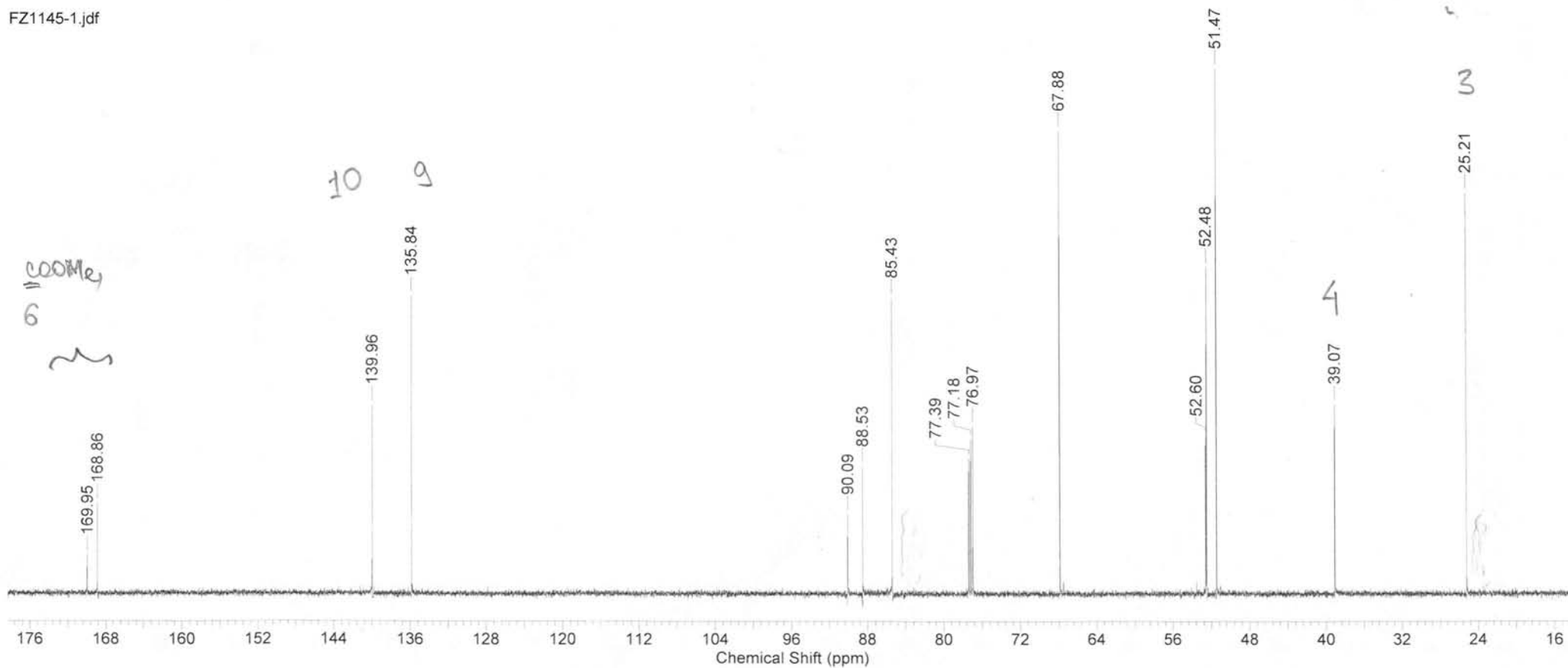


Formula	C ₁₃ H ₁₄ BrNO ₅	FW	344.1580
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE
Date Stamp	15 Apr 2010 13:39:01	Date	15 Apr 2010 13:40:05
Nucleus	13C	File Name	D:\NMR\14.04.10\FZ1145-1.jdf
Points Count	32768	Number of Transients	200
Solvent	CHLOROFORM-d	Origin	ECA 600
		Original Points Count	32768
		Receiver Gain	50.00
		Spectrum Offset (Hz)	15091.3428
		Sweep Width (Hz)	47348.49
		Temperature (degree C)	21.800

Compound 17c



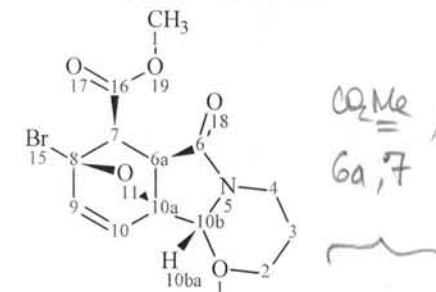
FZ1145-1.jdf



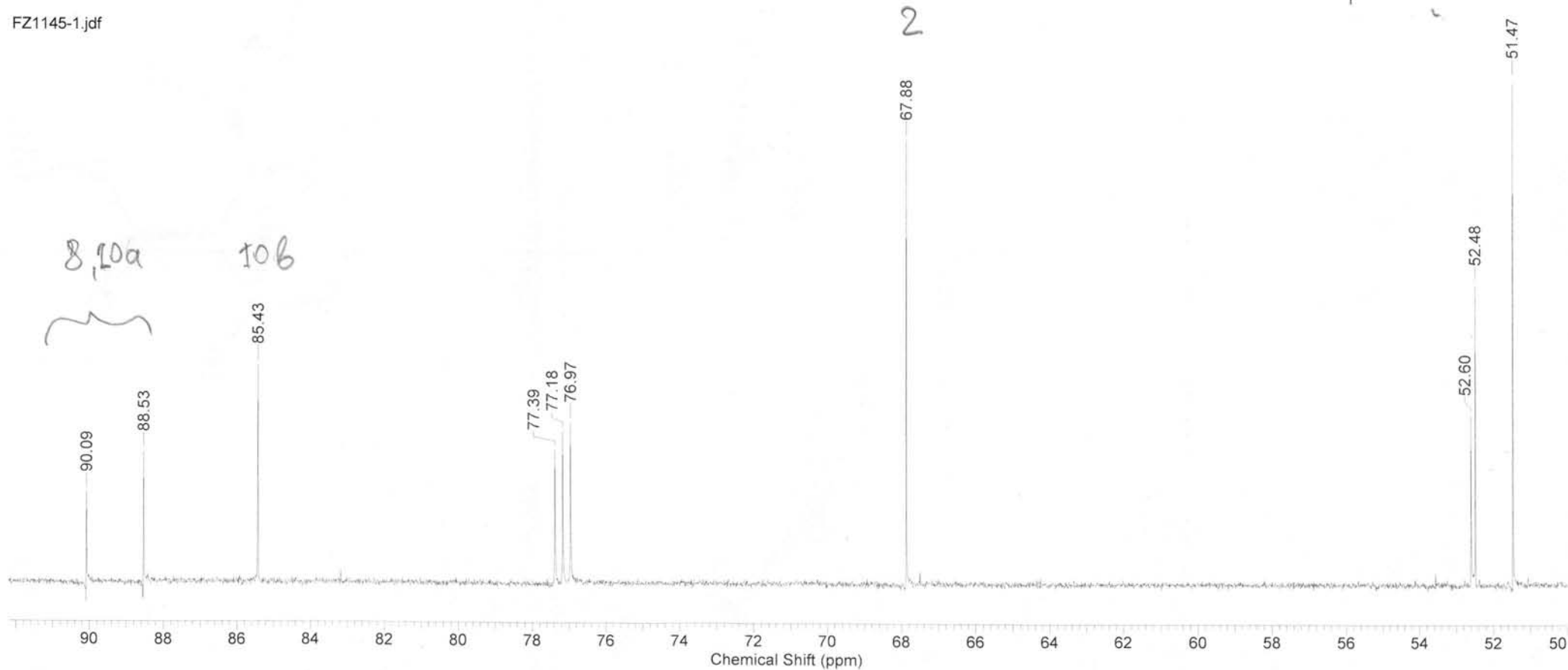
Formula C₁₃H₁₄BrNO₅ FW 344.1580

Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	15 Apr 2010 13:40:05
Date Stamp	15 Apr 2010 13:39:01	File Name	D:\NMR\14.04.10\FZ1145-1.jdf	Frequency (MHz)	150.91
Nucleus	13C	Number of Transients	200	Origin	ECA 600
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	15091.3428	Receiver Gain	50.00
		Sweep Width (Hz)	47348.49	Temperature (degree C)	21.800

Compound 17c



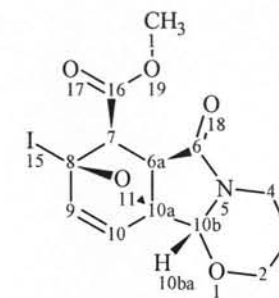
FZ1145-1.jdf



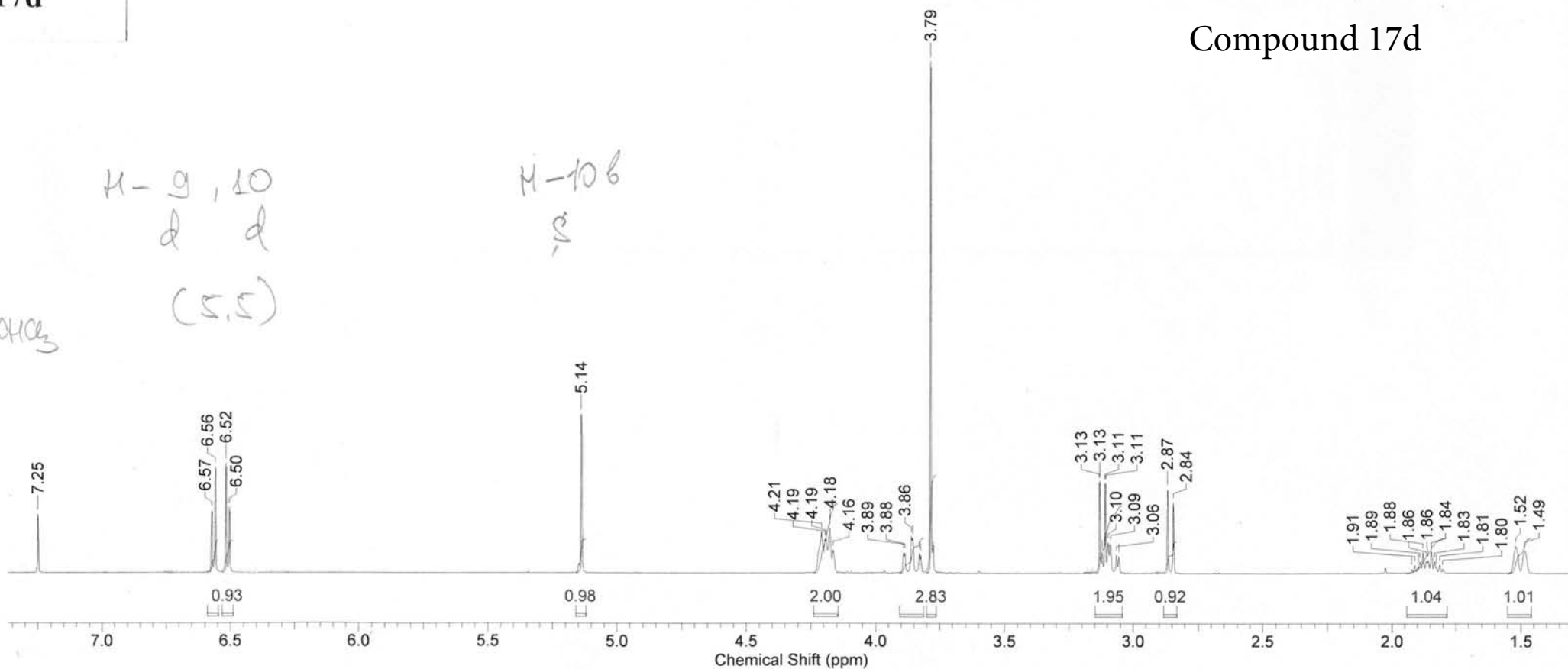
Formula	C ₁₃ H ₁₄ INO ₅	FW	391.1584
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Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	06 Jun 2012 09:08:00	Date Stamp	06 Jun 2012 12:57:17
File Name	D:\NMR\04.06.12\FZ2443-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	32
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	36.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2398.6931	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	22.900	Sweep Width (Hz)					7503.00

17d

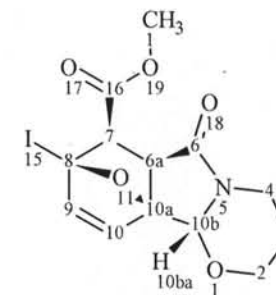


Compound 17d

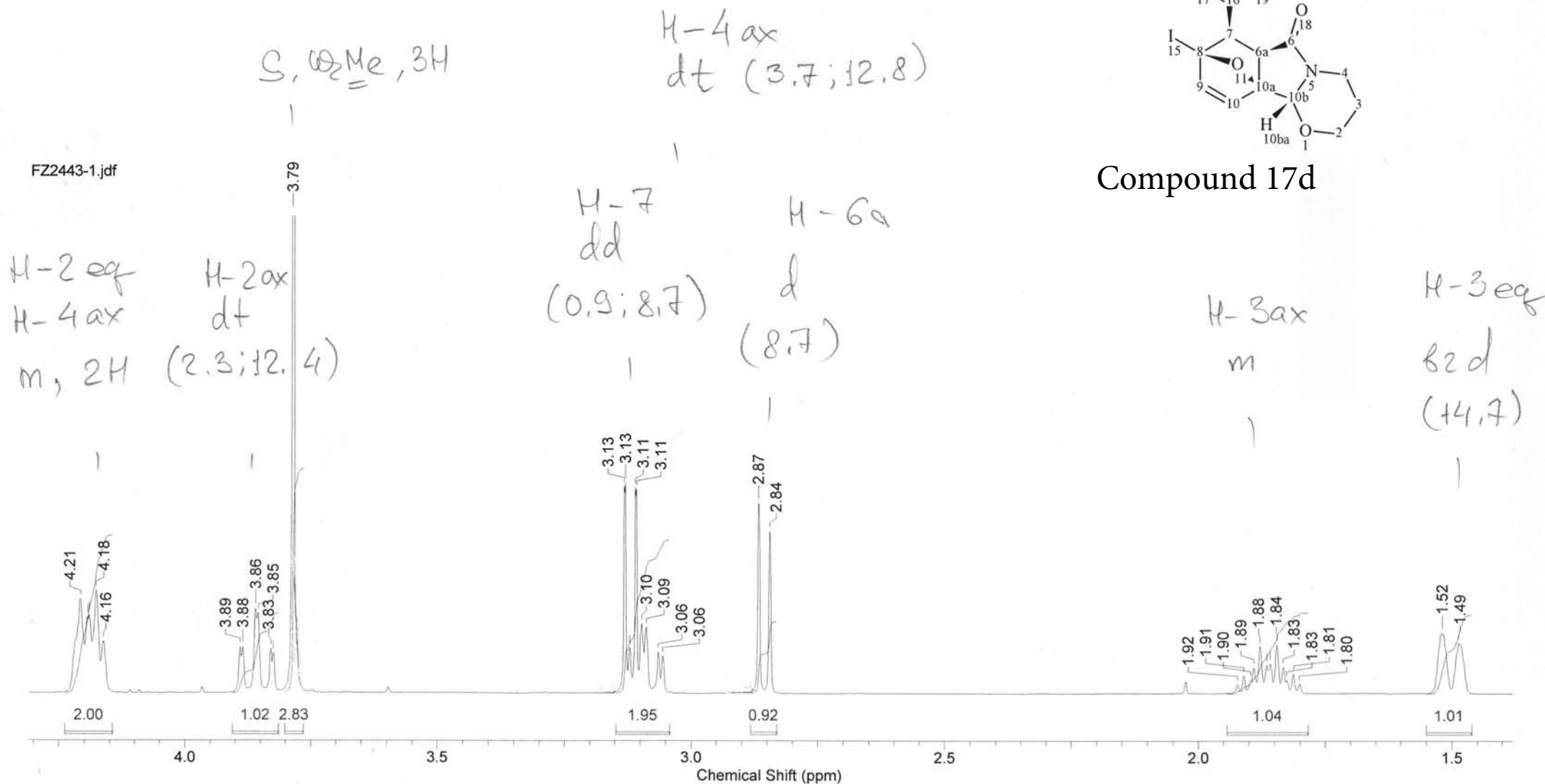


Formula	C ₁₃ H ₁₄ INO ₅	FW	391.1584
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Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	06 Jun 2012 09:08:00	Date Stamp	06 Jun 2012 12:57:17
File Name	D:\NMR\04.06.12\FZ2443-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	32
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	36.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2398.6931	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	22.900			Sweep Width (Hz)	7503.00		

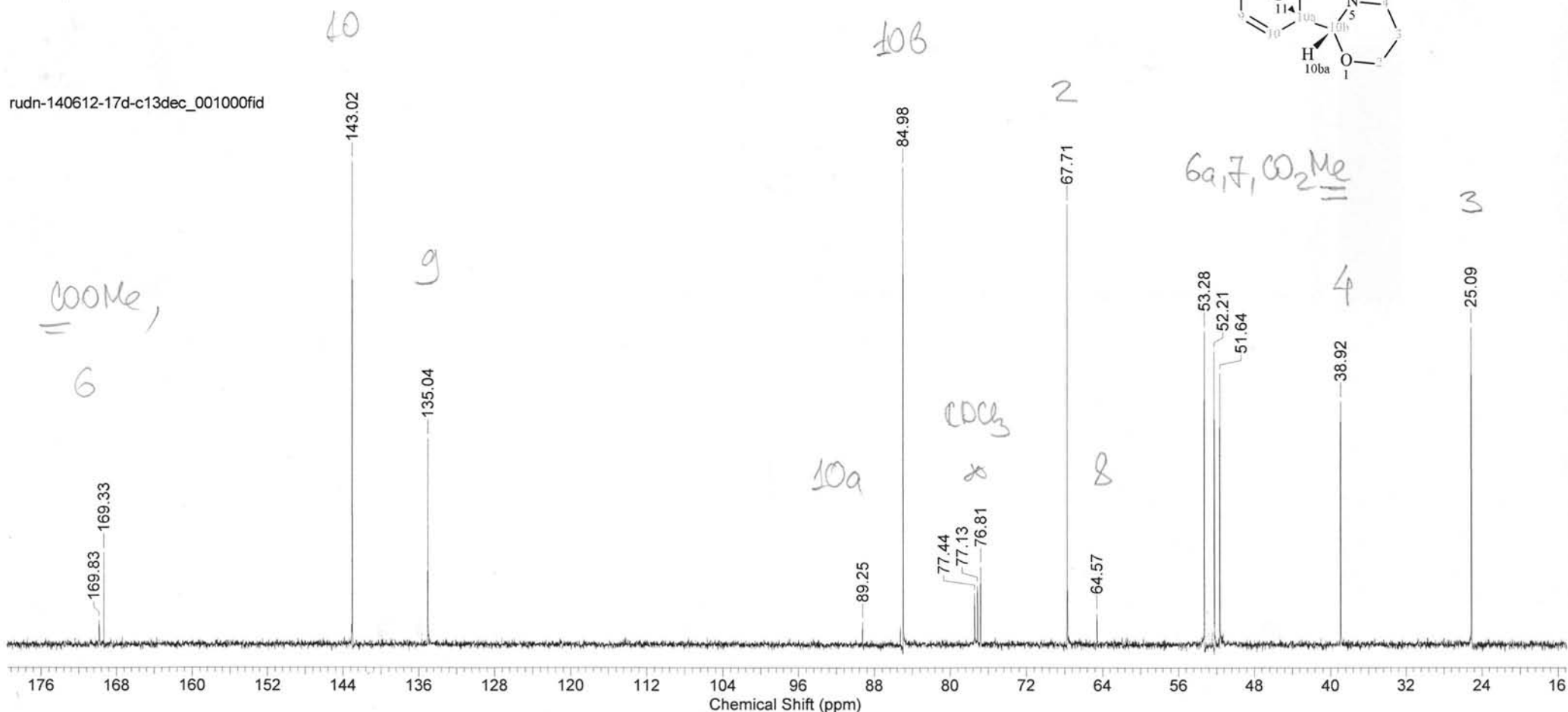
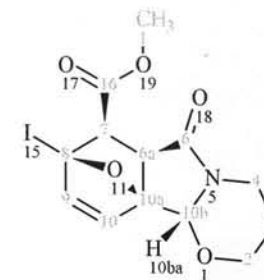


Compound 17d

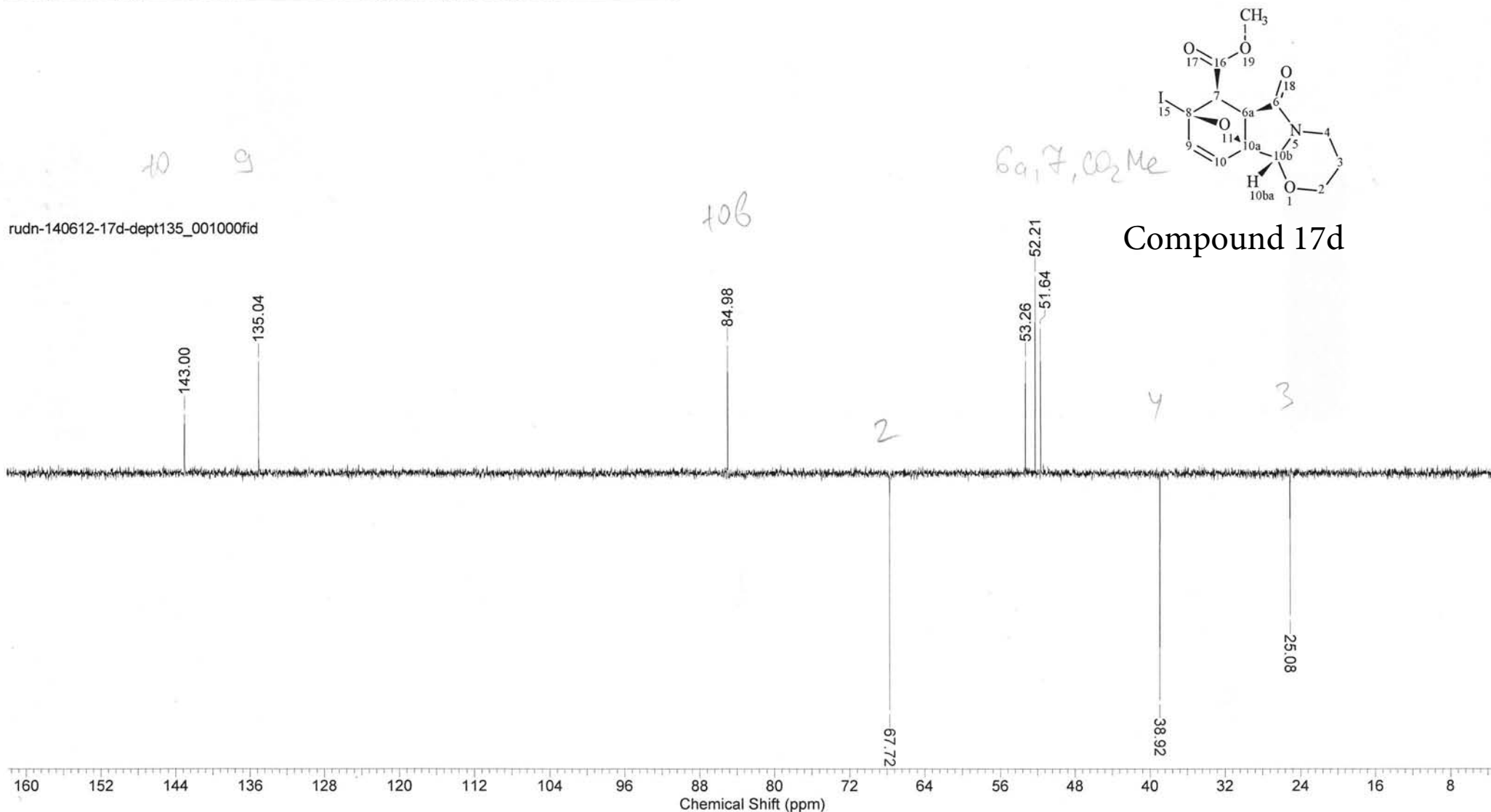


Formula C ₁₃ H ₁₄ INO ₅	FW 391.1584			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 26 Jun 2012 17:14:40		
Date Stamp 26 Jun 2012 17:14:40				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-140612-17d-c13dec\rudn-140612-17d-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 218	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent CHLOROFORM-d	Spectrum Offset (Hz) 11074.4697	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compound 17d



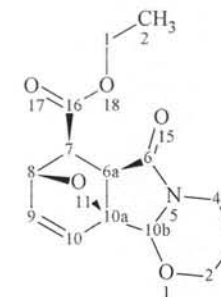
Formula C ₁₃ H ₁₄ INO ₅	FW 391.1584			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 26 Jun 2012 17:18:56		
Date Stamp 26 Jun 2012 17:18:56				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-140612-17d-dept135\rudn-140612-17d-dept135_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 156	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence dept135	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent CHLOROFORM-d	Spectrum Offset (Hz) 9624.0332	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			



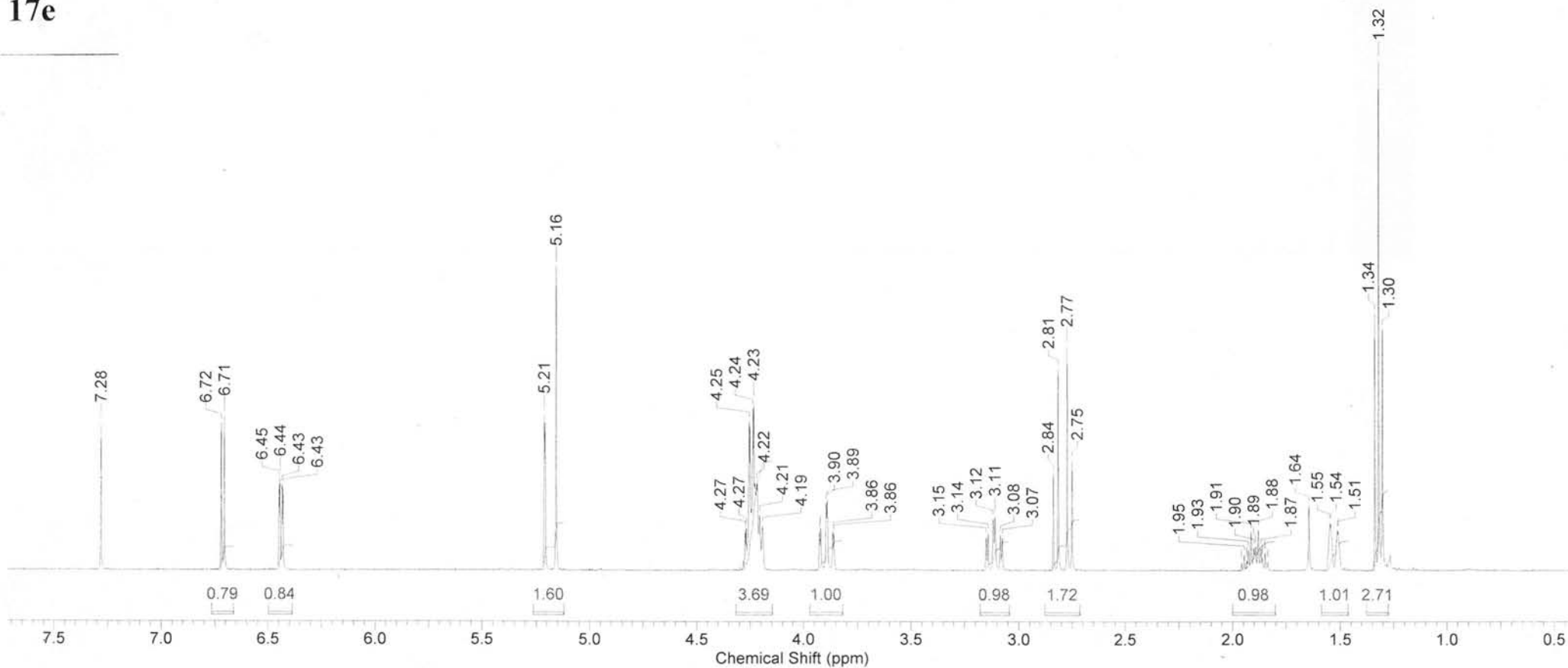
Formula $C_{14}H_{17}NO_5$ FW 279.2885

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	05 May 2012 09:16:46	Date Stamp	05 May 2012 13:06:05
File Name	D:\NMR\03.05.12\FZ2374-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	4
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	26.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	1998.9109	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	23.300			Sweep Width (Hz)	7503.00		

Compound 17e



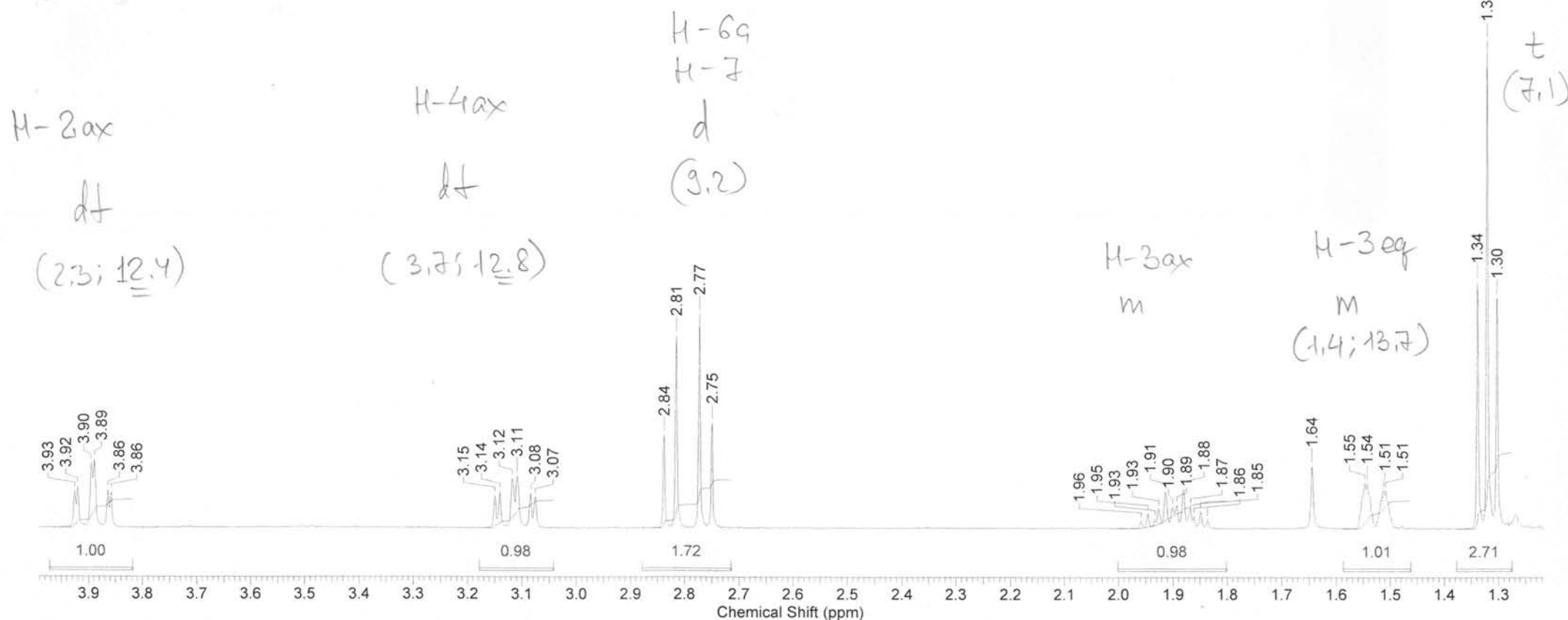
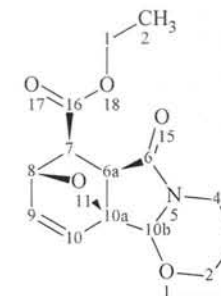
17e



Formula C₁₄H₁₇NO₅ FW 279.2885

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	05 May 2012 09:16:46	Date Stamp	05 May 2012 13:06:05
File Name	D:\NMR\03.05.12\FZ2374-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	4
Origin	ECS 400	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	26.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	1998.9109	Sweep Width (Hz)	7503.00
Temperature (degree C)	23.300						

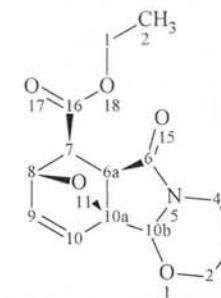
Compound 17e



Formula C₁₄H₁₇NO₅ FW 279.2885

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	05 May 2012 09:16:46	Date Stamp	05 May 2012 13:06:05
File Name	D:\NMR\03.05.12\FZ2374-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	4
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	26.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	1998.9109	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	23.300			Sweep Width (Hz)	7503.00		

Compound 17e



H-10
d
(5,8)

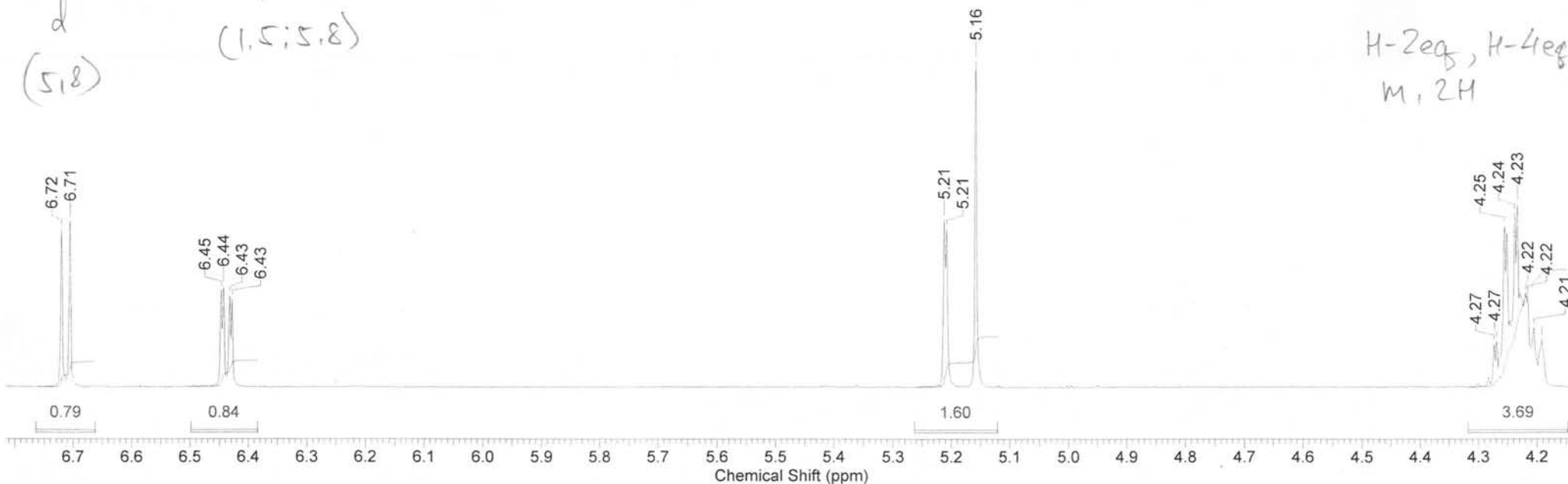
H-9
dd
(1.5; 5.8)

H-8
d
(1.5)

H-10B
s

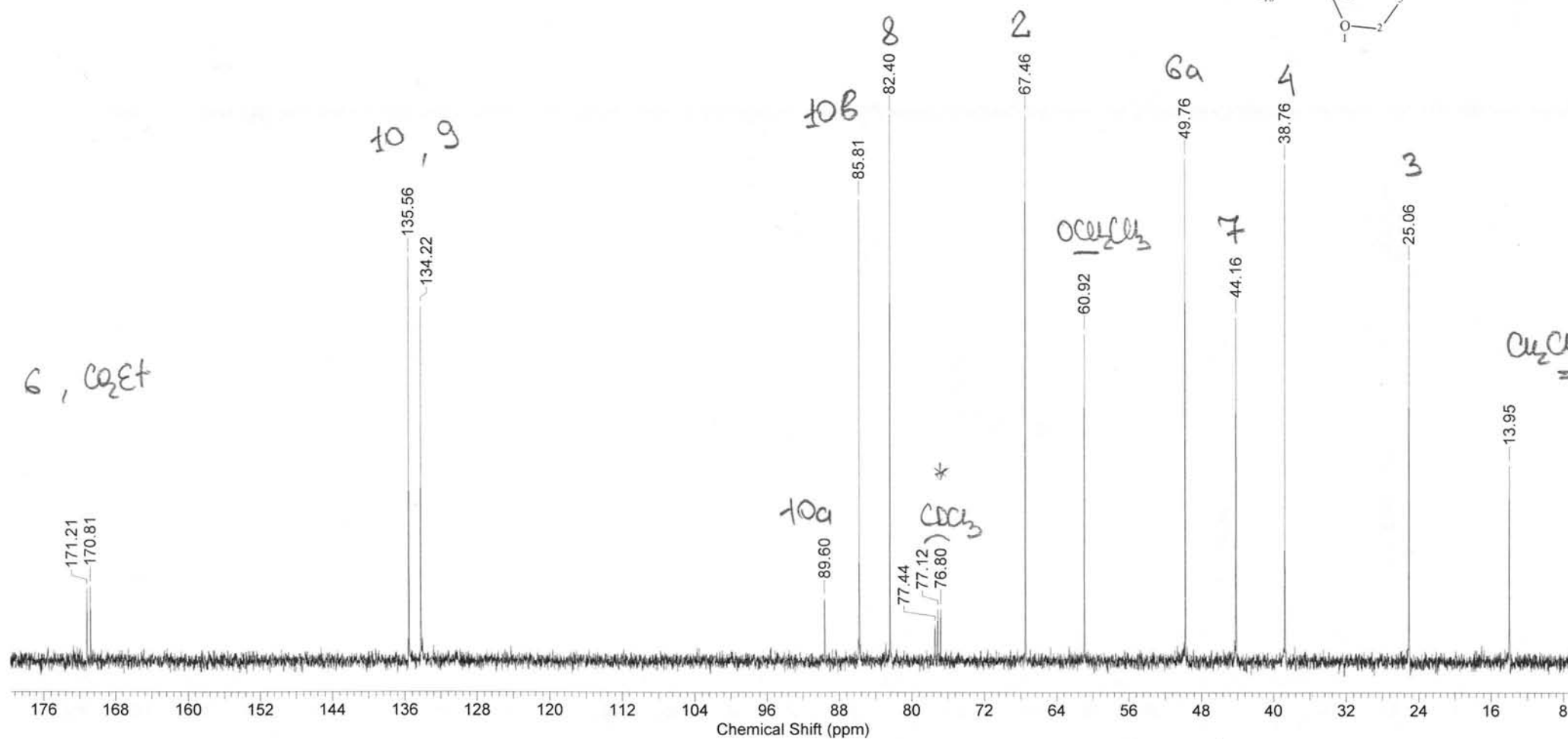
OCC₂CH₃
4.23, dq, 2H
(1.8; 7, 1)

H-2eq, H-4eq
m, 2H

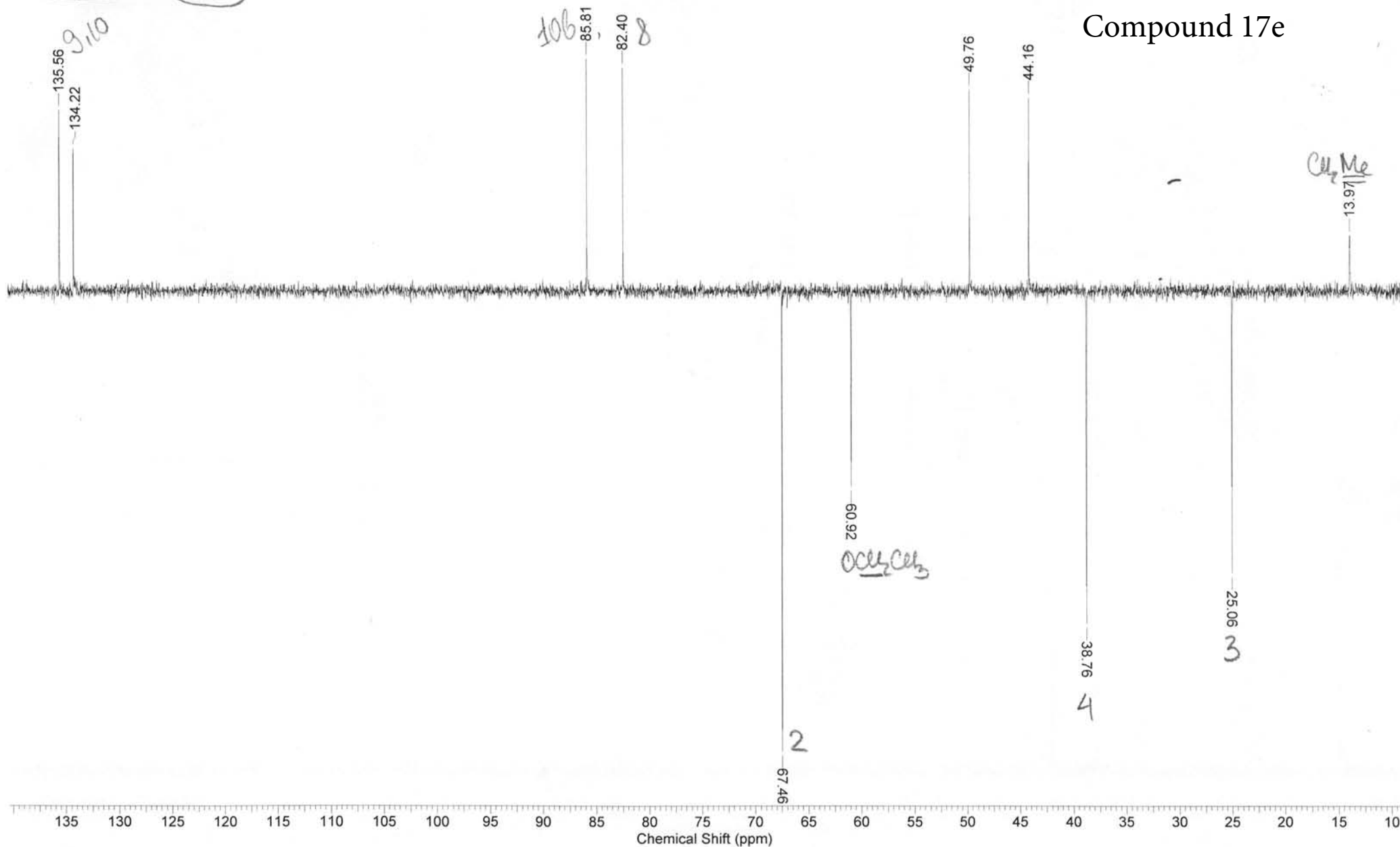


Acquisition Time (sec)	0.6226	Comment	Imported from UXMNR.	Date	29 Dec 2008 16:55:28
File Name	D:\NMR\13\Женя и Инга (10С конец 2008)\2nik_c13dec\2nik_c13dec_001000fid			Frequency (MHz)	100.62
Nucleus	13C	Number of Transients	77	Original Points Count	16384
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	26315.79
Temperature (degree C)	27.000				

Compound 17e

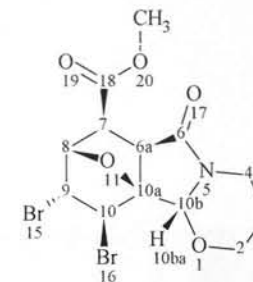


Acquisition Time (sec)	0.6226	Comment	Imported from UXMNR.		Date	29 Dec 2008 16:57:36	
File Name	D:\NMR\C_13\Женя и Инга (IOC конец 2008)\2nik_dept135\2nik_dept135_001000fid				Frequency (MHz)	100.62	
Nucleus	¹³ C	Number of Transients	84	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	CHLOROFORM-D	Sweep Width (Hz)	26315.79	Temperature (degree C)	27.000



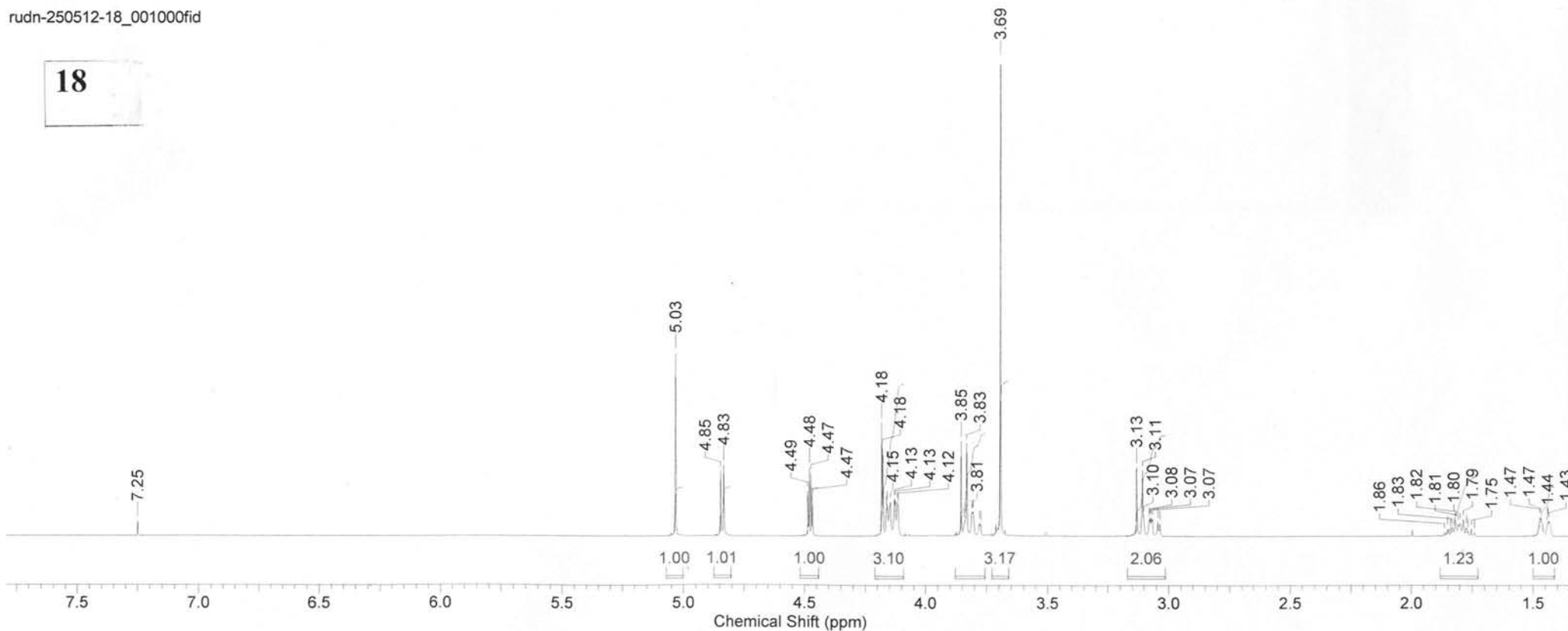
Formula C ₁₃ H ₁₅ Br ₂ NO ₅		FW 425.0699					
Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400				
Date Stamp	31 May 2012 15:49:20		Date	31 May 2012 15:49:20			
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-18\rudn-250512-18_001000fid		Frequency (MHz)	400.14			
Nucleus	1H	Number of Transients	4	Origin	spect	Original Points Count	16384
Owner	root	Points Count	16384	Pulse Sequence	zg	Receiver Gain	128.00
SW(cyclical) (Hz)	10204.08	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2602.0486	Sweep Width (Hz)	10203.46
Temperature (degree C)	27.000						

Compound 18



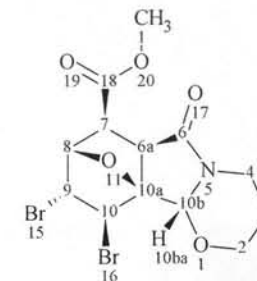
rudn-250512-18_001000fid

18

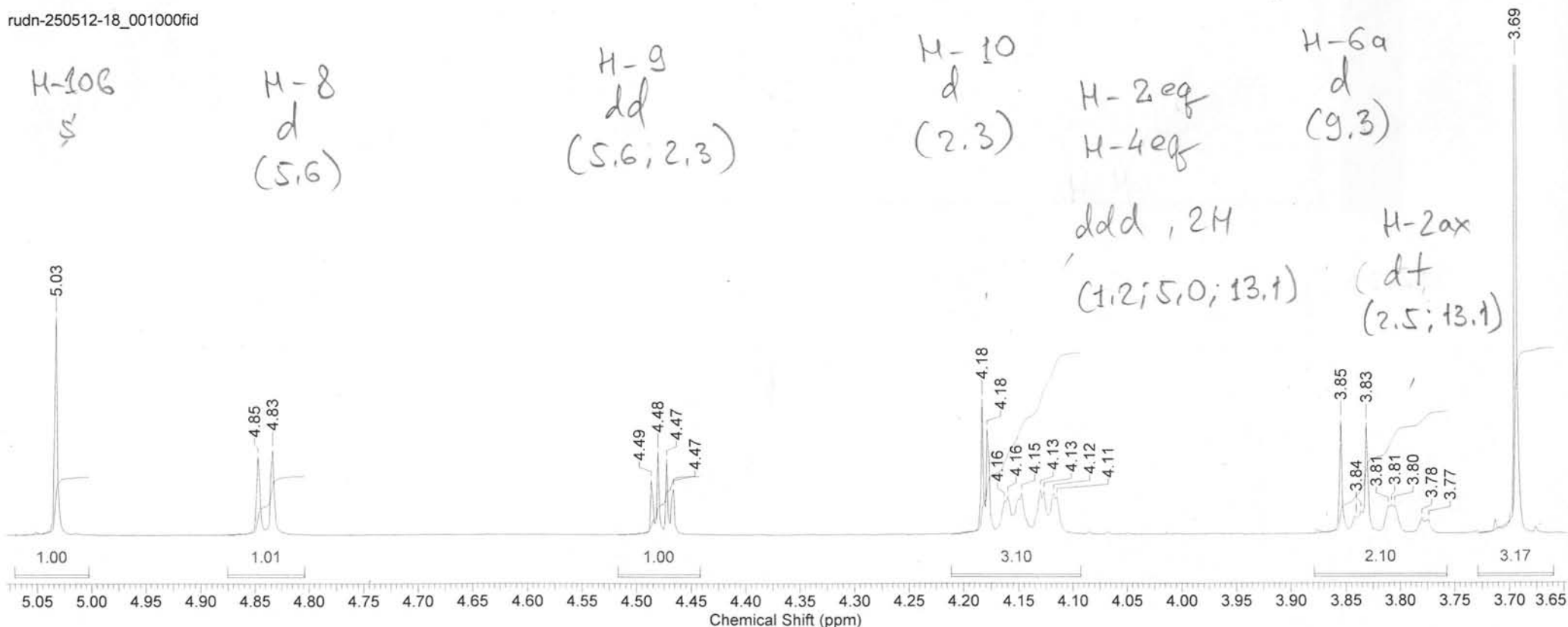


Formula C ₁₃ H ₁₅ Br ₂ NO ₅		FW 425.0699			
Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	31 May 2012 15:49:20
Date Stamp	31 May 2012 15:49:20			Frequency (MHz)	400.14
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-18\rudn-250512-18_001000fid			Original Points Count	16384
Nucleus	1H	Number of Transients	4	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zg
SW(cyclical) (Hz)	10204.08	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2602.0486
Temperature (degree C)	27.000			Sweep Width (Hz)	10203.46

Compound 18

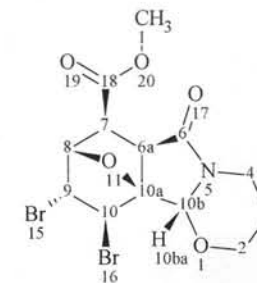


rudn-250512-18_001000fid



Formula C ₁₃ H ₁₅ Br ₂ NO ₅		FW 425.0699	
Acquisition Time (sec) 1.6056	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400		Date 31 May 2012 15:49:20
Date Stamp 31 May 2012 15:49:20			
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-18\rudn-250512-18_001000fid	Frequency (MHz) 400.14		Original Points Count 16384
Nucleus 1H	Number of Transients 4	Origin spect	Original Points Count 16384
Owner root	Points Count 16384	Pulse Sequence zg	Receiver Gain 128.00
SW(cyclical) (Hz) 10204.08	Solvent CHLOROFORM-d	Spectrum Offset (Hz) 2602.0486	Sweep Width (Hz) 10203.46
Temperature (degree C) 27.000			

Compound 18



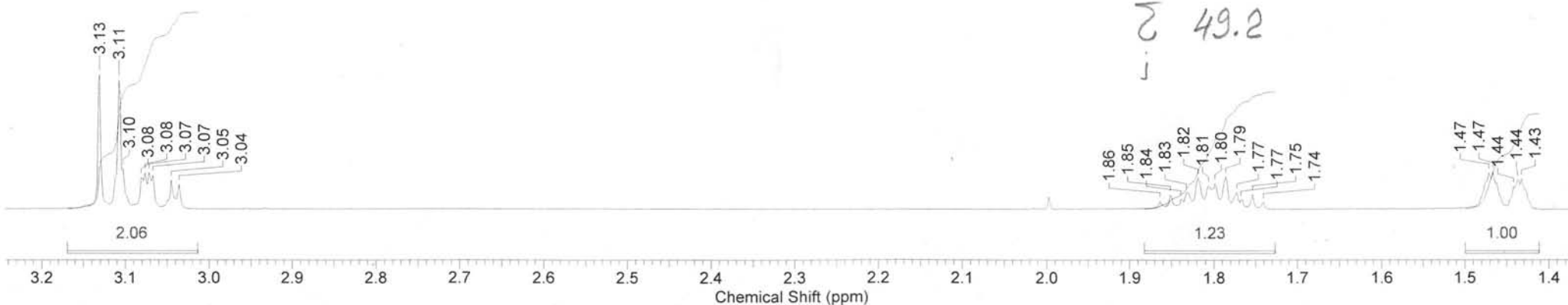
rudn-250512-18_001000fid

H-7
d
(9.3)

H-4ax
ddd
(3.7; 12.5; 13.1)

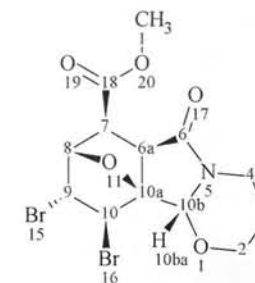
H-3ax
m
(5.0; 12.5; 13.1)

H-3eq
m

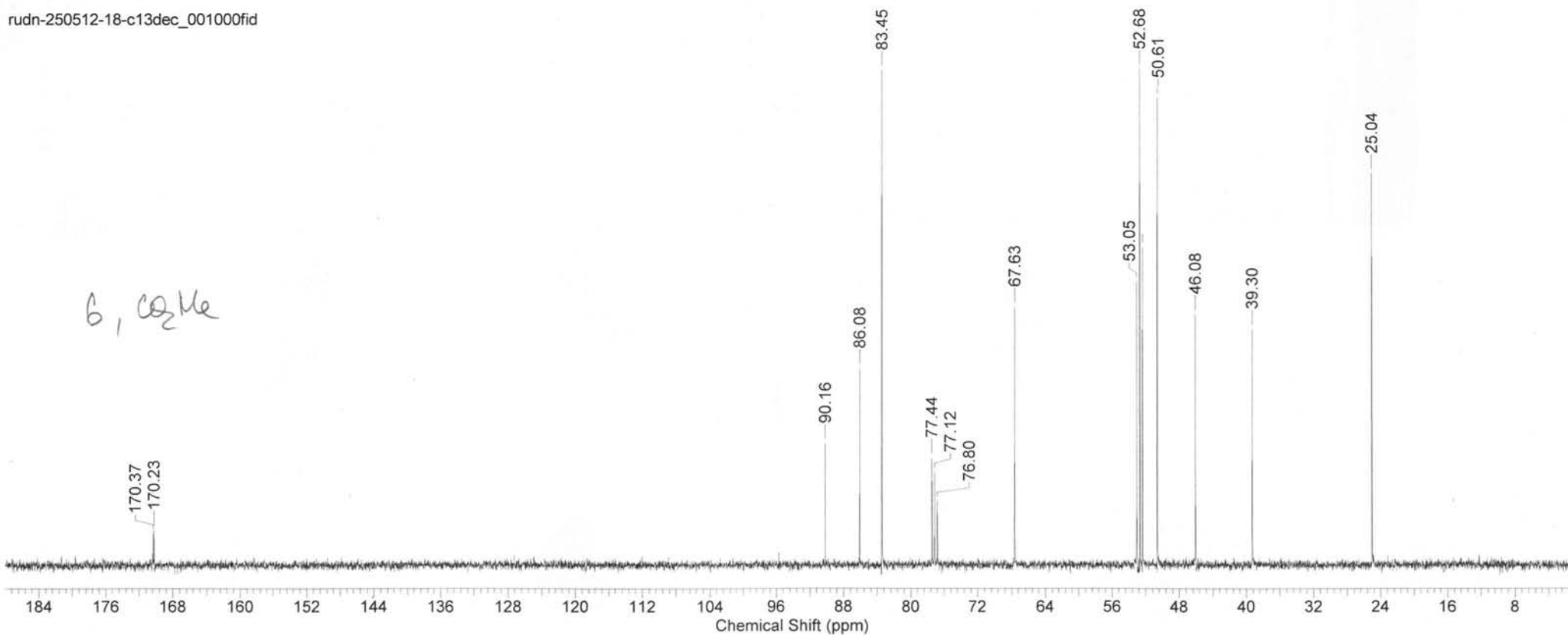


Formula C ₁₃ H ₁₅ Br ₂ NO ₅		FW 425.0699	
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400		Date 31 May 2012 15:51:28
Date Stamp 31 May 2012 15:51:28			
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-18-c13dec\rudn-250512-18-c13dec_001000fid			
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 337	Origin spect
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent CHLOROFORM-d	Spectrum Offset (Hz) 9631.5508
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000		

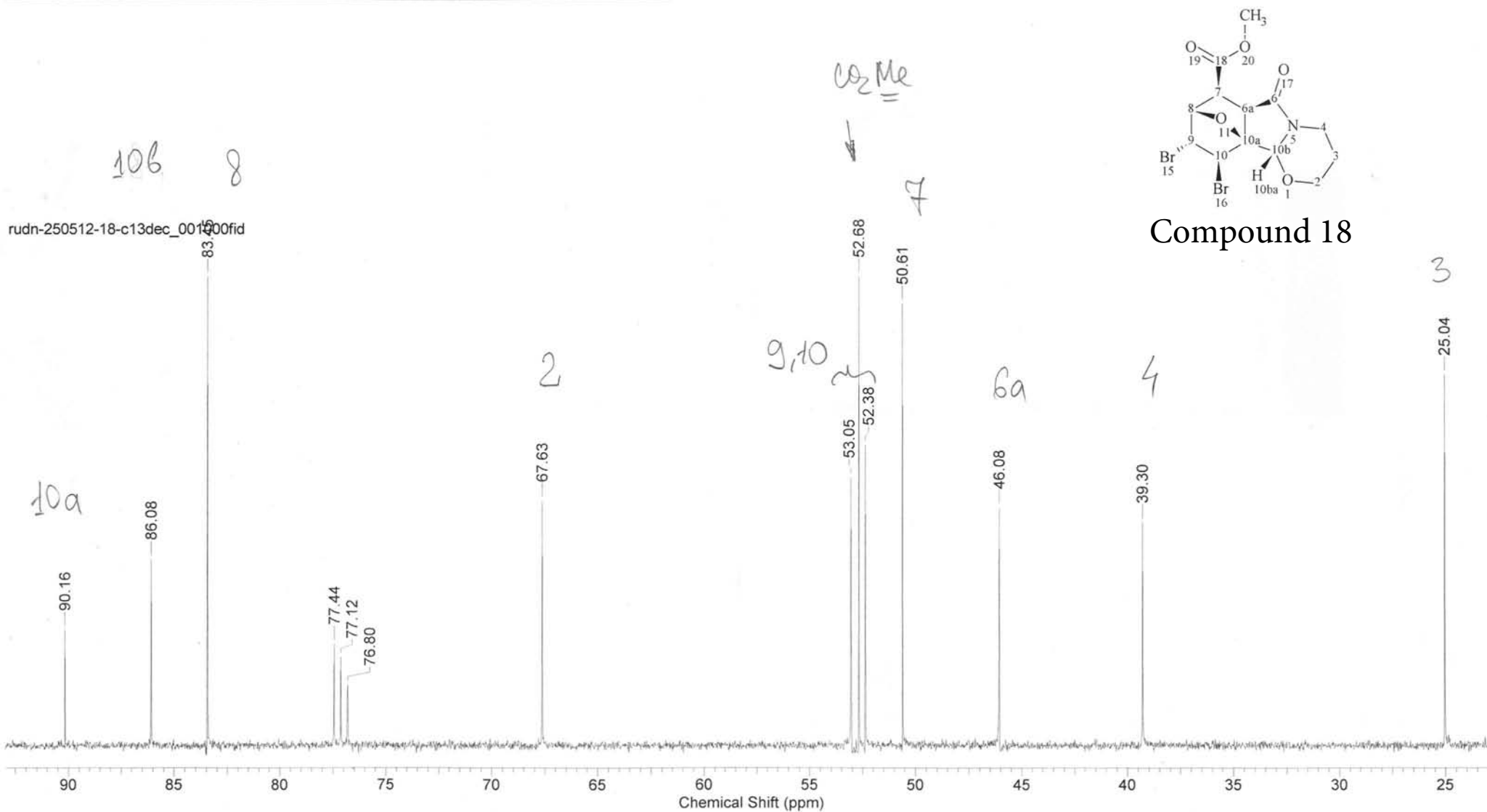
Compound 18



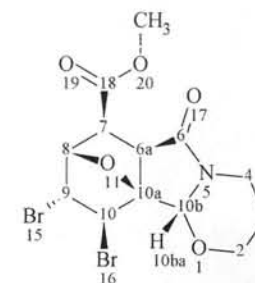
rudn-250512-18-c13dec_001000fid



Formula C ₁₃ H ₁₅ Br ₂ NO ₅		FW 425.0699					
Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	31 May 2012 15:51:28		
Date Stamp	31 May 2012 15:51:28						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-18-c13dec\rudn-250512-18-c13dec_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	337	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zgpg
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9631.5508
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				

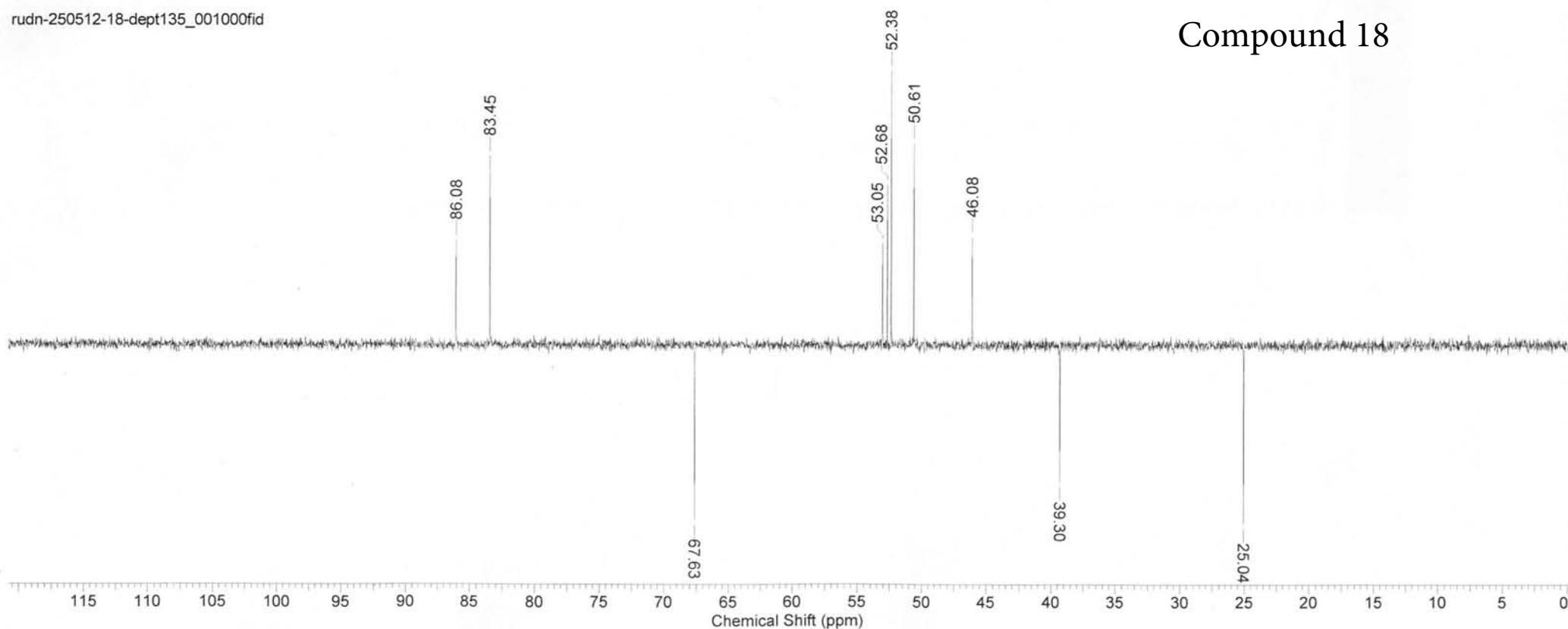


Formula C ₁₃ H ₁₅ Br ₂ NO ₅		FW 425.0699	
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400		Date 31 May 2012 15:57:52
Date Stamp 31 May 2012 15:57:52			
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-18-dept135\rudn-250512-18-dept135_001000fid			
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 252	Origin spect
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence dept135
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent CHLOROFORM-d	Spectrum Offset (Hz) 9631.5508
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000		



Compound 18

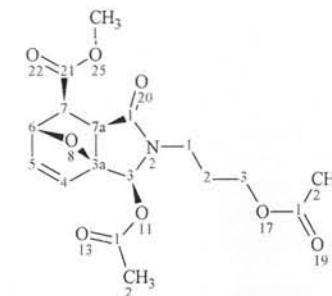
rudn-250512-18-dept135_001000fid



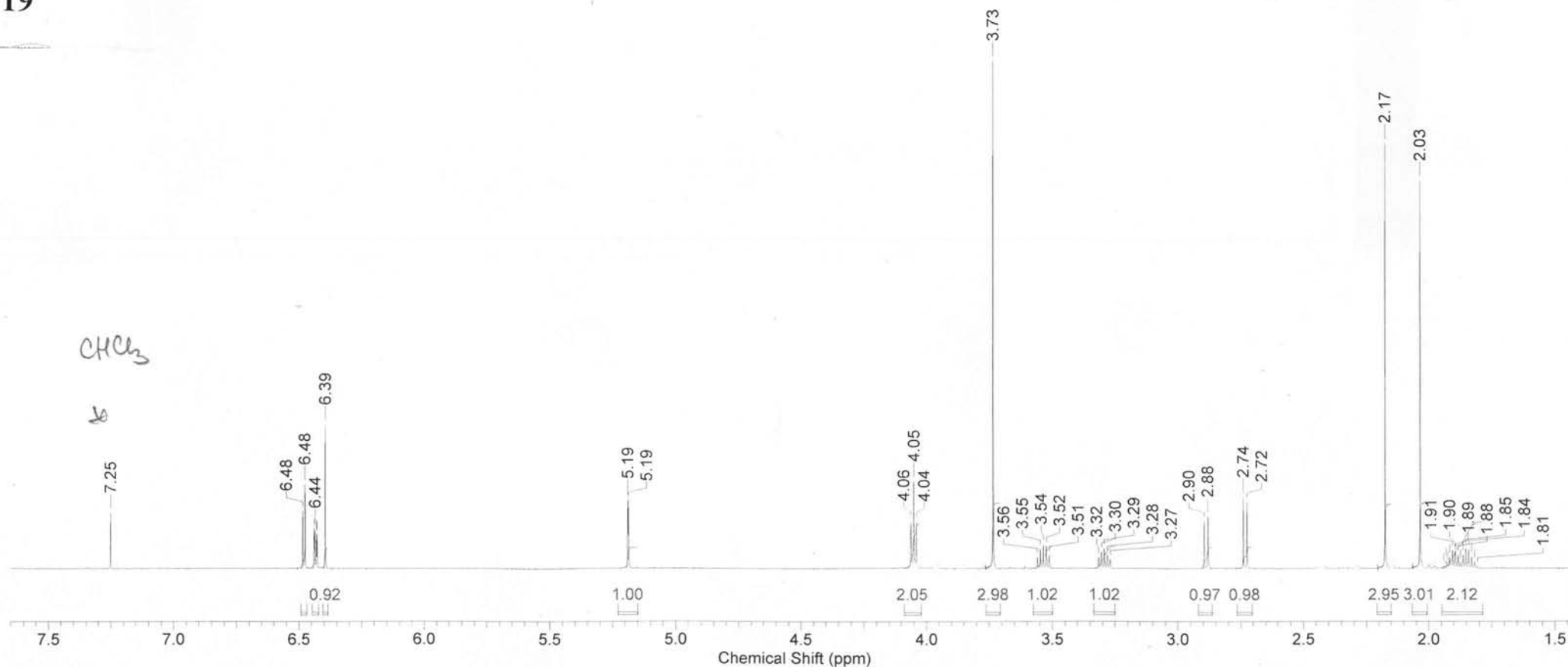
Formula C₁₇H₂₁NO₈ FW 367.3505

Acquisition Time (sec)	1.8193	Comment	single_pulse	Date	27 Apr 2009 12:30:02	Date Stamp	27 Apr 2009 12:27:30
File Name	D:\NMR\27.04.09\lz647-2.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	2
Origin	ECA 600	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	32.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3000.8616	Sweep Width (Hz)	9005.76
Temperature (degree C)	22.400						

Compound 19



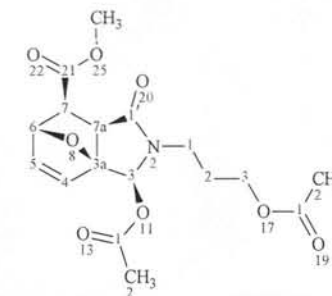
19



Formula C₁₇H₂₁NO₈ FW 367.3505

Acquisition Time (sec)	1.8193	Comment	single_pulse	Date	27 Apr 2009 12:30:02	Date Stamp	27 Apr 2009 12:27:30		
File Name	D:\NMR\27.04.09\ fz647-2.jdf		Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	2	
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384	Pulse Sequence	single_pulse.ex2
Receiver Gain	32.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3000.8616	Sweep Width (Hz)	9005.76		
Temperature (degree C)	22.400								

Compound 19



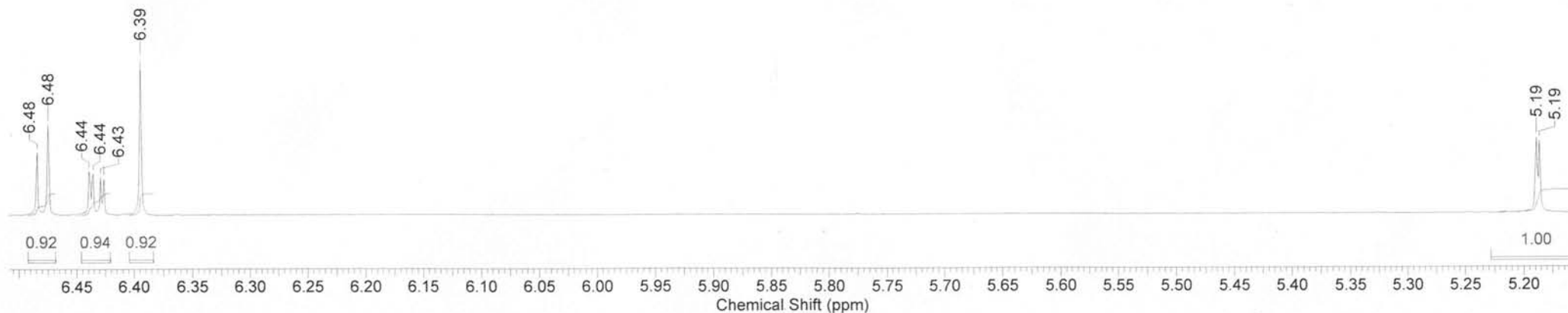
H-4
d
(5.9)

H-3, s

fz647-2.jdf

H-5
dd
(1.7; 5.9)

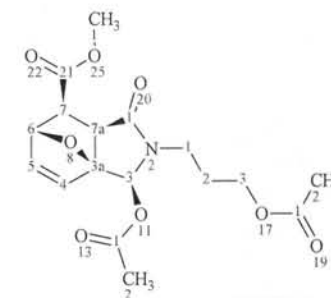
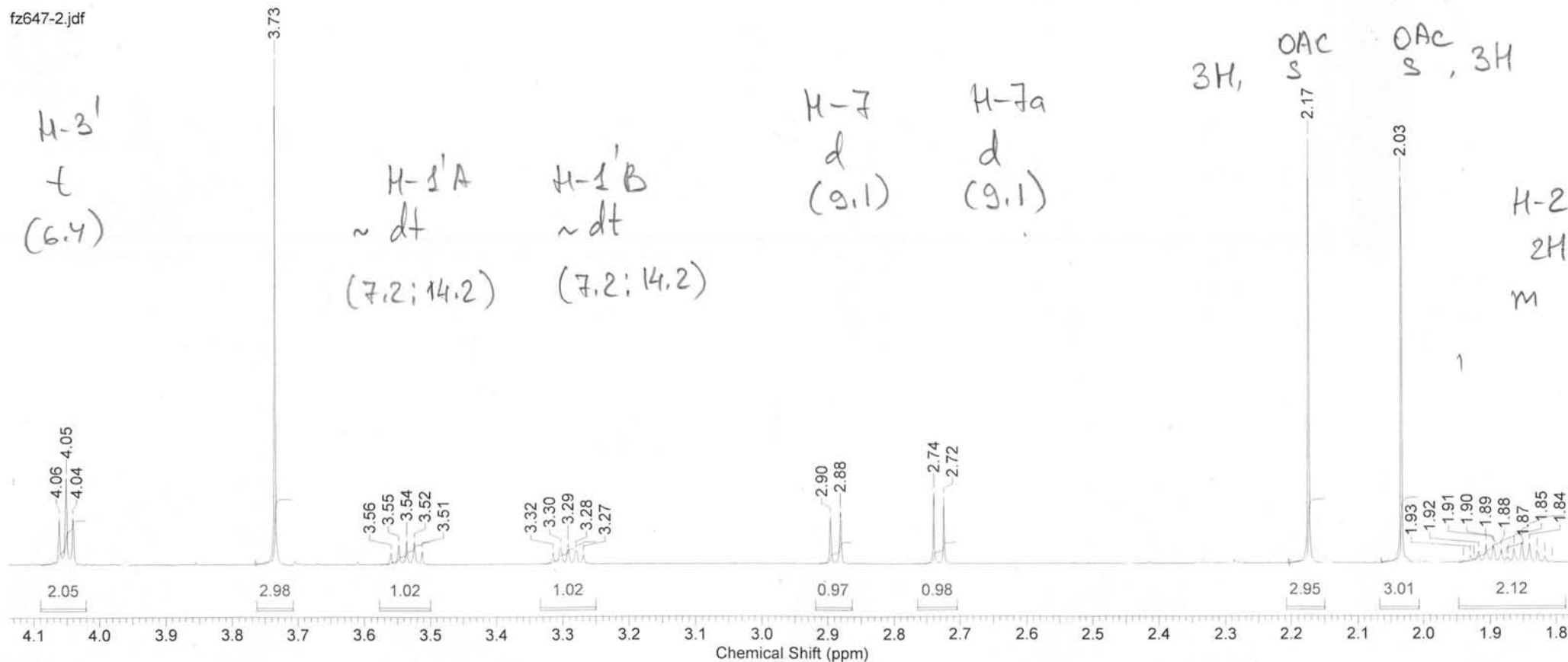
H-6
d
(1.7)



Formula C₁₇H₂₁NO₈ FW 367.3505

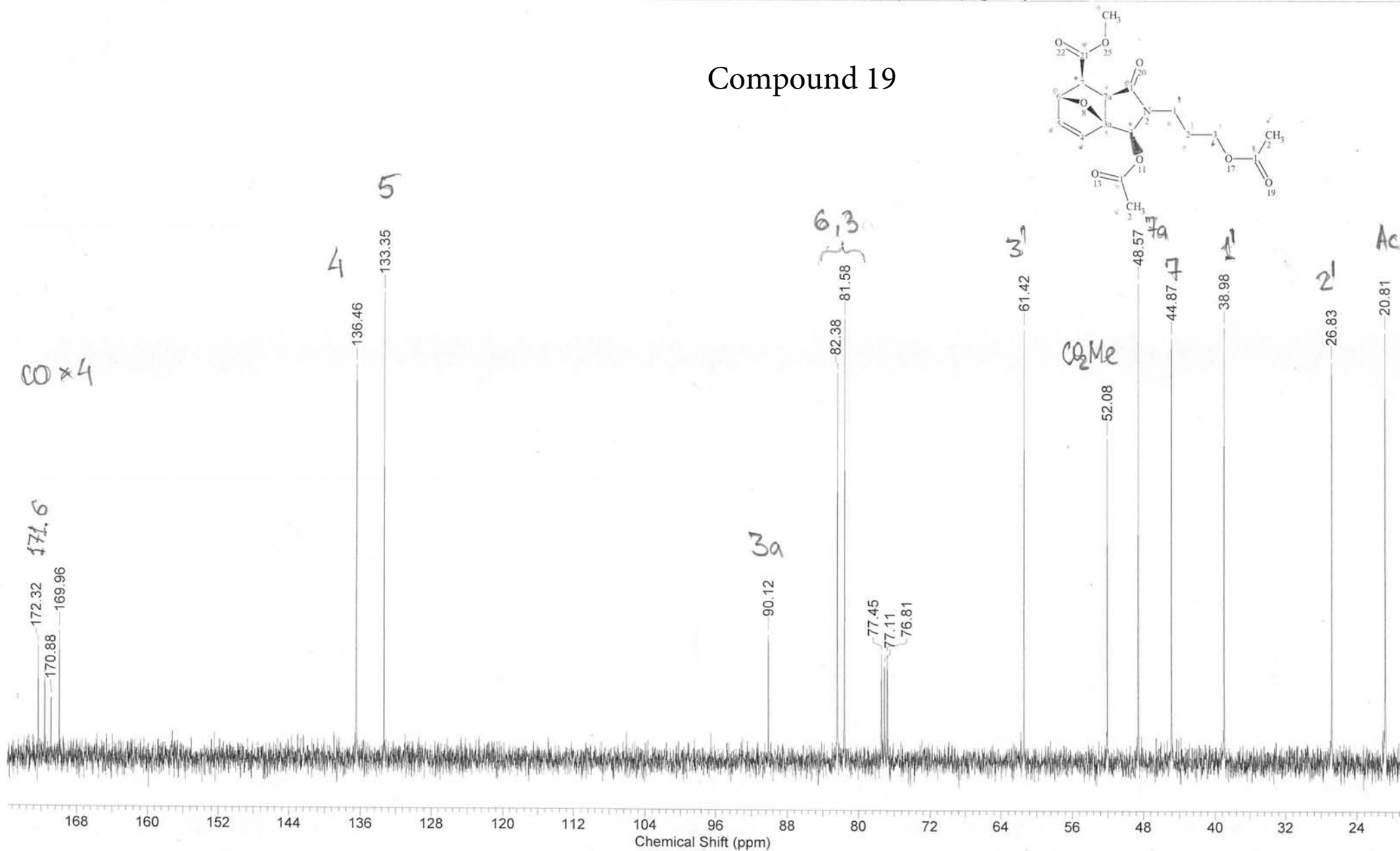
Acquisition Time (sec)	1.8193	Comment	single_pulse	Date	27 Apr 2009 12:30:02	Date Stamp	27 Apr 2009 12:27:30
File Name	D:\NMR\27.04.09\ fz647-2.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	2
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	32.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3000.8616	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	22.400					Sweep Width (Hz)	9005.76

Compound 19

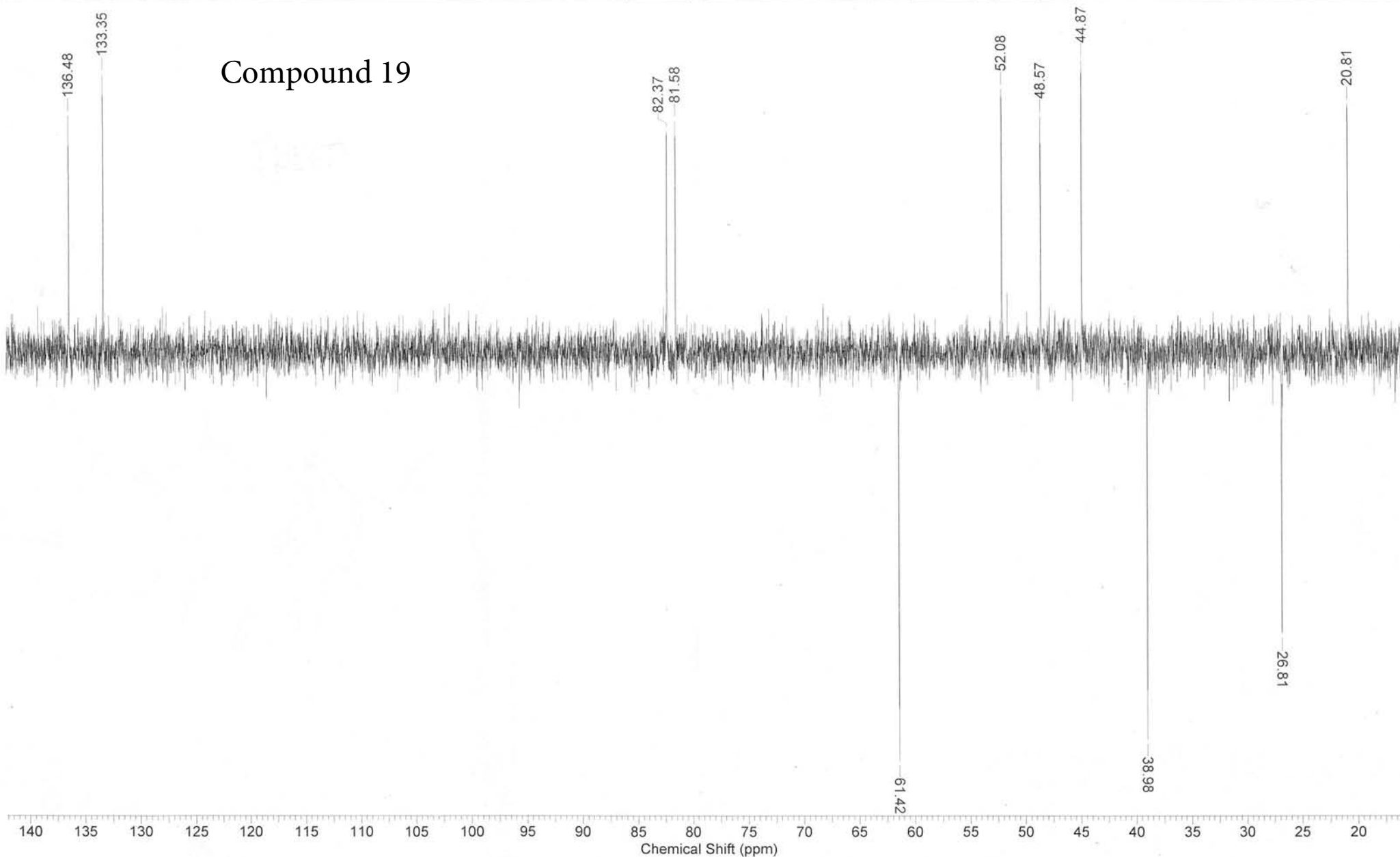
CO₂Me, s, 3H

Acquisition Time (sec)	0.6226	Comment	Imported from UXNMR.		Date	30 Apr 2009 14:49:36
File Name	D:\NMR\IC_13\30.04.09\7lazc13dec\7lazc13dec_001000fid	Frequency (MHz)	100.62	Nucleus	13C	
Number of Transients	192	Original Points Count	16384	Points Count	16384	
Solvent	CHLOROFORM-D	Sweep Width (Hz)	26315.79	Pulse Sequence	zgpg	
				Temperature (degree C)	27.000	

Compound 19



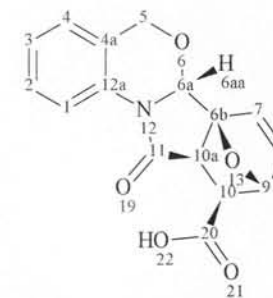
Acquisition Time (sec)	0.6226	Comment	Imported from UXMNR.		Date	30 Apr 2009 14:53:52
File Name	D:\NMR\13\30.04.09\7lazdept135\7lazdept135_001000fid	Frequency (MHz)	100.62	Nucleus	13C	
Number of Transients	63	Original Points Count	16384	Points Count	16384	Pulse Sequence dept135
Solvent	CHLOROFORM-D	Sweep Width (Hz)	26315.79	Temperature (degree C)	27.000	



Formula C₁₆H₁₃NO₅ FW 299.2781

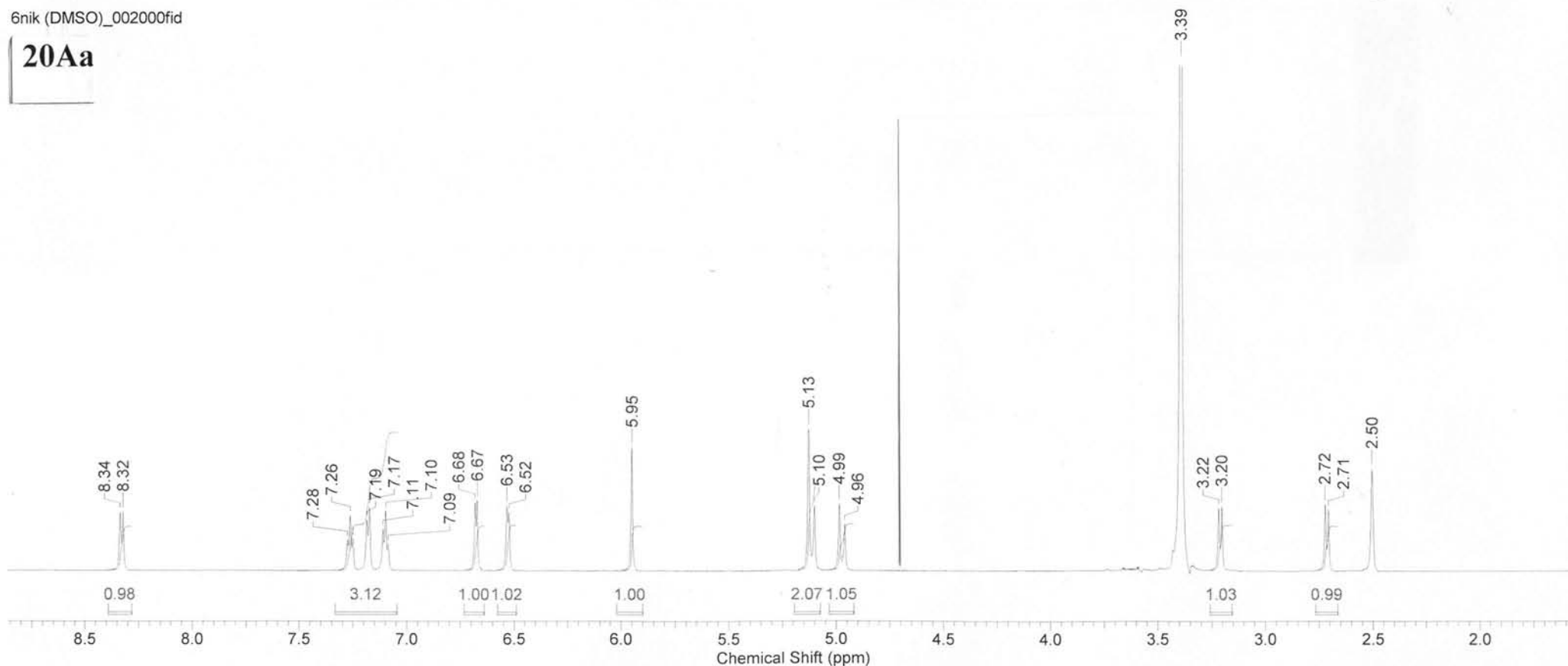
Acquisition Time (sec)	2.1845	Date	02 Feb 2009 06:56:00		Date Stamp	02 Feb 2009 06:56:00	
File Name	D:\NMR\13\Женя и Инга (ИОС конец 2008)\6nik (DMSO)\6nik (DMSO)_002000fid			Frequency (MHz)	600.22	Nucleus	1H
Number of Transients	4	Origin	spect	Original Points Count	32768	Owner	root
Pulse Sequence	zg	Receiver Gain	128.00	SW(cyclical) (Hz)	15000.00	Solvent	DMSO-d6
Sweep Width (Hz)	14999.54	Temperature (degree C)	22.500			Spectrum Offset (Hz)	3144.6580

Compound 20Aa



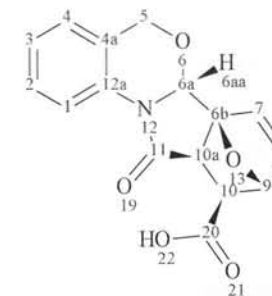
6nik (DMSO)_002000fid

20Aa



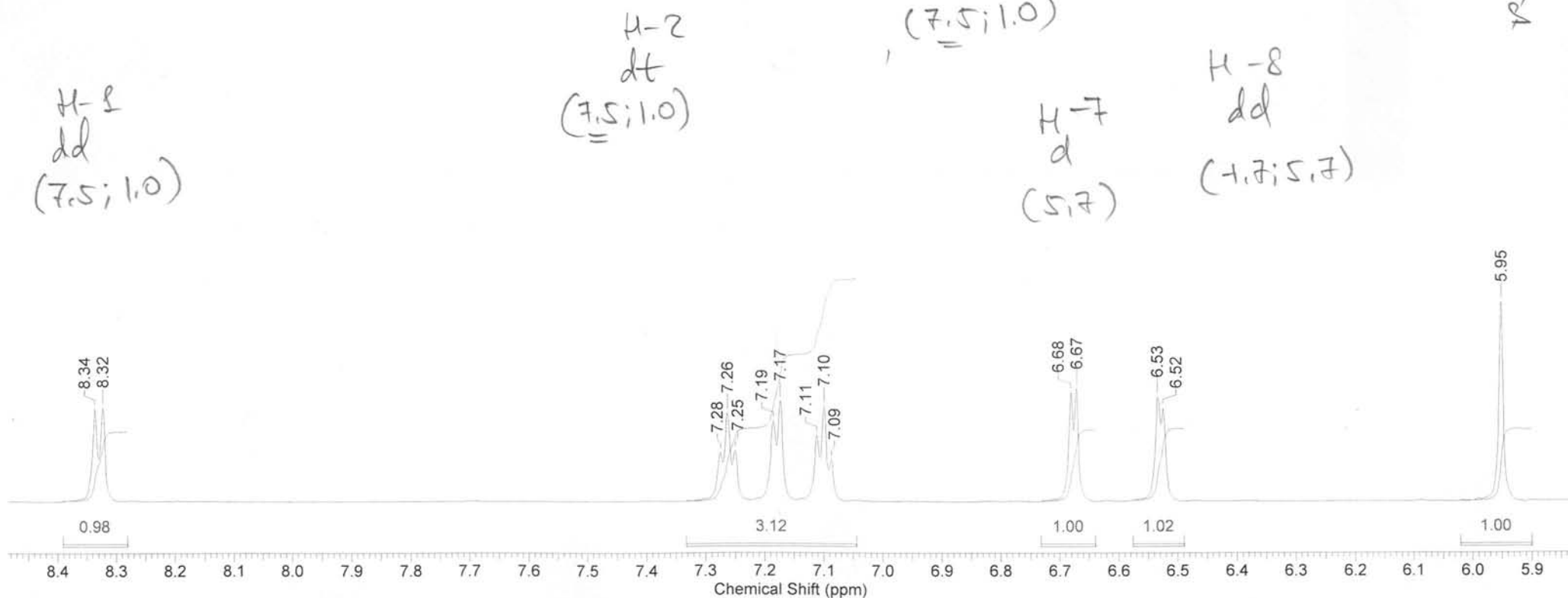
Formula	C ₁₆ H ₁₃ NO ₅	FW	299.2781
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Acquisition Time (sec)	2.1845	Date	02 Feb 2009 06:56:00	Date Stamp	02 Feb 2009 06:56:00		
File Name	D:\NMR\IC_13\Женя и Инга (IOC конец 2008)\6nik (DMSO)\6nik (DMSO)_002000fid			Frequency (MHz)	600.22	Nucleus	1H
Number of Transients	4	Origin	spect	Original Points Count	32768	Points Count	32768
Pulse Sequence	zg	Receiver Gain	128.00	SW(cyclical) (Hz)	15000.00	Solvent	DMSO-d6
Sweep Width (Hz)	14999.54	Temperature (degree C)	22.500			Spectrum Offset (Hz)	3144.6580



Compound 20Aa

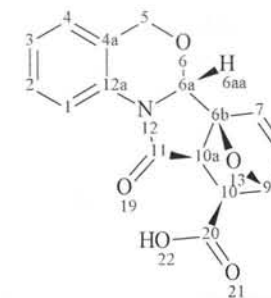
6nik (DMSO)_002000fid



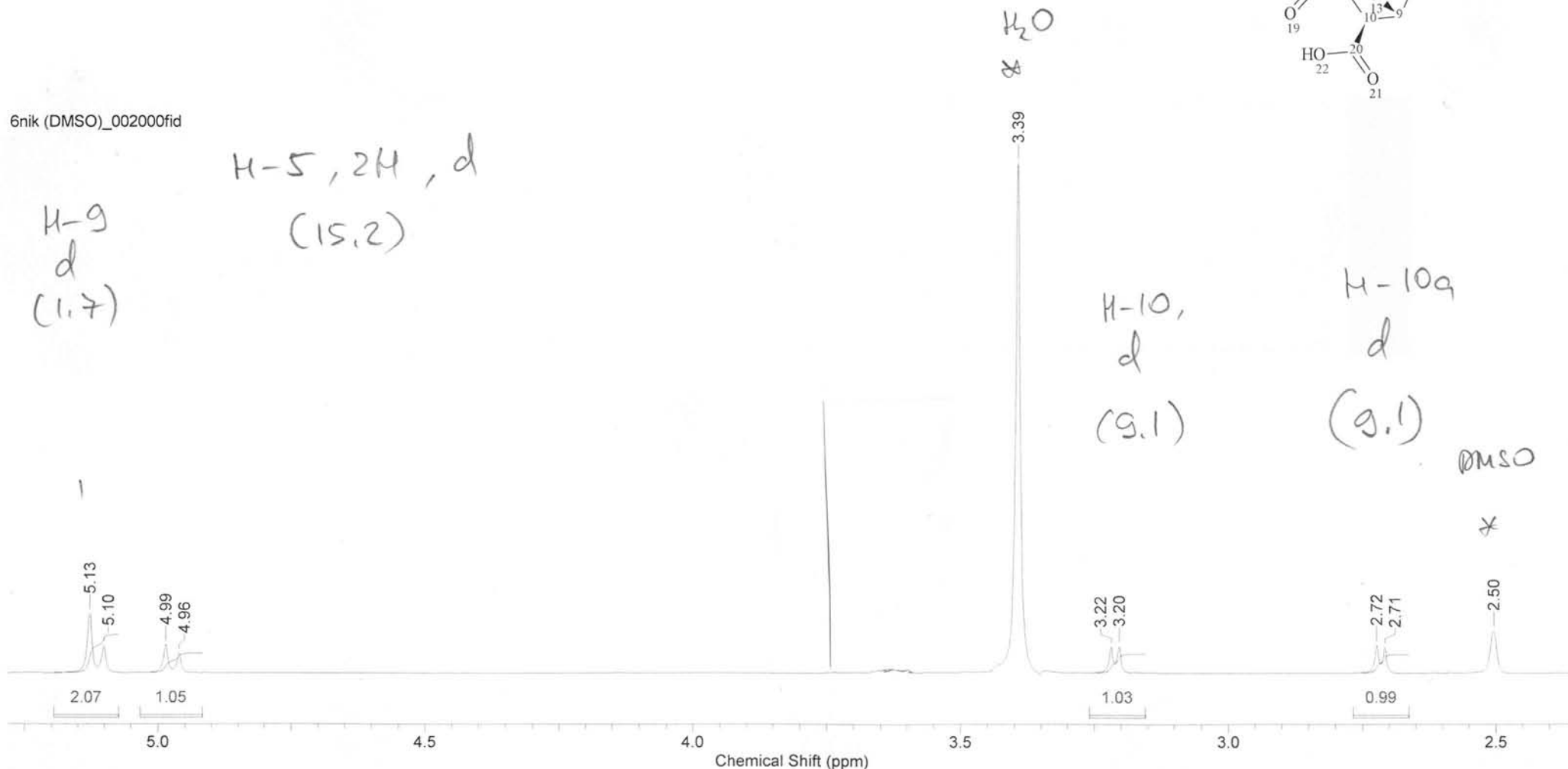
Formula $C_{16}H_{13}NO_5$ FW 299.2781

Acquisition Time (sec)	2.1845	Date	02 Feb 2009 06:56:00		Date Stamp	02 Feb 2009 06:56:00			
File Name	D:\NMR\IC_13\Женя и Инга (IOC конец 2008)\6nik (DMSO)\6nik (DMSO)_002000fid				Frequency (MHz)	600.22	Nucleus	1H	
Number of Transients	4	Origin	spect	Original Points Count	32768	Owner	root	Points Count	32768
Pulse Sequence	zg	Receiver Gain	128.00	SW(cyclical) (Hz)	15000.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3144.6580
Sweep Width (Hz)	14999.54	Temperature (degree C)	22.500						

Compound 20Aa

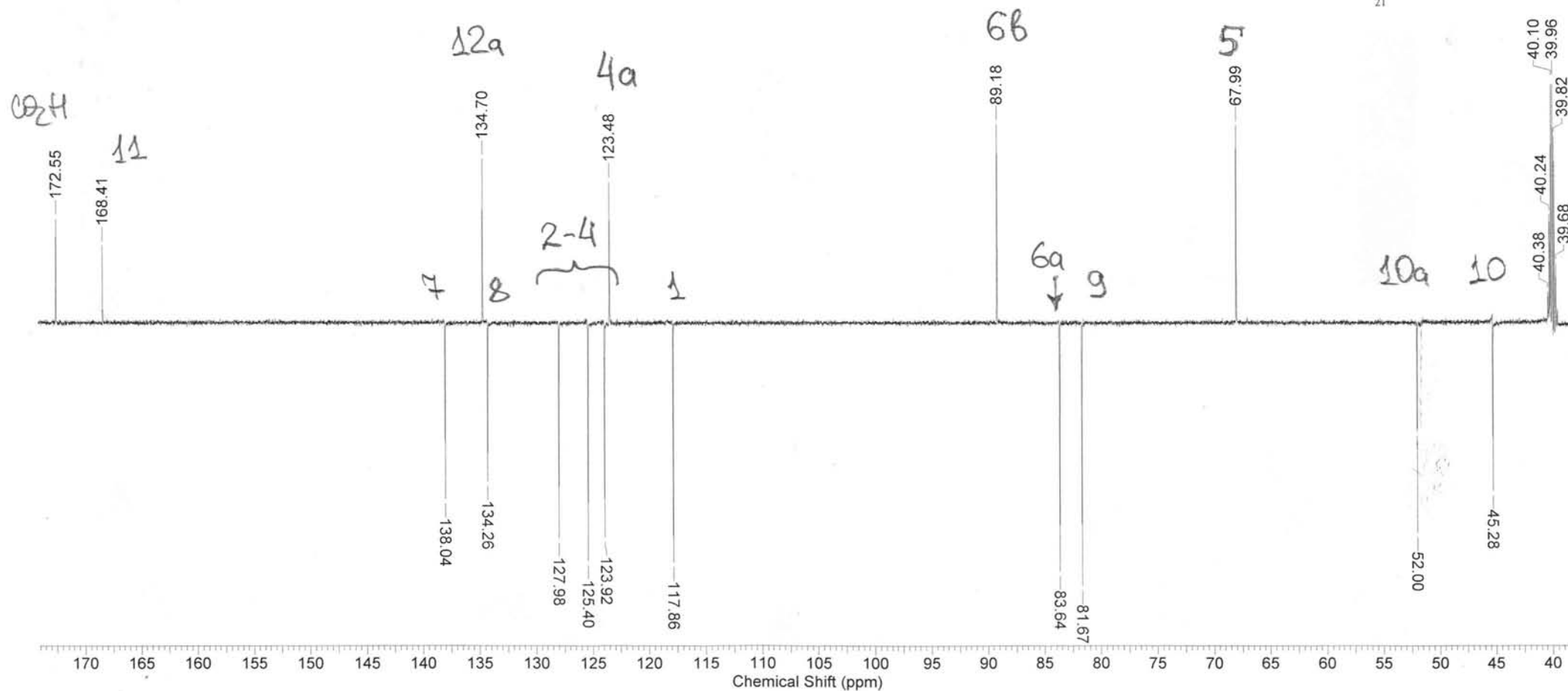
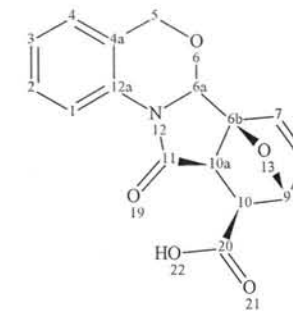


6nik (DMSO)_002000fid



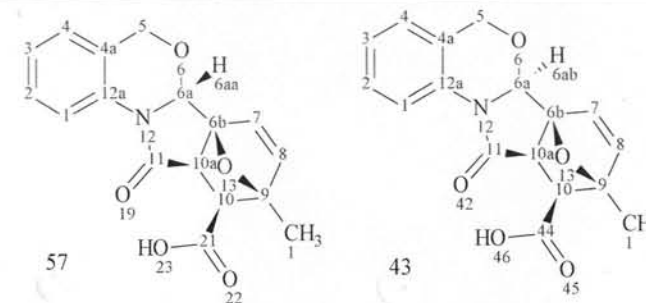
Acquisition Time (sec)	0.9044	Comment	APT	Date	02 Feb 2009 11:01:20
File Name	D:\NMR\IC_13\Женя и Инга (IOC конец 2008)\6nik (DMSO)\6nik (DMSO)_013000fid			Frequency (MHz)	150.94
Nucleus	13C	Number of Transients	5011	Original Points Count	32768
Pulse Sequence	apt	Solvent	CHLOROFORM-D	Sweep Width (Hz)	36231.88
Temperature (degree C)	21.800				

Compound 20Aa

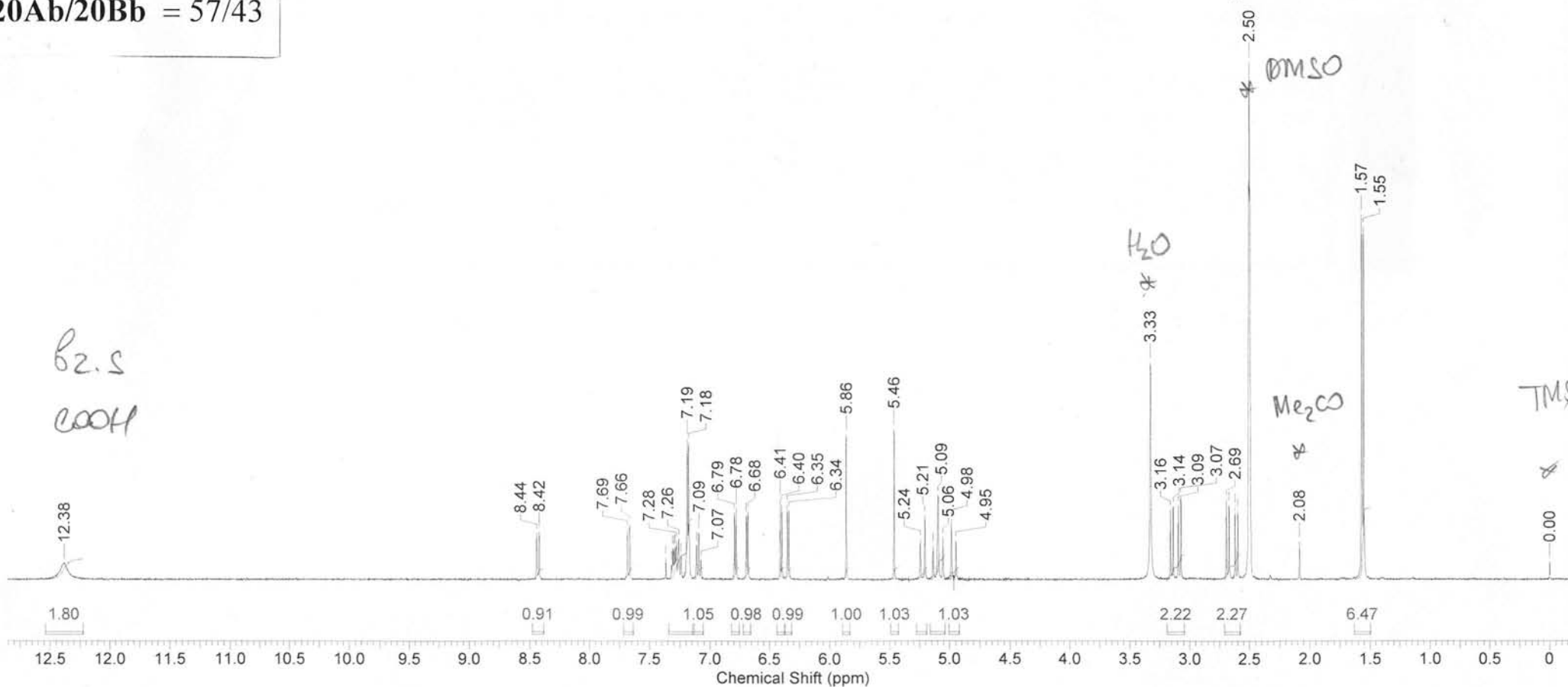


Formula C ₃₄ H ₃₀ N ₂ O ₁₀ ?		FW 626.6094+? (313.3047+313.3047+?+?)					
Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	22 May 2012 09:25:03	Date Stamp	22 May 2012 13:14:16
File Name	D:\NMR\21.05.12\FZ2408-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	4
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	20.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	1984.6338	Sweep Width (Hz)	7503.00
						Temperature (degree C)	24.500

Compounds 20Ab/20Bb

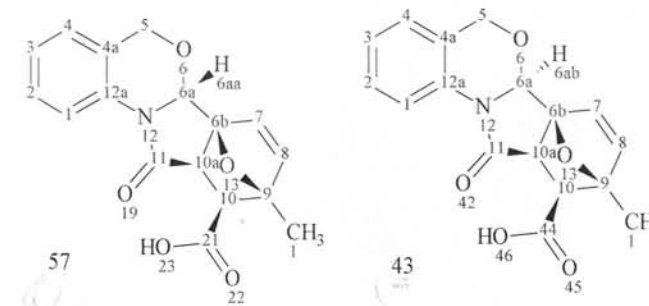


20Ab/20Bb = 57/43

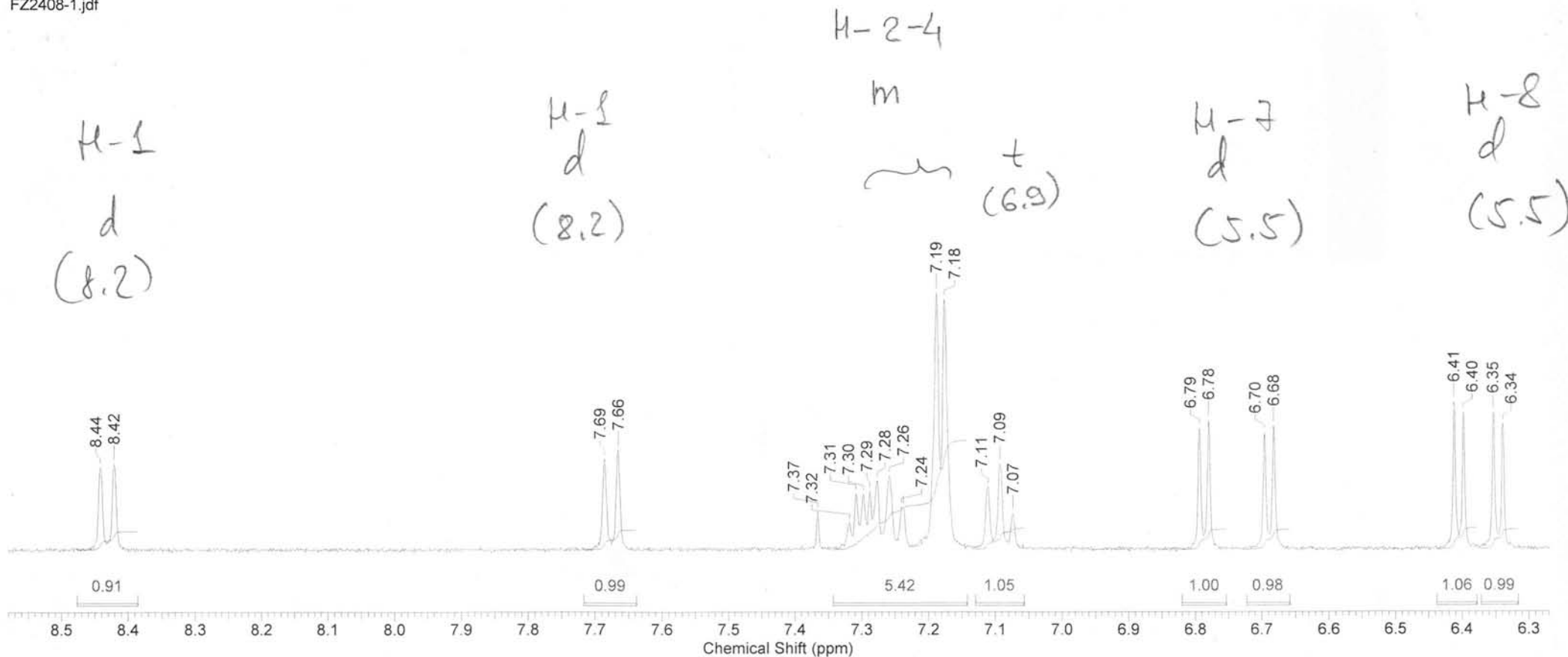


Formula C ₃₄ H ₃₀ N ₂ O ₁₀ ?		FW 626.6094+? (313.3047+313.3047+?+?)					
Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	22 May 2012 09:25:03	Date Stamp	22 May 2012 13:14:16
File Name	D:\NMR\21.05.12\FZ2408-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	4
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	20.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	1984.6338	Sweep Width (Hz)	7503.00
						Temperature (degree C)	24.500

Compounds 20Ab/20Bb

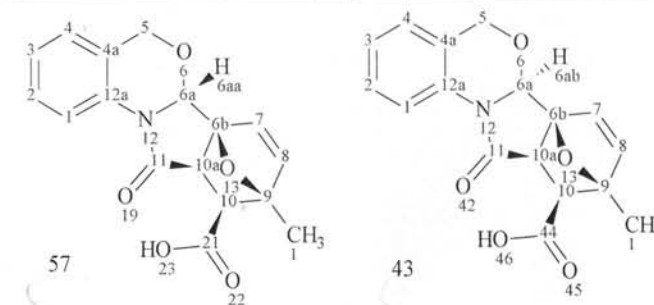


FZ2408-1.jdf

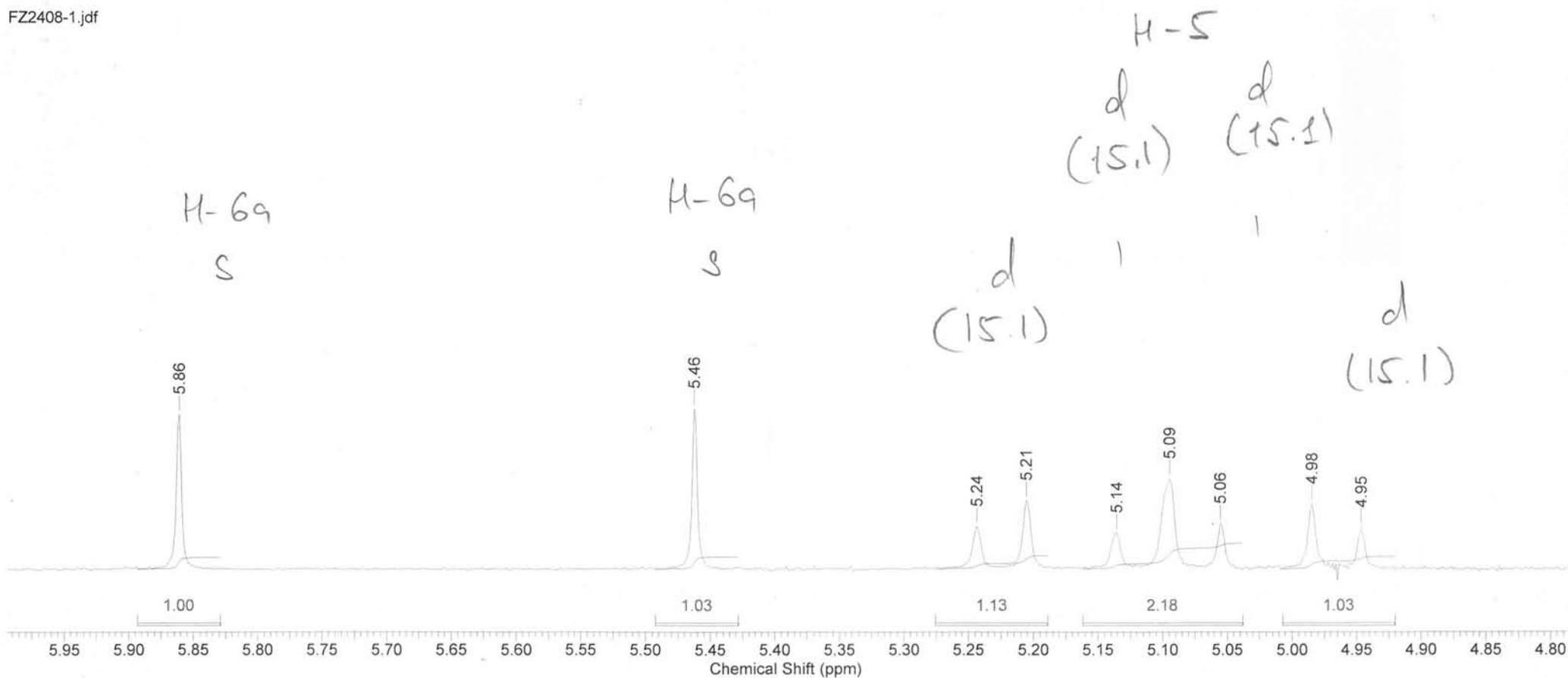


Formula C ₃₄ H ₃₀ N ₂ O ₁₀ ?		FW 626.6094+? (313.3047+313.3047+?+?)					
Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	22 May 2012 09:25:03	Date Stamp	22 May 2012 13:14:16
File Name	D:\NMR\21.05.12\FZ2408-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	4
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	20.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	1984.6338	Sweep Width (Hz)	7503.00
						Pulse Sequence	single_pulse.ex2
						Temperature (degree C)	24.500

Compounds 20Ab/20Bb

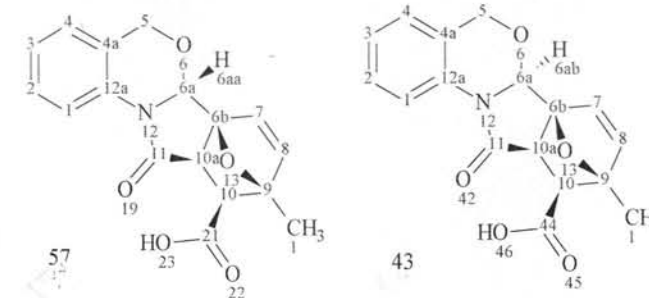


FZ2408-1.jdf

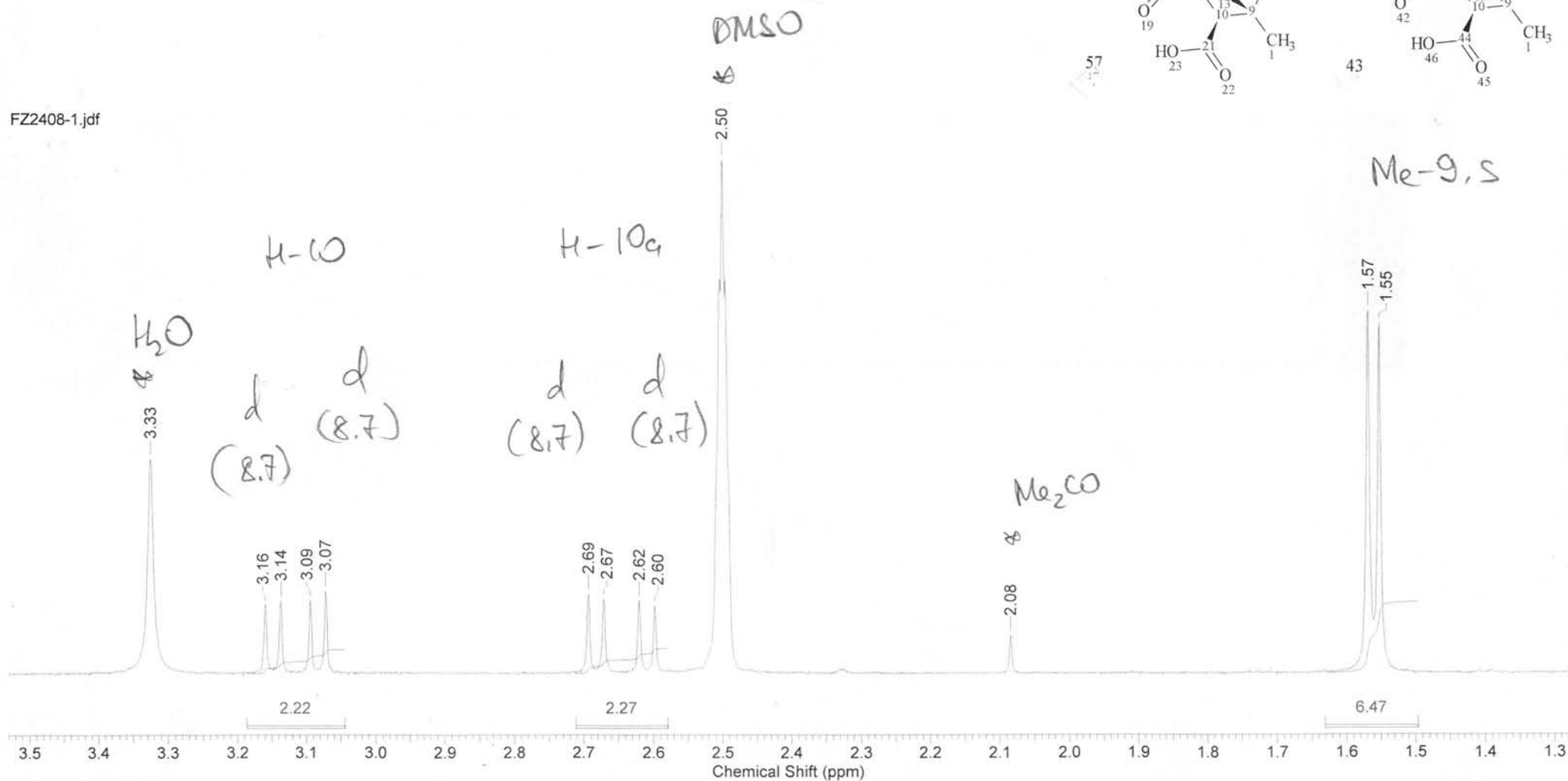


Formula C ₃₄ H ₃₀ N ₂ O ₁₀ ?		FW 626.6094+? (313.3047+313.3047+?+?)	
Acquisition Time (sec) 2.1837	Comment single_pulse	Date 22 May 2012 09:25:03	Date Stamp 22 May 2012 13:14:16
File Name D:\NMR\21.05.12\FZ2408-1.jdf		Frequency (MHz) 399.78	Nucleus 1H
Origin ECS 400	Original Points Count 16384	Owner delta	Points Count 16384
Receiver Gain 20.00	Solvent DMSO-d6	Spectrum Offset (Hz) 1984.6338	Sweep Width (Hz) 7503.00
			Number of Transients 4
			Pulse Sequence single_pulse.ex2
			Temperature (degree C) 24.500

Compounds 20Ab/20Bb

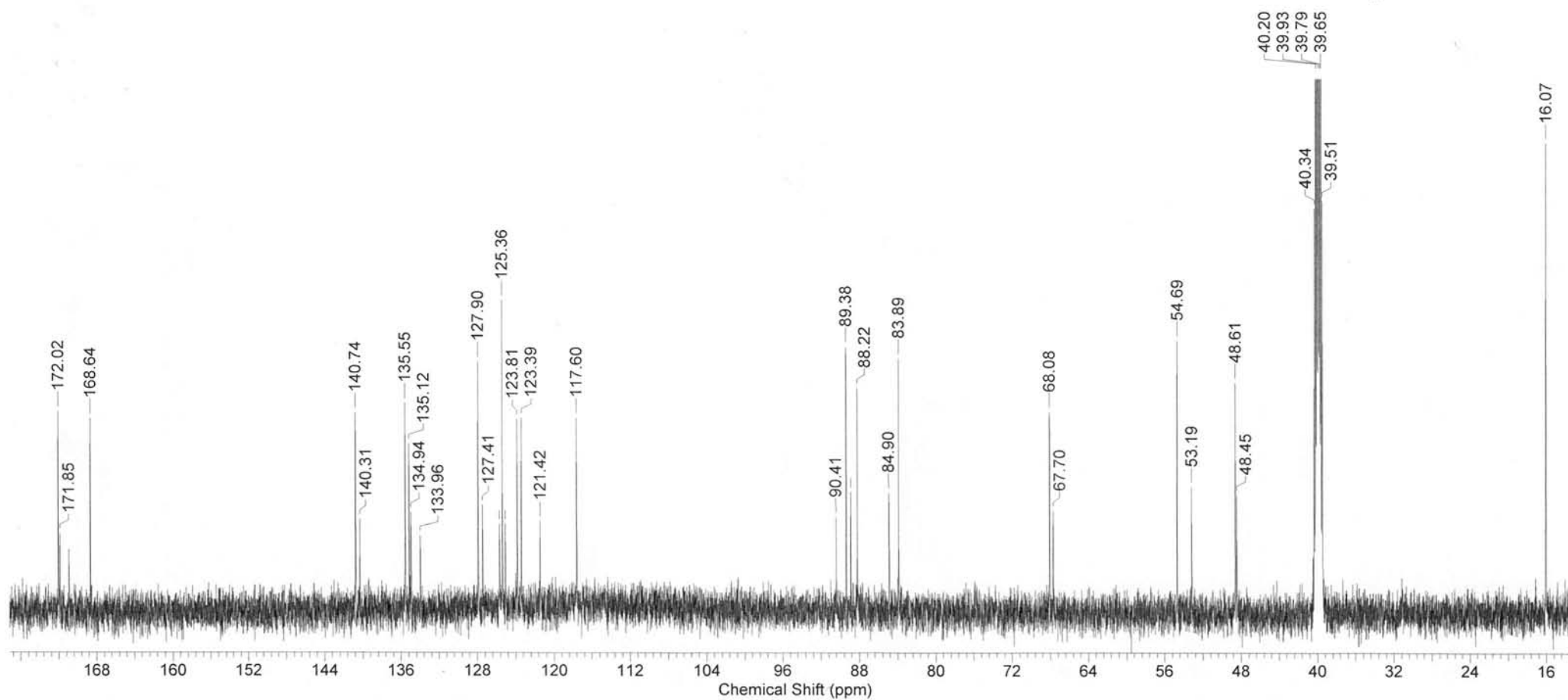
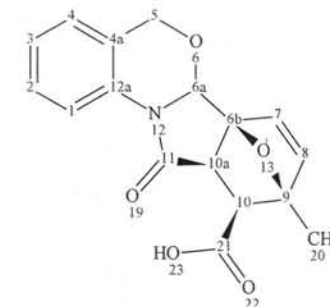


FZ2408-1.jdf



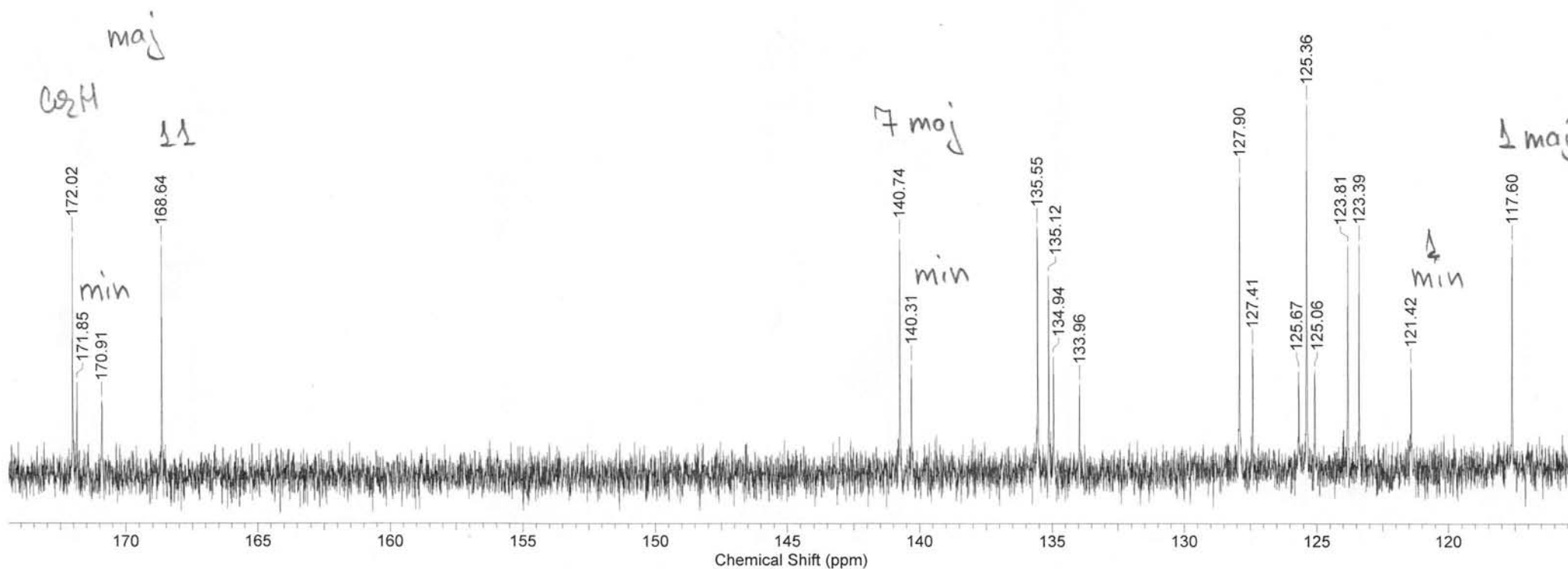
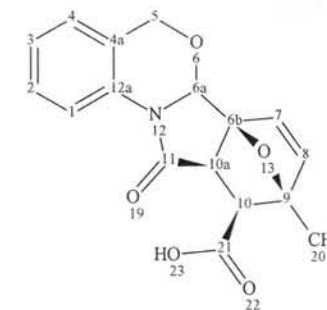
Acquisition Time (sec)	0.9044	Comment	fraction 24	Date	02 Feb 2009 13:41:20
File Name	D:\NMR\C_13\Женя и Инга (IOC конец 2008)\7nik (DMSO)\nik1d600\nik1d600_131000fid			Frequency (MHz)	150.94
Nucleus	13C	Number of Transients	778	Original Points Count	32768
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D	Sweep Width (Hz)	36231.88
Temperature (degree C)	21.000				

Compounds 20Ab/20Bb



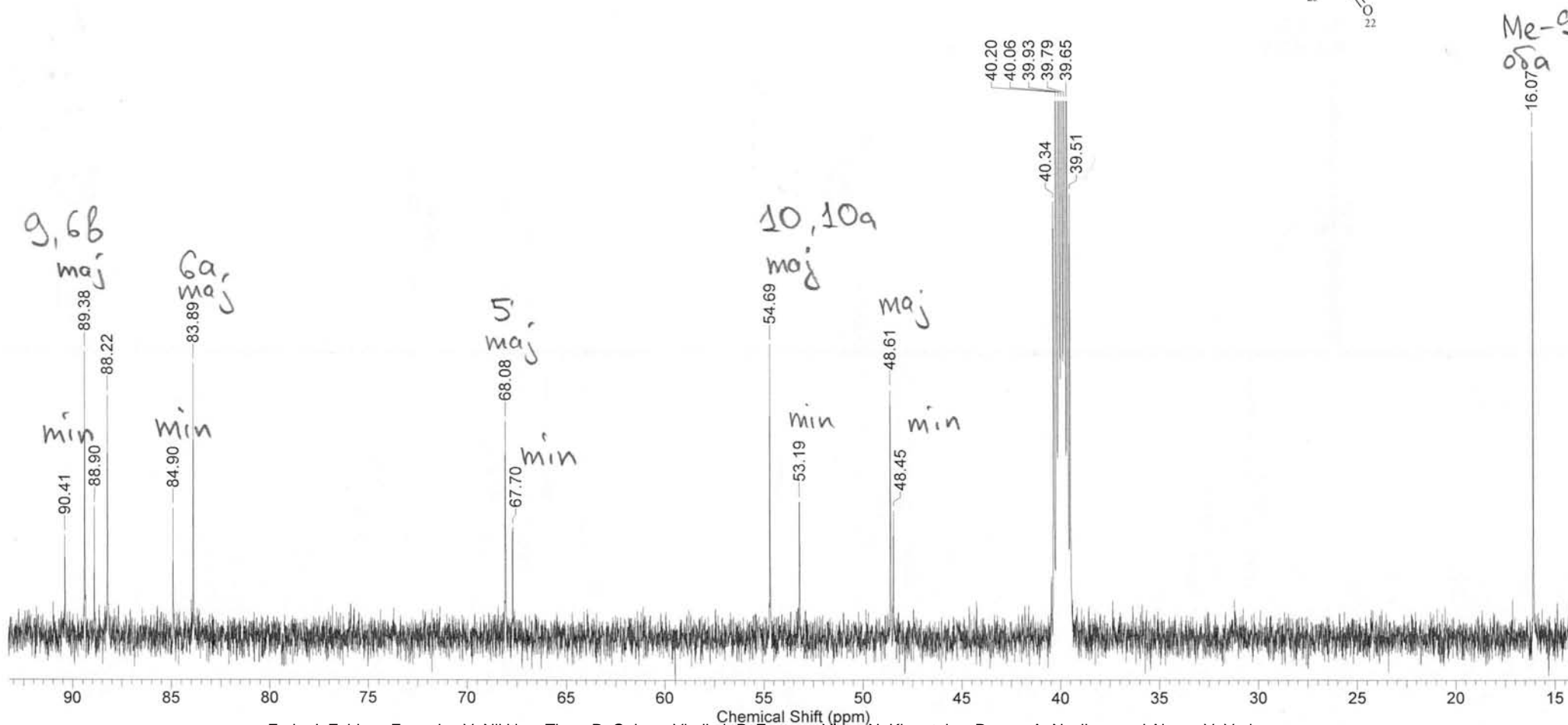
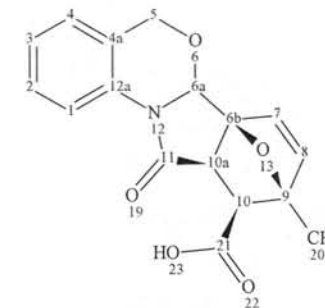
Acquisition Time (sec)	0.9044	Comment	fraction 24	Date	02 Feb 2009 13:41:20
File Name	D:\NMR\C_13\Женя и Инга (IOC конец 2008)\7nik (DMSO)\nik1d600\nik1d600_131000fid			Frequency (MHz)	150.94
Nucleus	13C	Number of Transients	778	Original Points Count	32768
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D	Points Count	32768
Temperature (degree C)	21.000			Sweep Width (Hz)	36231.88

Compounds 20Ab/20Bb



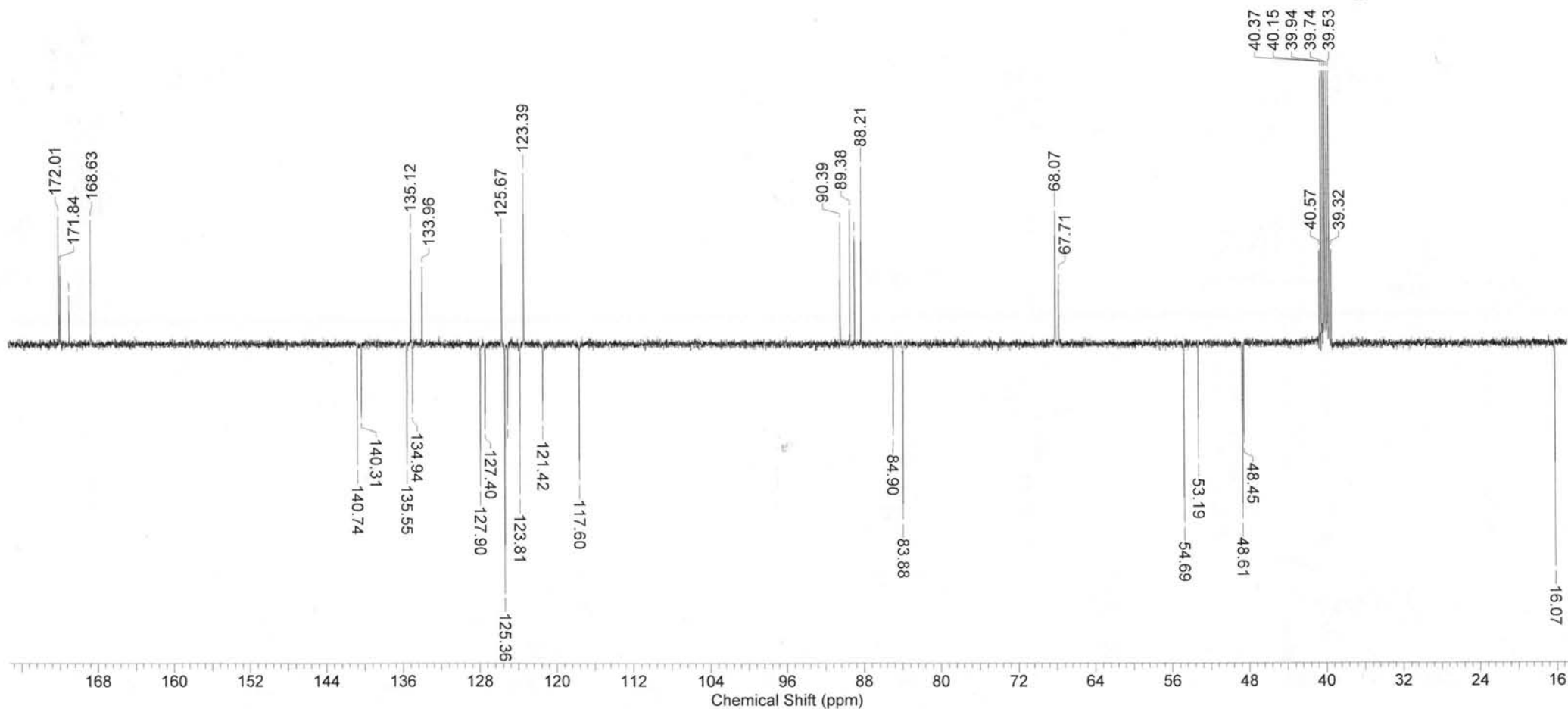
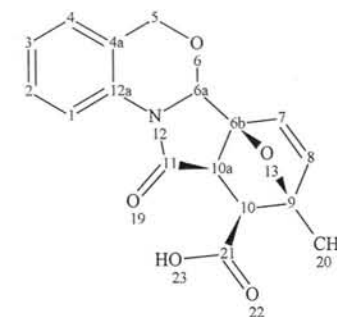
Acquisition Time (sec)	0.9044	Comment	fraction 24	Date	02 Feb 2009 13:41:20
File Name	D:\NMR\C_13\Женя и Инга (IOC конец 2008)\7nik (DMSO)\nik1d600\nik1d600_131000fid			Frequency (MHz)	150.94
Nucleus	13C	Number of Transients	778	Original Points Count	32768
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D	Sweep Width (Hz)	36231.88
Temperature (degree C)	21.000				

Compounds 20Ab/20Bb



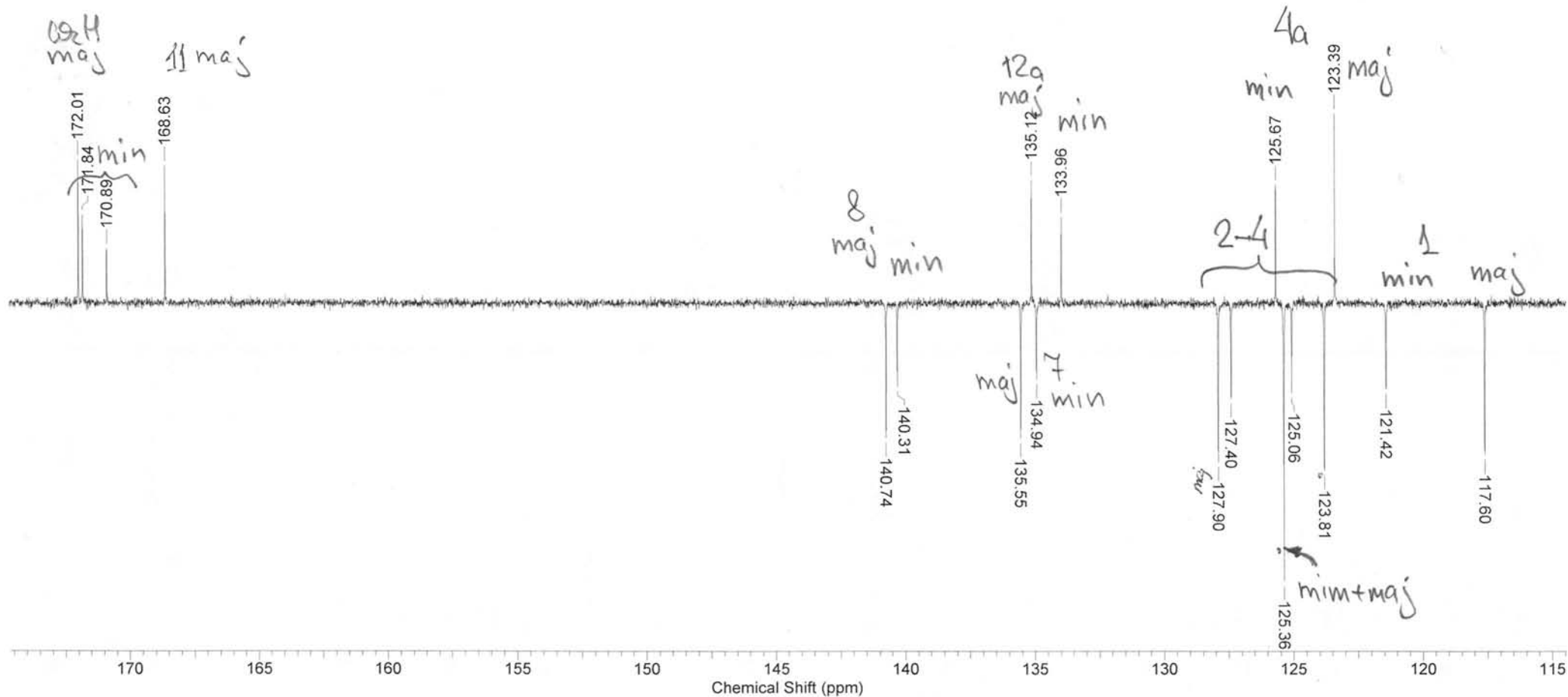
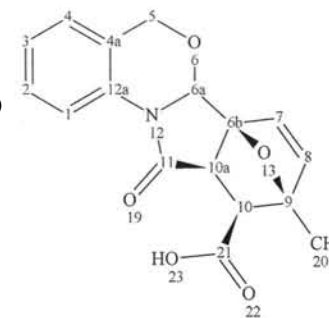
Acquisition Time (sec)	1.3631	Date	01 Feb 2009 11:39:44				
File Name	D:\NMR\13\Женя и Инга (IOC конец 2008)\7nik (DMSO)\7nik (DMSO)_131000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	19855	Original Points Count	32768	Points Count	32768
Pulse Sequence	jmod	Solvent	DMSO-D6	Sweep Width (Hz)	24038.46	Temperature (degree C)	27.000

Compounds 20Ab/20Bb



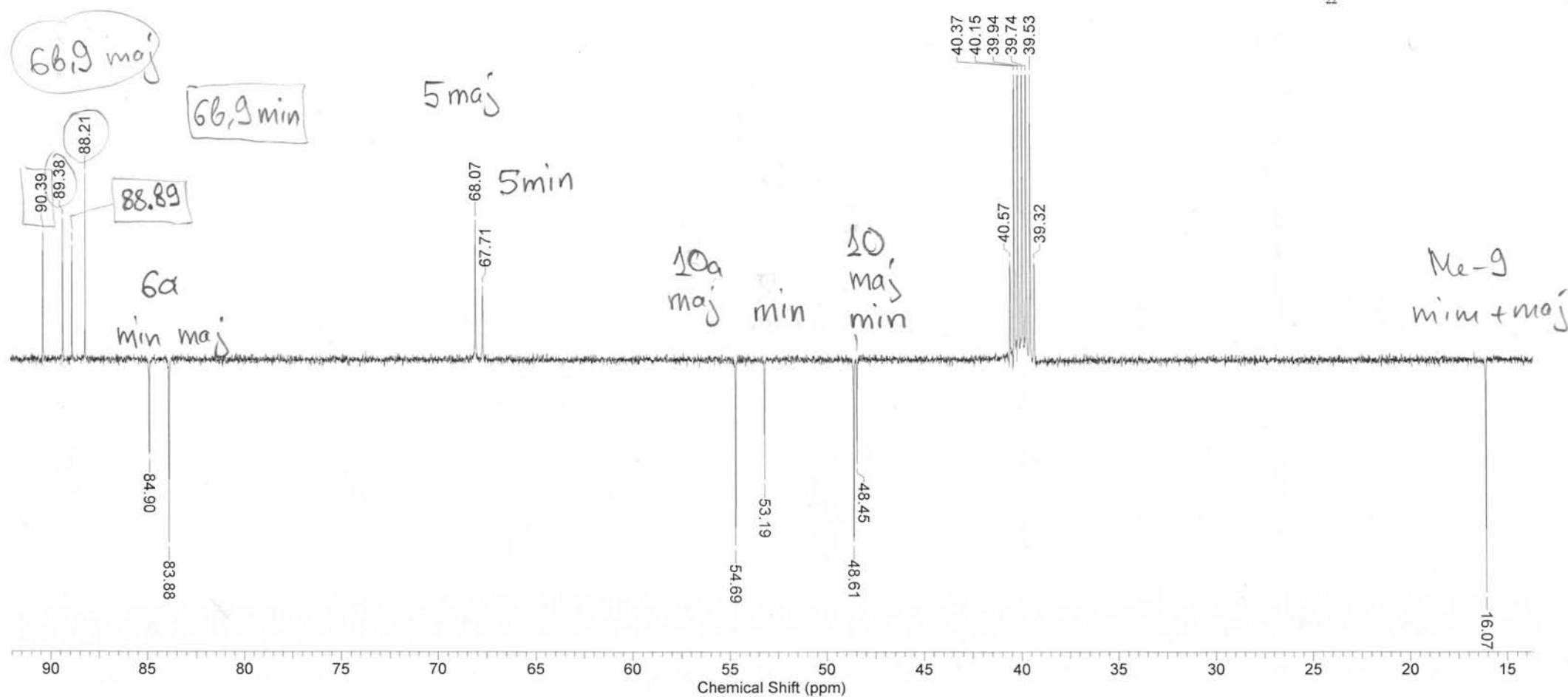
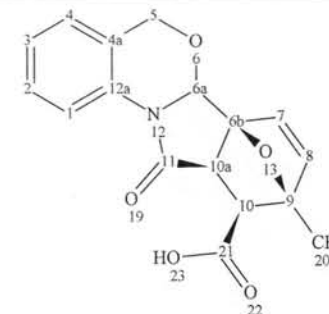
Acquisition Time (sec)	1.3631	Date	01 Feb 2009 11:39:44				
File Name	D:\NMR\13\Женя и Инга (IOC конец 2008)\7nik (DMSO)\7nik (DMSO)_131000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	19855	Original Points Count	32768	Points Count	32768
Pulse Sequence	jmod	Solvent	DMSO-D6	Sweep Width (Hz)	24038.46	Temperature (degree C)	27.000

Compounds 20Ab/20Bb



Acquisition Time (sec)	1.3631	Date	01 Feb 2009 11:39:44		
File Name	D:\NMR\13\Женя и Инга (IOC конец 2008)\7nik (DMSO)\7nik (DMSO)_131000fid			Frequency (MHz)	100.62
Nucleus	13C	Number of Transients	19855	Original Points Count	32768
Pulse Sequence	jmod	Solvent	DMSO-D6	Sweep Width (Hz)	24038.46
				Points Count	32768
				Temperature (degree C)	27.000

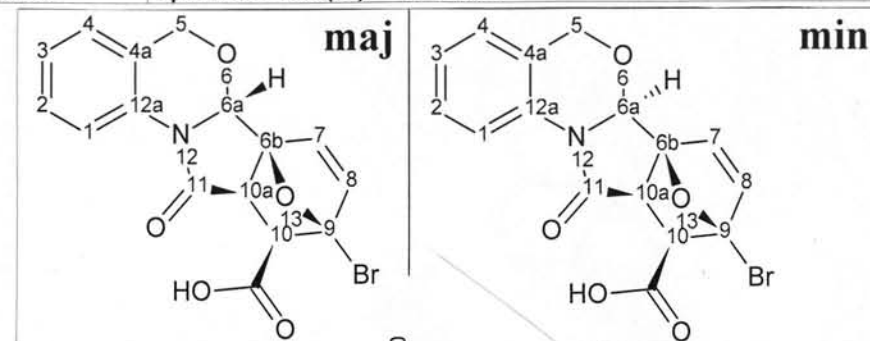
Compounds 20Ab/20Bb



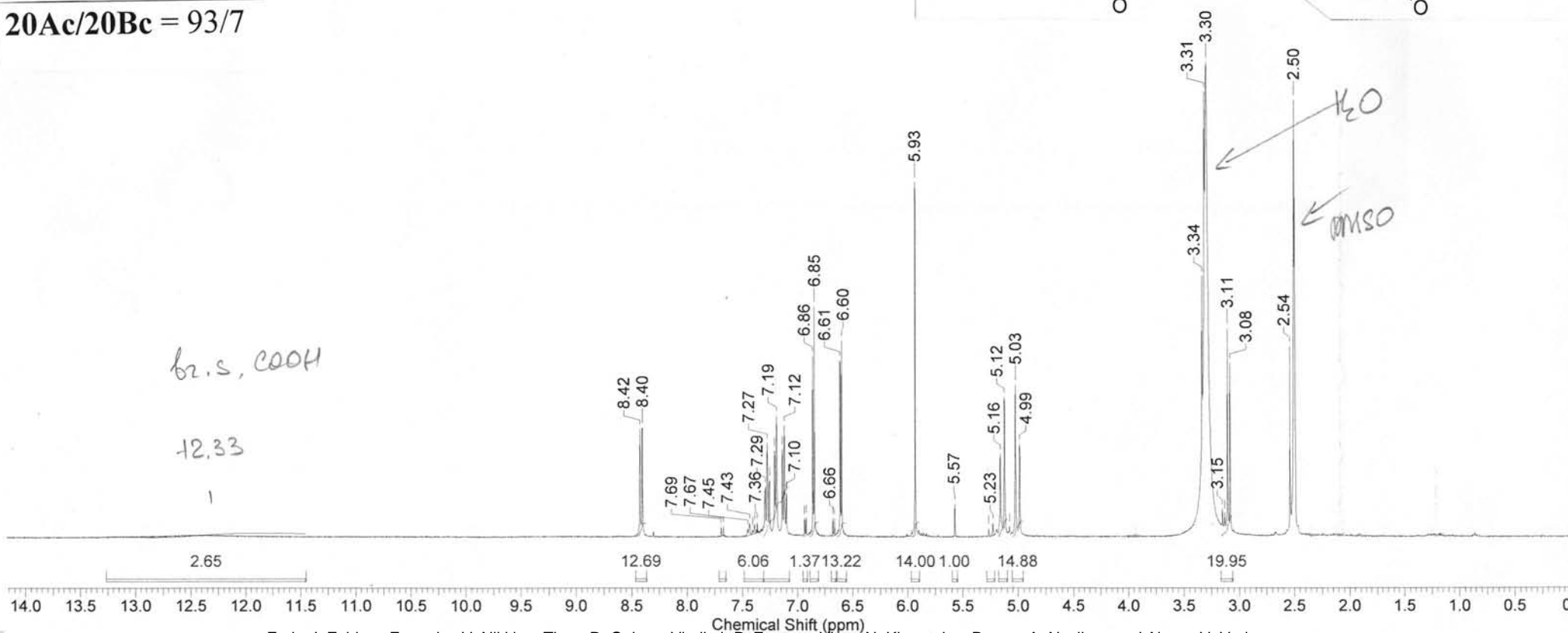
Formula C₁₆H₁₂BrNO₅ FW 378.1742

Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	08 Jun 2012 14:56:00	
Date Stamp	08 Jun 2012 14:56:00						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-20c_1\rudn-250512-20c_1_001000fid						
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	48	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zg
Receiver Gain	128.00	SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542
Sweep Width (Hz)	10416.03	Temperature (degree C)	32.000				

Compounds 20Ac/20Bc



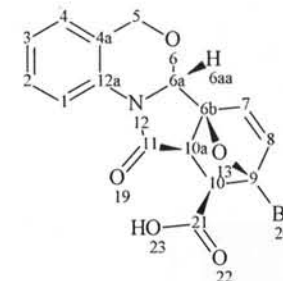
20Ac/20Bc = 93/7



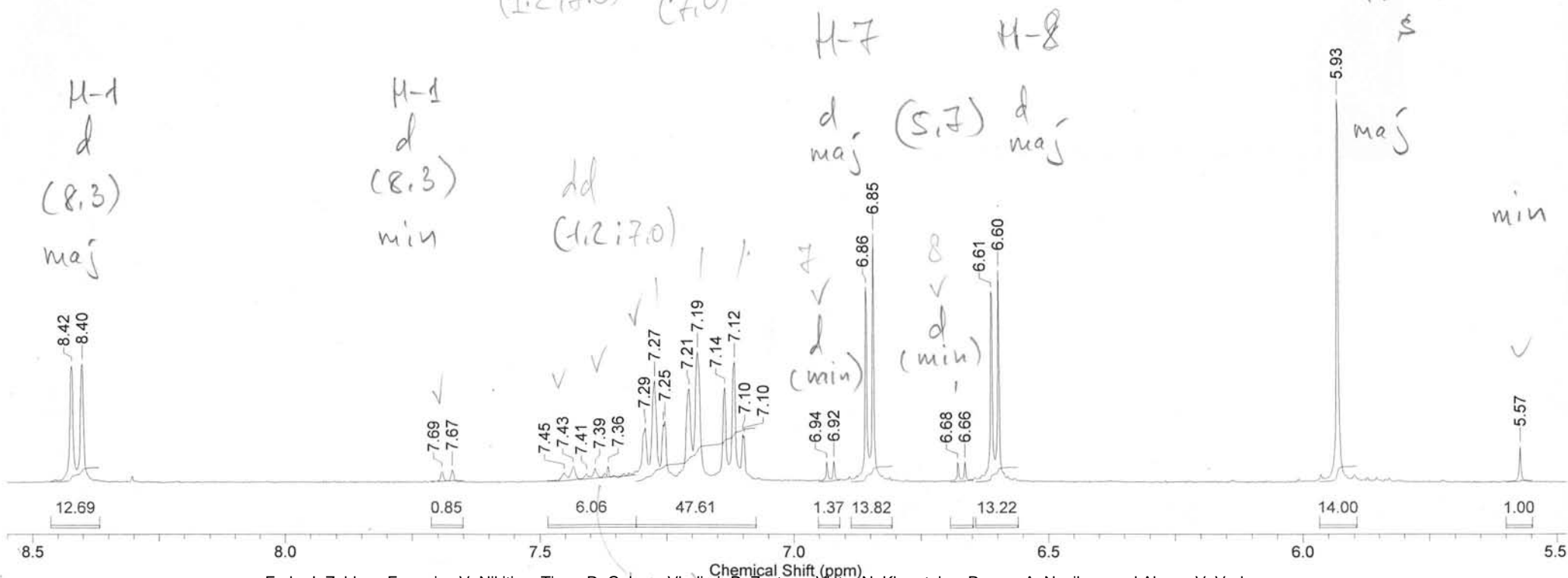
Formula $C_{16}H_{12}BrNO_5$ FW 378.1742

Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	08 Jun 2012 14:56:00
Date Stamp	08 Jun 2012 14:56:00				
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-20c_1\rudn-250512-20c_1_001000fid				
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	48
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	128.00	SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6
Sweep Width (Hz)	10416.03	Temperature (degree C)	32.000	Spectrum Offset (Hz)	2712.0542

Compounds 20Ac/20Bc

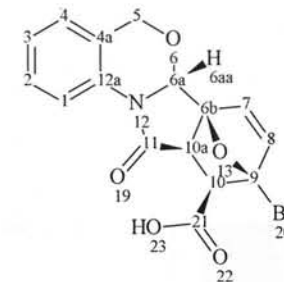


rudn-250512-20c_1_001000fid

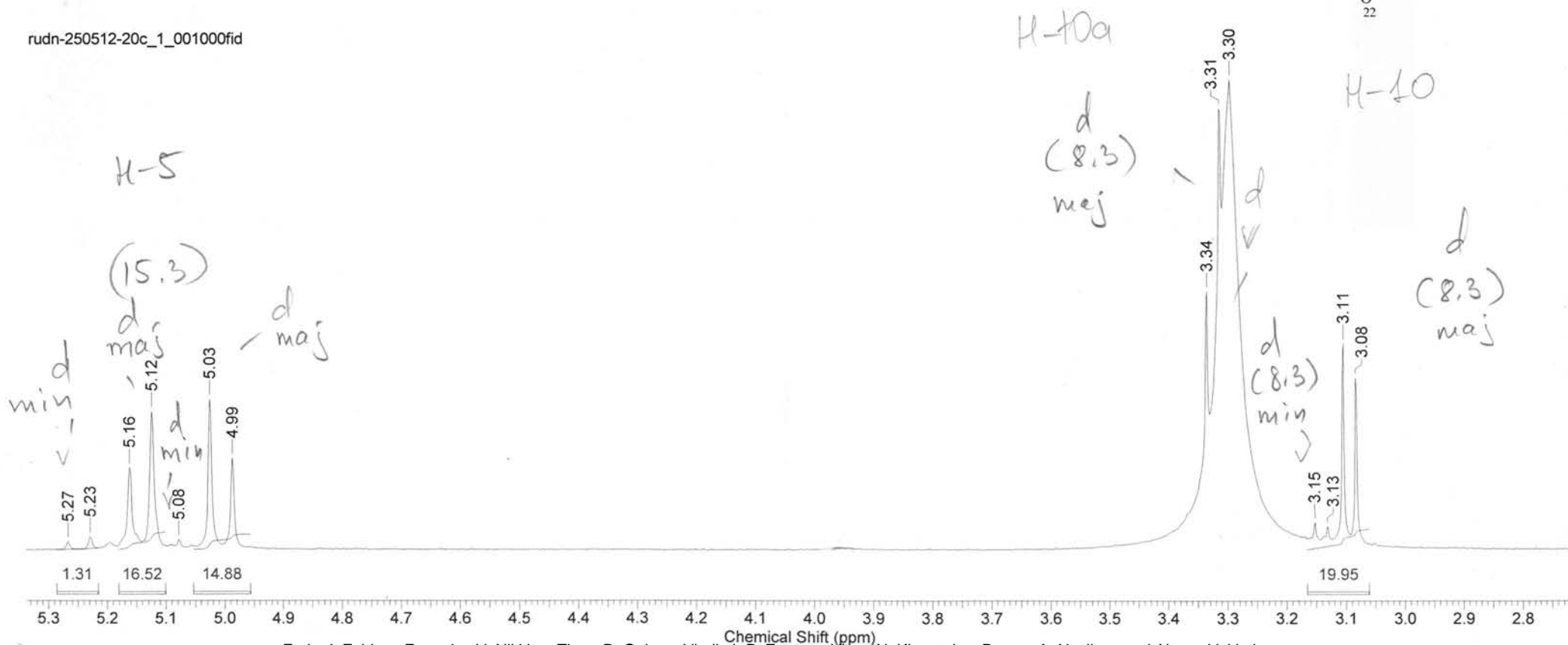


Formula C ₁₆ H ₁₂ BrNO ₅	FW 378.1742				
Acquisition Time (sec) 1.5729	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 08 Jun 2012 14:56:00			
Date Stamp 08 Jun 2012 14:56:00					
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-20c_1\rudn-250512-20c_1_001000fid					
Frequency (MHz) 400.14	Nucleus 1H	Number of Transients 48	Origin spect		
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zg		
Receiver Gain 128.00	SW(cyclical) (Hz) 10416.67	Solvent DMSO-d6	Spectrum Offset (Hz) 2712.0542		
Sweep Width (Hz) 10416.03	Temperature (degree C) 32.000				

Compounds 20Ac/20Bc

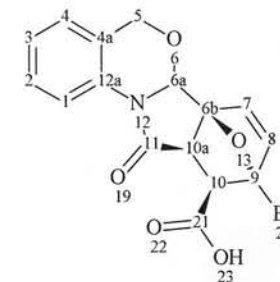


rudn-250512-20c_1_001000fid

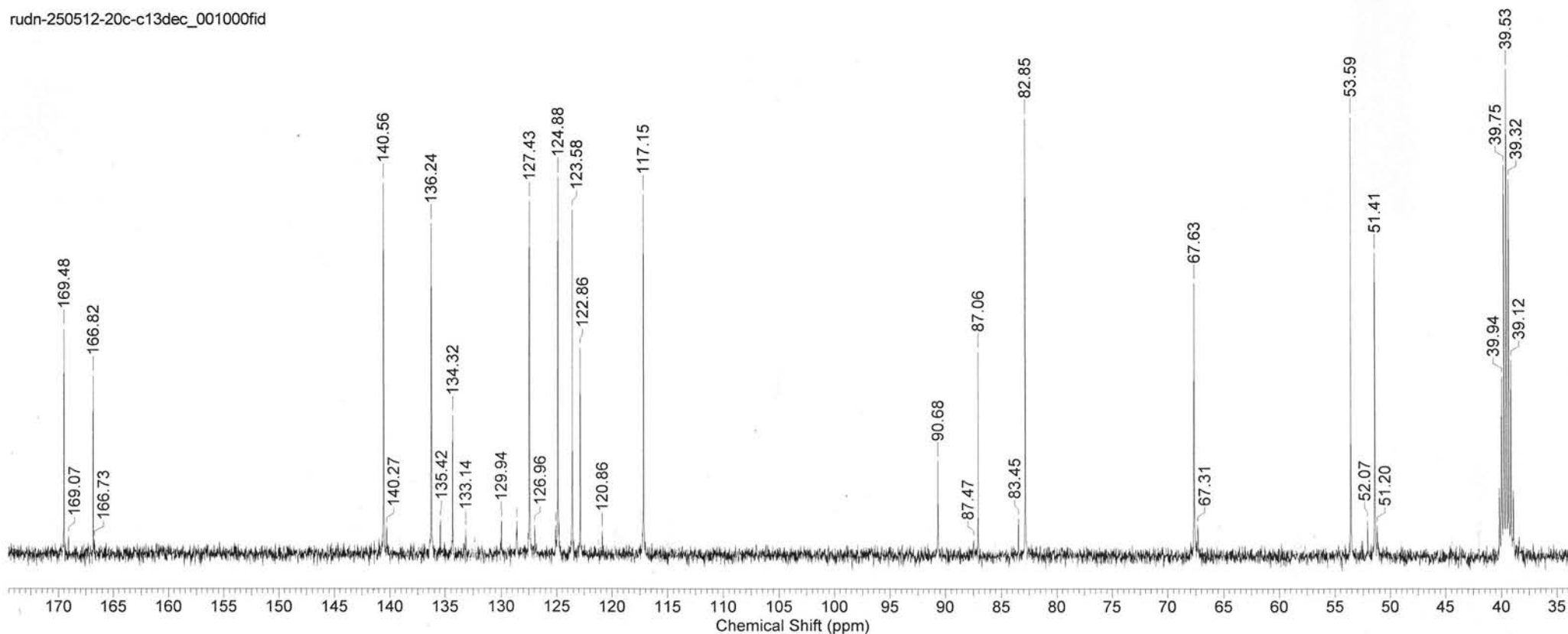


Formula C ₁₆ H ₁₂ BrNO ₅	FW 378.1742			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 31 May 2012 16:10:40		
Date Stamp 31 May 2012 16:10:40				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-20c-c13dec\rudn-250512-20c-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 2369	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10548.9570	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compounds 20Ac/20Bc

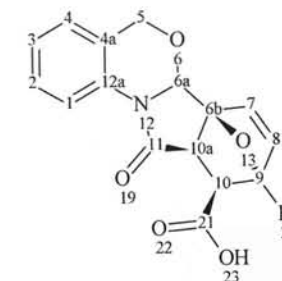


rudn-250512-20c-c13dec_001000fid

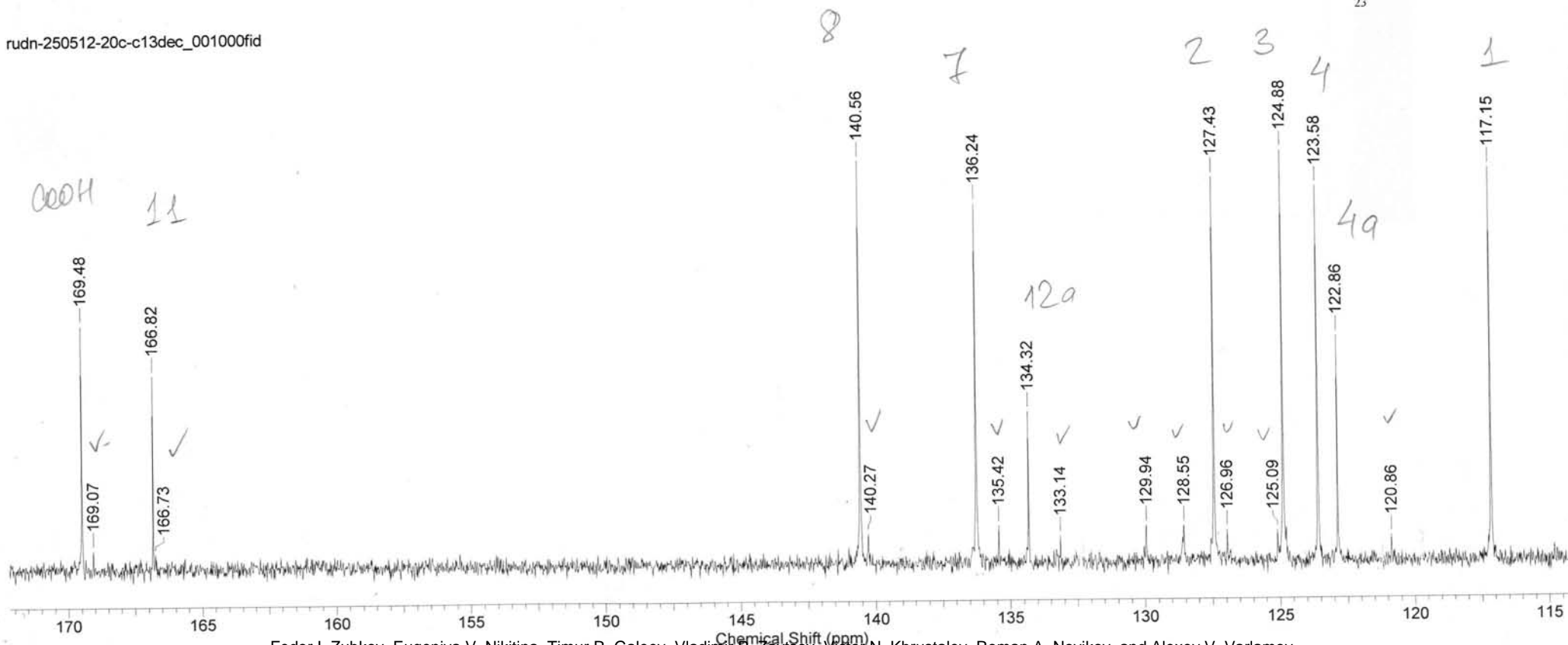


Formula C ₁₆ H ₁₂ BrNO ₅	FW 378.1742			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 31 May 2012 16:10:40		
Date Stamp 31 May 2012 16:10:40				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-20c-c13dec\rudn-250512-20c-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 2369	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10548.9570	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compounds 20Ac/20Bc

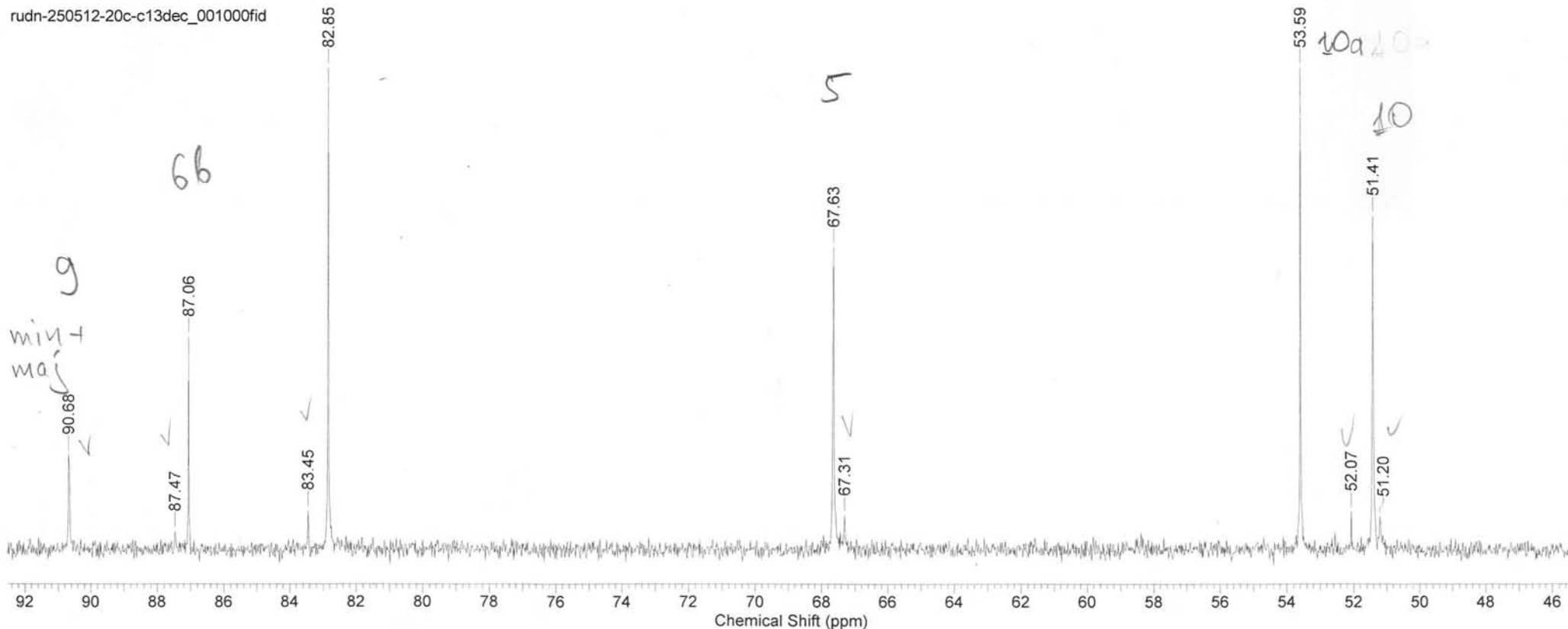
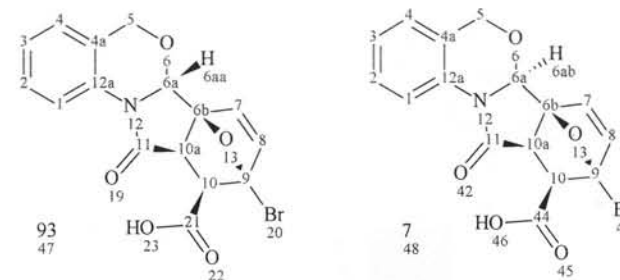


rudn-250512-20c-c13dec_001000fid



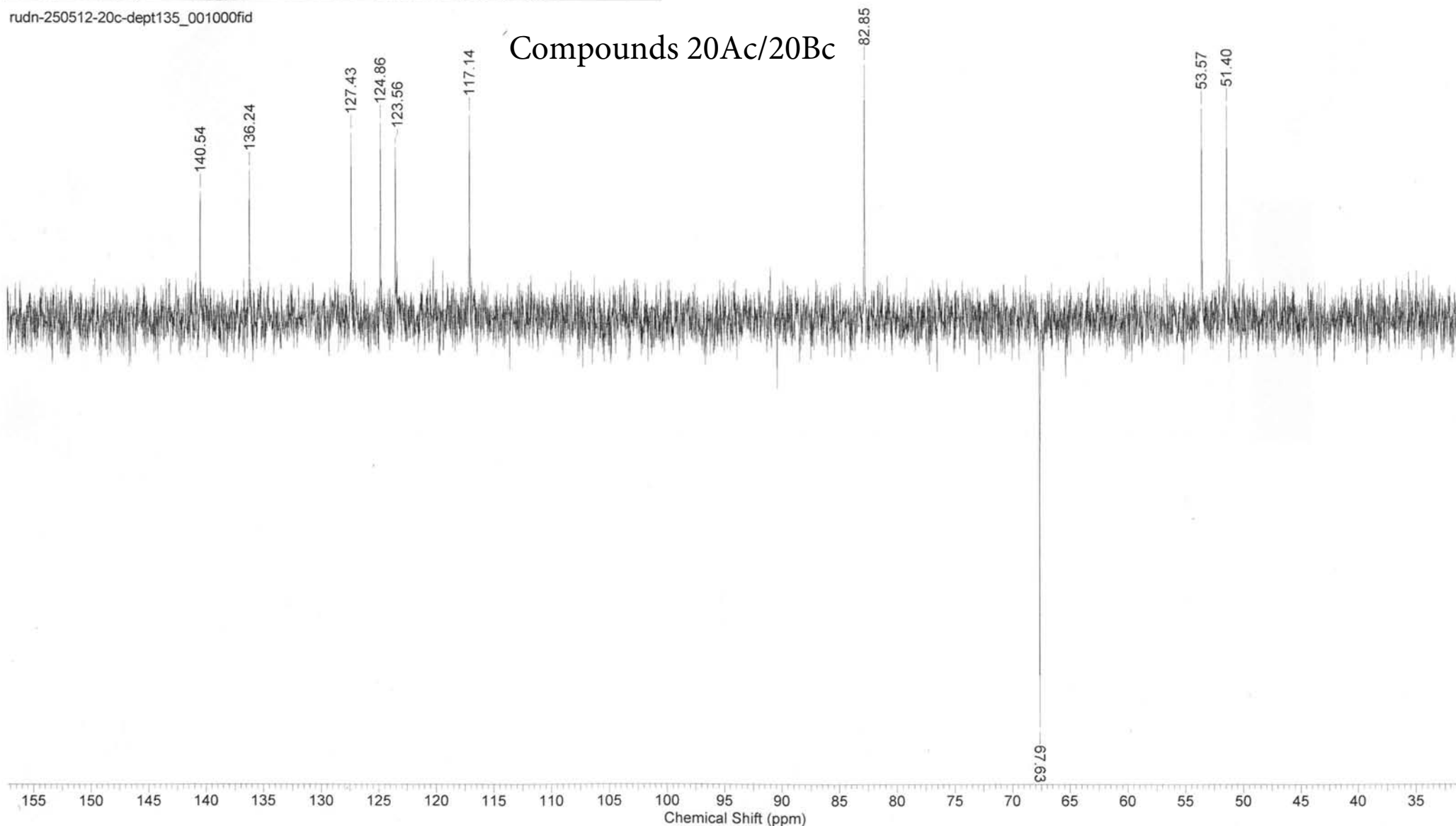
Formula C ₃₂ H ₂₄ Br ₂ N ₂ O ₁₀ ?		FW 756.3484+? (378.1742+378.1742+?+?)	
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400		Date 31 May 2012 16:10:40
Date Stamp 31 May 2012 16:10:40			
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-20c-c13dec\rudn-250512-20c-c13dec_001000fid			
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 2369	Origin spect
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10548.9570
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000		

Compounds 20Ac/20Bc



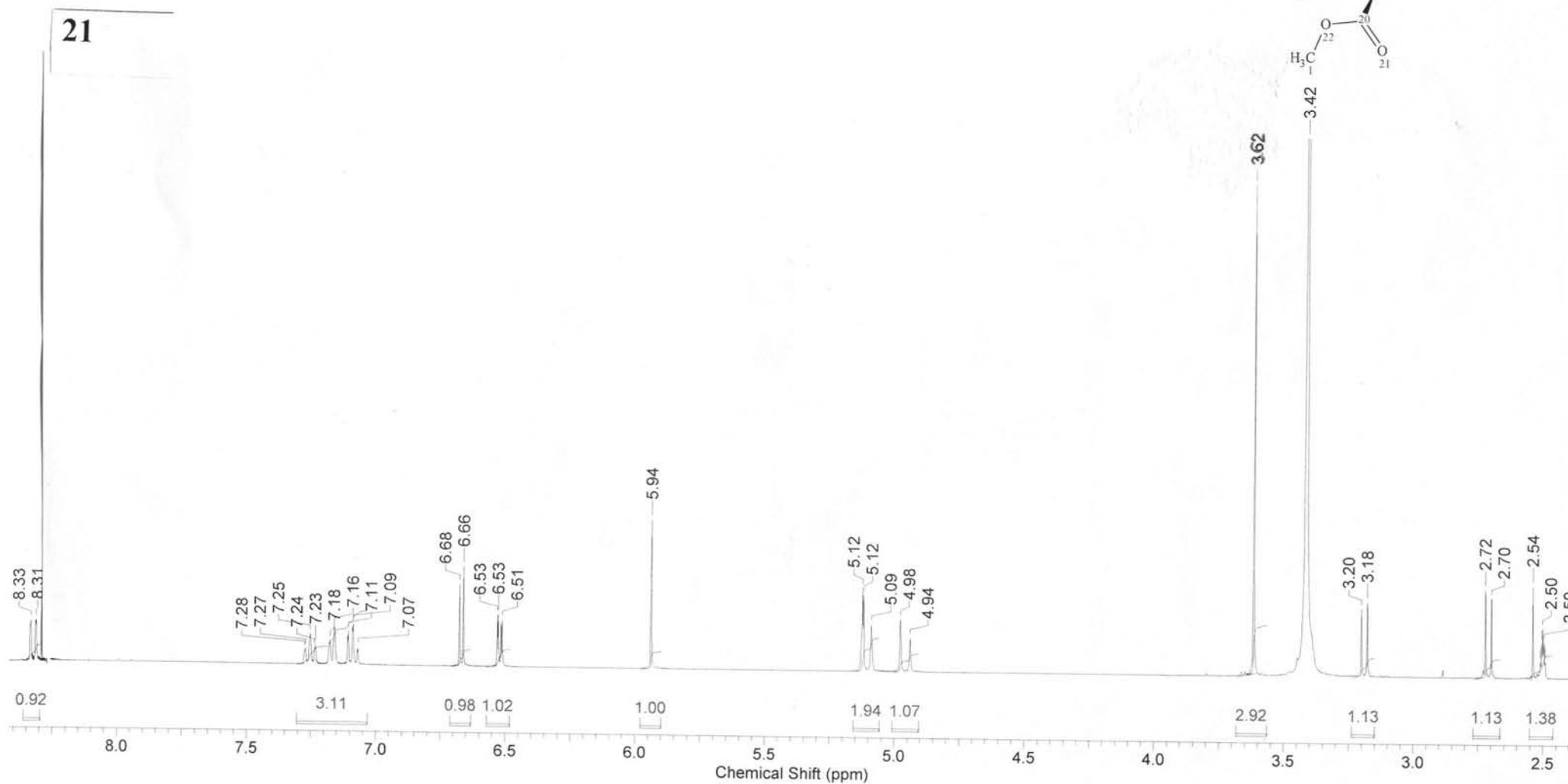
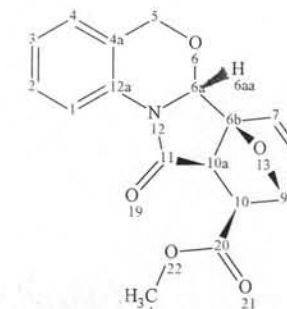
Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	31 May 2012 16:53:20	
Date Stamp	31 May 2012 16:53:20						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-20c-dept135\rudn-250512-20c-dept135_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	380	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	dept135
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9098.5479
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				

rudn-250512-20c-dept135_001000fid



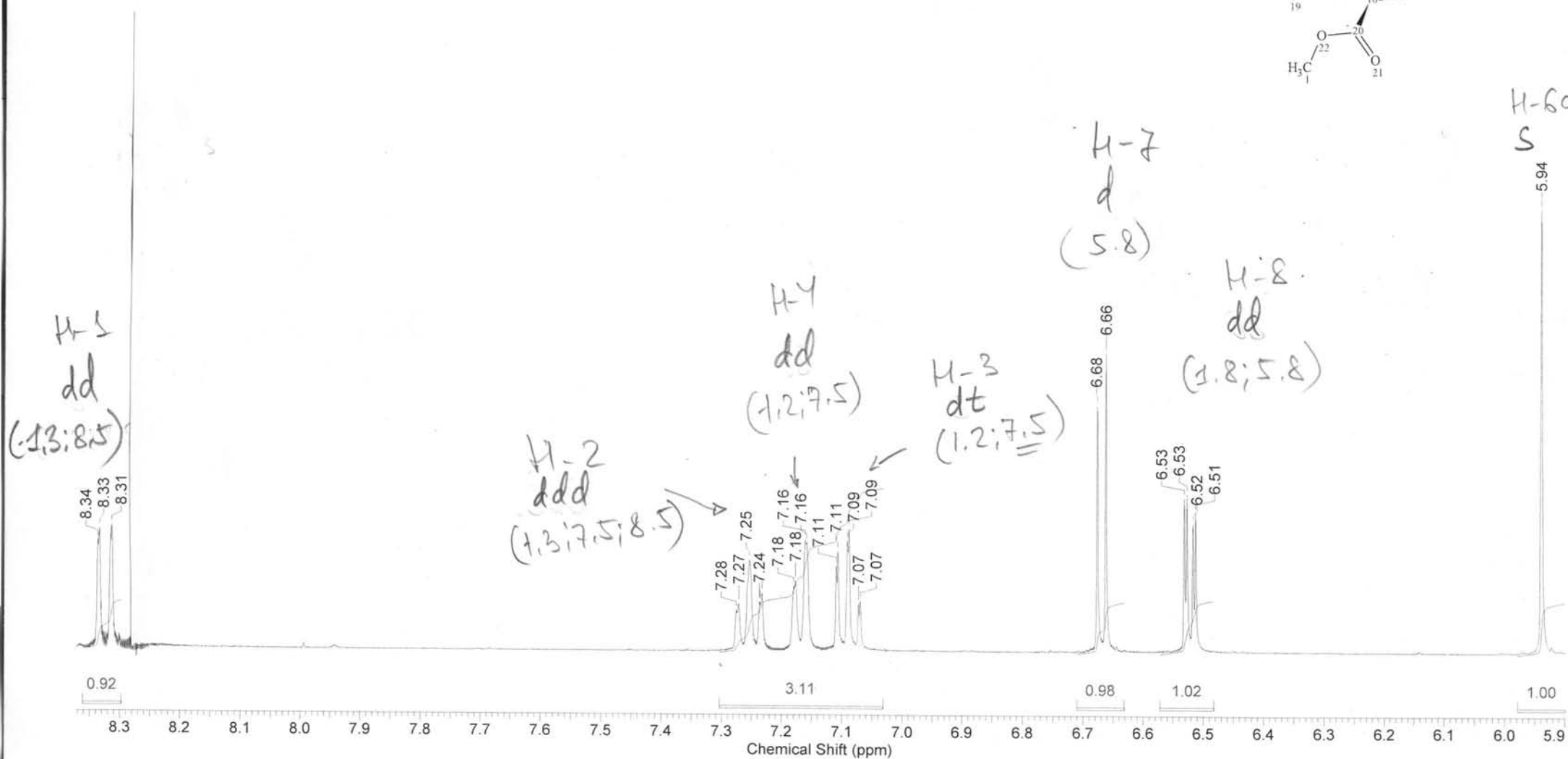
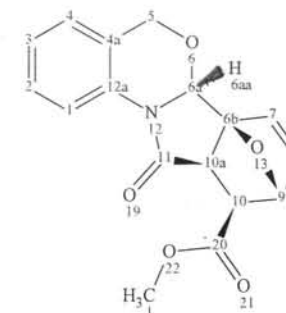
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File Name	C:\Users\Fedor\Desktop\08.10.09\fz799\fz799_001000fid		Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	8	
Original Points Count	16384	Points Count	262144	Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	10204.08
Temperature (degree C)	27.000								

Compound 21



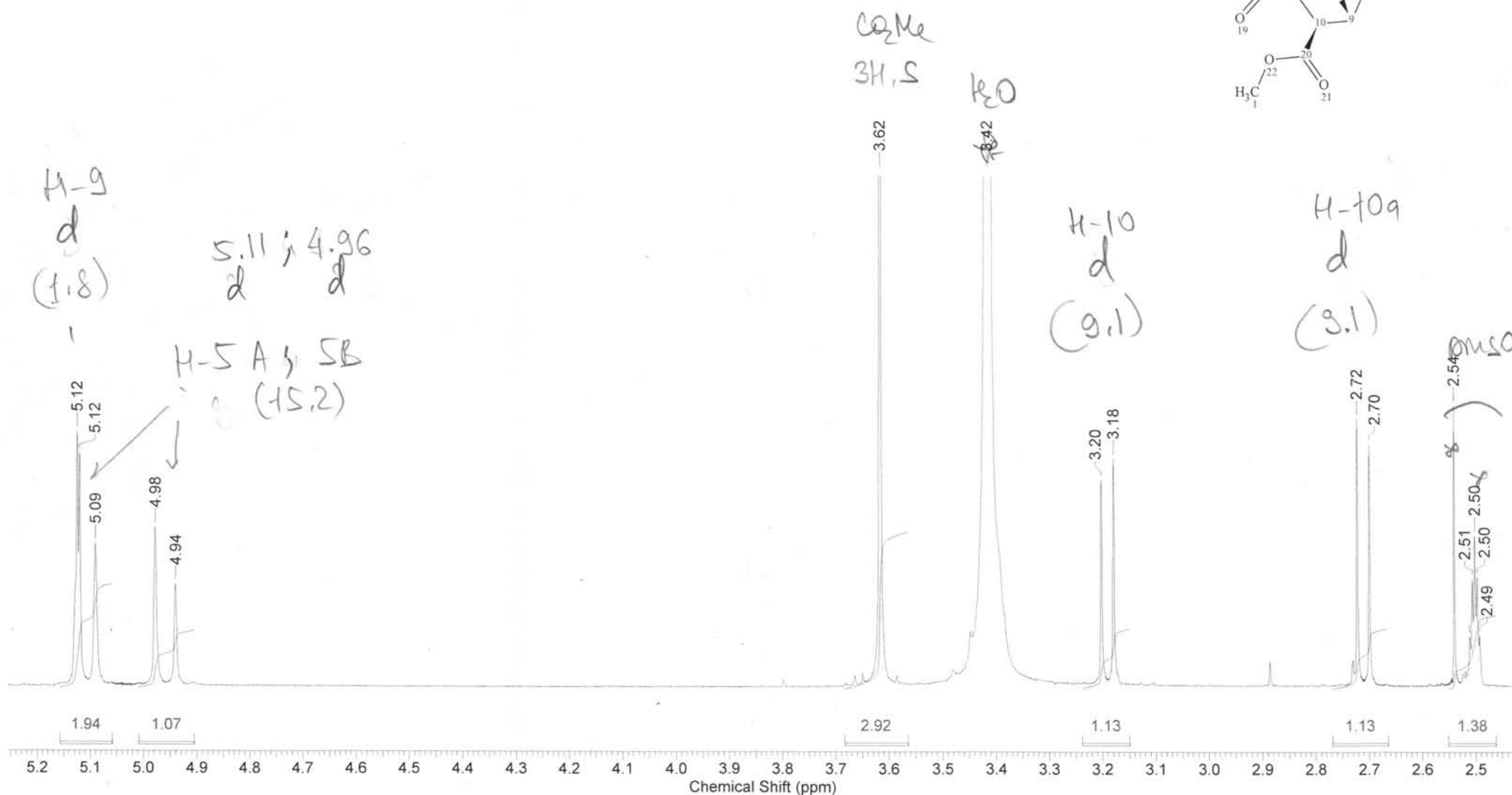
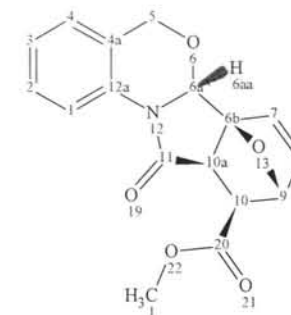
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File Name	C:\Users\Fedor\Desktop\08.10.09\799\799_001000fid	Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	8
Original Points Count	16384	Points Count	262144	Pulse Sequence	zg	Solvent	DMSO-D6
Temperature (degree C)	27.000					Sweep Width (Hz)	10204.08

Compound 21



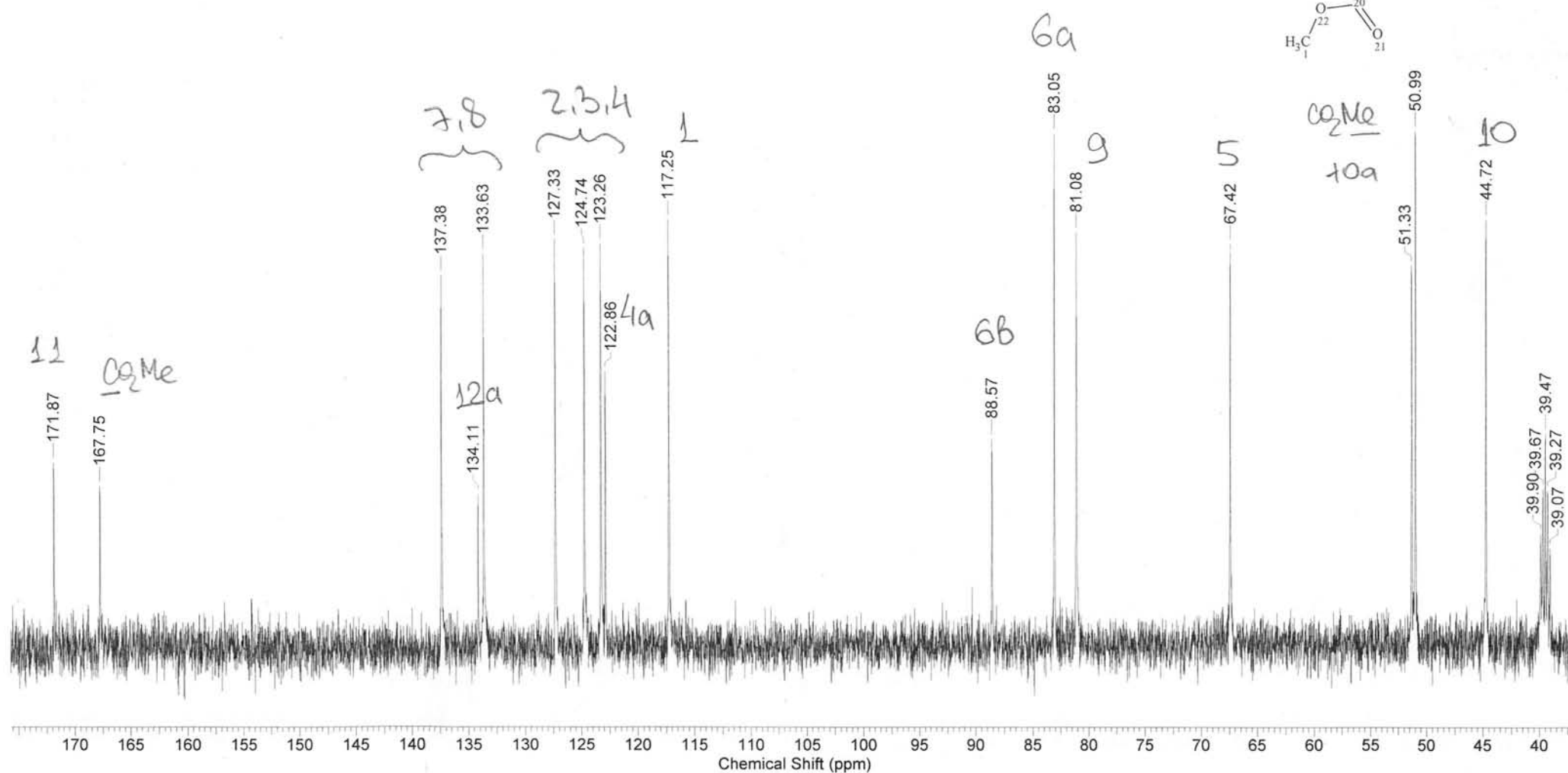
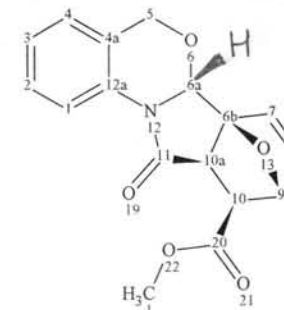
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File Name	C:\Users\Fedor\Desktop\08.10.09\799\799_001000fid	Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	8
Original Points Count	16384	Points Count	262144	Pulse Sequence	zg	Sweep Width (Hz)	10204.08
Temperature (degree C)	27.000						

Compound 21



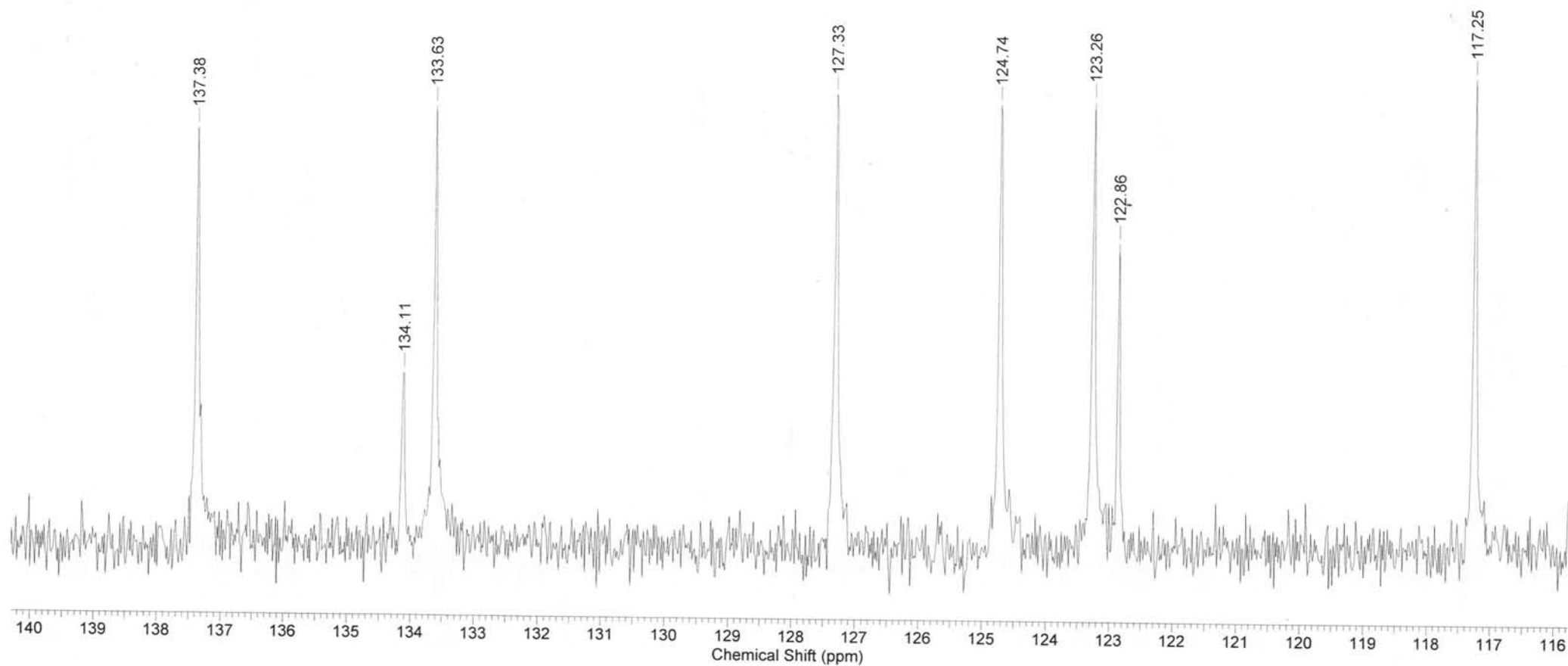
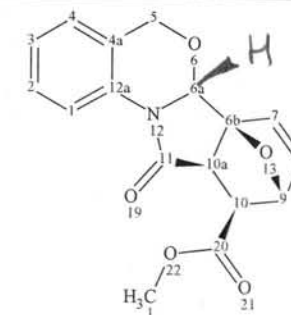
Acquisition Time (sec)	0.6226	Comment	Imported from UXNMR.		Date	29 Dec 2008 17:06:08	
File Name	D:\NMR\C_13\Женя и Инга (IOC конец 2008)\8nik_c13dec\8nik_c13dec_001000fid			Frequency (MHz)	100.62		
Nucleus	13C	Number of Transients	102	Original Points Count	16384	Points Count	16384
Pulse Sequence	zpgg	Solvent	DMSO-D6	Sweep Width (Hz)	26315.79	Temperature (degree C)	27.000

Compound 21



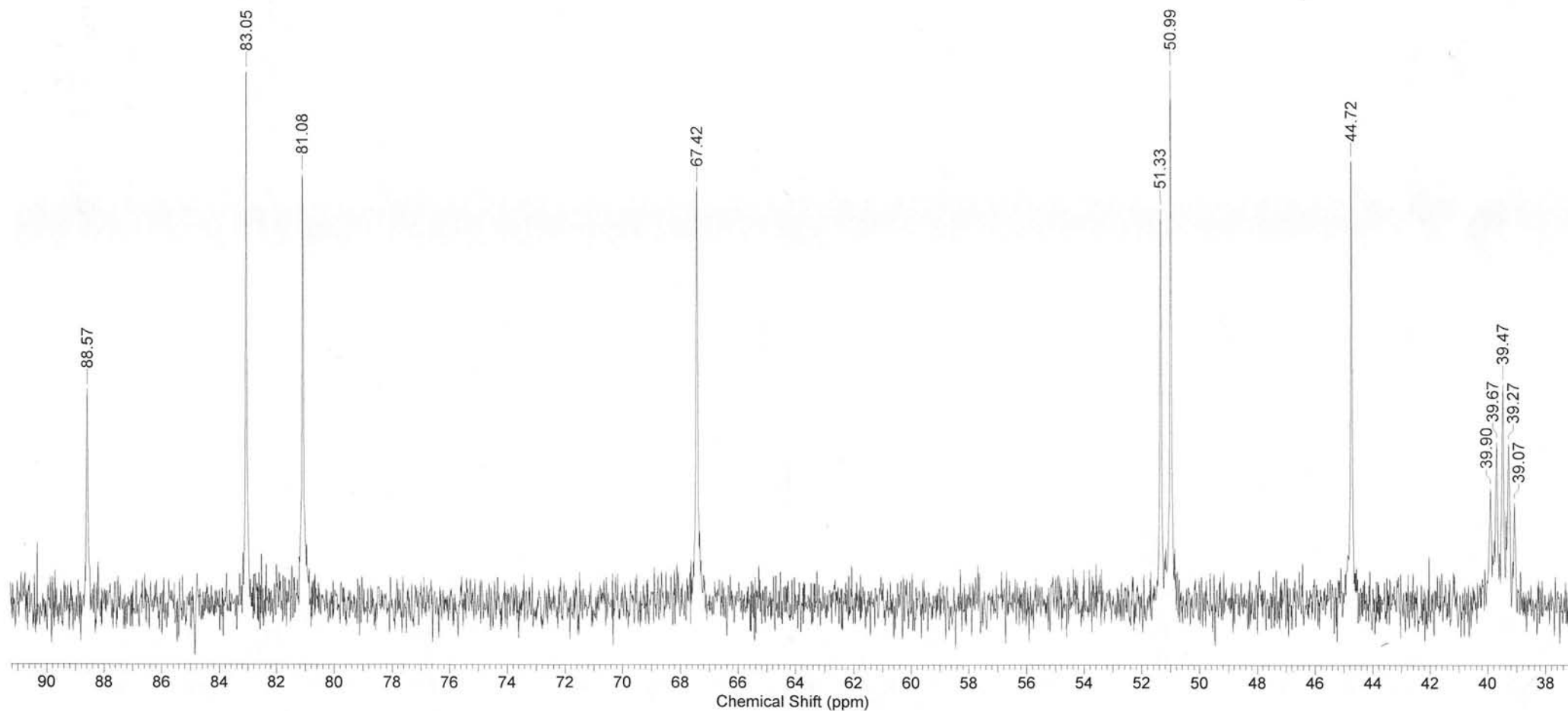
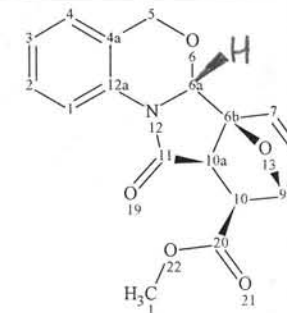
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File Name	D:\NMR\C_13\Женя и Инга (IOC конец 2008)\8nik_c13dec\8nik_c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	102	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	26315.79	Temperature (degree C)	27.000

Compound 21

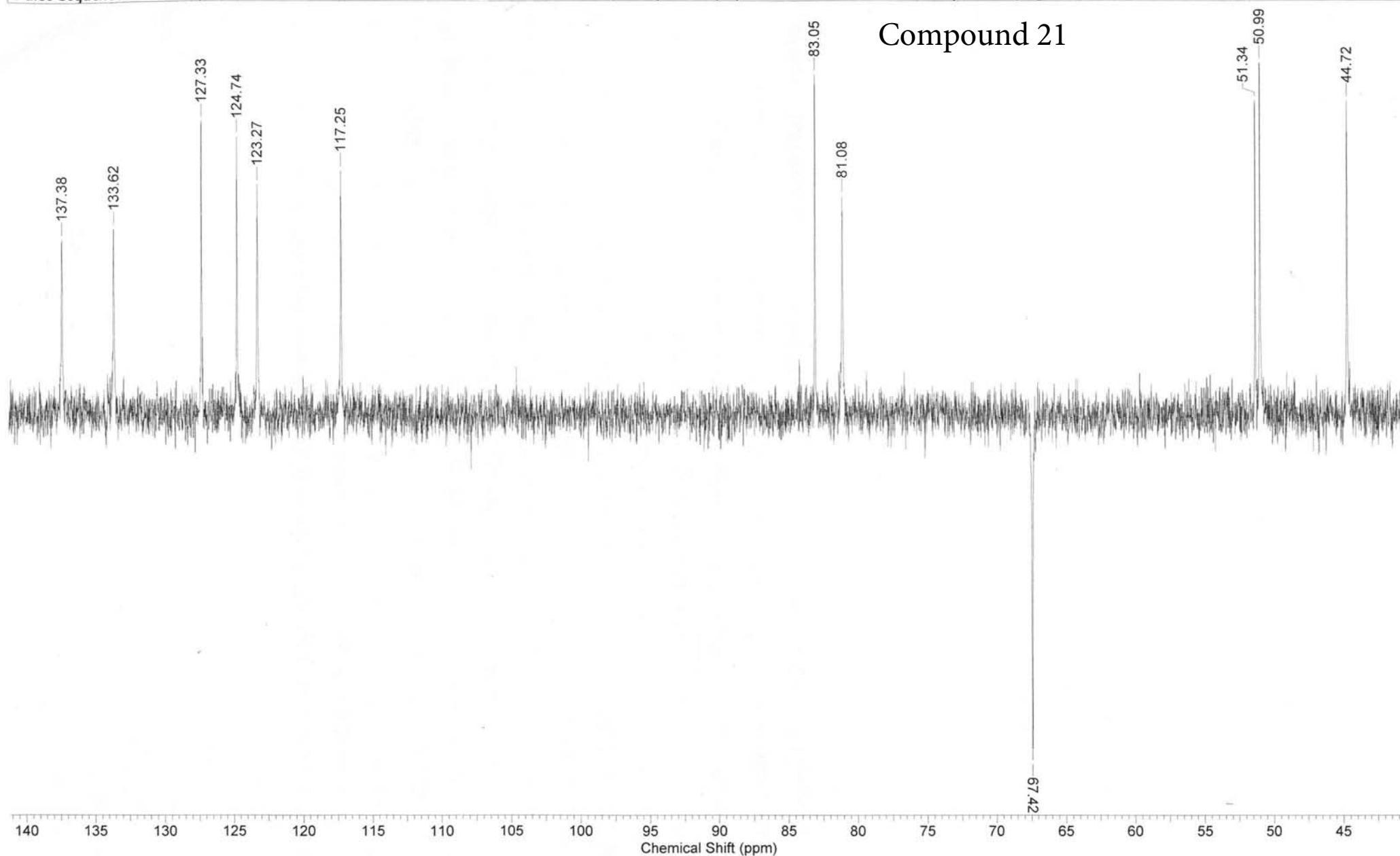


Acquisition Time (sec)	0.6226	Comment	Imported from UXMNR.		Date	29 Dec 2008 17:06:08	
File Name	D:\NMR\C_13\Женя и Инга (IOC конец 2008)\8nik_c13dec\8nik_c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	102	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	26315.79	Temperature (degree C)	27.000

Compound 21



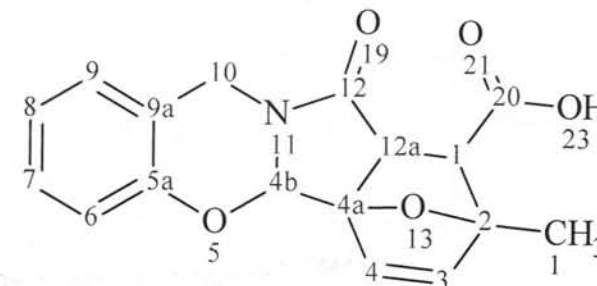
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Nucleus	13C	Number of Transients	70	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	CHLOROFORM-D	Sweep Width (Hz)	26315.79	Temperature (degree C)	27.000



Formula $C_{17}H_{15}NO_5$ FW 313.3047

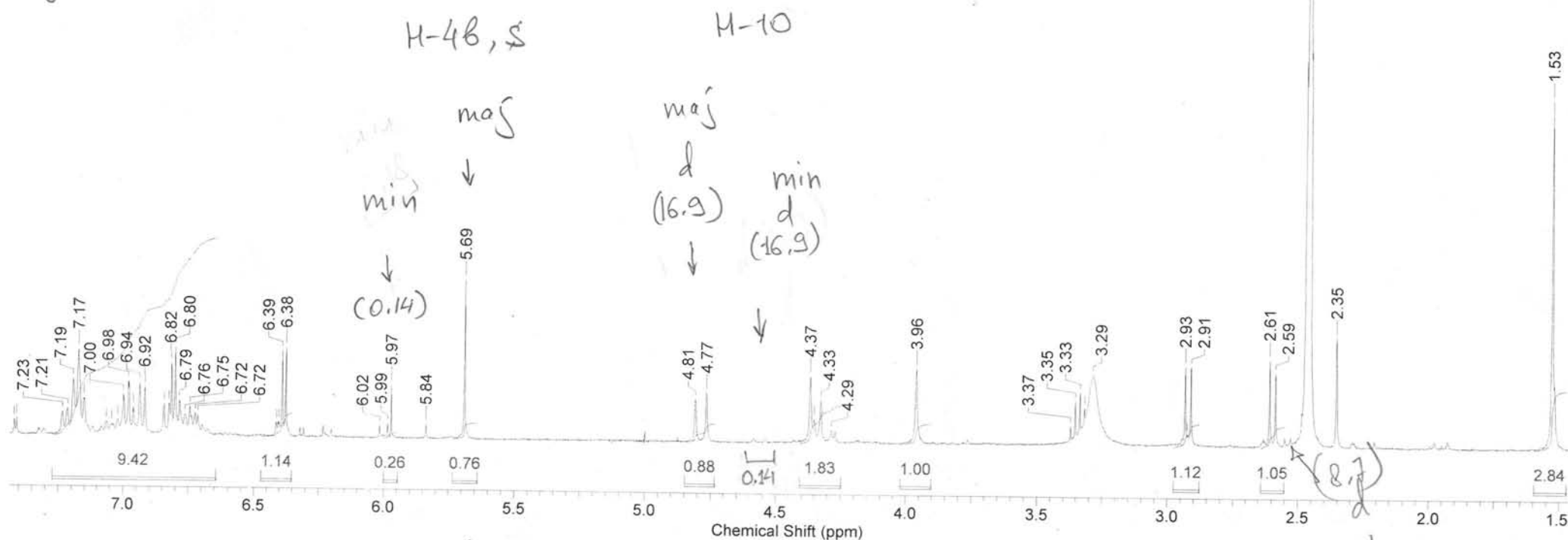
Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	28 Feb 2012 10:56:58	Date Stamp	28 Feb 2012 15:31:31
File Name	D:\NMR\21.02.12\FZ2241-1.jdf			Frequency (MHz)	399.78	Nucleus	1H
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	24.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	1998.9109	Sweep Width (Hz)	7503.00
						Temperature (degree C)	24.300

Compounds 22Ab/22Bb
before crystallization



22Ab/22Bb = 86/14

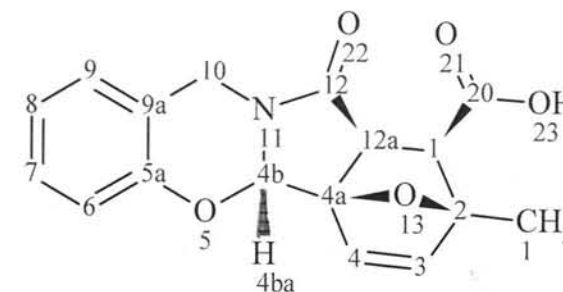
before
crystallization



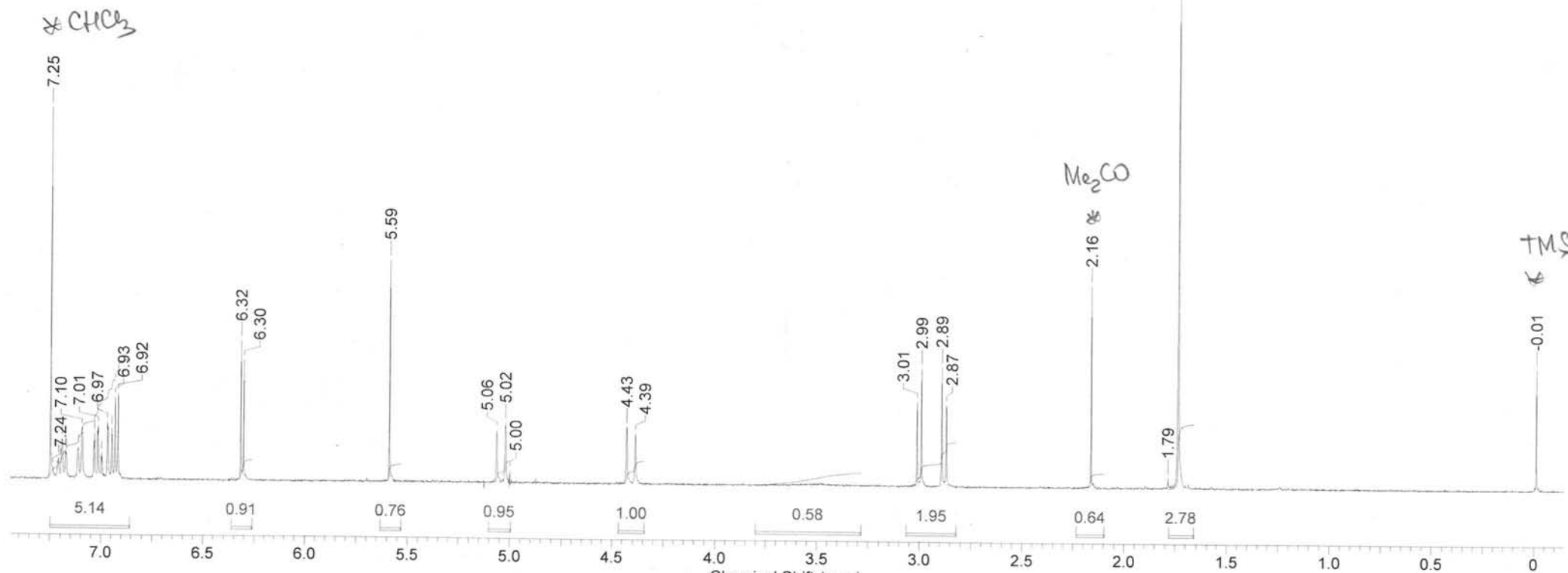
Formula $C_{17}H_{15}NO_5$ FW 313.3047

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	06 Mar 2012 09:39:46	Date Stamp	06 Mar 2012 14:14:34
File Name	D:\NMR\05.03.12\FZ2260.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	18.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	1998.9109	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	24.000			Sweep Width (Hz)	7503.00		

Compound 22Ab
after crystallization



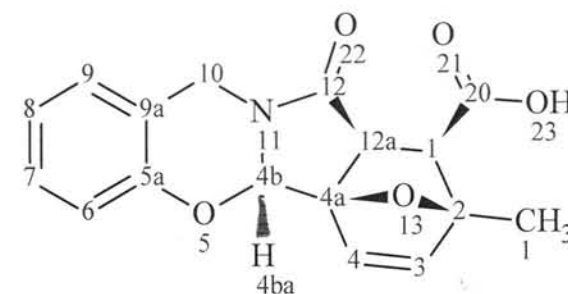
22Ab after crystallization



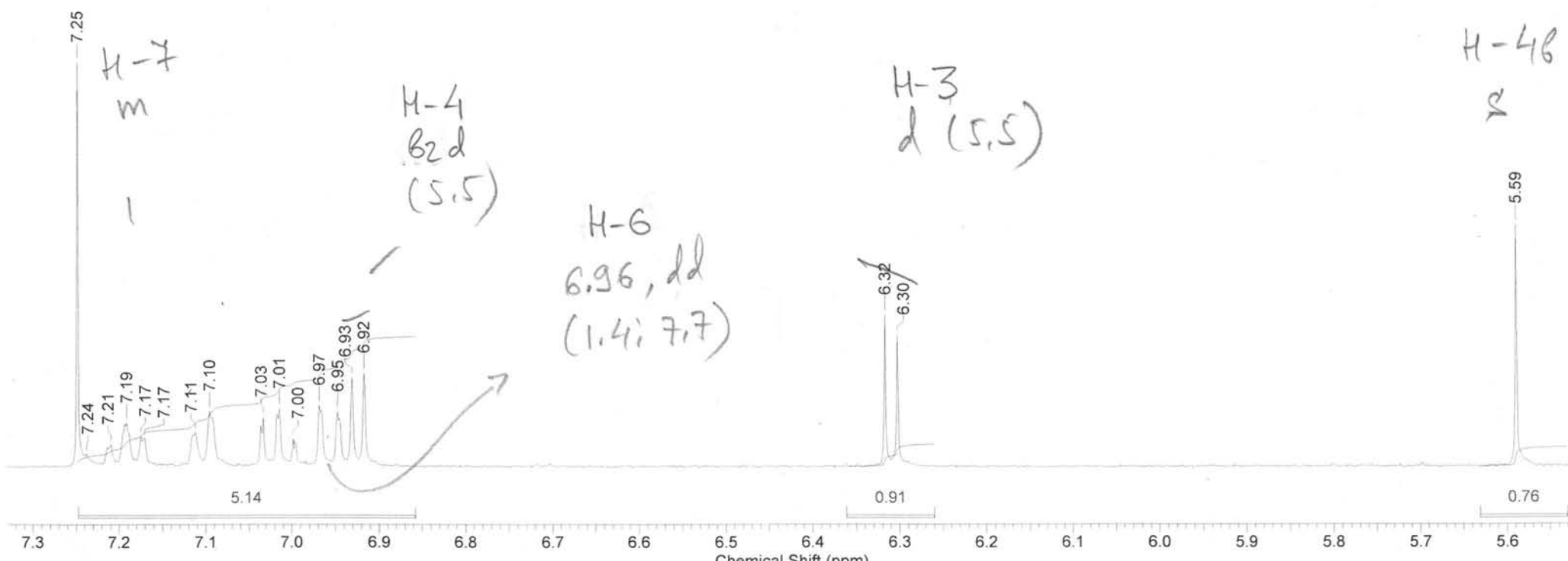
Formula C₁₇H₁₅NO₅ FW 313.3047

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	06 Mar 2012 09:39:46	Date Stamp	06 Mar 2012 14:14:34
File Name	D:\NMR\05.03.12\FZ2260.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	18.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	1998.9109	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	24.000	Sweep Width (Hz)	7503.00				

Compound 22Ab
after crystallization



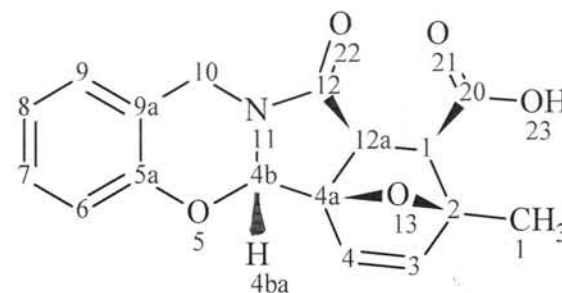
FZ2260.jdf



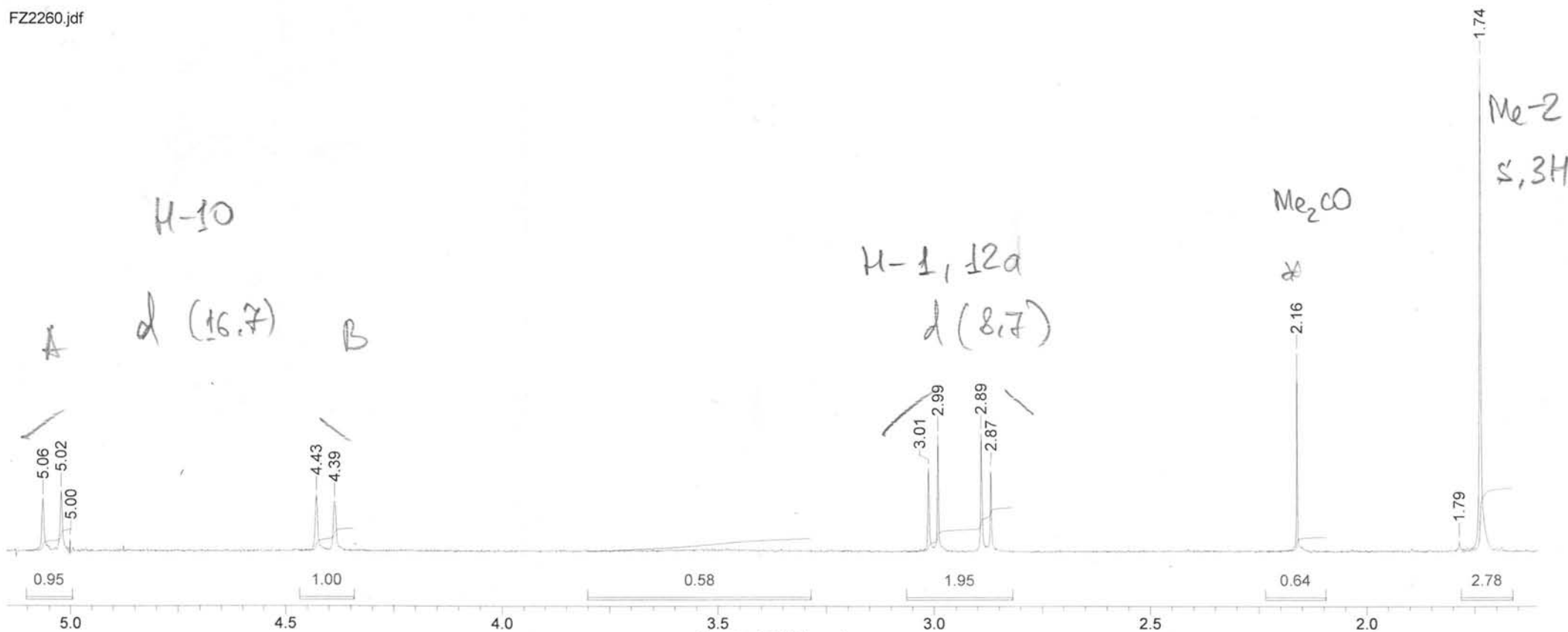
Formula C₁₇H₁₅NO₅ FW 313.3047

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	06 Mar 2012 09:39:46	Date Stamp	06 Mar 2012 14:14:34
File Name	D:\NMR\05.03.12\FZ2260.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	18.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	1998.9109	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	24.000	Sweep Width (Hz)					7503.00

Compound 22Ab
after crystallization



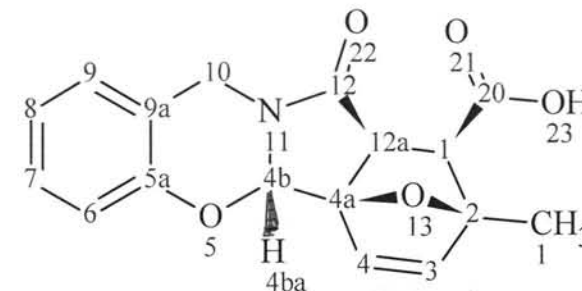
FZ2260.jdf



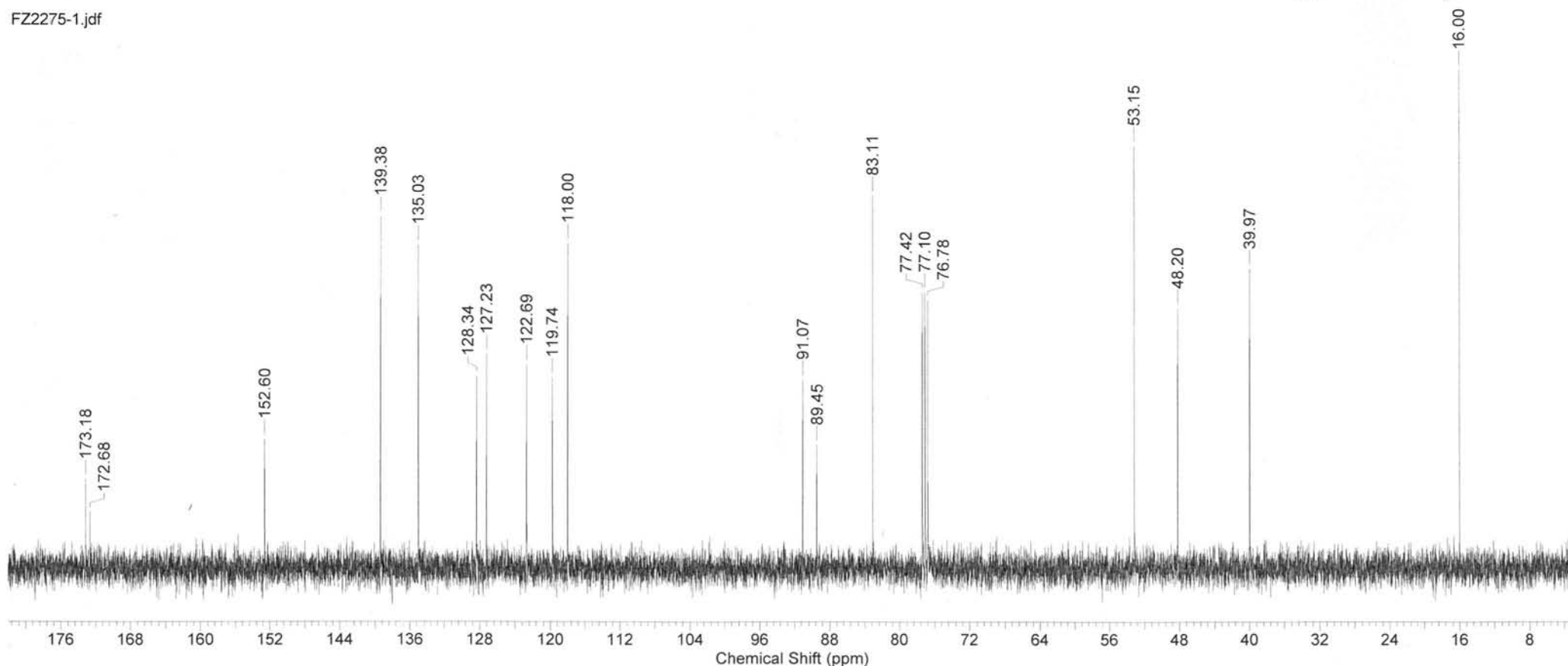
Formula C₁₇H₁₅NO₅ FW 313.3047

Acquisition Time (sec)	1.0433	Comment	single pulse decoupled gated NOE		Date	16 Mar 2012 07:14:06		
Date Stamp	16 Mar 2012 11:48:39	File Name	D:\NMR\12.03.12\FZ2275-1.jdf		Frequency (MHz)	100.53		
Nucleus	13C	Number of Transients	111	Origin	ECS 400	Original Points Count	32768	
Points Count	32768	Pulse Sequence	single_pulse_dec	Receiver Gain	50.00		Owner	delta
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10052.5303	Sweep Width (Hz)	31407.04	Temperature (degree C)		25.800

Compound 22Ab
after crystallization



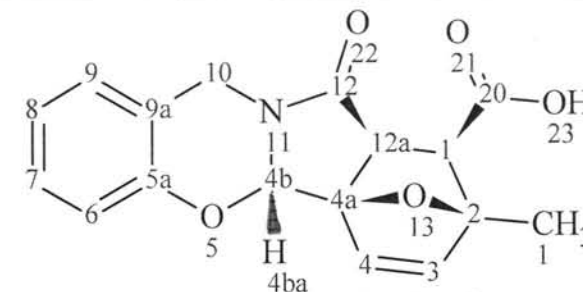
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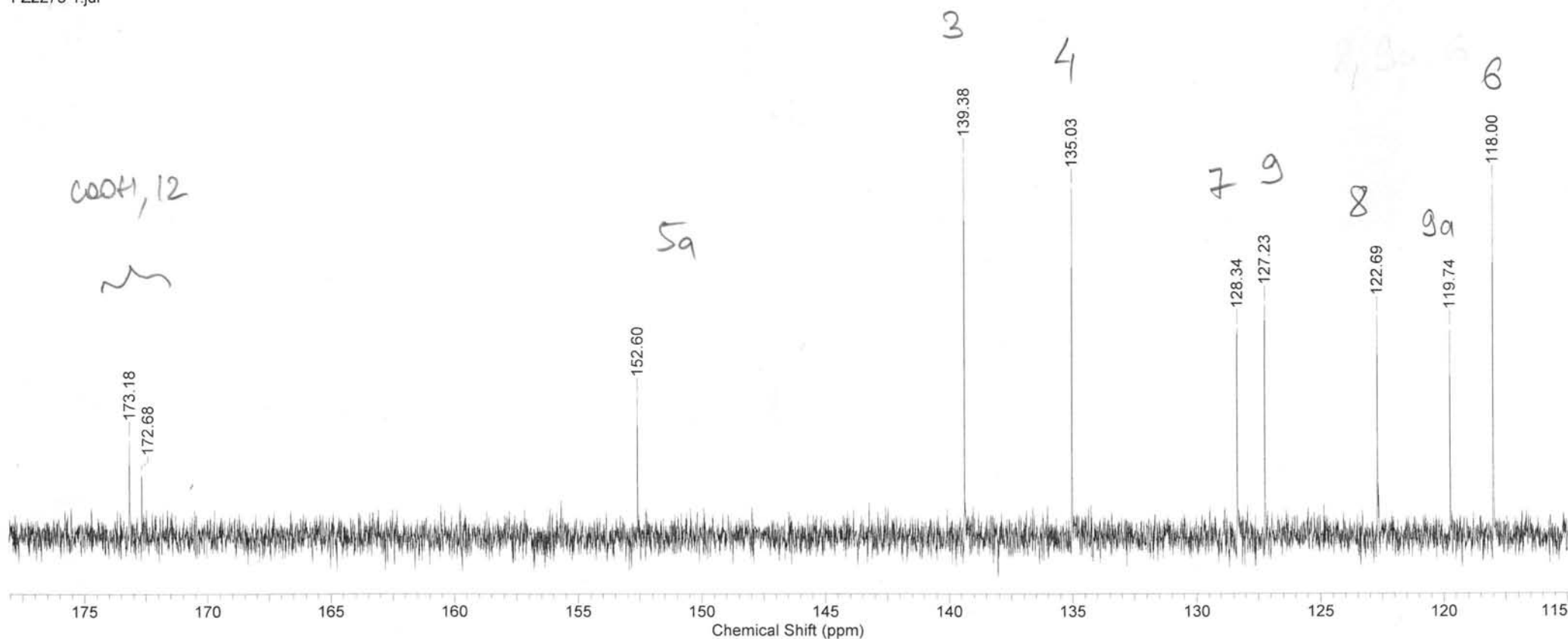
Formula C₁₇H₁₅NO₅ FW 313.3047

Acquisition Time (sec)	1.0433	Comment	single pulse decoupled gated NOE		Date	16 Mar 2012 07:14:06	
Date Stamp	16 Mar 2012 11:48:39	File Name	D:\NMR\12.03.12\FZ2275-1.jdf		Frequency (MHz)	100.53	
Nucleus	13C	Number of Transients	111	Origin	ECS 400	Original Points Count	32768
Points Count	32768	Pulse Sequence	single_pulse_dec		Receiver Gain	50.00	
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10052.5303	Sweep Width (Hz)	31407.04	Temperature (degree C) 25.800	

Compound 22Ab
after crystallization



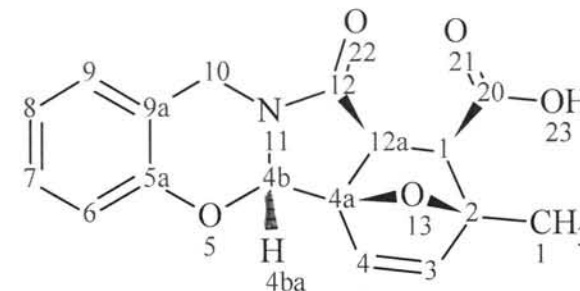
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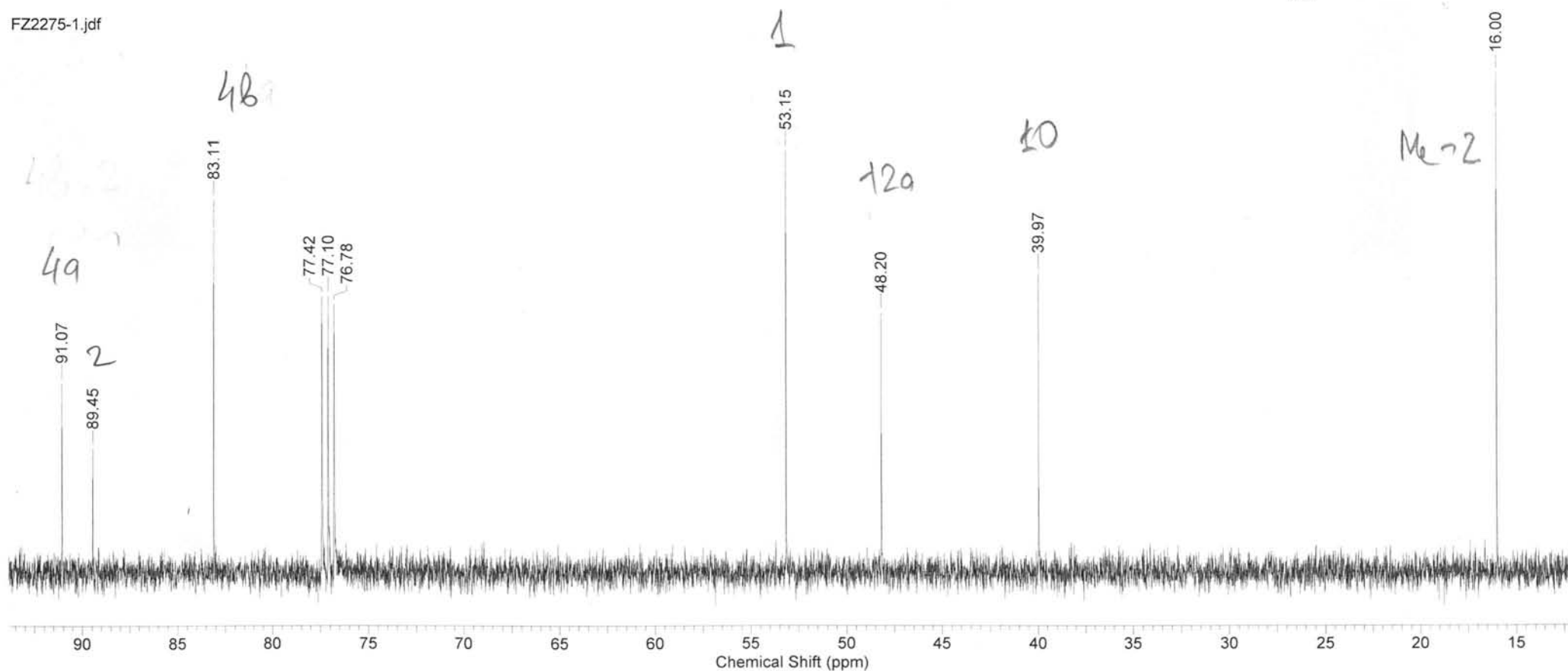
Formula C₁₇H₁₅NO₅ FW 313.3047

Acquisition Time (sec)	1.0433	Comment	single pulse decoupled gated NOE	Date	16 Mar 2012 07:14:06
Date Stamp	16 Mar 2012 11:48:39	File Name	D:\NMR\12.03.12\FZ2275-1.jdf	Frequency (MHz)	100.53
Nucleus	13C	Number of Transients	111	Origin	ECS 400
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10052.5303	Receiver Gain	50.00
		Sweep Width (Hz)	31407.04	Temperature (degree C)	25.800

Compound 22Ab
after crystallization

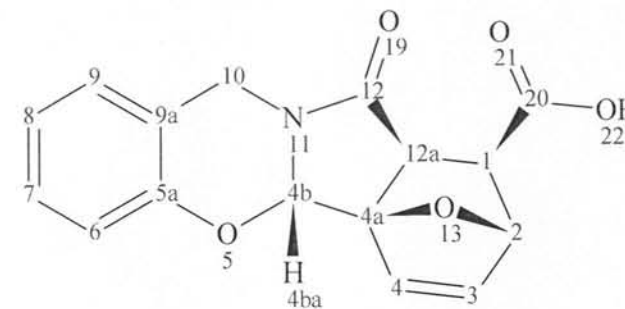


FZ2275-1.jdf

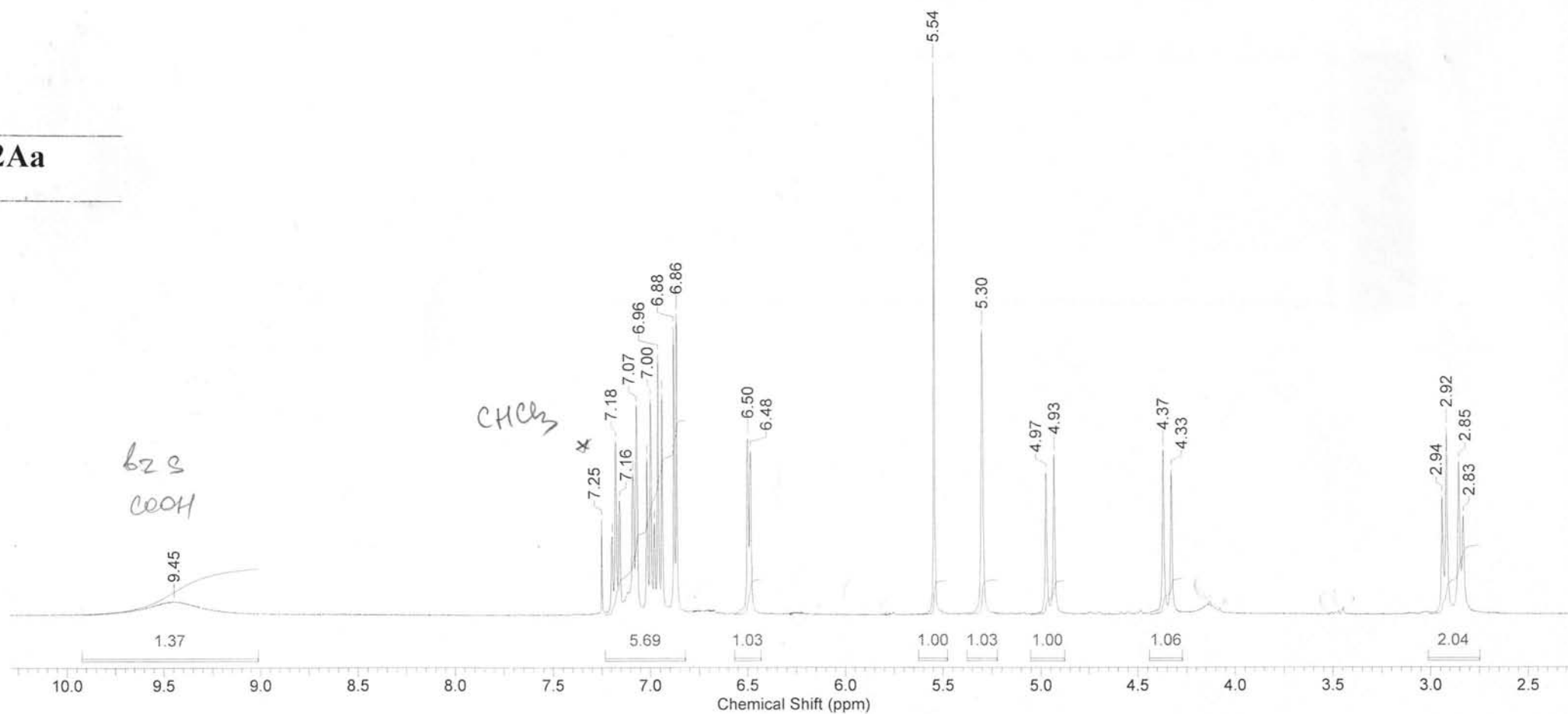


Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.		Date	10 Aug 2011 17:06:08	
File Name	C:\Users\Fedor\Desktop\05.08.11\rudn-050811-N2\rudn-050811-N2-1\rudn-050811-N2-1_001000fid				Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	16	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	10204.08	Temperature (degree C)	27.000

Compound 22Aa

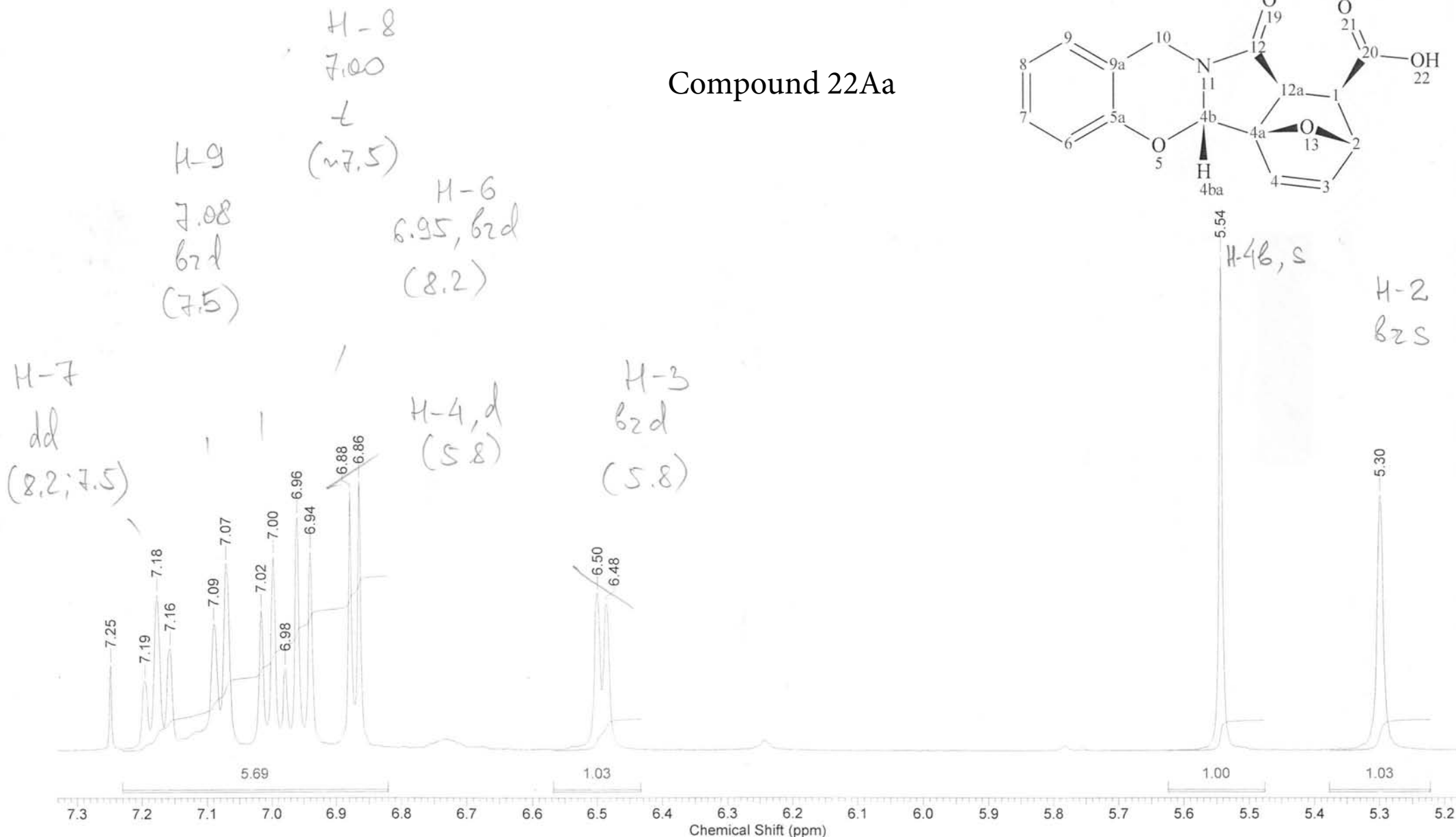
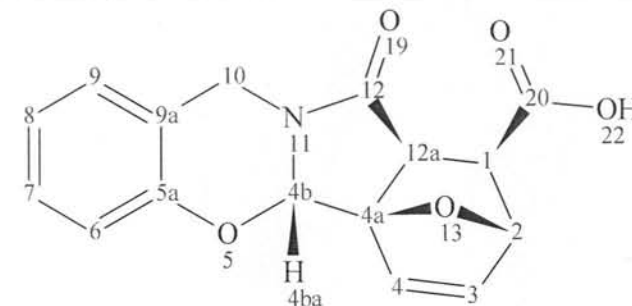


22Aa



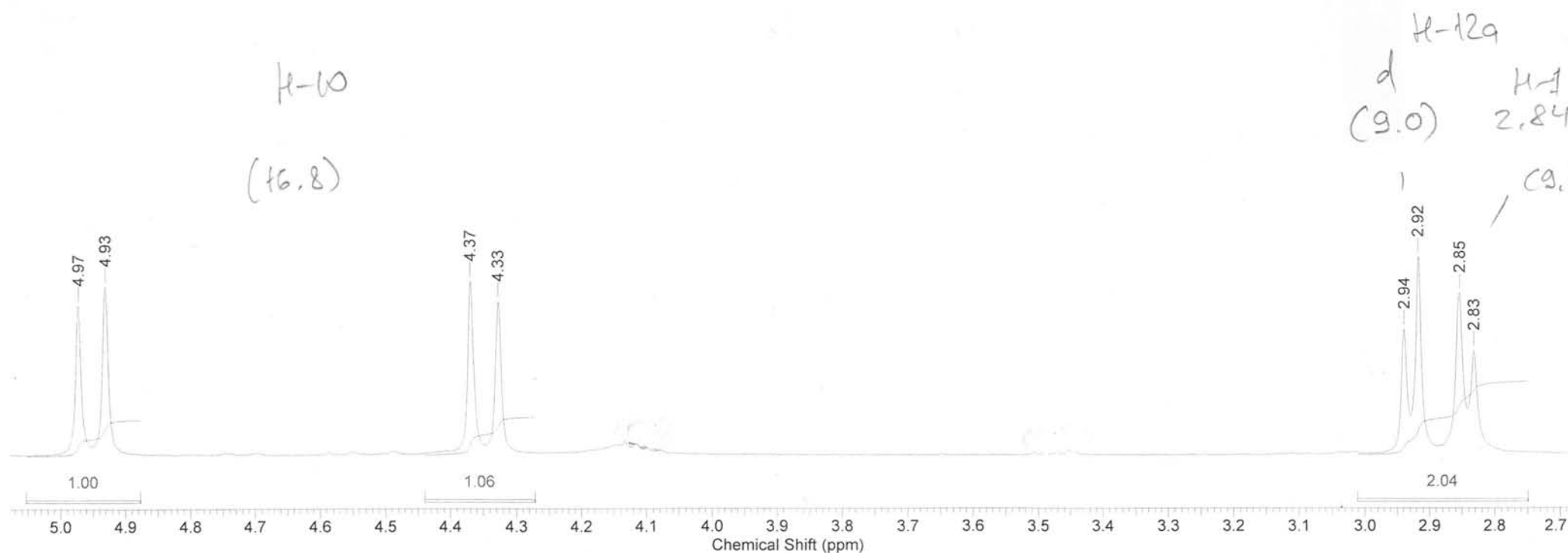
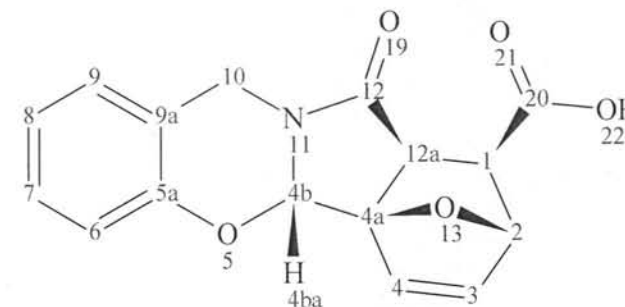
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File Name	C:\Users\Fedor\Desktop\05.08.11\rudn-050811-N2\rudn-050811-N2-1\rudn-050811-N2-1_001000fid				Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	16	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	10204.08	Temperature (degree C)	27.000

Compound 22Aa



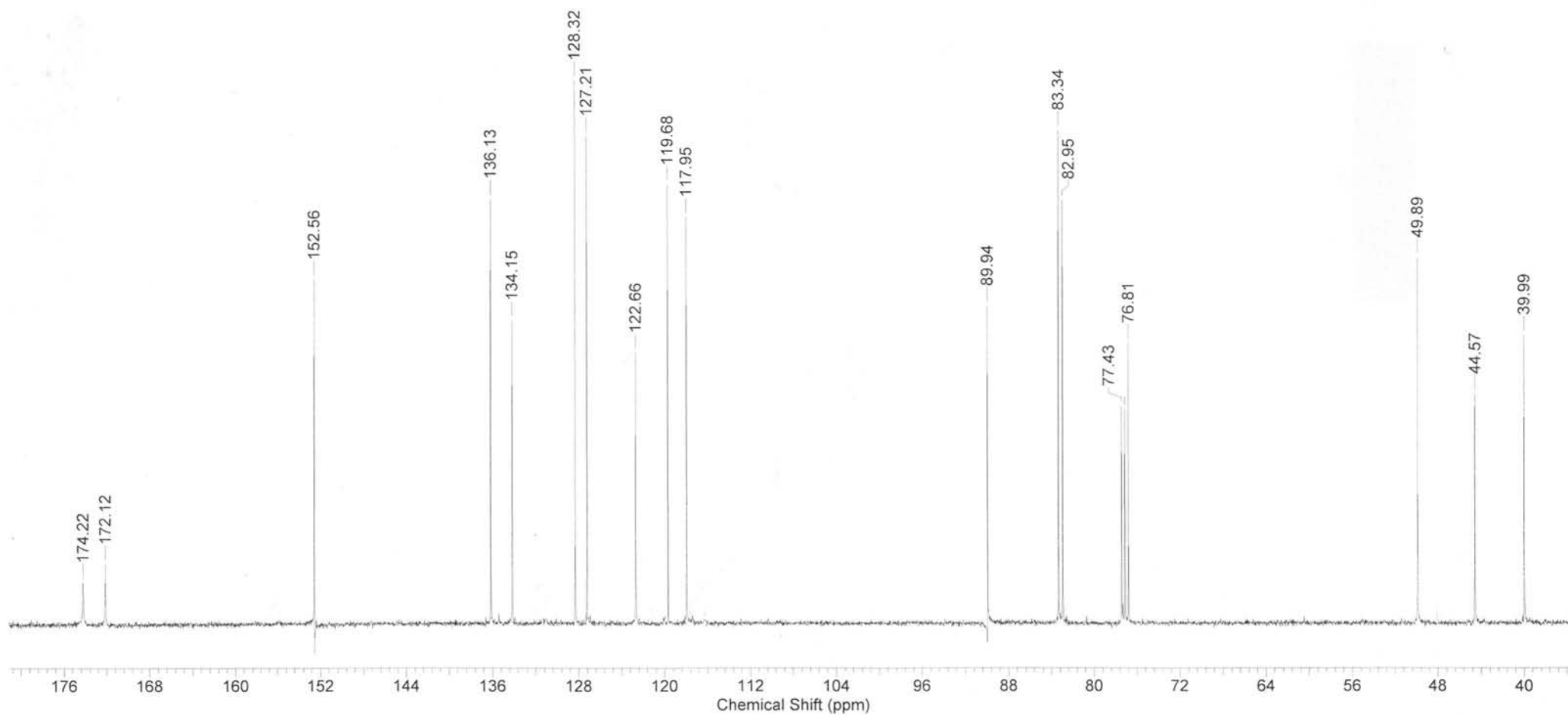
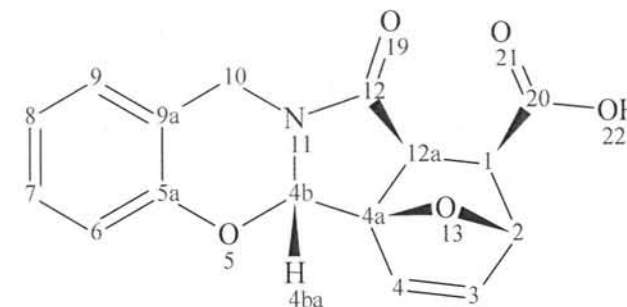
Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.		Date	10 Aug 2011 17:06:08	
File Name	C:\Users\Fedor\Desktop\05.08.11\rudn-050811-N2\rudn-050811-N2-1\rudn-050811-N2-1_001000fid				Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	16	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	10204.08	Temperature (degree C)	27.000

Compound 22Aa



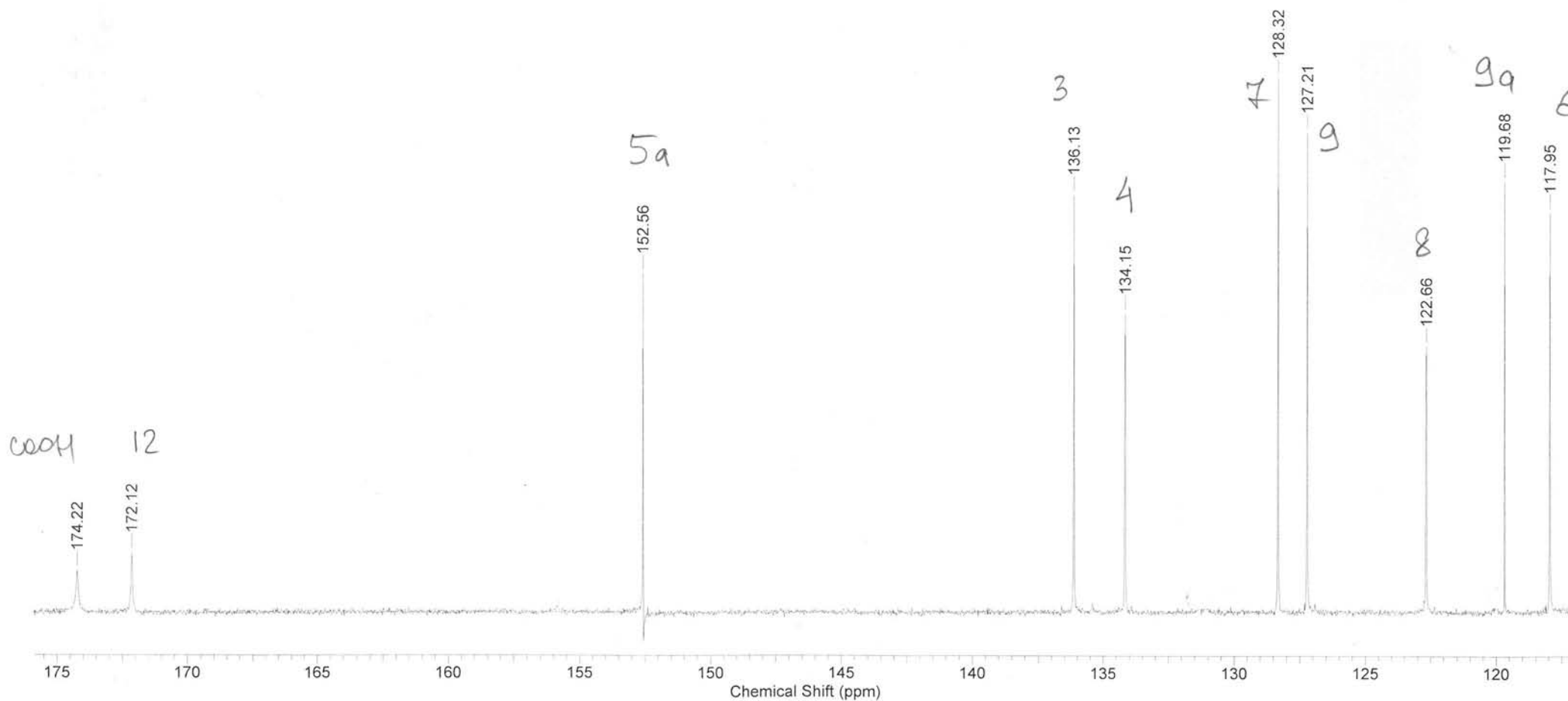
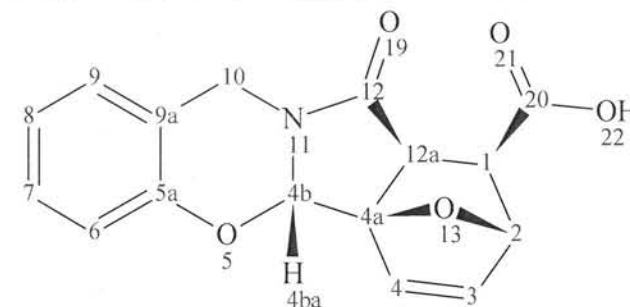
Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	10 Aug 2011 17:36:00	
File Name	C:\Users\Fedor\Desktop\05.08.11\rudn-050811-N2\rudn-050811-N2-c13dec\rudn-050811-N2-c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	2500	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compound 22Aa



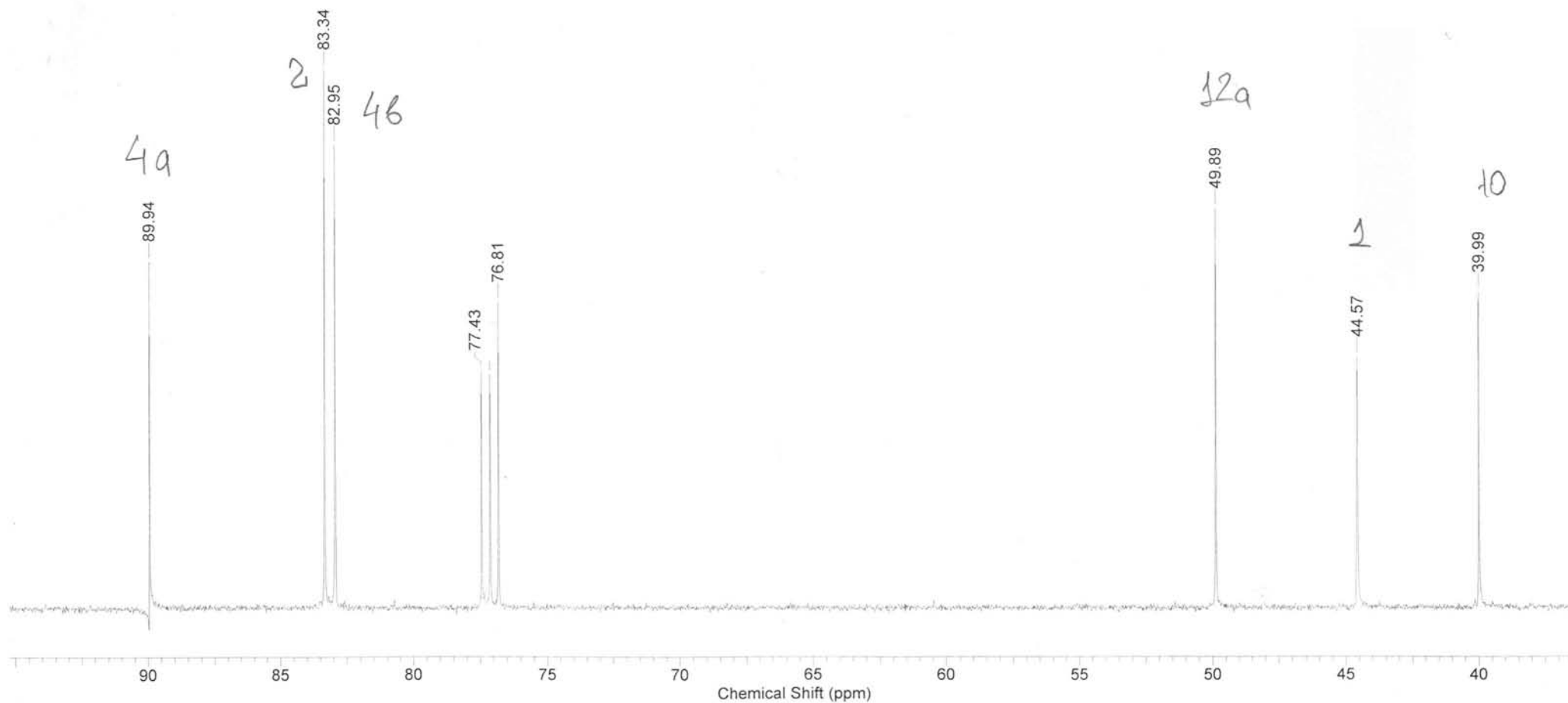
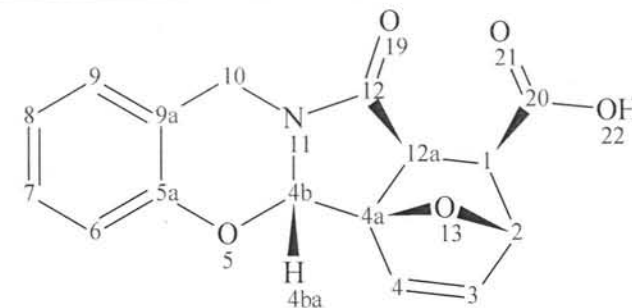
Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	10 Aug 2011 17:36:00	
File Name	C:\Users\Fedor\Desktop\05.08.11\rudn-050811-N2\rudn-050811-N2-c13dec\rudn-050811-N2-c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	2500	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compound 22Aa



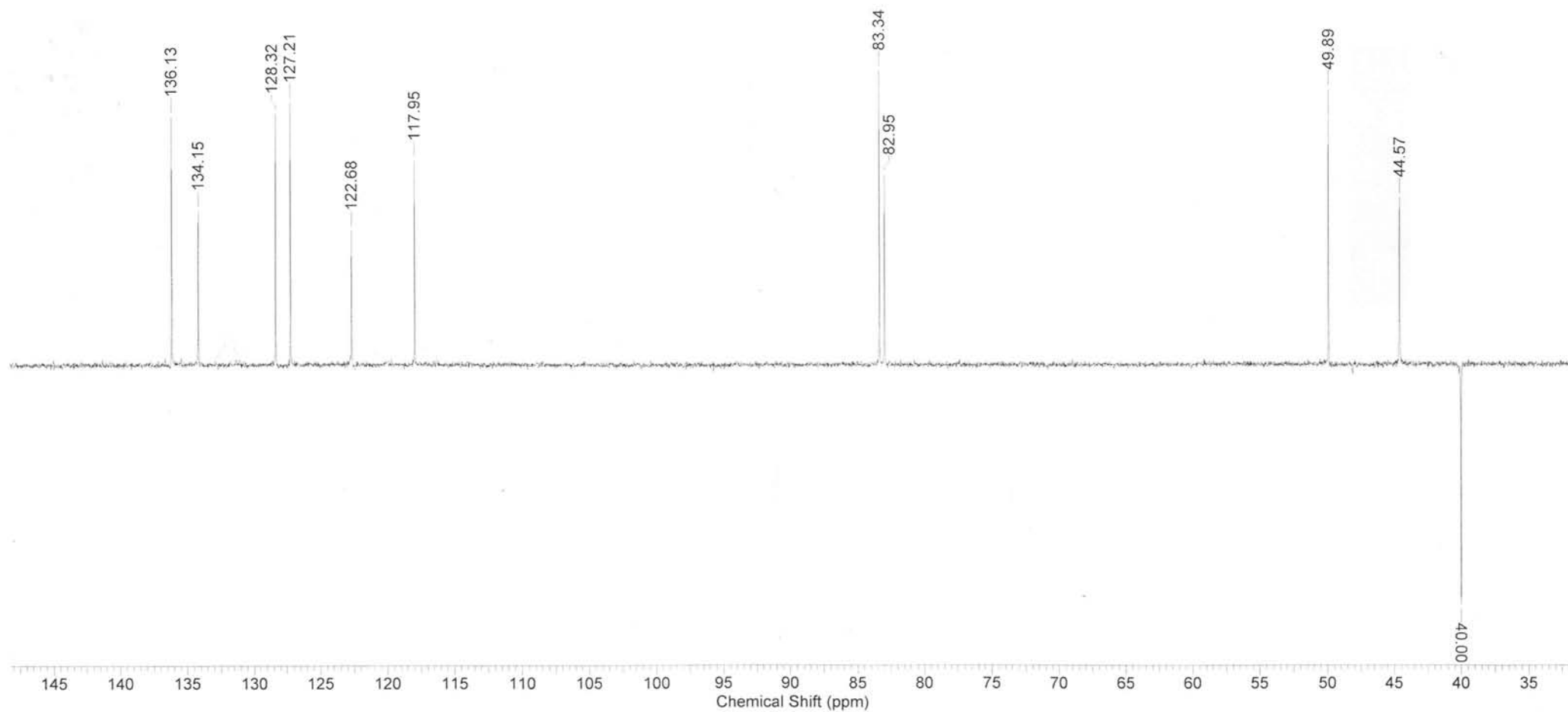
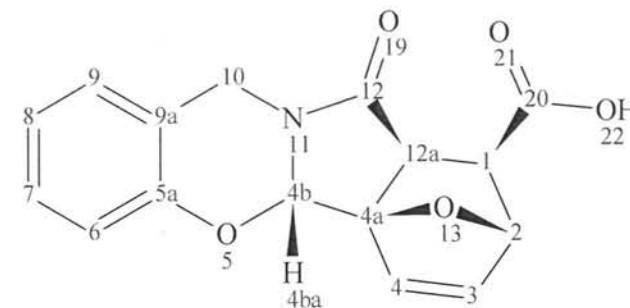
Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	10 Aug 2011 17:36:00	
File Name	C:\Users\Fedor\Desktop\05.08.11\rudn-050811-N2\rudn-050811-N2-c13dec\rudn-050811-N2-c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	2500	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compound 22Aa



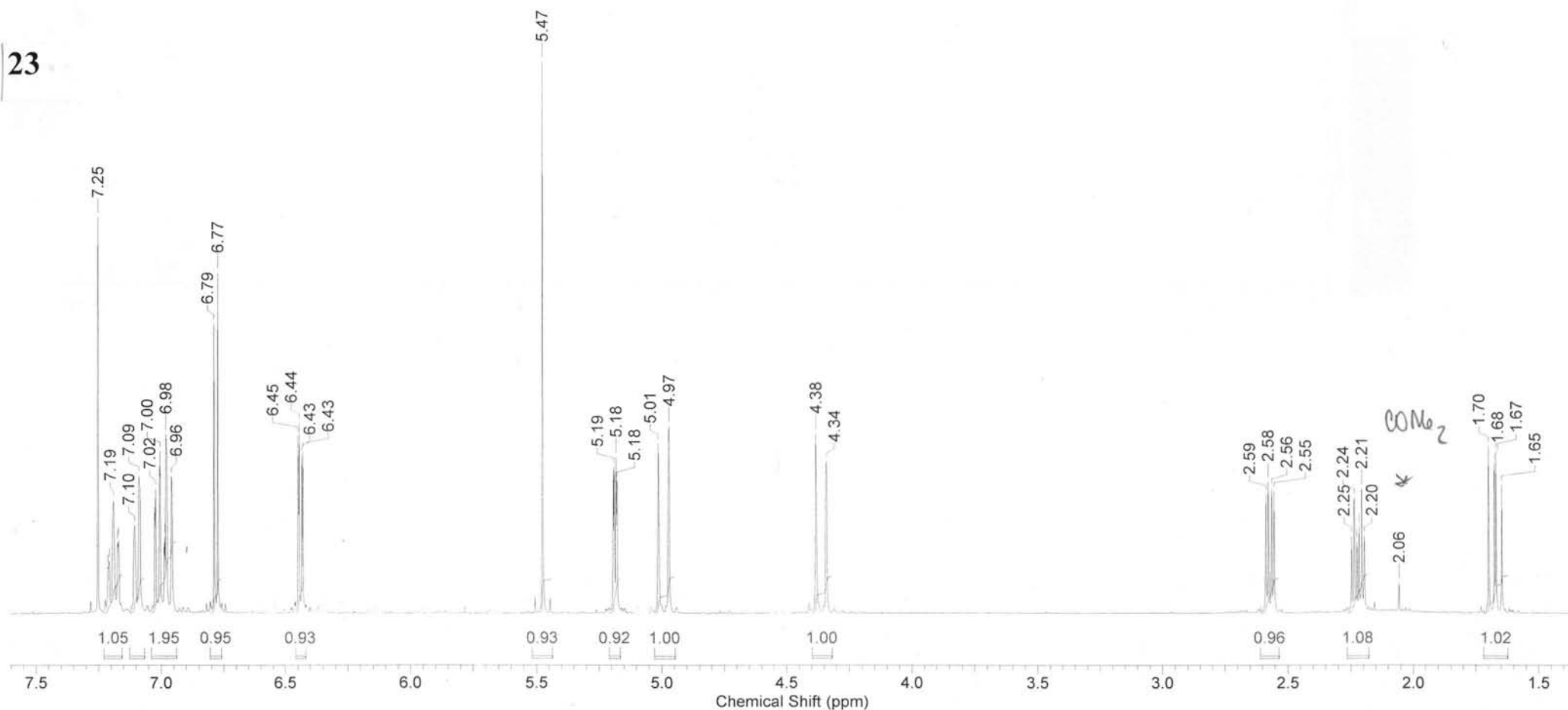
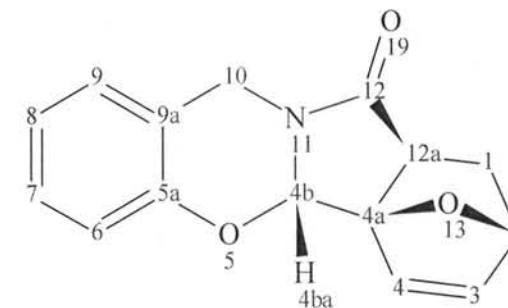
Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	10 Aug 2011 19:48:16	
File Name	C:\Users\Fedor\Desktop\05.08.11\rudn-050811-N2\rudn-050811-N2-dept135\rudn-050811-N2-dept135_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	2500	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	CHLOROFORM-D	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compound 22Aa



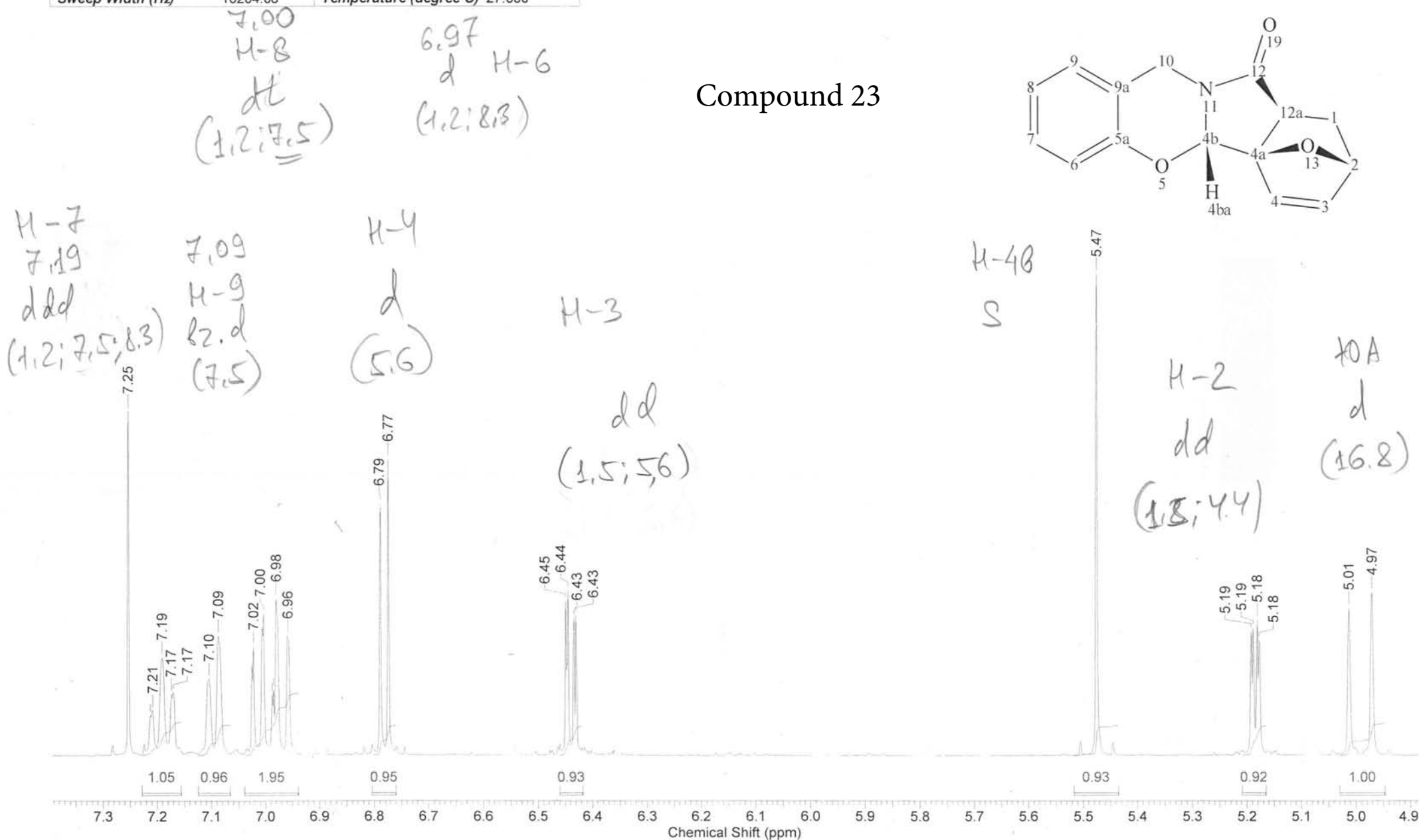
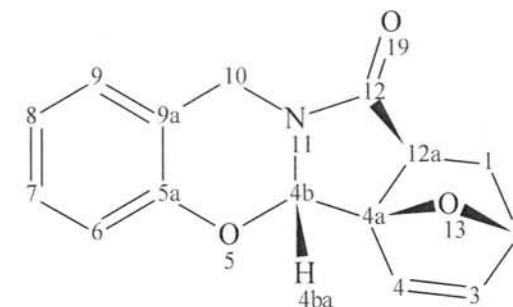
Acquisition Time (sec)	1.6056	Comment	Imported from UXNMR.		Date	07 Sep 2011 14:00:32	
File Name	D:\NMR\02.09.11\991\991_001000fid	Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	12
Original Points Count	16384	Points Count	16384	Pulse Sequence	zg	Solvent	CHLOROFORM-D
Sweep Width (Hz)	10204.08	Temperature (degree C)	27.000				

Compound 23



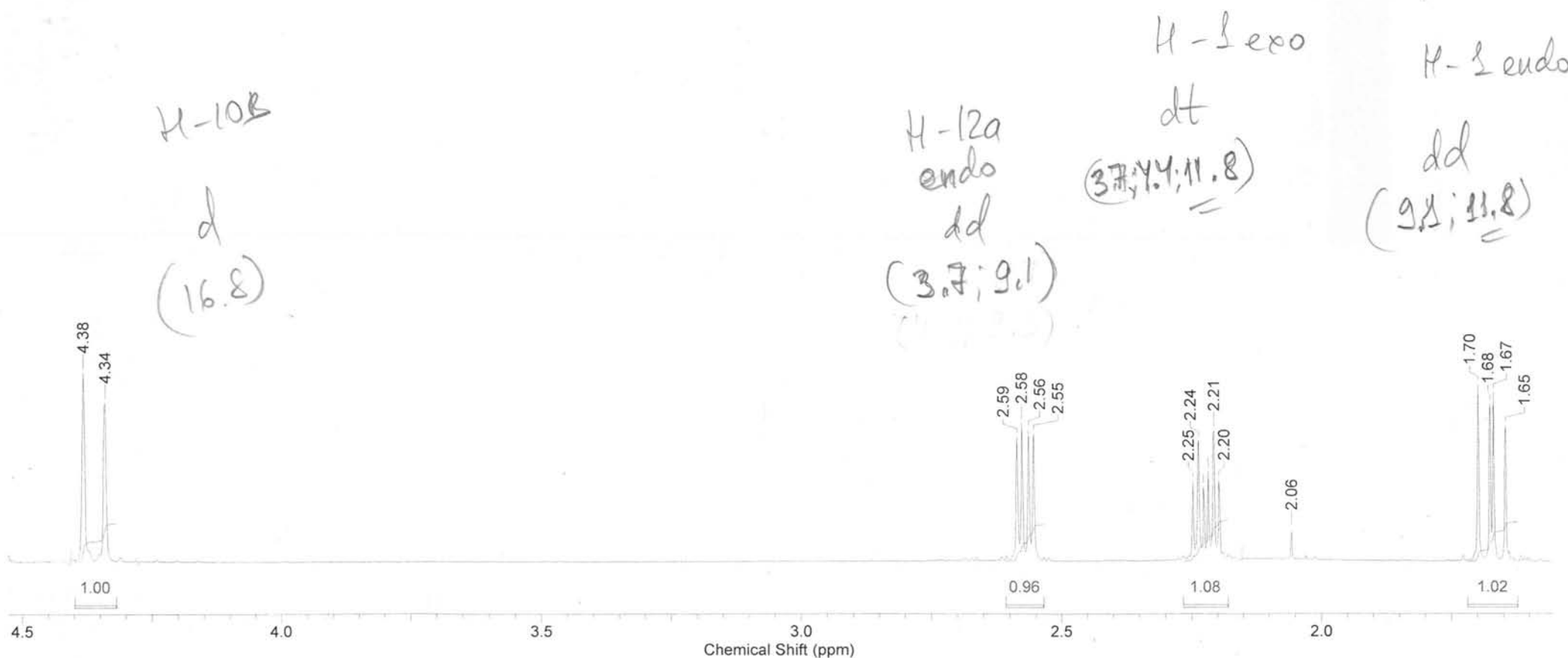
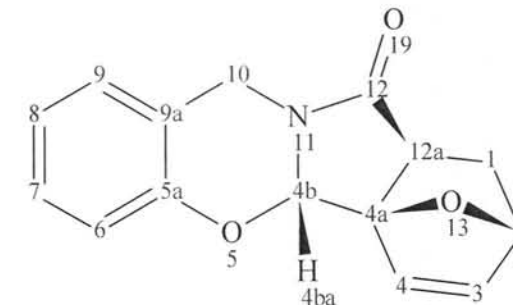
Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.		Date	07 Sep 2011 14:00:32	
File Name	D:\NMR\02.09.11\991\991_001000fid	Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	12
Original Points Count	16384	Points Count	16384	Pulse Sequence	zg	Solvent	CHLOROFORM-D
Sweep Width (Hz)	10204.08	Temperature (degree C)	27.000				

Compound 23



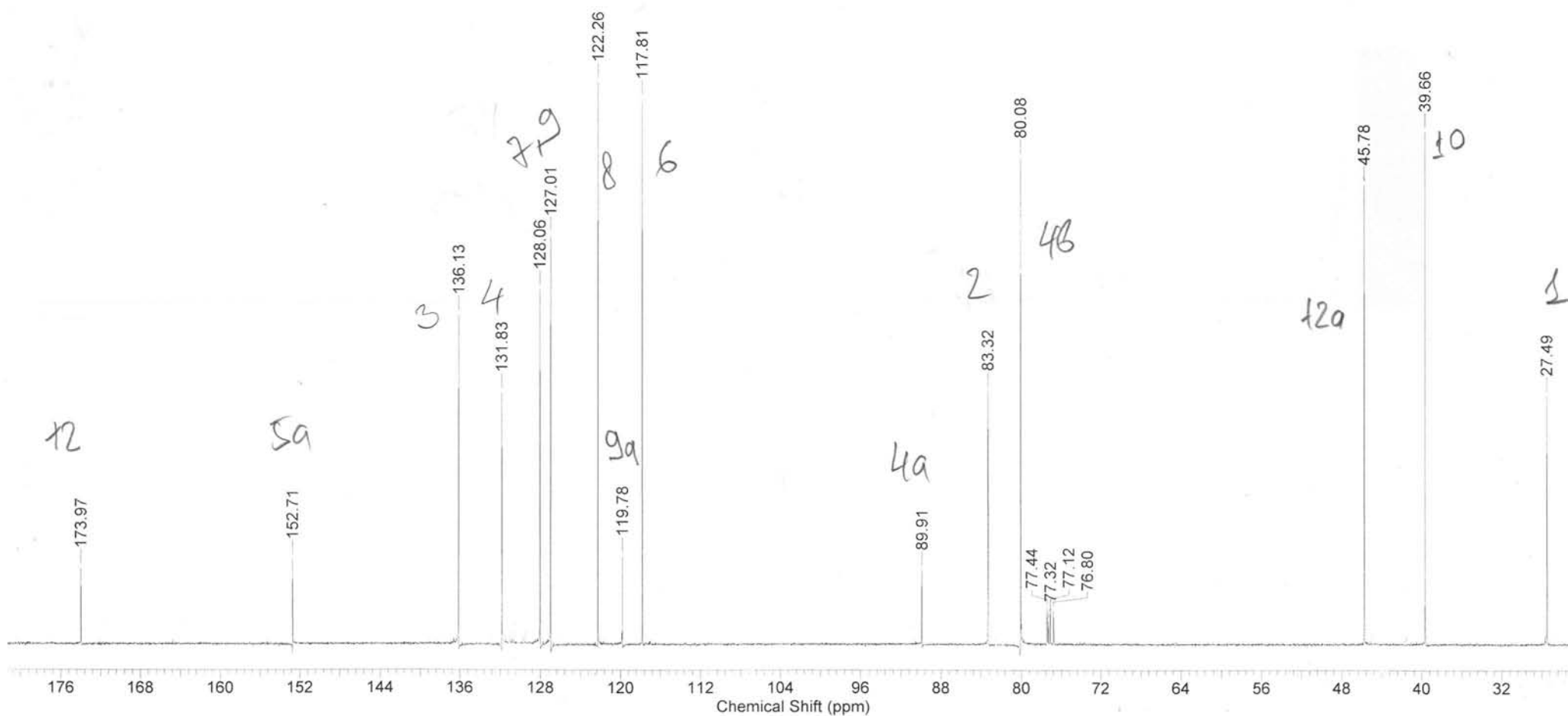
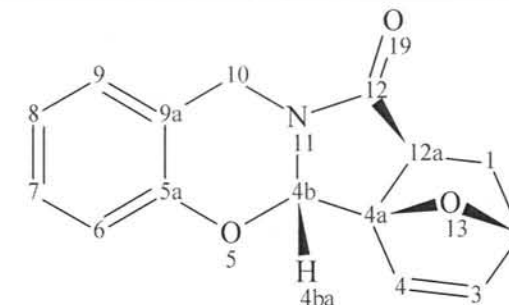
Acquisition Time (sec)	1.6056	Comment	Imported from UXNMR.		Date	07 Sep 2011 14:00:32	
File Name	D:\NMR\02.09.11\991\991_001000fid	Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	12
Original Points Count	16384	Points Count	16384	Pulse Sequence	zg	Solvent	CHLOROFORM-D
Sweep Width (Hz)	10204.08	Temperature (degree C)	27.000				

Compound 23

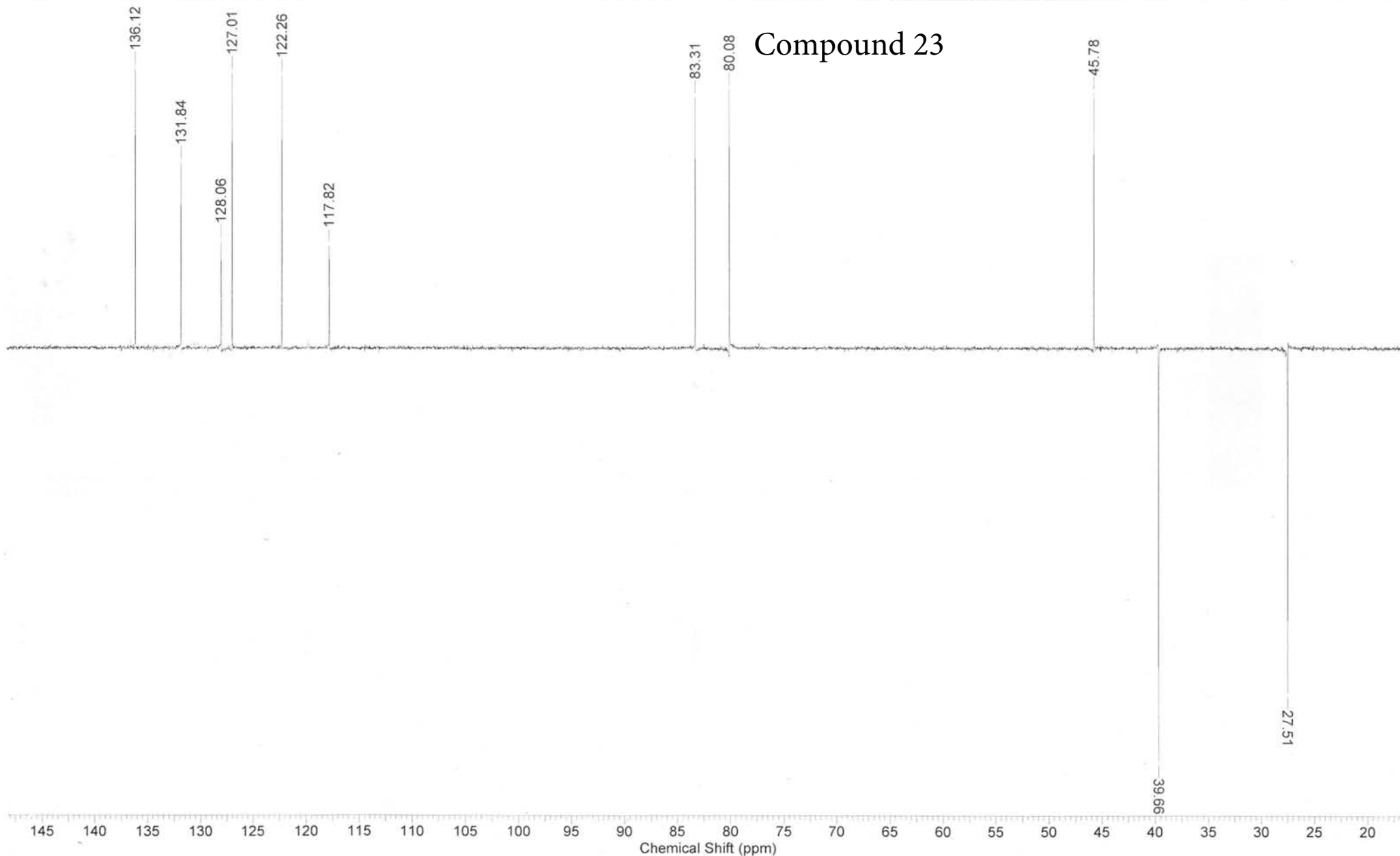


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File Name	D:\NMR\02.09.11\991-c13dec\991-c13dec_001000fid	Frequency (MHz)	100.62	Nucleus	13C		
Number of Transients	525	Original Points Count	16384	Points Count	16384	Pulse Sequence	zgpg
Solvent	CHLOROFORM-D	Sweep Width (Hz)	27777.78	Temperature (degree C)	27.000		

Compound 23



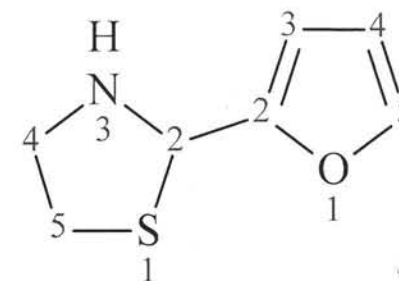
Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	07 Sep 2011 15:28:00	
File Name	D:\NMR\02.09.11\991-dept135\991-dept135_001000fid		Frequency (MHz)	100.62	Nucleus	13C	
Number of Transients	403	Original Points Count	16384	Points Count	16384	Pulse Sequence	dept135
Solvent	CHLOROFORM-D		Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000	



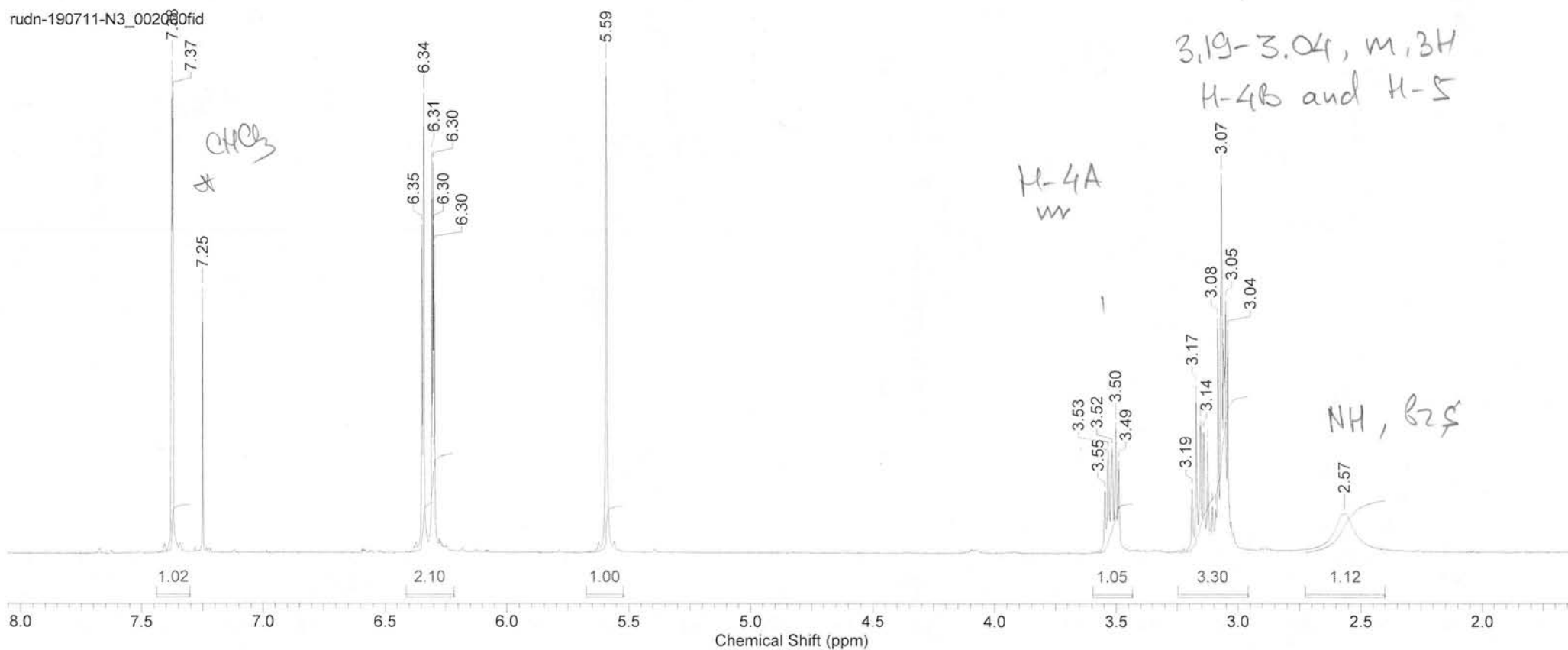
Formula C₇H₉NOS FW 155.2175

Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	21 Jul 2011 15:51:28
Date Stamp	21 Jul 2011 15:51:28	File Name	D:\NMR\19.07.11 (Poma)\rudn-190711-N3\rudn-190711-N3_002000fid	Origin	spect
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	12
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	512.00	SW(cyclical) (Hz)	10204.08	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2602.0486	Sweep Width (Hz)	10203.46	Temperature (degree C)	27.000

Initial for compound 24a



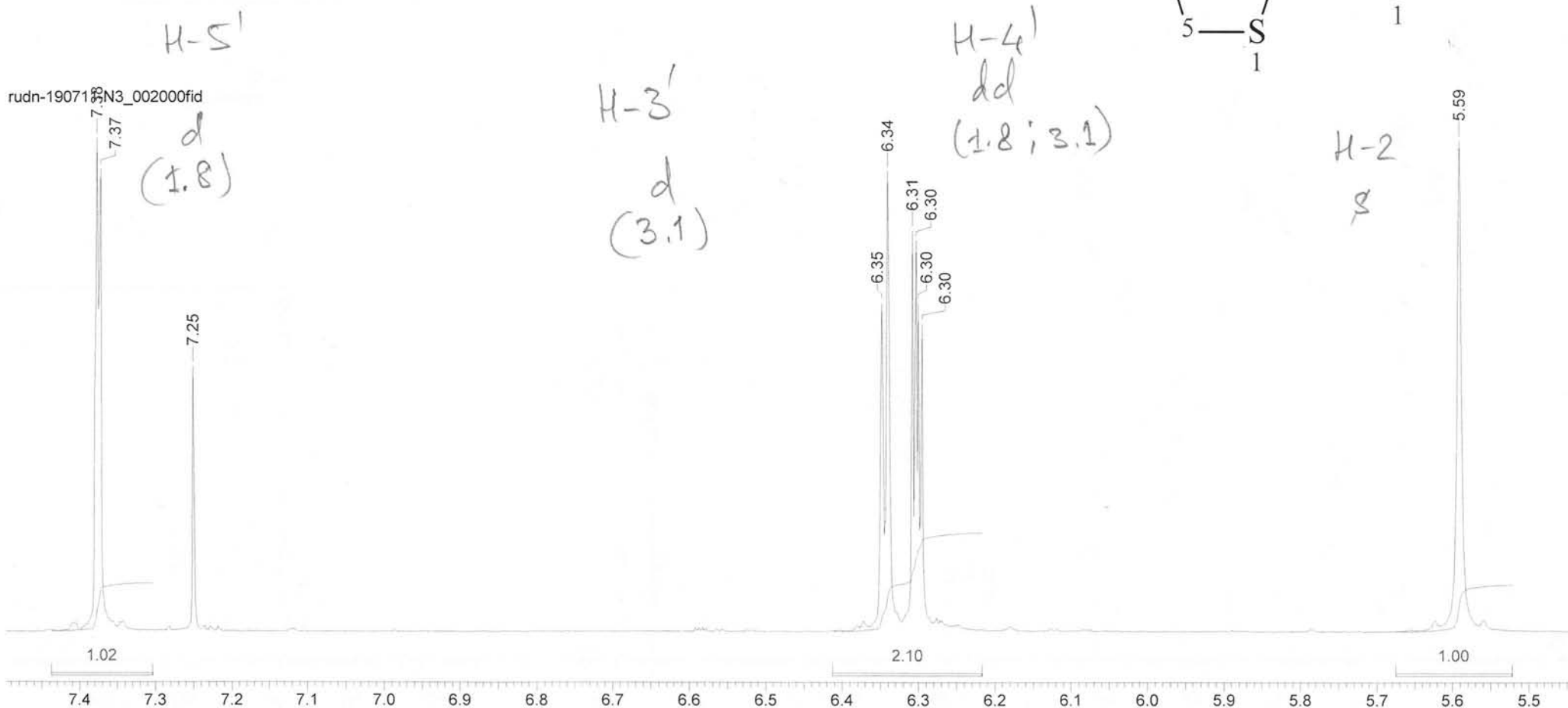
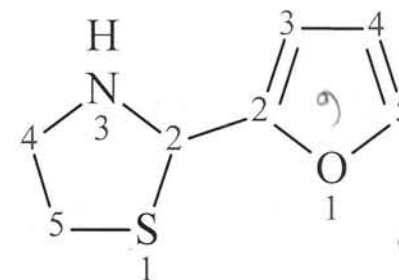
24a (initial)



Formula C₇H₉NOS FW 155.2175

Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	21 Jul 2011 15:51:28
Date Stamp	21 Jul 2011 15:51:28	File Name	D:\NMR\19.07.11 (Poma)\rudn-190711-N3\rudn-190711-N3_002000fid	Origin	spect
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	12
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	512.00	SW(cyclical) (Hz)	10204.08	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2602.0486	Sweep Width (Hz)	10203.46	Temperature (degree C)	27.000

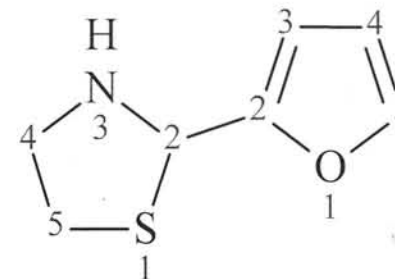
Initial for compound 24a



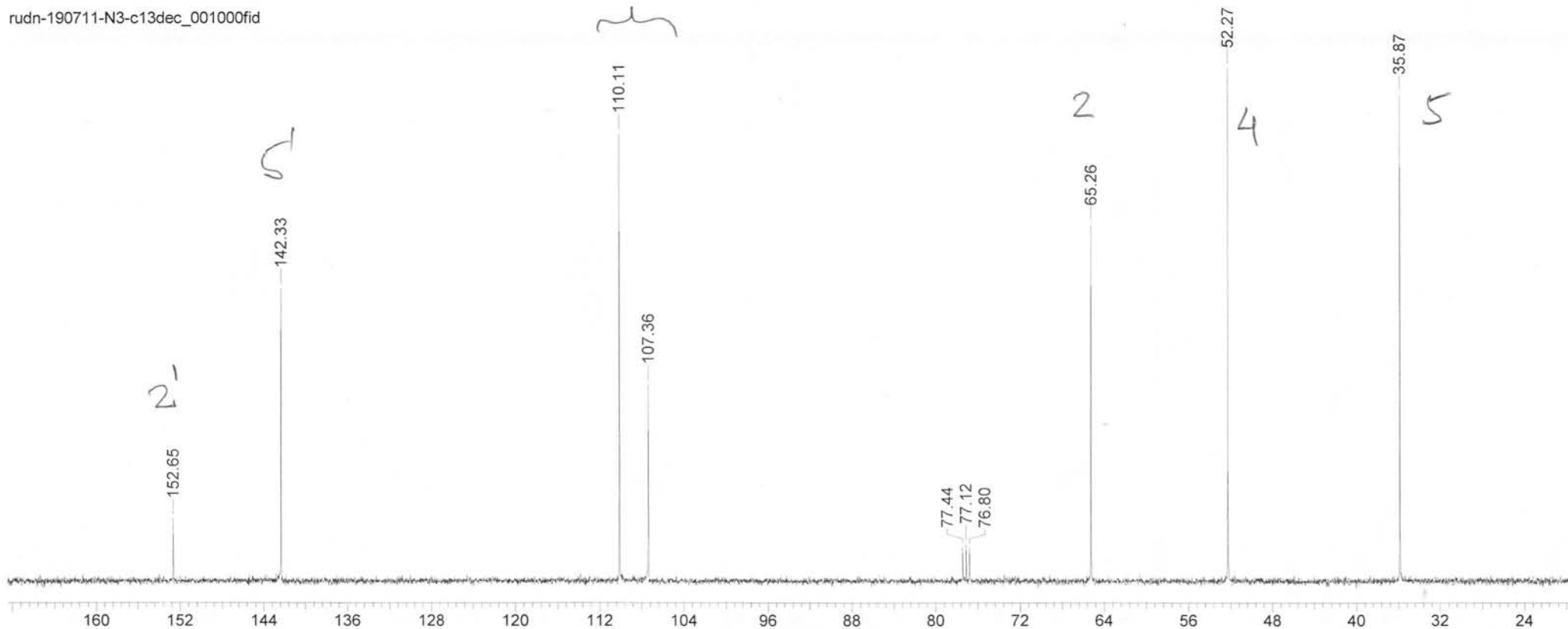
Formula C₇H₉NOS FW 155.2175

Acquisition Time (sec)	0.5898	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	21 Jul 2011 16:08:32
Date Stamp	21 Jul 2011 16:08:32	File Name	D:\NMR\19.07.11 (Poma)\rudn-190711-N3-c13dec\rudn-190711-N3-c13dec_001000fid	Number of Transients	203
Frequency (MHz)	100.62	Nucleus	13C	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	27777.78	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	9613.9424	Sweep Width (Hz)	27776.08	Temperature (degree C)	27.000

Initial for compound 24a

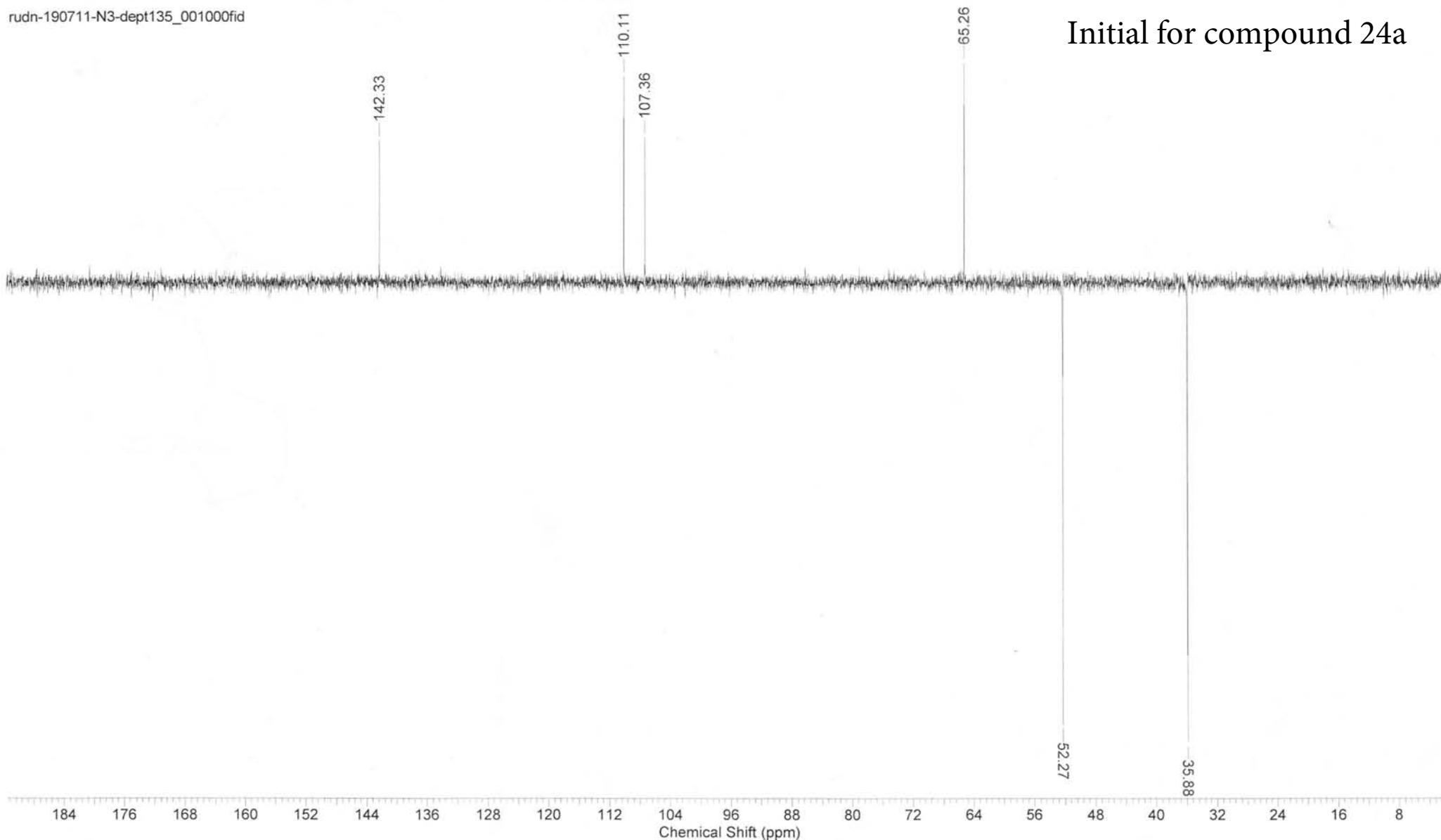


rudn-190711-N3-c13dec_001000fid



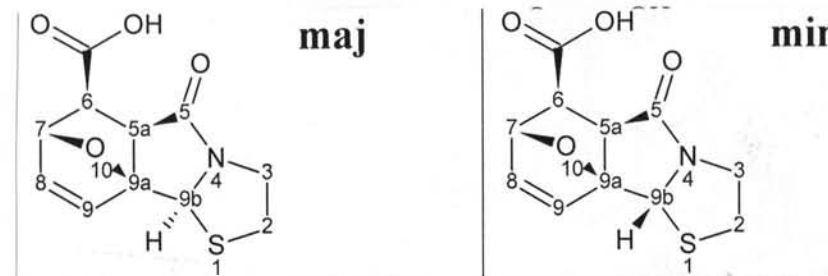
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Date Stamp	21 Jul 2011 16:12:48	File Name	D:\NMR\19.07.11 (Роман)\rudn-190711-N3-dept135\rudn-190711-N3-dept135_001000fid				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	209	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	dept135
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	9614.0205	Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000		

rudn-190711-N3-dept135_001000fid

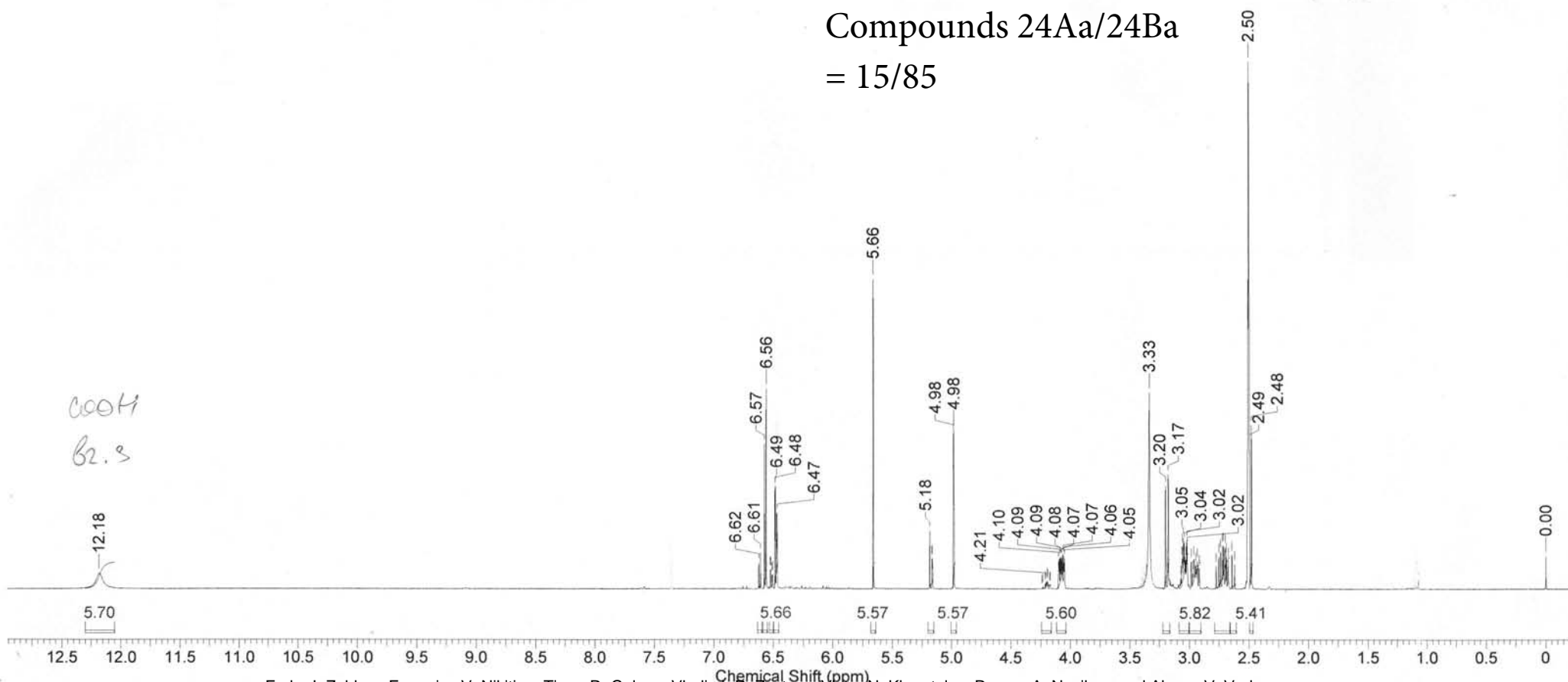


Formula	C ₁₁ H ₁₁ NO ₄ S	FW	253.2743
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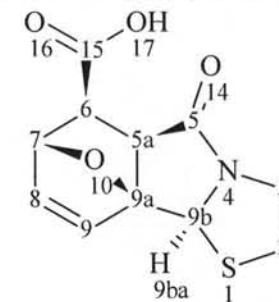
Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	06 Jun 2012 11:54:17	Date Stamp	06 Jun 2012 15:43:34
File Name	D:\NMR\04.06.12\FZ2444-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	9
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	36.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	2413.7561	Sweep Width (Hz)	7503.00
						Temperature (degree C)	22.900



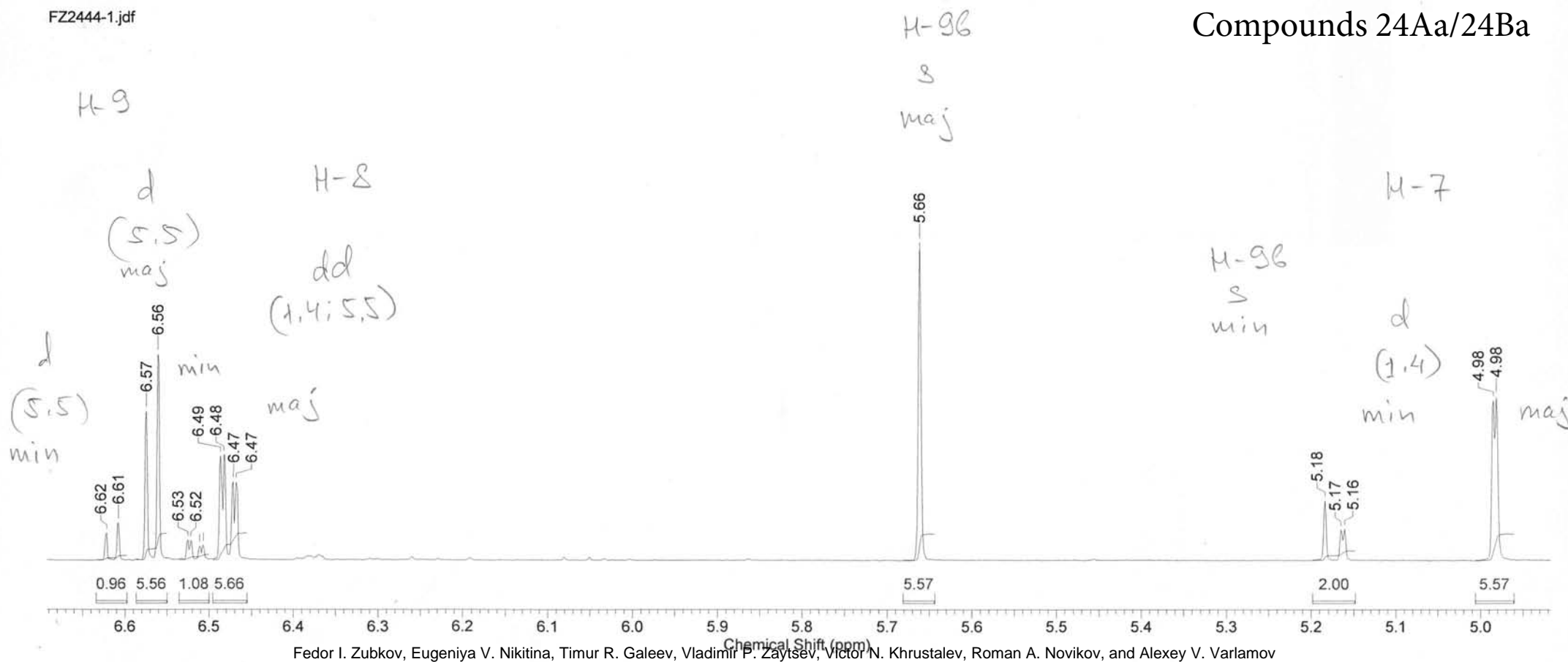
Compounds 24Aa/24Ba
= 15/85



Formula C ₁₁ H ₁₁ NO ₄ S	FW 253.2743						
Acquisition Time (sec) 2.1837	Comment single_pulse,	Date 06 Jun 2012 11:54:17	Date Stamp 06 Jun 2012 15:43:34				
File Name D:\NMR\04.06.12\FZ2444-1.jdf	Frequency (MHz) 399.78	Nucleus 1H	Number of Transients 9				
Origin ECS 400	Original Points Count 16384	Owner delta	Points Count 16384	Pulse Sequence single_pulse.ex2			
Receiver Gain 36.00	Solvent DMSO-d6	Spectrum Offset (Hz) 2413.7561	Sweep Width (Hz) 7503.00	Temperature (degree C) 22.900			



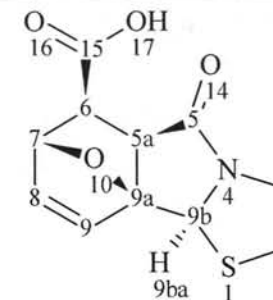
Compounds 24Aa/24Ba



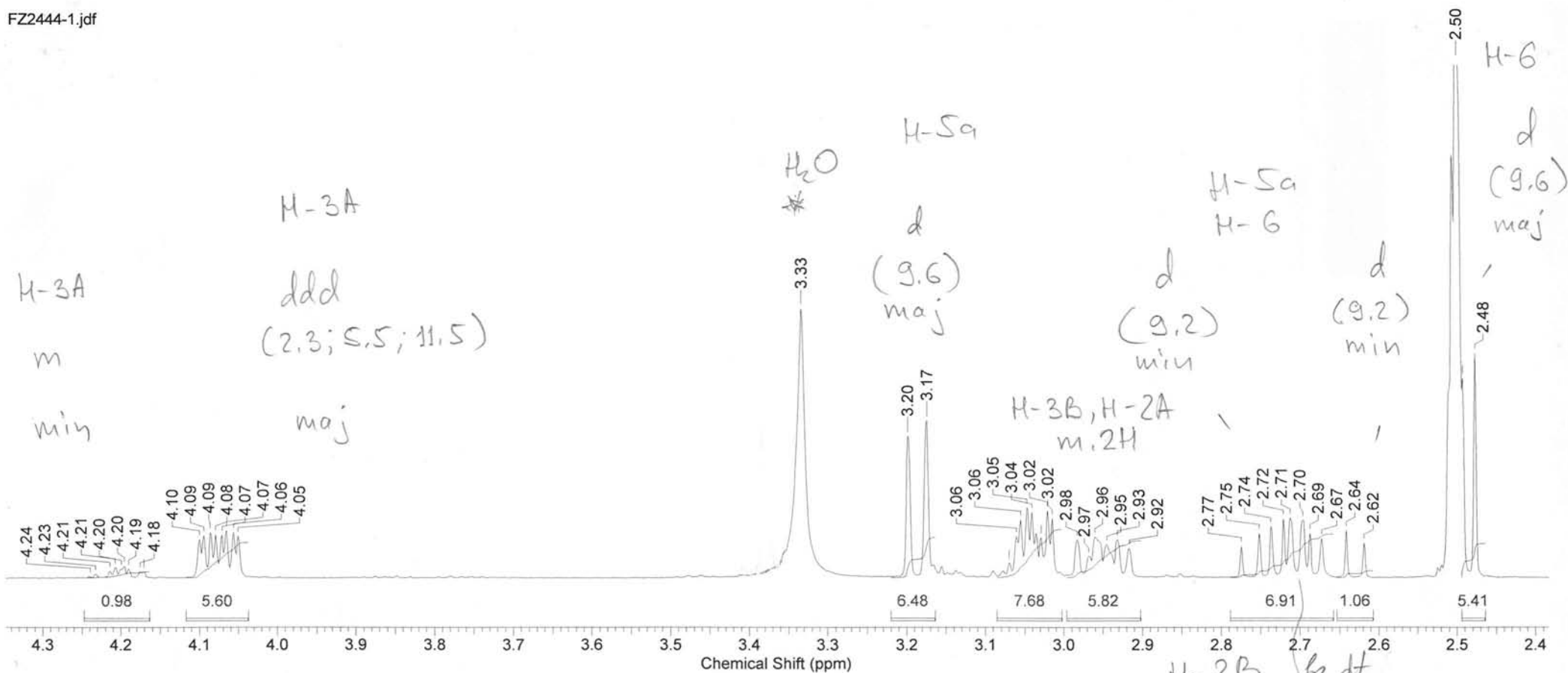
Formula C₁₁H₁₁NO₄S FW 253.2743

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	06 Jun 2012 11:54:17	Date Stamp	06 Jun 2012 15:43:34
File Name	D:\NMR\04.06.12\FZ2444-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	9
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	36.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	2413.7561	Sweep Width (Hz)	7503.00
						Temperature (degree C)	22.900

Compounds 24Aa/24Ba

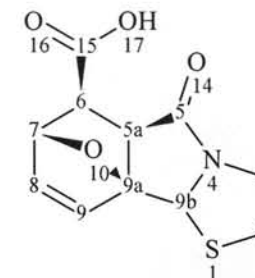


FZ2444-1.jdf

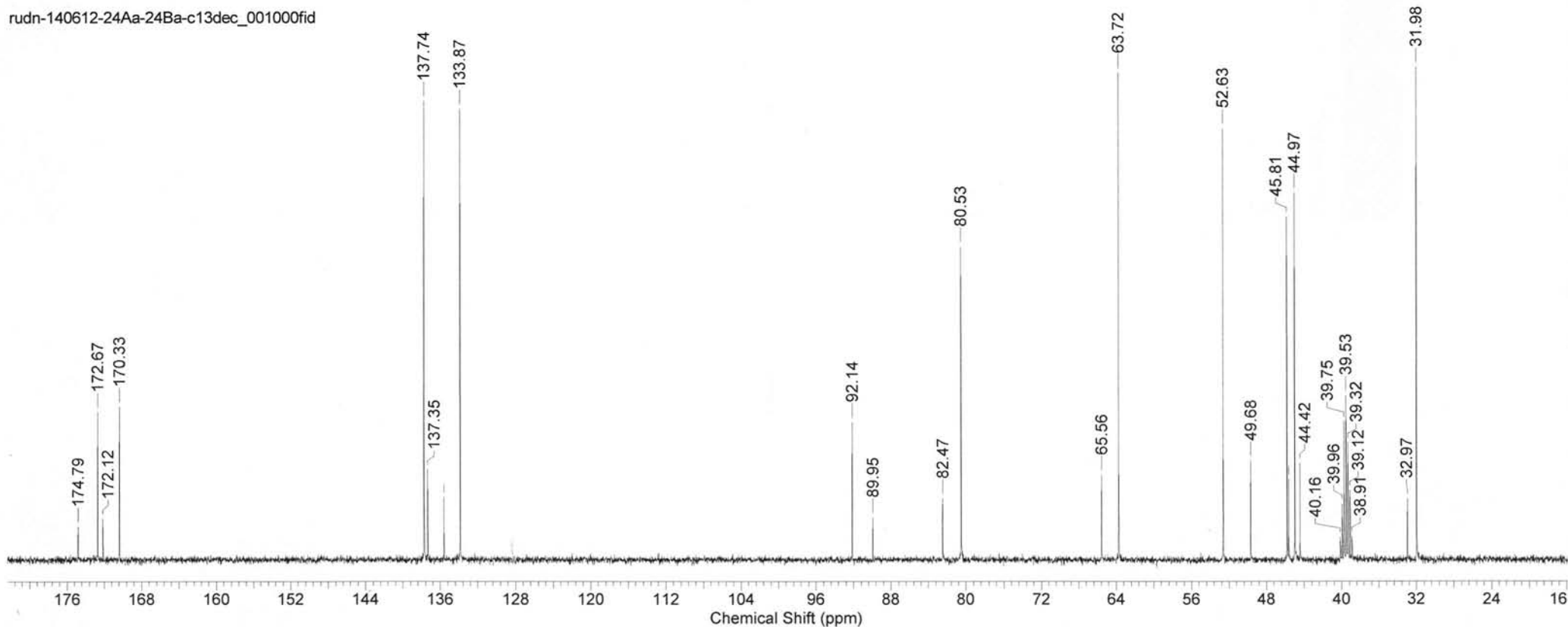


Formula C ₁₁ H ₁₁ NO ₄ S	FW 253.2743			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 26 Jun 2012 16:53:20		
Date Stamp 26 Jun 2012 16:53:20				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-140612-24Aa-24Ba-c13dec\rudn-140612-24Aa-24Ba-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 628	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10554.3486	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

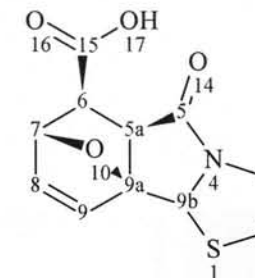
Compounds 24Aa/24Ba



rudn-140612-24Aa-24Ba-c13dec_001000fid

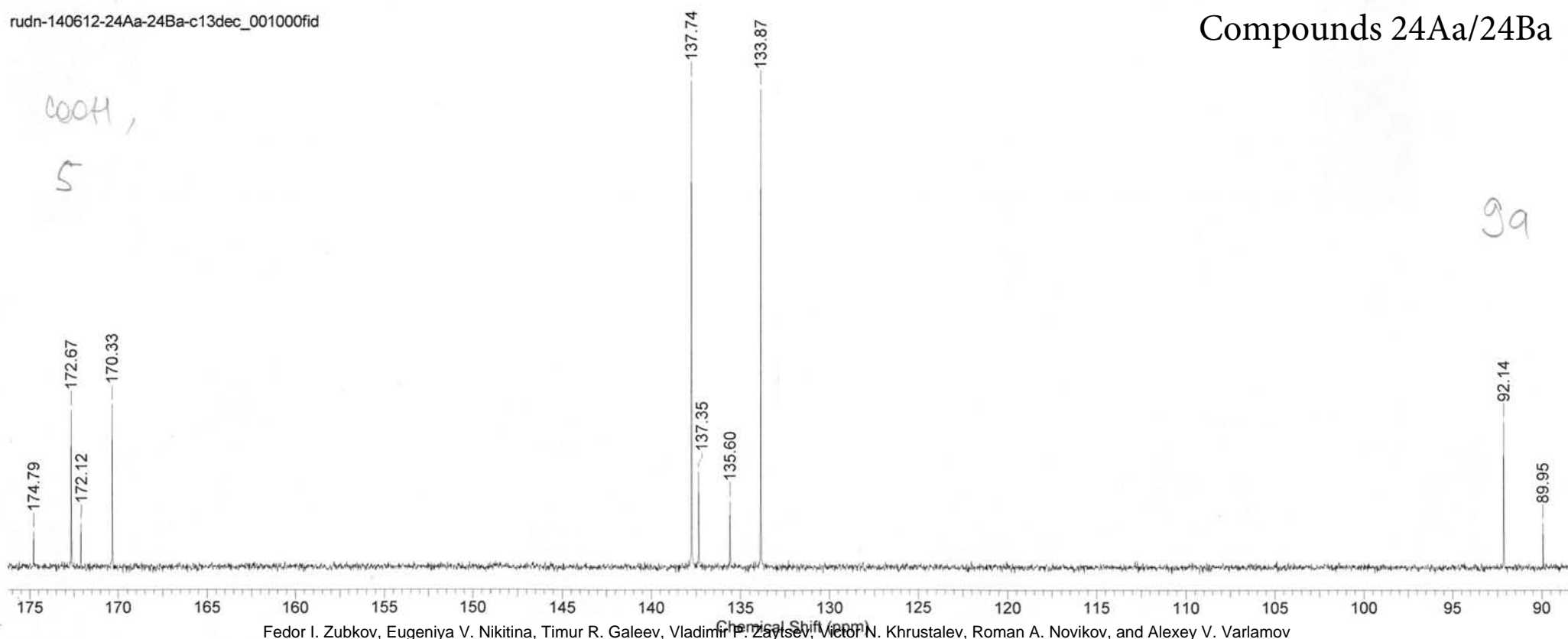


Formula C ₁₁ H ₁₁ NO ₄ S	FW 253.2743			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 26 Jun 2012 16:53:20		
Date Stamp 26 Jun 2012 16:53:20				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-140612-24Aa-24Ba-c13dec\rudn-140612-24Aa-24Ba-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 628	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10554.3486	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			



Compounds 24Aa/24Ba

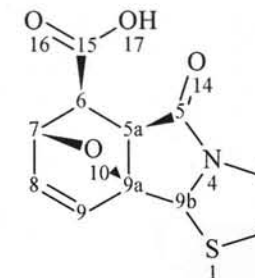
rudn-140612-24Aa-24Ba-c13dec_001000fid



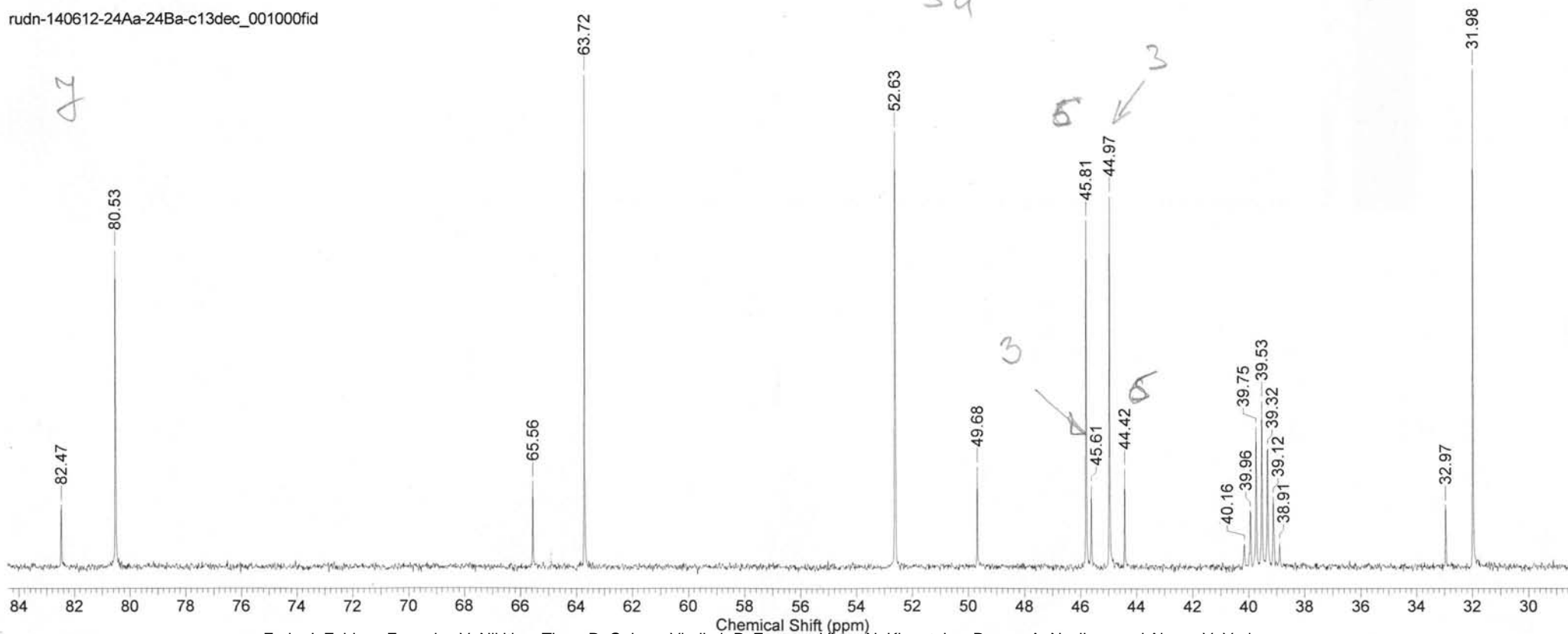
Formula C₁₁H₁₁NO₄S FW 253.2743

Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	26 Jun 2012 16:53:20	
Date Stamp	26 Jun 2012 16:53:20						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-140612-24Aa-24Ba-c13dec\rudn-140612-24Aa-24Ba-c13dec_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	628	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zgpg
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6	Spectrum Offset (Hz)	10554.3486
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				

Compounds 24Aa/24Ba

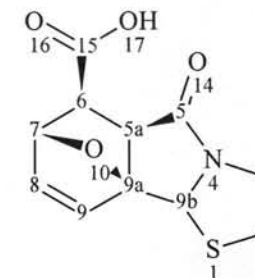


rudn-140612-24Aa-24Ba-c13dec_001000fid

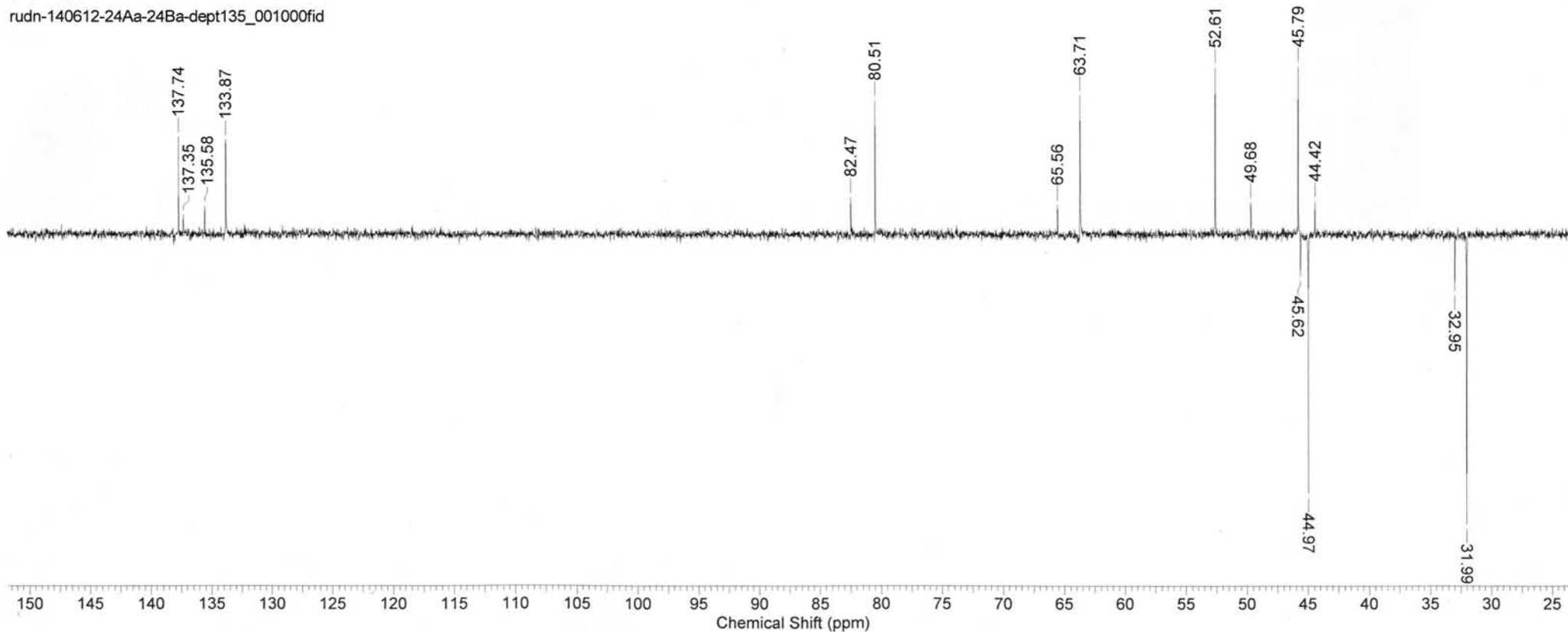


Formula C ₁₁ H ₁₁ NO ₄ S	FW 253.2743			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 26 Jun 2012 17:04:00		
Date Stamp 26 Jun 2012 17:04:00				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-140612-24Aa-24Ba-dept135\rudn-140612-24Aa-24Ba-dept135_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 347	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence dept135	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 9103.9404	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compounds 24Aa/24Ba

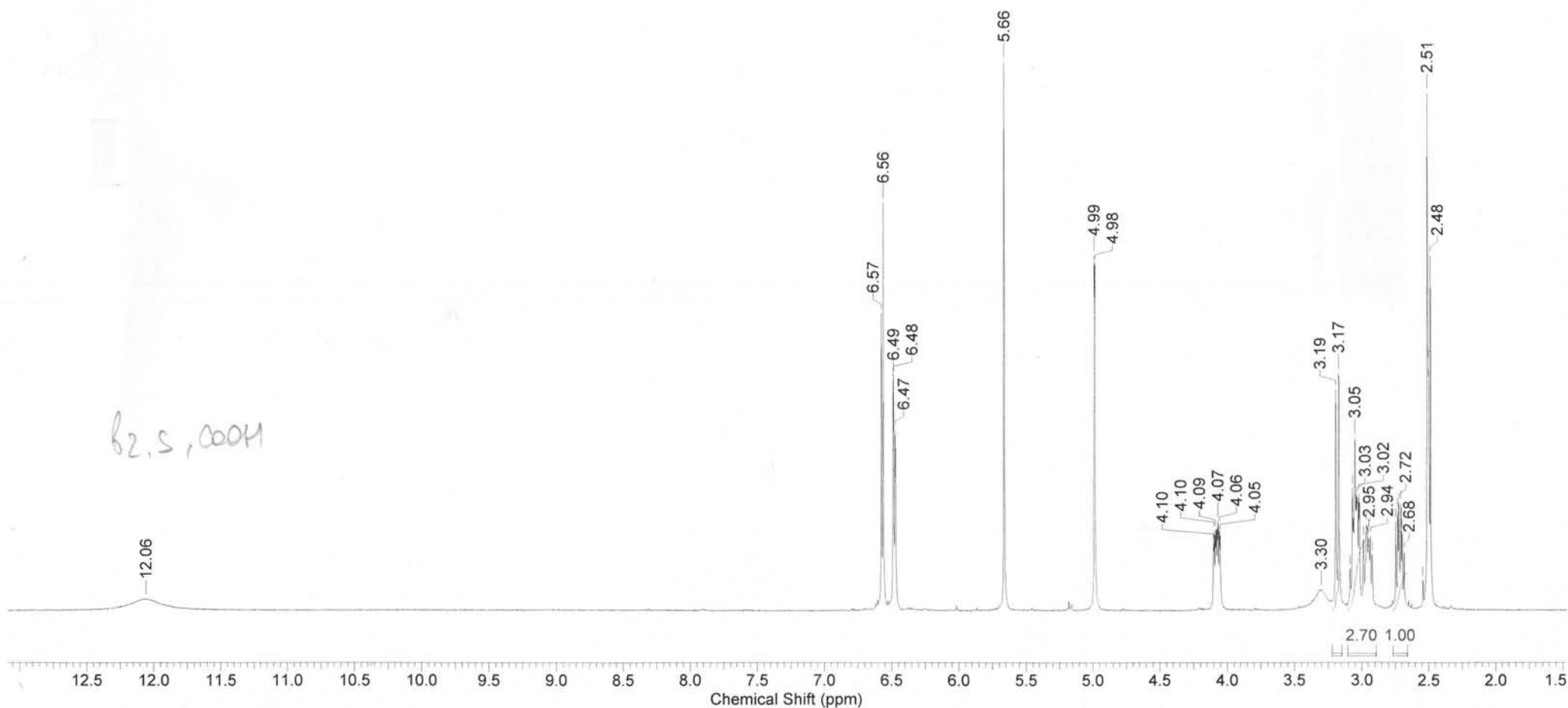
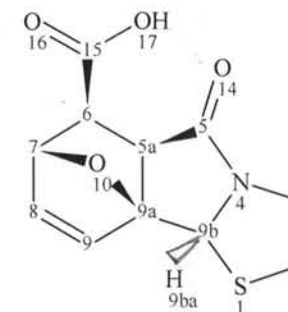


rudn-140612-24Aa-24Ba-dept135_001000fid



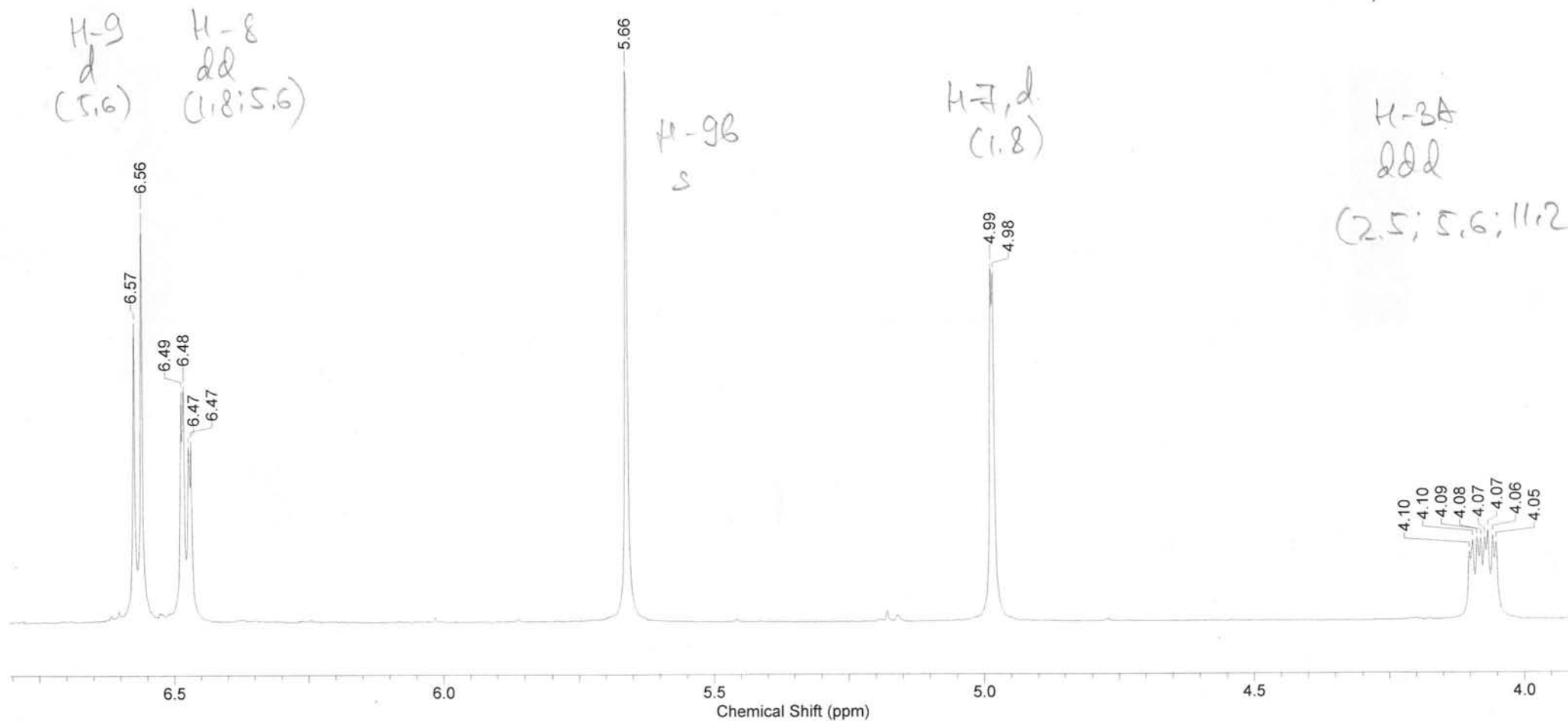
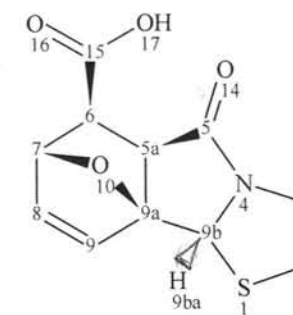
Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.		Date	15 Jul 2009 13:05:04	
File Name	D:\Тимур\Тимур (лето 2009)\rudn9\rudn9_001000fid	Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	4
Original Points Count	16384	Points Count	16384	Pulse Sequence	zg	Solvent	DMSO-D6
Temperature (degree C)	27.000					Sweep Width (Hz)	10204.08

Compound 24Ba



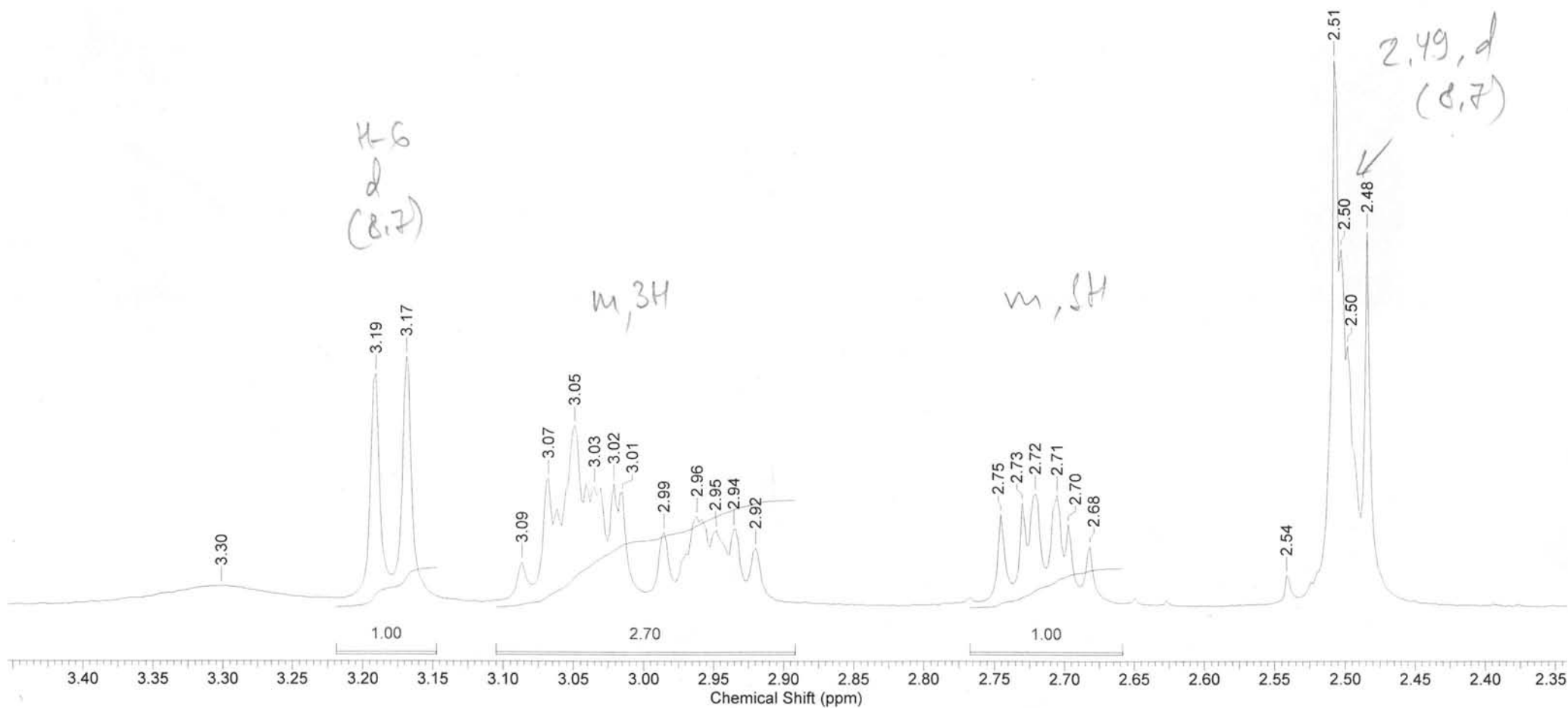
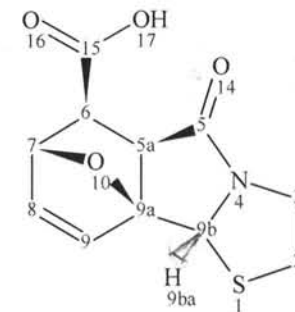
Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.		Date	15 Jul 2009 13:05:04	
File Name	D:\Тимур\Тимур (лето 2009)\rudn9\rudn9_001000fid	Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	4
Original Points Count	16384	Points Count	16384	Pulse Sequence	zg	Sweep Width (Hz)	10204.08
Temperature (degree C)	27.000						

Compound 24Ba



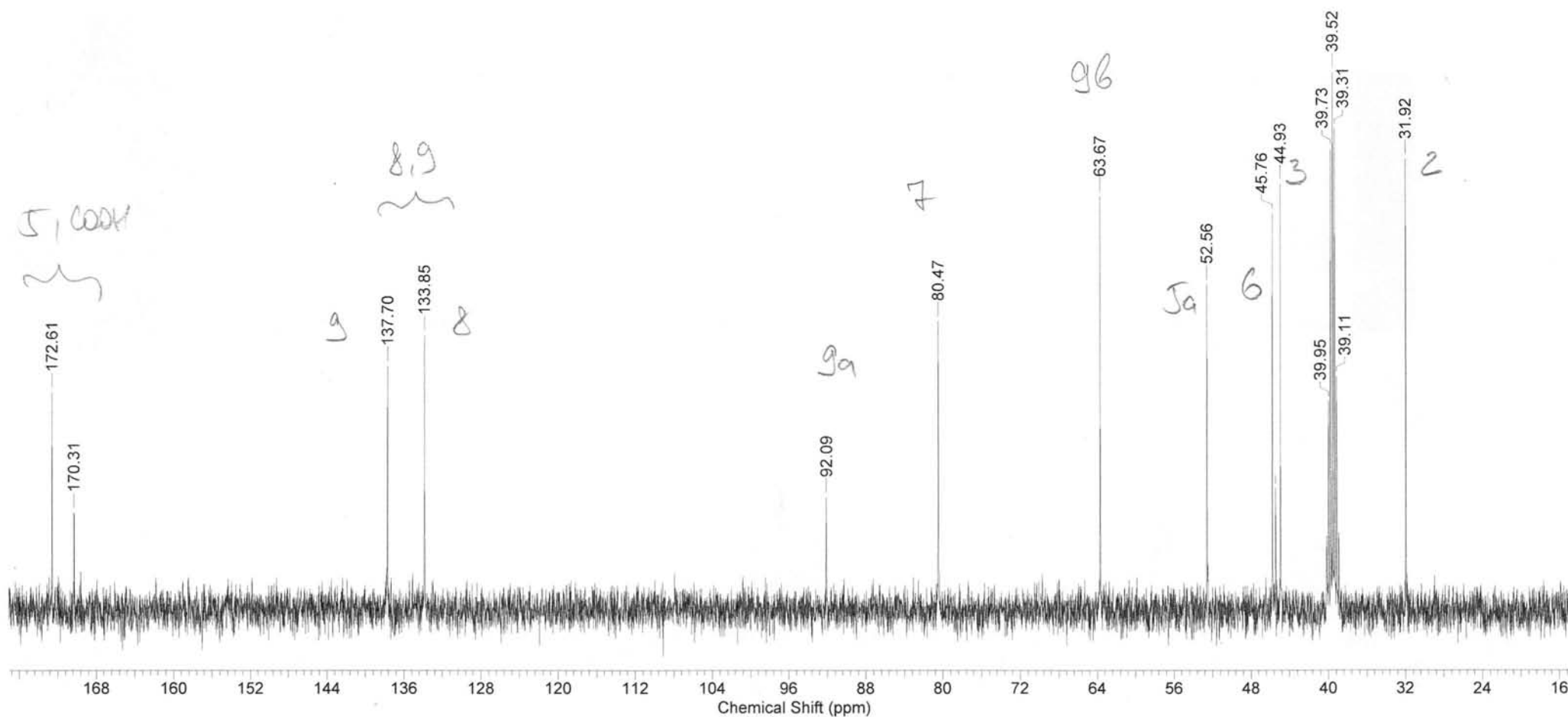
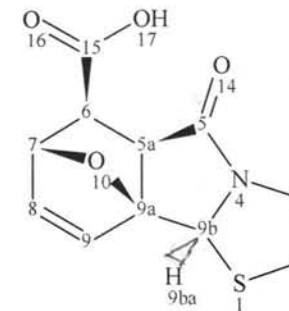
Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.		Date	15 Jul 2009 13:05:04	
File Name	D:\Тимур\Тимур (лето 2009)\rudn9\rudn9_001000fid	Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	4
Original Points Count	16384	Points Count	16384	Pulse Sequence	zg	Sweep Width (Hz)	10204.08
Temperature (degree C)	27.000						

Compound 24Ba



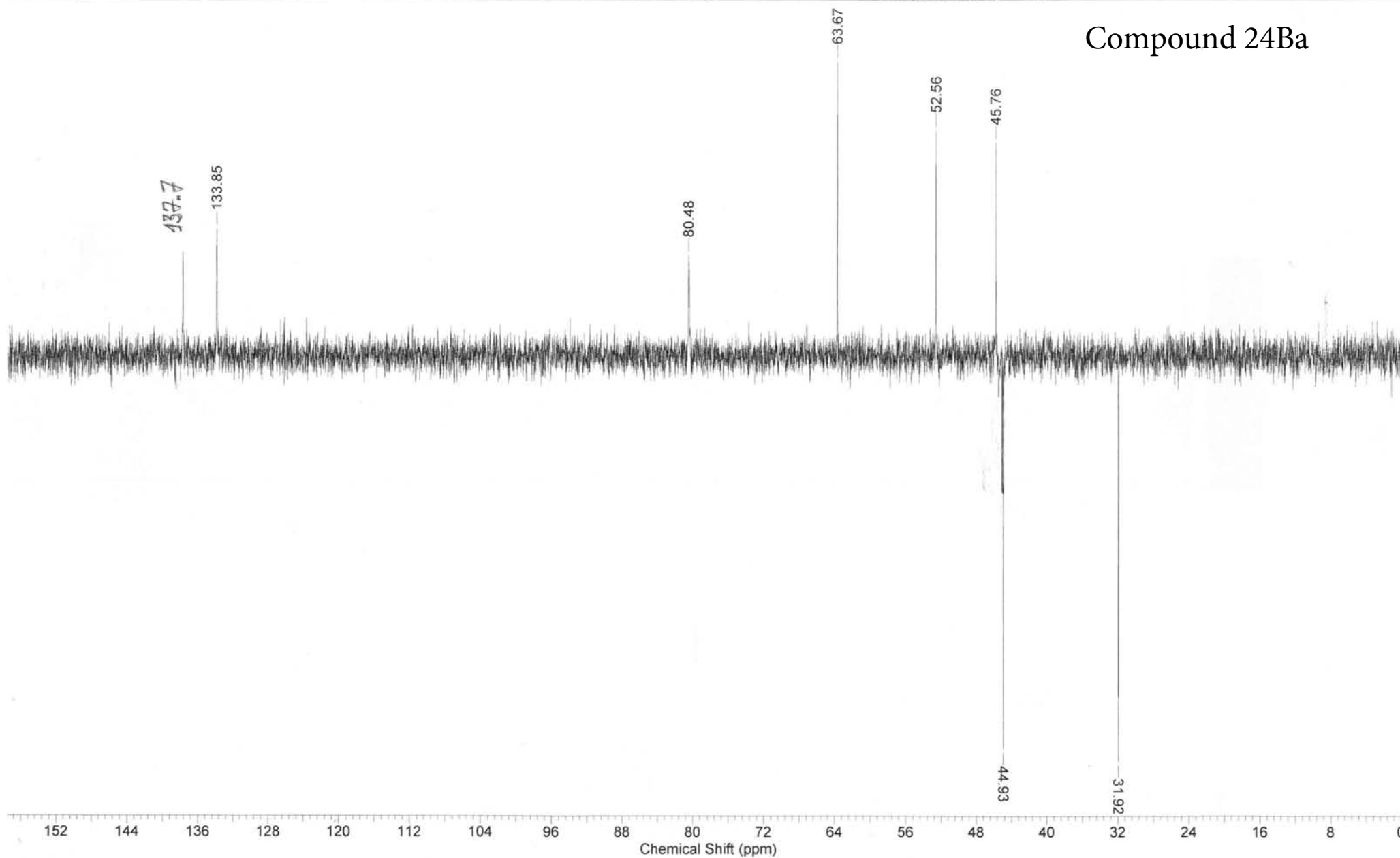
Acquisition Time (sec)	0.6226	Comment	Imported from UXMNR.		Date	15 Jul 2009 14:30:24	
File Name	D:\Тимур\Тимур (лето 2009)\rudn9c13dec\rudn9c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	112	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	26315.79	Temperature (degree C)	27.000

Compound 24Ba



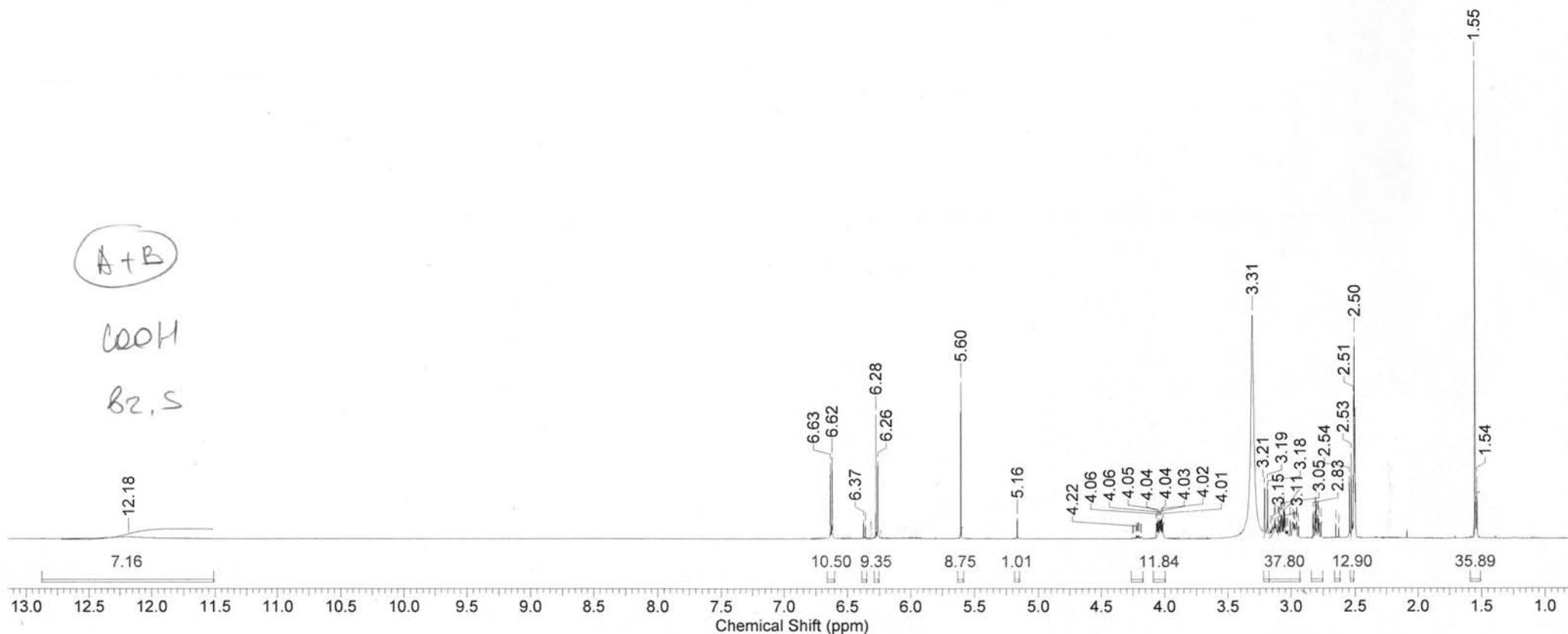
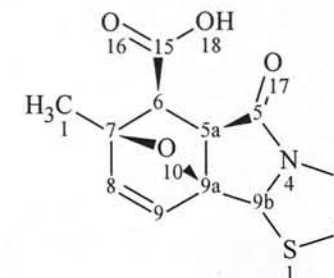
Acquisition Time (sec)	0.6226	Comment	Imported from UXMNR.		Date	15 Jul 2009 14:32:32	
File Name	D:\Timur\Тимур (лето 2009)\rudn9dept135\rudn9dept135_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	126	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	DMSO-d6	Sweep Width (Hz)	26315.79	Temperature (degree C)	27.000

Compound 24Ba



Formula C ₁₂ H ₁₃ NO ₄ S	FW 267.3009			
Acquisition Time (sec) 1.5729	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 06 Jul 2012 16:14:56		
Date Stamp 06 Jul 2012 16:14:56				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-24b\rudn-060712-24b_001000fid	Frequency (MHz) 400.14			
Nucleus 1H	Number of Transients 96	Origin spect	Original Points Count 16384	
Owner root	Points Count 16384	Pulse Sequence zg	Receiver Gain 128.00	
SW(cyclical) (Hz) 10416.67	Solvent DMSO-d6	Spectrum Offset (Hz) 2712.0542	Sweep Width (Hz) 10416.03	
Temperature (degree C) 32.000				

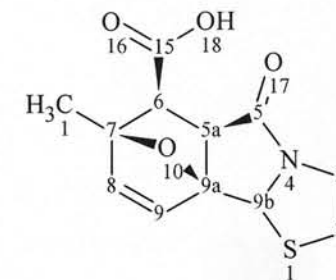
Compounds 24Ab/24Bb
10/90
after crystallization



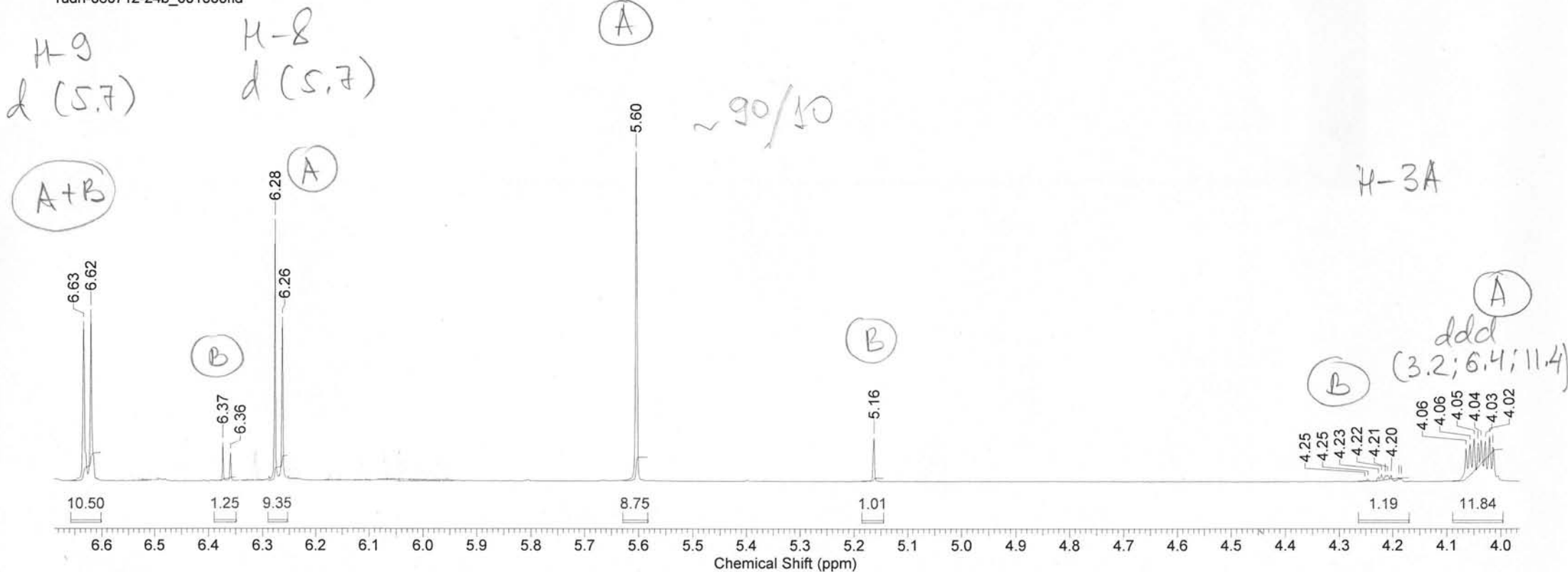
Formula	C ₁₂ H ₁₃ NO ₄ S	FW	267.3009
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Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	06 Jul 2012 16:14:56
Date Stamp	06 Jul 2012 16:14:56				
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-24b\rudn-060712-24b_001000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	96	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zg
SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542
Temperature (degree C)	32.000			Sweep Width (Hz)	10416.03

Compounds 24Ab/24Bb
after crystallization



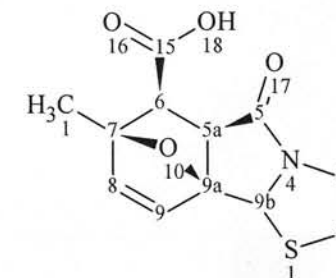
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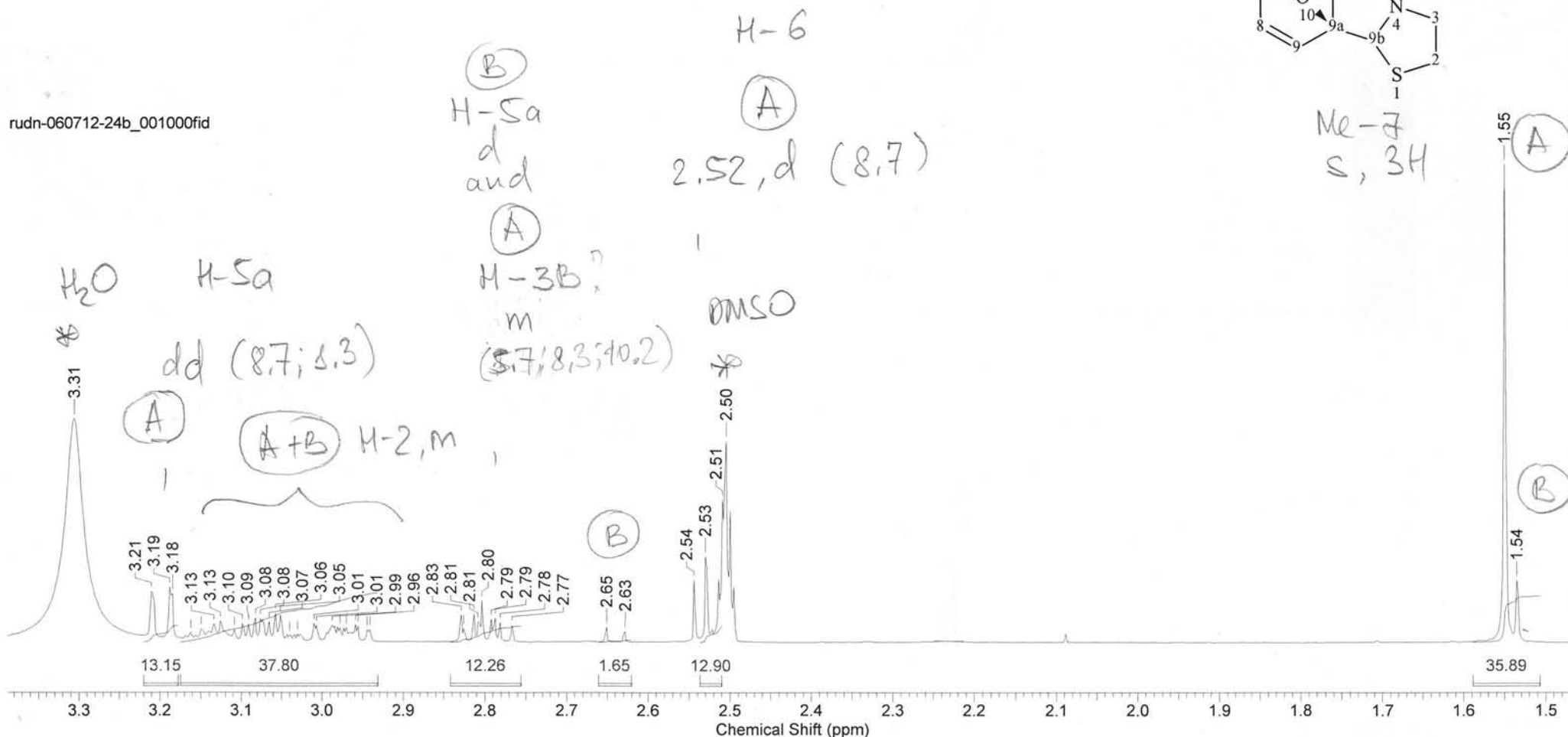
Formula	C ₁₂ H ₁₃ NO ₄ S	FW	267.3009
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Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	06 Jul 2012 16:14:56
Date Stamp	06 Jul 2012 16:14:56				
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-24b\rudn-060712-24b_001000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	96	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zg
SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542
Temperature (degree C)	32.000			Sweep Width (Hz)	10416.03

Compounds 24Ab/24Bb after crystallization

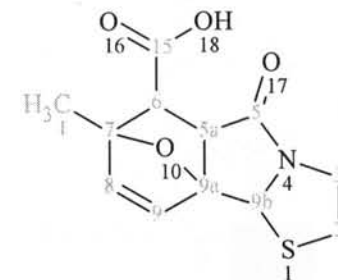


rudn-060712-24b_001000fid

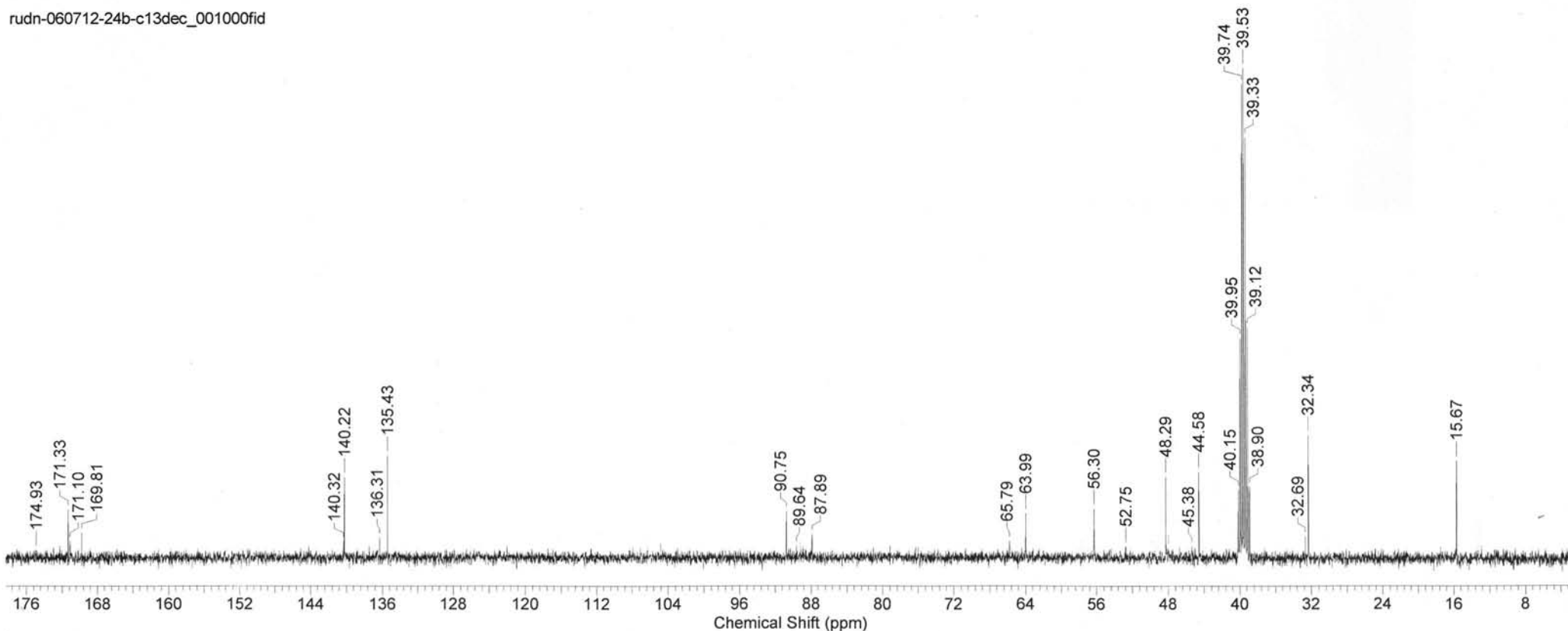


Formula C ₁₂ H ₁₃ NO ₄ S	FW 267.3009			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 06 Jul 2012 16:17:04		
Date Stamp 06 Jul 2012 16:17:04				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-24b-c13dec\rudn-060712-24b-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 2170	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10548.5127	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compounds 24Ab/24Bb
after crystallization



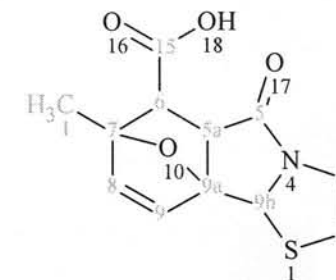
rudn-060712-24b-c13dec_001000fid



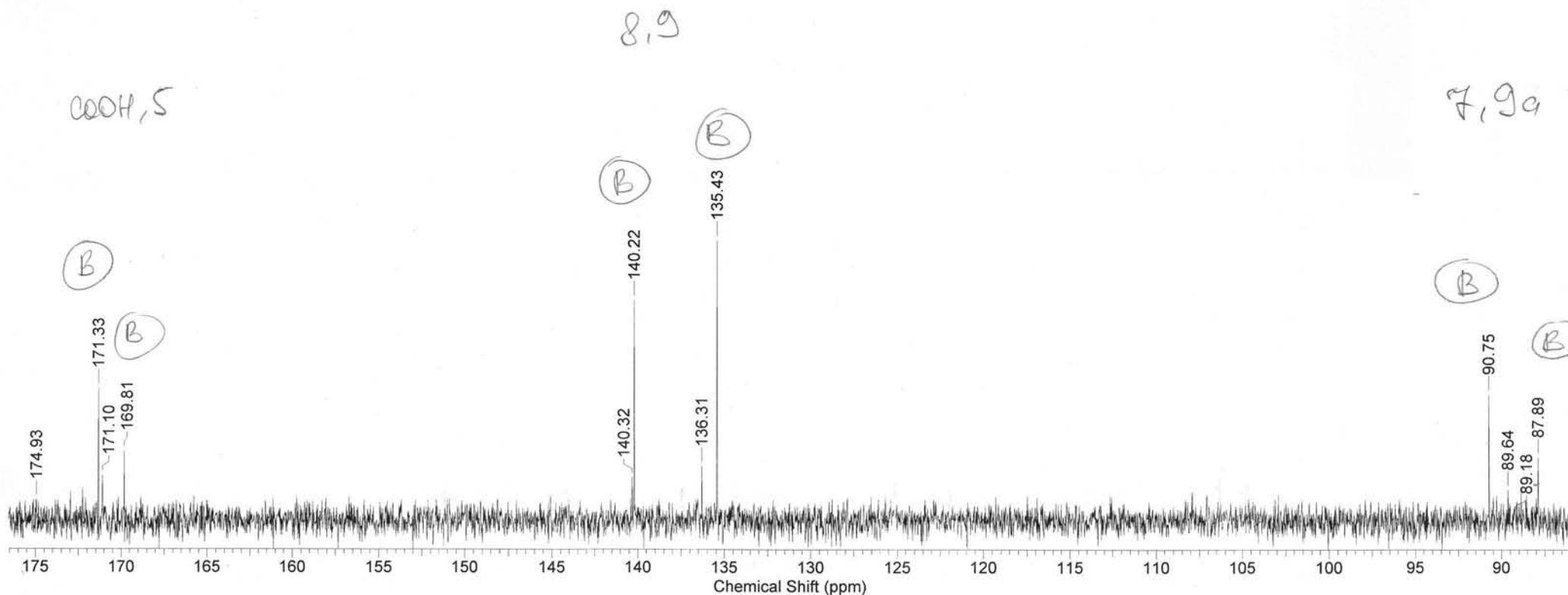
Formula	C ₁₂ H ₁₃ NO ₄ S	FW	267.3009
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	06 Jul 2012 16:17:04	
Date Stamp	06 Jul 2012 16:17:04						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-24b-c13dec\rudn-060712-24b-c13dec_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	2170	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zgpg
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6	Spectrum Offset (Hz)	10548.5127
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				

Compounds 24Ab/24Bb
after crystallization

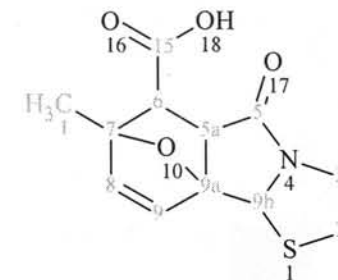


rudn-060712-24b-c13dec_001000fid

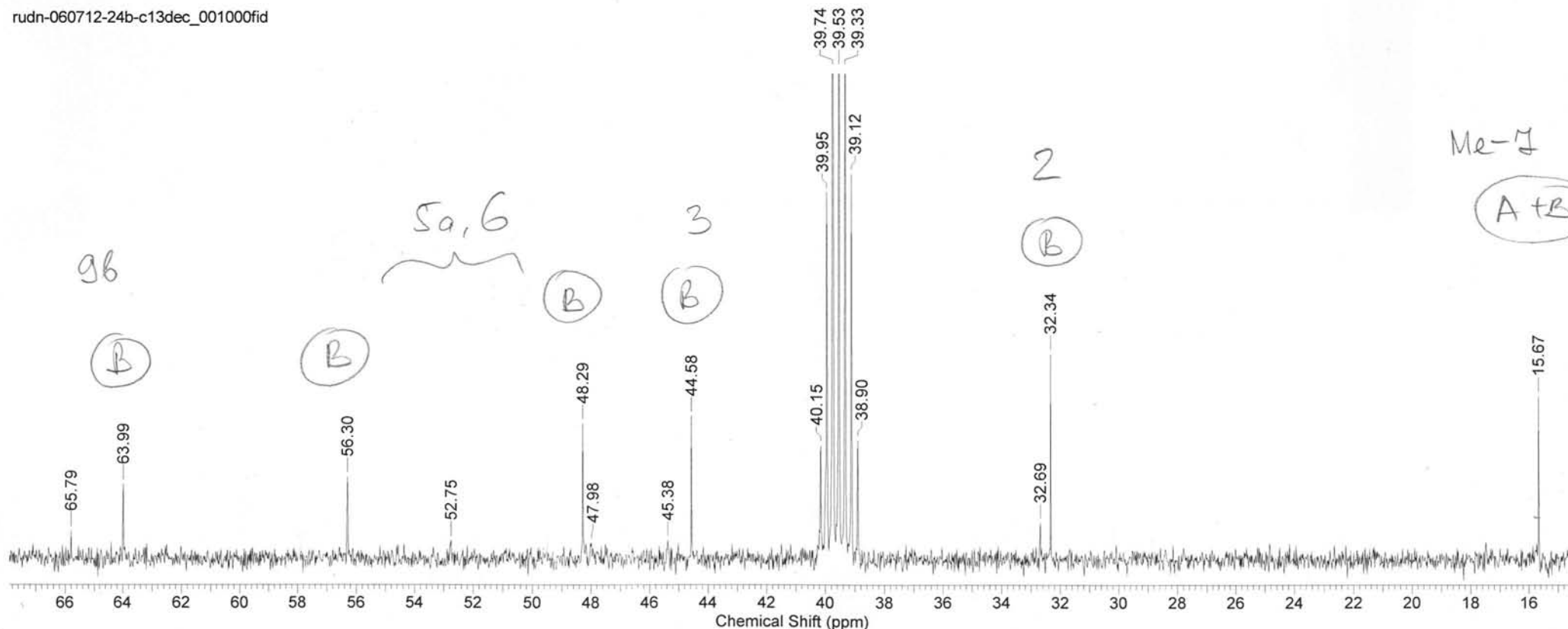


Formula C ₁₂ H ₁₃ NO ₄ S	FW 267.3009			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 06 Jul 2012 16:17:04		
Date Stamp 06 Jul 2012 16:17:04				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-24b-c13dec\rudn-060712-24b-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 2170	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10548.5127	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compounds 24Ab/24Bb
after crystallization

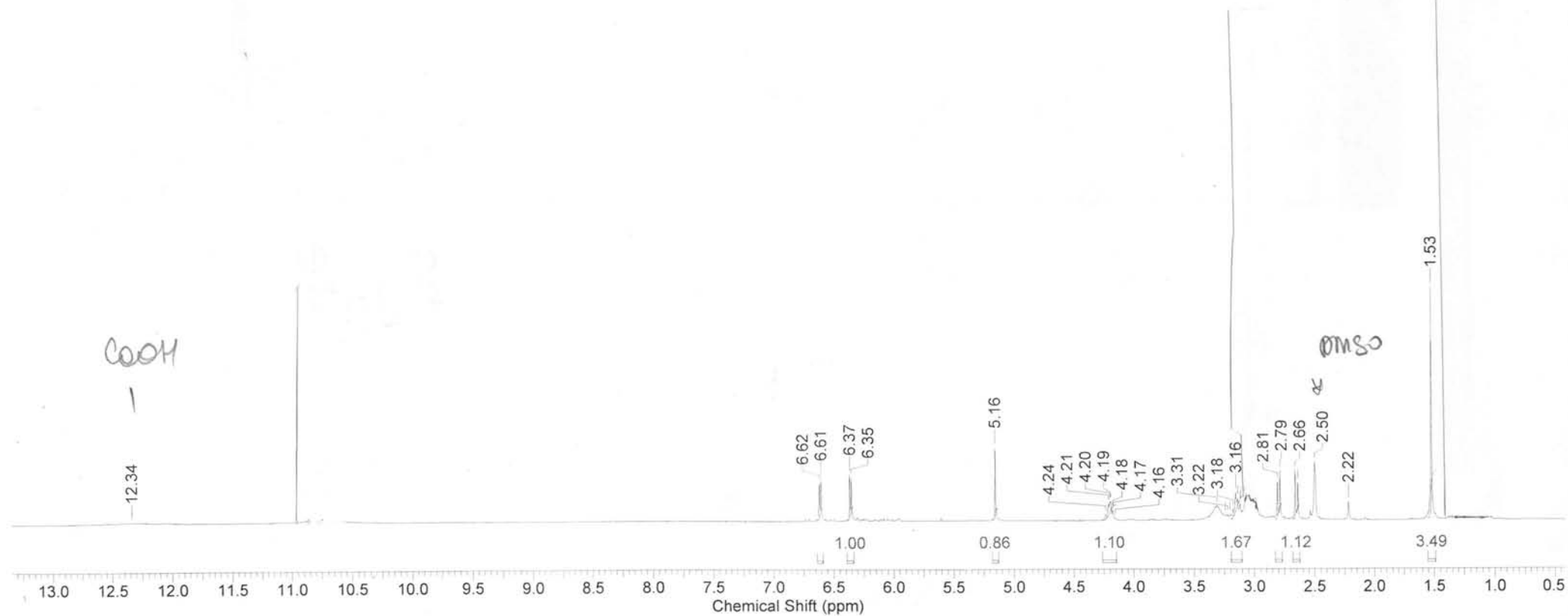
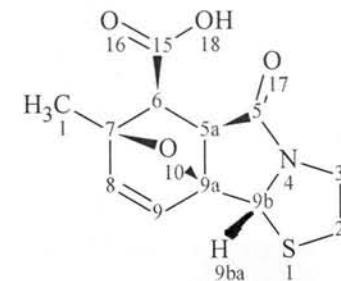


rudn-060712-24b-c13dec_001000fid



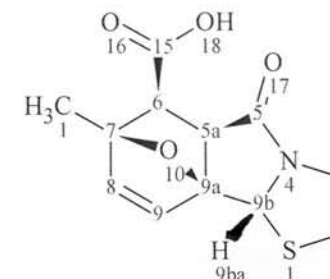
Formula	C ₁₂ H ₁₃ NO ₄ S	FW	267.3009
Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400
Date Stamp	12 Jul 2011 09:27:28		
File Name	D:\NMR\19.05.2011 C 13 Для Иры Статья в Тетраэдрон\N-3\rudn-0611-N3\rudn-0611-N3\rudn-0611-N3_001000fid		
Frequency (MHz)	400.14	Nucleus	1H
Original Points Count	16384	Owner	root
Receiver Gain	128.00	SW(cyclical) (Hz)	10416.67
Sweep Width (Hz)	10416.03	Temperature (degree C)	32.000
		Number of Transients	16
		Points Count	16384
		Origin	spect
		Pulse Sequence	zg
		Solvent	DMSO-d6
		Spectrum Offset (Hz)	2712.0542

Compound 24Ab

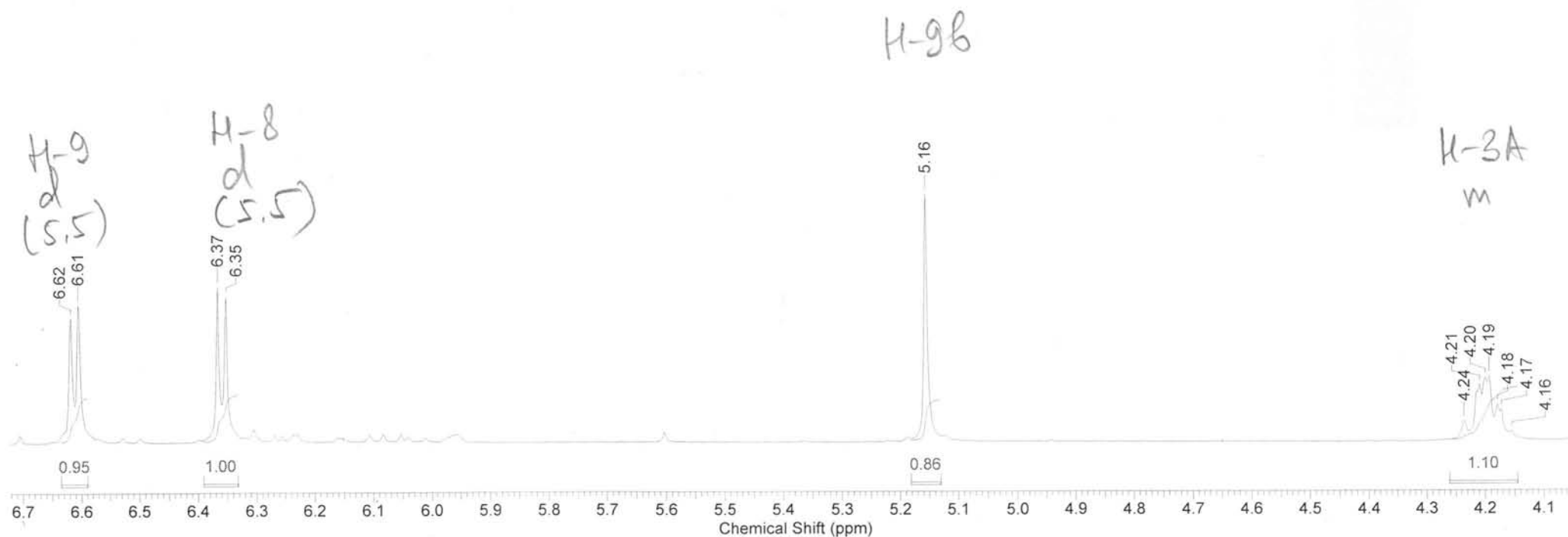


Formula	C ₁₂ H ₁₃ NO ₄ S	FW	267.3009
Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400
Date Stamp	12 Jul 2011 09:27:28	Date	12 Jul 2011 09:27:28
File Name	D:\NMR\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\N-3\rudn-0611-N3\rudn-0611-N3\rudn-0611-N3_001000fid		
Frequency (MHz)	400.14	Nucleus	1H
Original Points Count	16384	Number of Transients	16
Receiver Gain	128.00	Owner	root
Sweep Width (Hz)	10416.03	Points Count	16384
		Solvent	DMSO-d6
		Pulse Sequence	zg
		SW(cyclical) (Hz)	10416.67
		Spectrum Offset (Hz)	2712.0542
		Temperature (degree C)	32.000

Compound 24Ab

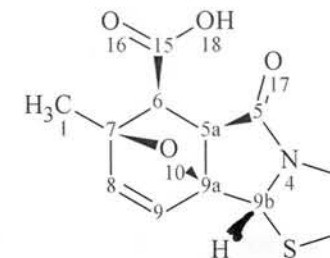


rudn-0611-N3_001000fid

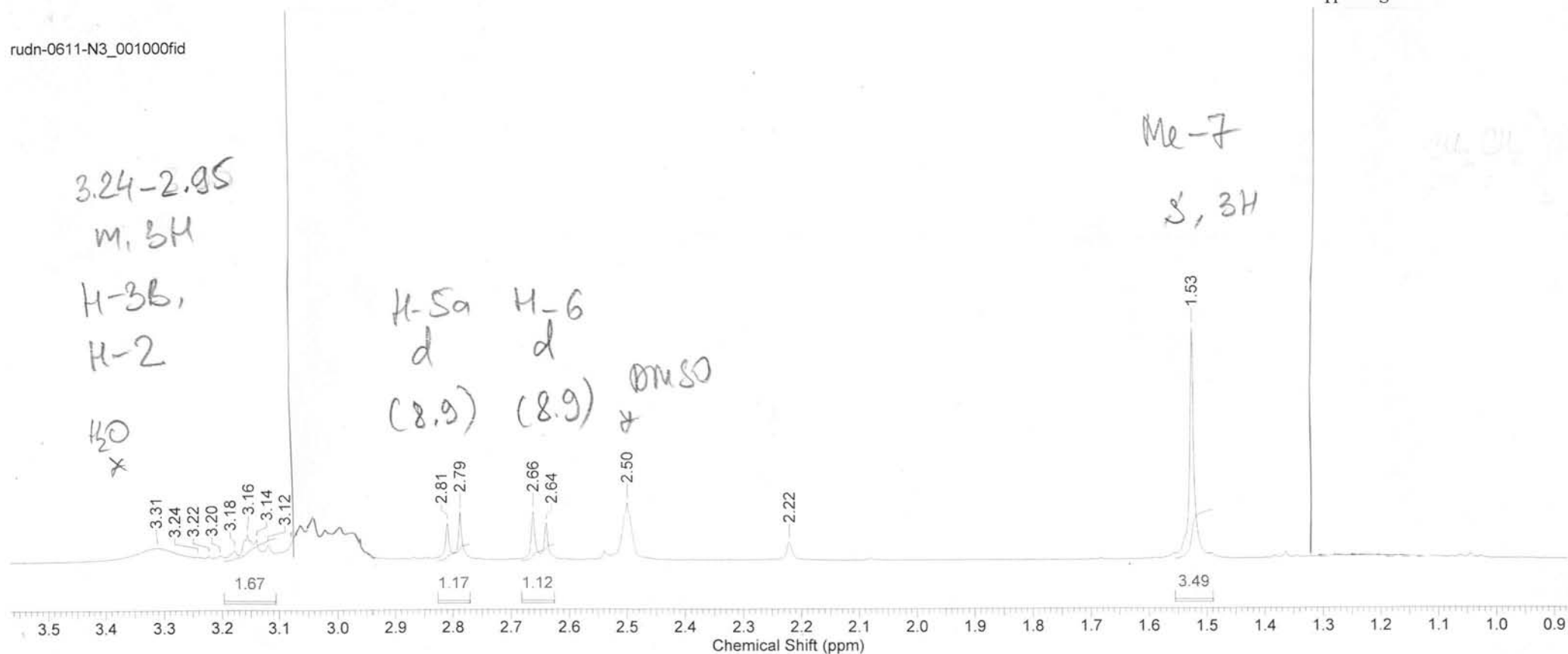


Formula	C ₁₂ H ₁₃ NO ₄ S	FW	267.3009
Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400
Date Stamp	12 Jul 2011 09:27:28	Date	12 Jul 2011 09:27:28
File Name	D:\NMR\19.05.2011 C 13 Для Иры Статья в Тетраэдрон\N-3\rudn-0611-N3\rudn-0611-N3\rudn-0611-N3_001000fid		
Frequency (MHz)	400.14	Nucleus	1H
Original Points Count	16384	Number of Transients	16
Receiver Gain	128.00	Owner	root
Sweep Width (Hz)	10416.03	Points Count	16384
		Pulse Sequence	zg
		Solvent	DMSO-d6
		Spectrum Offset (Hz)	2712.0542
		SW(cyclical) (Hz)	10416.67
		Temperature (degree C)	32.000

Compound 24Ab

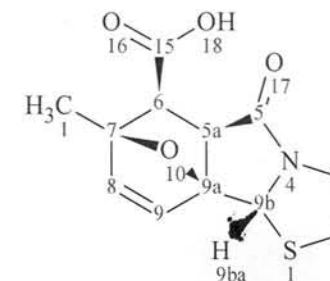


rudn-0611-N3_001000fid

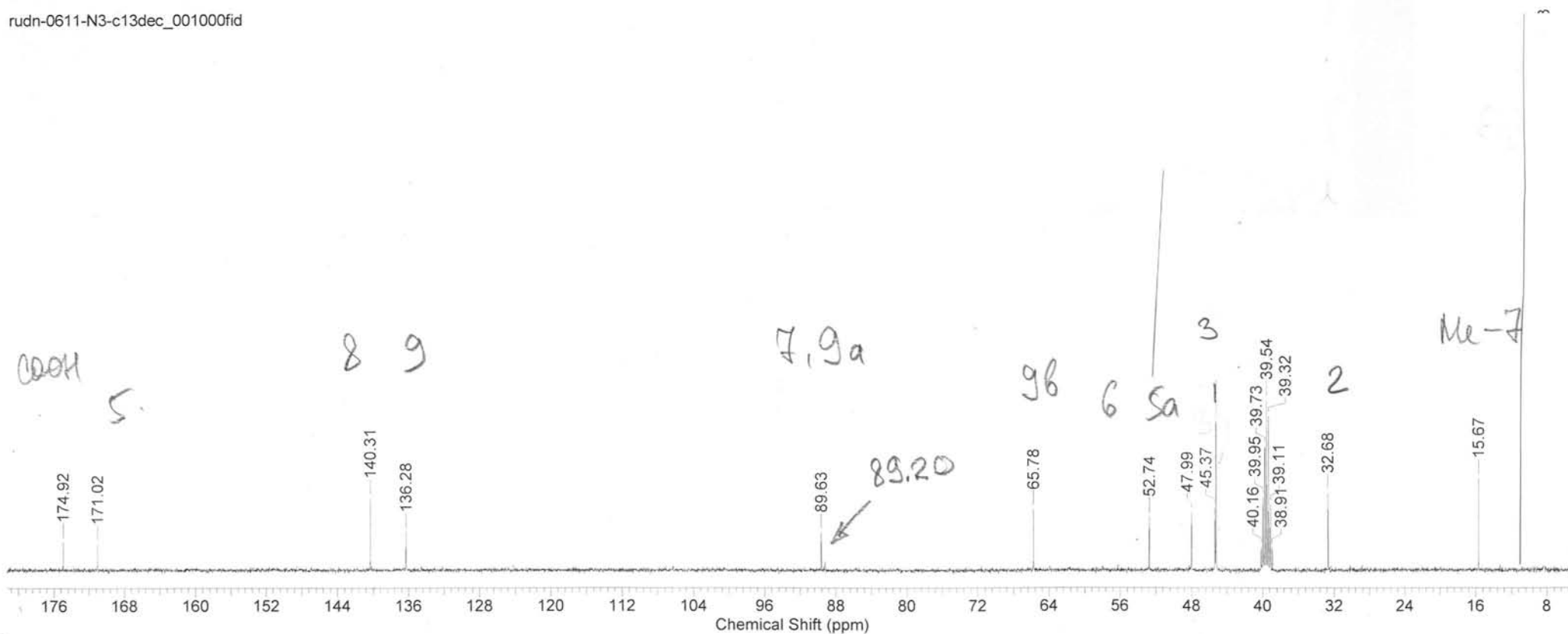


Formula	C ₁₂ H ₁₃ NO ₄ S	FW	267.3009
Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400
Date Stamp	12 Jul 2011 09:38:08	Date	12 Jul 2011 09:38:08
File Name	D:\NMR\19.05.2011 C 13 Для Иры Статья в Тетраэдрон\N-3\rudn-0611-N3-c13dec\rudn-0611-N3-c13dec\rudn-0611-N3-c13dec_001000fid		
Frequency (MHz)	100.62	Nucleus	13C
Original Points Count	16384	Number of Transients	2000
Receiver Gain	32768.00	Origin	spect
Sweep Width (Hz)	29409.97	Owner	root
		Points Count	16384
		Pulse Sequence	zgpg
		Solvent	DMSO-d6
		Spectrum Offset (Hz)	10547.6182
		Temperature (degree C)	27.000

Compound 24Ab



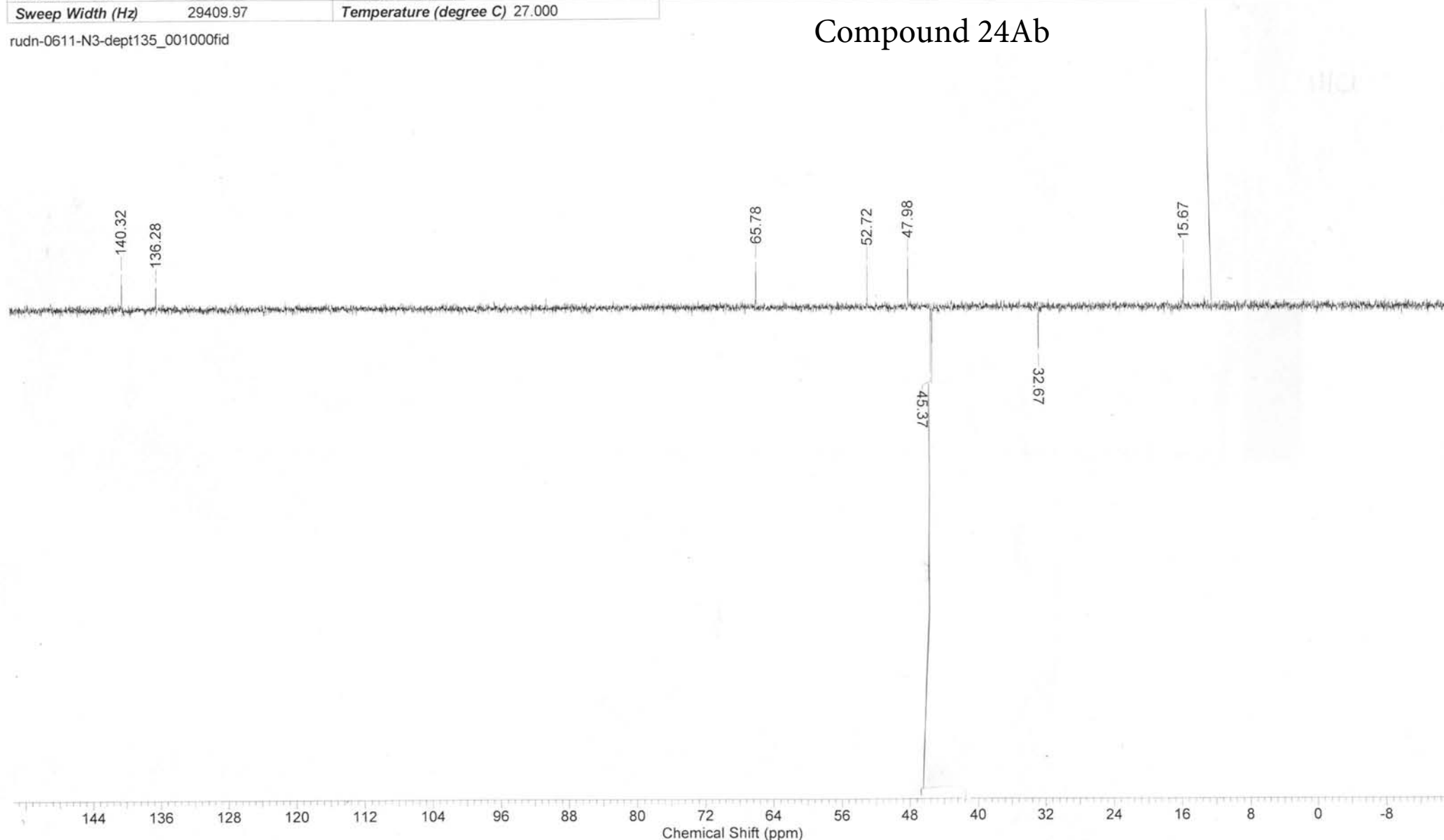
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	12 Jul 2011 10:46:24	
Date Stamp	12 Jul 2011 10:46:24	File Name	D:\NMR\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\N-3\rudn-0611-N3-dept135\rudn-0611-N3-dept135\rudn-0611-N3-dept135_001000fid				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	2000	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	dept135
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6	Spectrum Offset (Hz)	9097.1982
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				

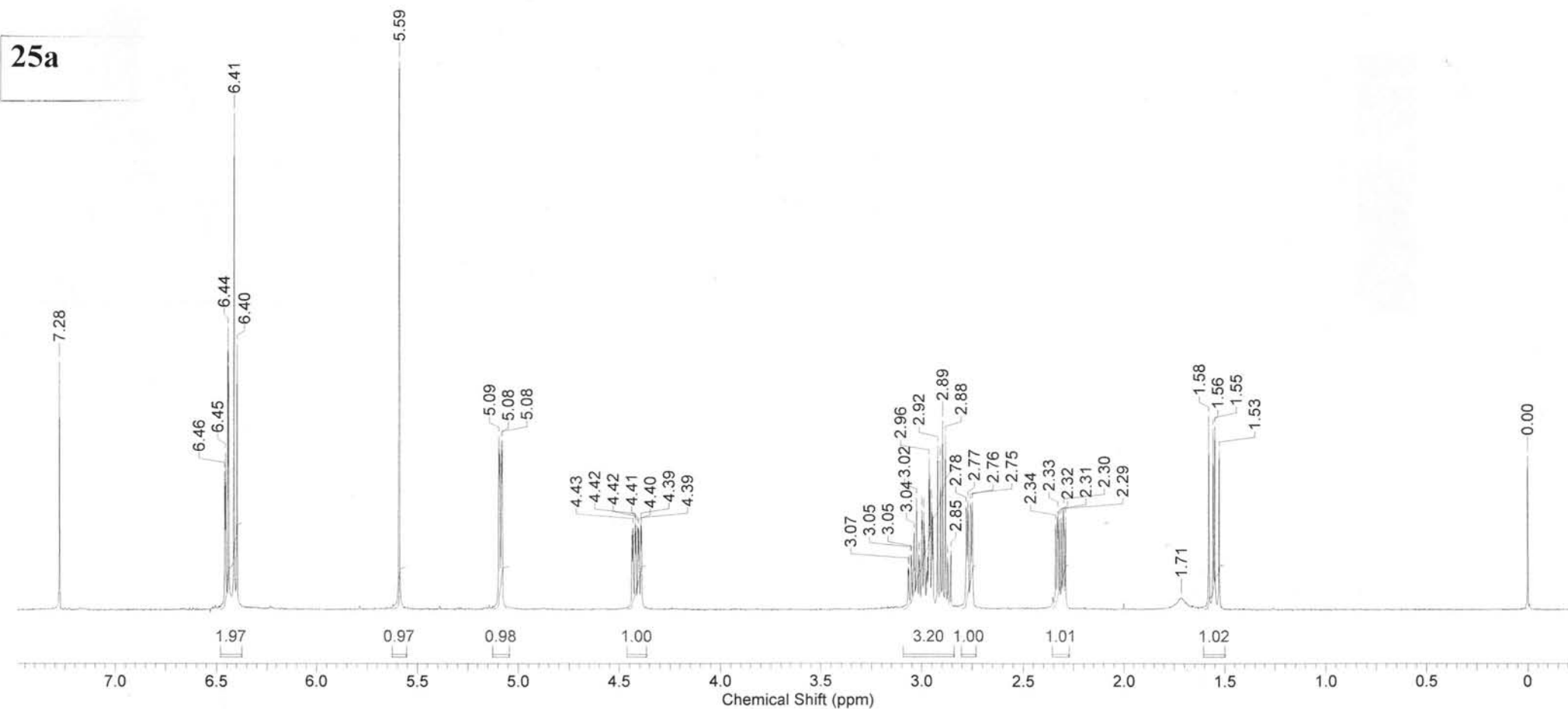
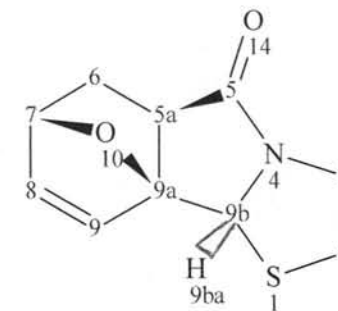
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Compound 24Ab



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File Name	D:\Тимур\Тимур (лето 2009)\rudn8\rudn8_001000fid	Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	4
Original Points Count	16384	Points Count	16384	Pulse Sequence	zg	Solvent	CHLOROFORM-D
Sweep Width (Hz)	10204.08	Temperature (degree C)	27.000				

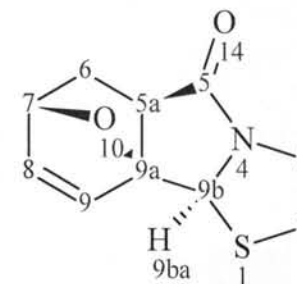
Compound 25a



Formula C₁₀H₁₁NO₂S FW 209.2648

Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	15 Jul 2009 12:50:08	
Date Stamp	15 Jul 2009 12:50:08	File Name	D:\NMR\C_13\Тимур (лето 2009)\rudn8\rudn8_001000fid				
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	4	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zg
Receiver Gain	512.00	SW(cyclical) (Hz)	10204.08	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2612.4158	Sweep Width (Hz)	10203.46	Temperature (degree C)	27.000		

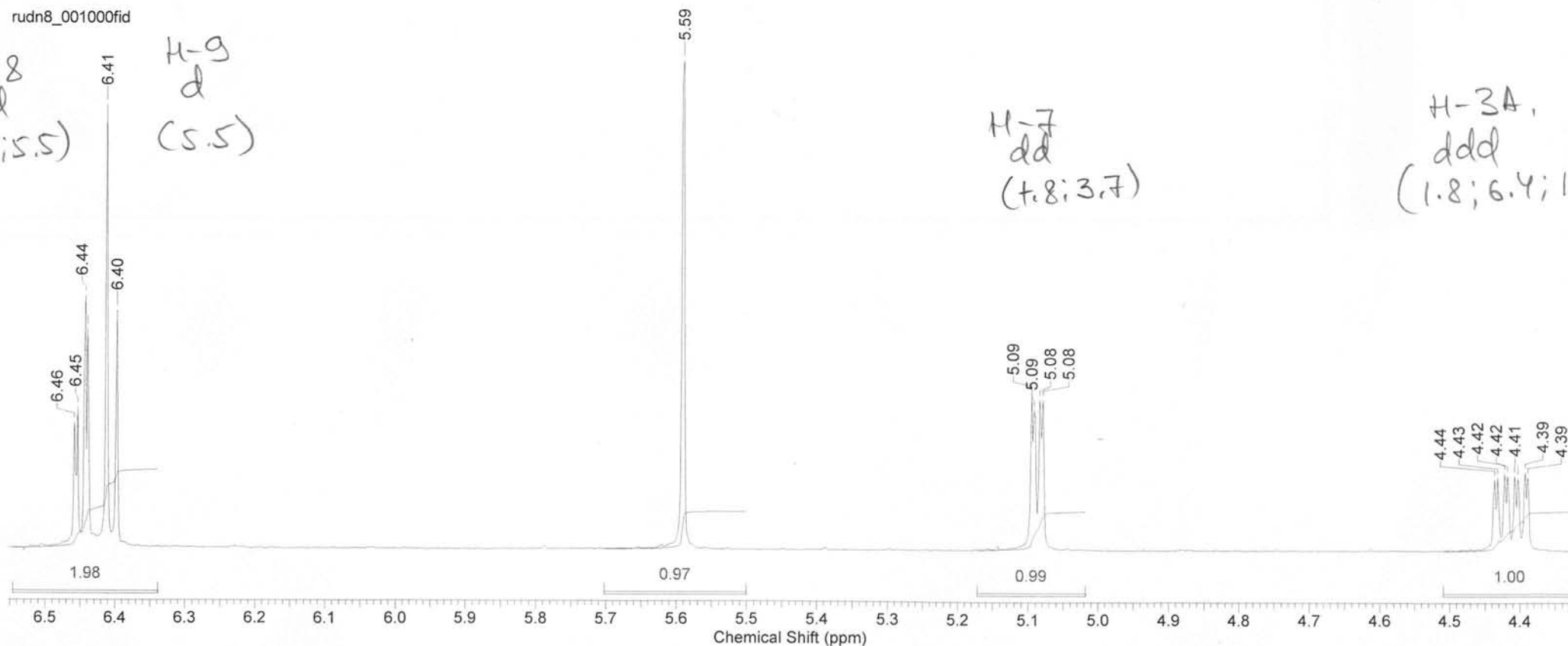
Compound 25a



H-9b

s

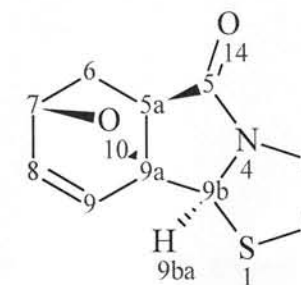
rudn8_001000fid

H-8
dd
(1.8;5.5)H-9
d
(5.5)H-7
dd
(4.8;3.7)H-3A,
ddd
(1.8;6.4;11.9)

Formula C₁₀H₁₁NO₂S FW 209.2648

Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	15 Jul 2009 12:50:08	
Date Stamp	15 Jul 2009 12:50:08	File Name	D:\NMR\C_13\Тимур (лето 2009)\rudn8\rudn8_001000fid				
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	4	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zg
Receiver Gain	512.00	SW(cyclical) (Hz)	10204.08	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2612.4158	Sweep Width (Hz)	10203.46	Temperature (degree C)	27.000		

Compound 25a



H-2A
ddd
(1.8; 6.4; 11.0)

rudn8_001000fid

H-2B
(6.4; 11.0)

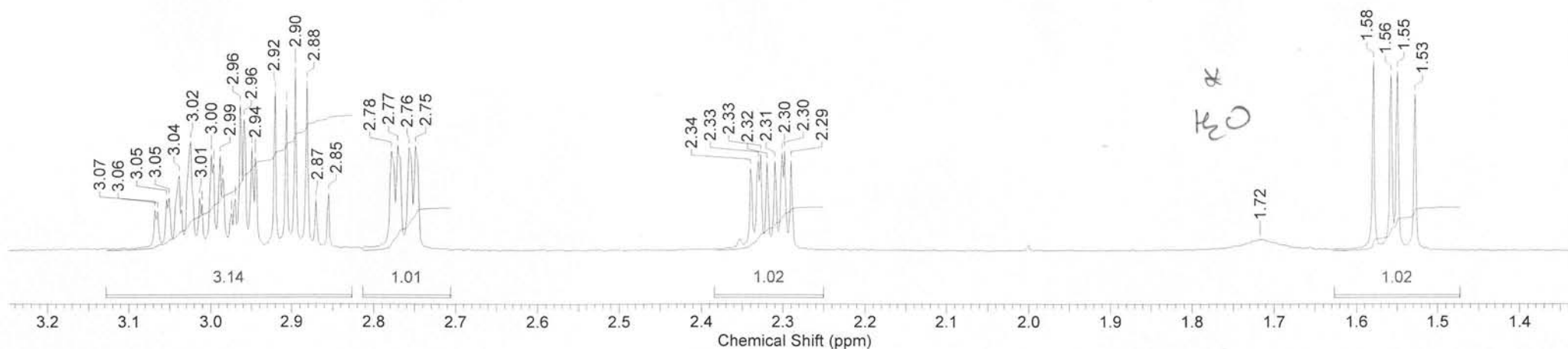
dt

H-3B
m

H-5a endo
bz dd
(3.7; 8.3)

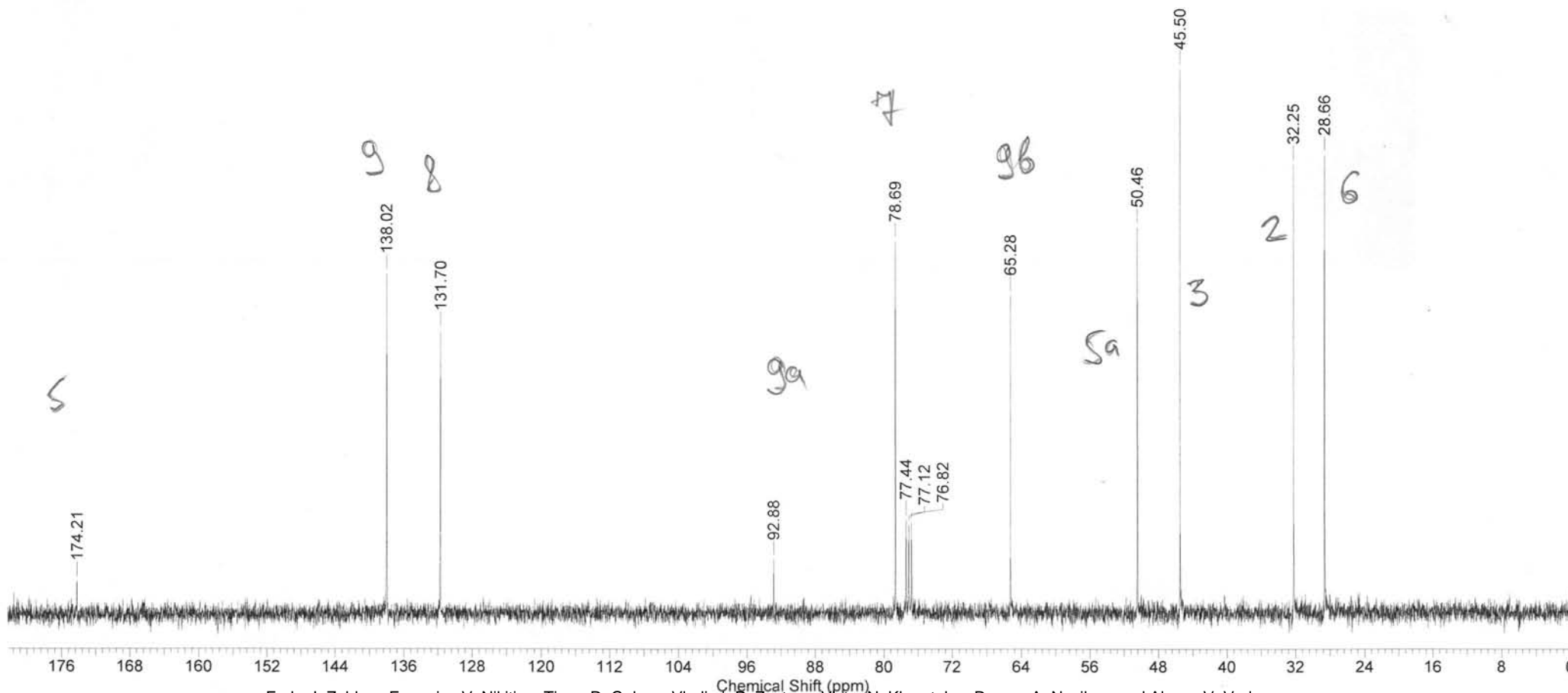
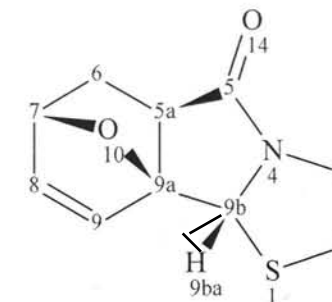
H-6 exo
ddd
(3.7; 5.0; 11.9)

H-6 endo
dd
(8.3; 11.9)



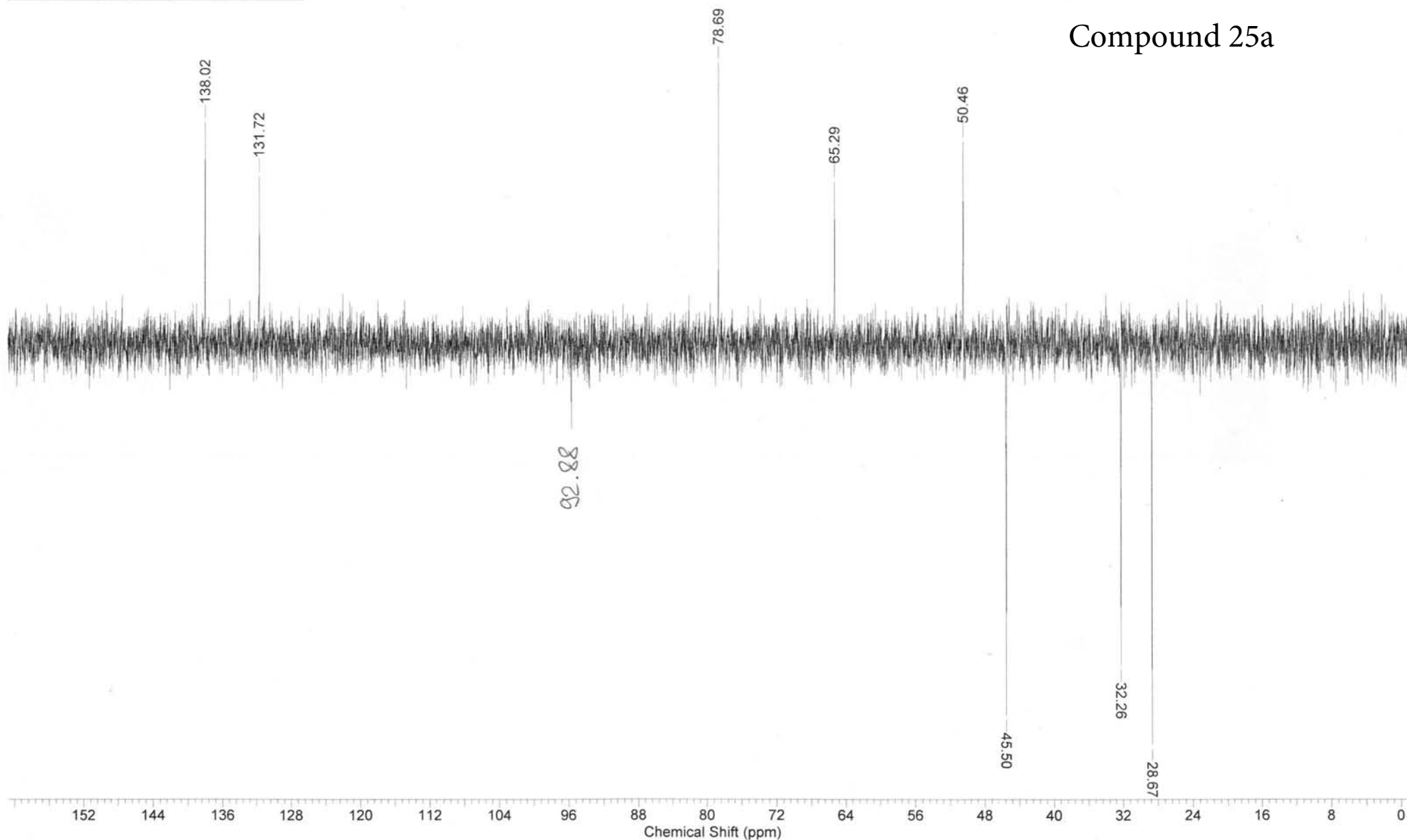
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File Name	D:\Тимур\Тимур (лето 2009)\rudn8c13dec\rudn8c13dec_001000fid			Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	282	Original Points Count	16384	
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D		Points Count	16384
Temperature (degree C)	27.000				Sweep Width (Hz)	26315.79

Compound 25a



Acquisition Time (sec)	0.6226	Comment	Imported from UXMNR.		Date	15 Jul 2009 15:10:56	
File Name	D:\Timur\Тимур (лето 2009)\rudn8dept135\rudn8dept135_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	96	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	CHLOROFORM-D		Sweep Width (Hz)	26315.79	
Temperature (degree C)	27.000						

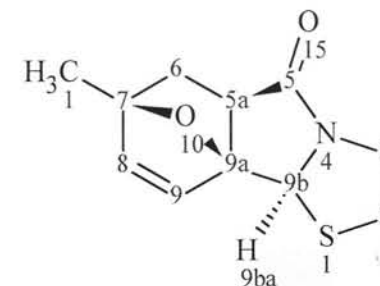
Compound 25a



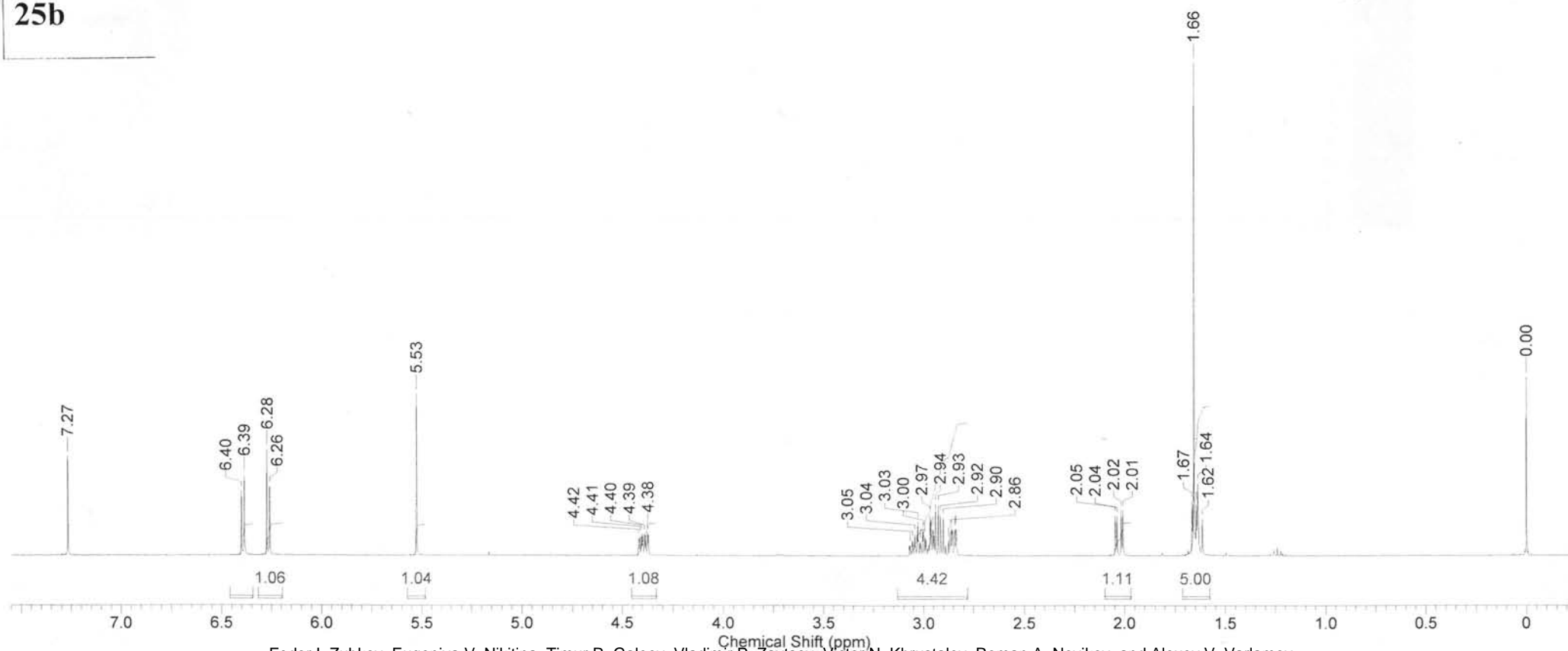
Formula C₁₁H₁₃NO₂S FW 223.2914

Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	07 Apr 2010 16:51:12
Date Stamp	07 Apr 2010 16:51:12	File Name	D:\NMR\IC_13\07.04.10 (В основном аддукты с DMAD на пиперидонах)\N848\N848_001000fid		
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	12
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	1024.00	SW(cyclical) (Hz)	10204.08	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2608.9912	Sweep Width (Hz)	10203.46	Temperature (degree C)	27.000
				Origin	spect
				Pulse Sequence	zg

Compound 25b



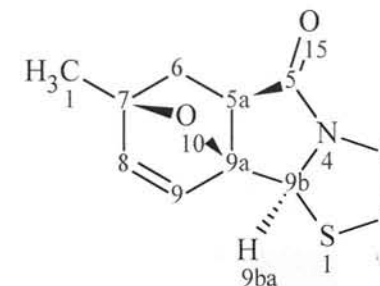
25b



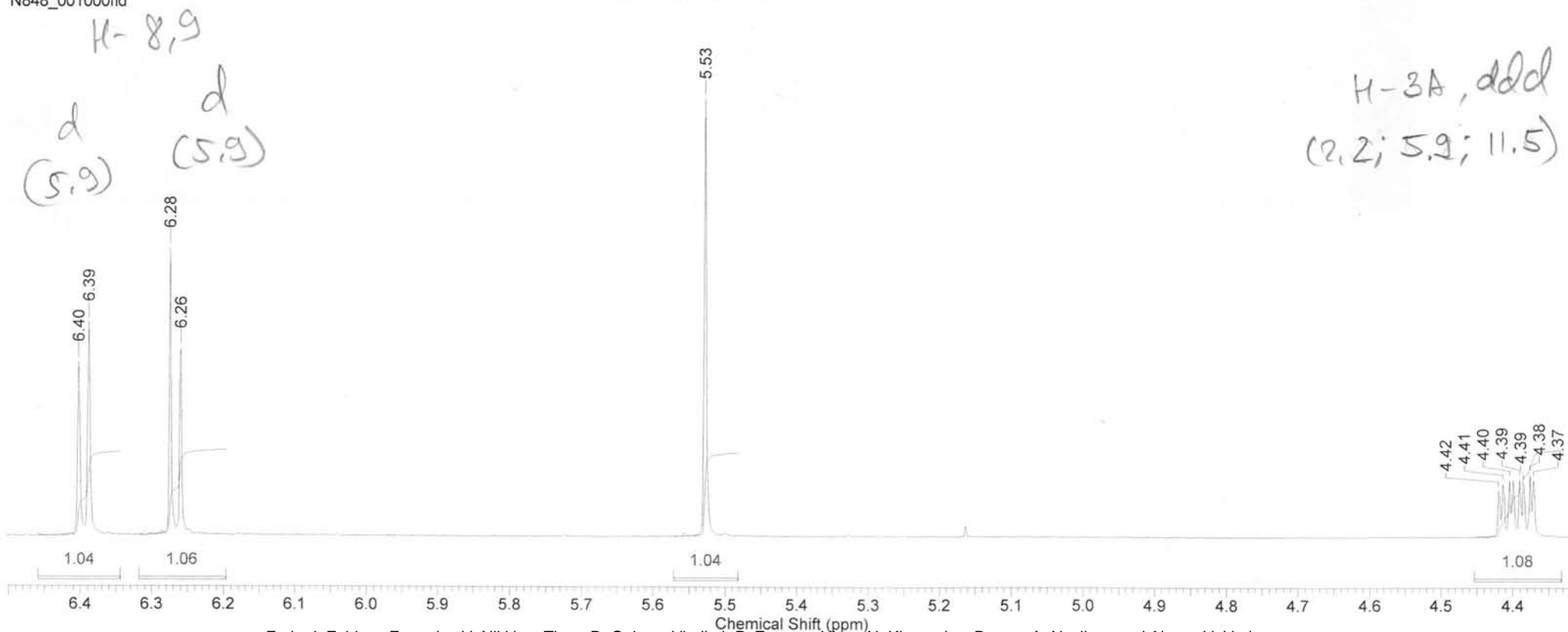
Formula C₁₁H₁₃NO₂S FW 223.2914

Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	07 Apr 2010 16:51:12
Date Stamp	07 Apr 2010 16:51:12	File Name	D:\NMR\IC_13\07.04.10 (В основном аддукты с DMAD на пиперидонах)\N848\N848_001000fid		
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	12
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	1024.00	SW(cyclical) (Hz)	10204.08	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2608.9912	Sweep Width (Hz)	10203.46	Temperature (degree C)	27.000
				Origin	spect
				Pulse Sequence	zg

Compound 25b



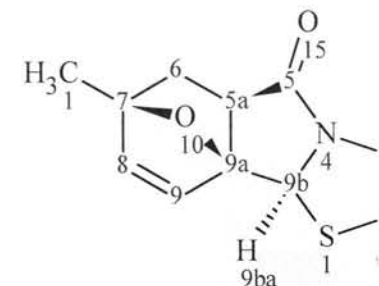
N848_001000fid



Formula C₁₁H₁₃NO₂S FW 223.2914

Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	07 Apr 2010 16:51:12	
Date Stamp	07 Apr 2010 16:51:12	File Name	D:\NMR\C_13\07.04.10 (В основном аддукты с DMAD на пиперидонах)\N848\N848_001000fid				
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	12	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zg
Receiver Gain	1024.00	SW(cyclical) (Hz)	10204.08	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2608.9912	Sweep Width (Hz)	10203.46	Temperature (degree C)	27.000		

Compound 25b



N848_001000fid

H-5a
2.86, ddd
(1.2; 3.3; 8.7)

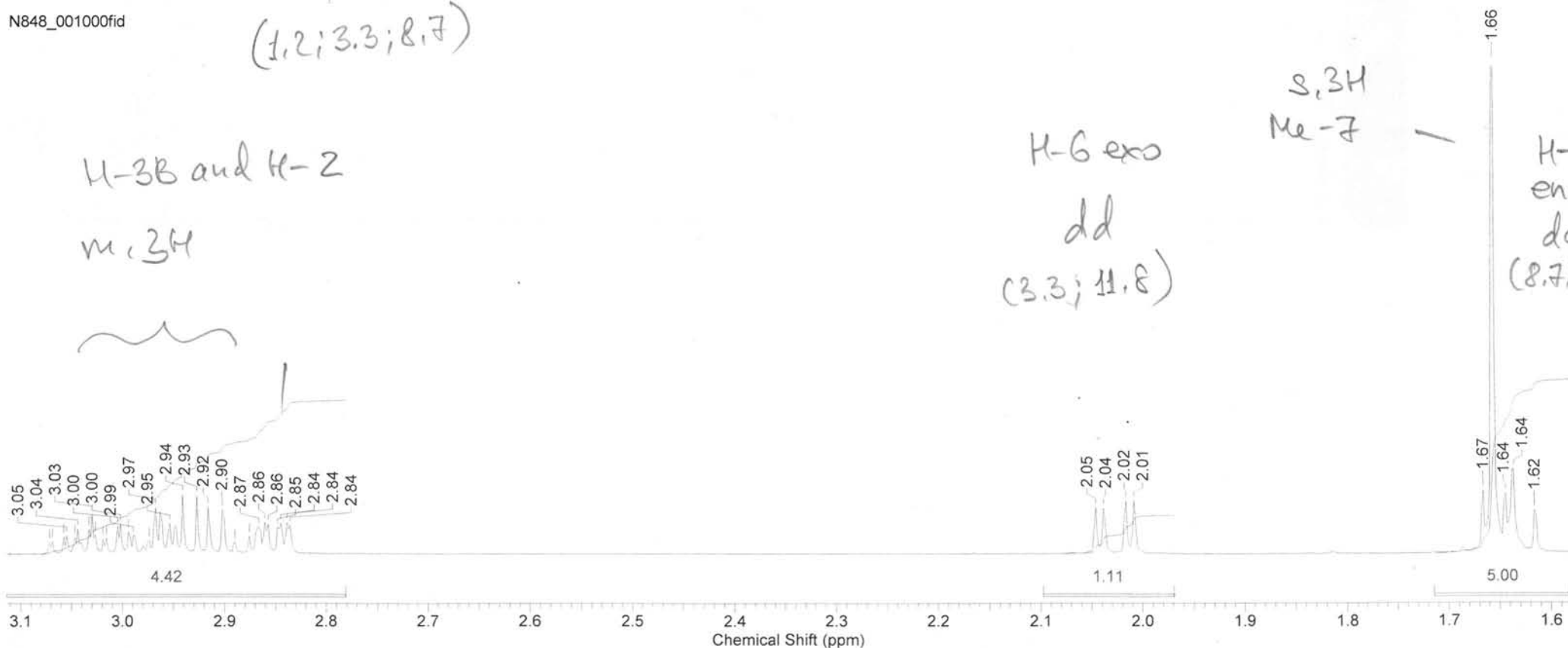
H-3B and H-2

m, 3H

H-6 exo
dd
(3.3; 11.8)

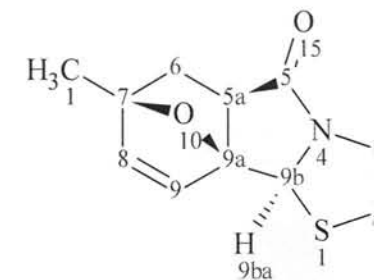
s, 3H
Me-7

H-6 endo
dd
(8.7; 11.8)

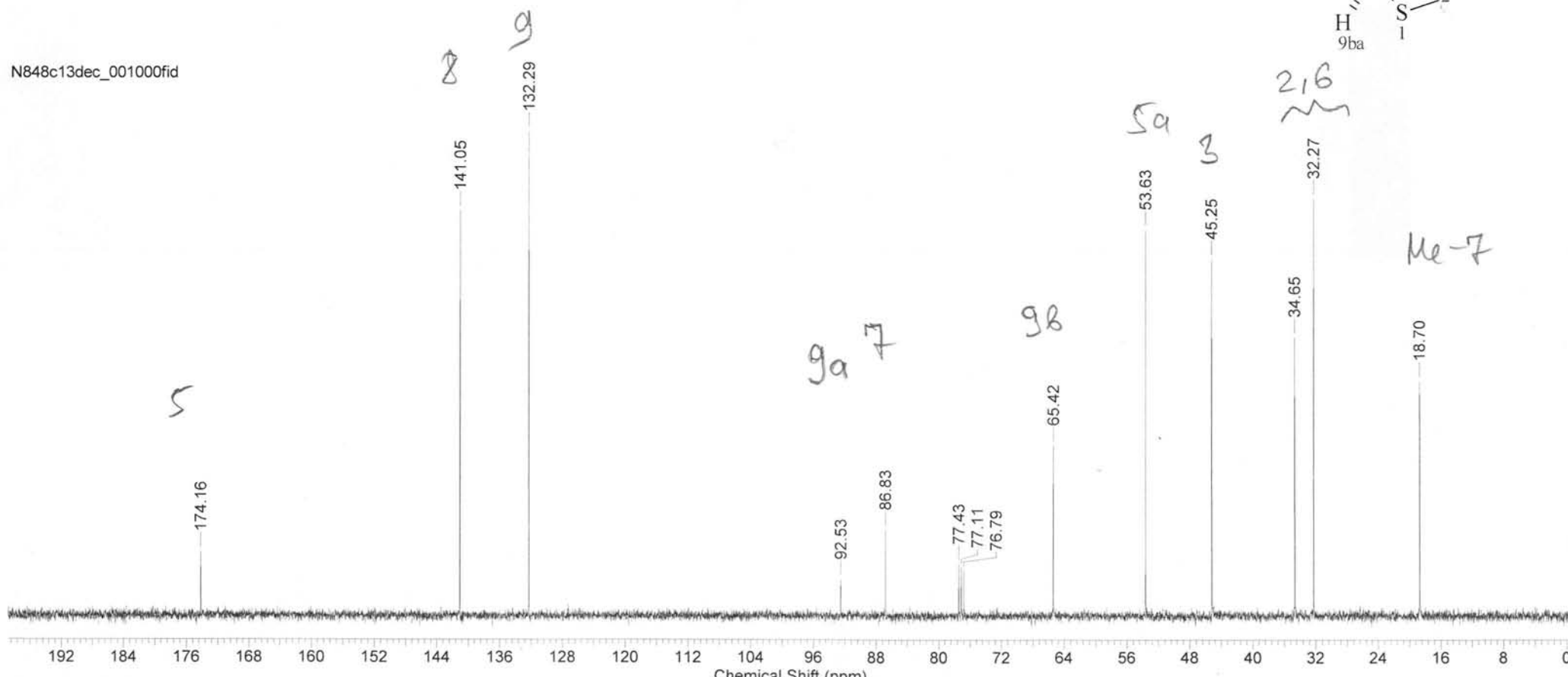


Formula	C ₁₁ H ₁₃ NO ₂ S	FW	223.2914				
Acquisition Time (sec)	0.6226	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400				
Date Stamp	07 Apr 2010 17:44:32	Date	07 Apr 2010 17:44:32				
File Name	D:\NMR\13\07.04.10 (В основном аддукты с DMAD на пиперидонах)\N848c13dec\N848c13dec_001000fid		Frequency (MHz)	100.62			
Nucleus	13C	Number of Transients	128	Origin	spect	Original Points Count	16384
Owner	root	Points Count	16384	Pulse Sequence	zgpg	Receiver Gain	32768.00
SW(cyclical) (Hz)	26315.79	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9619.4717	Sweep Width (Hz)	26314.18
Temperature (degree C)	27.000						

Compound 25b

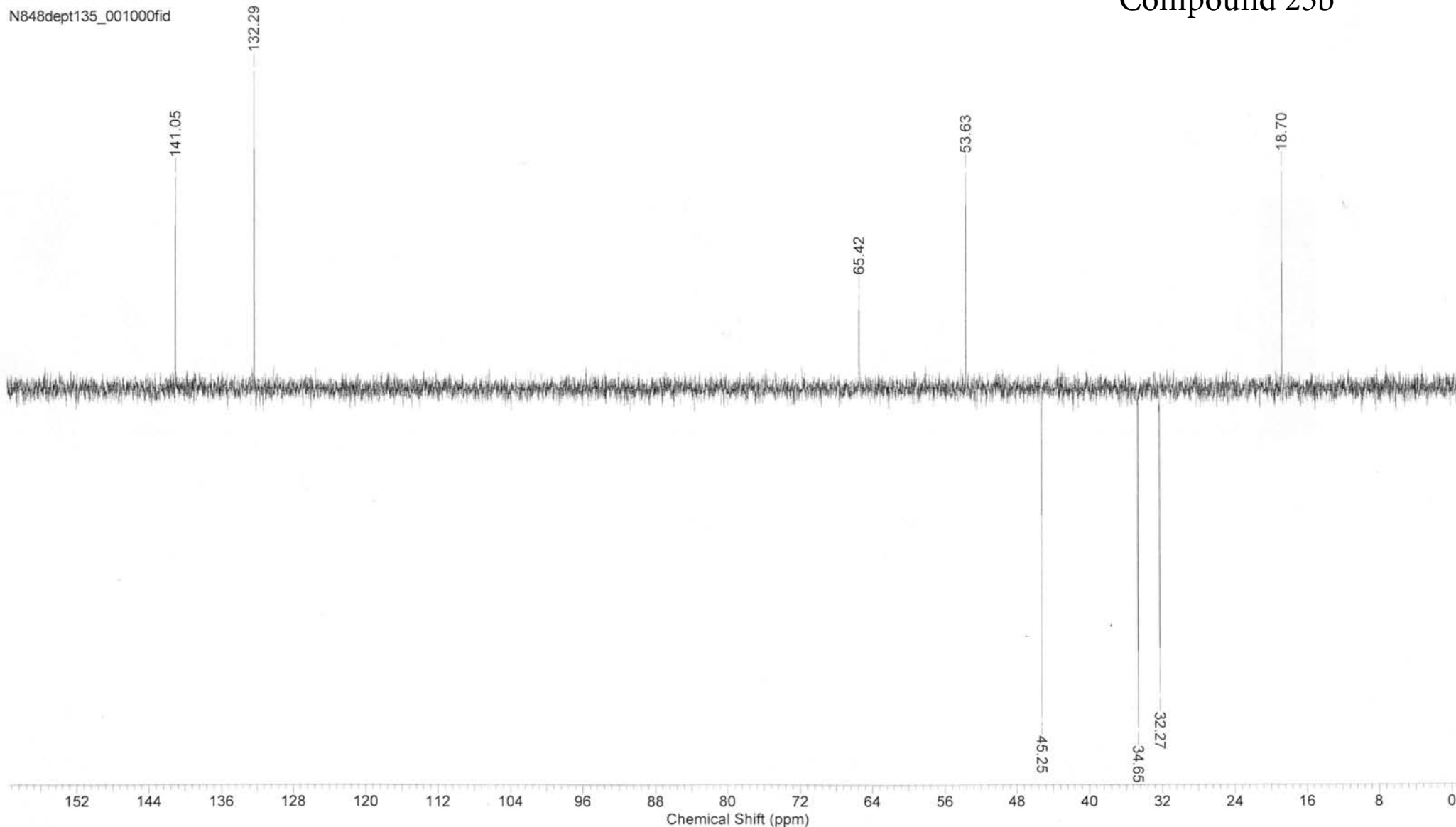


N848c13dec_001000fid



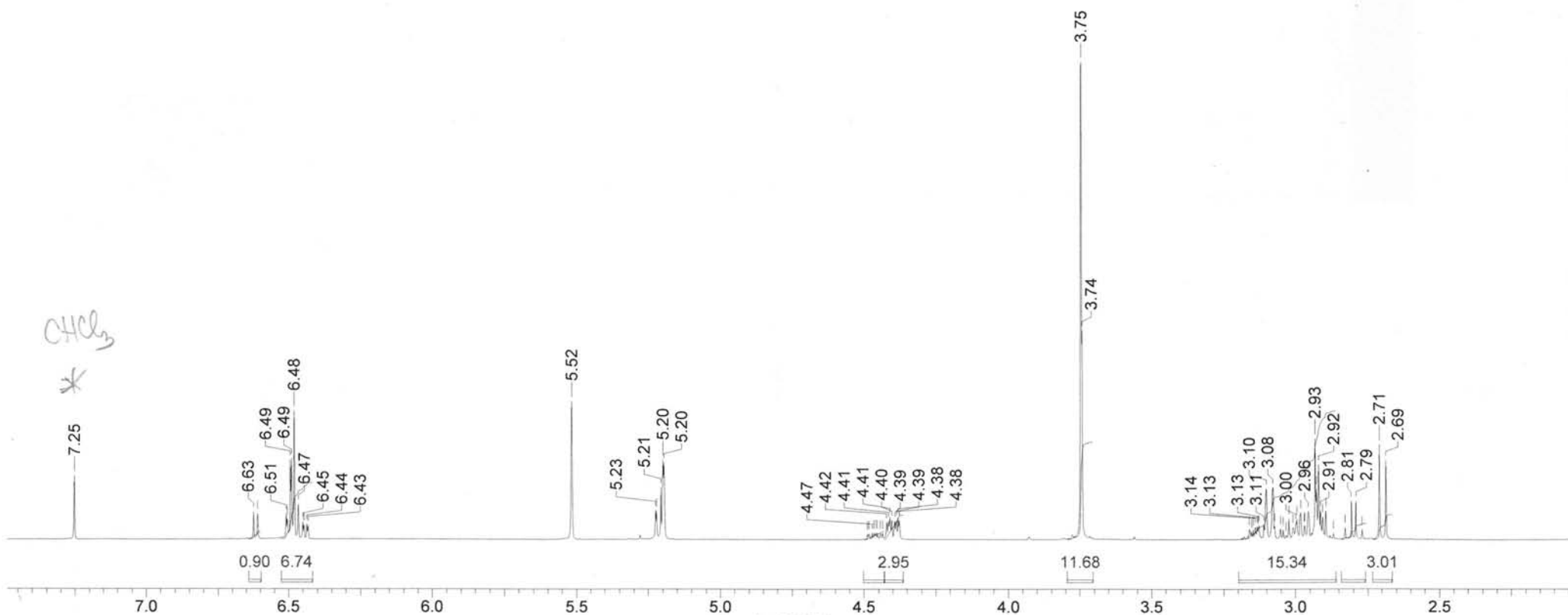
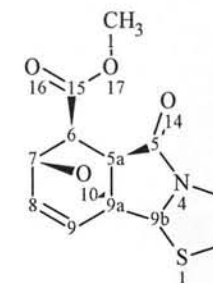
Acquisition Time (sec)	0.6226	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	07 Apr 2010 17:48:48	
Date Stamp	07 Apr 2010 17:48:48						
File Name	D:\NMR\13\07.04.10 (В основном аддукты с DMAD на пиперидонах)\N848dept135\N848dept135_001000fid			Frequency (MHz)	100.62		
Nucleus	13C	Number of Transients	74	Origin	spect	Original Points Count	16384
Owner	root	Points Count	16384	Pulse Sequence	dept135	Receiver Gain	32768.00
SW(cyclical) (Hz)	26315.79	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9619.4814	Sweep Width (Hz)	26314.18
Temperature (degree C)	27.000						

Compound 25b



Formula C ₁₂ H ₁₃ NO ₄ S	FW 267.3009			
Acquisition Time (sec) 1.6056	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 06 Jul 2012 15:17:20		
Date Stamp 06 Jul 2012 15:17:20				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-26a\rudn-060712-26a_001000fid	Frequency (MHz) 400.14			
Nucleus 1H	Number of Transients 18	Origin spect	Original Points Count 16384	
Owner root	Points Count 16384	Pulse Sequence zg	Receiver Gain 512.00	
SW(cyclical) (Hz) 10204.08	Solvent CHLOROFORM-d	Spectrum Offset (Hz) 2602.0486	Sweep Width (Hz) 10203.46	
Temperature (degree C) 27.000				

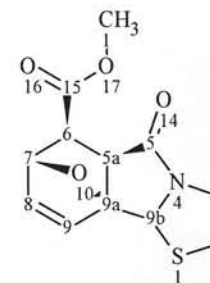
Compounds 26Aa/26Ba
25/75
after crystallization



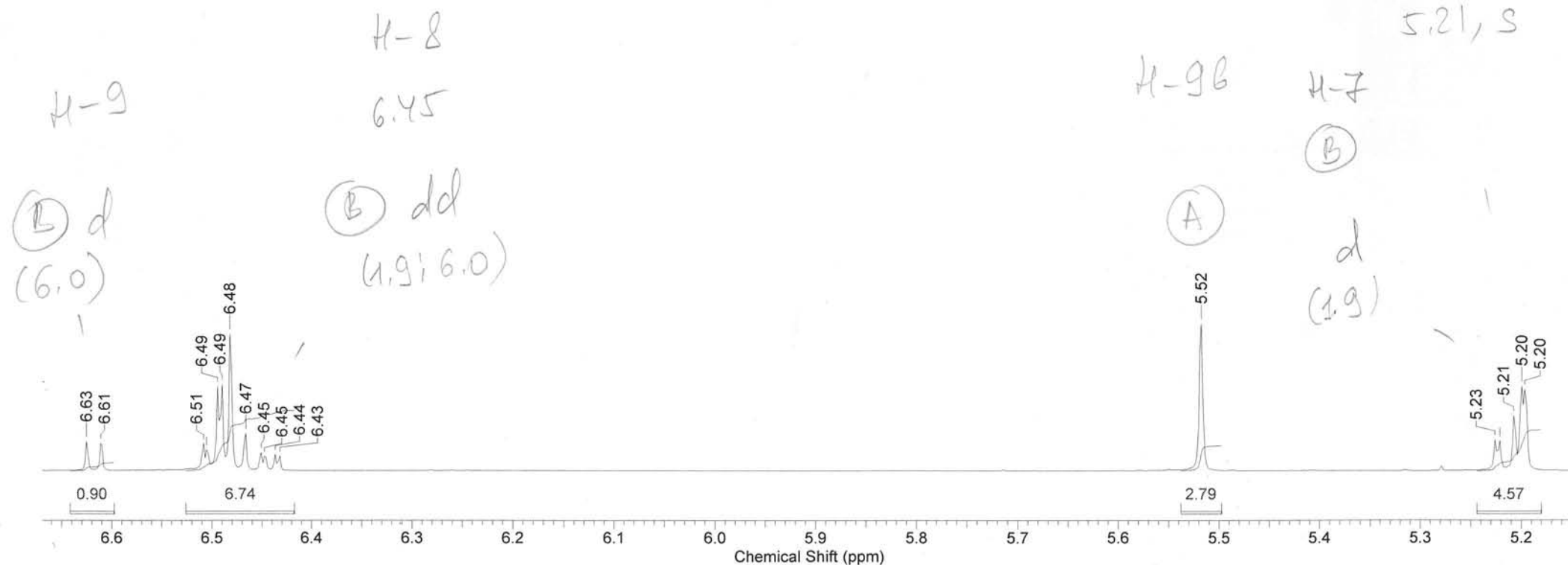
Formula	C ₁₂ H ₁₃ NO ₄ S	FW	267.3009
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Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	06 Jul 2012 15:17:20
Date Stamp	06 Jul 2012 15:17:20				
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-26a\rudn-060712-26a_001000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	18	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zg
SW(cyclical) (Hz)	10204.08	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2602.0486
Temperature (degree C)	27.000			Sweep Width (Hz)	10203.46

Compounds 26Aa/26Ba
after crystallization

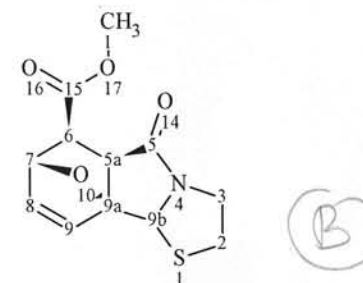


rudn-060712-26a_001000fid

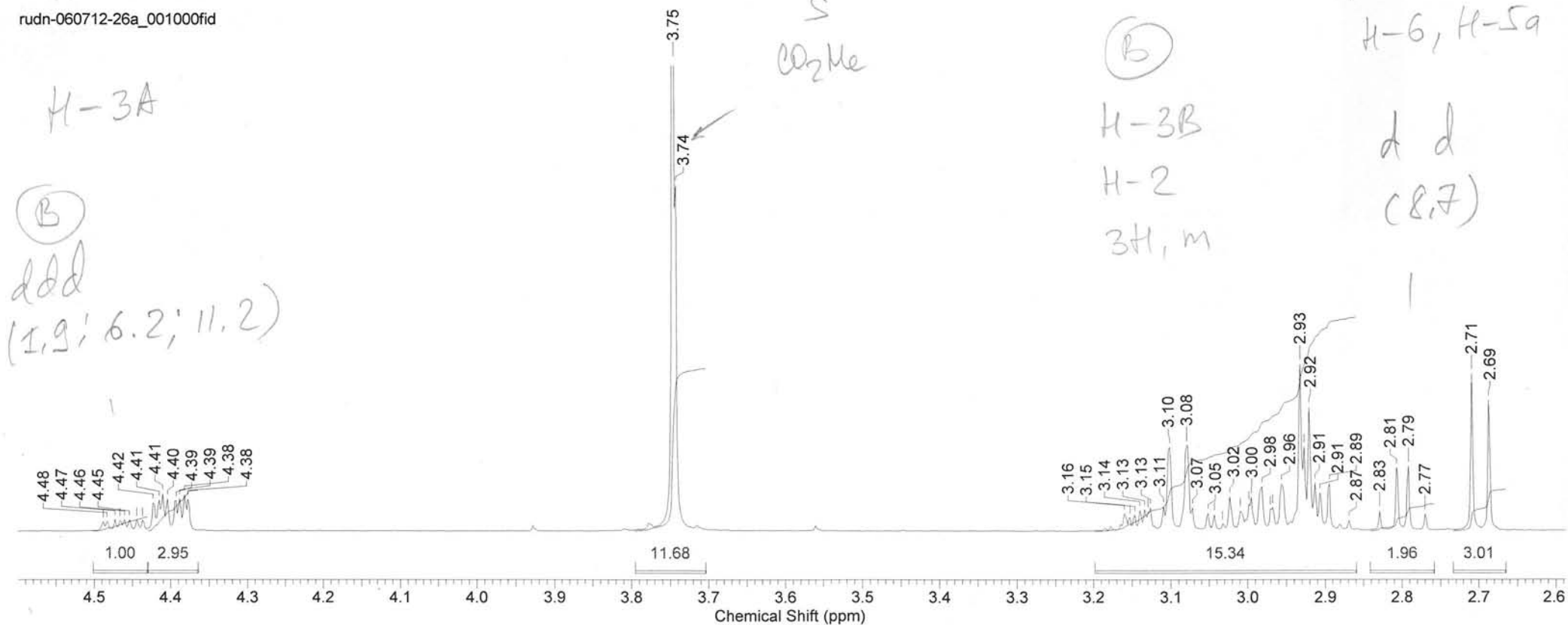


Formula C ₁₂ H ₁₃ NO ₄ S	FW 267.3009			
Acquisition Time (sec) 1.6056	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 06 Jul 2012 15:17:20		
Date Stamp 06 Jul 2012 15:17:20				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-26a\rudn-060712-26a_001000fid	Frequency (MHz) 400.14			
Nucleus 1H	Number of Transients 18	Origin spect	Original Points Count 16384	
Owner root	Points Count 16384	Pulse Sequence zg	Receiver Gain 512.00	
SW(cyclical) (Hz) 10204.08	Solvent CHLOROFORM-d	Spectrum Offset (Hz) 2602.0486	Sweep Width (Hz) 10203.46	
Temperature (degree C) 27.000				

Compounds 26Aa/26Ba
after crystallization



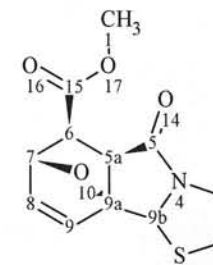
rudn-060712-26a_001000fid



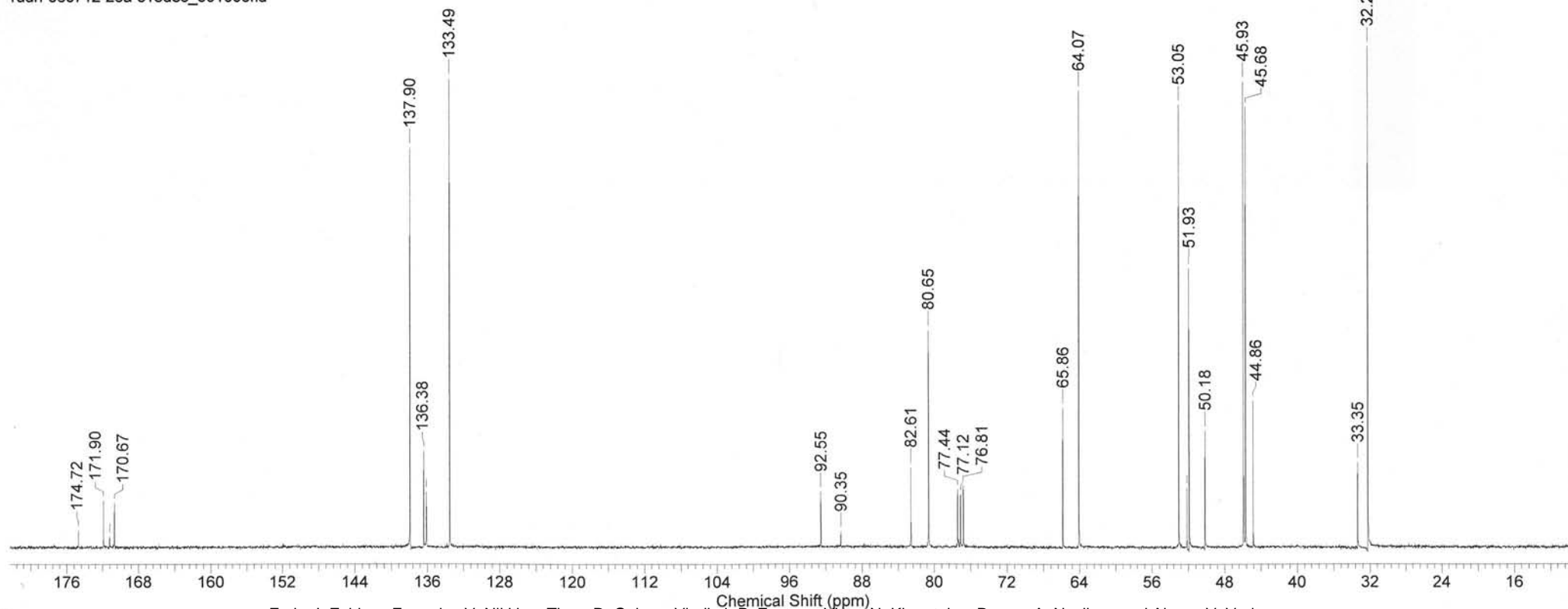
Formula	C ₁₂ H ₁₃ NO ₄ S	FW	267.3009
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	06 Jul 2012 15:21:36	
Date Stamp	06 Jul 2012 15:21:36						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-26a-c13dec\rudn-060712-26a-c13dec_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	1724	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zgpg
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9618.5391
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				

Compounds 26Aa/26Ba
after crystallization



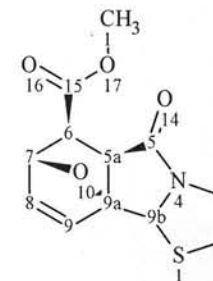
rudn-060712-26a-c13dec_001000fid



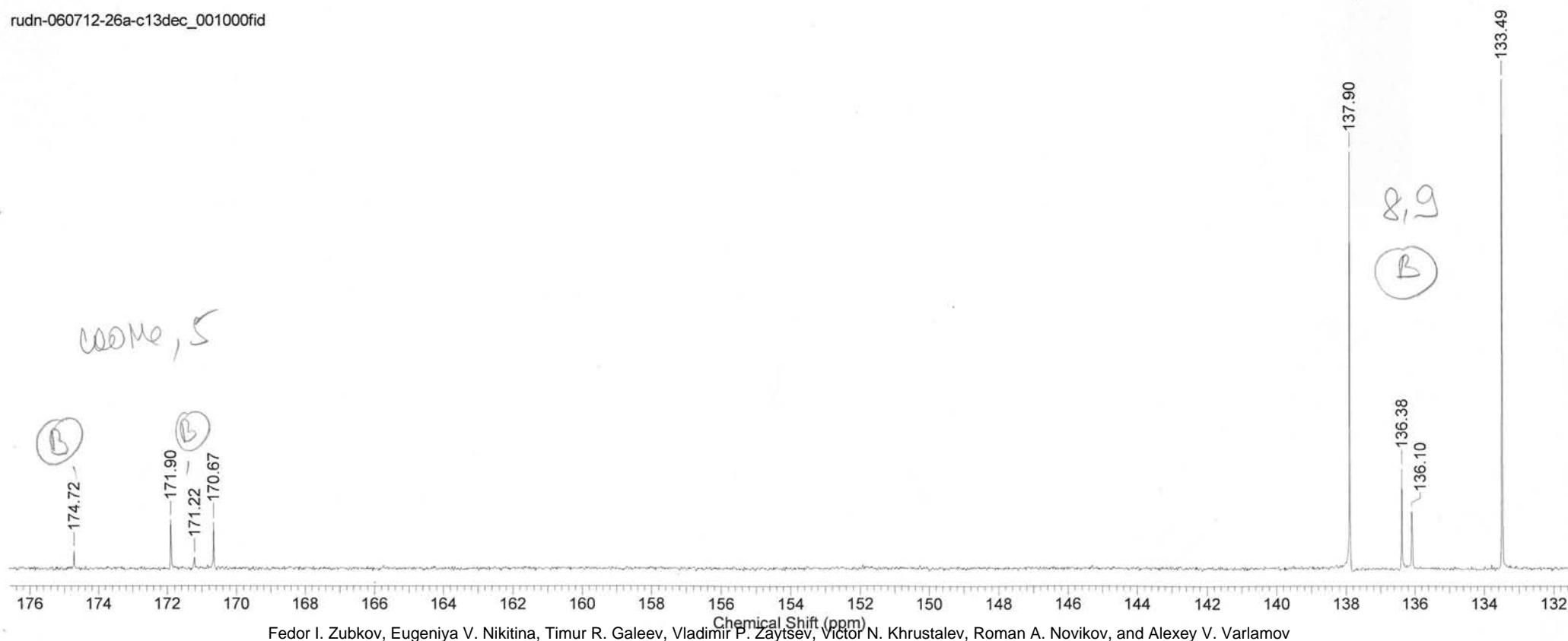
Formula	C ₁₂ H ₁₃ NO ₄ S	FW	267.3009
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	06 Jul 2012 15:21:36	
Date Stamp	06 Jul 2012 15:21:36						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-26a-c13dec\rudn-060712-26a-c13dec_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	1724	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zgpg
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9618.5391
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				

Compounds 26Aa/26Ba
after crystallization

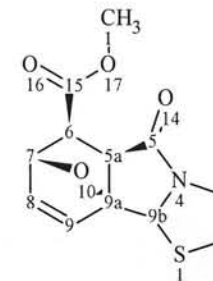


rudn-060712-26a-c13dec_001000fid

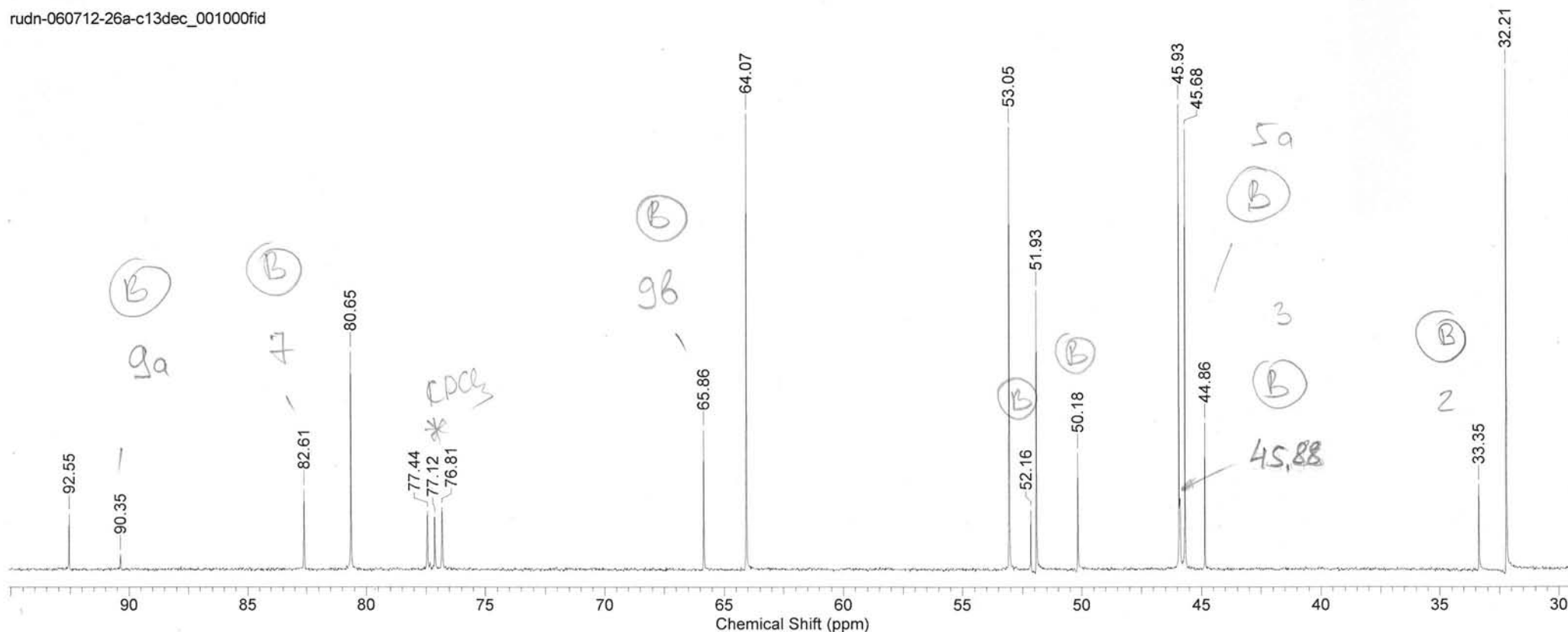


Formula C ₁₂ H ₁₃ NO ₄ S	FW 267.3009			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 06 Jul 2012 15:21:36		
Date Stamp 06 Jul 2012 15:21:36				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-26a-c13dec\rudn-060712-26a-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 1724	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent CHLOROFORM-d	Spectrum Offset (Hz) 9618.5391	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compounds 26Aa/26Ba
after crystallization



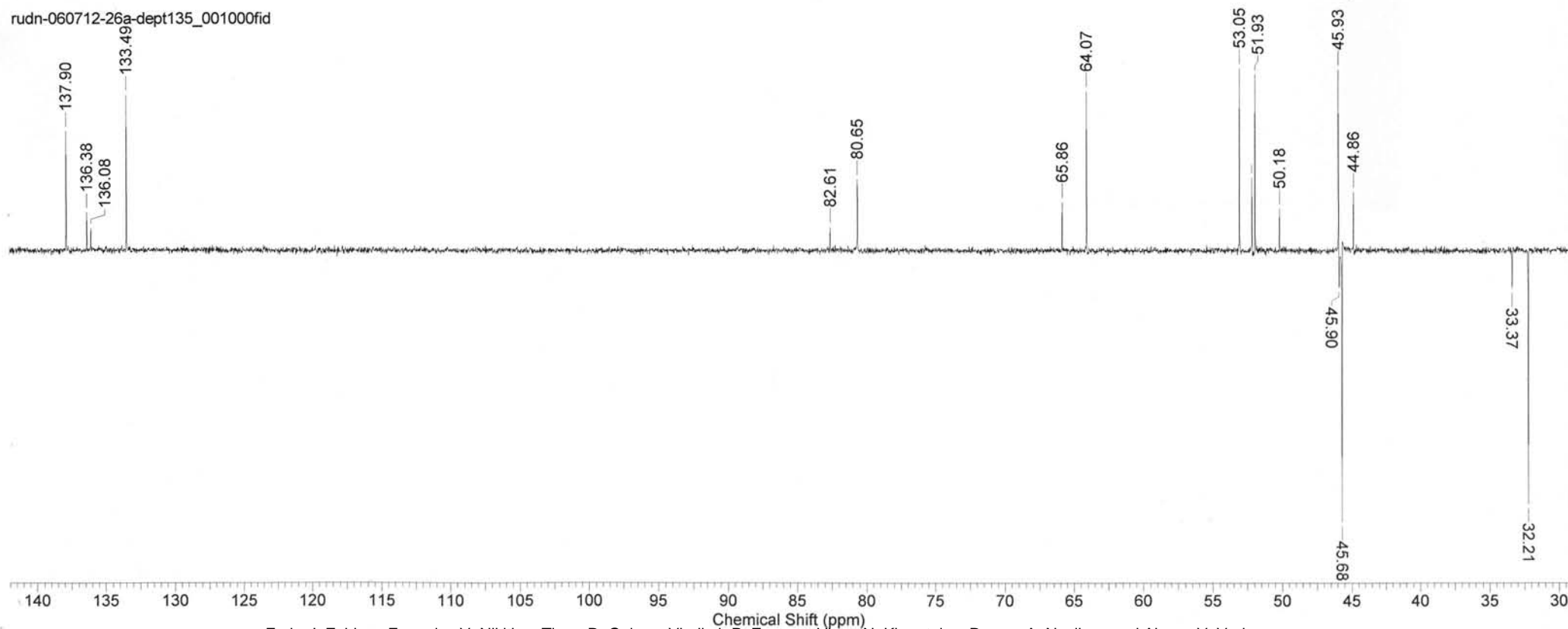
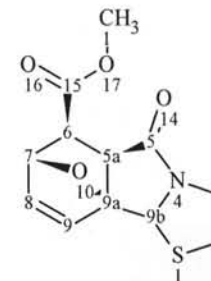
rudn-060712-26a-c13dec_001000fid



Formula	C ₁₂ H ₁₃ NO ₄ S	FW	267.3009
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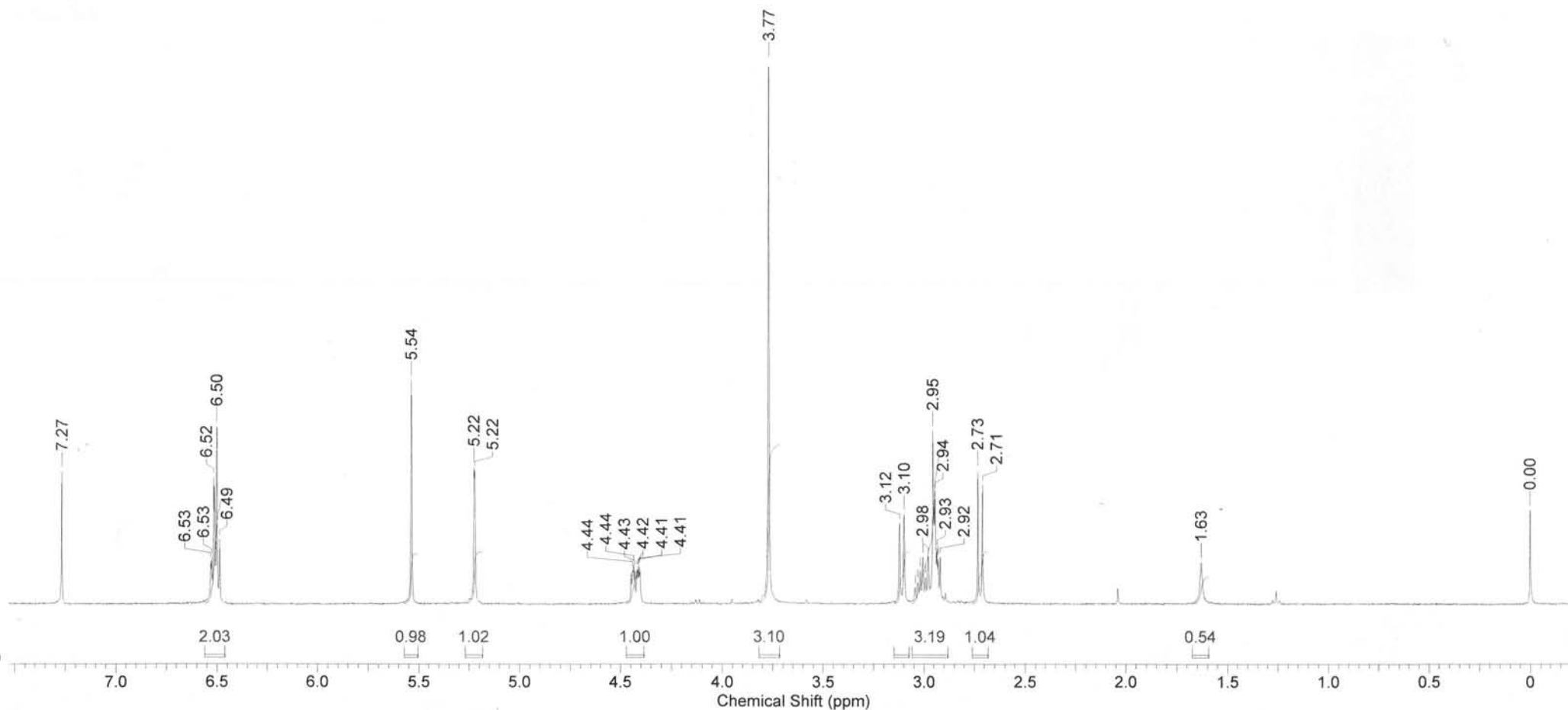
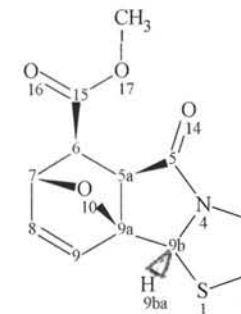
Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	06 Jul 2012 15:53:36	
Date Stamp	06 Jul 2012 15:53:36						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-26a-dept135\rudn-060712-26a-dept135_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	597	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	dept135
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9618.5283
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				

Compounds 26Aa/26Ba
after crystallization



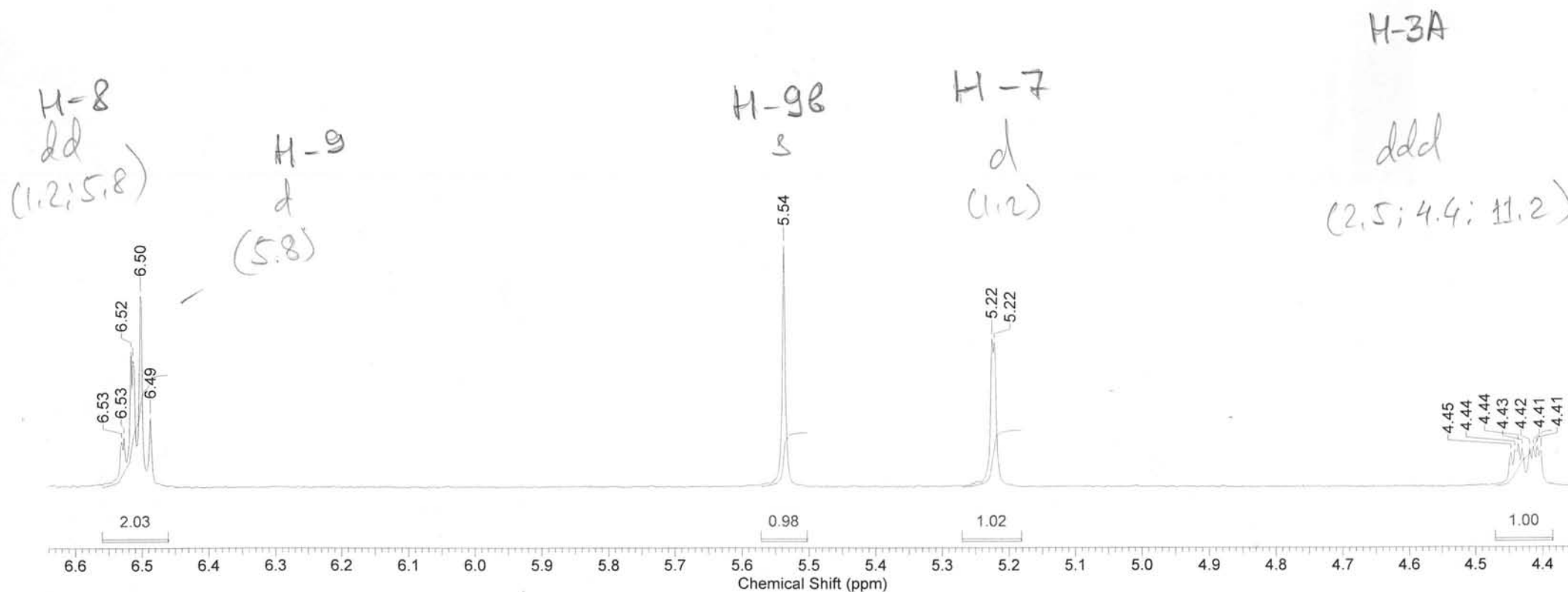
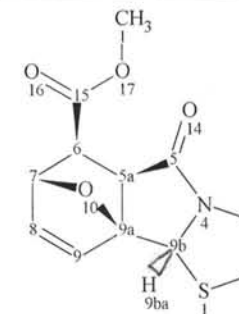
Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.		Date	15 Jul 2009 13:00:48
File Name	D:\Timur\Тимур (лето 2009)\rudn10\rudn10_001000fid	Frequency (MHz)	400.14	Nucleus	1H	
Number of Transients	4	Original Points Count	16384	Points Count	16384	
Solvent	CHLOROFORM-D	Sweep Width (Hz)	10204.08	Temperature (degree C)	27.000	
				Pulse Sequence	zg	

Compound 26Ba



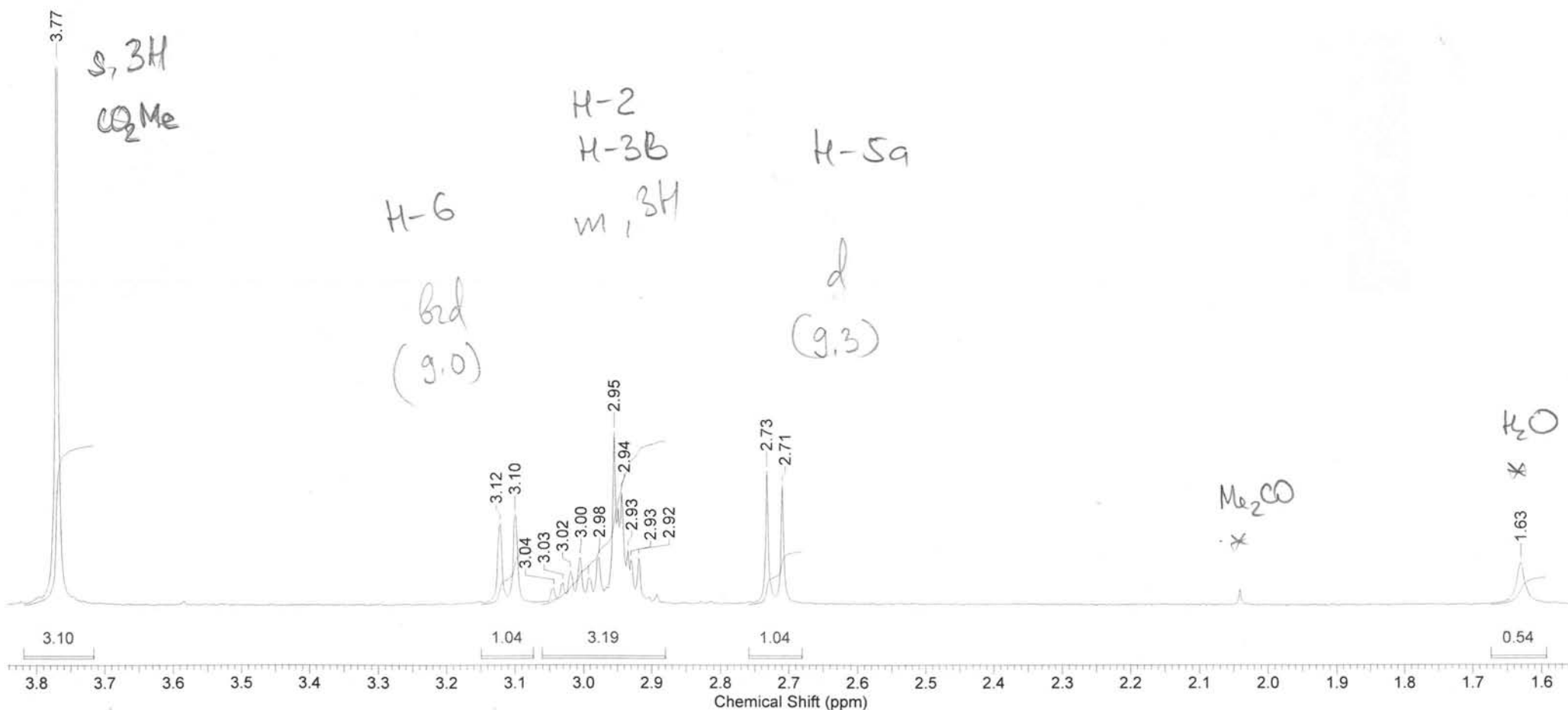
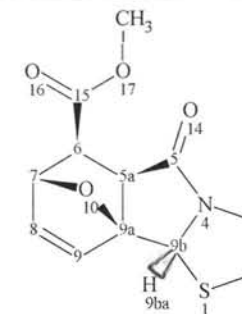
Acquisition Time (sec)	1.6056	Comment	Imported from UXNMR.		Date	15 Jul 2009 13:00:48
File Name	D:\Тимур\Тимур (лето 2009)\rudn10\rudn10_001000fid	Frequency (MHz)	400.14	Nucleus	1H	
Number of Transients	4	Original Points Count	16384	Points Count	16384	
Solvent	CHLOROFORM-D	Sweep Width (Hz)	10204.08	Temperature (degree C)	27.000	
				Pulse Sequence	zg	

Compound 26Ba



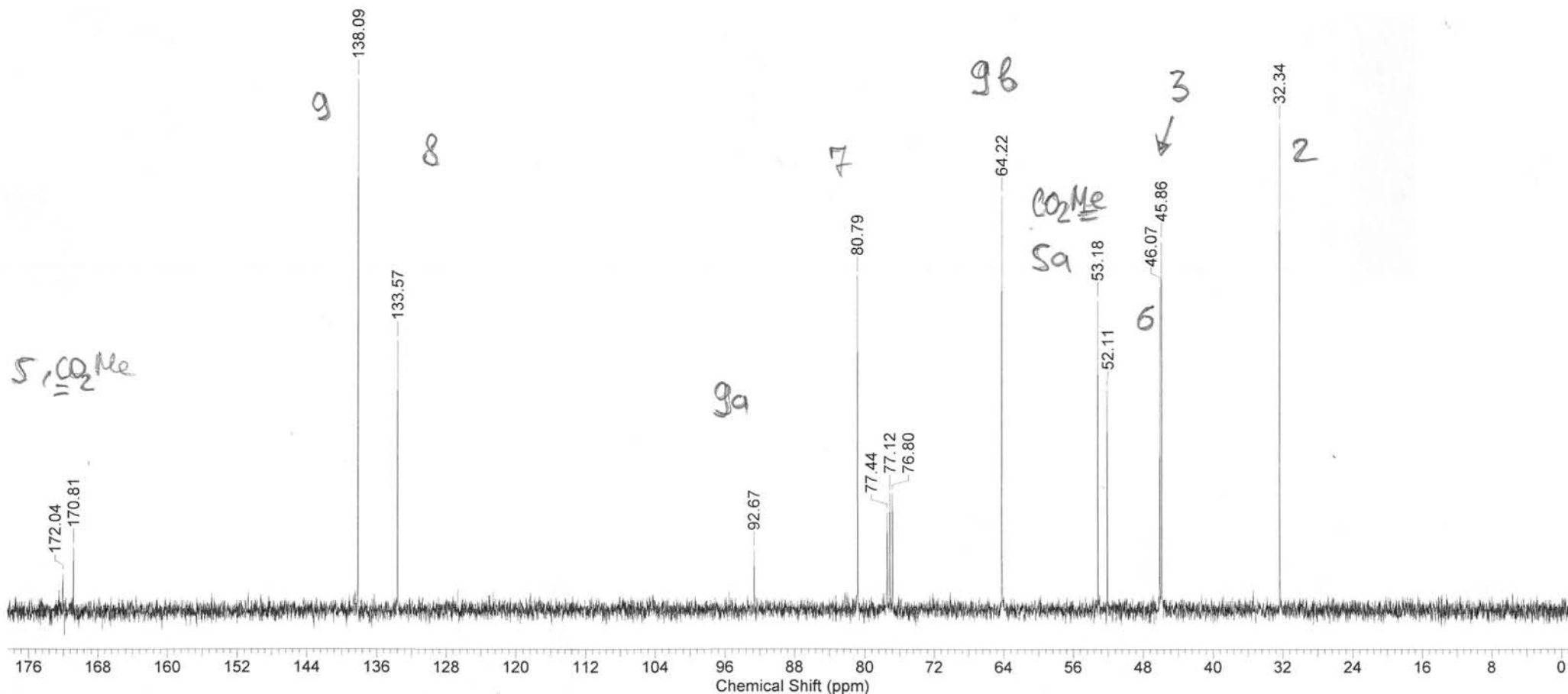
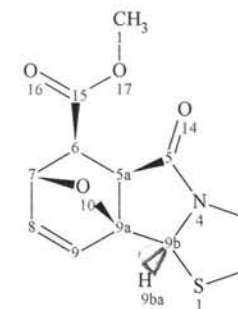
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File Name	D:\Тимур\Тимур (лето 2009)\rudn10\rudn10_001000fid	Frequency (MHz)	400.14	Nucleus	1H	
Number of Transients	4	Original Points Count	16384	Points Count	16384	
Solvent	CHLOROFORM-D	Sweep Width (Hz)	10204.08	Temperature (degree C)	27.000	
				Pulse Sequence	zg	

Compound 26Ba



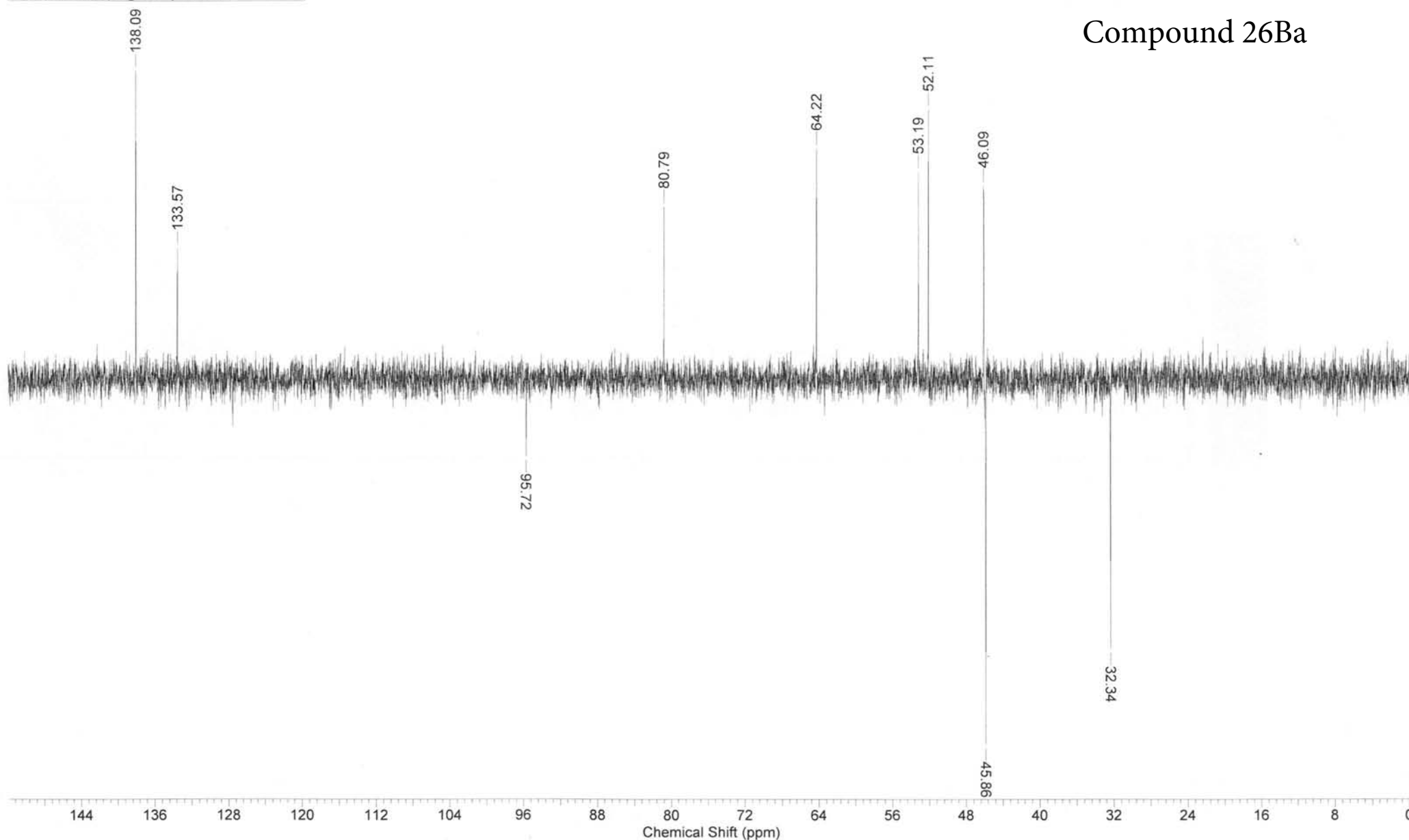
Acquisition Time (sec)	0.6226	Comment	Imported from UXNMR.		Date	15 Jul 2009 15:13:04	
File Name	D:\Тимур\Тимур (лето 2009)\rudn10c13dec\rudn10c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	292	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D		Sweep Width (Hz)	26315.79	
Temperature (degree C)	27.000						

Compound 26Ba



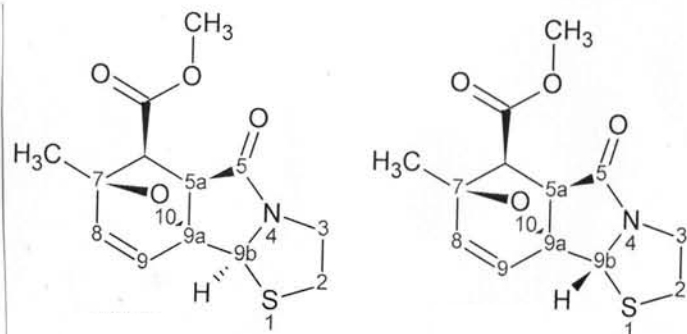
Acquisition Time (sec)	0.6226	Comment	Imported from UXMNR.	Date	15 Jul 2009 15:19:28
File Name	D:\Тимур\Тимур (лето 2009)\rudn10dept135\rudn10dept135_001000fid			Frequency (MHz)	100.62
Nucleus	13C	Number of Transients	116	Original Points Count	16384
Pulse Sequence	dept135	Solvent	CHLOROFORM-D	Points Count	16384
Temperature (degree C)	27.000			Sweep Width (Hz)	26315.79

Compound 26Ba

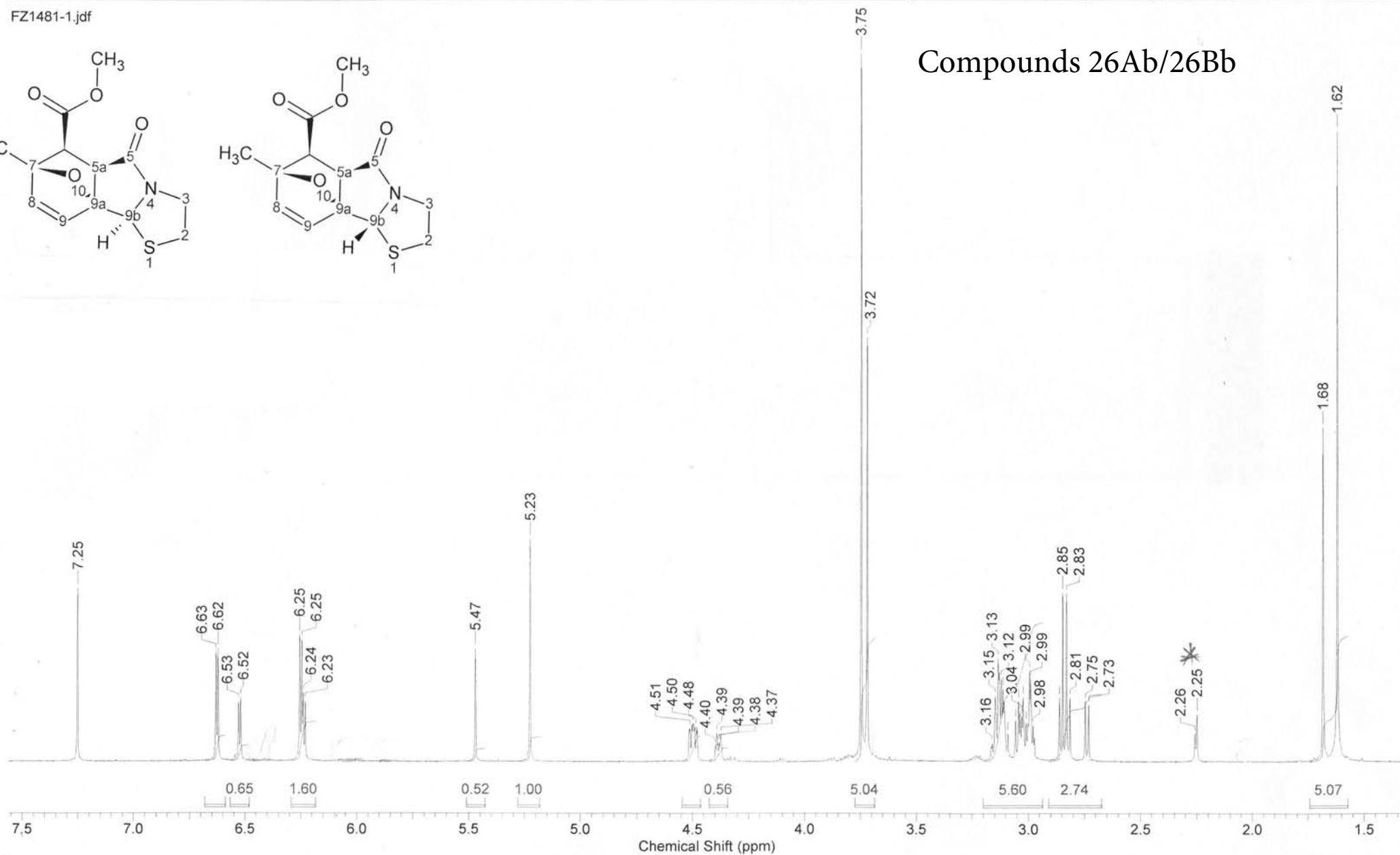


Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	23 Nov 2010 14:38:05	Date Stamp	23 Nov 2010 13:50:36
File Name	D:\NMR\22.11.10\FZ1481-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	10
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3601.0339	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	11261.26

FZ1481-1.jdf



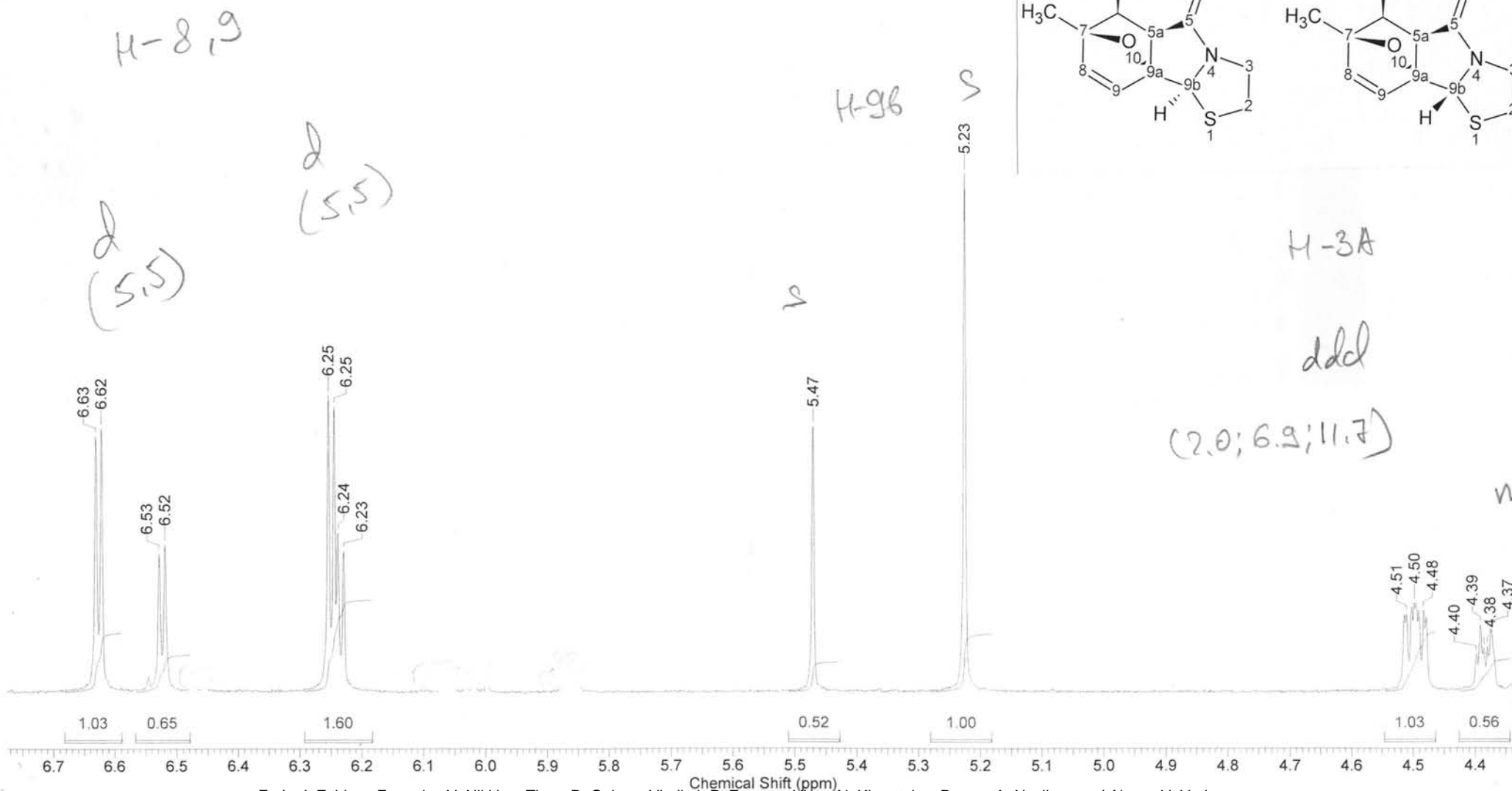
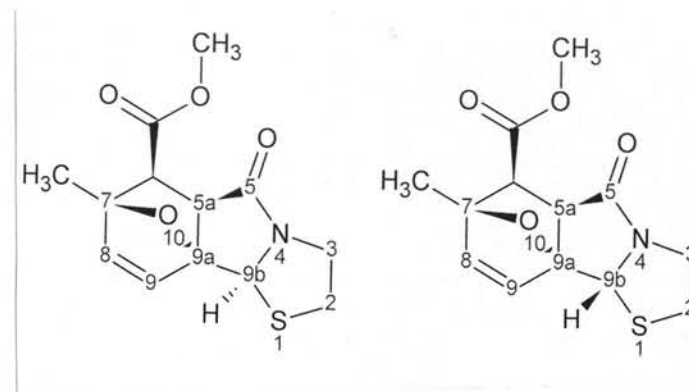
Compounds 26Ab/26Bb



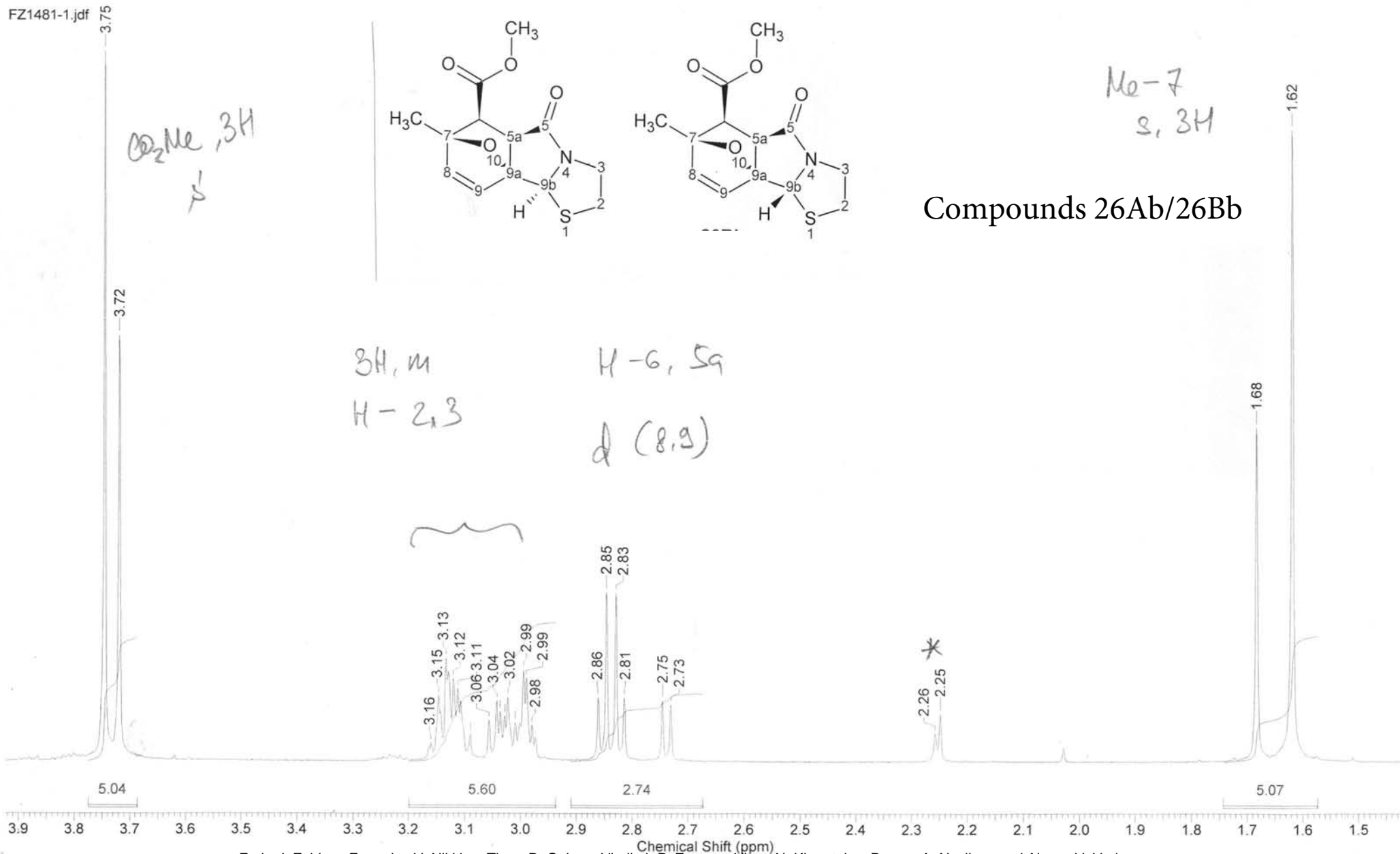
Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	23 Nov 2010 14:38:05	Date Stamp	23 Nov 2010 13:50:36
File Name	D:\NMR\22.11.10\FZ1481-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	10
Origin	ECA 600	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3601.0339	Sweep Width (Hz)	11261.26

FZ1481-1.jdf

Compounds 26Ab/26Bb



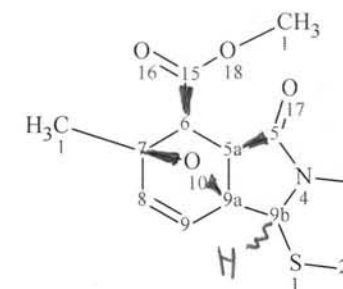
Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	23 Nov 2010 14:38:05	Date Stamp	23 Nov 2010 13:50:36
File Name	D:\NMR\22.11.10\FZ1481-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	10
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3601.0339	Pulse Sequence	single_pulse.ex2
				Sweep Width (Hz)	11261.26		



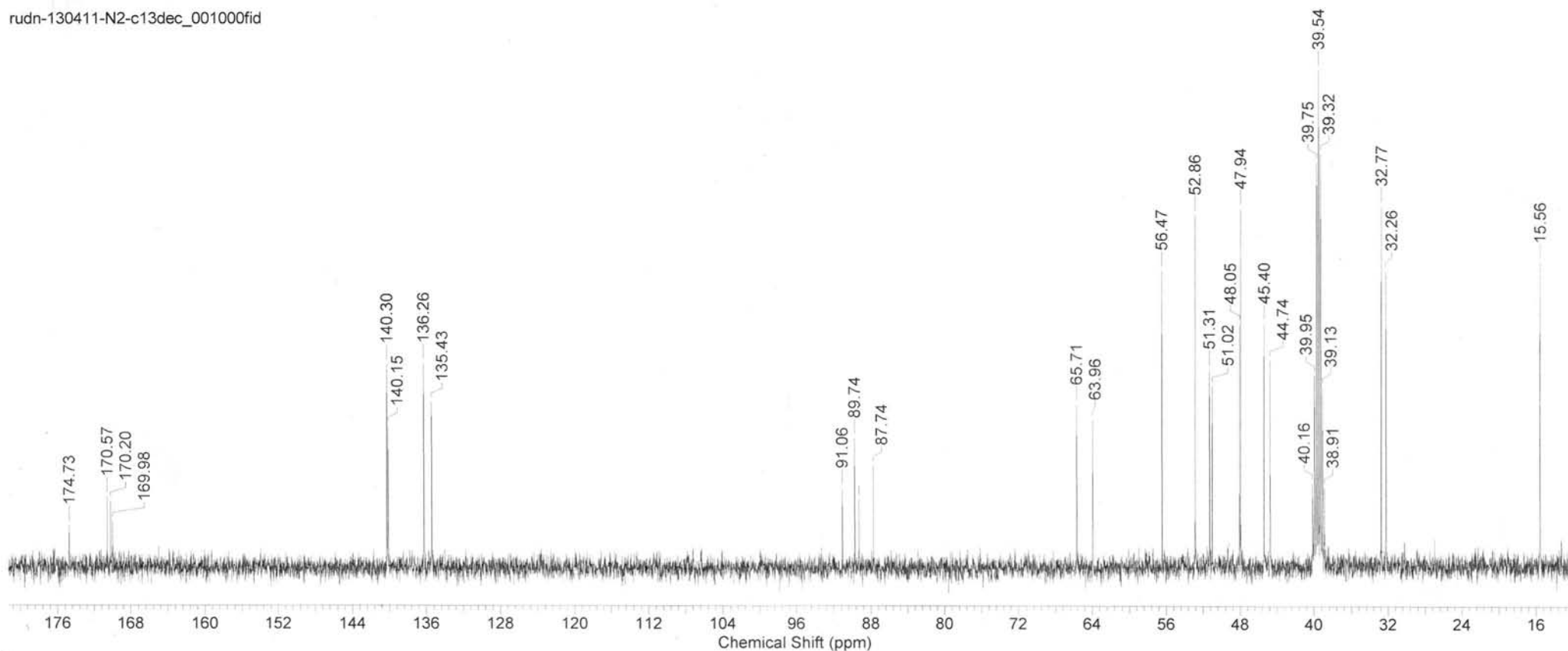
Formula $C_{13}H_{15}NO_4S$ FW 281.3275

Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	14 Apr 2011 05:56:16
Date Stamp	14 Apr 2011 05:56:16	File Name	D:\NMR\13.04.2011 C-13\rudn-130411-N2-c13dec\rudn-130411-N2-c13dec_001000fid		
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	650
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6
Sweep Width (Hz)	29409.97	Temperature (degree C)	32.000	Pulse Sequence	zgpg
				Spectrum Offset (Hz)	10547.6182

Compounds 26Ab/26Bb



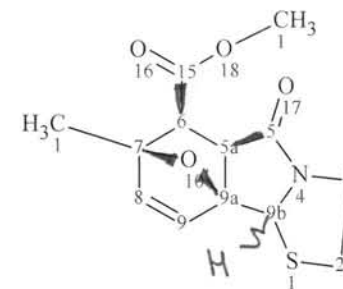
rudn-130411-N2-c13dec_001000fid



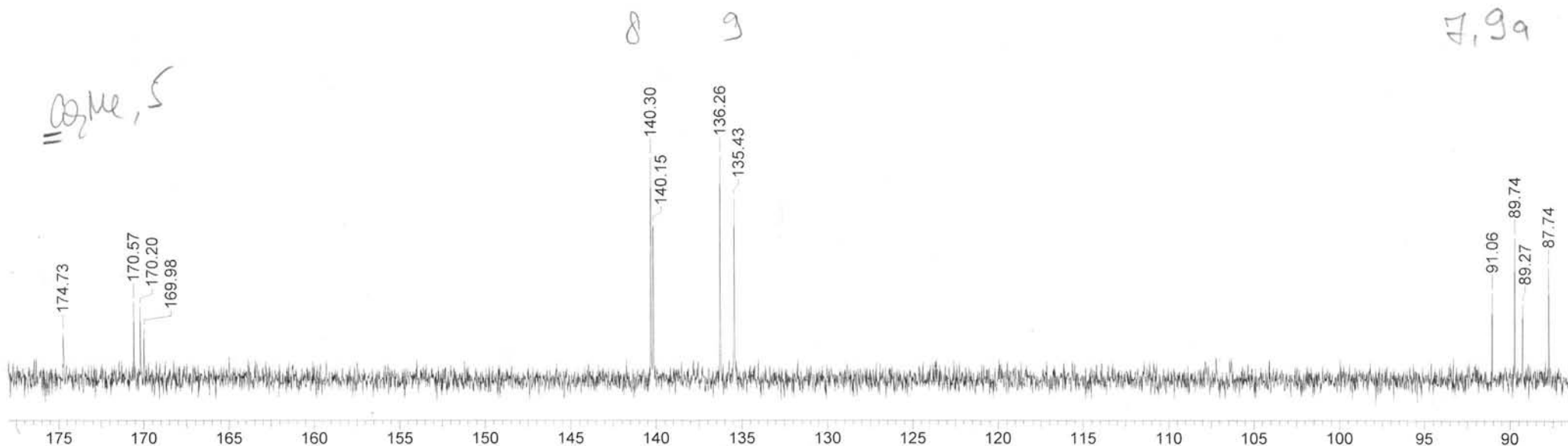
Formula C₁₃H₁₅NO₄S FW 281.3275

Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	14 Apr 2011 05:56:16	
Date Stamp	14 Apr 2011 05:56:16	File Name	D:\NMR\13.04.2011 C-13\rudn-130411-N2-c13dec\rudn-130411-N2-c13dec_001000fid				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	650	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zgpg
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6	Spectrum Offset (Hz)	10547.6182
Sweep Width (Hz)	29409.97	Temperature (degree C)	32.000				

Compounds 26Ab/26Bb

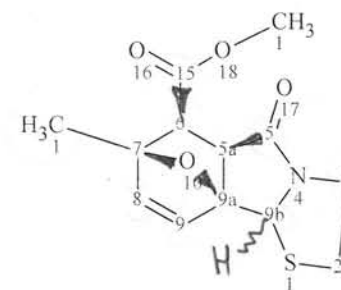


rudn-130411-N2-c13dec_001000fid

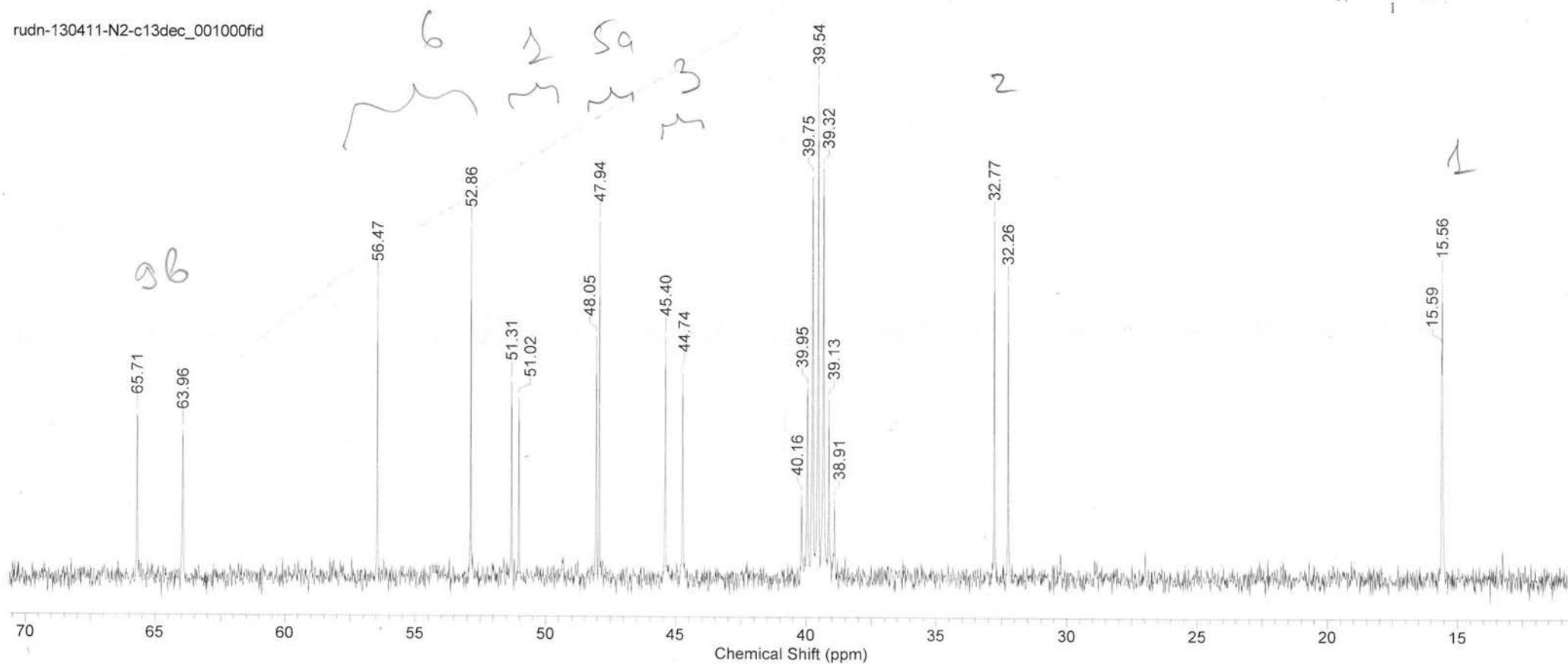


Formula	C ₁₃ H ₁₅ NO ₄ S	FW	281.3275
Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400
Date Stamp	14 Apr 2011 05:56:16	File Name	D:\NMR\13.04.2011 C-13\rudn-130411-N2-c13dec\rudn-130411-N2-c13dec_001000fid
Frequency (MHz)	100.62	Nucleus	13C
Original Points Count	16384	Number of Transients	650
Receiver Gain	32768.00	Origin	spect
Sweep Width (Hz)	29409.97	Points Count	16384
		Pulse Sequence	zgpg
		Solvent	DMSO-d6
		Spectrum Offset (Hz)	10547.6182
		Temperature (degree C)	32.000

Compounds 26Ab/26Bb

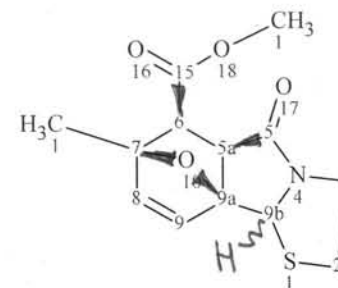


rudn-130411-N2-c13dec_001000fid

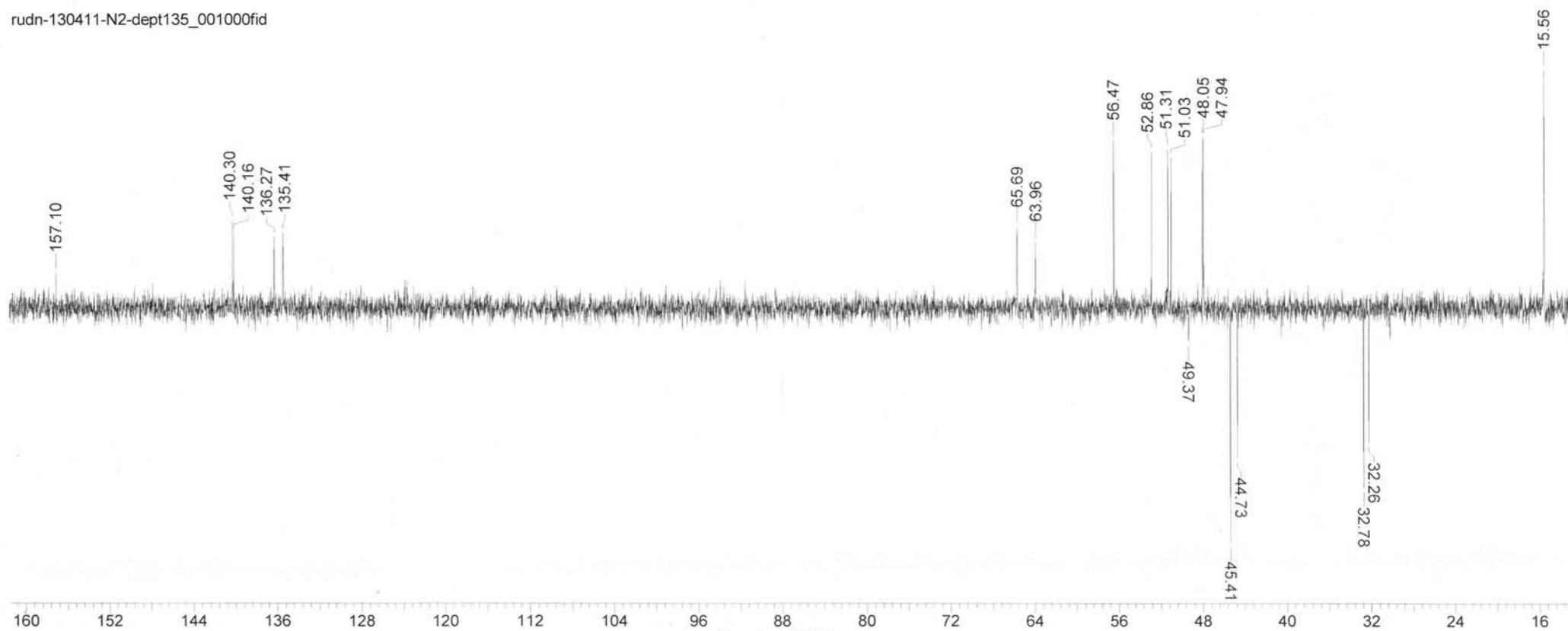


Formula	C ₁₃ H ₁₅ NO ₄ S	FW	281.3275		
Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	14 Apr 2011 06:11:12
Date Stamp	14 Apr 2011 06:11:12	File Name	D:\NMR\13.04.2011 C-13\rudn-130411-N2-dept135\rudn-130411-N2-dept135_001000fid		
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	575
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6
Sweep Width (Hz)	29409.97	Temperature (degree C)	32.000	Pulse Sequence	dept135
				Spectrum Offset (Hz)	9097.1982

Compounds 26Ab/26Bb

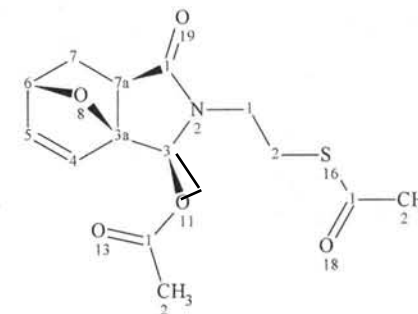


rudn-130411-N2-dept135_001000fid

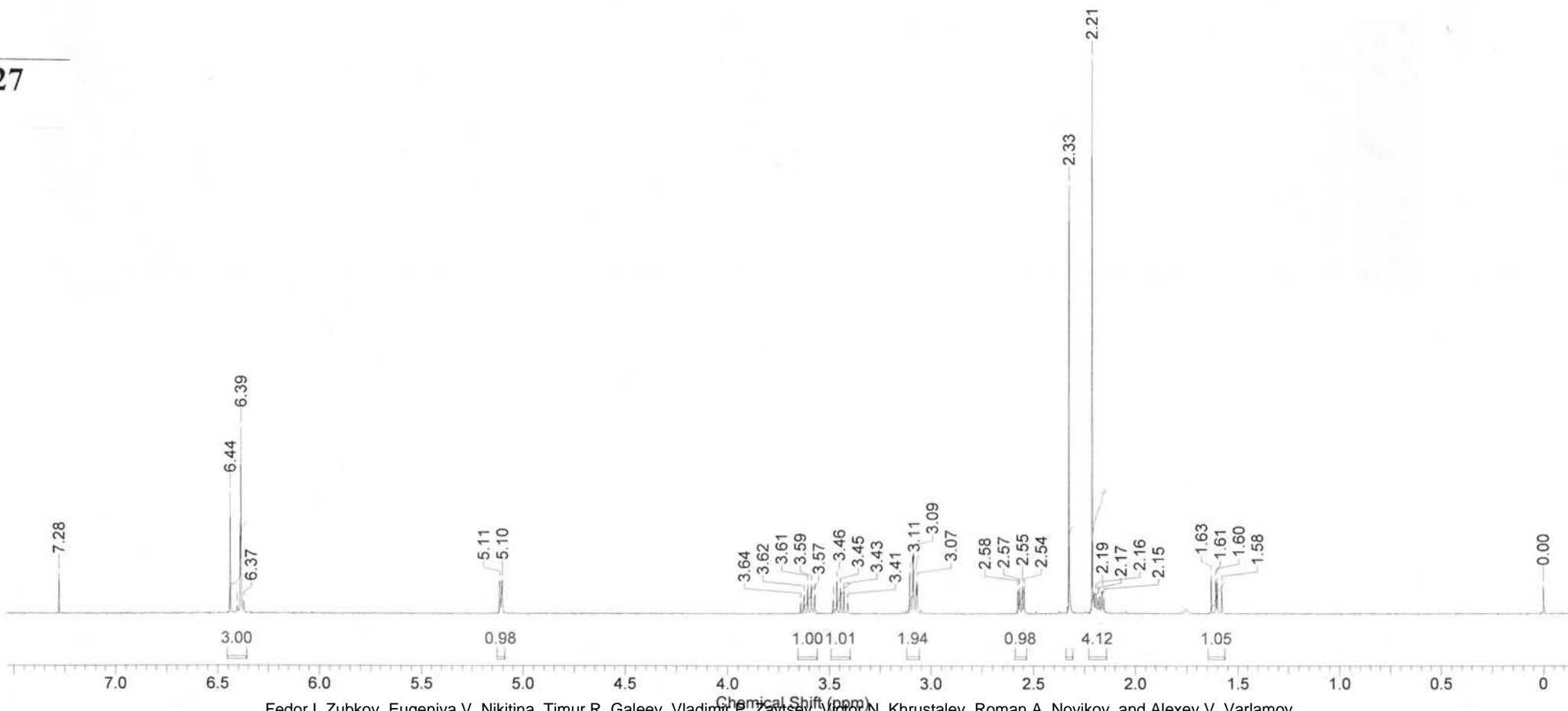


Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.		Date	15 Jul 2009 12:41:36	
File Name	D:\Тимур\Тимур (лето 2009)\rudn11\rudn11_001000fid	Frequency (MHz)	400.14	Nucleus	1H		
Number of Transients	4	Original Points Count	16384	Points Count	16384	Pulse Sequence	zg
Solvent	CHLOROFORM-D	Sweep Width (Hz)	10204.08	Temperature (degree C)	27.000		

Compound 27

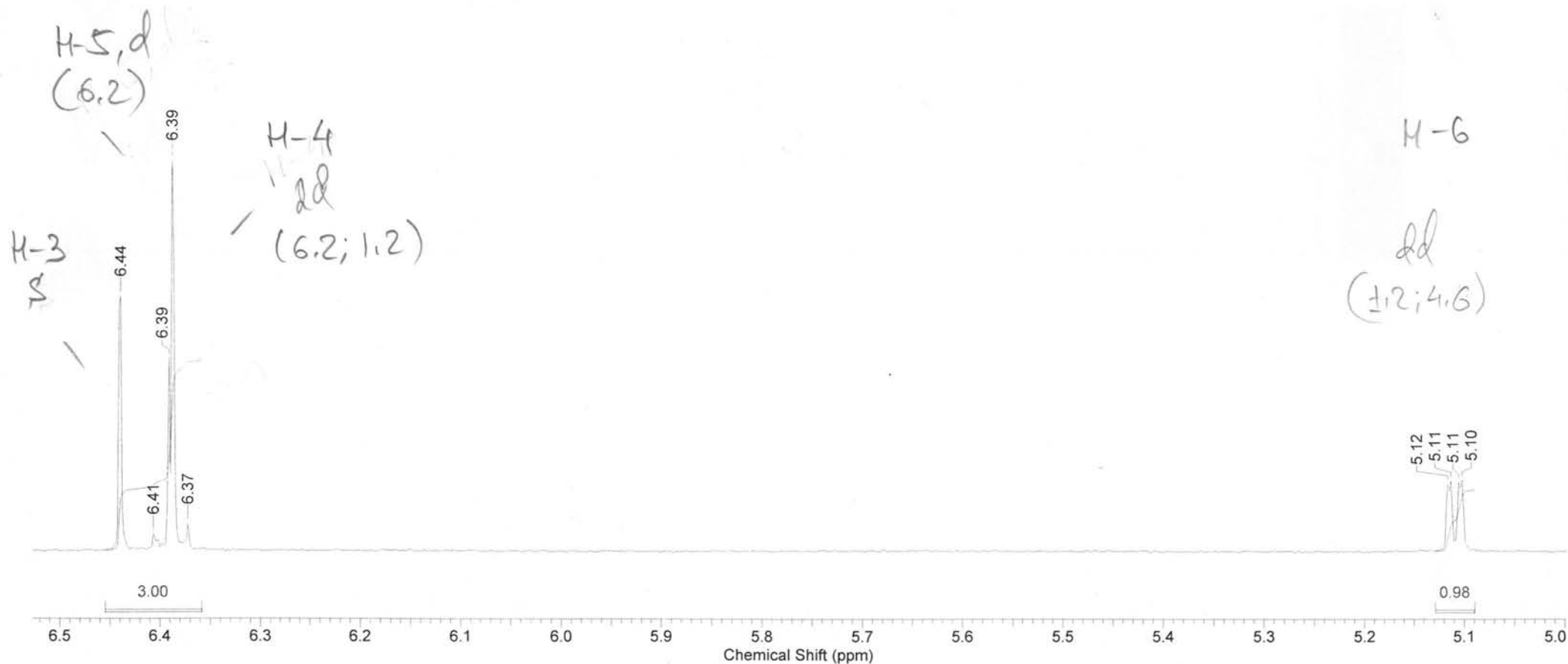
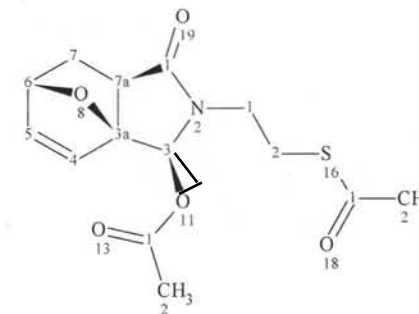


27



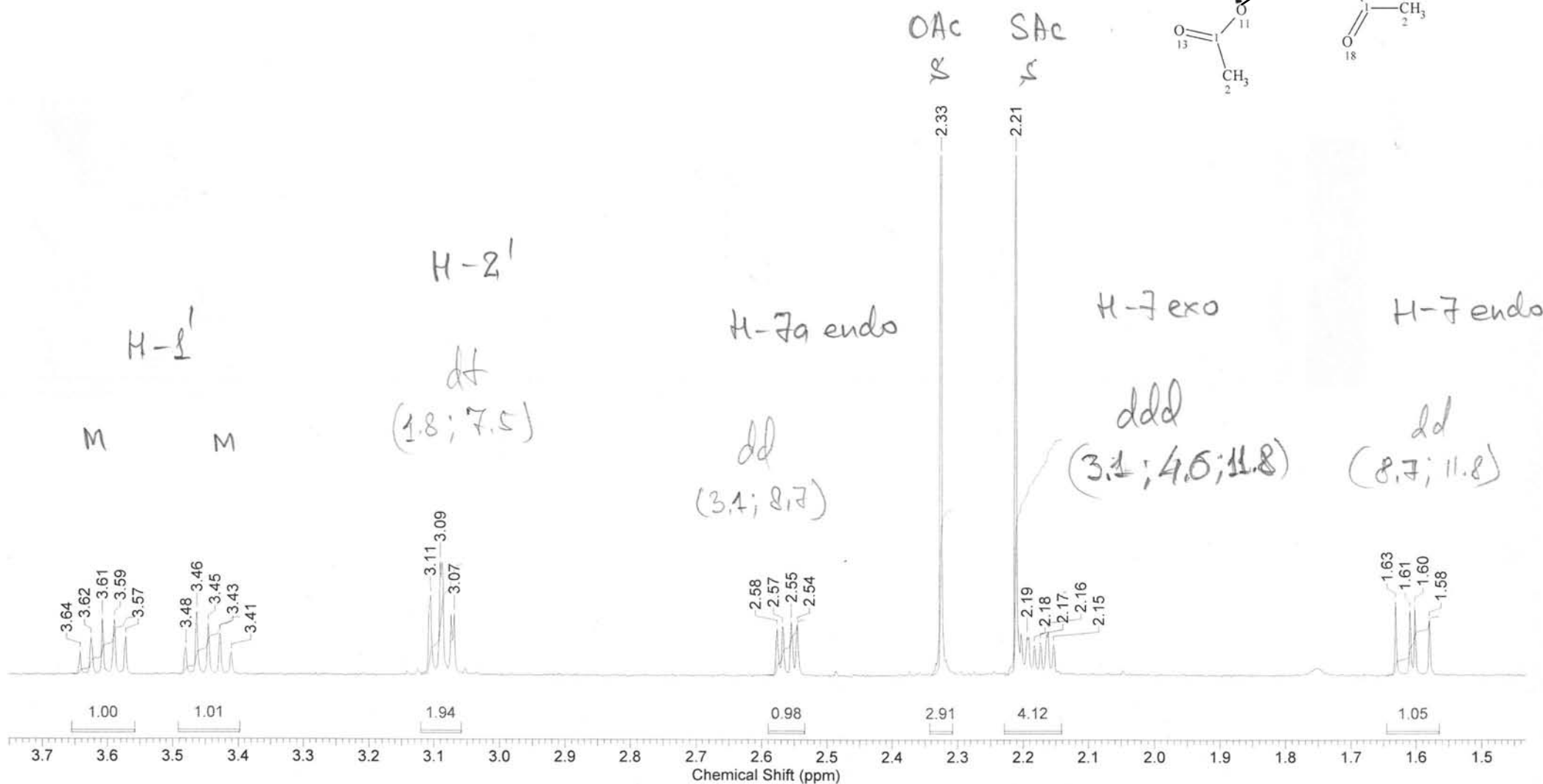
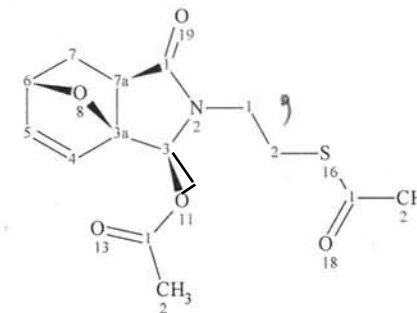
Acquisition Time (sec)	1.6056	Comment	Imported from UXNMR.		Date	15 Jul 2009 12:41:36
File Name	D:\Тимур\Тимур (лето 2009)\rudn11\rudn11_001000fid	Frequency (MHz)	400.14	Nucleus	1H	
Number of Transients	4	Original Points Count	16384	Points Count	16384	
Solvent	CHLOROFORM-D	Sweep Width (Hz)	10204.08	Pulse Sequence	zg	
				Temperature (degree C)	27.000	

Compound 27



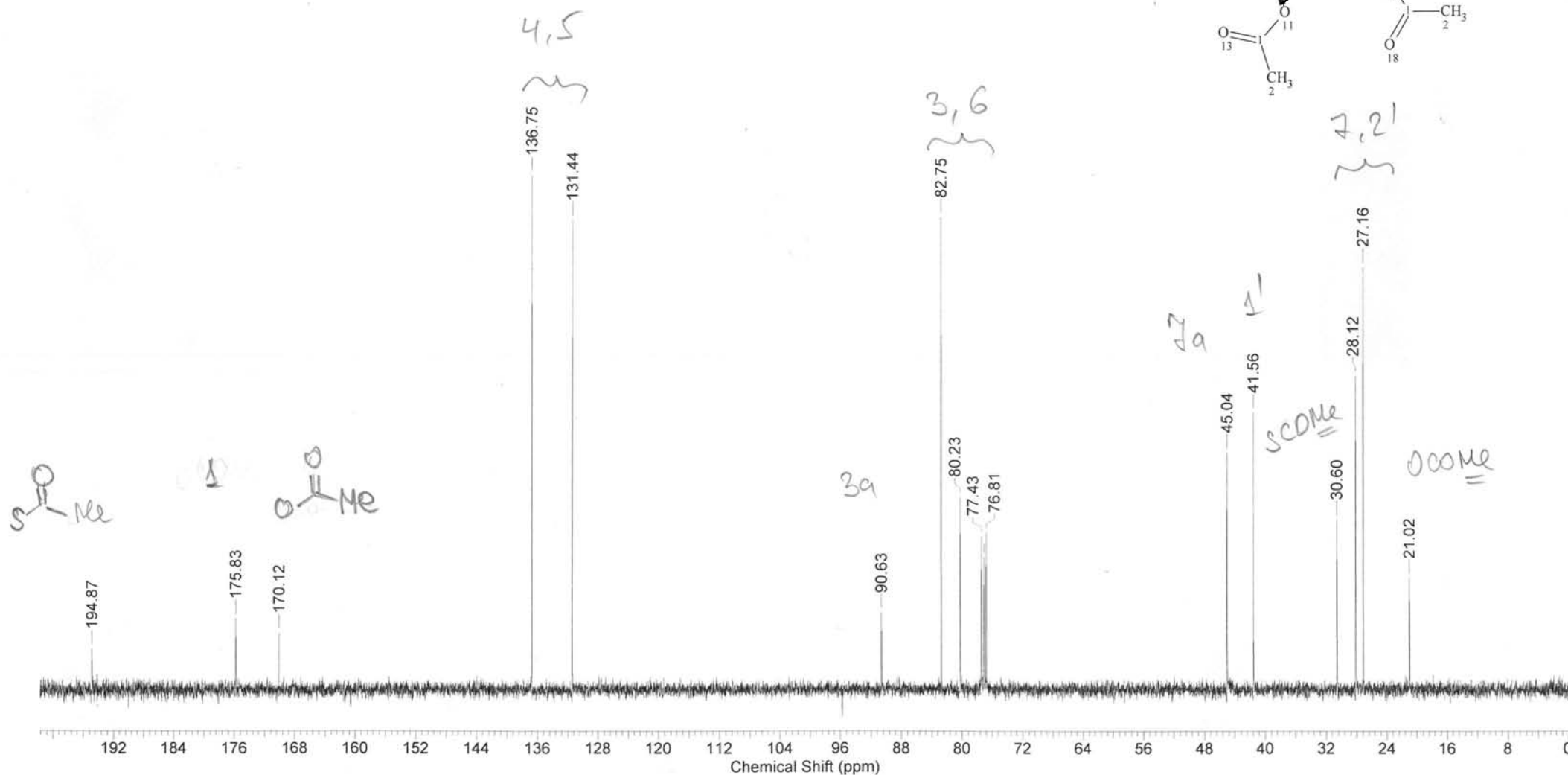
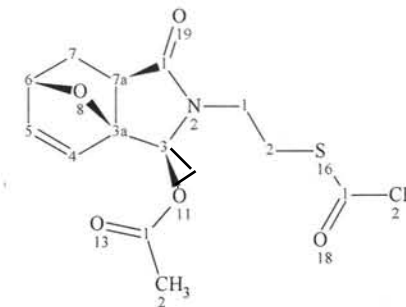
Acquisition Time (sec)	1.6056	Comment	Imported from UXNMR.		Date	15 Jul 2009 12:41:36
File Name	D:\Timur\Тимур (лето 2009)\rudn11\rudn11_001000fid	Frequency (MHz)	400.14	Nucleus	1H	
Number of Transients	4	Original Points Count	16384	Points Count	16384	
Solvent	CHLOROFORM-D	Sweep Width (Hz)	10204.08	Pulse Sequence	zg	
				Temperature (degree C)	27.000	

Compound 27



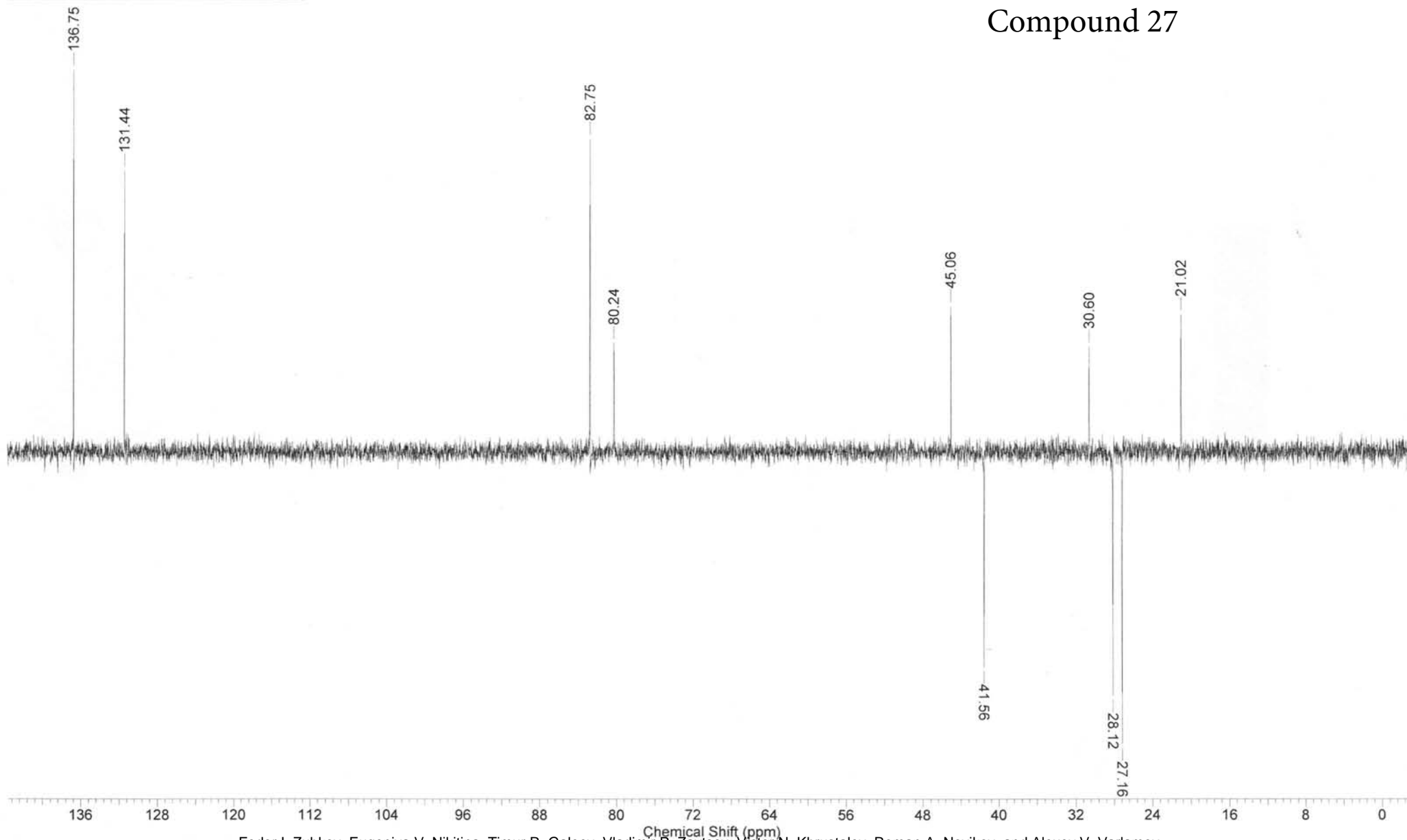
Acquisition Time (sec)	0.6226	Comment	Imported from UXMNR.	Date	15 Jul 2009 16:32:00
File Name	D:\Timur\Тимур (лето 2009)\rudn11c13dec\rudn11c13dec_001000fid			Frequency (MHz)	100.62
Nucleus	13C	Number of Transients	276	Original Points Count	16384
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D	Points Count	16384
Temperature (degree C)	27.000			Sweep Width (Hz)	26315.79

Compound 27



Acquisition Time (sec)	0.6226	Comment	Imported from UXMNR.		Date	15 Jul 2009 16:40:32	
File Name	D:\Тимур\Тимур (лето 2009)\rudn11dept135\rudn11dept135_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	176	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	CHLOROFORM-D		Sweep Width (Hz)	26315.79	
Temperature (degree C)	27.000						

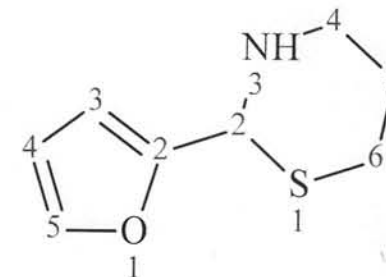
Compound 27



Formula C₈H₁₁NOS FW 169.2440

Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	21 Jul 2011 16:00:00
Date Stamp	21 Jul 2011 16:00:00	File Name	D:\NMR\19.07.11 (Poma)\rudn-190711-N4\rudn-190711-N4_001000fid	Number of Transients	16
Frequency (MHz)	400.14	Nucleus	1H	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	512.00	SW(cyclical) (Hz)	10204.08	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2602.0486	Sweep Width (Hz)	10203.46	Temperature (degree C)	27.000

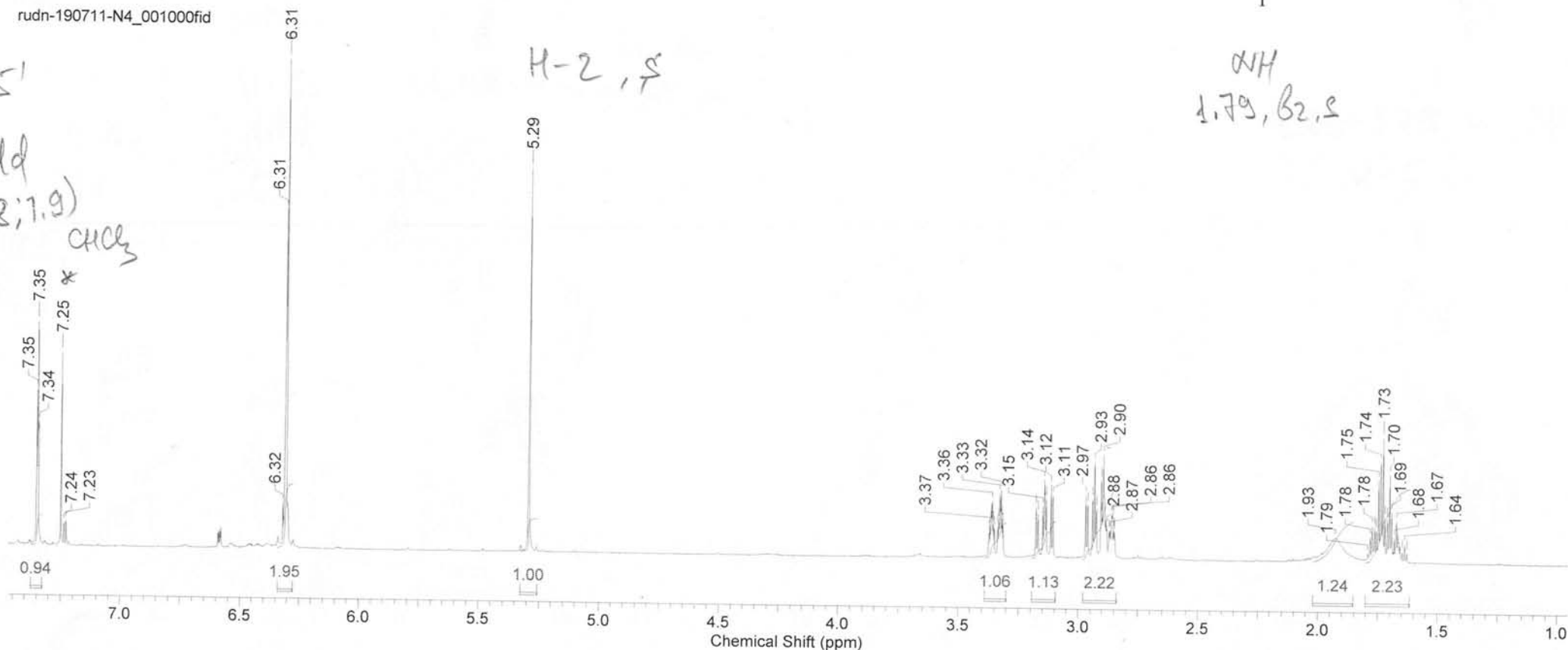
Compound 30a



30a

H-3' and H-4'
6.32 - 6.30
m, 2H

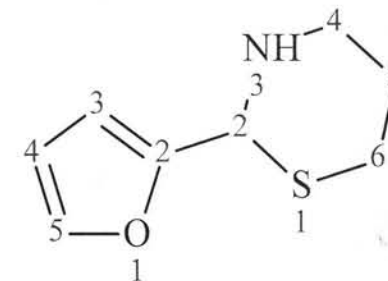
rudn-190711-N4_001000fid



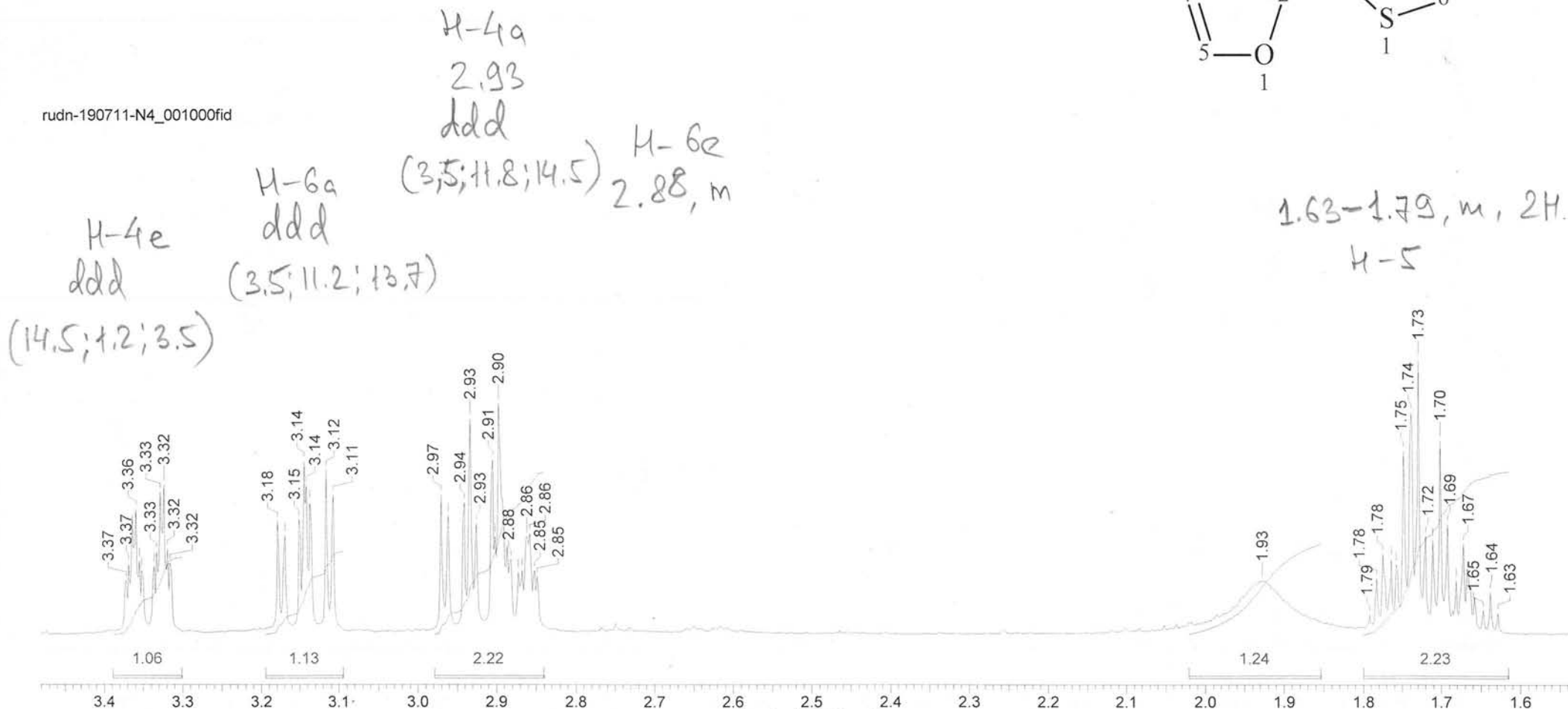
Formula C₈H₁₁NOS FW 169.2440

Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	21 Jul 2011 16:00:00
Date Stamp	21 Jul 2011 16:00:00	File Name	D:\NMR\19.07.11 (Poma)\rudn-190711-N4\rudn-190711-N4_001000fid		
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	16
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	512.00	SW(cyclical) (Hz)	10204.08	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2602.0486	Sweep Width (Hz)	10203.46	Temperature (degree C)	27.000

Compound 30a



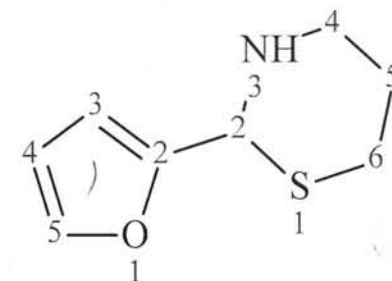
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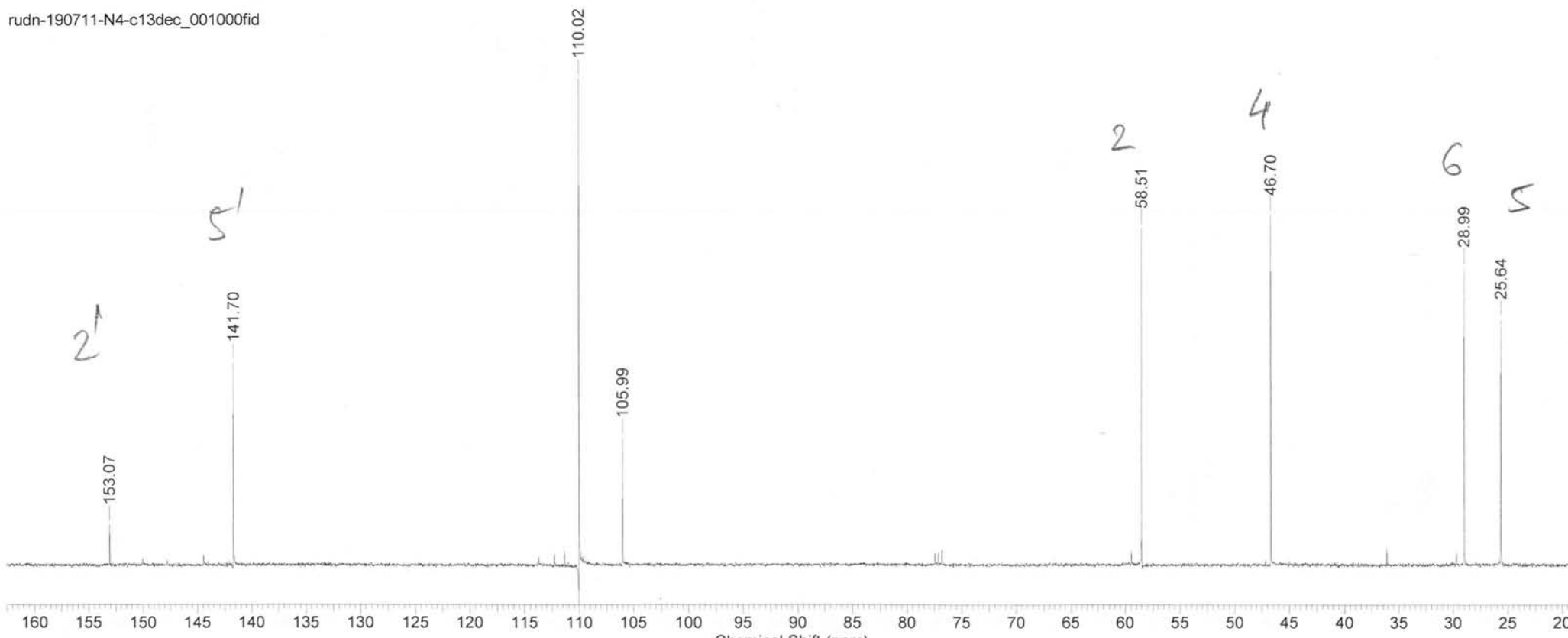
Formula	C ₈ H ₁₁ NOS	FW	169.2440
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Acquisition Time (sec)	0.5898	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	21 Jul 2011 16:19:12
Date Stamp	21 Jul 2011 16:19:12	File Name	D:\NMR\19.07.11 (Poma)\rudn-190711-N4-c13dec\rudn-190711-N4-c13dec_001000fid		
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	219
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	27777.78	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	9608.4277	Sweep Width (Hz)	27776.08	Temperature (degree C)	27.000

Compound 30a

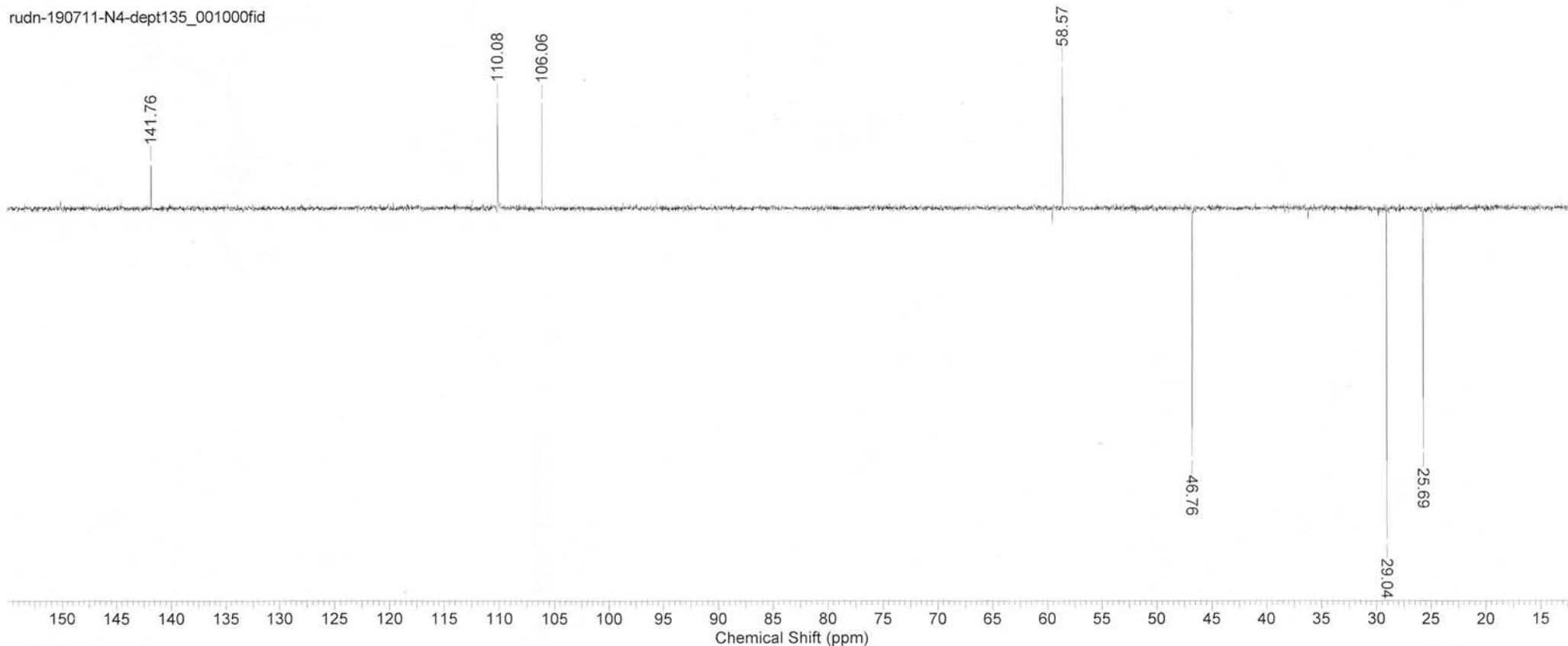
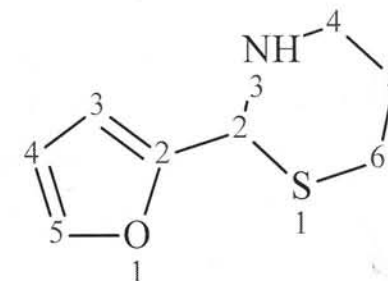


rudn-190711-N4-c13dec_001000fid



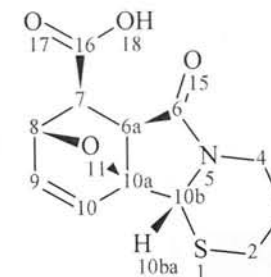
Formula C ₈ H ₁₁ NOS	FW 169.2440			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 21 Jul 2011 16:23:28		
Date Stamp 21 Jul 2011 16:23:28	File Name D:\NMR\19.07.11 (Рома)\rudn-190711-N4-dept135\rudn-190711-N4-dept135_001000fid			
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 301	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence dept135	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent CHLOROFORM-d		
Spectrum Offset (Hz) 9614.0205	Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000		

Compound 30a

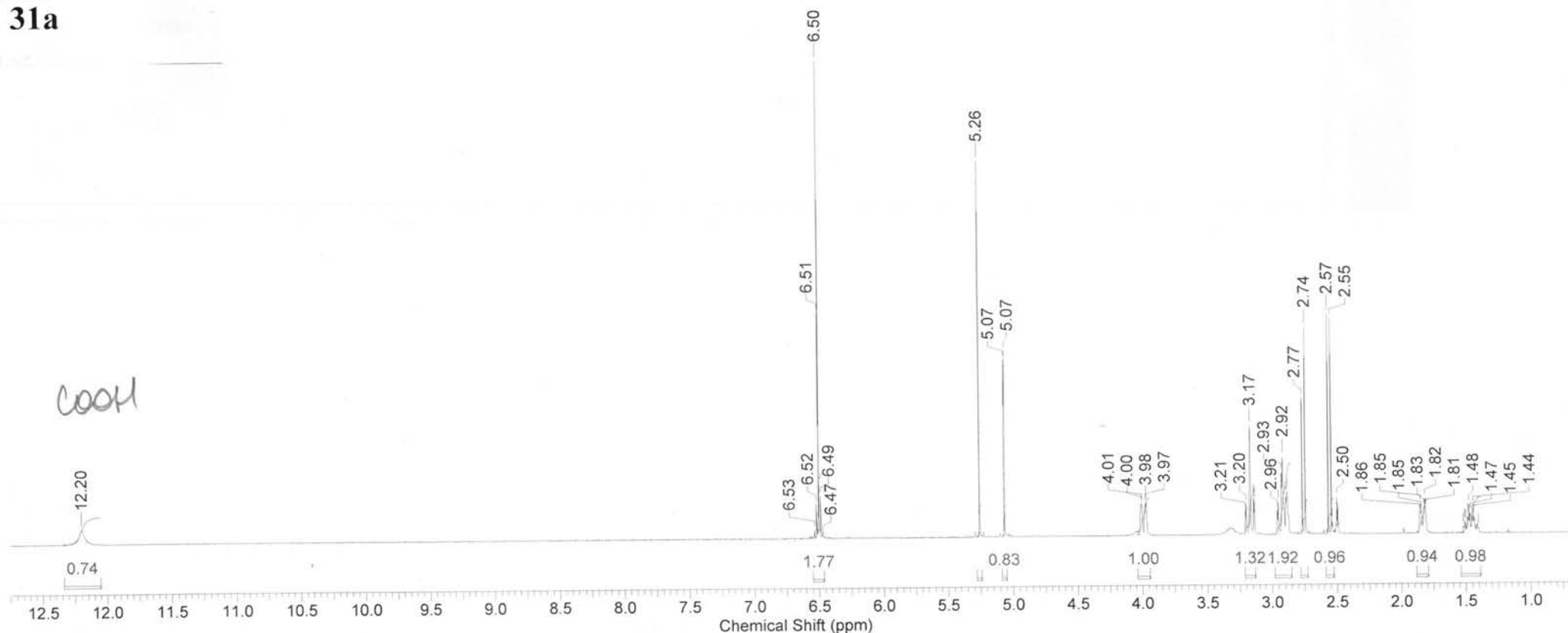


Formula	C ₁₂ H ₁₃ NO ₄ S	FW	267.3009
Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400
Date Stamp	08 Jul 2011 07:45:04	Date	08 Jul 2011 07:45:04
File Name	D:\NMR\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\rudn-0611-N13\rudn-0611-N13\rudn-0611-N13\rudn-0611-N13_001000fid		
Frequency (MHz)	400.14	Nucleus	1H
Original Points Count	16384	Owner	root
Receiver Gain	128.00	SW(cyclical) (Hz)	10416.67
Sweep Width (Hz)	10416.03	Temperature (degree C)	32.000
		Number of Transients	8
		Points Count	16384
		Solvent	DMSO-d6
		Origin	spect
		Pulse Sequence	zg
		Spectrum Offset (Hz)	2712.0542

Compound 31a



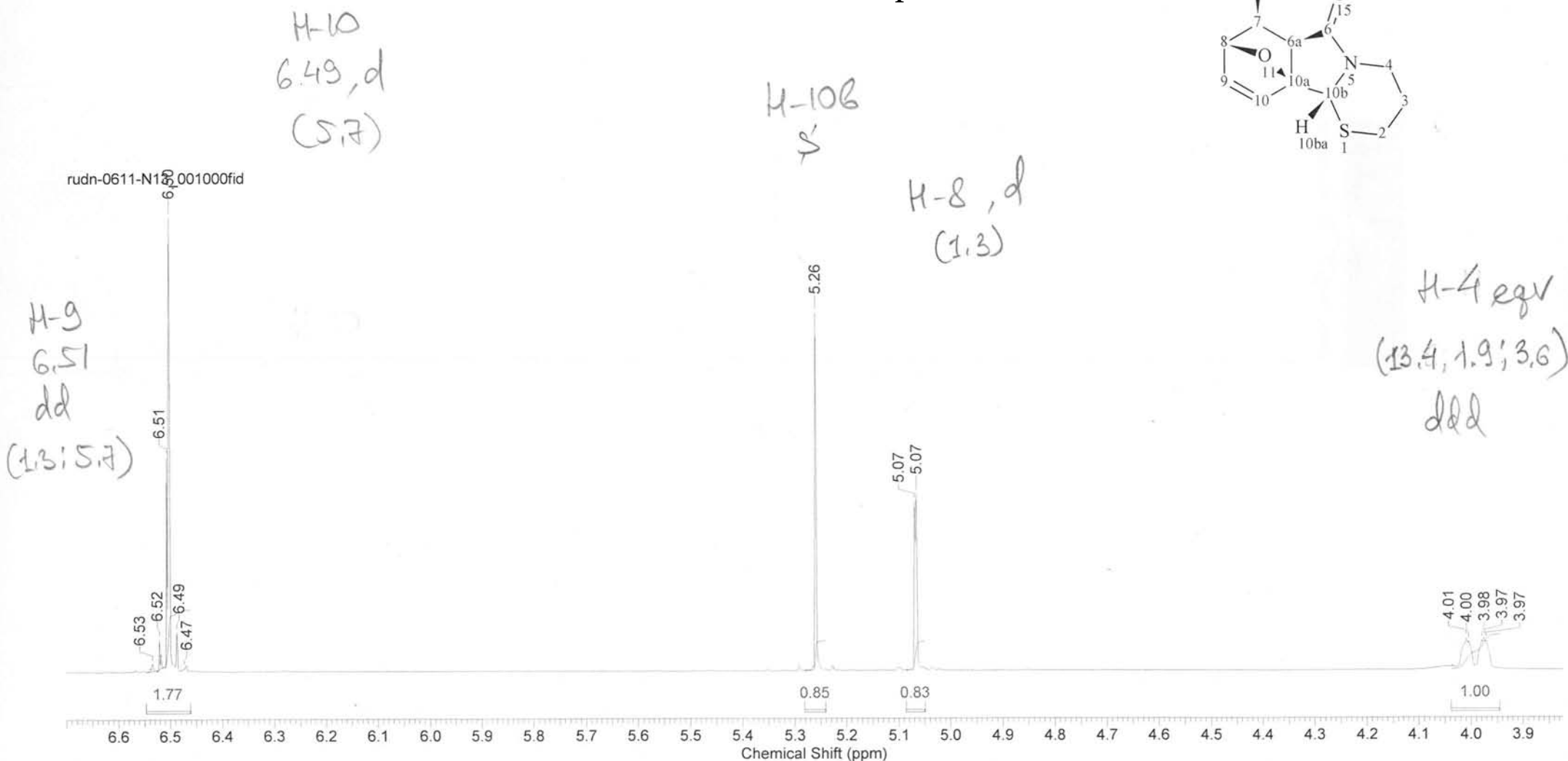
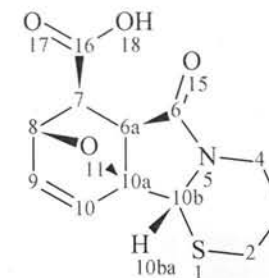
31a



Formula C₁₂H₁₃NO₄S FW 267.3009

Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	08 Jul 2011 07:45:04
Date Stamp	08 Jul 2011 07:45:04				
File Name	D:\NMR\19.05.2011 C 13 Для Иры Статья в Тетраэдрон\rudn-0611-N13\rudn-0611-N13\rudn-0611-N13\rudn-0611-N13_001000fid				
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	8
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	128.00	SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6
Sweep Width (Hz)	10416.03	Temperature (degree C)	32.000	Spectrum Offset (Hz)	2712.0542

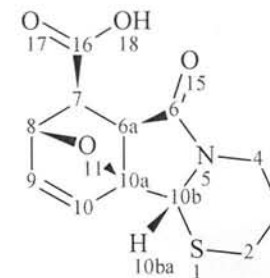
Compound 31a



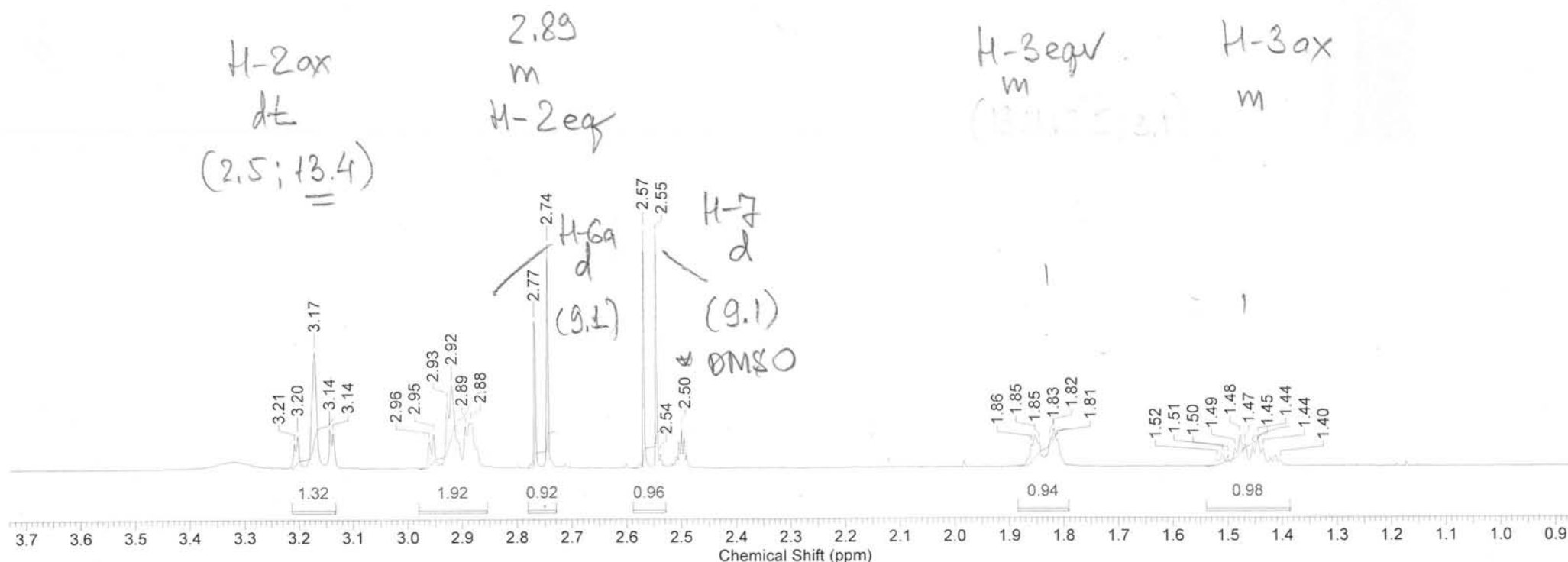
Formula C₁₂H₁₃NO₄S FW 267.3009

Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	08 Jul 2011 07:45:04
Date Stamp	08 Jul 2011 07:45:04					
File Name	D:\NMR\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\rudn-0611-N13\rudn-0611-N13\rudn-0611-N13\rudn-0611-N13_001000fid					
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	8	Origin spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence zg
Receiver Gain	128.00	SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz) 2712.0542
Sweep Width (Hz)	10416.03	Temperature (degree C)	32.000			

Compound 31a

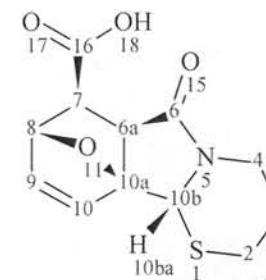


rudn-0611-N13_001000fid

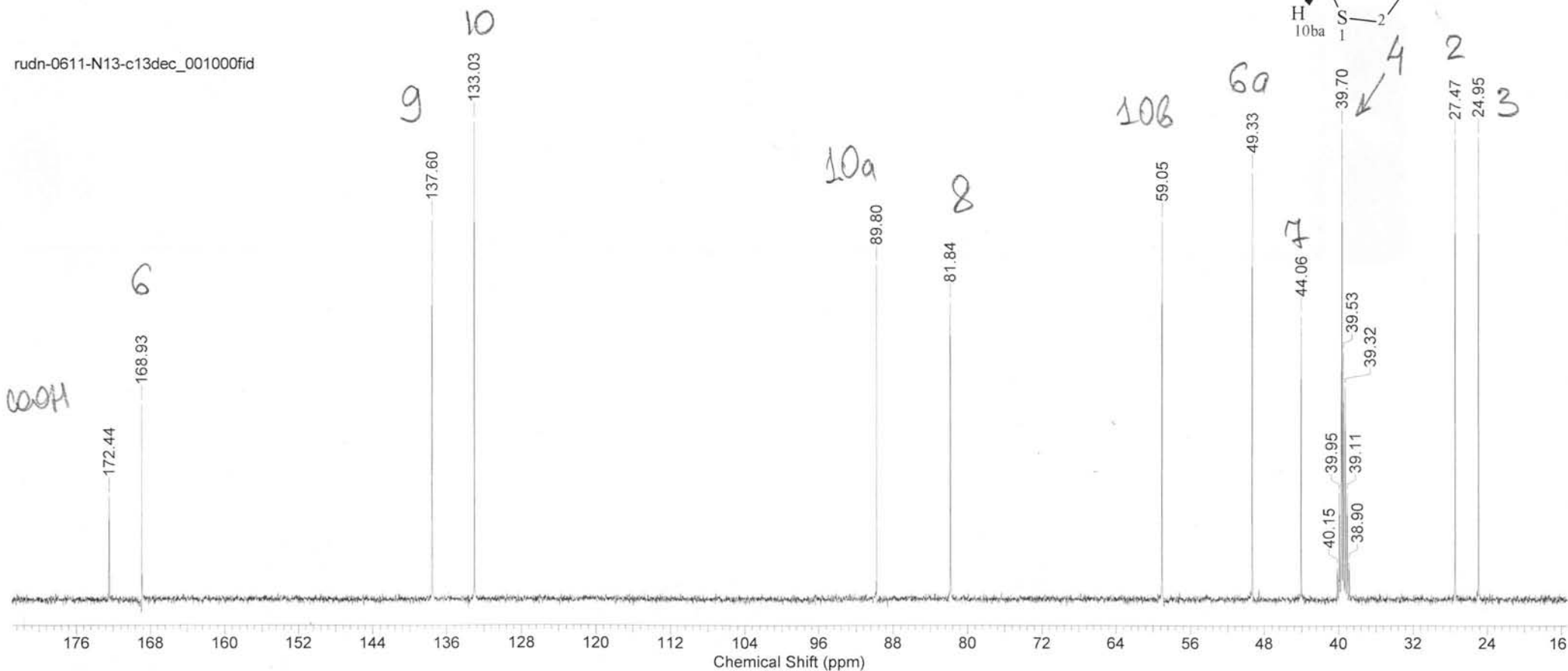


Formula C ₁₂ H ₁₃ NO ₄ S	FW 267.3009			
Acquisition Time (sec) 0.5243	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 08 Jul 2011 07:49:20		
Date Stamp 08 Jul 2011 07:49:20				
File Name D:\NMR\19.05.2011 C 13 Для Иры Статья в Тетраэдрон\rudn-0611-N13\rudn-0611-N13-c13dec\rudn-0611-N13-c13dec\rudn-0611-N13-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 750	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 31250.00	Solvent DMSO-d6	Spectrum Offset (Hz) 10553.1045	
Sweep Width (Hz) 31248.09	Temperature (degree C) 27.000			

Compound 31a

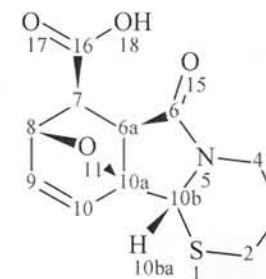


rudn-0611-N13-c13dec_001000fid

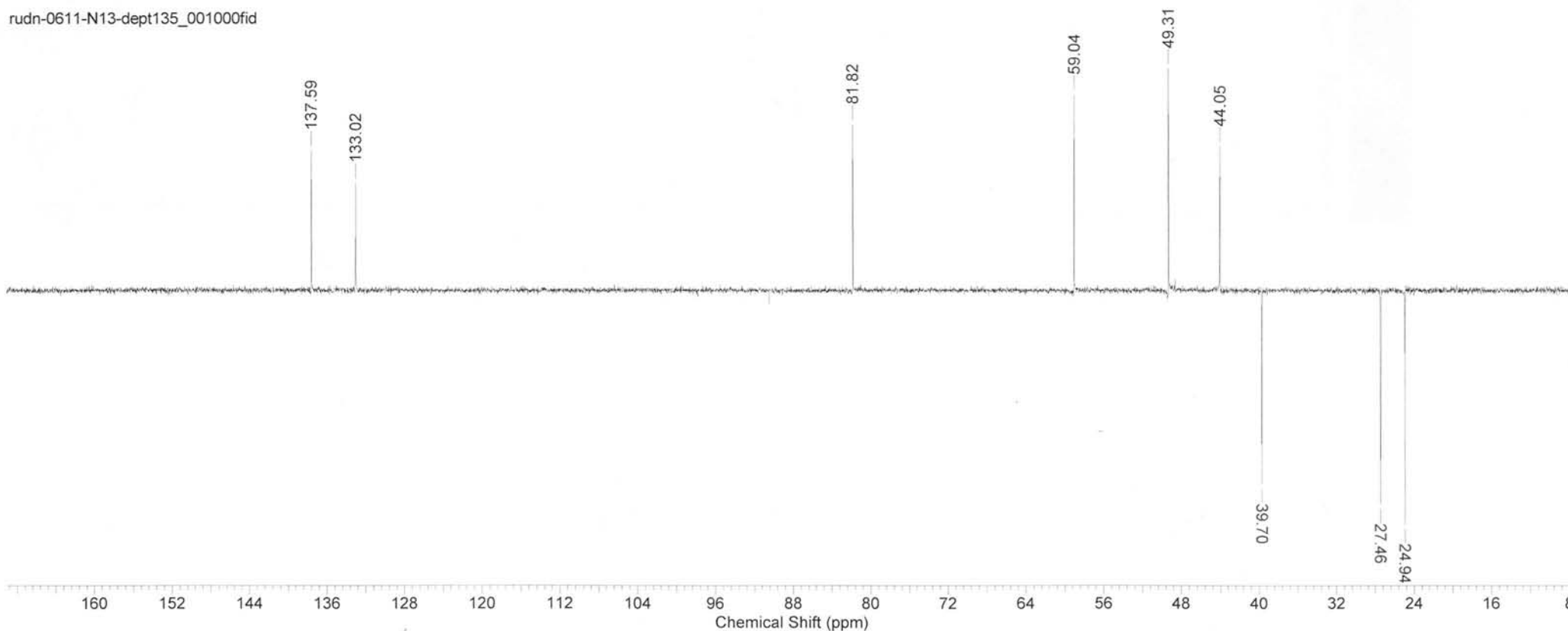


Formula C ₁₂ H ₁₃ NO ₄ S	FW 267.3009			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400		Date 08 Jul 2011 08:29:52	
Date Stamp 08 Jul 2011 08:29:52				
File Name D:\NMR\19.05.2011 C 13 Для Иры Статья в Тетраэдрон\rudn-0611-N13\rudn-0611-N13-dept135\rudn-0611-N13-dept135\rudn-0611-N13-dept135_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 750	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence dept135	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 9102.5918	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compound 31a

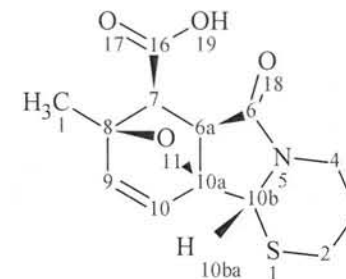


rudn-0611-N13-dept135_001000fid

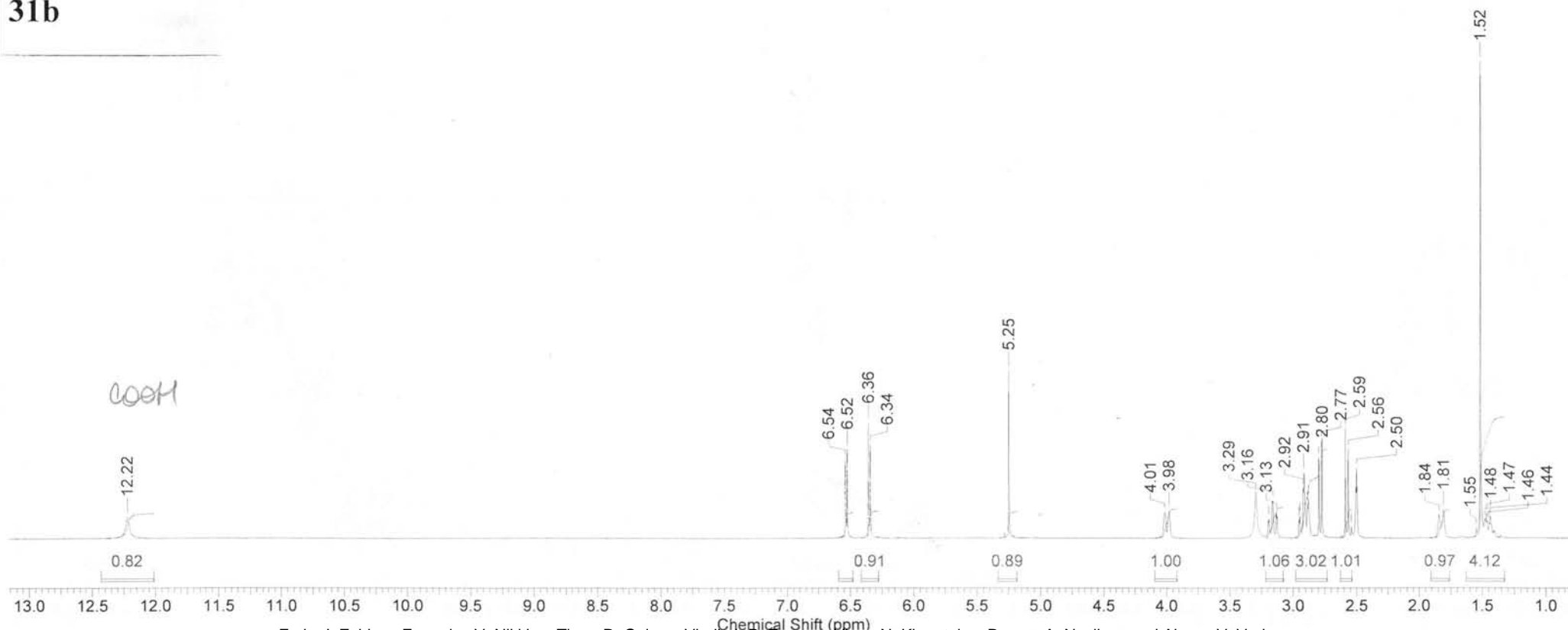


Formula C ₁₃ H ₁₅ NO ₄ S		FW 281.3275					
Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400				
Date Stamp	14 Jul 2011 10:05:52	Date	14 Jul 2011 10:05:52				
File Name	D:\NMR\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\rudn-0611-N41\rudn-0611-N41_001000fid		Frequency (MHz)	400.14			
Nucleus	1H	Number of Transients	12	Origin	spect	Original Points Count	16384
Owner	root	Points Count	16384	Pulse Sequence	zg	Receiver Gain	256.00
SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542	Sweep Width (Hz)	10416.03
Temperature (degree C)	32.000						

Compound 31b



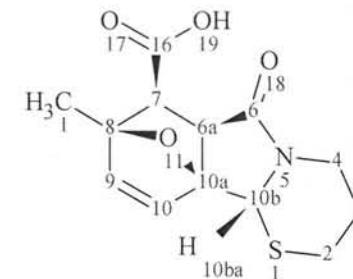
31b



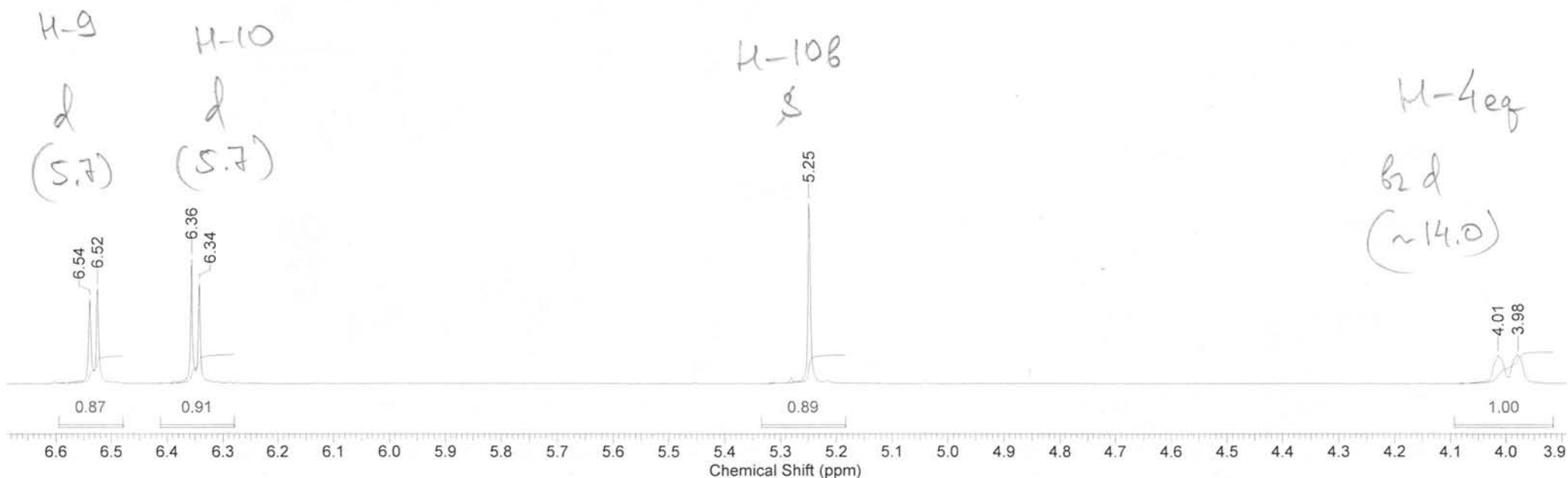
Formula C₁₃H₁₅NO₄S FW 281.3275

Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	14 Jul 2011 10:05:52	
Date Stamp	14 Jul 2011 10:05:52						
File Name	D:\NMR\19.05.2011 C 13 Для Иры Статья в Тетраэдрон\rudn-0611-N41\rudn-0611-N41_001000fid			Frequency (MHz)	400.14		
Nucleus	1H	Number of Transients	12	Origin	spect	Original Points Count	16384
Owner	root	Points Count	16384	Pulse Sequence	zg	Receiver Gain	256.00
SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542	Sweep Width (Hz)	10416.03
Temperature (degree C)	32.000						

Compound 31b



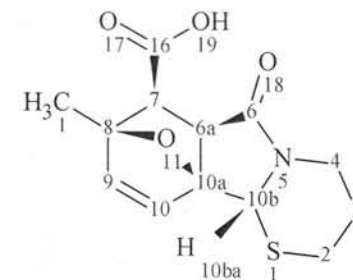
rudn-0611-N41_001000fid



Formula C₁₃H₁₅NO₄S FW 281.3275

Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	14 Jul 2011 10:05:52	
Date Stamp	14 Jul 2011 10:05:52						
File Name	D:\NMR\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\rudn-0611-N41\rudn-0611-N41_001000fid				Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	12	Origin	spect	Original Points Count	16384
Owner	root	Points Count	16384	Pulse Sequence	zg	Receiver Gain	256.00
SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542	Sweep Width (Hz)	10416.03
Temperature (degree C)	32.000						

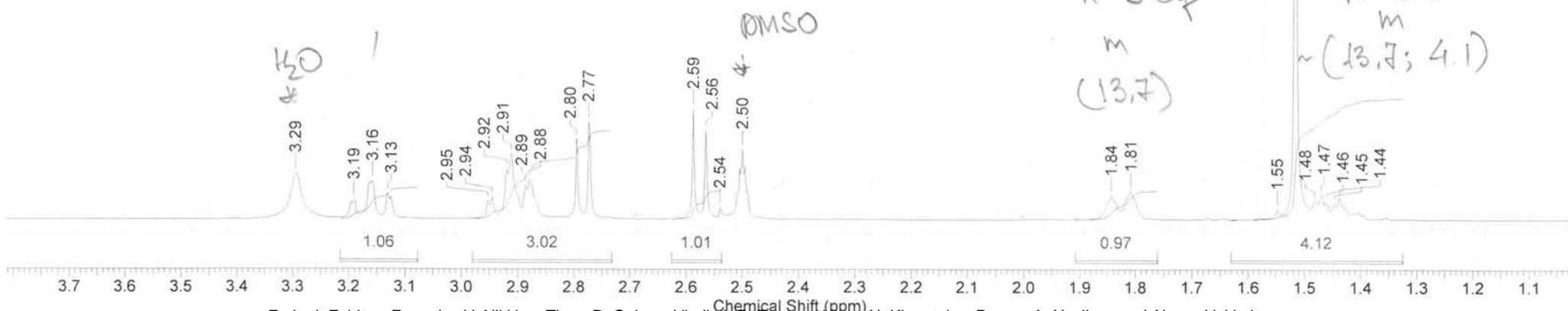
Compound 31b



rudn-0611-N41_001000fid

H-4ax, H-2eq
2.95-2.88
m, 2H

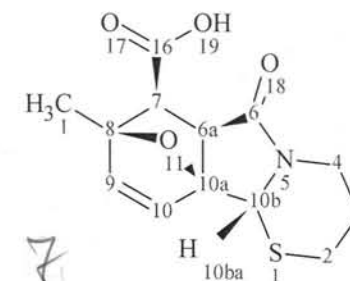
H-2ax dt (7.9; 13.5)
H-6a d (8.9)
H-7 d (8.9)



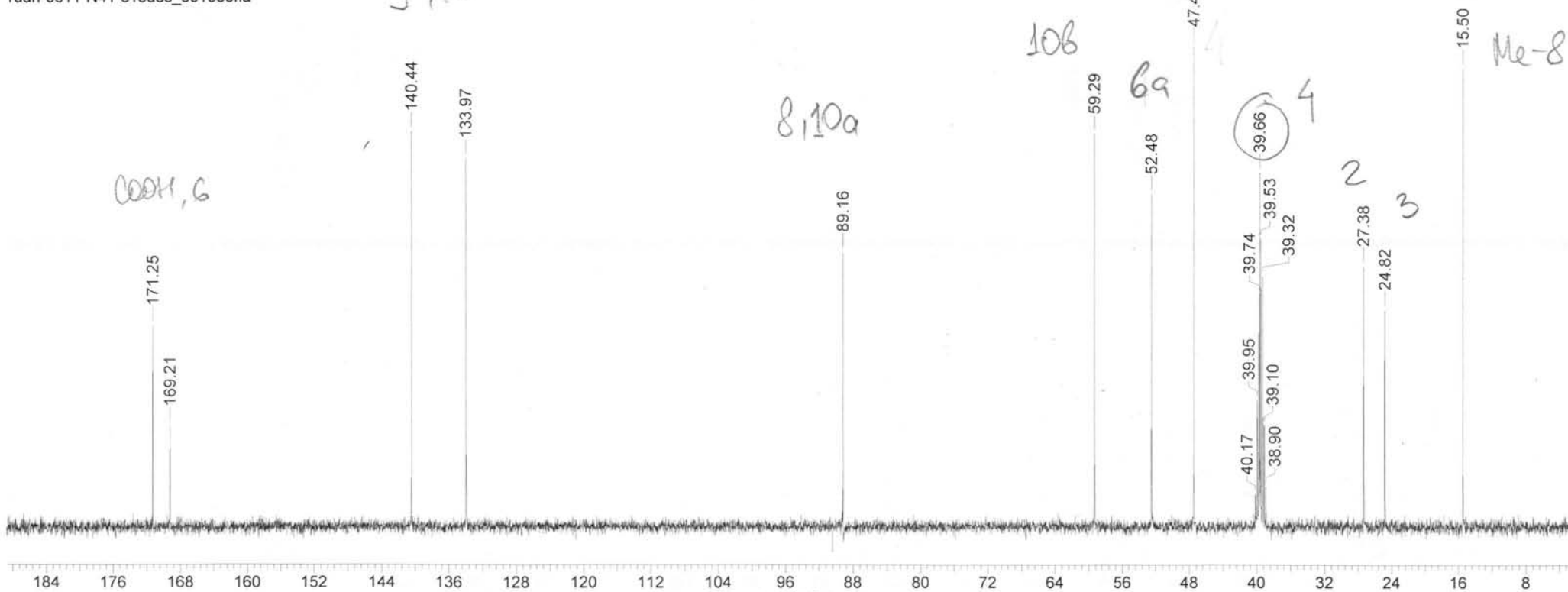
Formula C₁₃H₁₅NO₄S FW 281.3275

Acquisition Time (sec)	0.5898	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	14 Jul 2011 10:12:16	
Date Stamp	14 Jul 2011 10:12:16						
File Name	D:\NMR\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\rudn-0611-N41-c13dec\rudn-0611-N41-c13dec_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	435	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zgpg
Receiver Gain	32768.00	SW(cyclical) (Hz)	27777.78	Solvent	DMSO-d6	Spectrum Offset (Hz)	9099.9072
Sweep Width (Hz)	27776.08	Temperature (degree C)	27.000				

Compound 31b

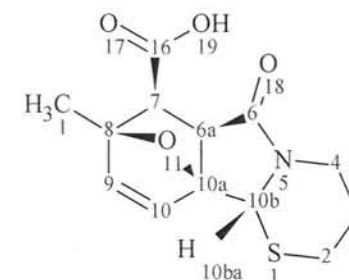


rudn-0611-N41-c13dec_001000fid

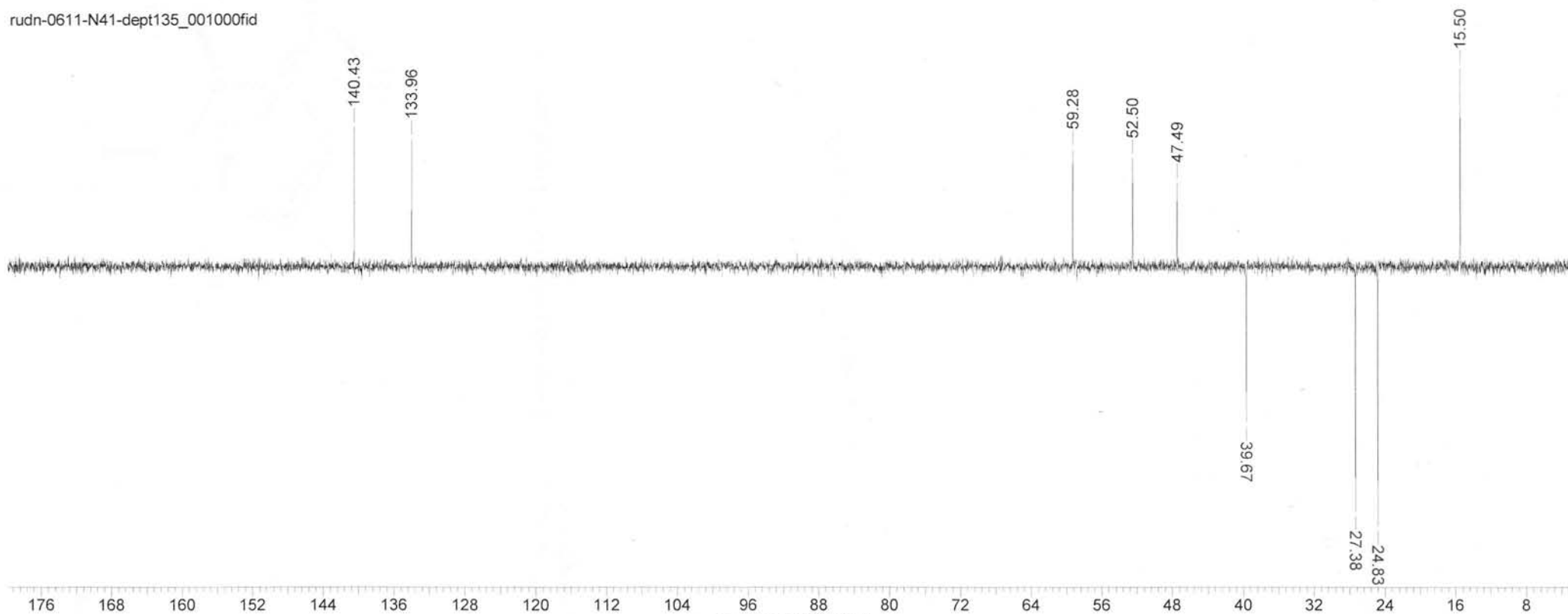


Formula C ₁₃ H ₁₅ NO ₄ S	FW 281.3275				
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 14 Jul 2011 10:22:56			
Date Stamp 14 Jul 2011 10:22:56					
File Name D:\NMR\19.05.2011 C 13 Для Иры Статья в Тетраэдрон\rudn-0611-N41-dept135\rudn-0611-N41-dept135_001000fid					
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 462	Origin spect		
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence dept135		
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent CHLOROFORM-d	Spectrum Offset (Hz) 9099.9863		
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000				

Compound 31b



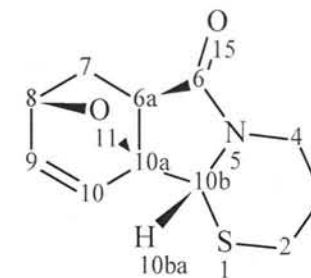
rudn-0611-N41-dept135_001000fid



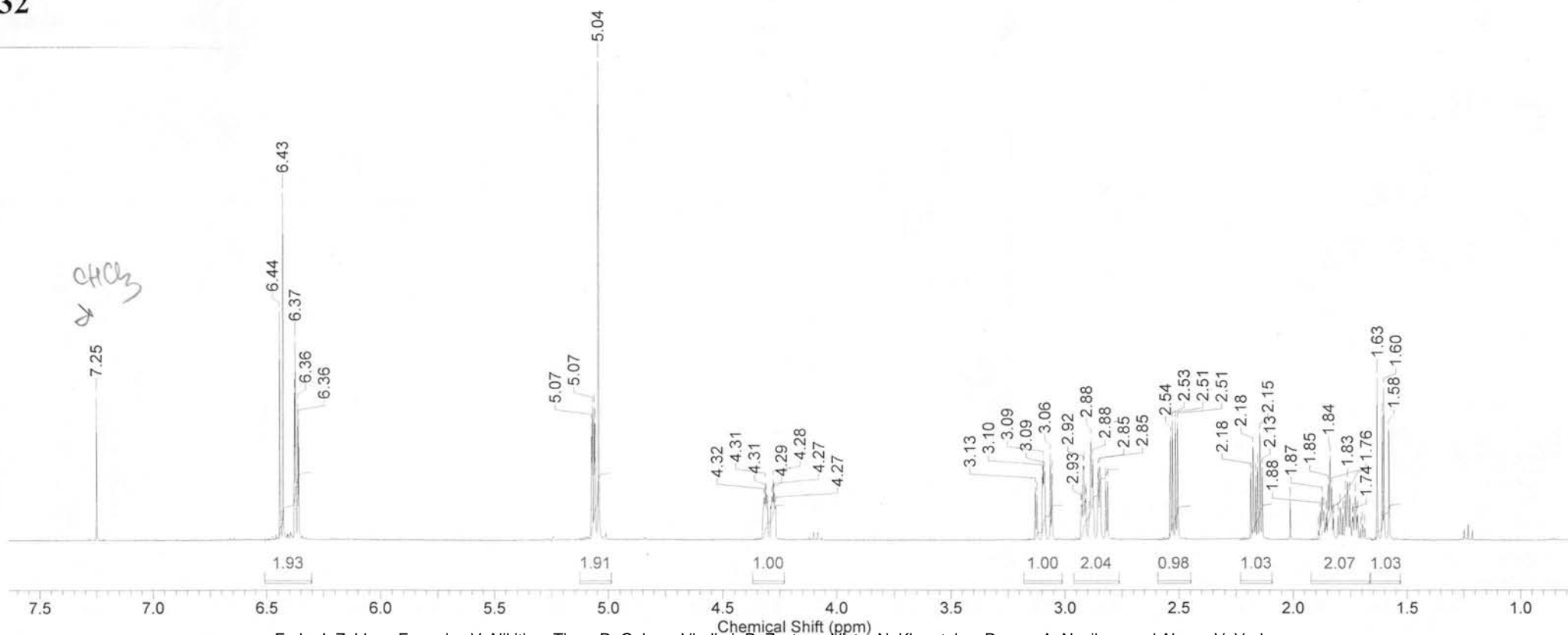
Formula $C_{11}H_{13}NO_2S$ FW 223.2914

Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	14 Jul 2011 08:53:20
Date Stamp	14 Jul 2011 08:53:20				
File Name	D:\NMR\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\rudn-0611-N14\rudn-0611-N14_002000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	16	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zg
SW(cyclical) (Hz)	10204.08	Solvent	CHLOROFORM-d	Receiver Gain	512.00
Sweep Width (Hz)	10203.46	Temperature (degree C)	27.000	Spectrum Offset (Hz)	2602.0486

Compound 32



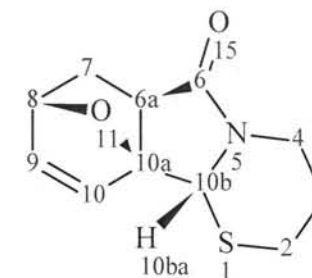
32



Formula $C_{11}H_{13}NO_2S$ FW 223.2914

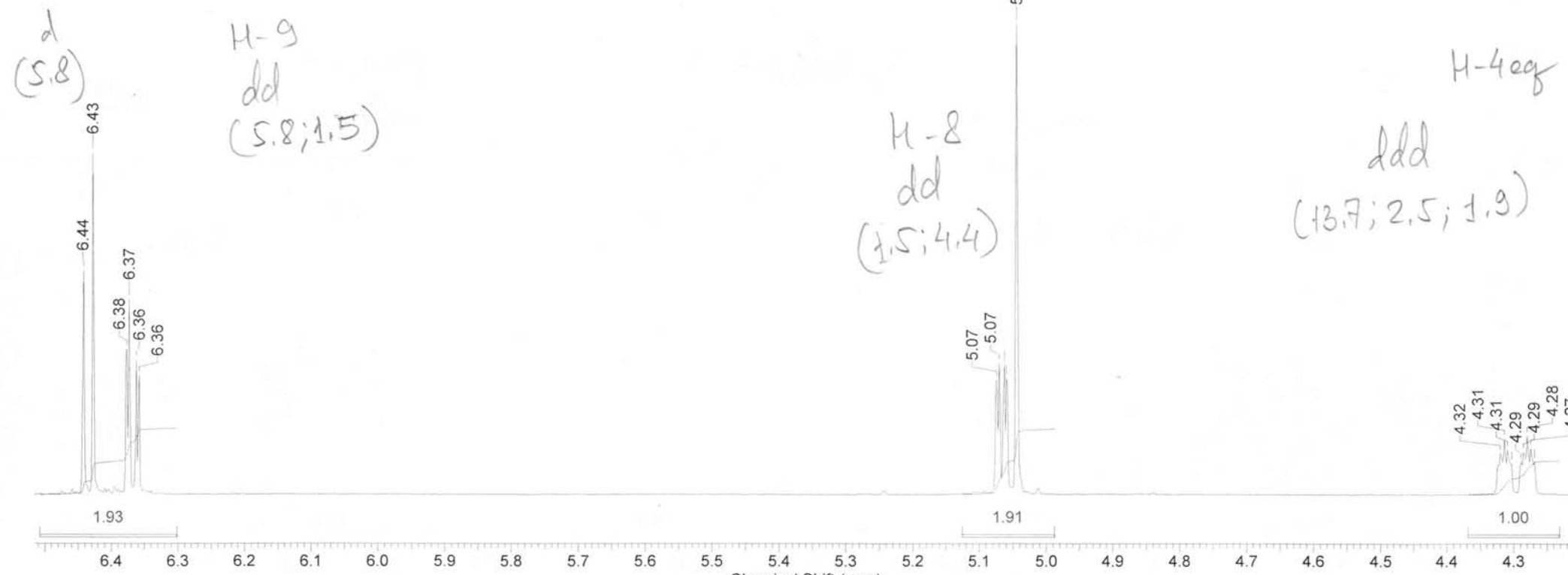
Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	14 Jul 2011 08:53:20
Date Stamp	14 Jul 2011 08:53:20				
File Name	D:\NMR\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\rudn-0611-N14\rudn-0611-N14_002000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	16	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zg
SW(cyclical) (Hz)	10204.08	Solvent	CHLOROFORM-d	Receiver Gain	512.00
Sweep Width (Hz)	10203.46	Temperature (degree C)	27.000	Spectrum Offset (Hz)	2602.0486

Compound 32



H-10

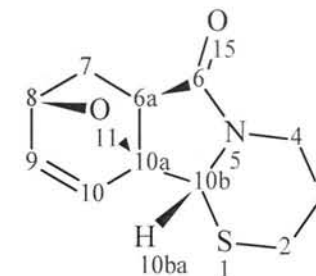
rudn-0611-N14_002000fid



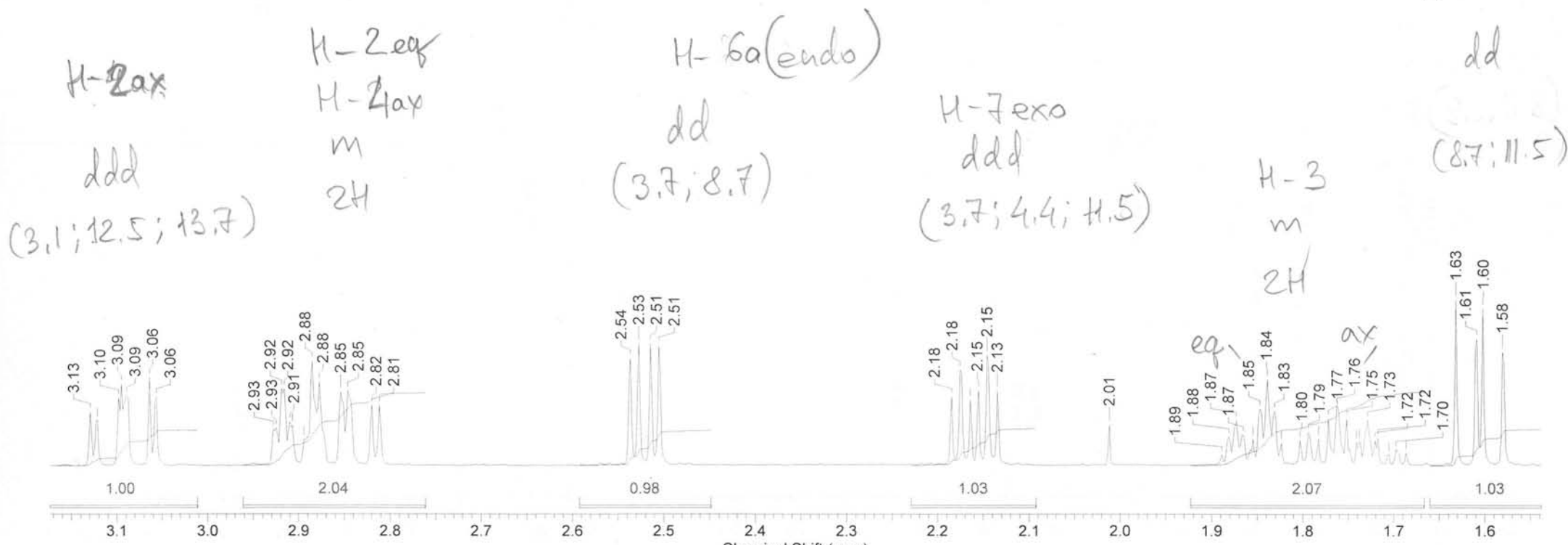
Formula C₁₁H₁₃NO₂S FW 223.2914

Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	14 Jul 2011 08:53:20	
Date Stamp	14 Jul 2011 08:53:20						
File Name	D:\NMR\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\rudn-0611-N14\rudn-0611-N14_002000fid			Frequency (MHz)	400.14		
Nucleus	1H	Number of Transients	16	Origin	spect	Original Points Count	16384
Owner	root	Points Count	16384	Pulse Sequence	zg	Receiver Gain	512.00
SW(cyclical) (Hz)	10204.08	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	2602.0486	
Sweep Width (Hz)	10203.46	Temperature (degree C)	27.000				

Compound 32

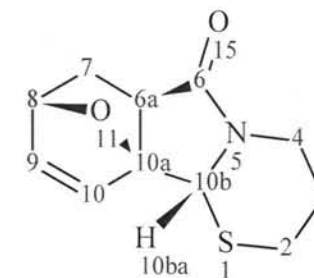


rudn-0611-N14_002000fid

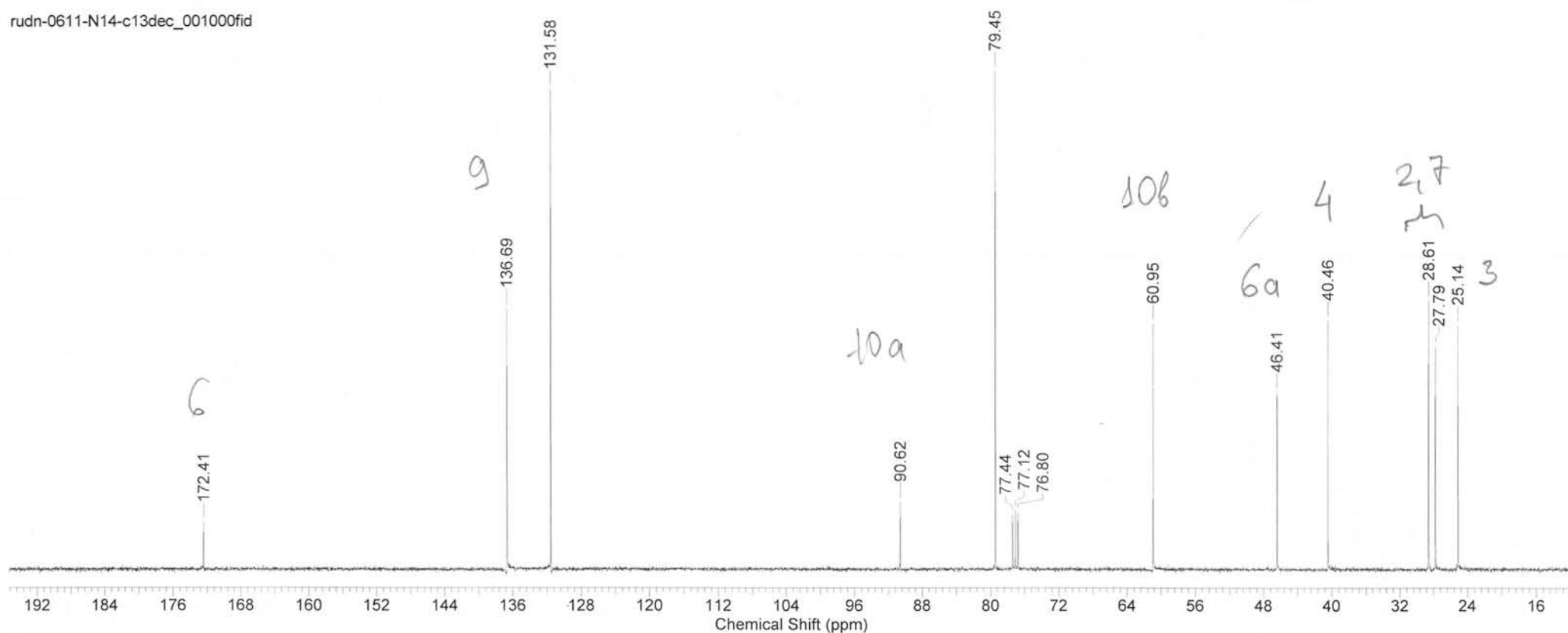


Formula	C ₁₁ H ₁₃ NO ₂ S	FW	223.2914				
Acquisition Time (sec)	0.5898	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400				
Date Stamp	14 Jul 2011 08:59:44	Date	14 Jul 2011 08:59:44				
File Name	D:\NMR\19.05.2011 C 13 Для Иры Статья в Тетраэдрон\rudn-0611-N14-c13dec\rudn-0611-N14-c13dec_001000fid		Frequency (MHz)	100.62			
Nucleus	13C	Number of Transients	523	Origin	spect	Original Points Count	16384
Owner	root	Points Count	16384	Pulse Sequence	zgpg	Receiver Gain	32768.00
SW(cyclical) (Hz)	27777.78	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9622.8369	Sweep Width (Hz)	27776.08
Temperature (degree C)	27.000						

Compound 32

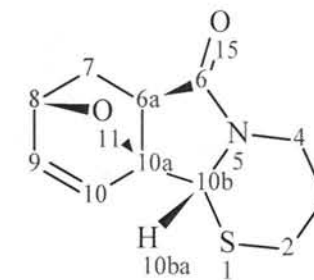


rudn-0611-N14-c13dec_001000fid

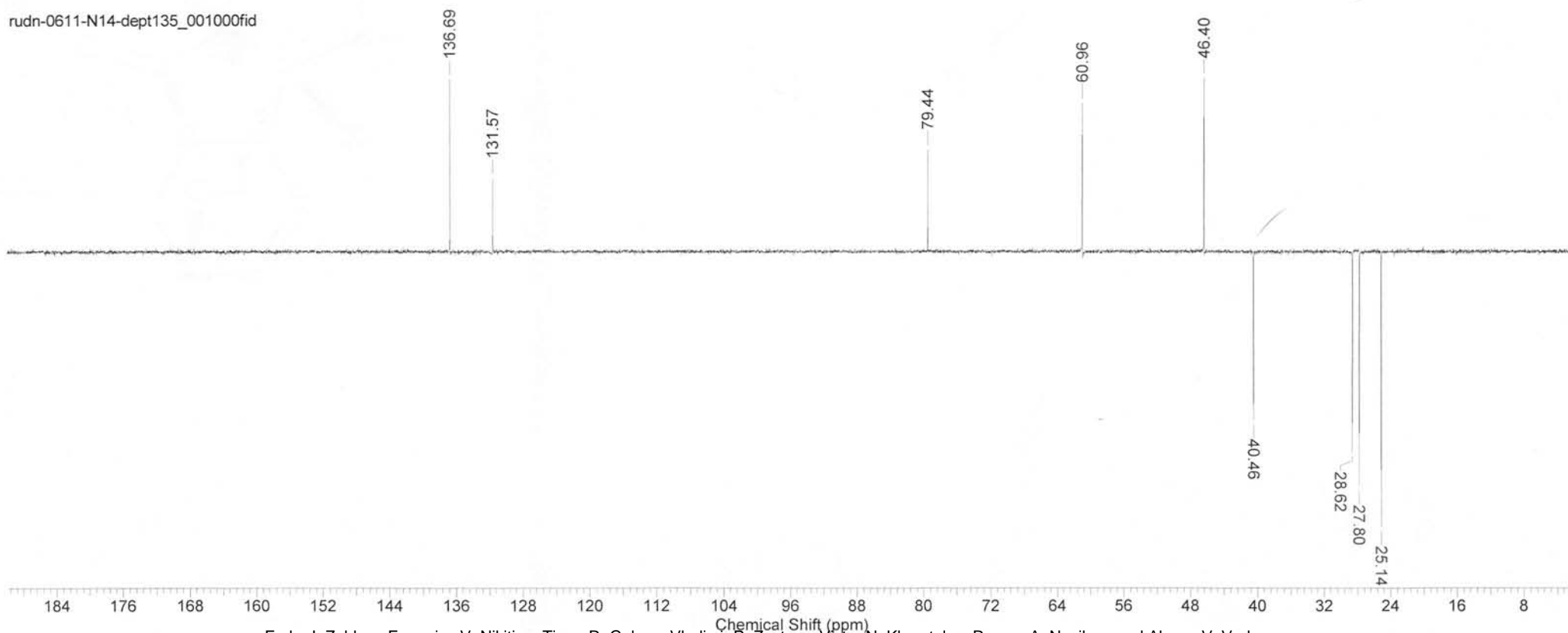


Formula C ₁₁ H ₁₃ NO ₂ S		FW 223.2914				
Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	14 Jul 2011 09:10:24
Date Stamp	14 Jul 2011 09:10:24					
File Name	D:\NMR\19.05.2011 C 13 Для Иры Статья в Тетраэдрон\rudn-0611-N14-dept135\rudn-0611-N14-dept135_001000fid			Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	1058	Origin	spect	
Owner	root	Points Count	16384	Pulse Sequence	dept135	
SW(cyclical) (Hz)	29411.77	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9622.9170	
Temperature (degree C)	27.000			Receiver Gain	32768.00	
				Sweep Width (Hz)	29409.97	

Compound 32



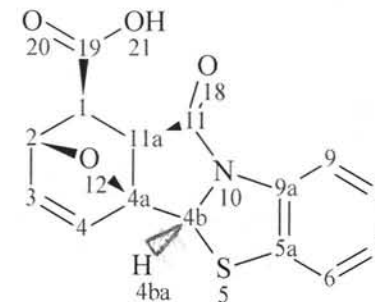
rudn-0611-N14-dept135_001000fid



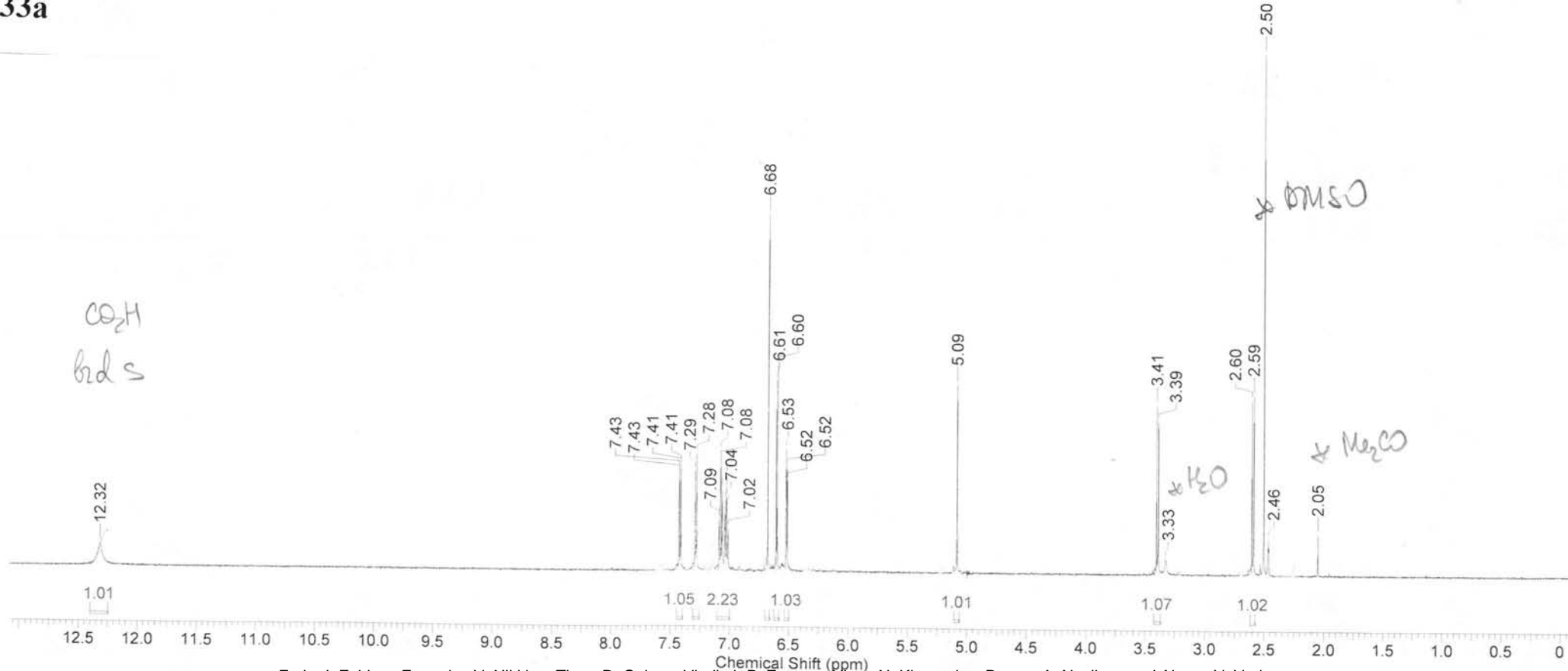
Formula C₁₅H₁₁NO₄S FW 301.3171

Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	13 Oct 2010 11:00:43	Date Stamp	13 Oct 2010 10:13:08
File Name	D:\NMR\11.10.2010\FZ1390-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	20.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3000.8616	Sweep Width (Hz)	11261.26
						Temperature (degree C)	18.800

Compound 33a



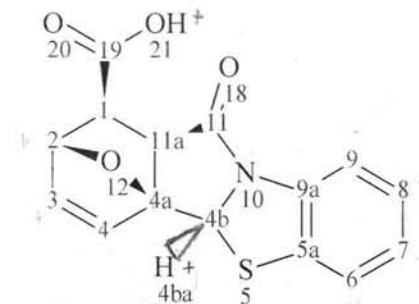
33a



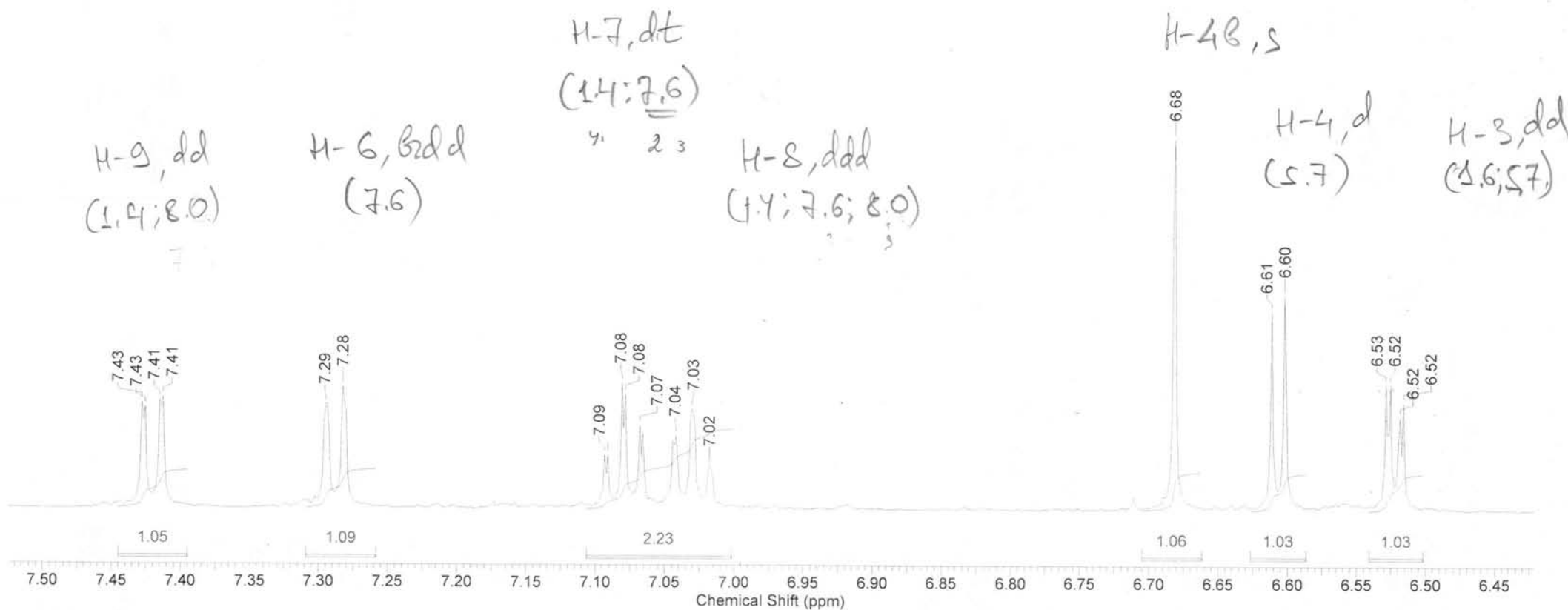
Formula $C_{15}H_{11}NO_4S$ FW 301.3171

Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	13 Oct 2010 11:00:43	Date Stamp	13 Oct 2010 10:13:08
File Name	D:\NMR\11.10.2010\FZ1390-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	20.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3000.8616	Sweep Width (Hz)	11261.26
						Temperature (degree C)	18.800

Compound 33a



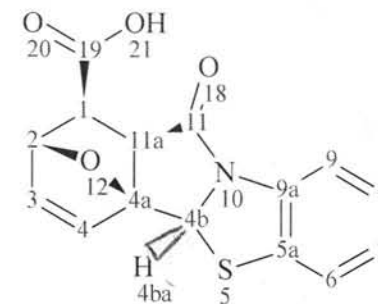
FZ1390-1.jdf



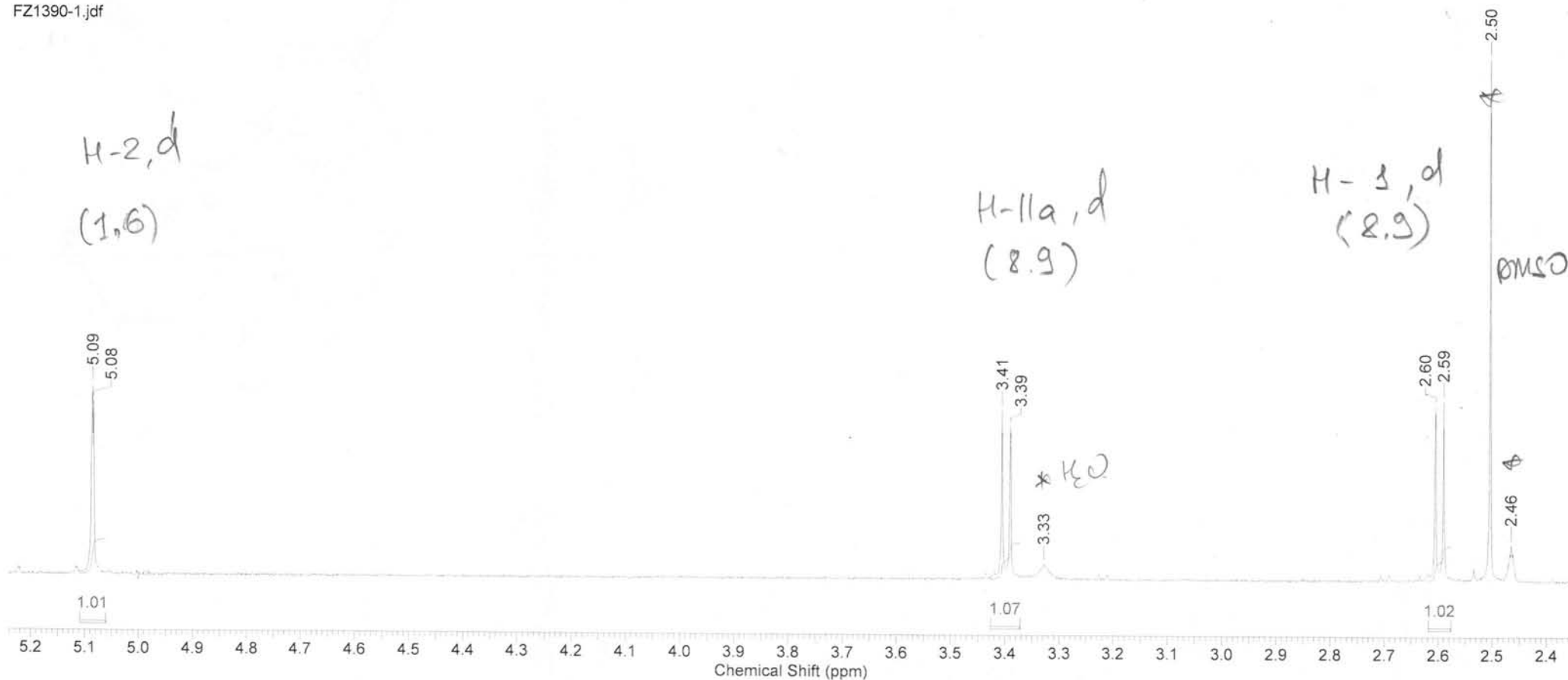
Formula C₁₅H₁₁NO₄S FW 301.3171

Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	13 Oct 2010 11:00:43	Date Stamp	13 Oct 2010 10:13:08
File Name	D:\NMR\11.10.2010\FZ1390-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	20.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3000.8616	Sweep Width (Hz)	11261.26
						Temperature (degree C)	18.800

Compound 33a



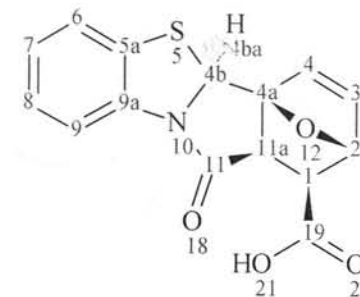
FZ1390-1.jdf



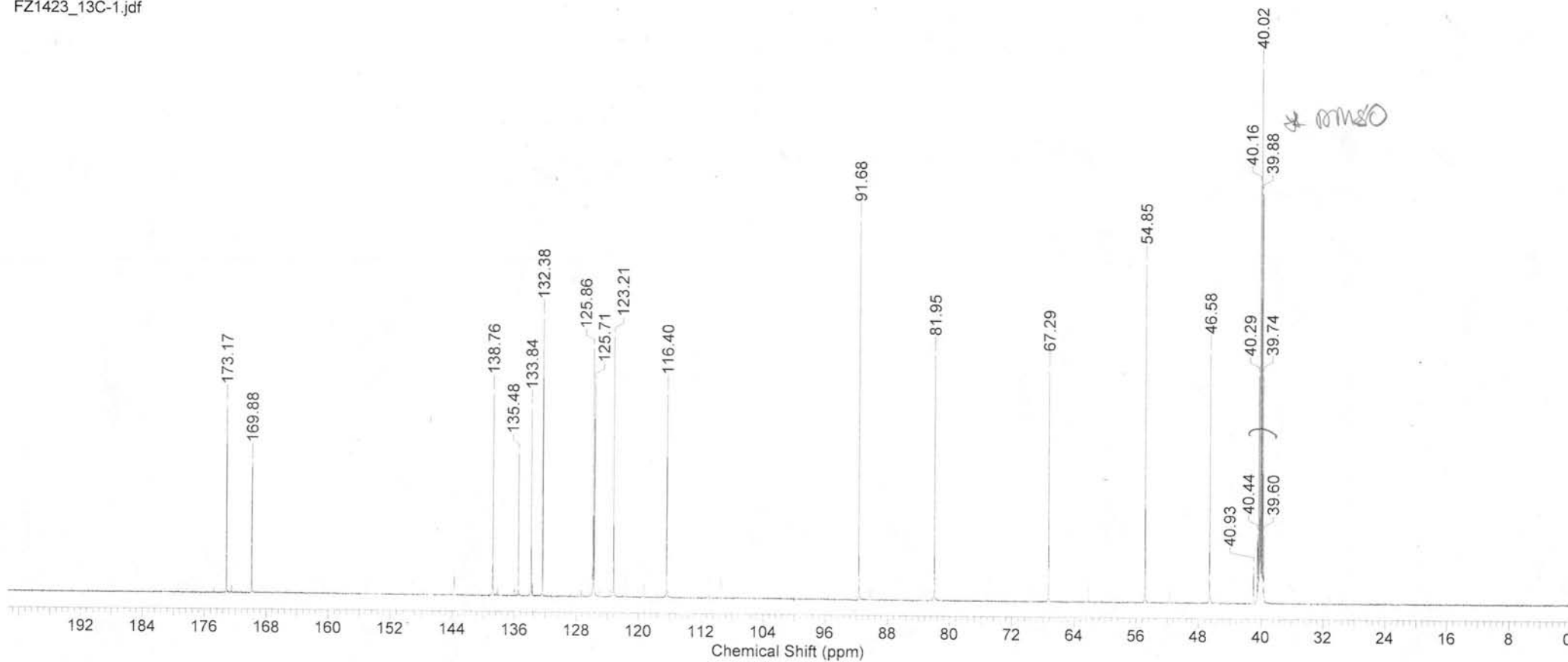
Formula C₁₅H₁₁NO₄S FW 301.3171

Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	27 Oct 2010 08:52:03
Date Stamp	27 Oct 2010 08:04:42	File Name	D:\NMR\22.10.10\FZ1423_13C-1.jdf	Frequency (MHz)	150.91
Nucleus	13C	Number of Transients	10000	Origin	ECA 600
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49	Receiver Gain	56.00
		Temperature (degree C)	22.300	Solvent	DMSO-d6

Compound 33a



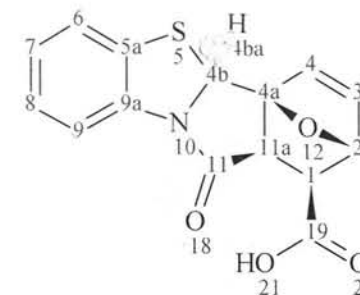
FZ1423_13C-1.jdf



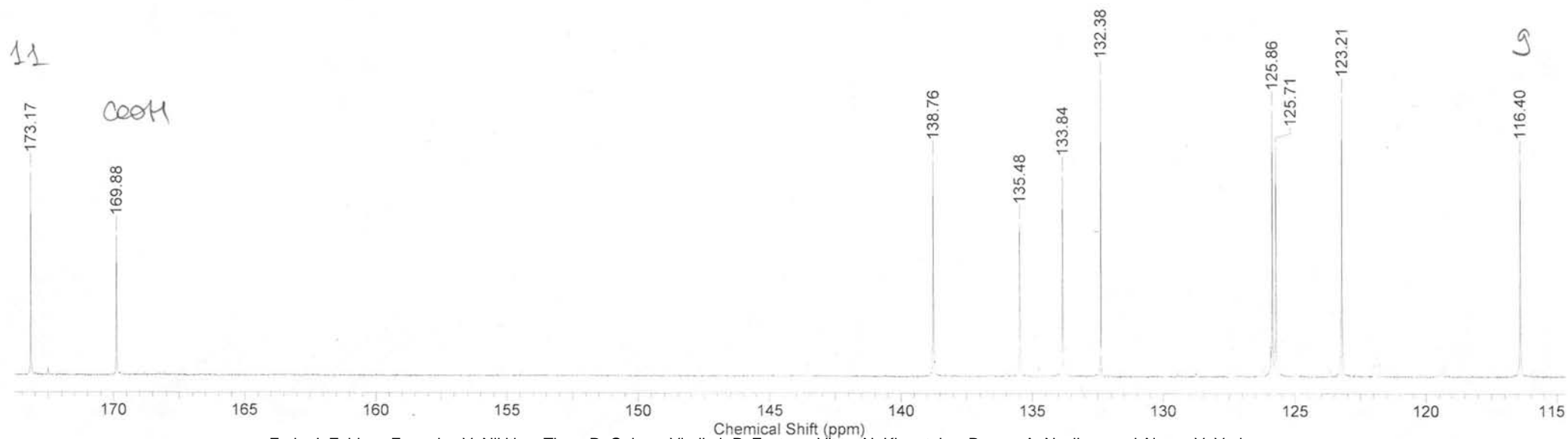
Formula C₁₅H₁₁NO₄S FW 301.3171

Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	27 Oct 2010 08:52:03	
Date Stamp	27 Oct 2010 08:04:42	File Name	D:\NMR\22.10.10\FZ1423_13C-1.jdf		Frequency (MHz)	150.91	
Nucleus	13C	Number of Transients	10000	Origin	ECA 600	Original Points Count	32768
Points Count	32768	Pulse Sequence	single_pulse_dec	Receiver Gain	56.00	Owner	delta
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49	Temperature (degree C)	22.300	Solvent	DMSO-d6

Compound 33a



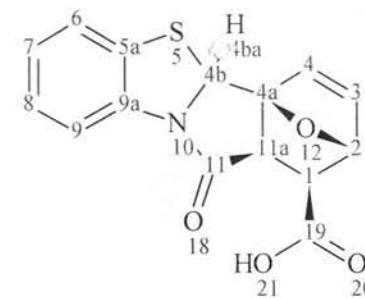
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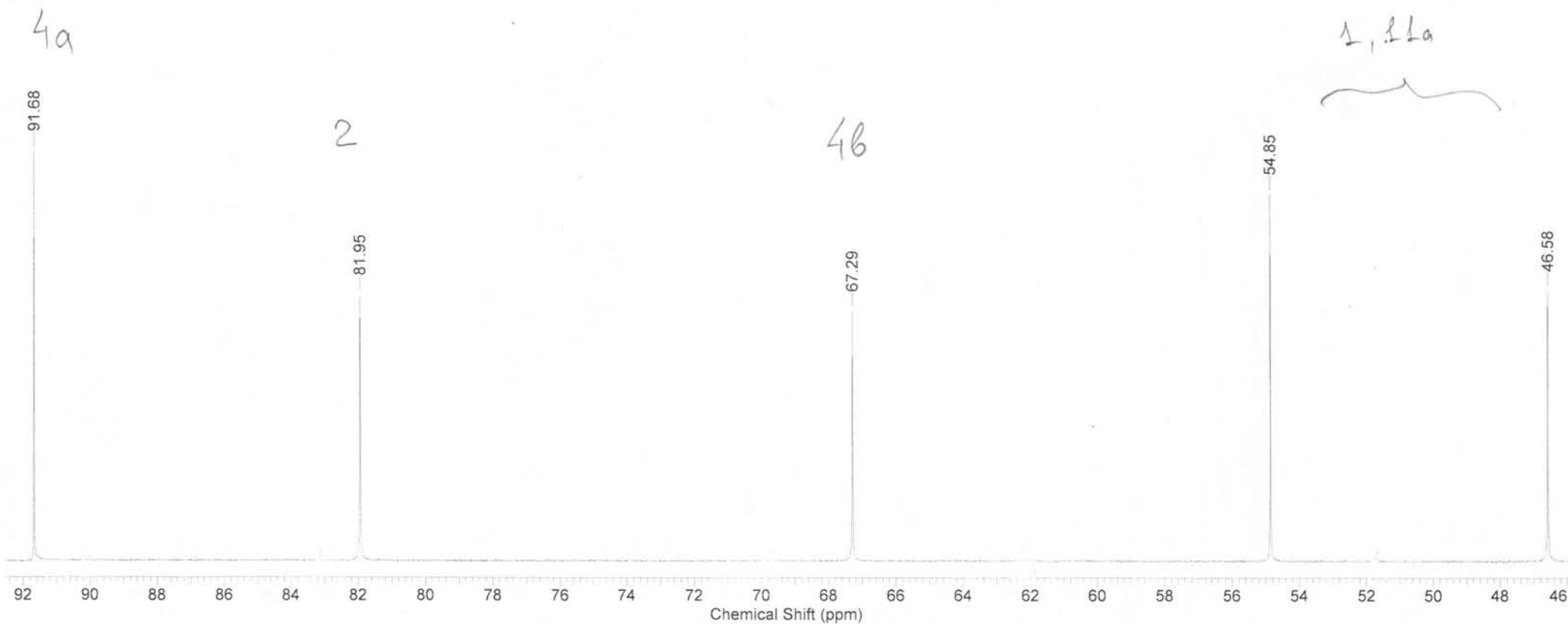
Formula C₁₅H₁₁NO₄S FW 301.3171

Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	27 Oct 2010 08:52:03
Date Stamp	27 Oct 2010 08:04:42	File Name	D:\NMR\22.10.10\FZ1423_13C-1.jdf	Frequency (MHz)	150.91
Nucleus	13C	Number of Transients	10000	Origin	ECA 600
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49	Receiver Gain	56.00
		Temperature (degree C)	22.300	Owner	delta
				Solvent	DMSO-d6

Compound 33a



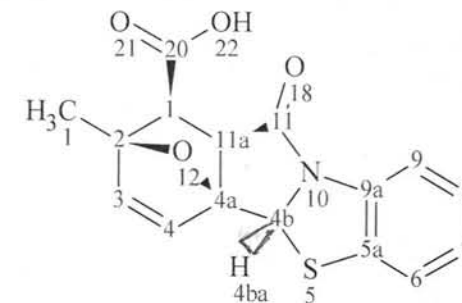
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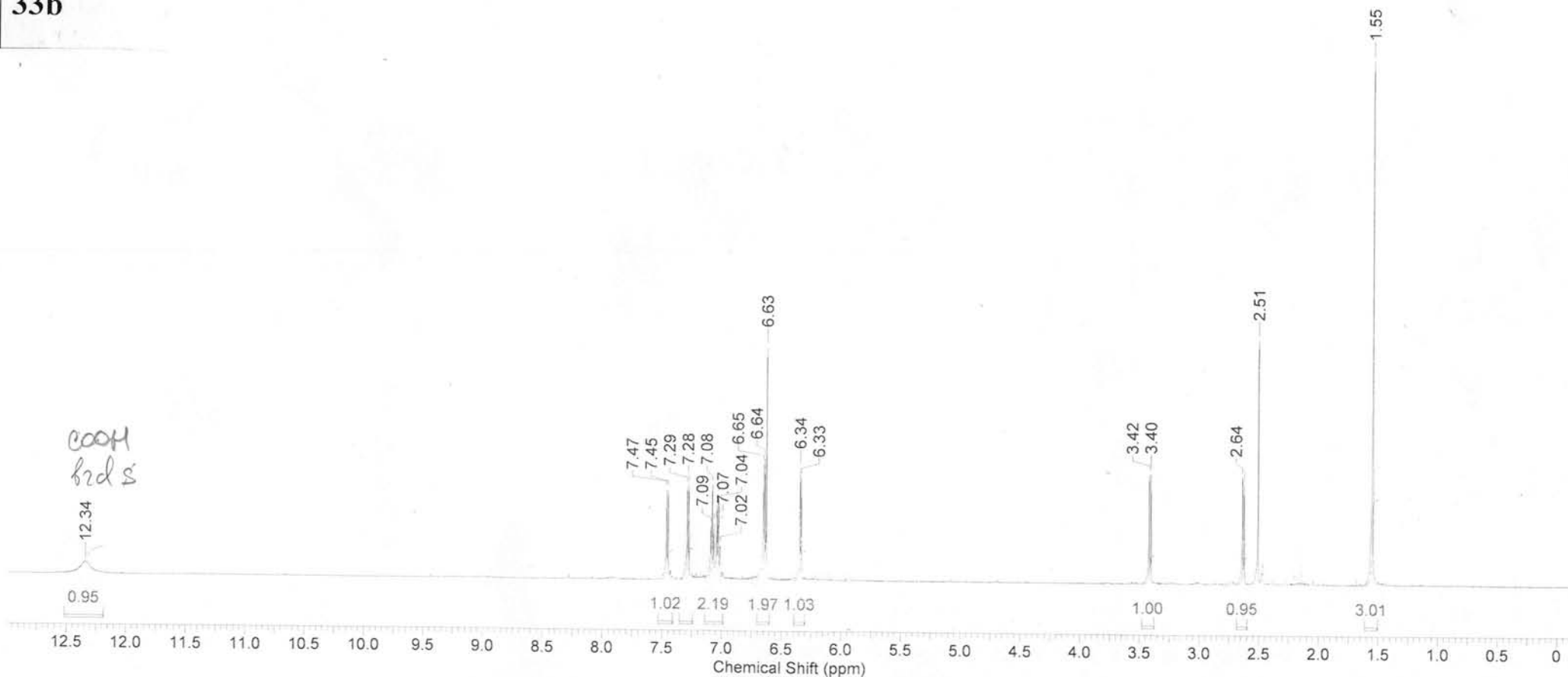
Formula C₁₆H₁₃NO₄S FW 315.3437

Acquisition Time (sec)	1.0905	Comment	single_pulse	Date	07 Dec 2010 12:22:41		Date Stamp	07 Dec 2010 11:34:24		
File Name	D:\NMR\06.12.10\FZ1525-1.jdf		Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	10		
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384		Pulse Sequence	single_pulse.ex2
Receiver Gain	44.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	4201.2061	Sweep Width (Hz)	15024.04			

Compound 33b



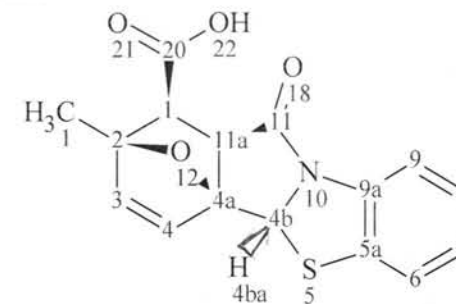
33b



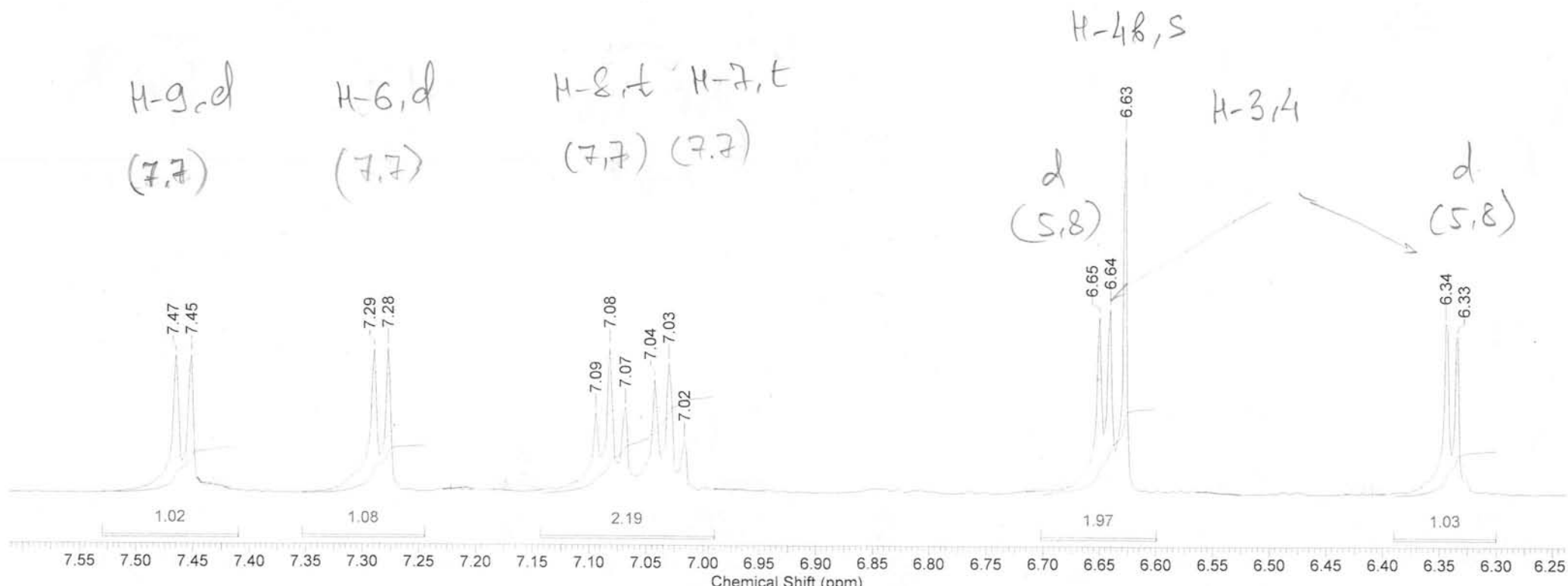
Formula C₁₆H₁₃NO₄S FW 315.3437

Acquisition Time (sec)	1.0905	Comment	single_pulse	Date	07 Dec 2010 12:22:41	Date Stamp	07 Dec 2010 11:34:24
File Name	D:\NMR\06.12.10\FZ1525-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	10
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	44.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	4201.2061	Sweep Width (Hz)	15024.04
						Pulse Sequence	single_pulse.ex2

Compound 33b



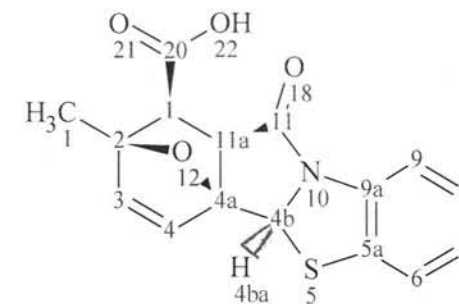
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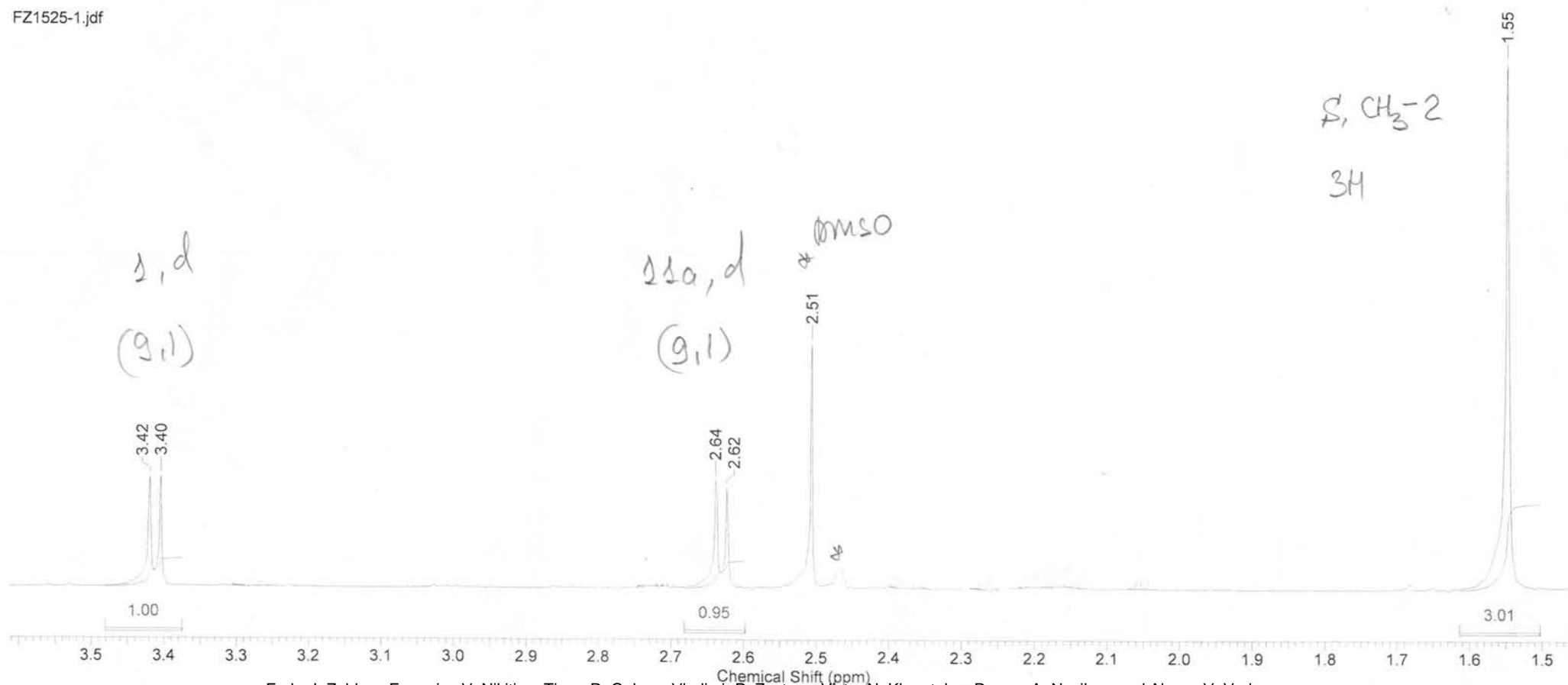
Formula C₁₆H₁₃NO₄S FW 315.3437

Acquisition Time (sec)	1.0905	Comment	single_pulse	Date	07 Dec 2010 12:22:41	Date Stamp	07 Dec 2010 11:34:24
File Name	D:\NMR\06.12.10\FZ1525-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	10
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	44.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	4201.2061	Sweep Width (Hz)	15024.04
						Pulse Sequence	single_pulse.ex2

Compound 33b



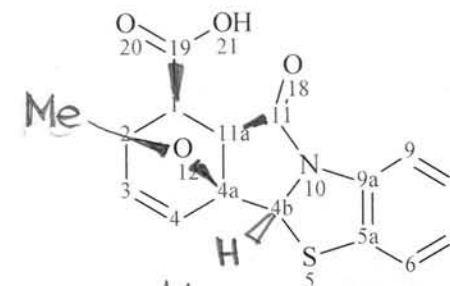
FZ1525-1.jdf



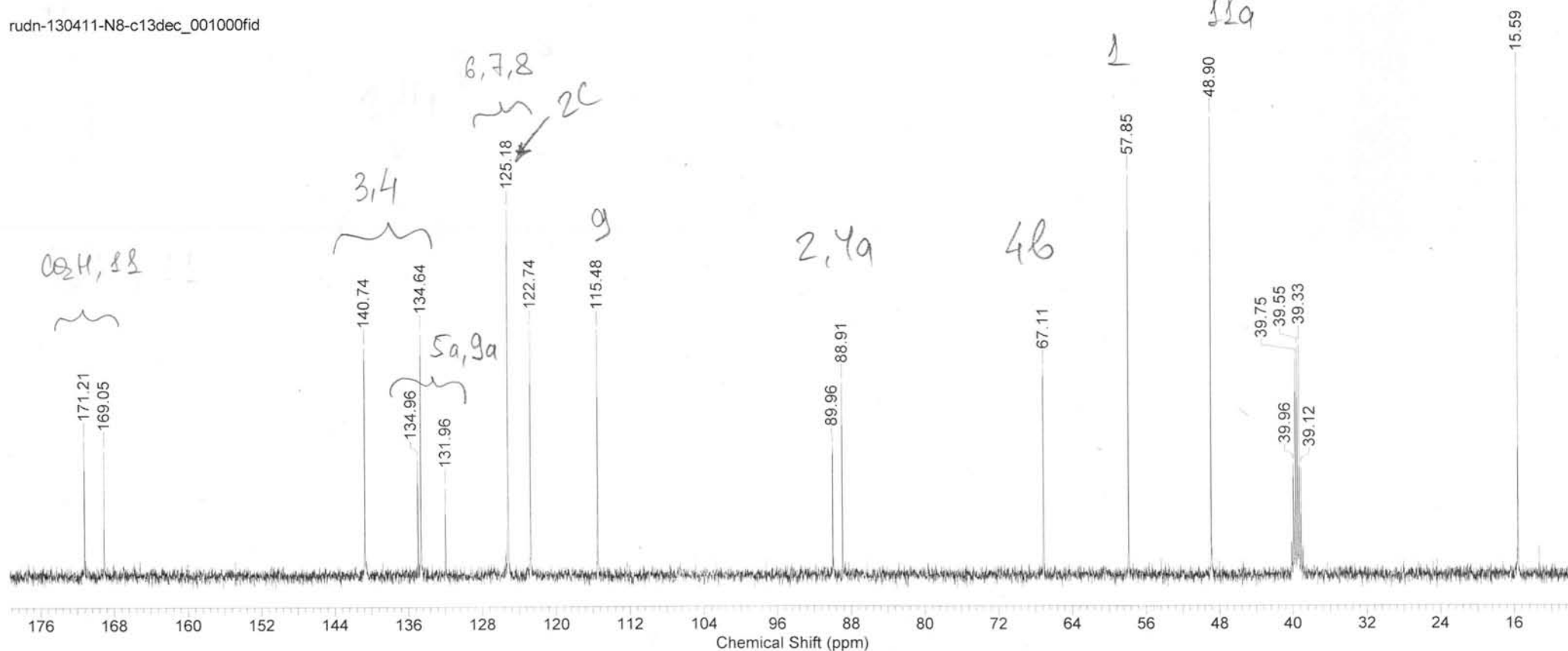
Formula C₁₅H₁₁NO₄S FW 301.3171

Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	14 Apr 2011 06:49:36
Date Stamp	14 Apr 2011 06:49:36	File Name	D:\NMR\13.04.2011 C-13\rudn-130411-N8-c13dec\rudn-130411-N8-c13dec_001000fid		
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	299
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6
Sweep Width (Hz)	29409.97	Temperature (degree C)	32.000	Spectrum Offset (Hz)	10552.5586

Compound 33b



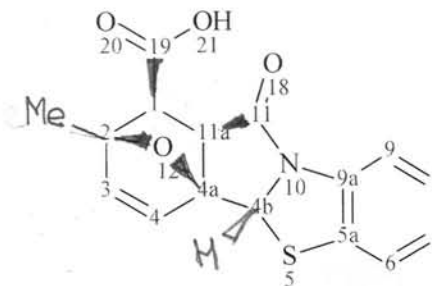
rudn-130411-N8-c13dec_001000fid



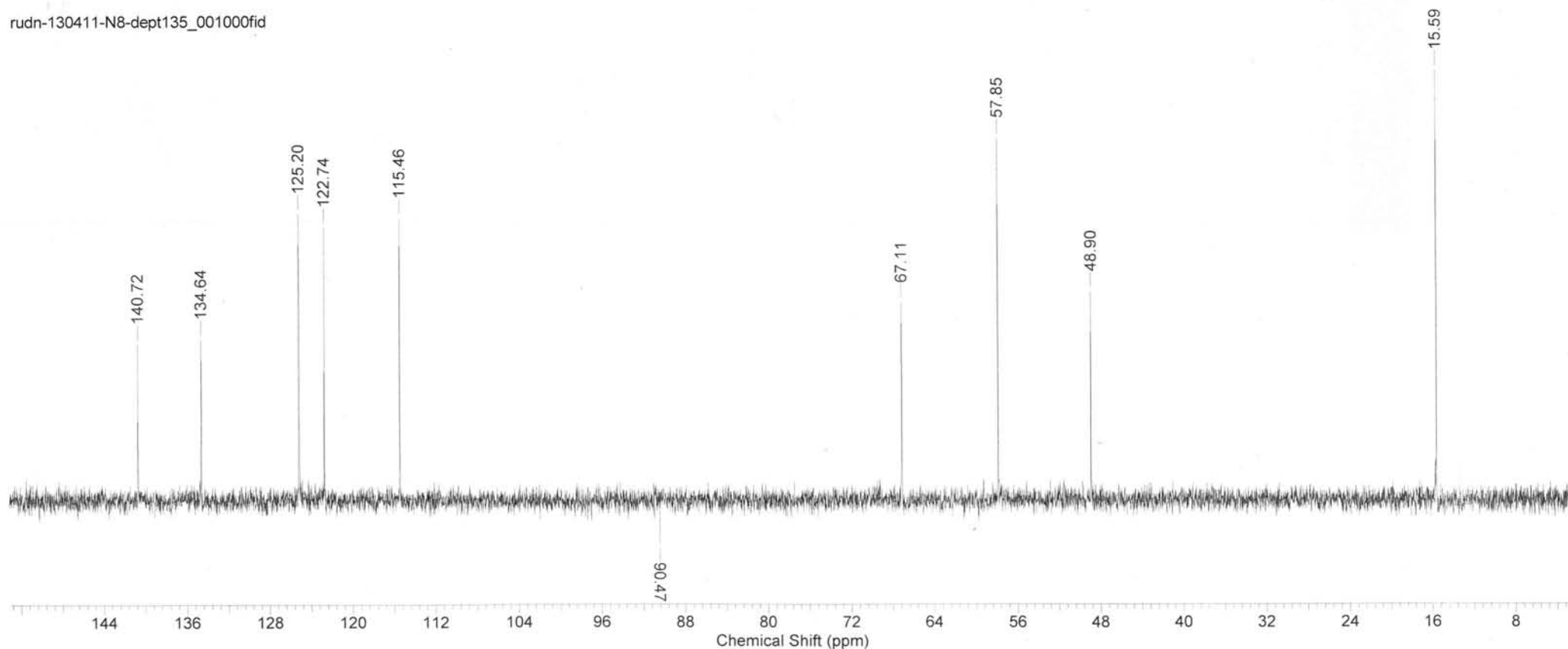
Formula C₁₅H₁₁NO₄S FW 301.3171

Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	14 Apr 2011 06:56:00
Date Stamp	14 Apr 2011 06:56:00	File Name	D:\NMR\13.04.2011 C-13\rudn-130411-N8-dept135\rudn-130411-N8-dept135_001000fid	Origin	spect
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	201
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Pulse Sequence	dept135
Sweep Width (Hz)	29409.97	Temperature (degree C)	32.000	Solvent	DMSO-d6
				Spectrum Offset (Hz)	9102.1396

Compound 33b

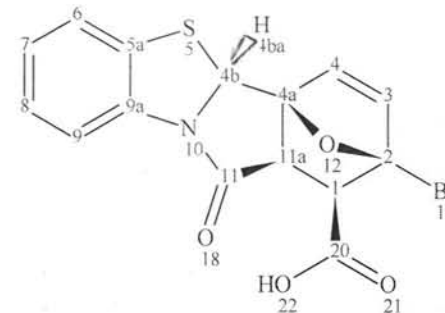


rudn-130411-N8-dept135_001000fid

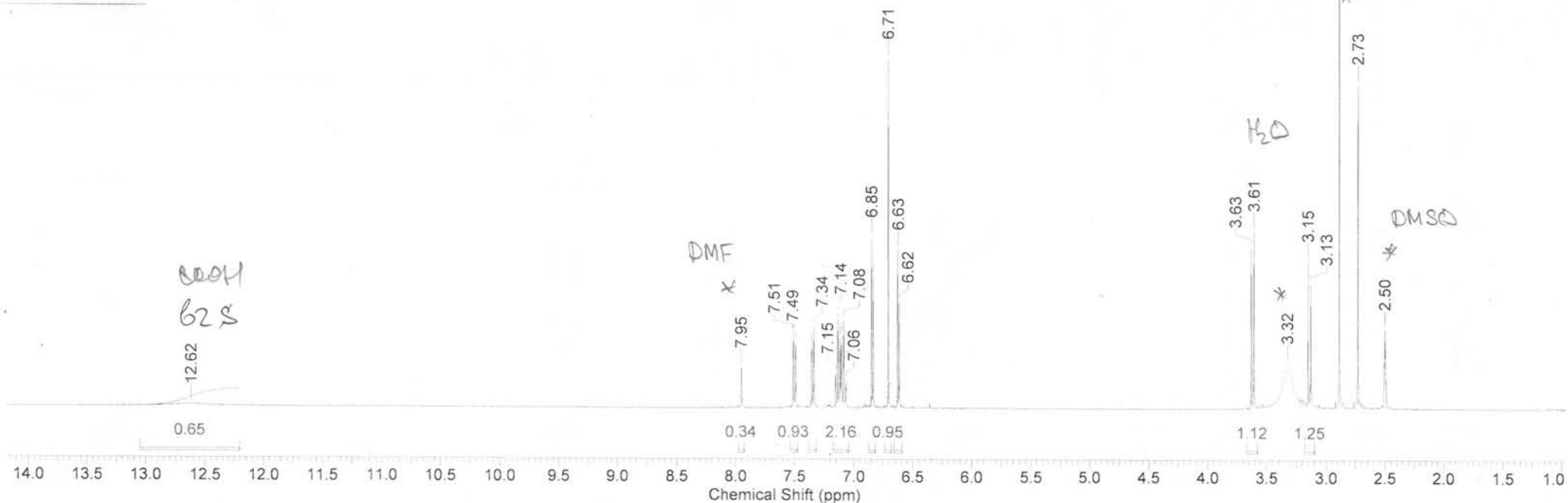


Acquisition Time (sec)	1.5729	Comment	Imported from UXMNR.		Date	04 Feb 2011 15:23:44	
File Name	D:\NMR\31.01.11\z1646\z1646_001000fid	Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	16
Original Points Count	16384	Points Count	16384	Pulse Sequence	zg	Solvent	DMSO-D6
Temperature (degree C)	27.000					Sweep Width (Hz)	10416.67

Compound 33c

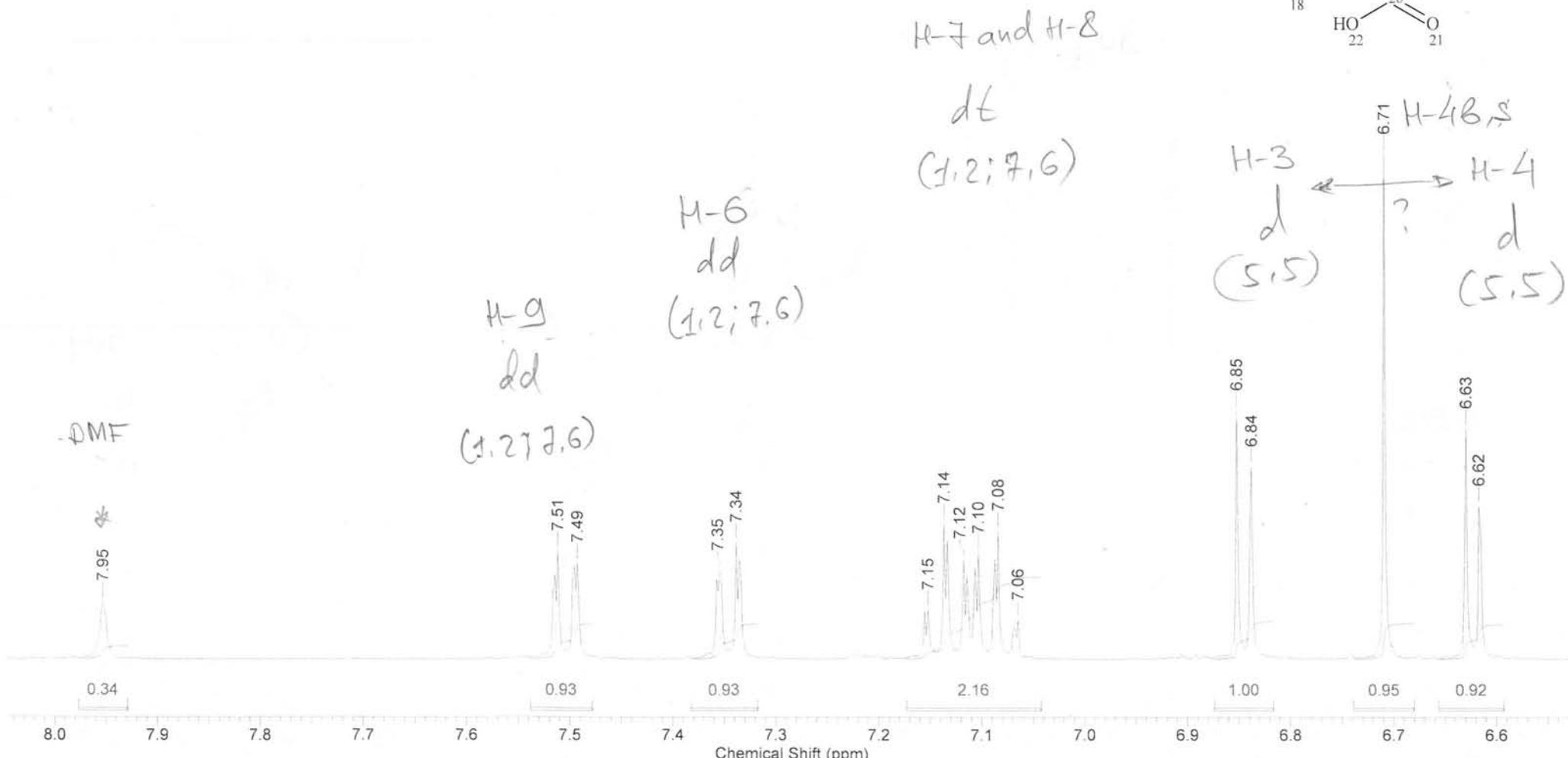
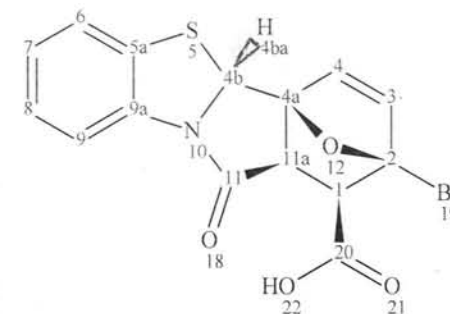


33c



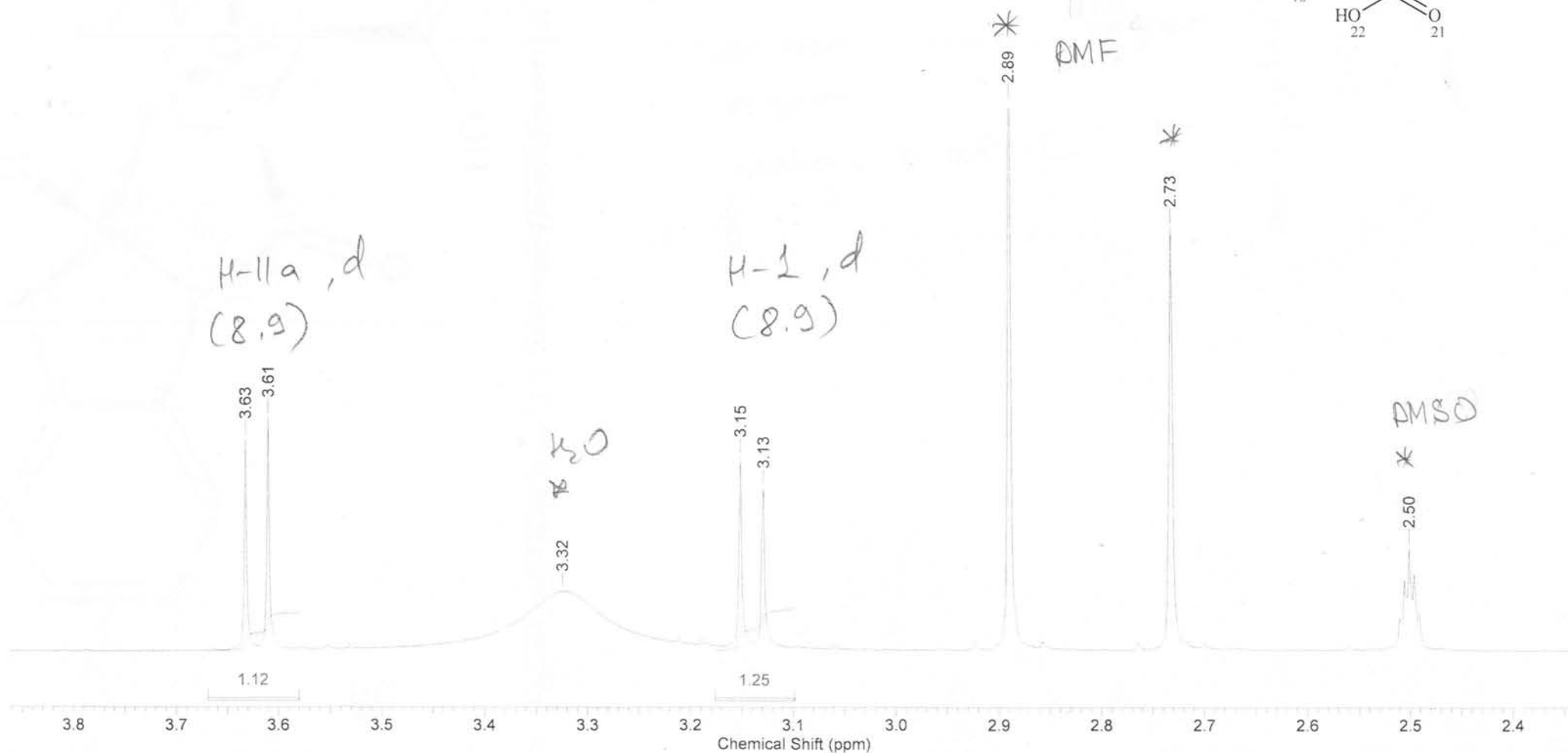
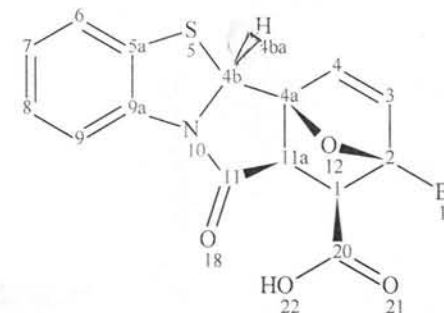
Acquisition Time (sec)	1.5729	Comment	Imported from UXMNR.		Date	04 Feb 2011 15:23:44	
File Name	D:\NMR\31.01.11\z1646\z1646_001000fid	Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	16
Original Points Count	16384	Points Count	16384	Pulse Sequence	zg	Sweep Width (Hz)	10416.67
Temperature (degree C)	27.000						

Compound 33c



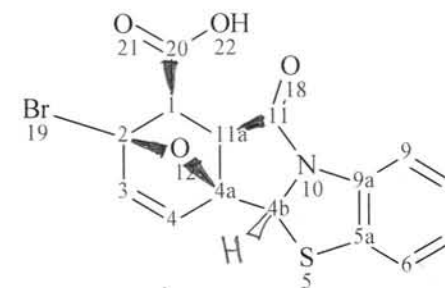
Acquisition Time (sec)	1.5729	Comment	Imported from UXNMR.		Date	04 Feb 2011 15:23:44	
File Name	D:\NMR\31.01.11\1646\1646_001000fid	Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	16
Original Points Count	16384	Points Count	16384	Pulse Sequence	zg	Solvent	DMSO-D6
Temperature (degree C)	27.000					Sweep Width (Hz)	10416.67

Compound 33c

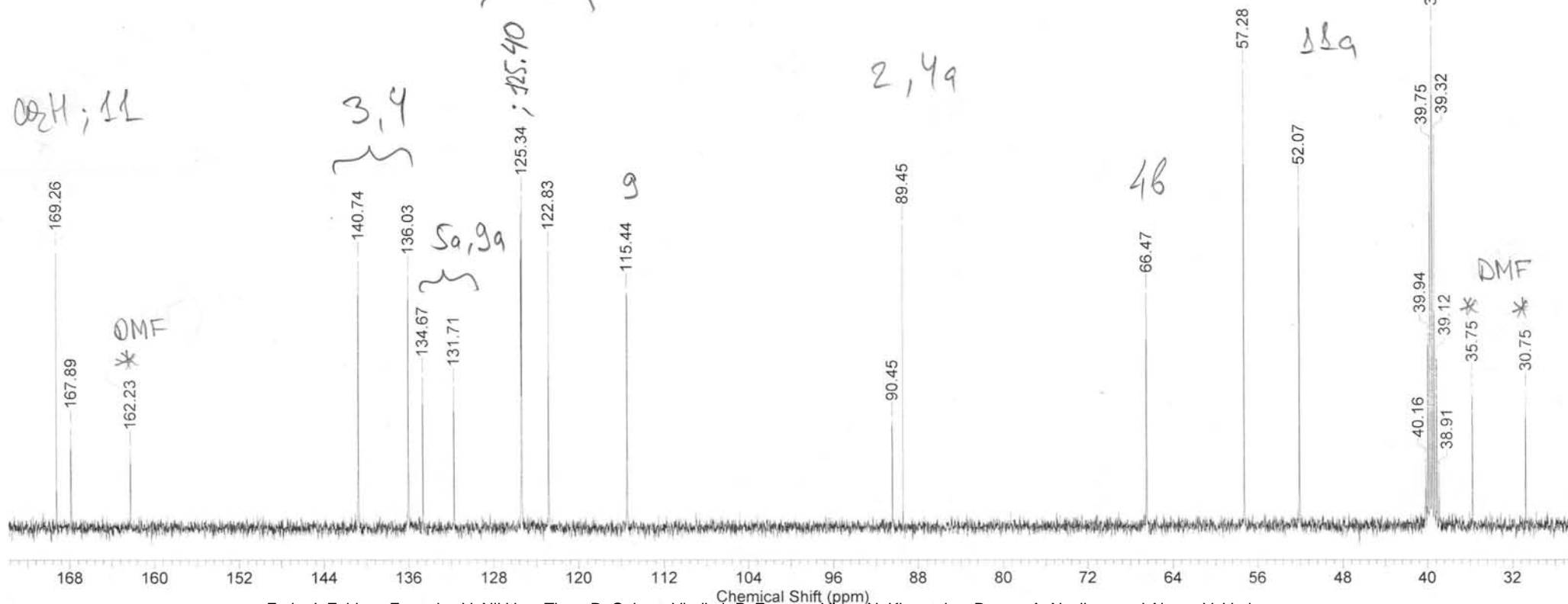


Formula C ₁₅ H ₁₀ BrNO ₄ S		FW 380.2132					
Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	15 Apr 2011 08:12:48		
Date Stamp	15 Apr 2011 08:12:48	File Name	D:\NMR\13.04.2011 C-13\rudn-130411-N9-c13dec\rudn-130411-N9-c13dec_001000fid				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	977	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zgpg
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6	Spectrum Offset (Hz)	10548.9658
Sweep Width (Hz)	29409.97	Temperature (degree C)	90.000				

Compound 33c

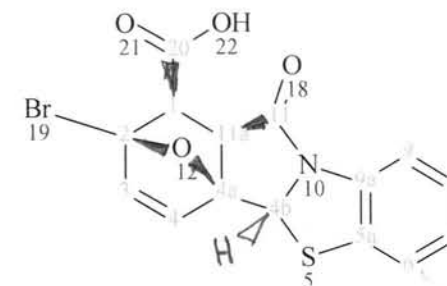


rudn-130411-N9-c13dec_001000fid

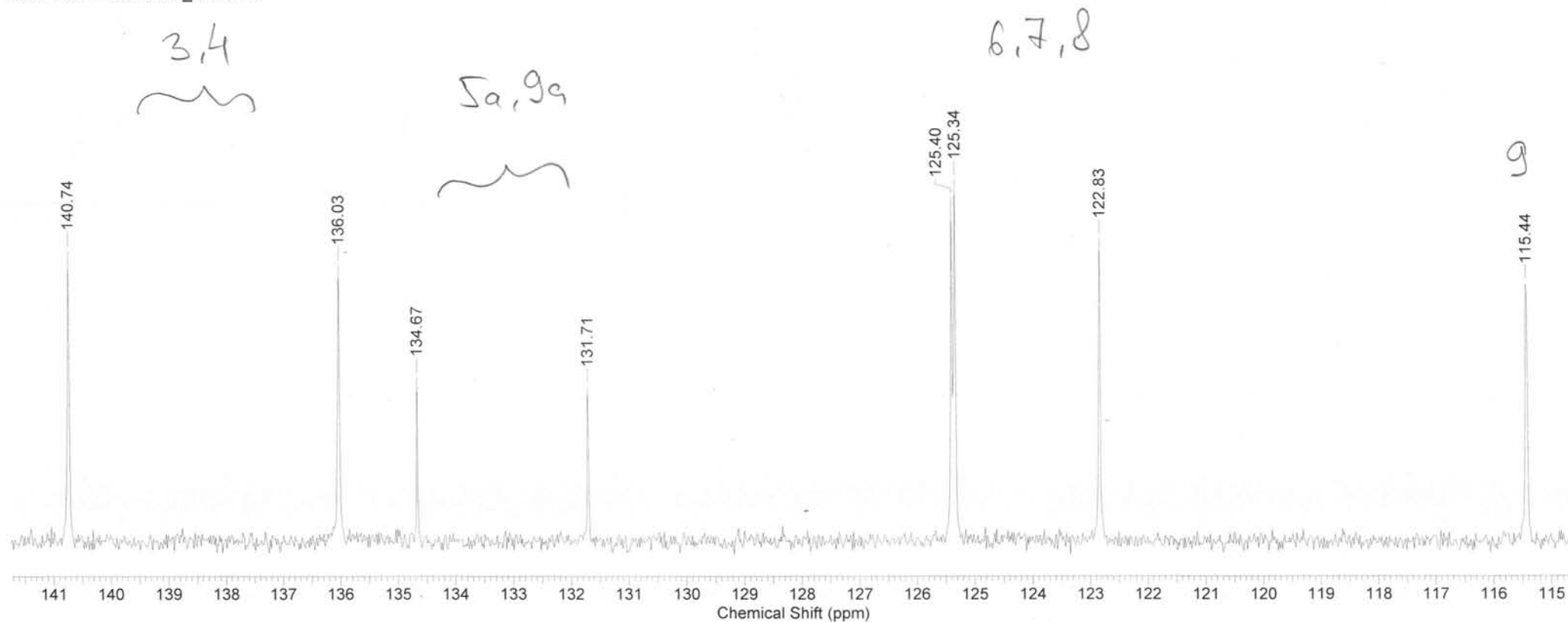


Formula C ₁₅ H ₁₀ BrNO ₄ S		FW 380.2132	
Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400
Date Stamp	15 Apr 2011 08:12:48	File Name	D:\NMR\13.04.2011 C-13\rudn-130411-N9-c13dec\rudn-130411-N9-c13dec_001000fid
Frequency (MHz)	100.62	Nucleus	13C
Original Points Count	16384	Number of Transients	977
Receiver Gain	32768.00	Origin	spect
Sweep Width (Hz)	29409.97	Owner	root
		Points Count	16384
		Pulse Sequence	zgpg
		Solvent	DMSO-d6
		Spectrum Offset (Hz)	10548.9658
		Temperature (degree C)	90.000

Compound 33c

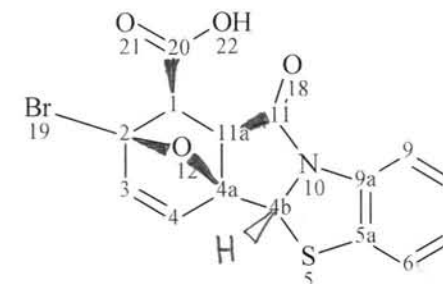


rudn-130411-N9-c13dec_001000fid

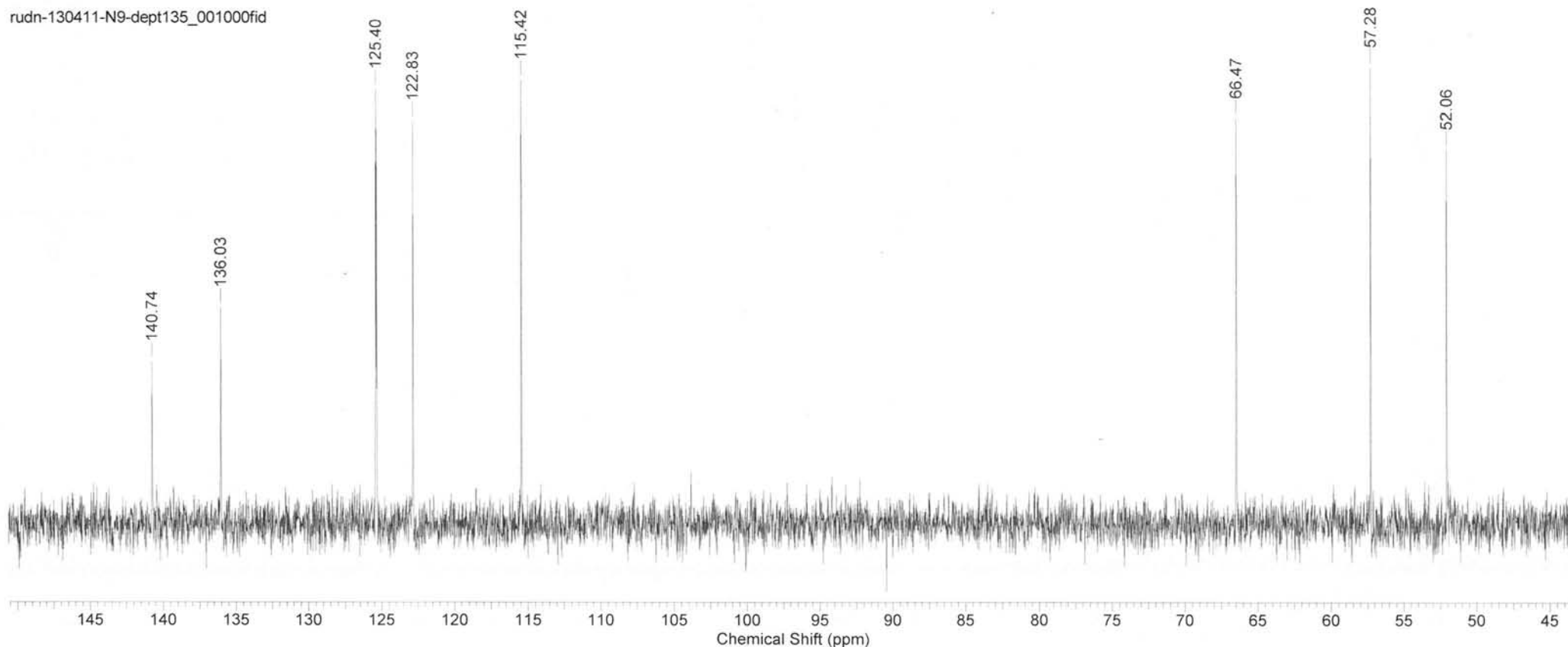


Formula C ₁₅ H ₁₀ BrNO ₄ S		FW 380.2132	
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 15 Apr 2011 08:36:16	
Date Stamp 15 Apr 2011 08:36:16	File Name D:\NMR\13.04.2011 C-13\rudn-130411-N9-dept135\rudn-130411-N9-dept135_001000fid		
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 443	Origin spect
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence dept135
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 9098.5479
Sweep Width (Hz) 29409.97	Temperature (degree C) 90.000		

Compound 33c

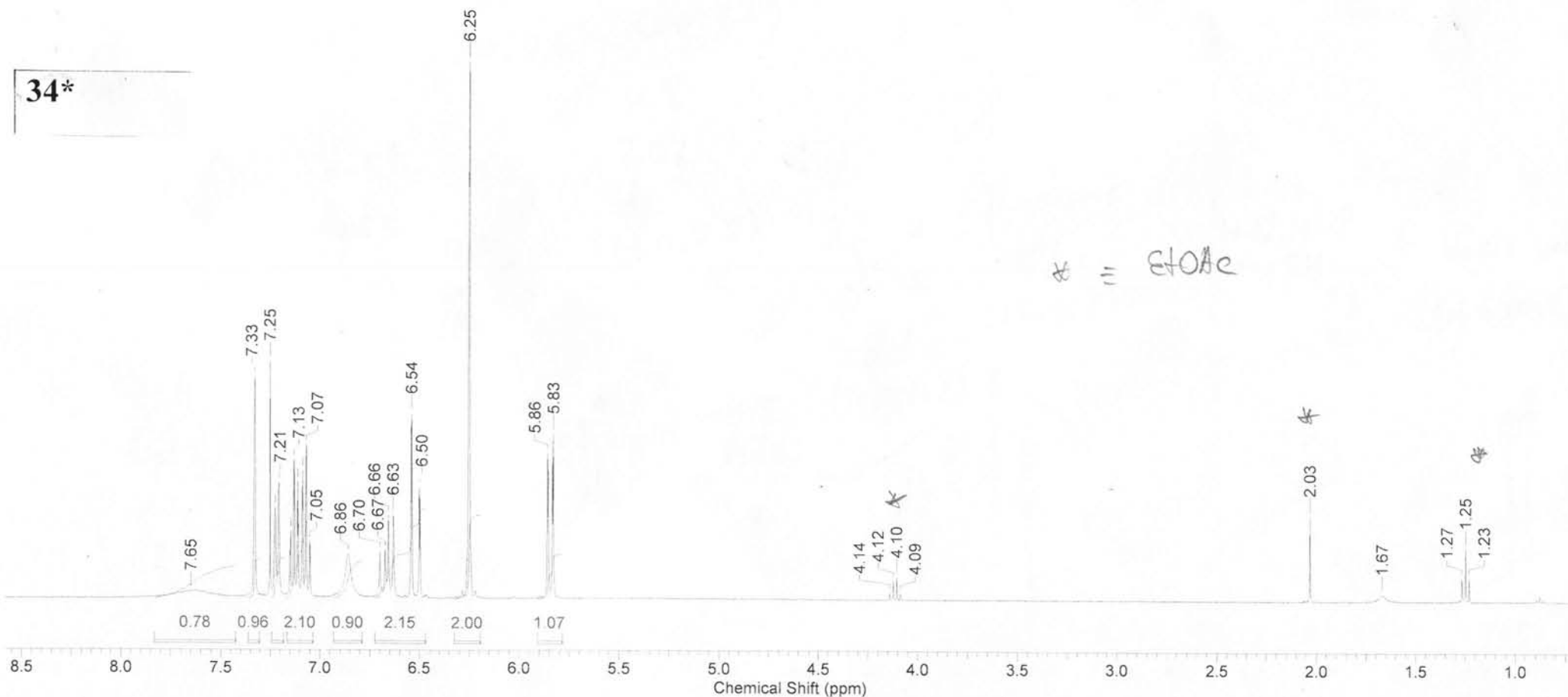
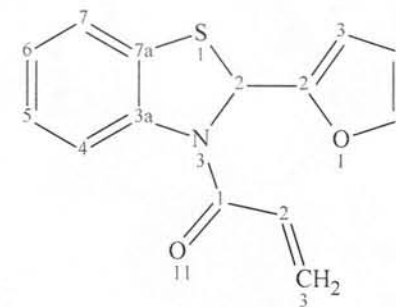


rudn-130411-N9-dept135_001000fid



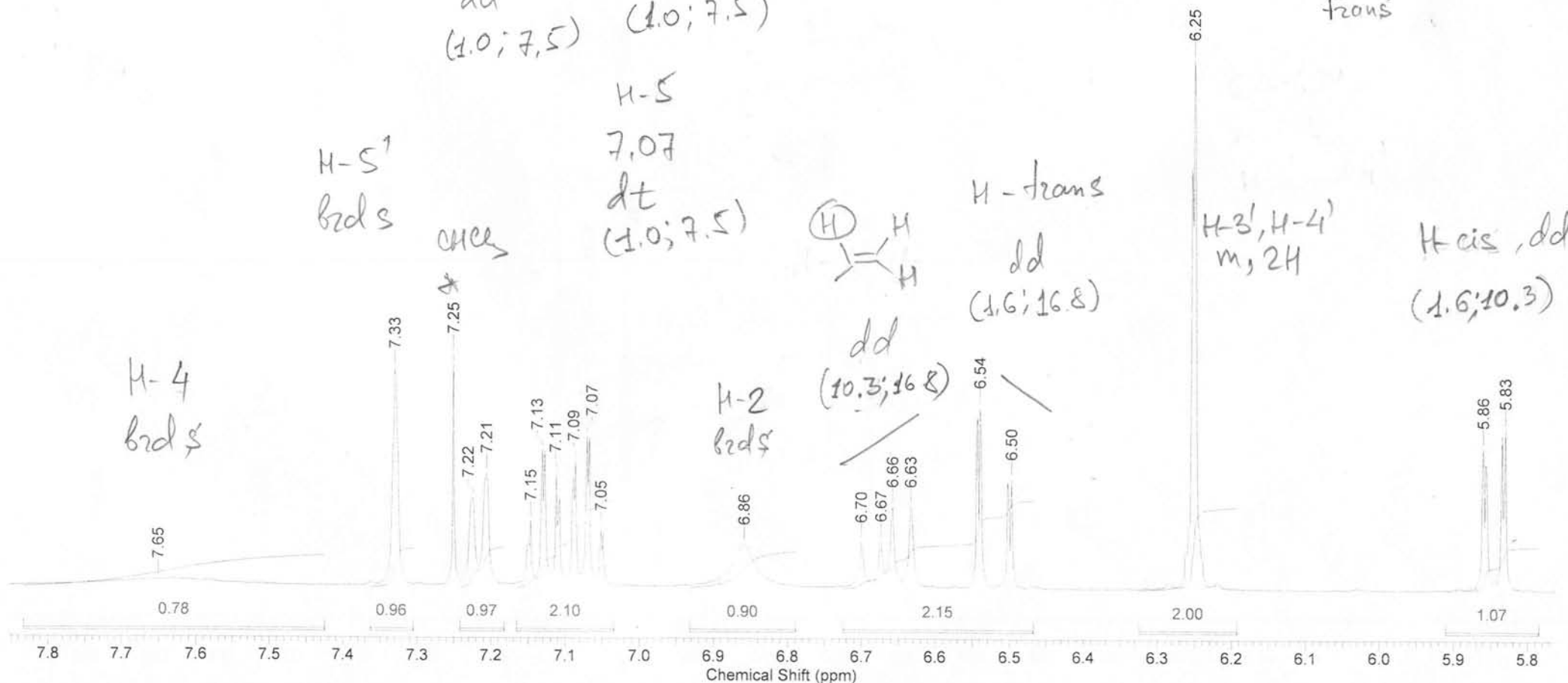
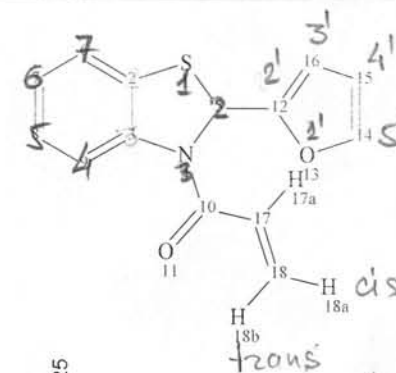
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File Name	C:\Users\Fedor\Desktop\31.01.11-1\1614\1614_001000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	32	Original Points Count	16384
Pulse Sequence	zg	Solvent	CHLOROFORM-D	Points Count	16384
Temperature (degree C)	27.000			Sweep Width (Hz)	10204.08

Compound 34*



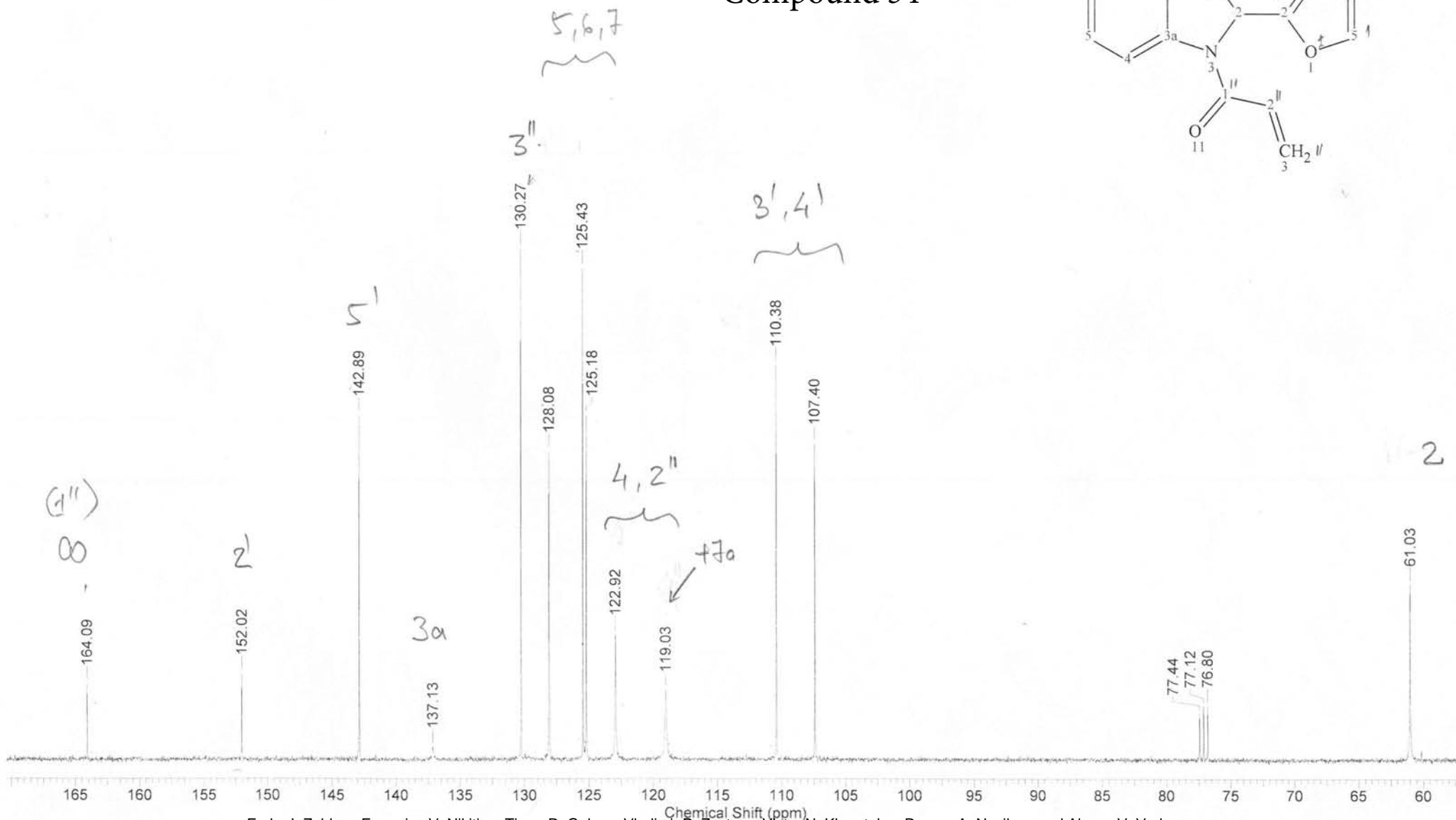
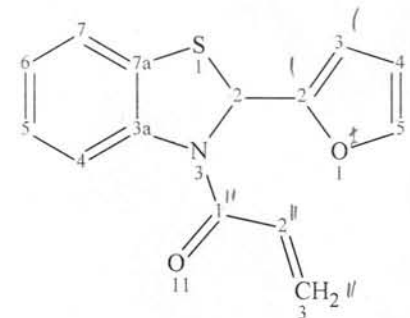
Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.		Date	31 Jan 2011 14:06:56	
File Name	C:\Users\Fedor\Desktop\31.01.11-1\1614\1614_001000fid			Frequency (MHz)	400.14		
Nucleus	1H	Number of Transients	32	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	CHLOROFORM-D		Sweep Width (Hz)	10204.08	
Temperature (degree C)	27.000						

Compound 34*



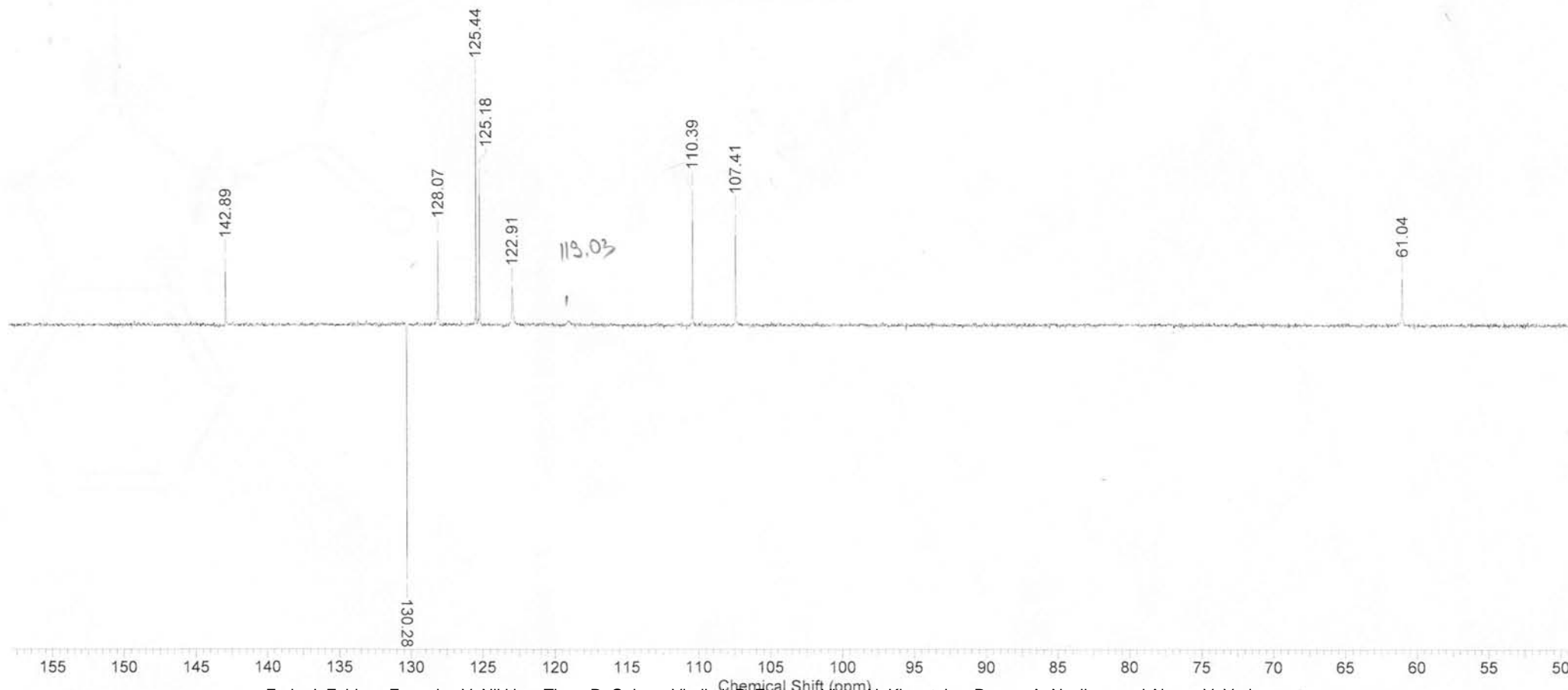
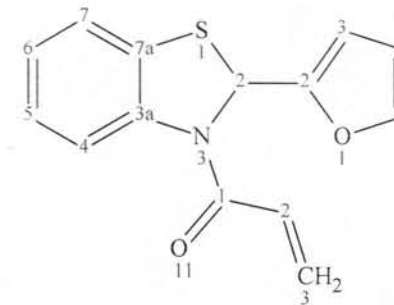
Acquisition Time (sec)	0.5898	Comment	Imported from UXMNR.	Date	31 Jan 2011 14:47:28
File Name	C:\Users\Fedor\Desktop\31.01.11-1\1fz1614c13dec\1fz1614c13dec_002000fid			Frequency (MHz)	100.62
Nucleus	¹³ C	Number of Transients	360	Original Points Count	16384
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D	Points Count	16384
Temperature (degree C)	27.000			Sweep Width (Hz)	27777.78

Compound 34*



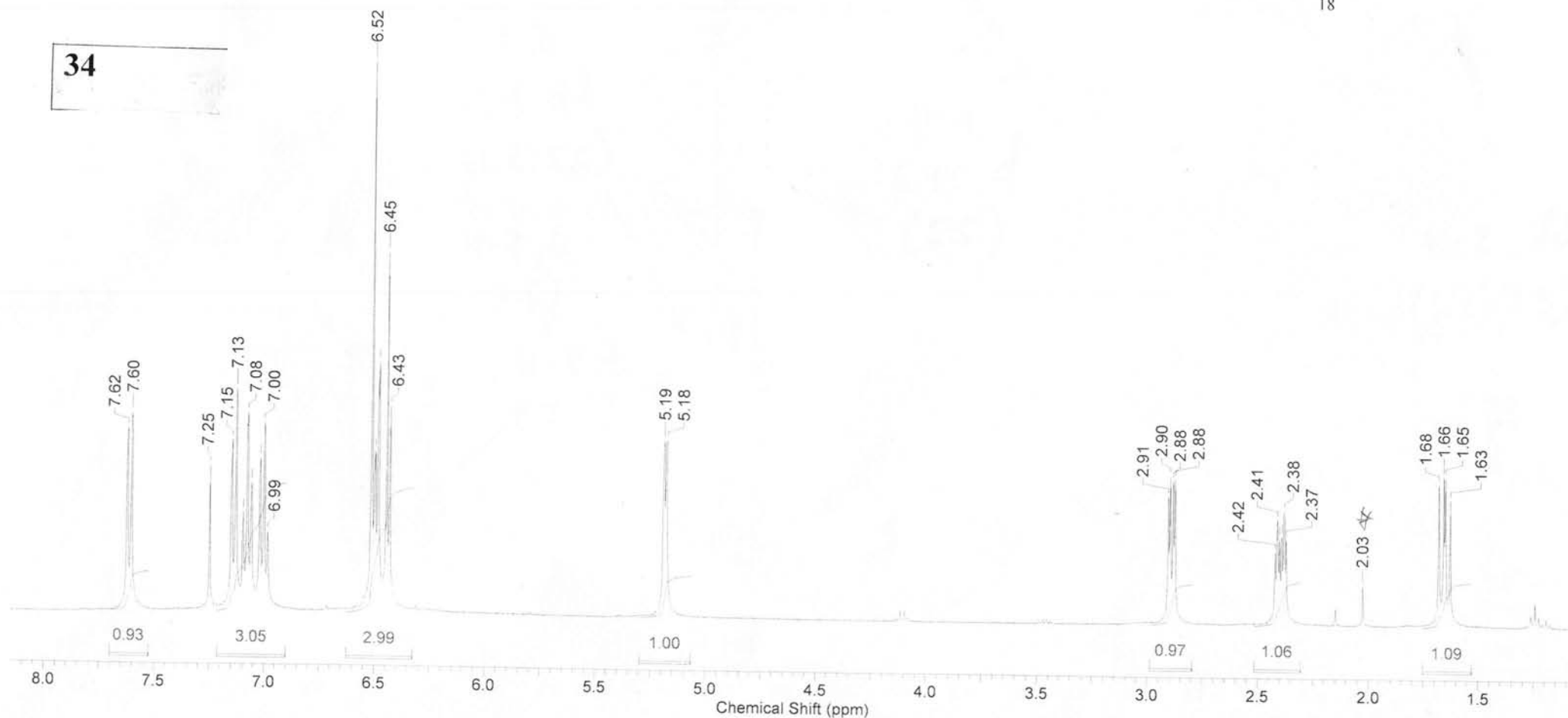
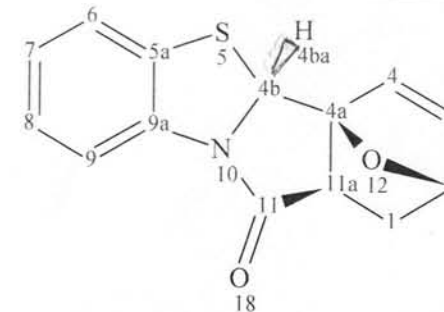
Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	31 Jan 2011 14:56:00	
File Name	C:\Users\Fedor\Desktop\31.01.11-1\lz1614dept135\lz1614dept135_002000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	539	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	CHLOROFORM-D		Sweep Width (Hz)	29411.77	
Temperature (degree C)	27.000						

Compound 34*

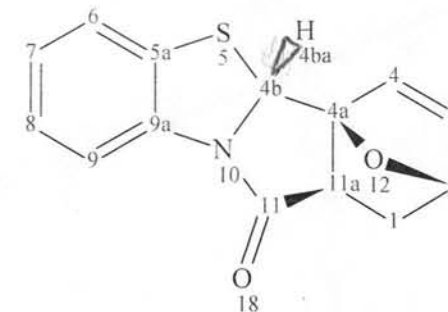


Acquisition Time (sec)	1.6056	Comment	Imported from UXNMR.		Date	24 Jan 2011 18:05:52	
File Name	C:\Users\Fedor\Desktop\27.12.10\1z1612\1z1612_001000fid		Frequency (MHz)	400.14	Nucleus	1H	
Number of Transients	40	Original Points Count	16384	Points Count	16384	Pulse Sequence	zg
Solvent	CHLOROFORM-D		Sweep Width (Hz)	10204.08	Temperature (degree C)	27.000	

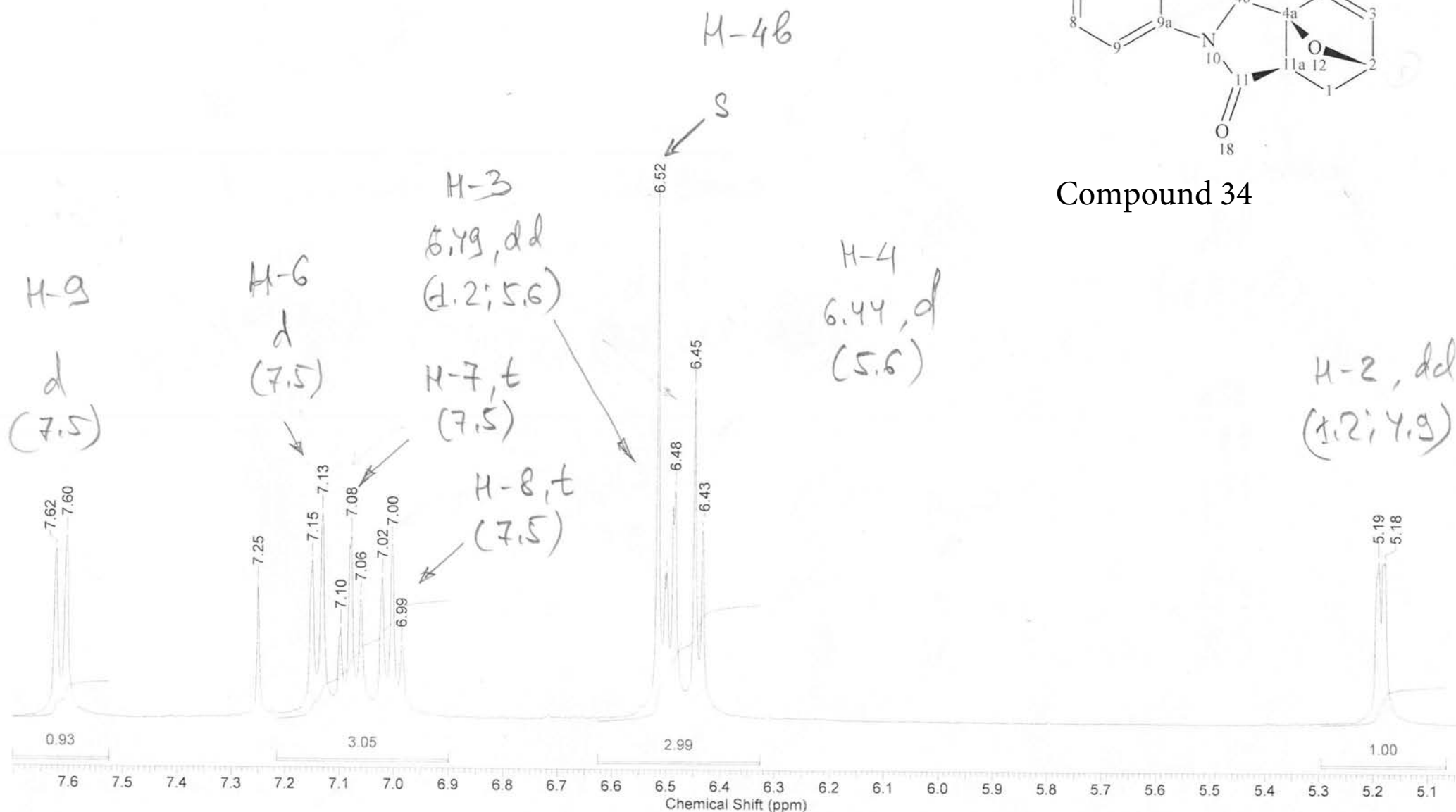
Compound 34



Acquisition Time (sec)	1.6056	Comment	Imported from UXNMR.		Date	24 Jan 2011 18:05:52
File Name	C:\Users\Fedor\Desktop\27.12.10\fvz1612\fvz1612_001000fid	Frequency (MHz)	400.14	Nucleus	1H	
Number of Transients	40	Original Points Count	16384	Points Count	16384	
Solvent	CHLOROFORM-D	Sweep Width (Hz)	10204.08	Pulse Sequence	zg	
				Temperature (degree C)	27.000	

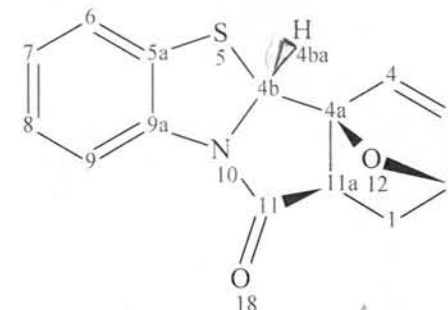


Compound 34



Acquisition Time (sec)	1.6056	Comment	Imported from UJXNMR.		Date	24 Jan 2011 18:05:52
File Name	C:\Users\Fedor\Desktop\27.12.10\lz1612\lz1612_001000fid	Frequency (MHz)	400.14	Nucleus	1H	
Number of Transients	40	Original Points Count	16384	Points Count	16384	
Solvent	CHLOROFORM-D	Sweep Width (Hz)	10204.08	Pulse Sequence	zg	
				Temperature (degree C)	27.000	

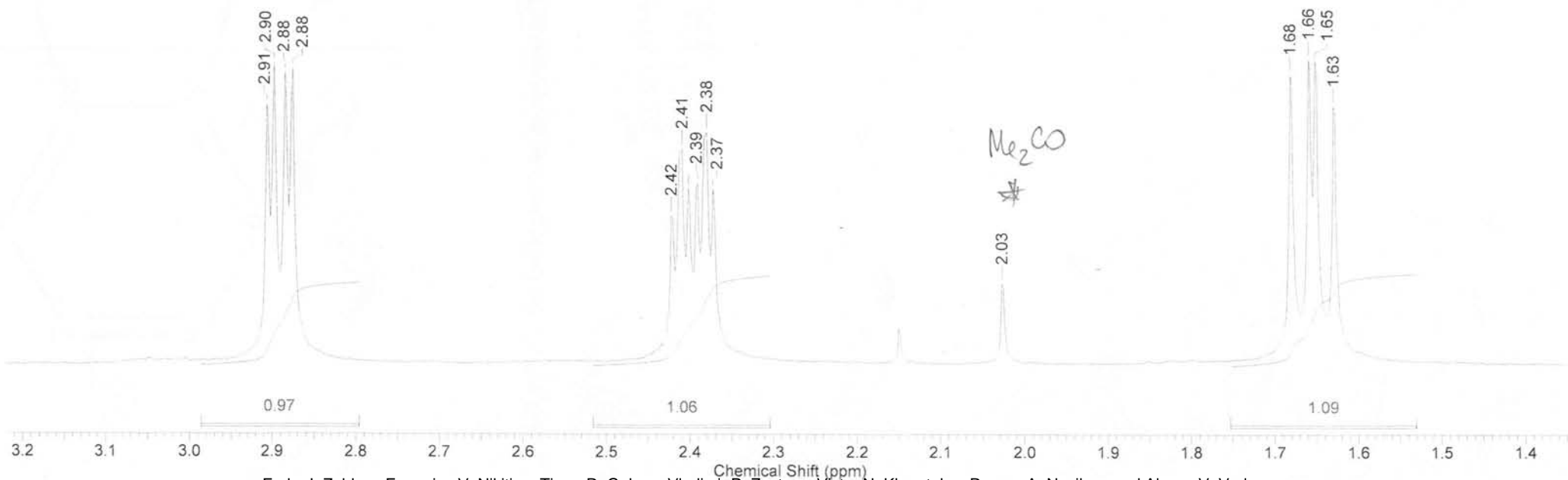
Compound 34



H-11a endo
dd
(3.7; 8.7)

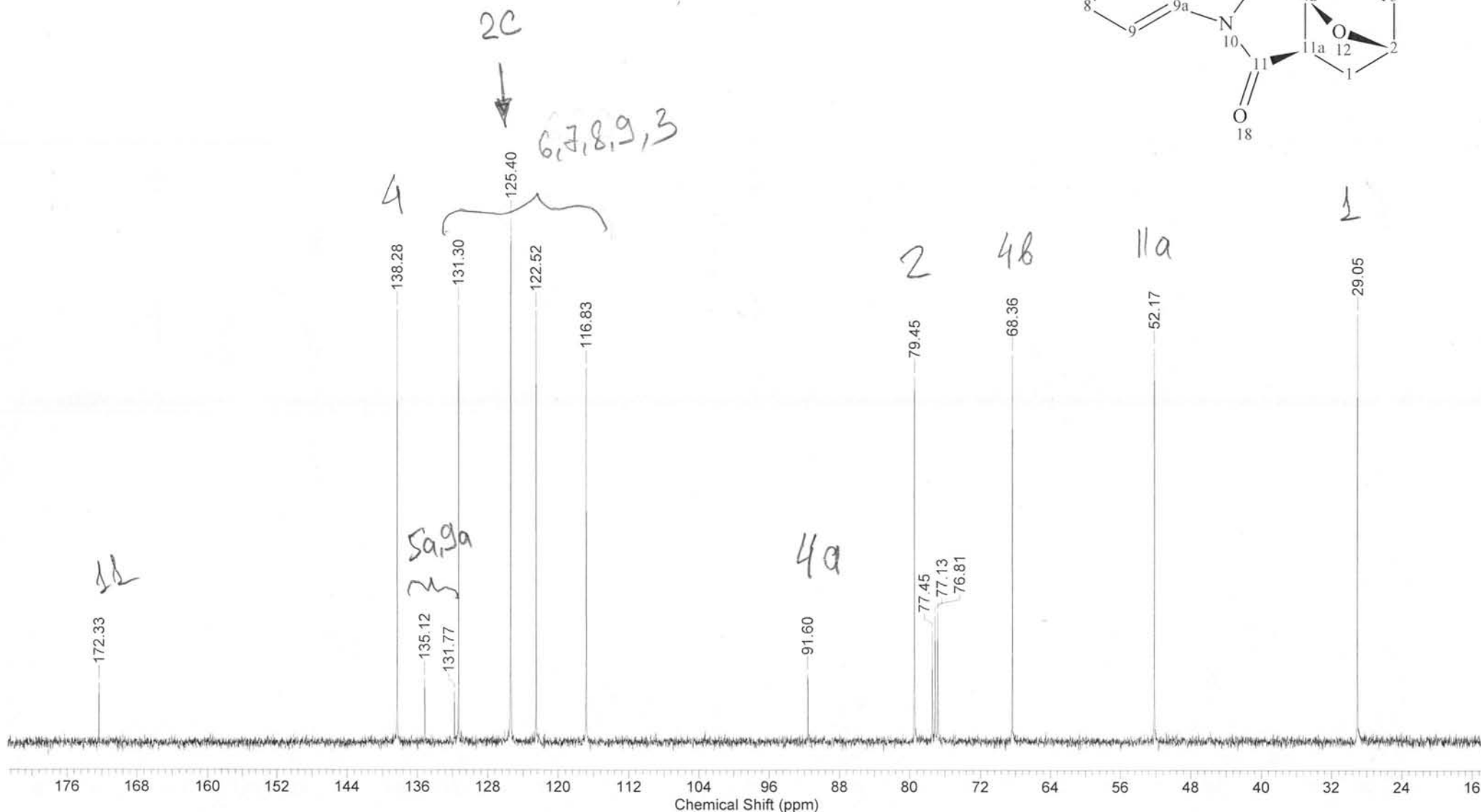
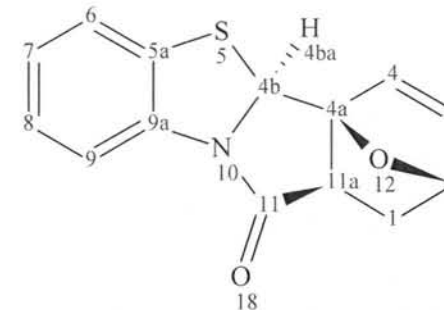
H-1 exo
ddd
(3.7; 11.8; 4.9)

H-2 endo
dd
(8.7; 11.8)



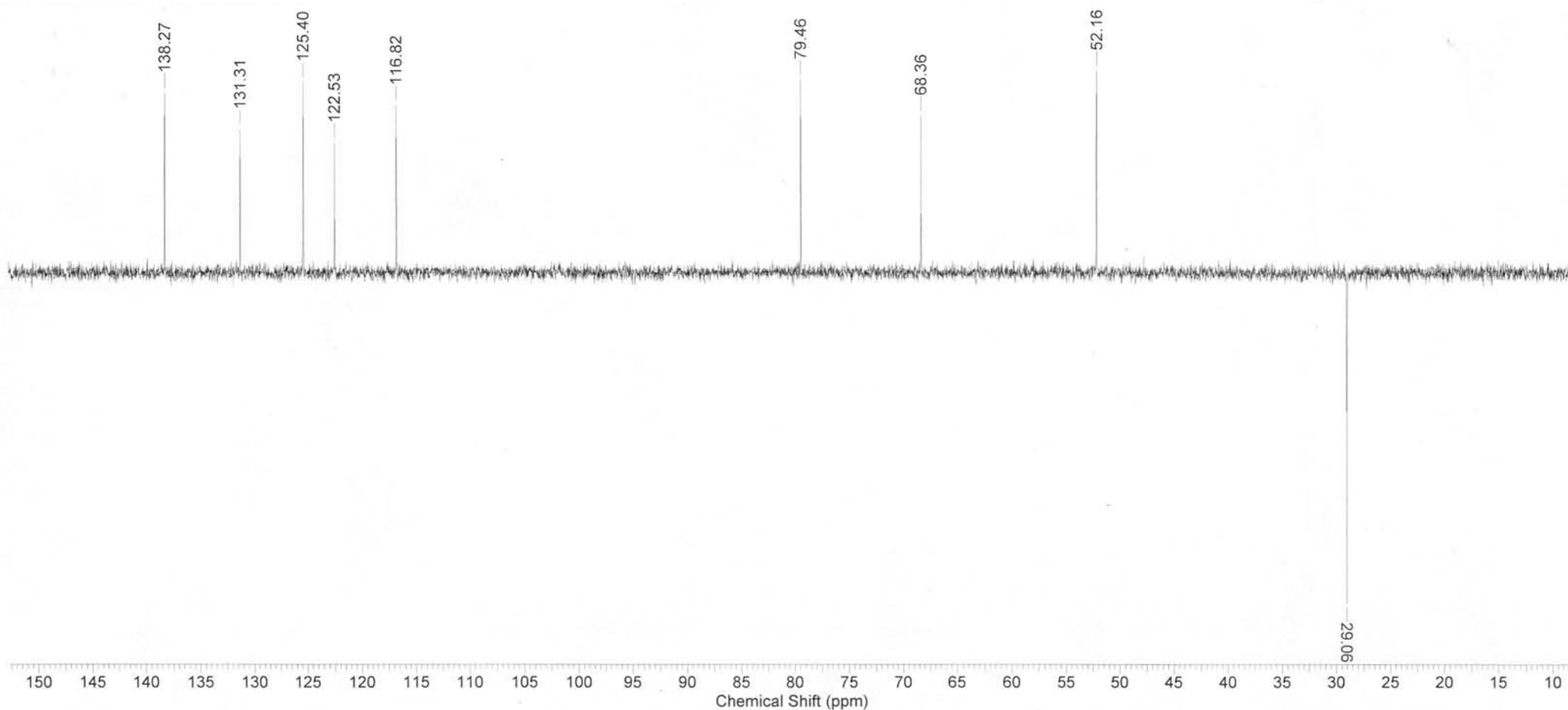
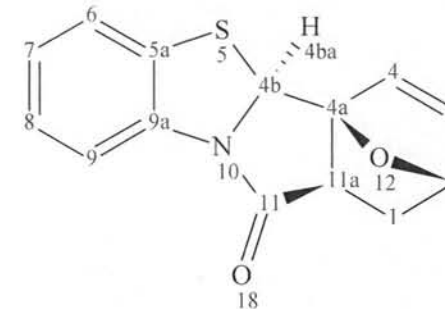
Acquisition Time (sec)	0.5898	Comment	Imported from UXNMR.		Date	14 Jul 2011 09:36:00	
File Name	D:\NMR\19.05.2011 C 13 Для Иры Статья в Тетраэдрон\rudn-0611-N2-c13dec\rudn-0611-N2-c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	746	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	27777.78	Temperature (degree C)	27.000

Compound 34



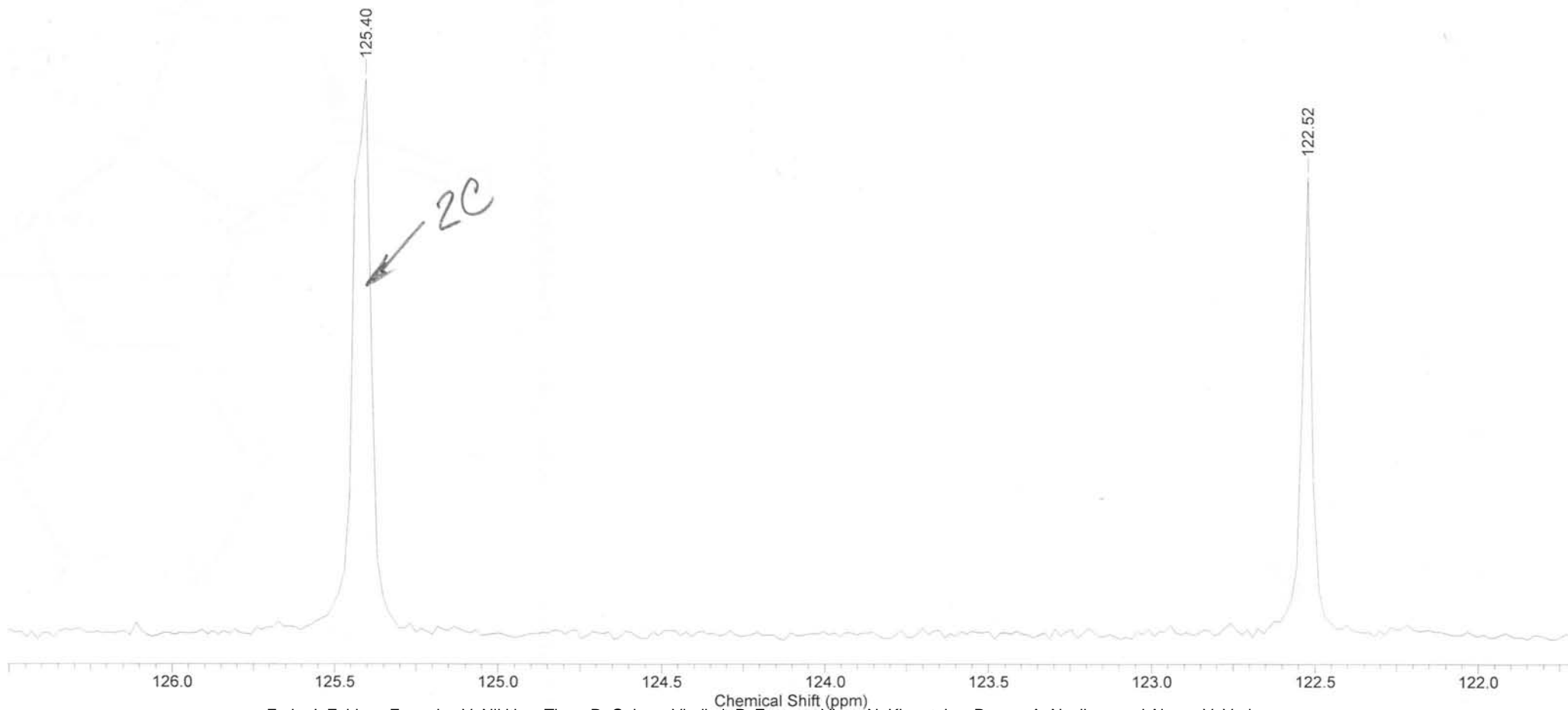
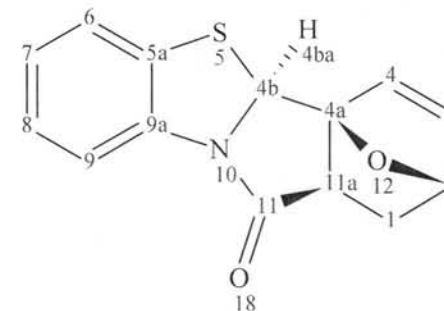
Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	14 Jul 2011 09:53:04	
File Name	D:\NMR\19.05.2011 C 13 Для Иры Статья в Тетраэдрон\rudn-0611-N2-dept135\rudn-0611-N2-dept135_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	432	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	CHLOROFORM-D	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compound 34



Acquisition Time (sec)	0.5898	Comment	Imported from UXMNR.		Date	14 Jul 2011 09:36:00	
File Name	D:\NMR\19.05.2011 C 13 Для Иры Статья в Тетраэдрон\rudn-0611-N2-c13dec\rudn-0611-N2-c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	746	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	27777.78	Temperature (degree C)	27.000

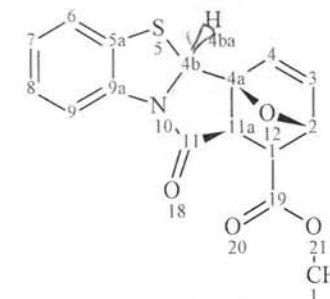
Compound 34



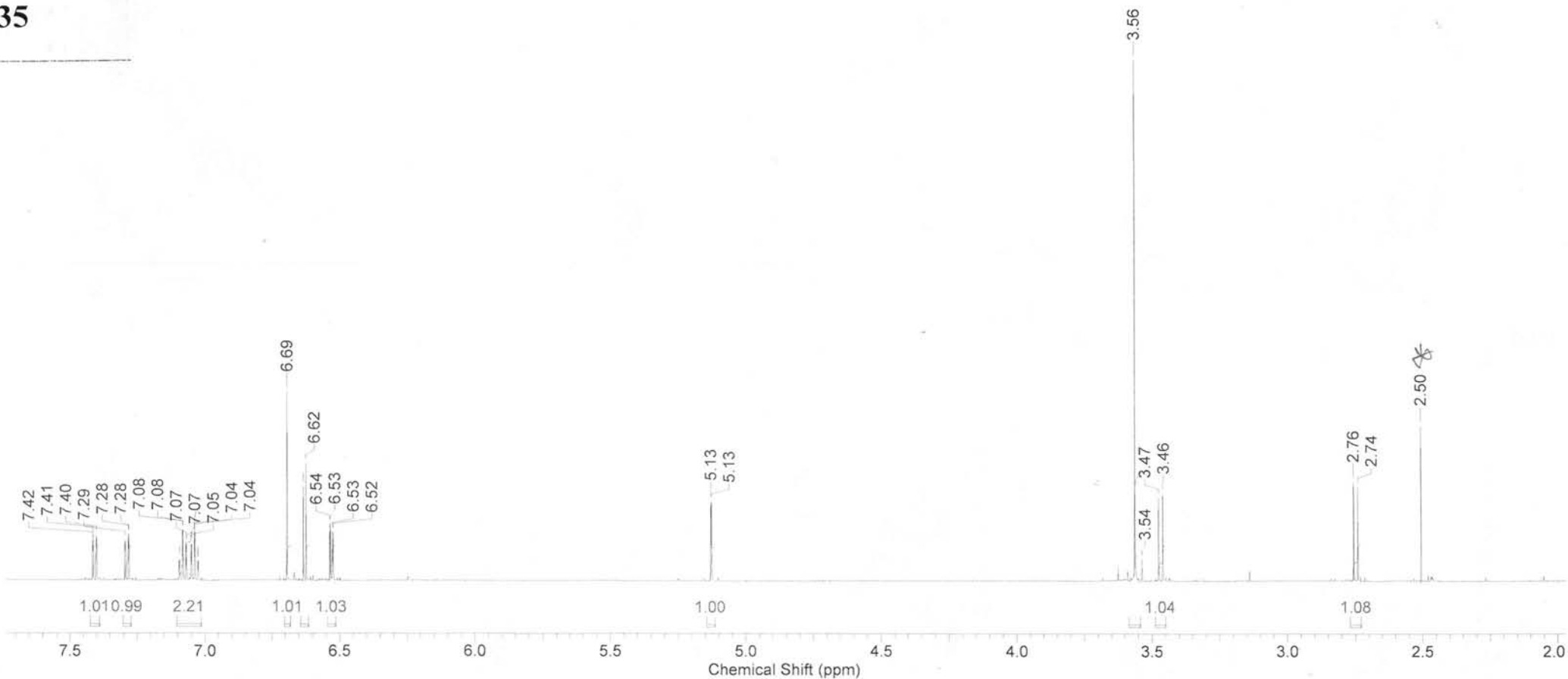
Formula $C_{16}H_{13}NO_4S$ FW 315.3437

Acquisition Time (sec)	2.9098	Comment	single_pulse	Date	18 Oct 2010 15:17:16	Date Stamp	18 Oct 2010 14:29:45
File Name	D:\NMR\18.10.2010\fz1399-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	2
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	36.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3000.8616	Sweep Width (Hz)	11261.26
						Temperature (degree C)	21.100

Compound 35



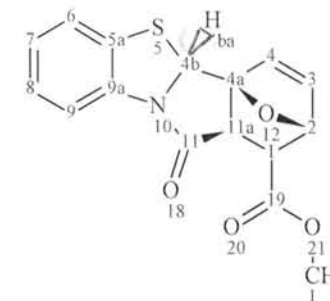
35



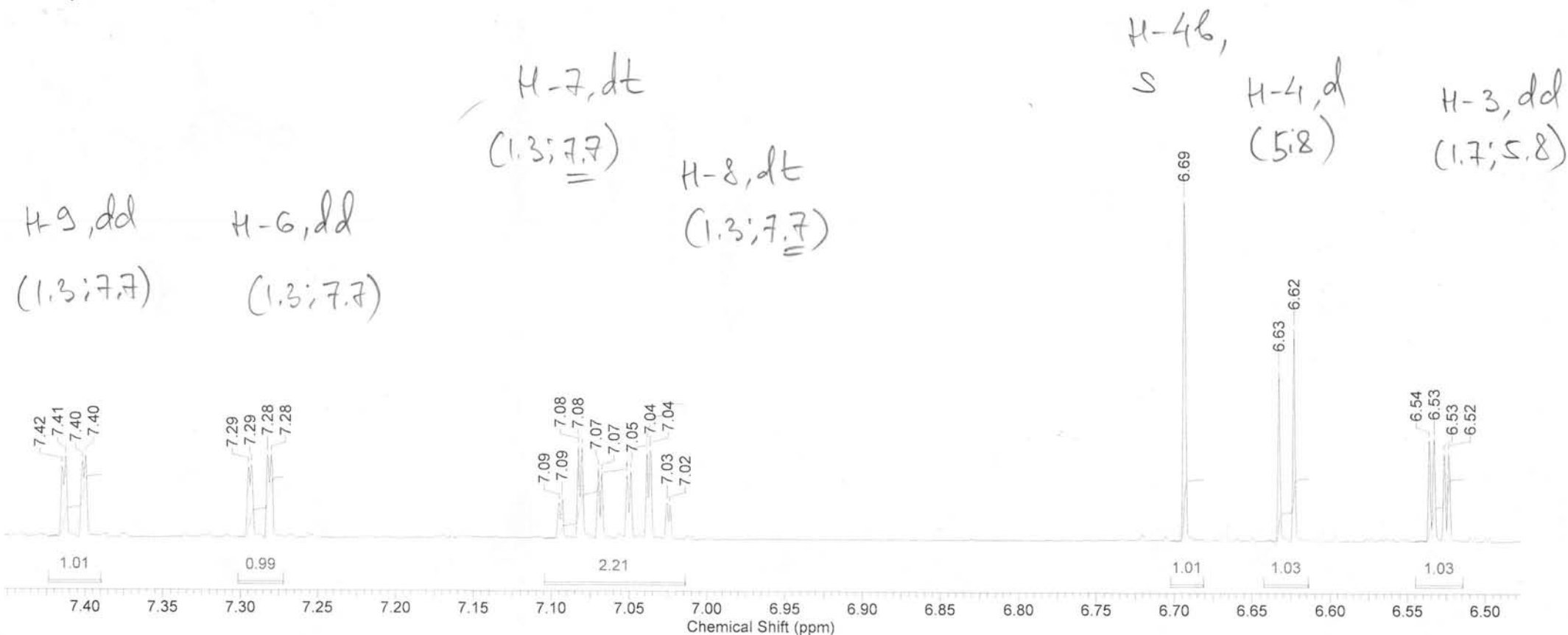
Formula $C_{16}H_{13}NO_4S$ FW 315.3437

Acquisition Time (sec)	2.9098	Comment	single_pulse	Date	18 Oct 2010 15:17:16	Date Stamp	18 Oct 2010 14:29:45		
File Name	D:\NMR\18.10.2010\fvz1399-1.jdf		Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	2	
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single_pulse.ex2
Receiver Gain	36.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3000.8616	Sweep Width (Hz)	11261.26	Temperature (degree C)	21.100

Compound 35

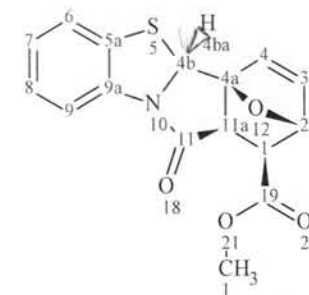


fvz1399-1.jdf

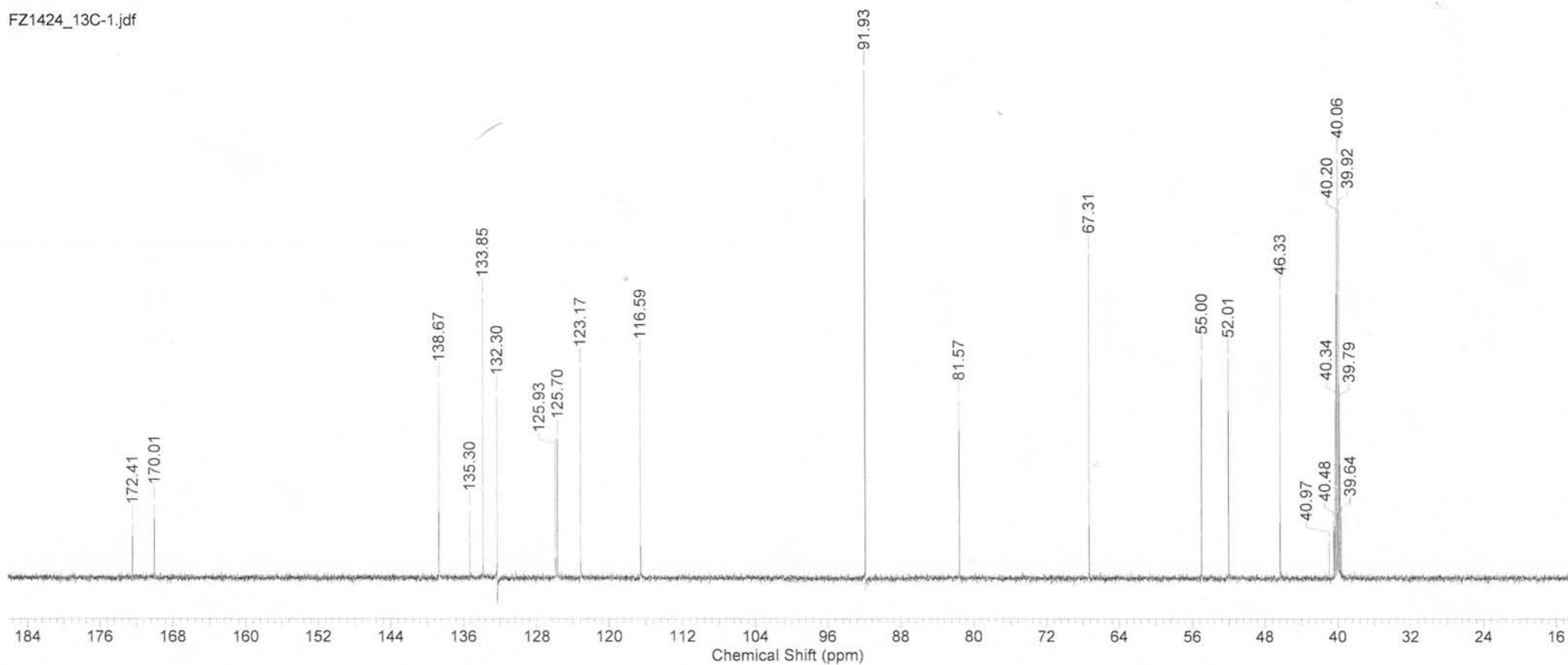


Formula	C ₁₆ H ₁₃ NO ₄ S	FW	315.3437
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE
Date Stamp	03 Nov 2010 12:49:03	File Name	D:\NMR\22.10.10\FZ1424_13C-1.jdf
Nucleus	13C	Number of Transients	130
Points Count	32768	Origin	ECA 600
Spectrum Offset (Hz)	15091.3428	Original Points Count	32768
		Pulse Sequence	single_pulse_dec
		Receiver Gain	56.00
		Sweep Width (Hz)	47348.49
		Temperature (degree C)	24.100
		Date	03 Nov 2010 13:36:58
		Frequency (MHz)	150.91
		Owner	delta
		Solvent	DMSO-d6

Compound 35



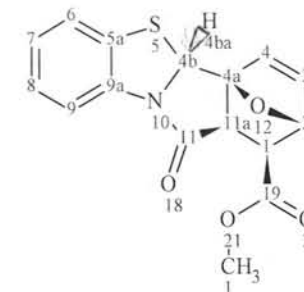
FZ1424_13C-1.jdf



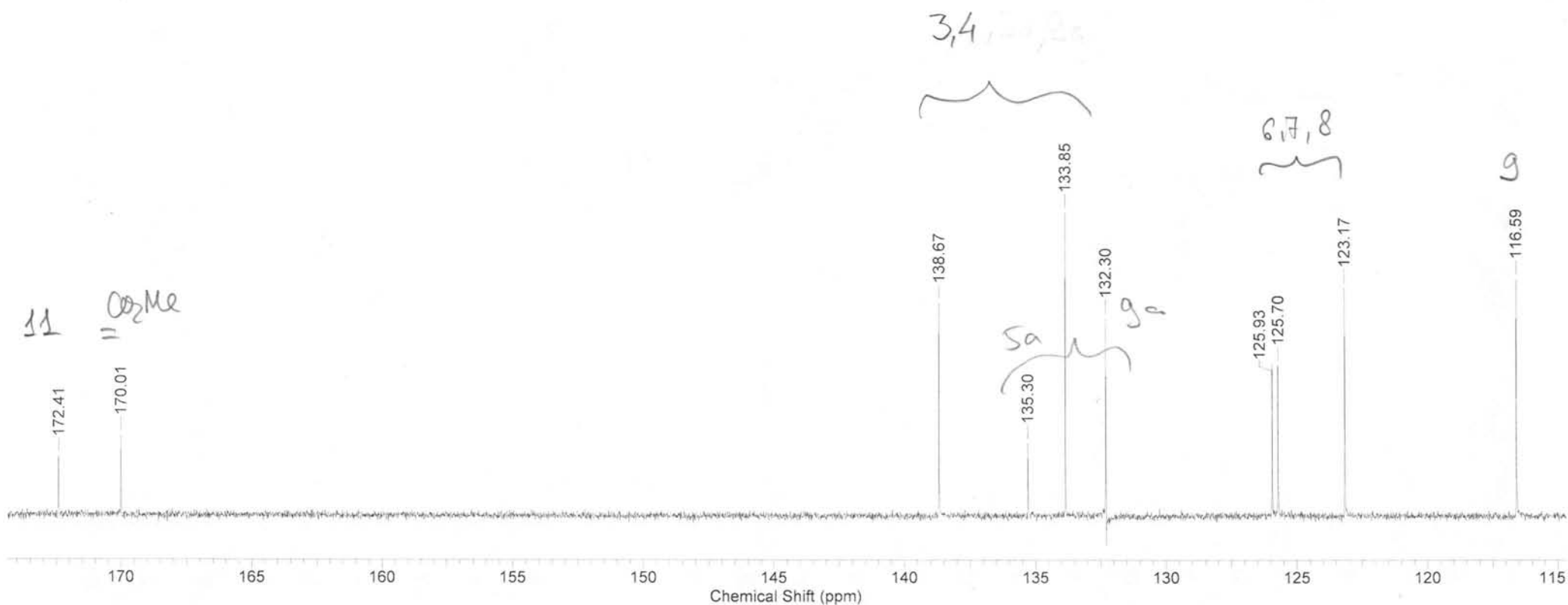
Formula C₁₆H₁₃NO₄S FW 315.3437

Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	03 Nov 2010 13:36:58
Date Stamp	03 Nov 2010 12:49:03	File Name	D:\NMR\22.10.10\FZ1424_13C-1.jdf	Frequency (MHz)	150.91
Nucleus	13C	Number of Transients	130	Origin	ECA 600
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49	Receiver Gain	56.00
		Temperature (degree C)	24.100	Owner	delta
				Solvent	DMSO-d6

Compound 35



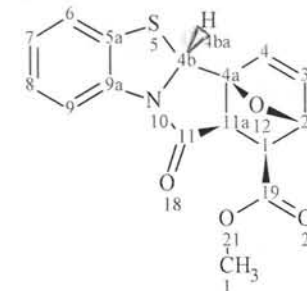
FZ1424_13C-1.jdf



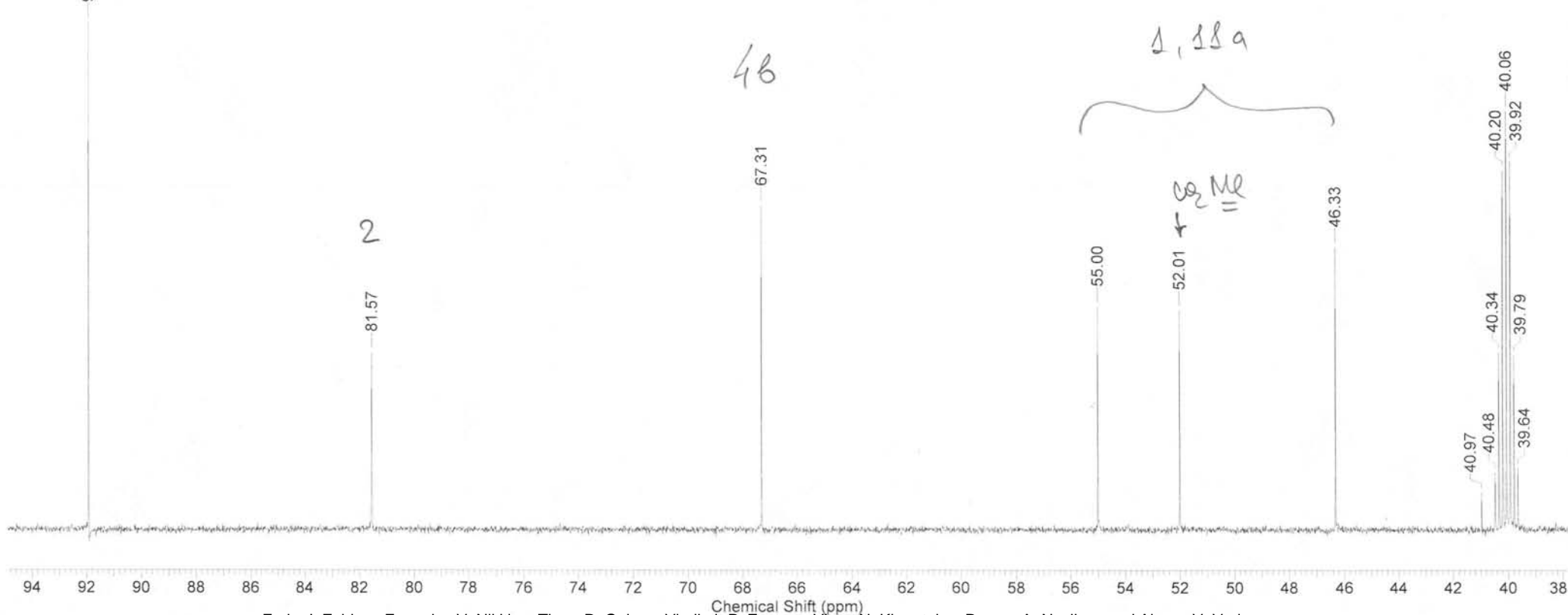
Formula C₁₈H₁₃NO₄S FW 315.3437

Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	03 Nov 2010 13:36:58
Date Stamp	03 Nov 2010 12:49:03	File Name	D:\NMR\22.10.10\FZ1424_13C-1.jdf	Frequency (MHz)	150.91
Nucleus	13C	Number of Transients	130	Origin	ECA 600
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49	Receiver Gain	56.00
		Temperature (degree C)	24.100	Owner	delta
				Solvent	DMSO-d6

Compound 35

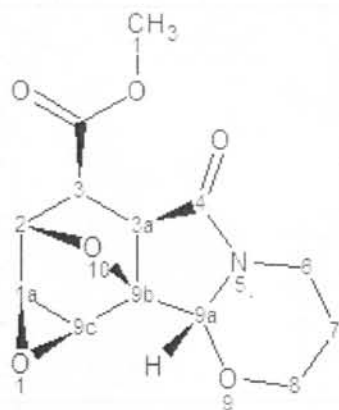


FZ1424_13C-1.jdf



600MHz,
CDCl₃, ¹H

Compound 36a



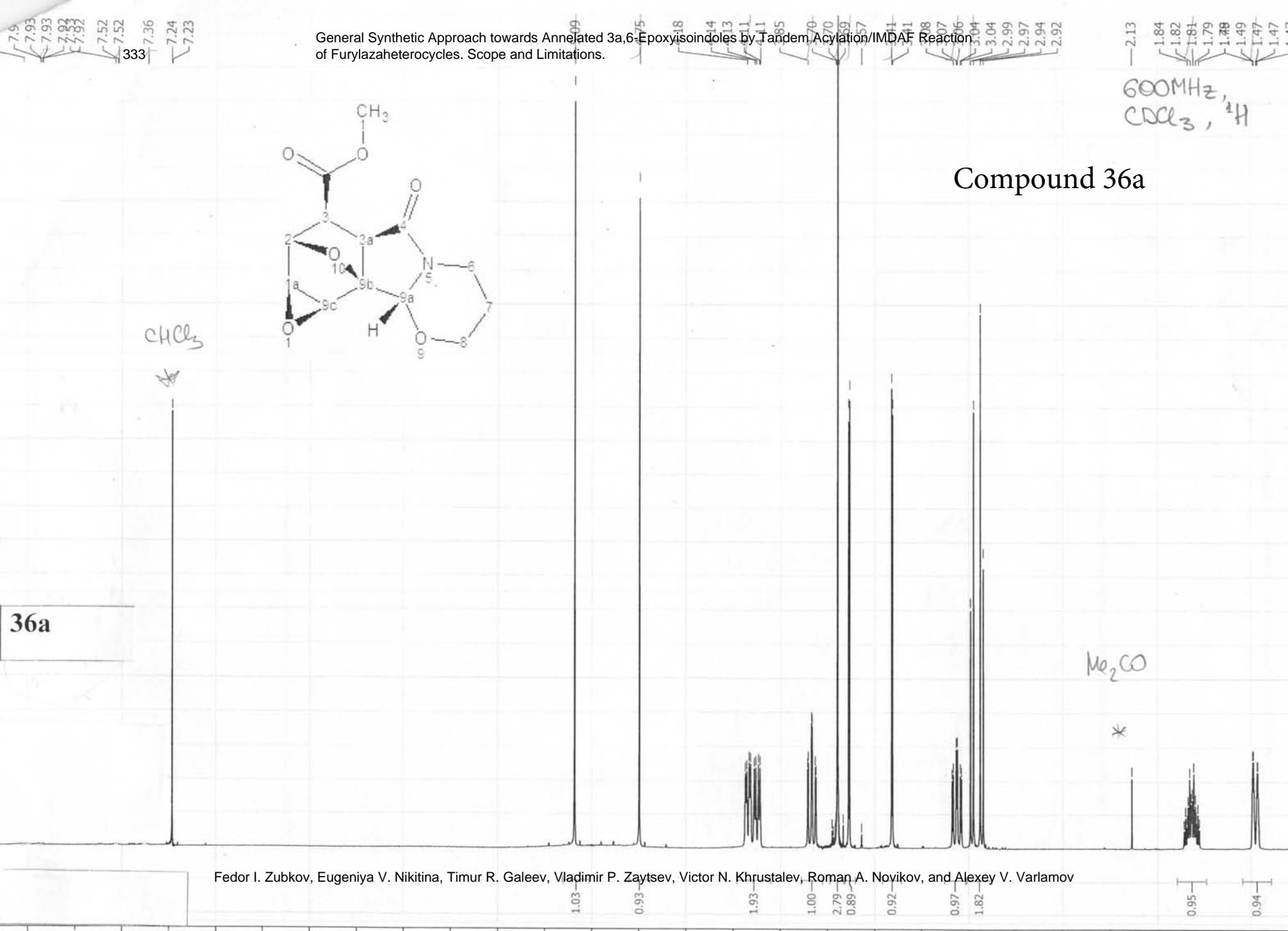
CHCl₃

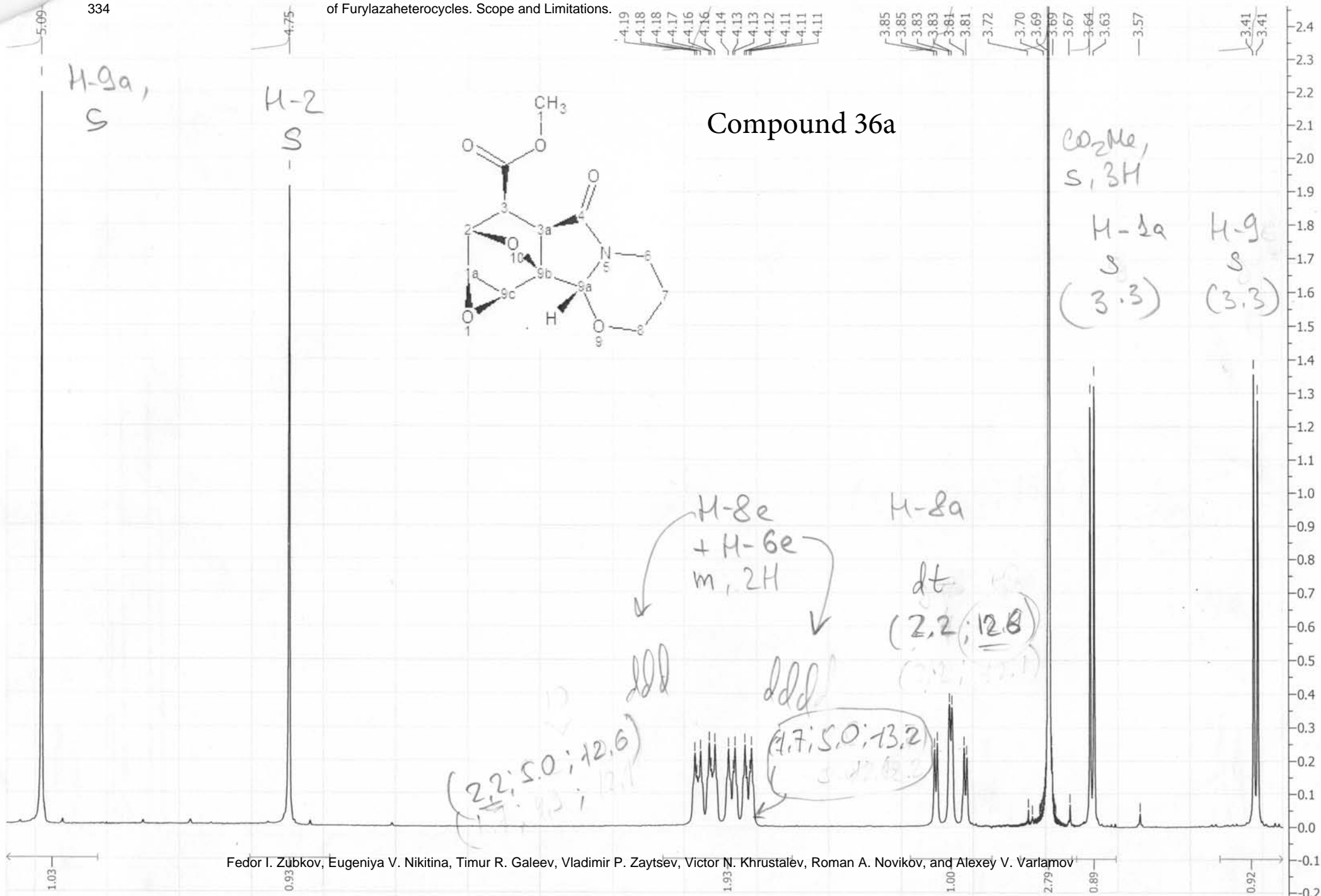


36a

Me₂CO

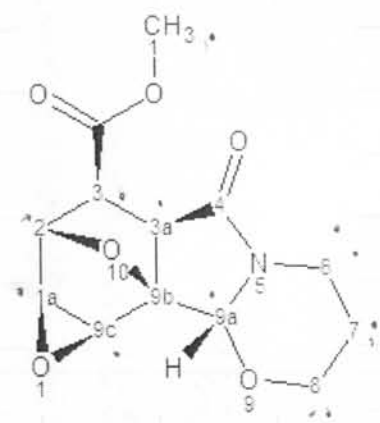
*





3.07
3.06
3.04
3.04
2.99
2.97
2.94
2.92

H-3a ↔ H-3a
d
(9.5) d
(9.5)



Compound 36a

2.13

1.86
1.85
1.84
1.84
1.83
1.82
1.81
1.81
1.80
1.79
1.79
1.78

1.50
1.49
1.49
1.47
1.47
1.47

H-6ax
ddd
3.8; 12.6
13.2

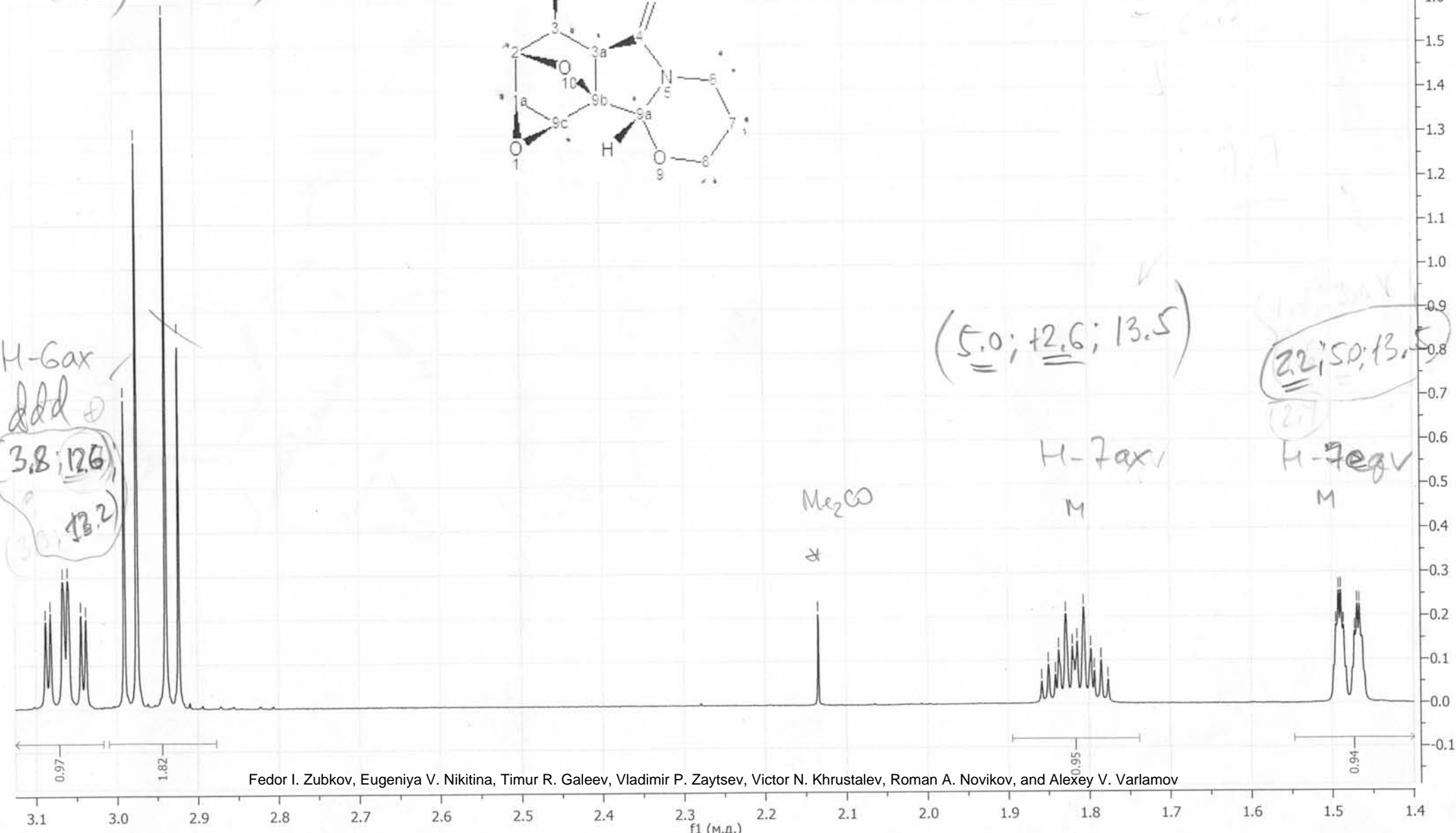
(5.0; 12.6; 13.5)

(2.2; 5.0; 13.5)

H-7ax
M

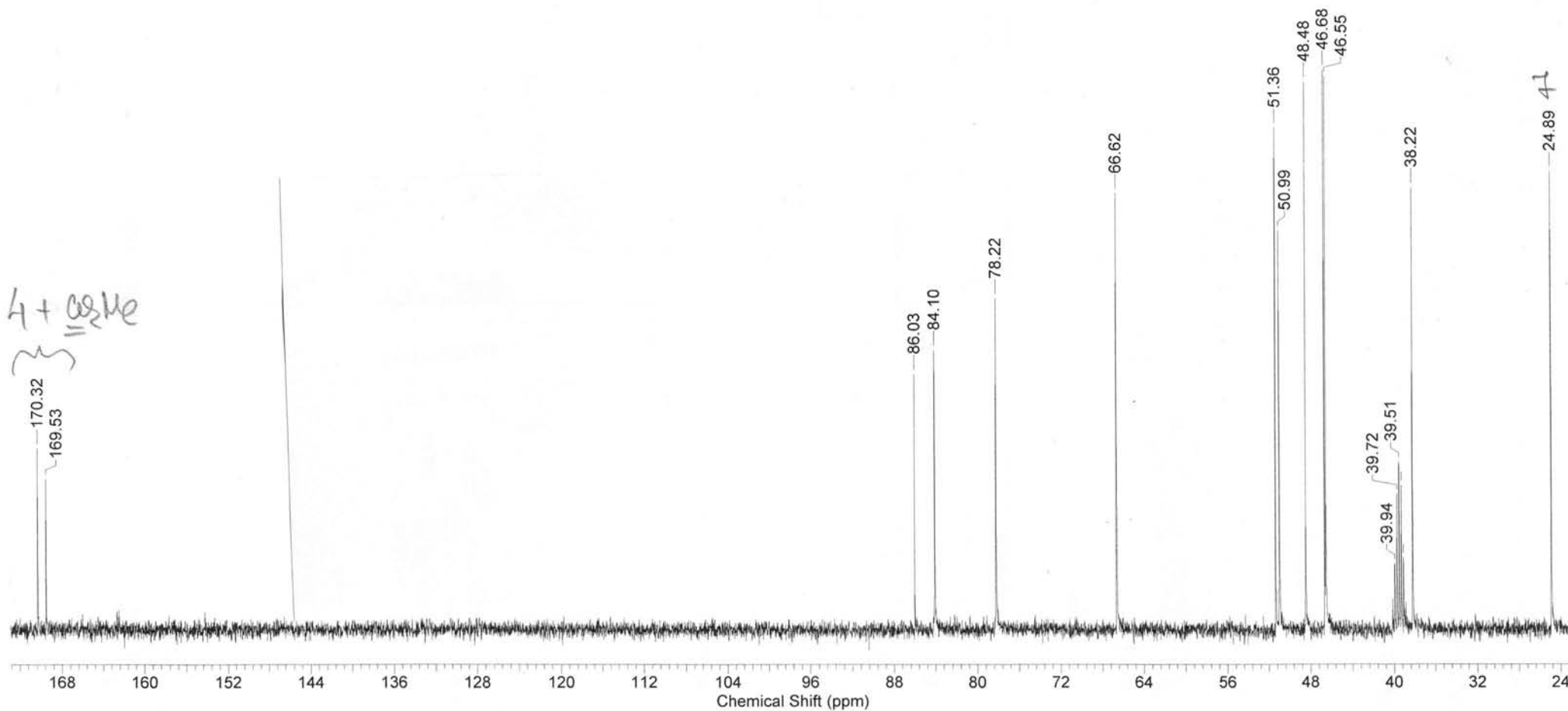
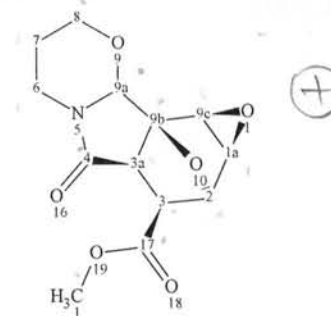
H-7eq
M

Me₂CO
*



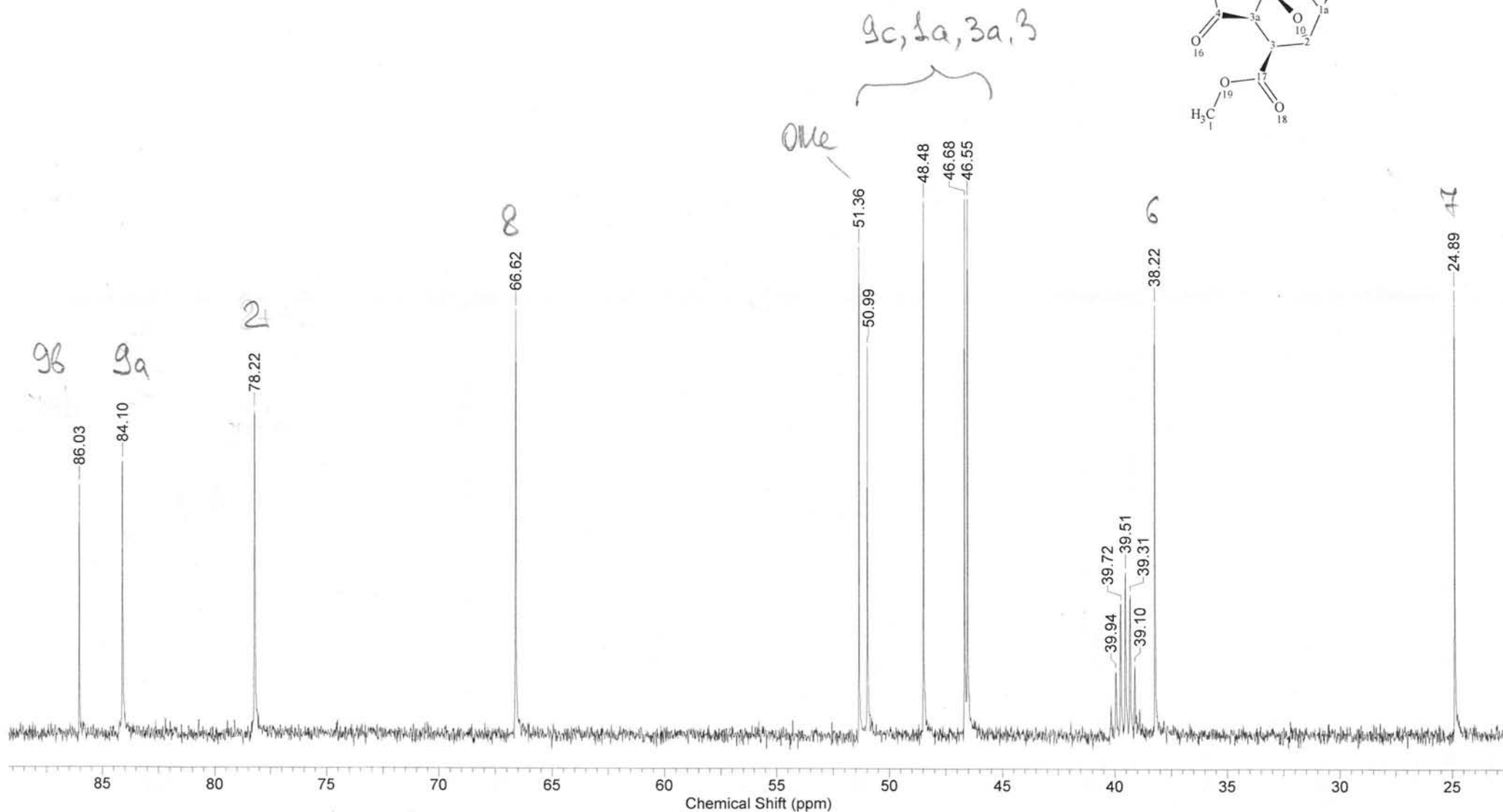
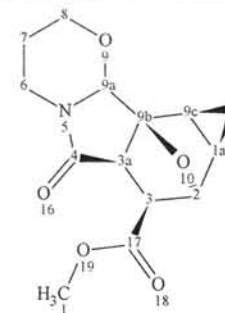
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File Name	D:\NMR\13\NMR 13 C IOC конец 2009\4laz_c13dec\4laz_c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	223	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	26315.79	Temperature (degree C)	27.000

Compound 36a

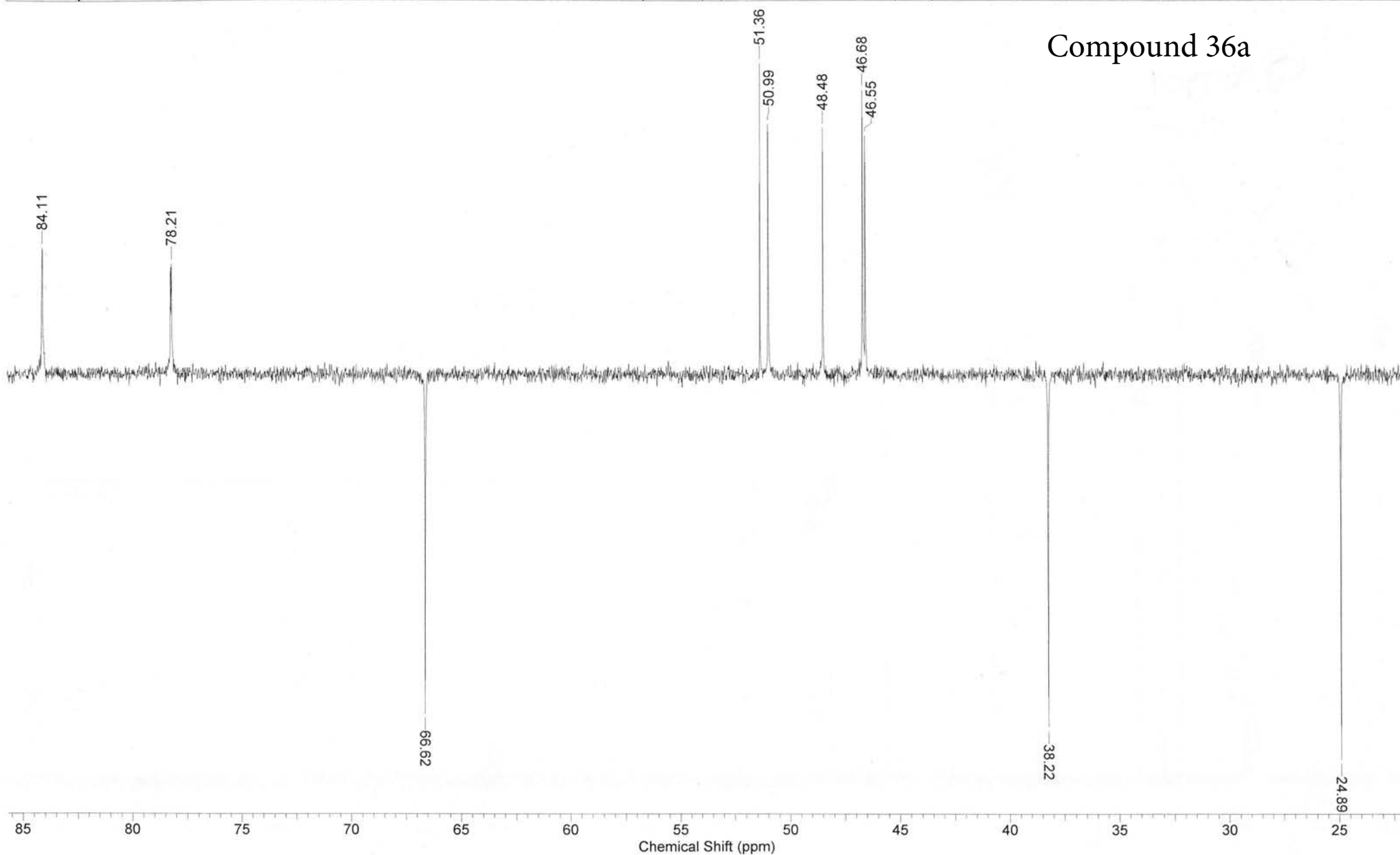


Acquisition Time (sec)	0.6226	Comment	Imported from UXNMR.		Date	22 Dec 2008 13:49:52	
File Name	D:\NMR\C_13\NMR 13 C IOC конец 2009\4laz_c13dec\4laz_c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	223	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	26315.79	Temperature (degree C)	27.000

Compound 36a

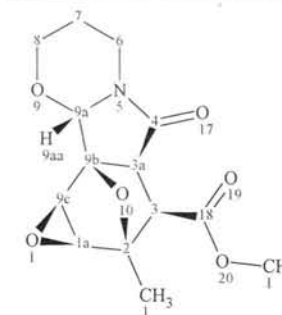


Acquisition Time (sec)	0.6226	Comment	Imported from UXMNR.		Date	22 Dec 2008 13:56:16
File Name	D:\NMR\13\NMR 13 C IOC конец 2009\4laz_dept135\4laz_dept135_001000fid			Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	176	Original Points Count	16384	
Pulse Sequence	dept135	Solvent	DMSO-D6	Sweep Width (Hz)	26315.79	
				Temperature (degree C)	27.000	

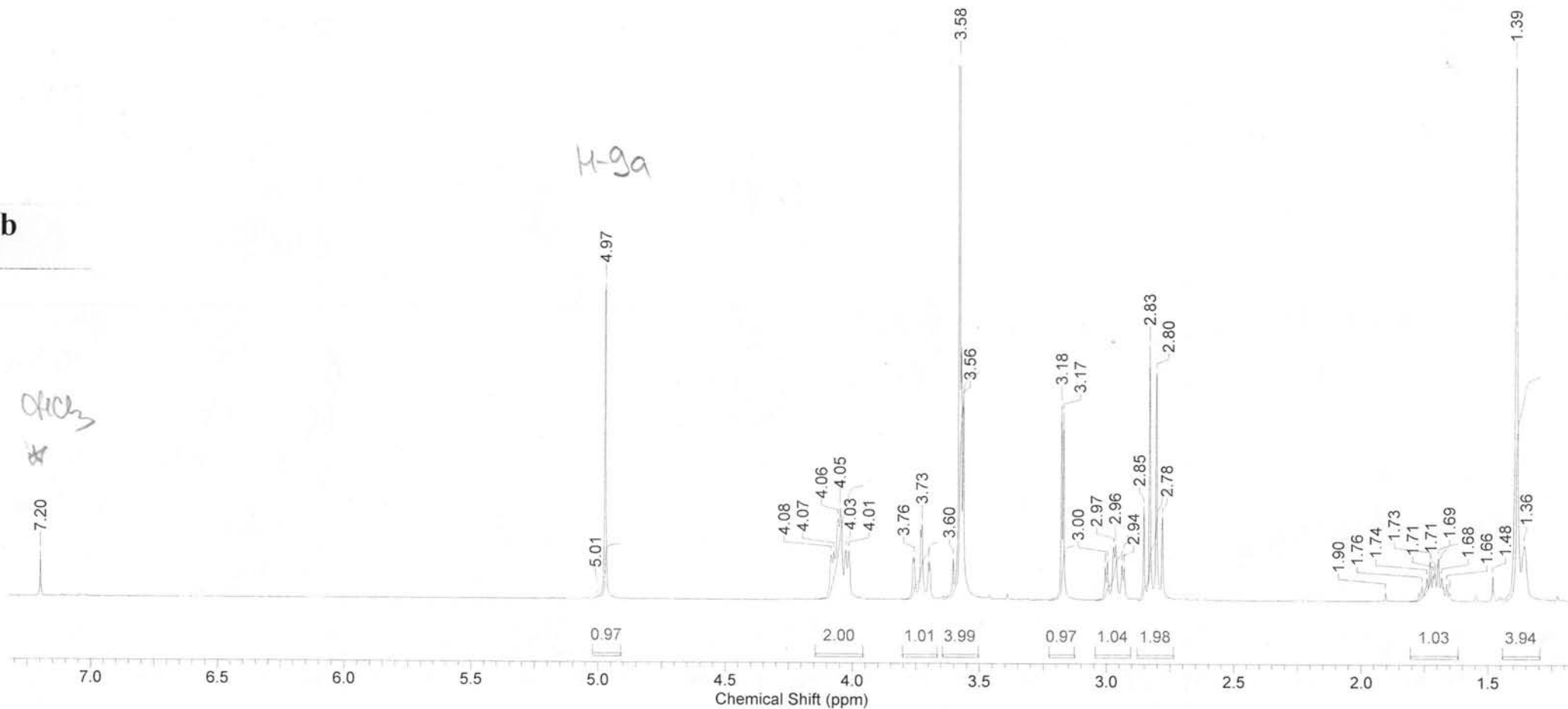


Acquisition Time (sec)	1.6056	Comment	Imported from UXNMR.		Date	19 Jun 2009 16:59:44
File Name	C:\Users\Fedor\Desktop\19.06.09\laz20\laz20_001000fid	Frequency (MHz)	400.14	Nucleus	1H	
Number of Transients	4	Original Points Count	16384	Points Count	16384	
Solvent	CHLOROFORM-D	Sweep Width (Hz)	10204.08	Pulse Sequence	zg	
				Temperature (degree C)	27.000	

Compound 36b

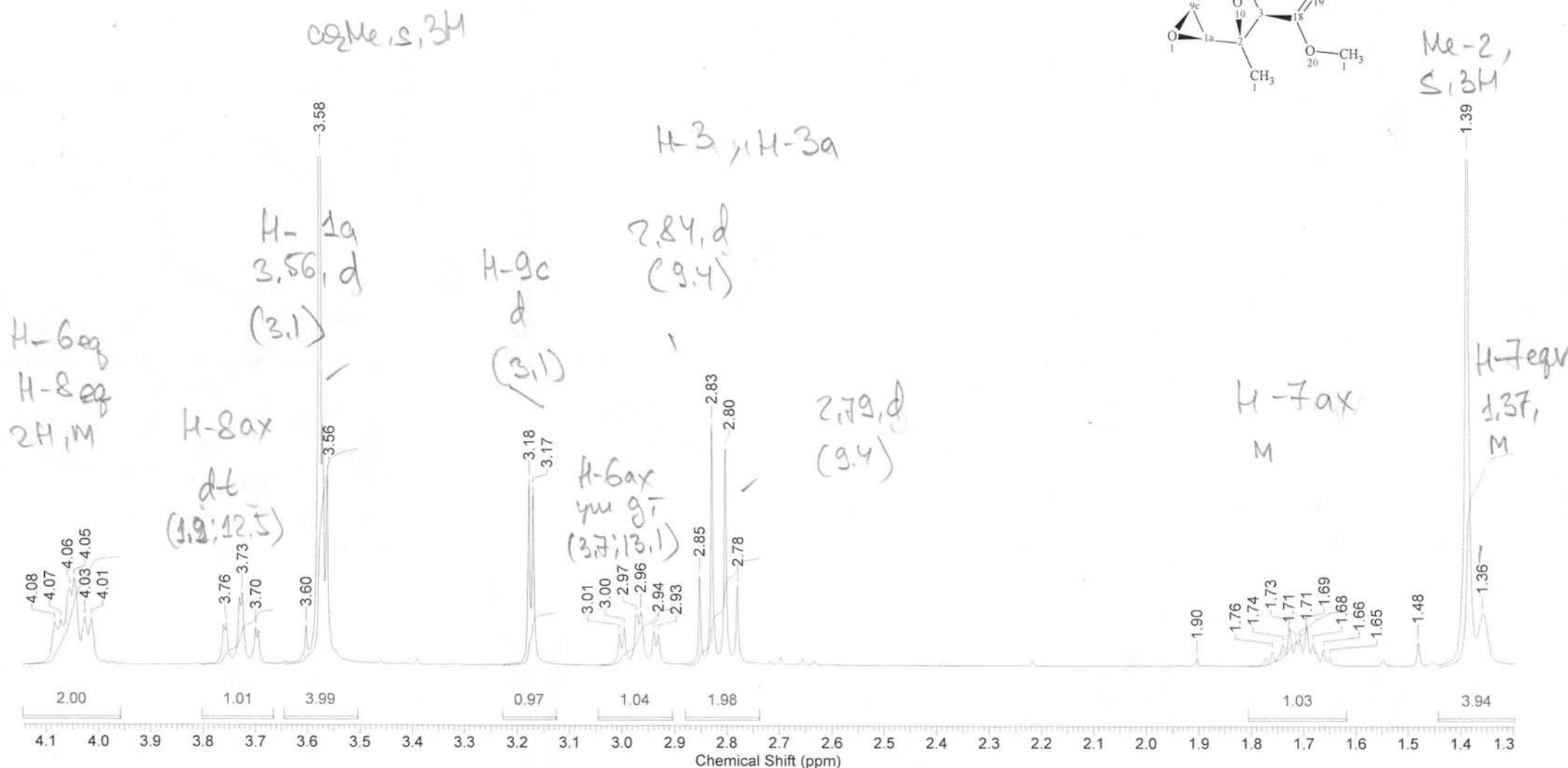
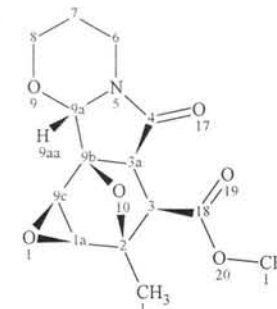


36b



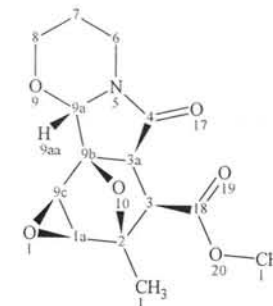
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File Name	C:\Users\Fedor\Desktop\19.06.09\laz20\laz20_001000fid	Frequency (MHz)	400.14	Nucleus	1H	
Number of Transients	4	Original Points Count	16384	Points Count	16384	
Solvent	CHLOROFORM-D	Sweep Width (Hz)	10204.08	Pulse Sequence	zg	
				Temperature (degree C)	27.000	

Compound 36b



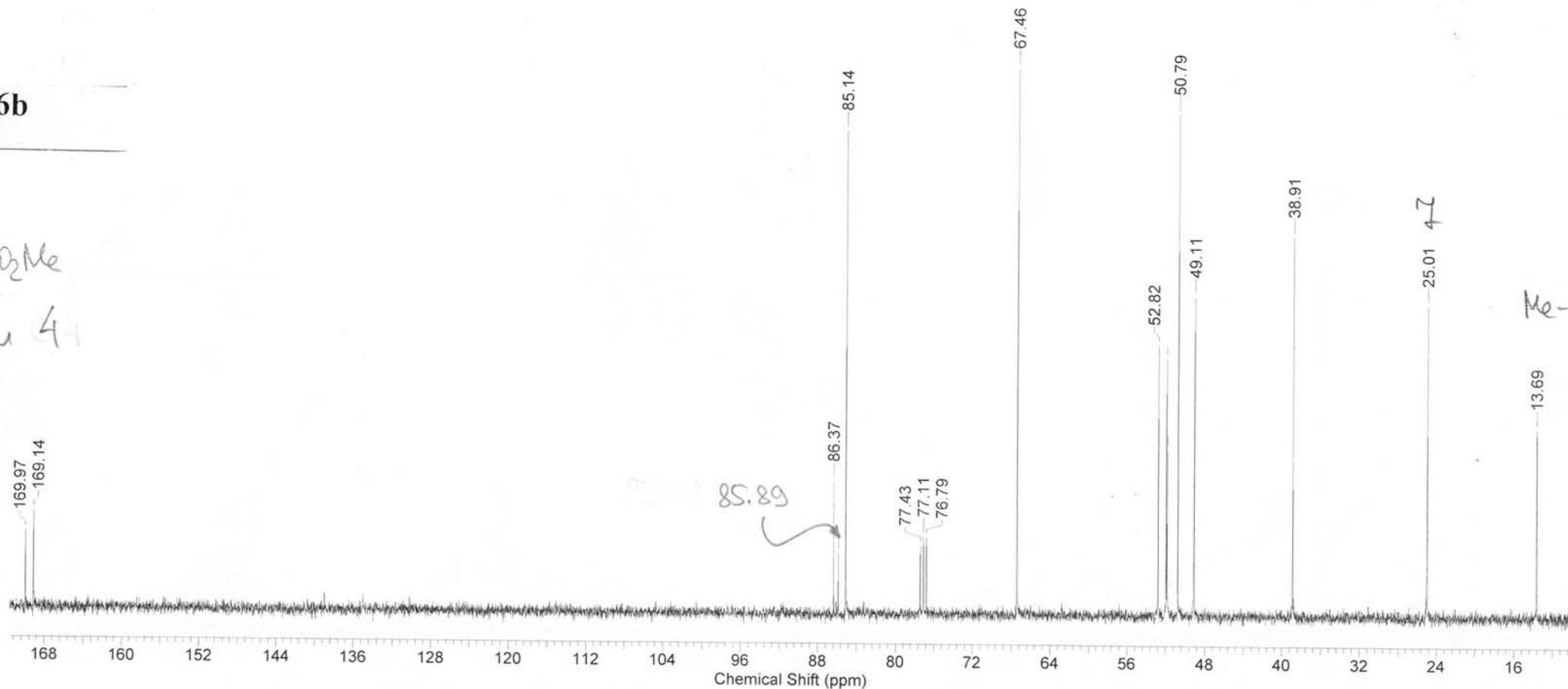
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File Name	C:\Users\Fedor\Desktop\19.06.09\laz20c13dec\laz20c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	144	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D		Sweep Width (Hz)	26315.79	
Temperature (degree C)	27.000						

Compound 36b



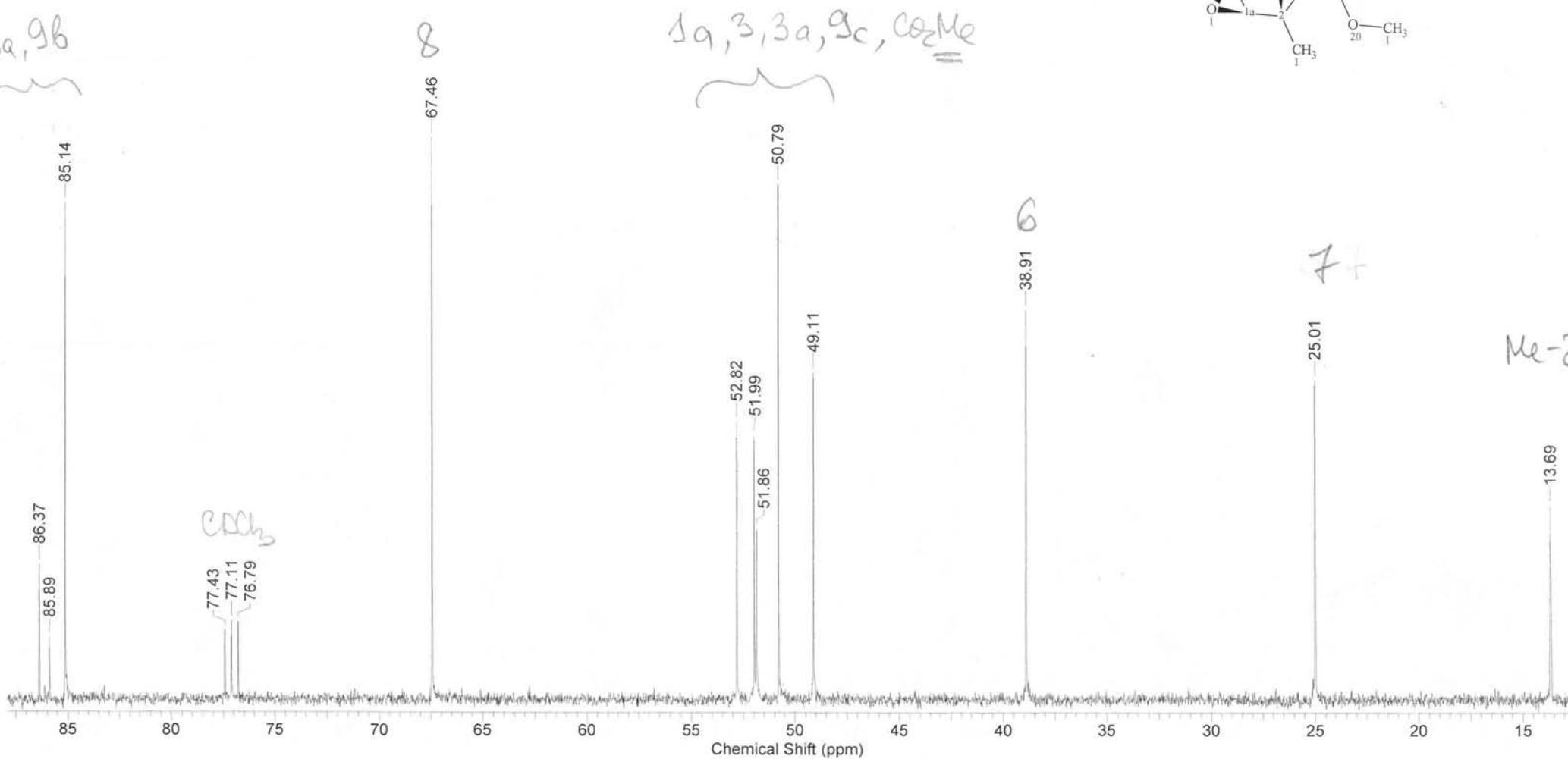
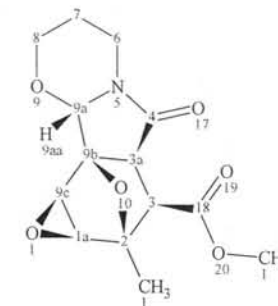
36b

CO₂Me
= u 4



Acquisition Time (sec)	0.6226	Comment	Imported from UXNMR.		Date	19 Jun 2009 16:59:44	
File Name	C:\Users\Fedor\Desktop\19.06.09\laz20c13dec\laz20c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	144	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D		Sweep Width (Hz)	26315.79	
Temperature (degree C)	27.000						

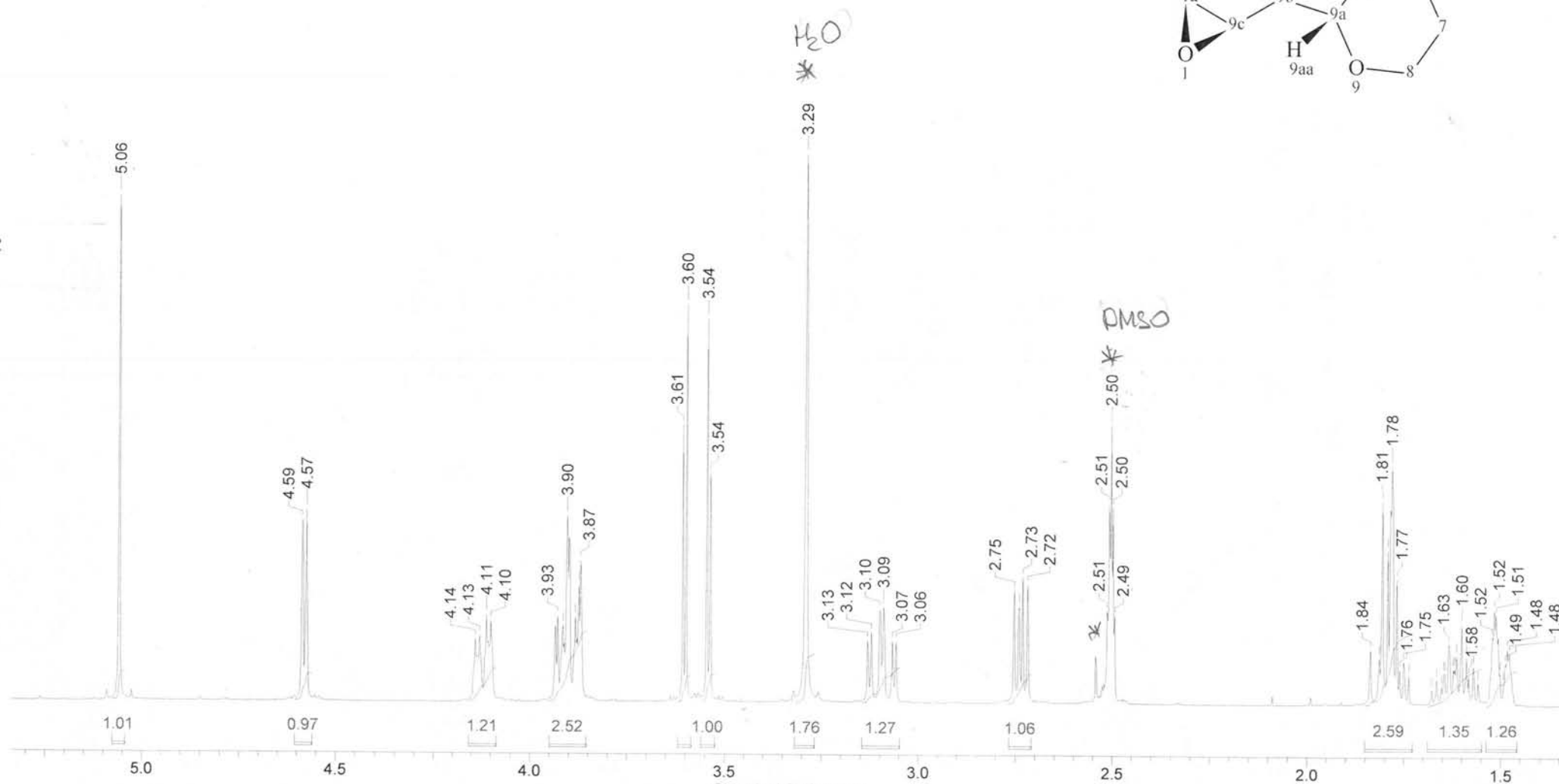
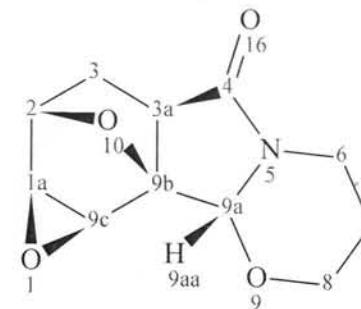
Compound 36b



13 May 2011

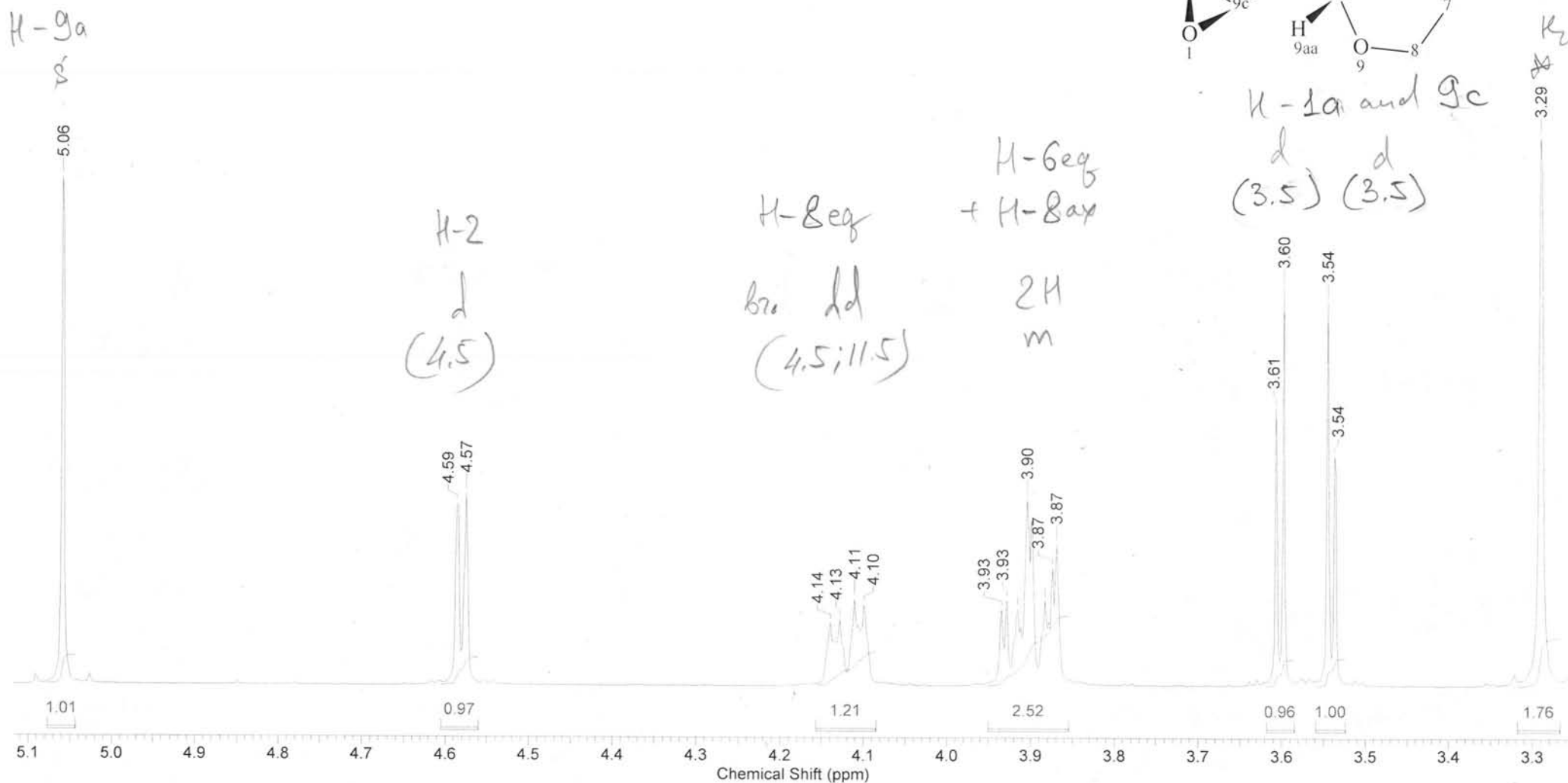
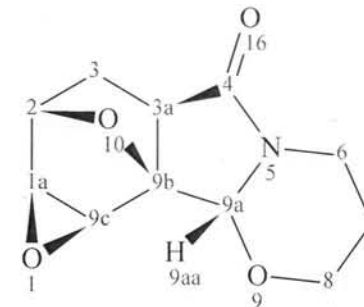
Acquisition Time (sec)	1.5729	Comment	Imported from UXNMR.		Date	06 May 2011 10:20:48	
File Name	D:\NMR\C_13\29.04.11 (C-13 Poma)\rudn-290411-N15\rudn-290411-N15_002000fid			Frequency (MHz)	400.14		
Nucleus	1H	Number of Transients	12	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	10416.67	Temperature (degree C)	32.000

Compound 36c



Acquisition Time (sec)	1.5729	Comment	Imported from UXNMR.		Date	06 May 2011 10:20:48	
File Name	D:\NMR\C_13\29.04.11 (C-13 Рома)\rudn-290411-N15\rudn-290411-N15_002000fid				Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	12	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	10416.67	Temperature (degree C)	32.000

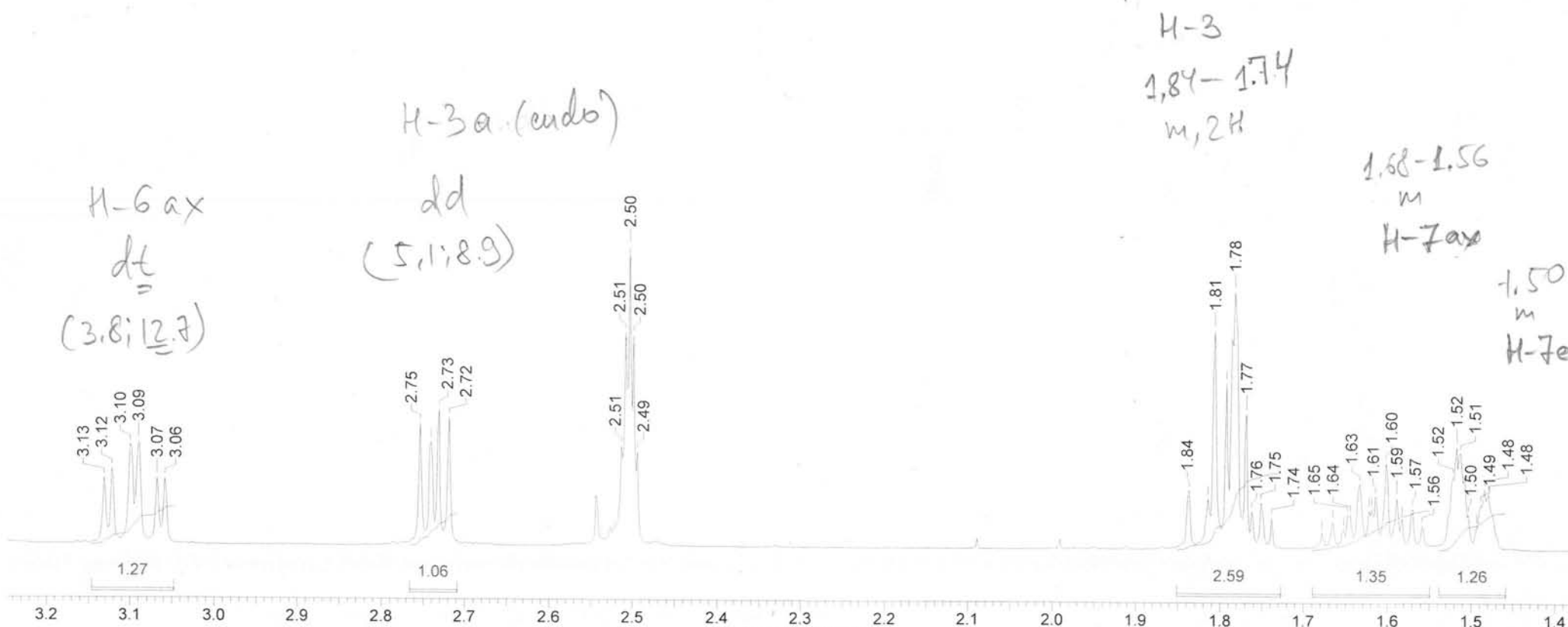
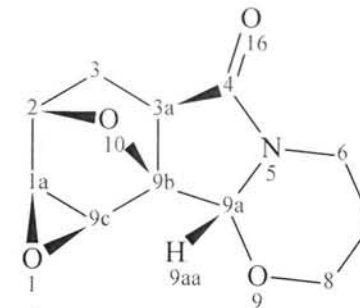
Compound 36c



13 May 2011

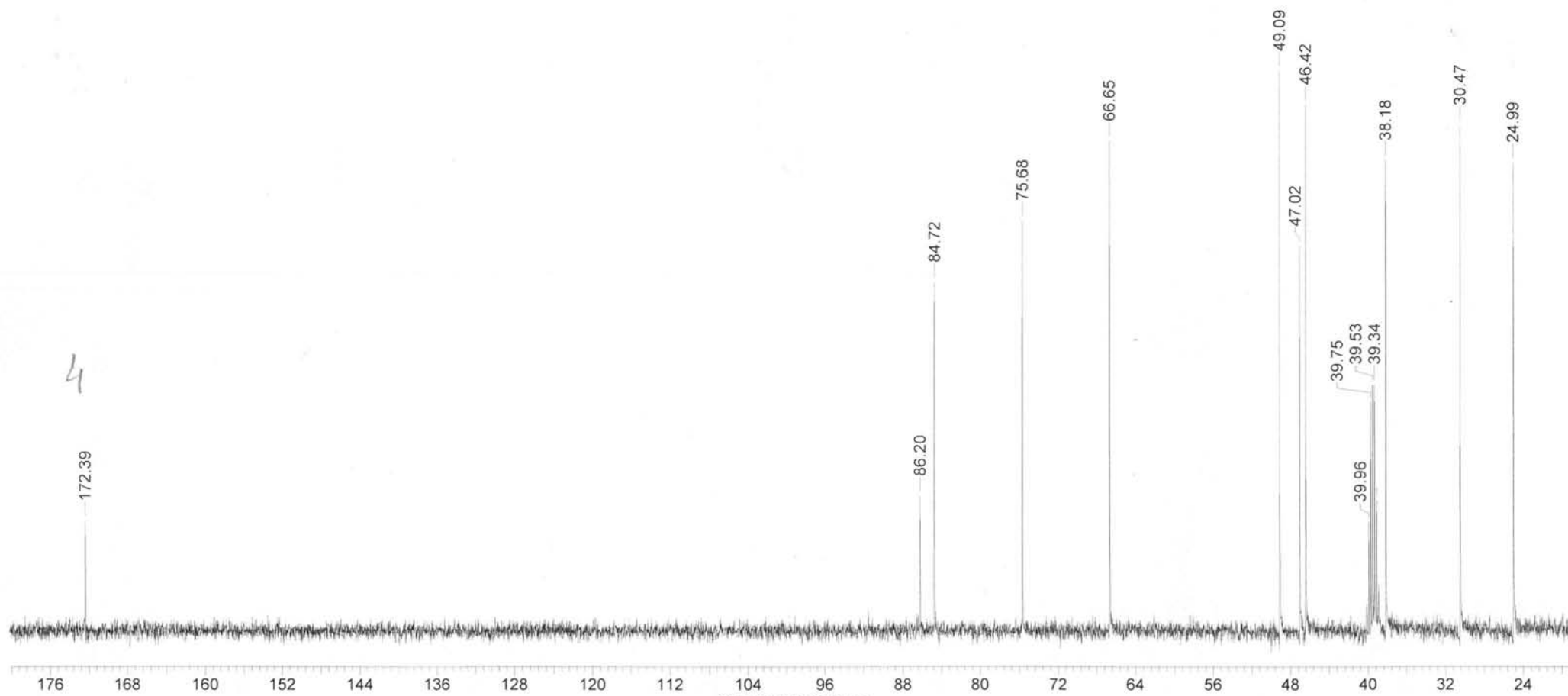
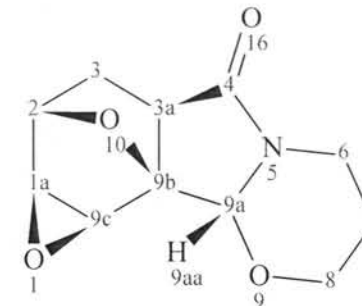
Acquisition Time (sec)	1.5729	Comment	Imported from UXMNR.		Date	06 May 2011 10:20:48	
File Name	D:\NMR\C_13\29.04.11 (C-13 Рома)\rudn-290411-N15\rudn-290411-N15_002000fid				Frequency (MHz)	400.14	
Nucleus	¹ H	Number of Transients	12	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	10416.67	Temperature (degree C)	32.000

Compound 36c



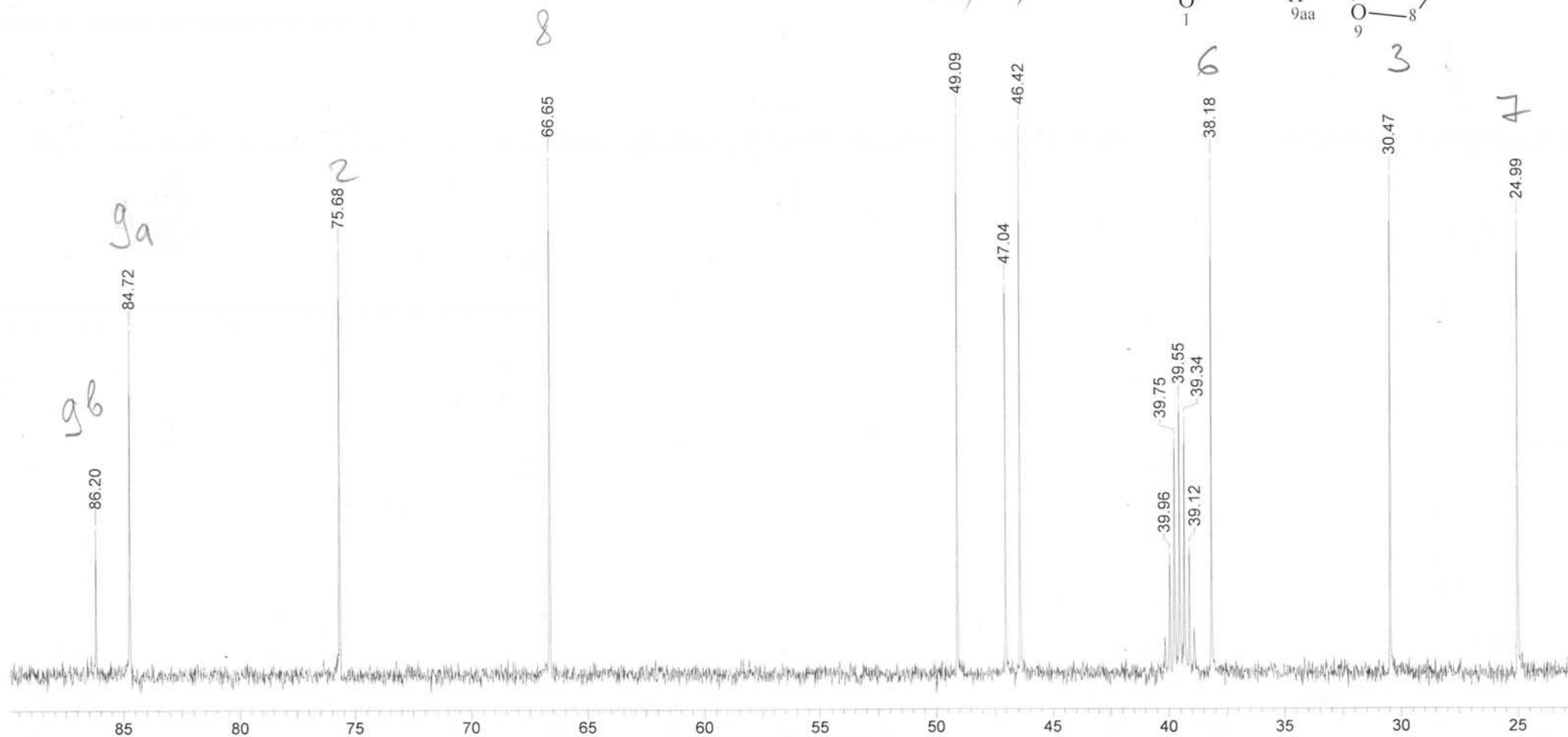
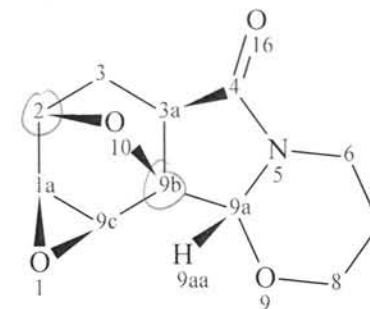
Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.			Date	06 May 2011 11:24:48
File Name	D:\NMR\C_13\29.04.11 (C-13 Рома)\rudn-290411-N15-c13dec\rudn-290411-N15-c13dec_001000fid					Frequency (MHz)	100.62
Nucleus	13C	Number of Transients	239	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compound 36c



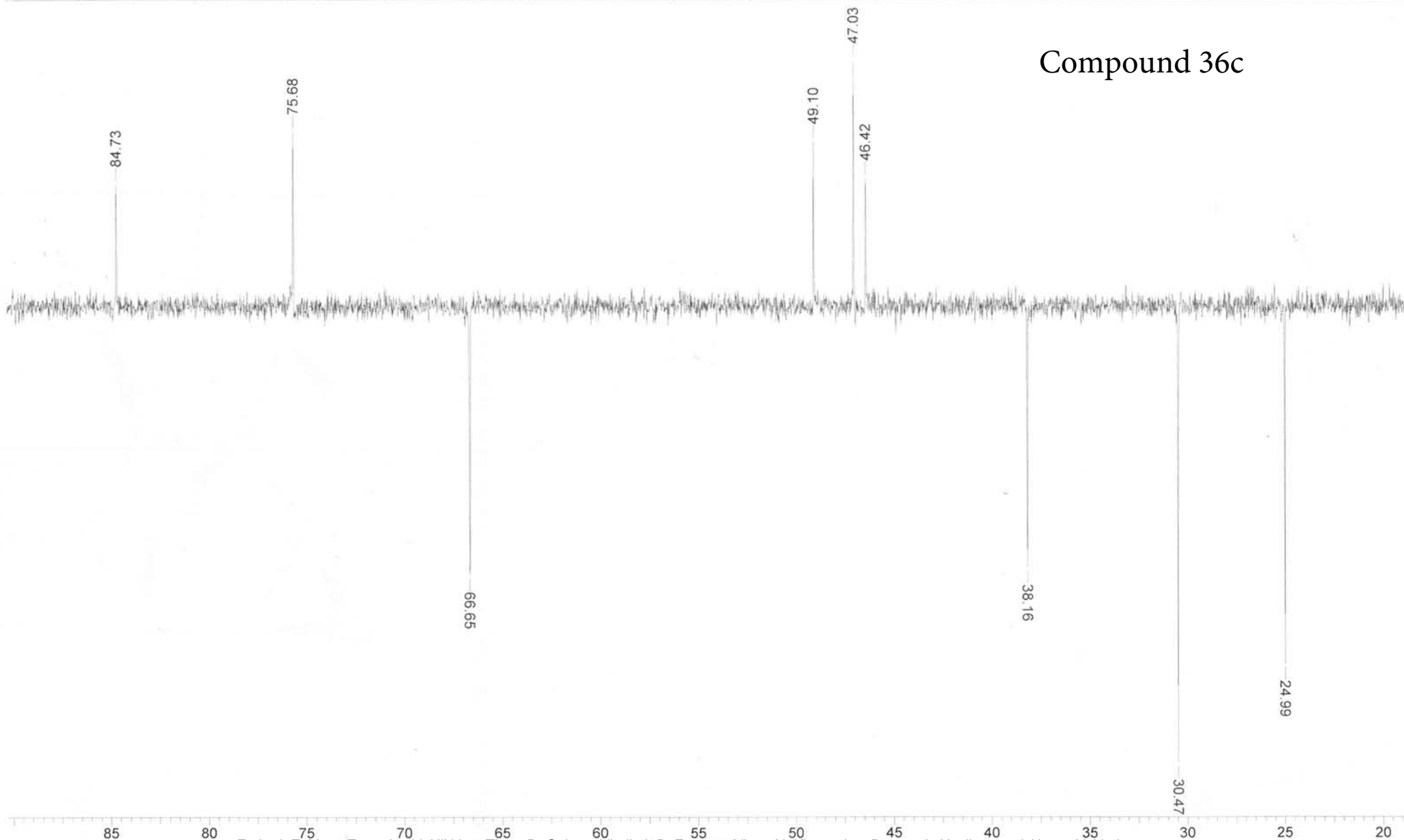
Acquisition Time (sec)	0.5571	Comment	Imported from UXNMR.		Date	06 May 2011 11:24:48	
File Name	D:\NMR\C_13\29.04.11 (C-13 Poma)\rudn-290411-N15-c13dec\rudn-290411-N15-c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	239	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compound 36c



13 May 2011

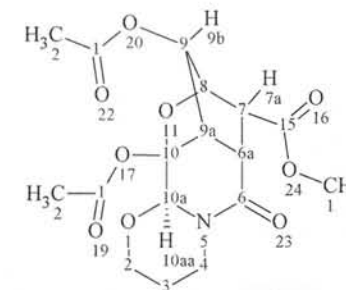
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File Name	D:\NMR\C_13\29.04.11 (C-13 Poma)\rudn-290411-N15-dept135\rudn-290411-N15-dept135_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	184	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	32.000



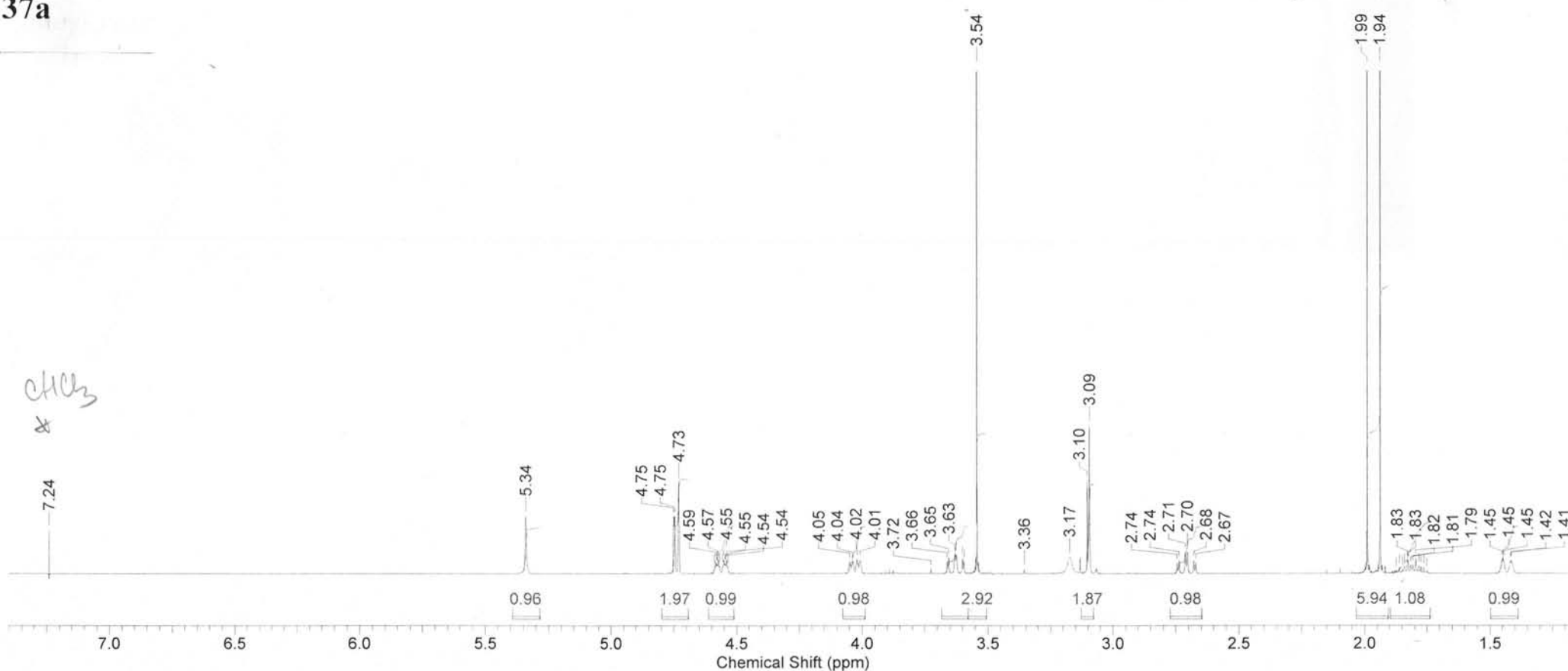
Formula	C ₁₇ H ₂₁ NO ₉	FW	383.3499
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Date Stamp	Dec 13 2007	File Name	D:\NMR\IC_13\ТУРЧИН зима 2007-08\Гузель № 15\Guzel15\FZGuz15-h_131207				
Frequency (MHz)	399.96	Nucleus	1H	Number of Transients	32	Original Points Count	29999
Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	40.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	1611.3262	Sweep Width (Hz)	5999.70	Temperature (degree C)	29.000		

Compound 37a

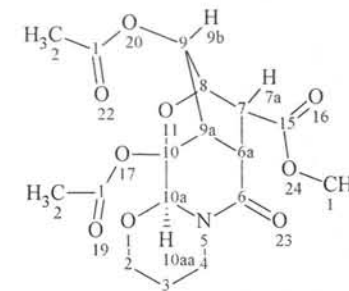


37a



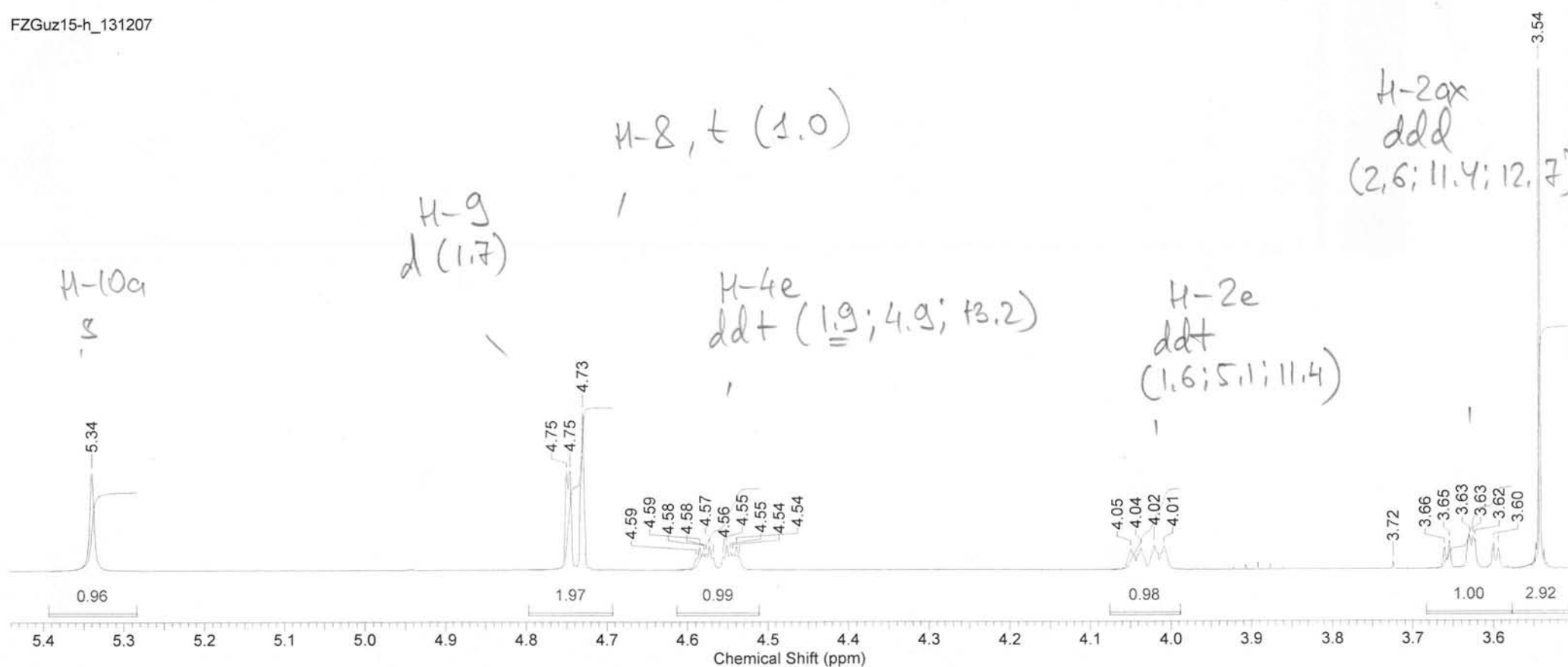
Formula C ₁₇ H ₂₁ NO ₉		FW 383.3499			
Acquisition Time (sec)	5.0001	Comment	ENOTHERA-56_02.12.05	Date	Dec 13 2007
Date Stamp	Dec 13 2007	File Name	D:\NMR\13\ТУРЧИН зима 2007-08\Гузель № 15\Guzel15\FZGuz15-h_131207		
Frequency (MHz)	399.96	Nucleus	1H	Number of Transients	32
Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	40.00
Spectrum Offset (Hz)	1611.3262	Sweep Width (Hz)	5999.70	Temperature (degree C)	29.000
				Original Points Count	29999
				Solvent	CHLOROFORM-d

Compound 37a



OME
s, 3H

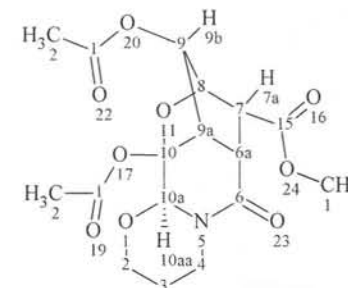
FZGuz15-h_131207



Formula C₁₇H₂₁NO₉ FW 383.3499

Acquisition Time (sec)	5.0001	Comment	ENOTHERA-56_02.12.05		Date	Dec 13 2007	
Date Stamp	Dec 13 2007	File Name	D:\NMR\IC_13\ТУРЧИН зима 2007-08\Гузелъ № 15\Guzel15\FZGuz15-h_131207				
Frequency (MHz)	399.96	Nucleus	1H	Number of Transients	32	Original Points Count	29999
Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	40.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	1611.3262	Sweep Width (Hz)	5999.70	Temperature (degree C)	29.000		

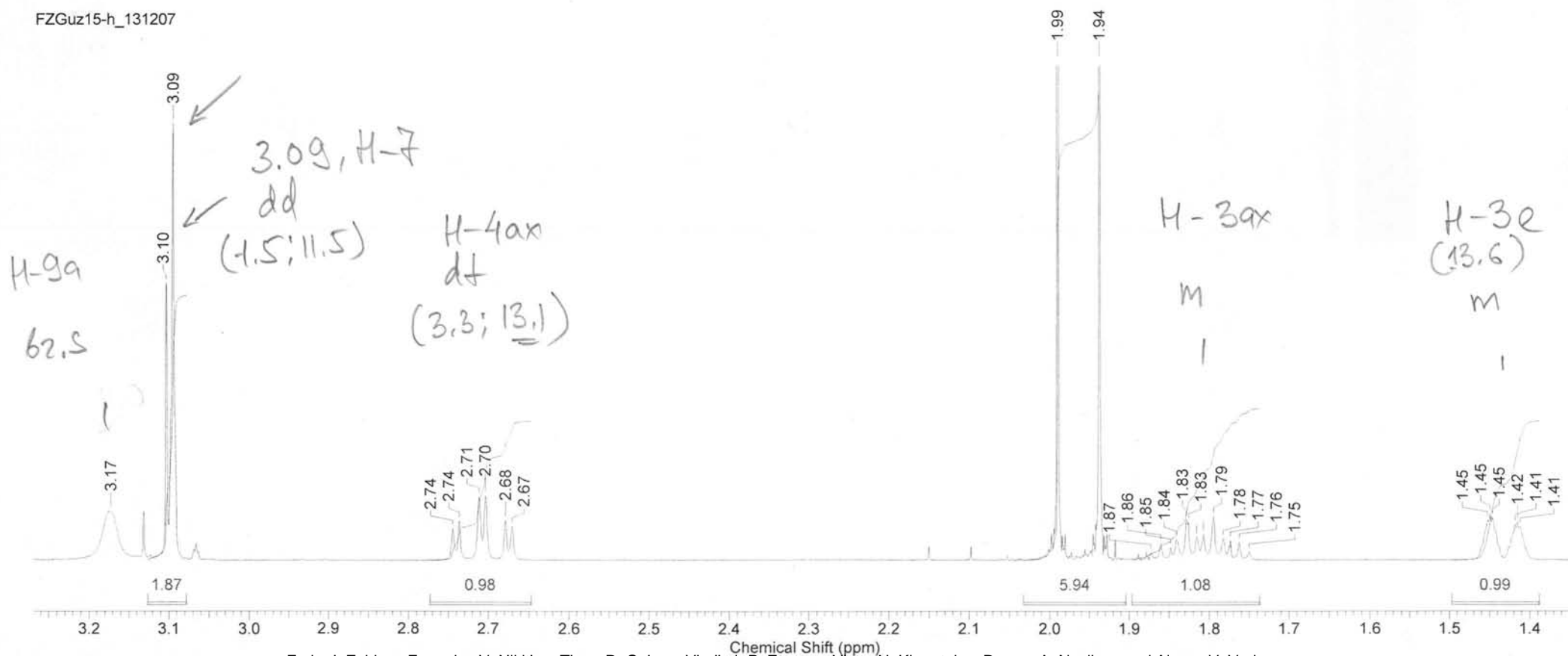
Compound 37a



3.10, H-6a
dd (4.5; 11.5)

s, COMe x2

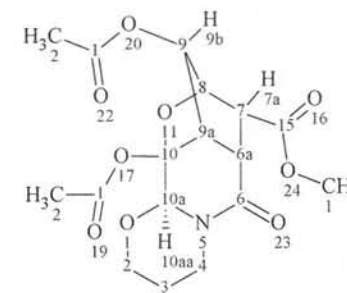
FZGuz15-h_131207



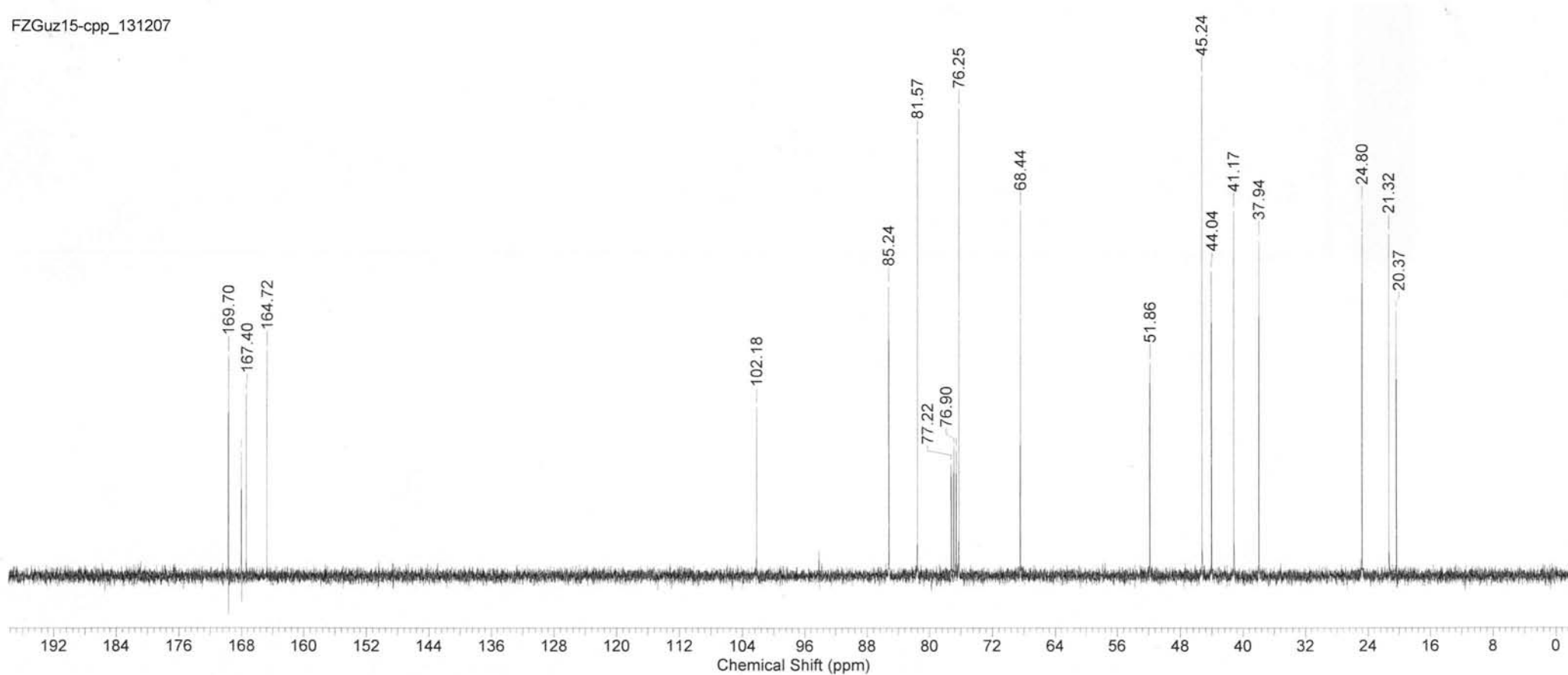
Formula C₁₇H₂₁NO₉ FW 383.3499

Acquisition Time (sec)	1.0000	Comment	13C OBSERVE	Date	Dec 13 2007	Date Stamp	Dec 13 2007
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Nucleus	13C	Number of Transients	8192	Original Points Count	27009	Points Count	32768
Pulse Sequence	s2pul	Receiver Gain	58.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	9466.8164	Sweep Width (Hz)	27008.78	Temperature (degree C)	29.000		

Compound 37a



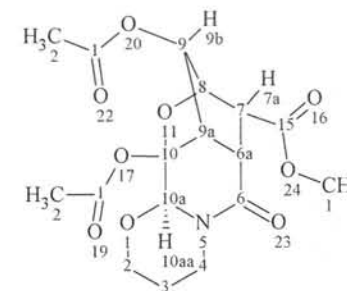
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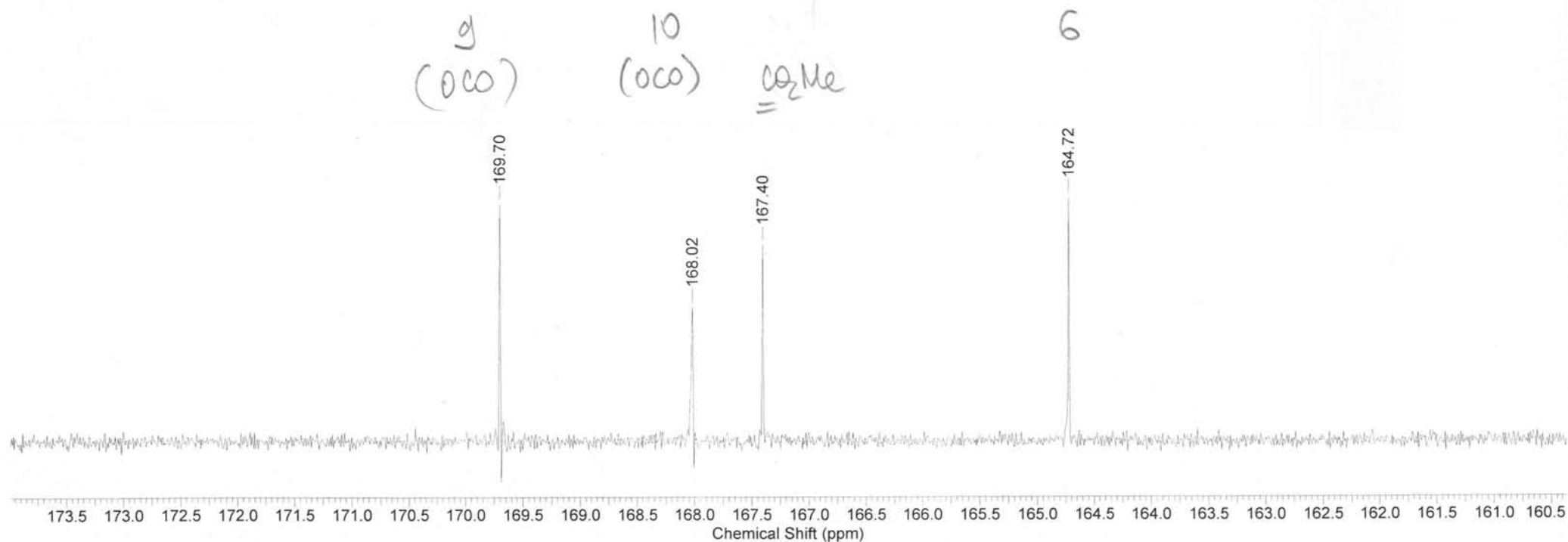
Formula C₁₇H₂₁NO₉ FW 383.3499

Acquisition Time (sec)	1.0000	Comment	13C OBSERVE	Date	Dec 13 2007	Date Stamp	Dec 13 2007
File Name	D:\NMR\13\ТУРЧИН зима 2007-08\Гузель № 15\Guzel15\FZGuz15-cpp_131207					Frequency (MHz)	100.58
Nucleus	13C	Number of Transients	8192	Original Points Count	27009	Points Count	32768
Pulse Sequence	s2pul	Receiver Gain	58.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	9466.8164	Sweep Width (Hz)	27008.78	Temperature (degree C)	29.000		

Compound 37a



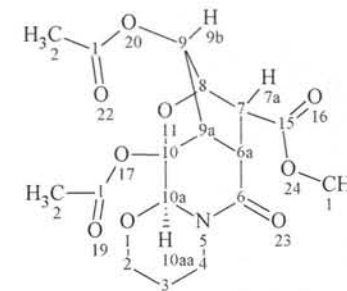
FZGuz15-cpp_131207



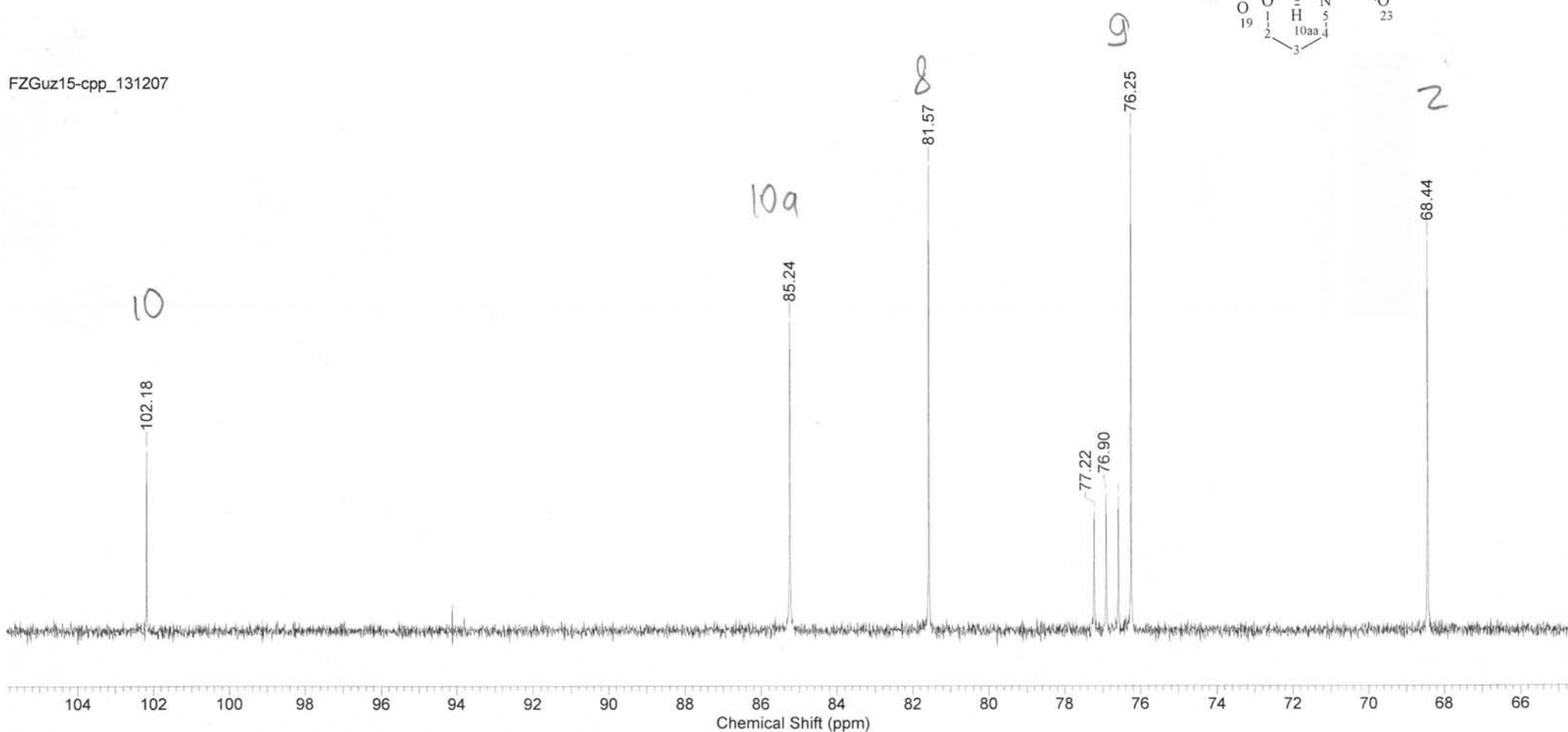
Formula C₁₇H₂₁NO₉ FW 383.3499

Acquisition Time (sec)	1.0000	Comment	13C OBSERVE	Date	Dec 13 2007	Date Stamp	Dec 13 2007
File Name	D:\NMR\13\ТУРЧИН зима 2007-08\Гузелъ № 15\Guzel15\FZGuz15-cpp_131207			Frequency (MHz)	100.58		
Nucleus	13C	Number of Transients	8192	Original Points Count	27009	Points Count	32768
Pulse Sequence	s2pul	Receiver Gain	58.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	9466.8164	Sweep Width (Hz)	27008.78	Temperature (degree C)	29.000		

Compound 37a



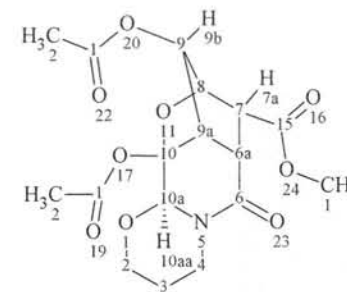
FZGuz15-cpp_131207



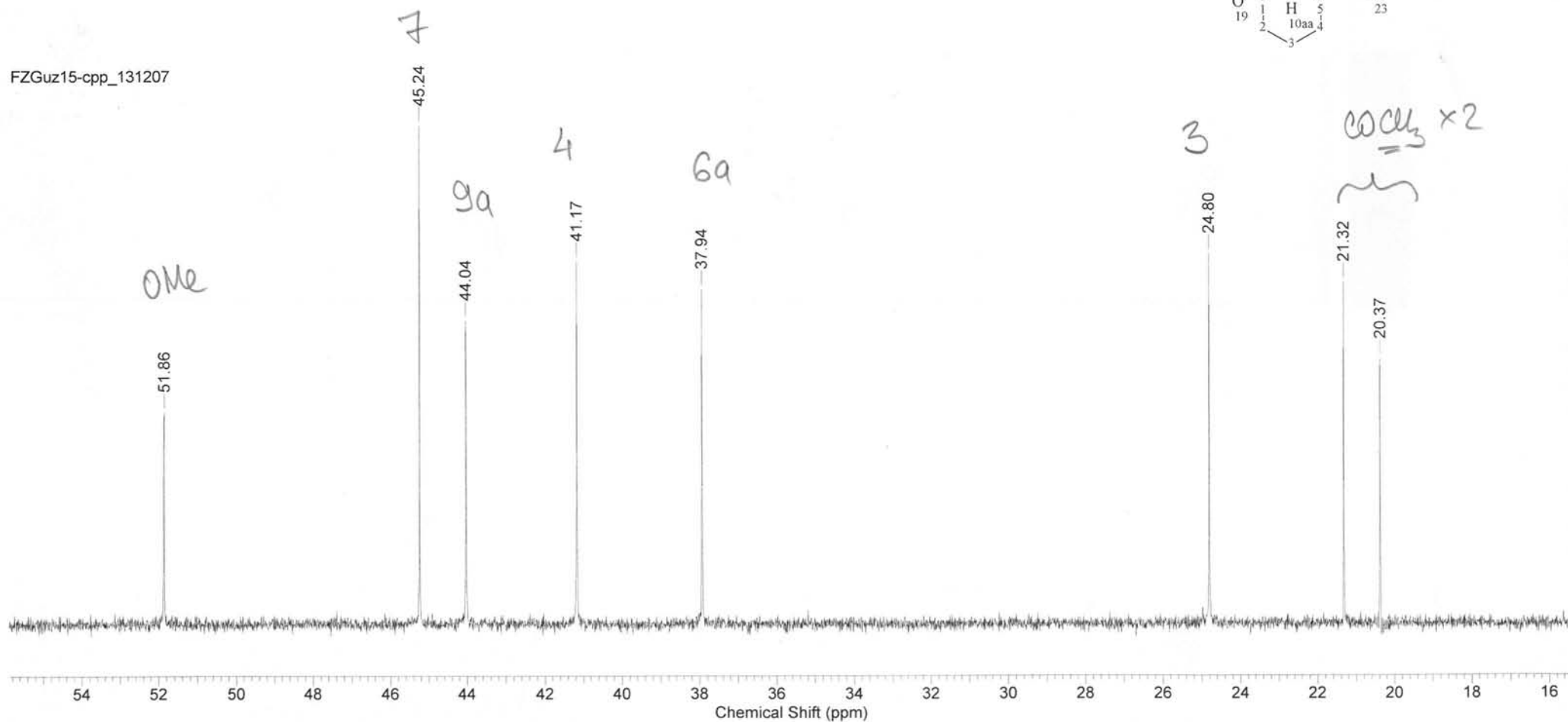
Formula $C_{17}H_{21}NO_9$ FW 383.3499

Acquisition Time (sec)	1.0000	Comment	13C OBSERVE	Date	Dec 13 2007	Date Stamp	Dec 13 2007
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Nucleus	13C	Number of Transients	8192	Original Points Count	27009	Points Count	32768
Pulse Sequence	s2pul	Receiver Gain	58.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	9466.8164	Sweep Width (Hz)	27008.78	Temperature (degree C)	29.000		

Compound 37a



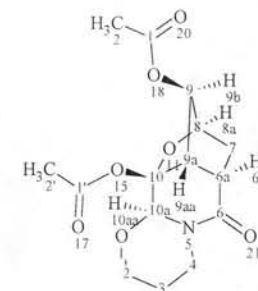
FZGuz15-cpp_131207



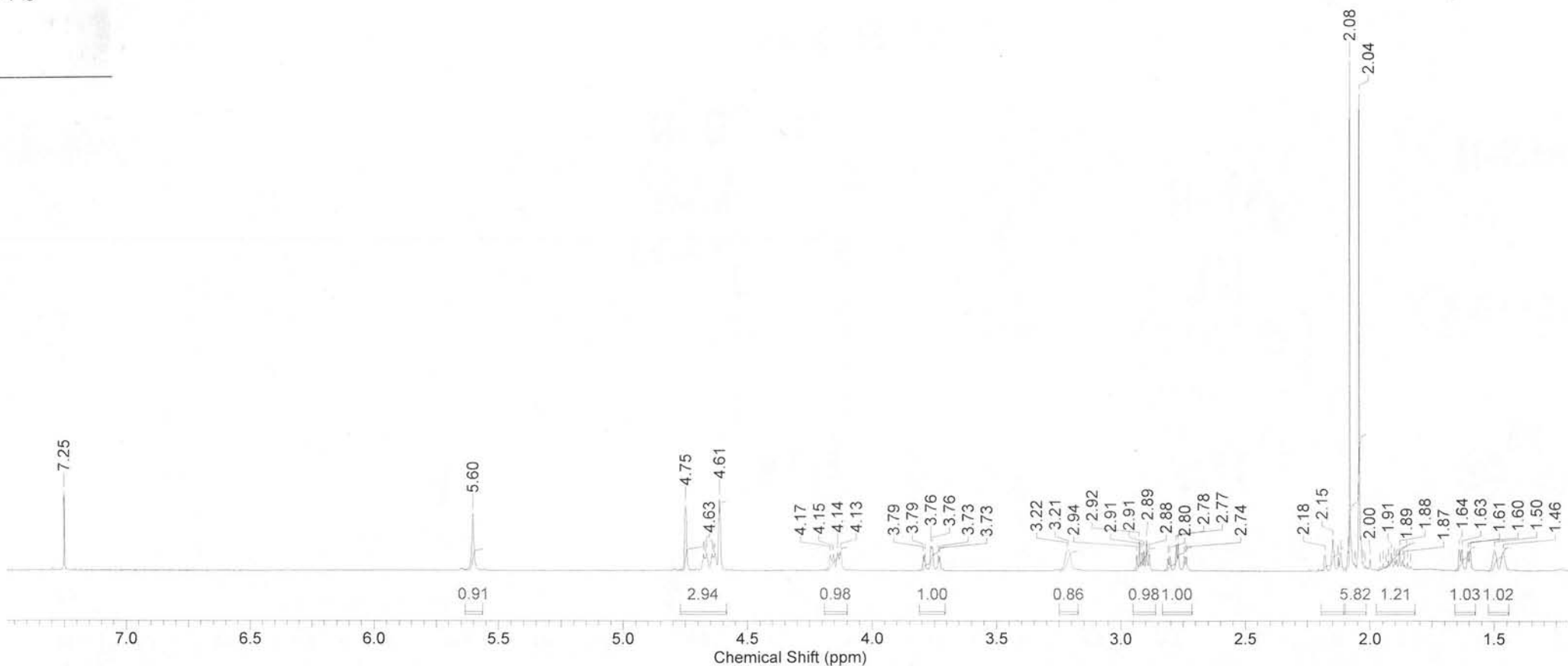
Formula $C_{15}H_{19}NO_7$ FW 325.3139

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	17 May 2011 11:43:12	Date Stamp	17 May 2011 15:31:23
File Name	D:\NMR\16.05.11\FZ1857-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	10
Origin	ECS 400	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2398.6931	Sweep Width (Hz)	7503.00
Temperature (degree C)	19.000						

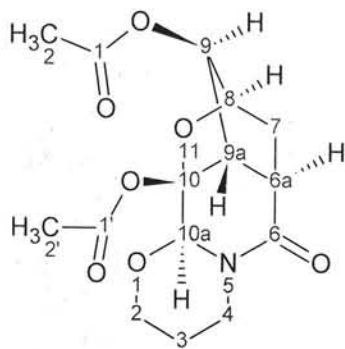
Compound 37b



37b



Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.	Date	09 Jun 2011 17:53:04
File Name	C:\Users\Fedor\Desktop\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\N-10\rudn-300511-N10\rudn-300511-N10\rudn-300511-N10_001000fid				
Frequency (MHz)	400.14	Nucleus	¹ H	Number of Transients	32
Points Count	16384	Pulse Sequence	zg	Solvent	CHLOROFORM-D
Temperature (degree C)	27.000			Original Points Count	16384
				Sweep Width (Hz)	10204.08



4e,4a 13.1

4e,3e 1.9

4e,3a 5.0

4a,3e 3.1

4a,3a 13.1

3e,3a 13.7

2e,2a 12.5

2e,3a 5.0

2e,3e ~1.0

2a,3a ~12.5

2a,3e 2.5

9a,6a 3.1

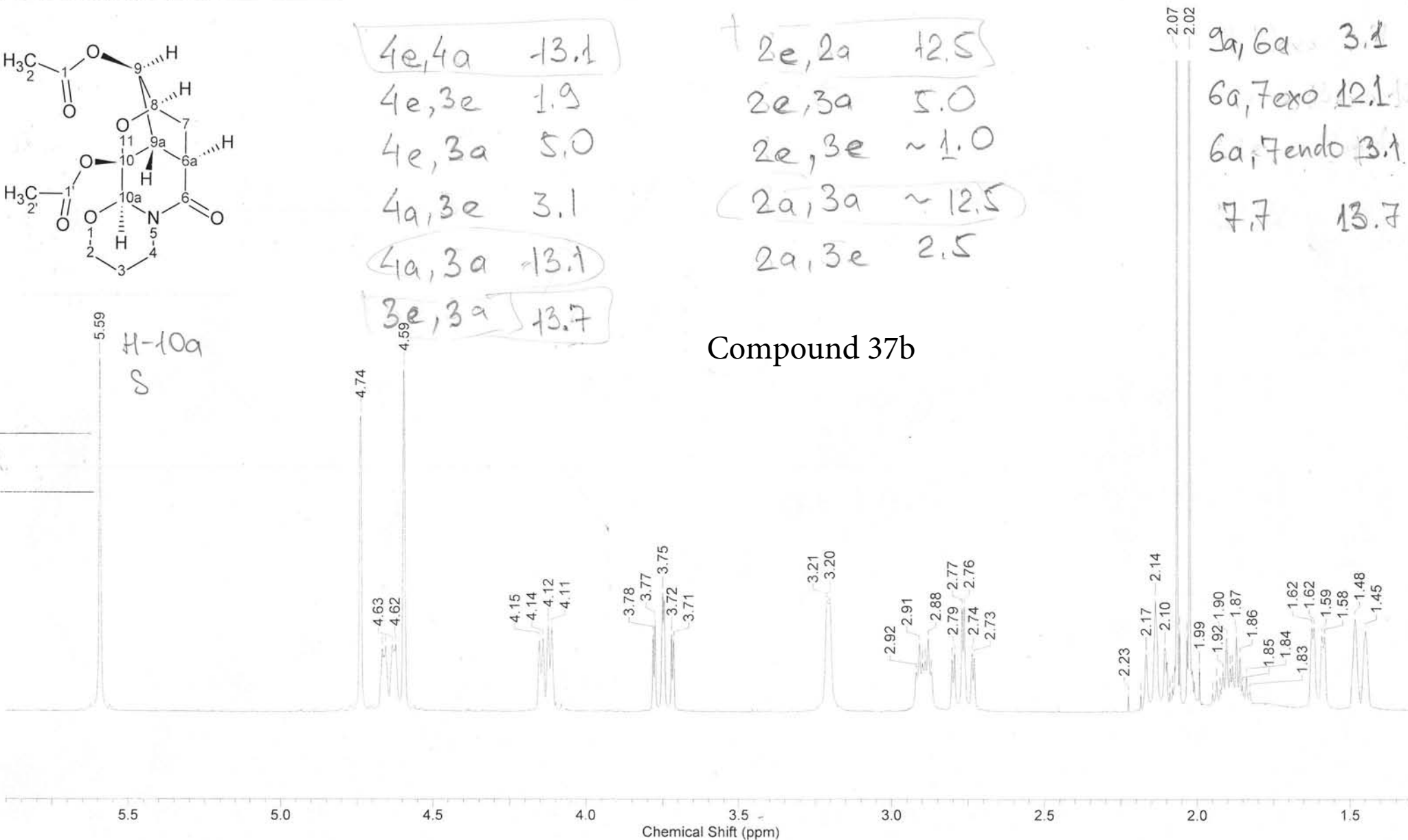
6a,7exo 12.1-12.1

6a,7endo 3.1

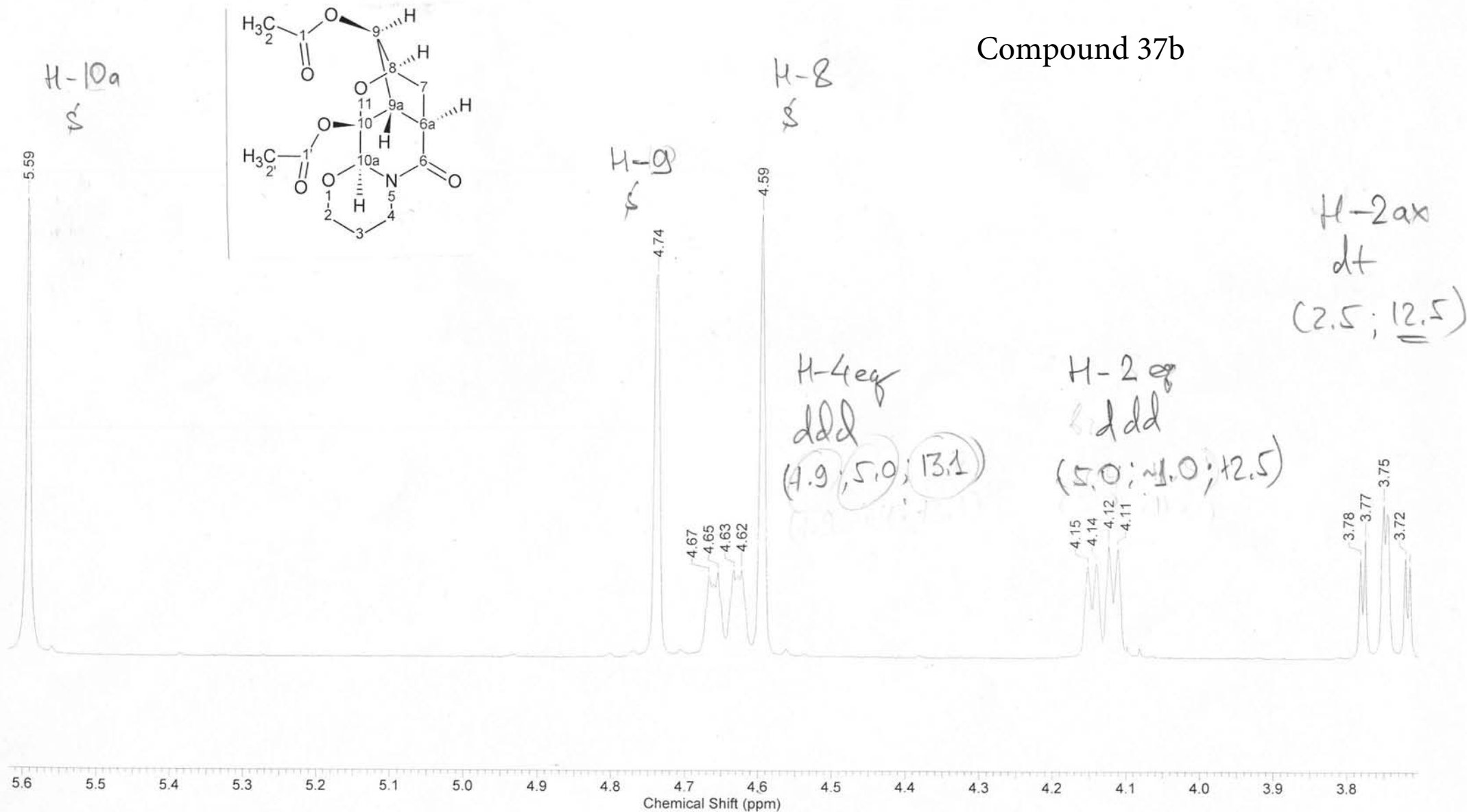
7.7 13.7

Compound 37b

37b

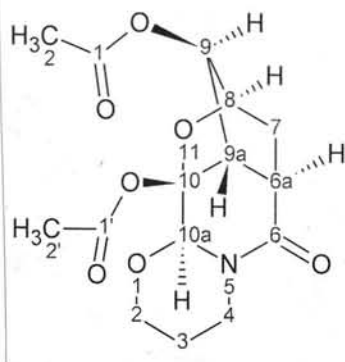


Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.	Date	09 Jun 2011 17:53:04
File Name	C:\Users\Fedor\Desktop\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\N-10\rudn-300511-N10\rudn-300511-N10\rudn-300511-N10_001000fid				
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	32
Points Count	16384	Pulse Sequence	zg	Solvent	CHLOROFORM-D
Temperature (degree C)	27.000			Original Points Count	16384
				Sweep Width (Hz)	10204.08



15 Jun 2011

Acquisition Time (sec)	1.6056	Comment	Imported from UXNMR.	Date	09 Jun 2011 17:53:04
File Name	C:\Users\Fedor\Desktop\19.05.2011 С 13 Для Иры Статья в Тетраэдрон\N-10\rudn-300511-N10\rudn-300511-N10\rudn-300511-N10_001000fid				
Frequency (MHz)	400.14	Nucleus	¹ H	Number of Transients	32
Points Count	16384	Pulse Sequence	zg	Solvent	CHLOROFORM-D
Temperature (degree C)	27.000			Original Points Count	16384
				Sweep Width (Hz)	10204.08



CO Me - 9

CO Me - 10

Compound 37b

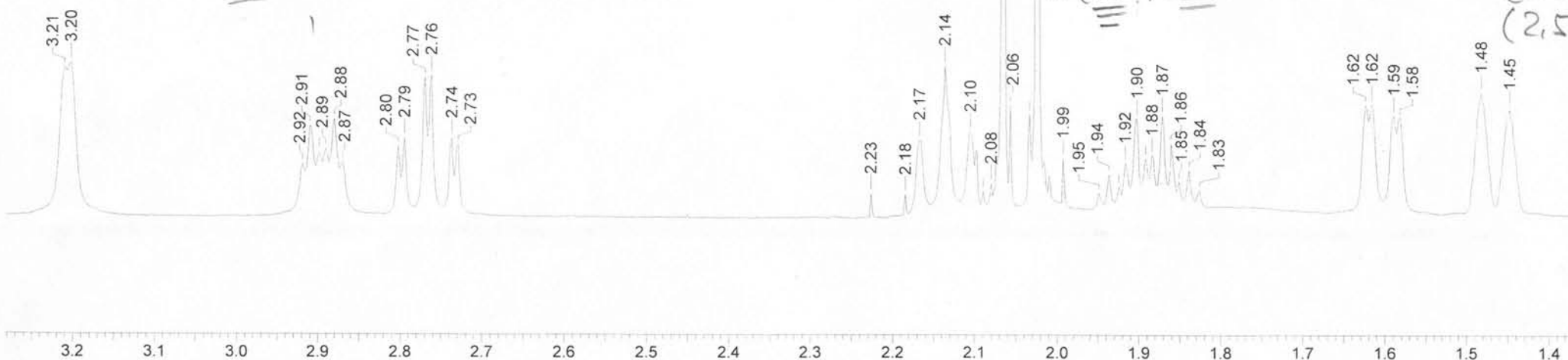
H-9a, b, d
(3.1)H-6a
dt

(3.1; 12.1)

H-4ax
dt
(3.1; 13.1)H-7exo
dd
(12.1; 13.7)H-3ax
tg

n(13.7; 5.0)

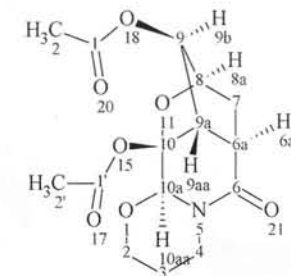
H-7endo H-3eq
m
(13.7)
dd
(1.9)
(3.1)
(1.0)
(2.5)



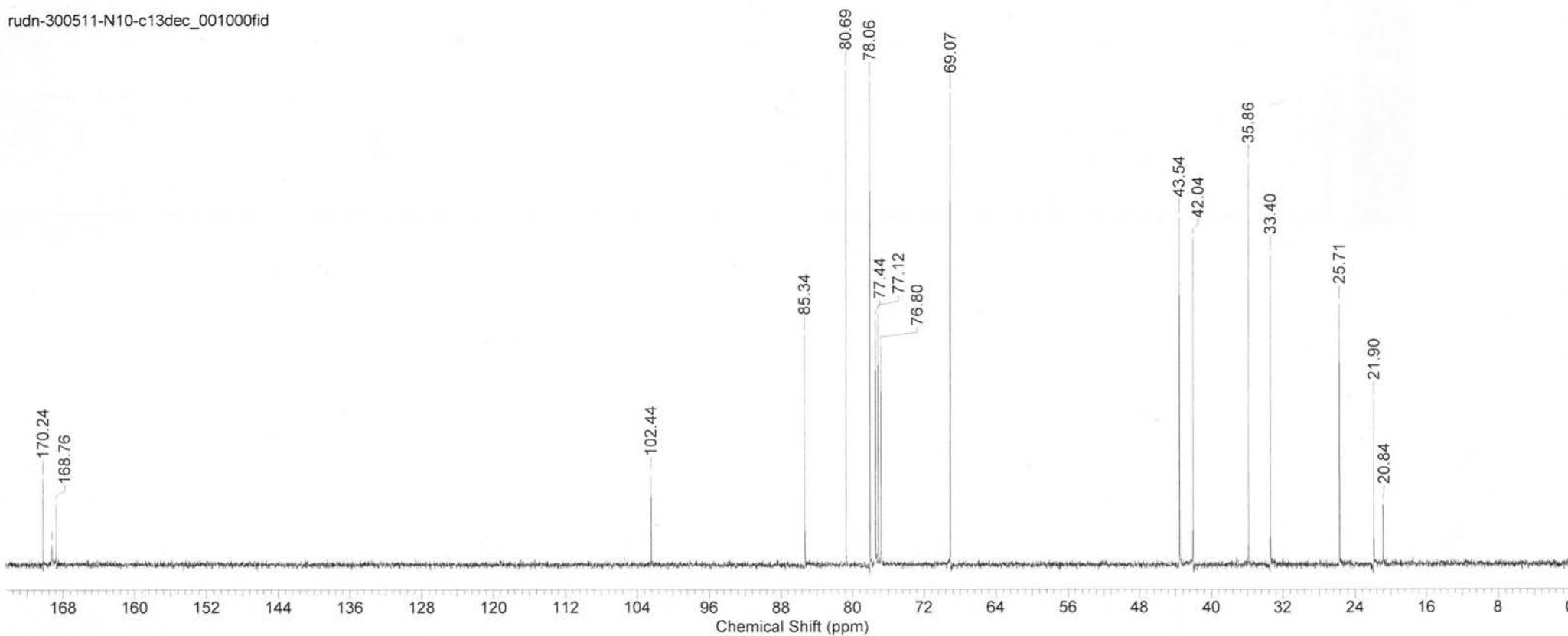
Formula $C_{15}H_{19}NO_7$ FW 325.3139

Acquisition Time (sec)	0.5898	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	09 Jun 2011 18:08:00
Date Stamp	09 Jun 2011 18:08:00				
File Name	D:\NMR\19.05.2011 C 13 Для Иры Статья в Тетраэдрон\N-10\rudn-300511-N10-c13dec\rudn-300511-N10-c13dec\rudn-300511-N10-c13dec_001000fid				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	3000
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	27777.78	Solvent	CHLOROFORM-d
Sweep Width (Hz)	27776.08	Temperature (degree C)	27.000	Spectrum Offset (Hz)	9637.6885

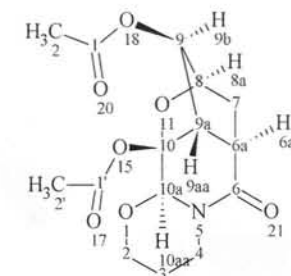
Compound 37b



rudn-300511-N10-c13dec_001000fid



Formula C ₁₅ H ₁₉ NO ₇	FW 325.3139			
Acquisition Time (sec) 0.5898	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 09 Jun 2011 18:08:00		
Date Stamp 09 Jun 2011 18:08:00				
File Name D:\NMR\19.05.2011 C 13 Для Иры Статья в Тетраэдрон\N-10\rudn-300511-N10-c13dec\rudn-300511-N10-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 3000	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpgg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 27777.78	Solvent CHLOROFORM-d	Spectrum Offset (Hz) 9637.6885	
Sweep Width (Hz) 27776.08	Temperature (degree C) 27.000			

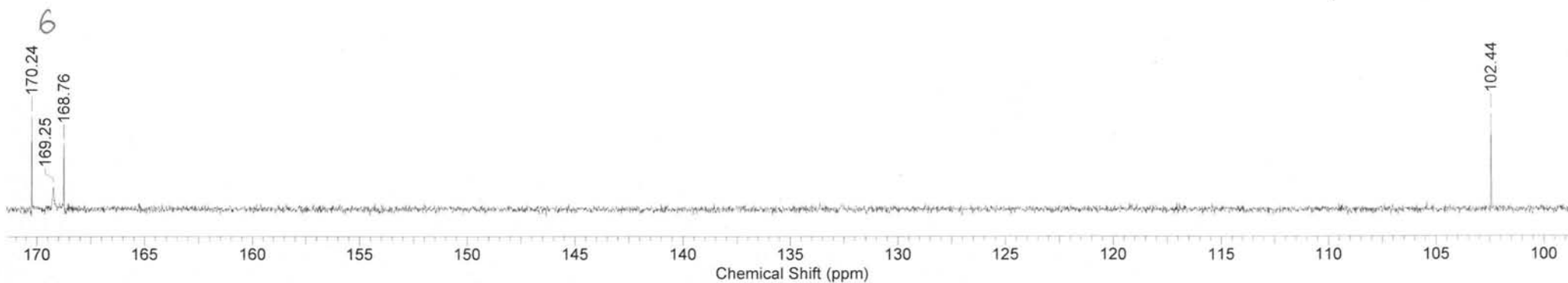


rudn-300511-N10-c13dec_001000fid

Compound 37b

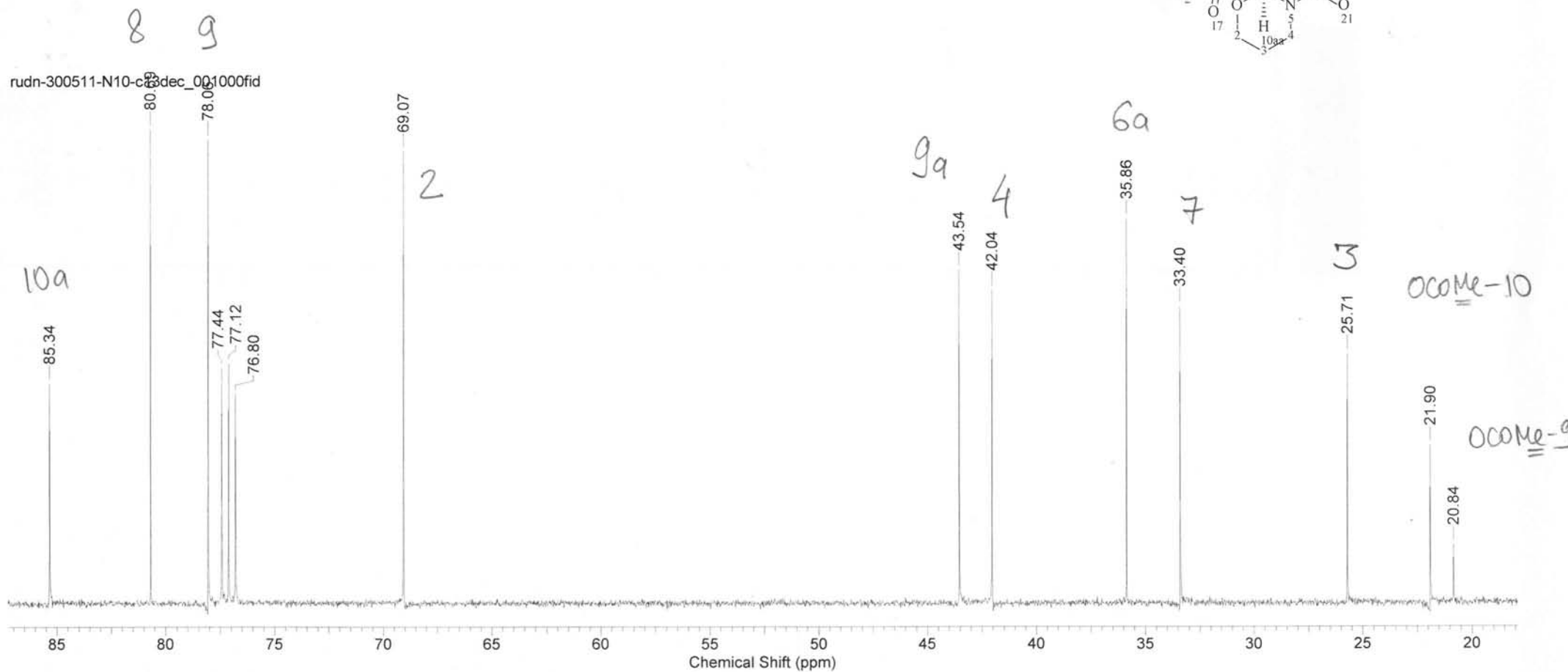
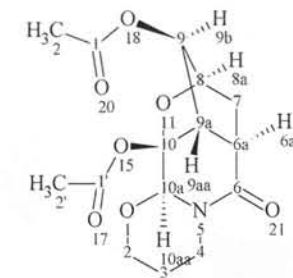
OCOME
9

OCOME
10



Formula C ₁₅ H ₁₉ NO ₇	FW 325.3139			
Acquisition Time (sec) 0.5898	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 09 Jun 2011 18:08:00		
Date Stamp 09 Jun 2011 18:08:00				
File Name D:\NMR\19.05.2011 C 13 Для Иры Статья в Тетраэдрон\N-10\rudn-300511-N10-c13dec\rudn-300511-N10-c13dec\rudn-300511-N10-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 3000	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 27777.78	Solvent CHLOROFORM-d	Spectrum Offset (Hz) 9637.6885	
Sweep Width (Hz) 27776.08	Temperature (degree C) 27.000			

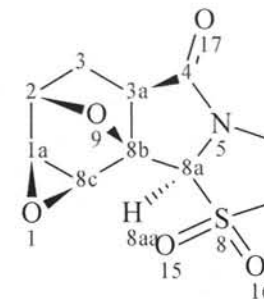
Compound 37b



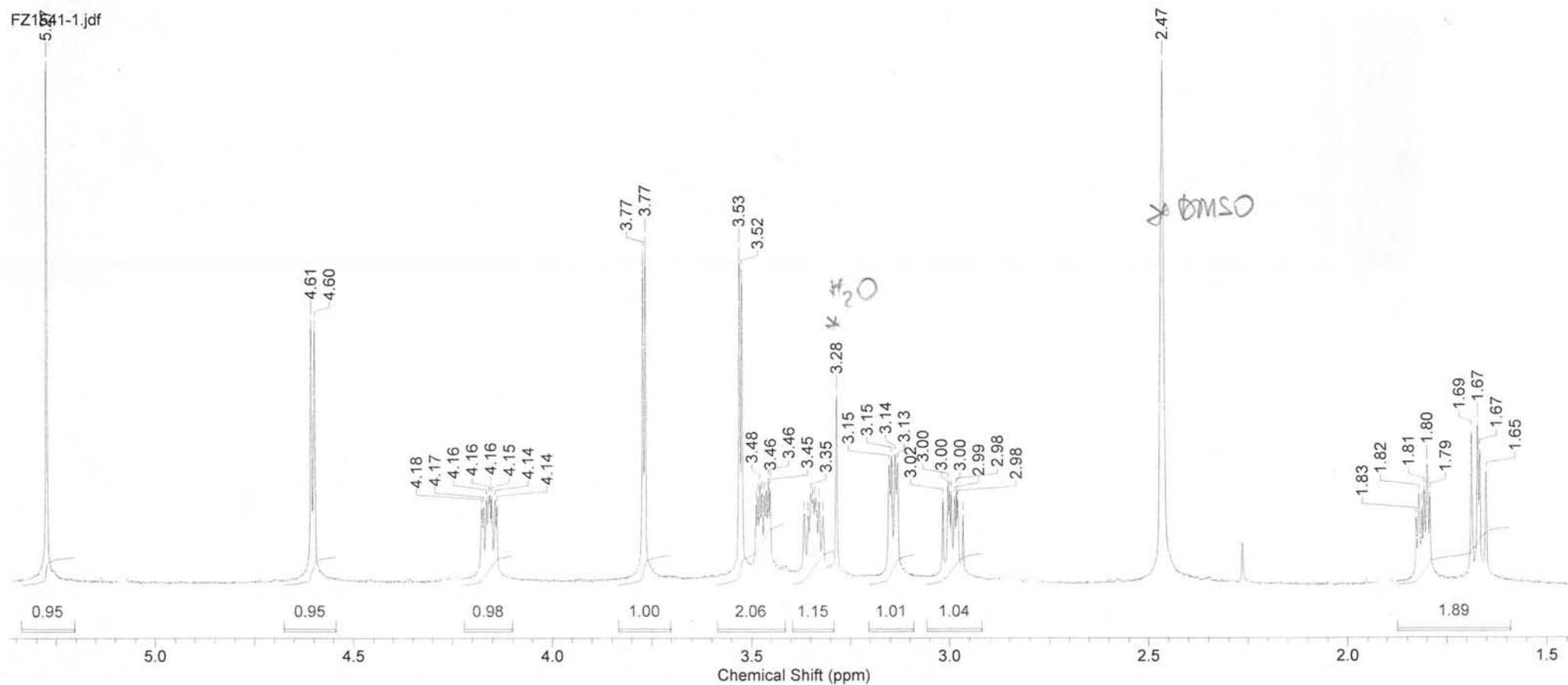
Formula C₁₀H₁₁NO₅S FW 257.2630

Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	16 Dec 2010 14:33:23	Date Stamp	16 Dec 2010 13:45:15
File Name	D:\NMR\13.12.10\FZ1541-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	10
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	54.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3601.0339	Sweep Width (Hz)	11261.26
						Pulse Sequence	single_pulse.ex2

Compound 38a



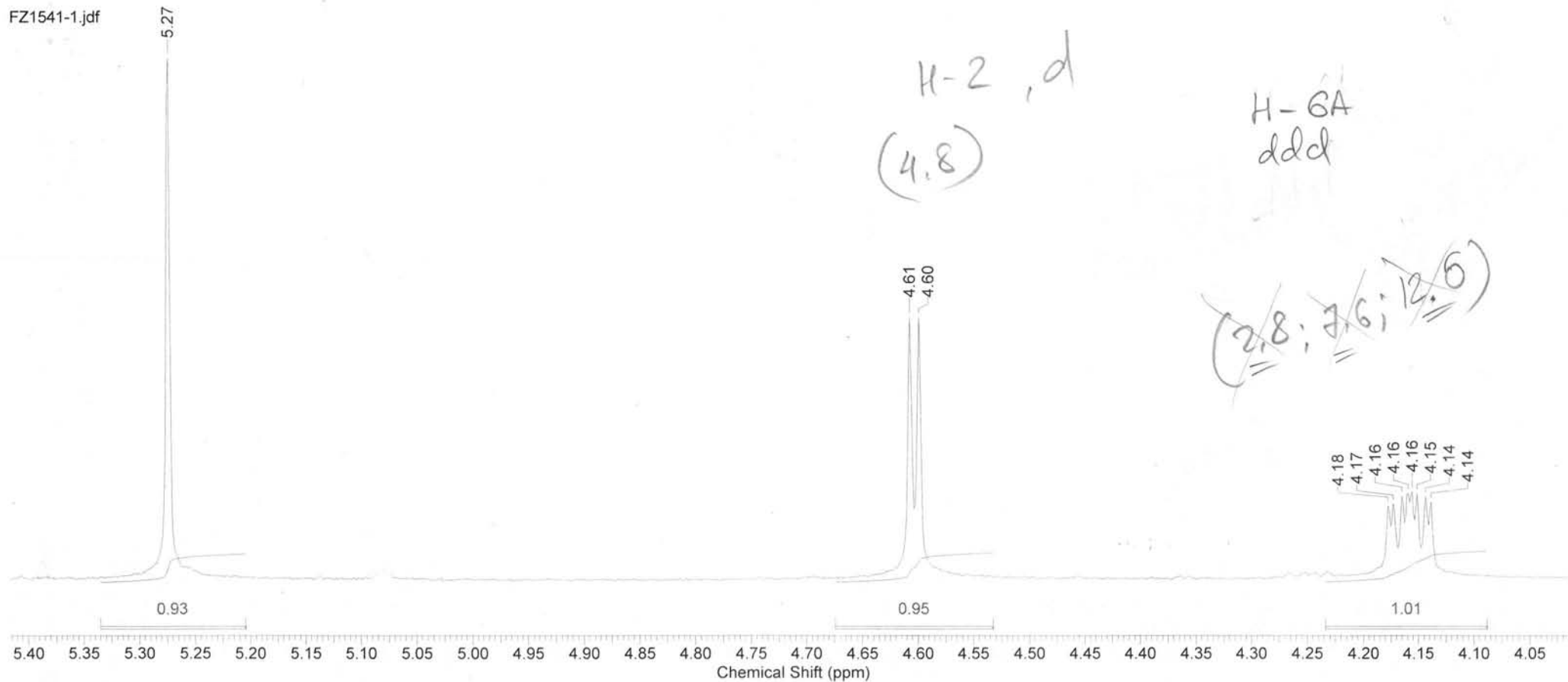
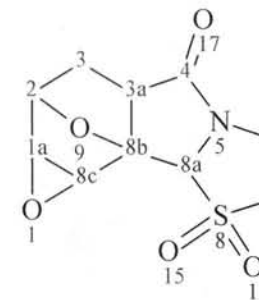
38a



Formula C₁₀H₁₁NO₅S FW 257.2630

Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	16 Dec 2010 14:33:23		Date Stamp	16 Dec 2010 13:45:15		
File Name	D:\NMR\13.12.10\FZ1541-1.jdf			Frequency (MHz)	600.17	Nucleus	1H		Number of Transients	10
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384		Pulse Sequence	single_pulse.ex2
Receiver Gain	54.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3601.0339	Sweep Width (Hz)	11261.26			

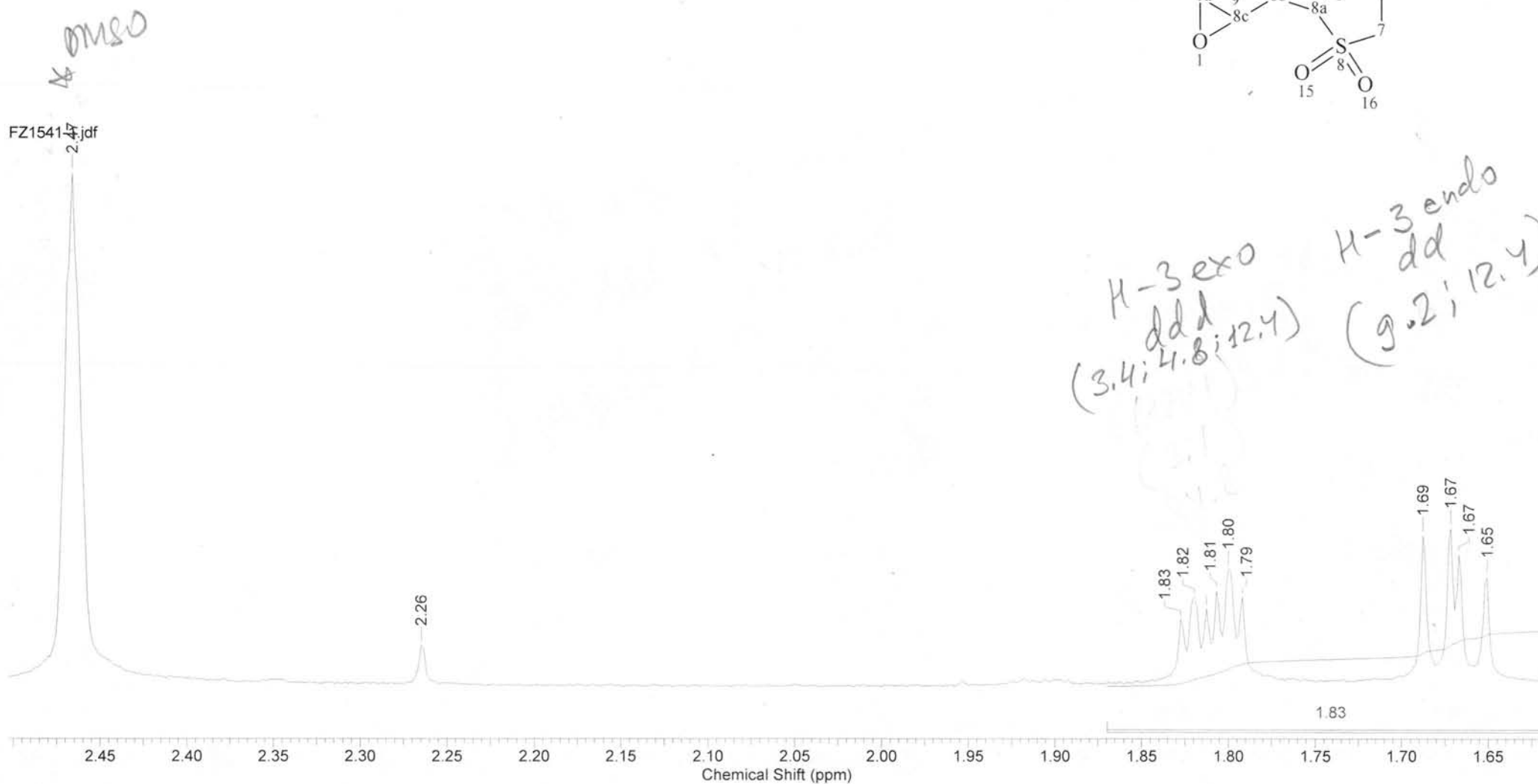
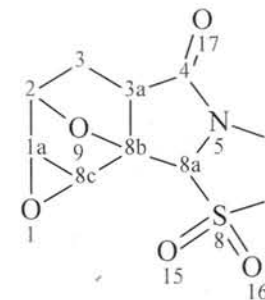
Compound 38a



Formula C₁₀H₁₁NO₅S FW 257.2630

Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	16 Dec 2010 14:33:23		Date Stamp	16 Dec 2010 13:45:15	
File Name	D:\NMR\13.12.10\FZ1541-1.jdf			Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	10
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384	Pulse Sequence	single_pulse.ex2
Receiver Gain	54.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3601.0339	Sweep Width (Hz)	11261.26		

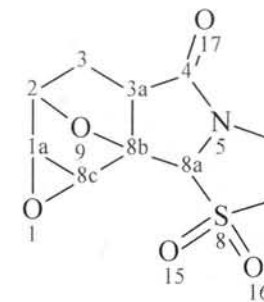
Compound 38a



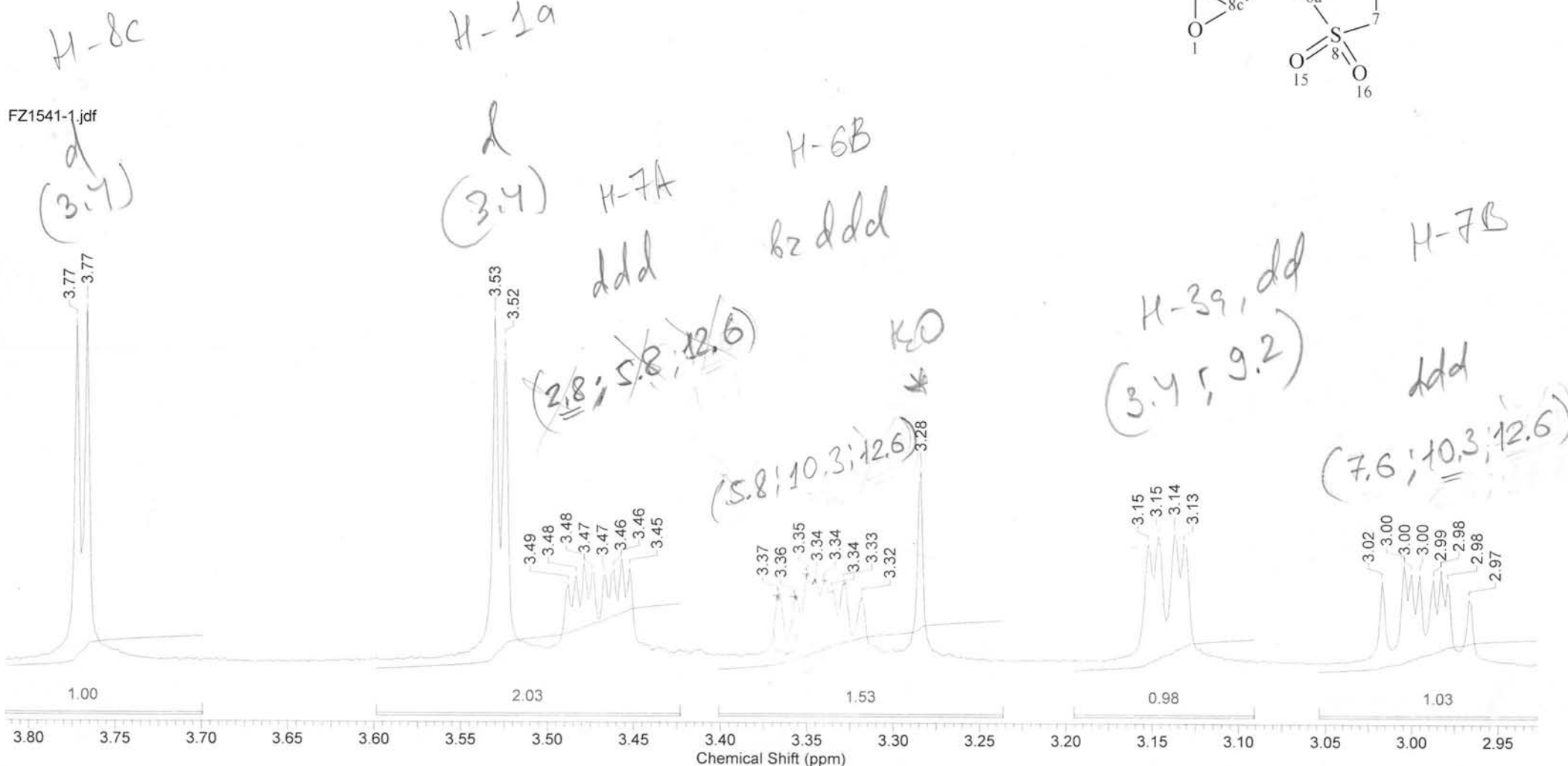
Formula C₁₀H₁₁NO₅S FW 257.2630

Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	16 Dec 2010 14:33:23	Date Stamp	16 Dec 2010 13:45:15
File Name	D:\NMR\13.12.10\FZ1541-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	10
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	54.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3601.0339	Sweep Width (Hz)	11261.26
						Pulse Sequence	single_pulse.ex2

Compound 38a

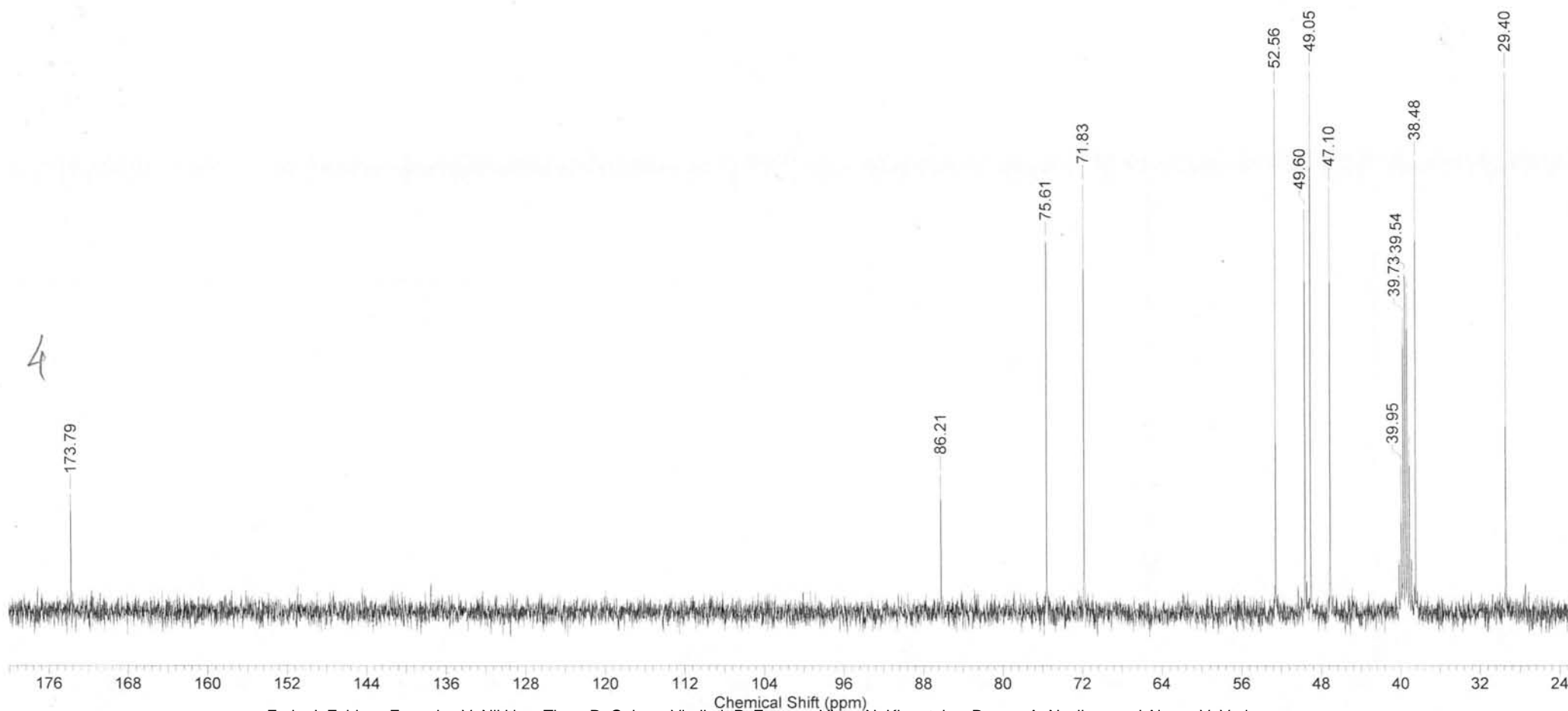
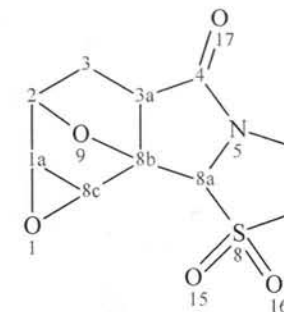


FZ1541-1.jdf

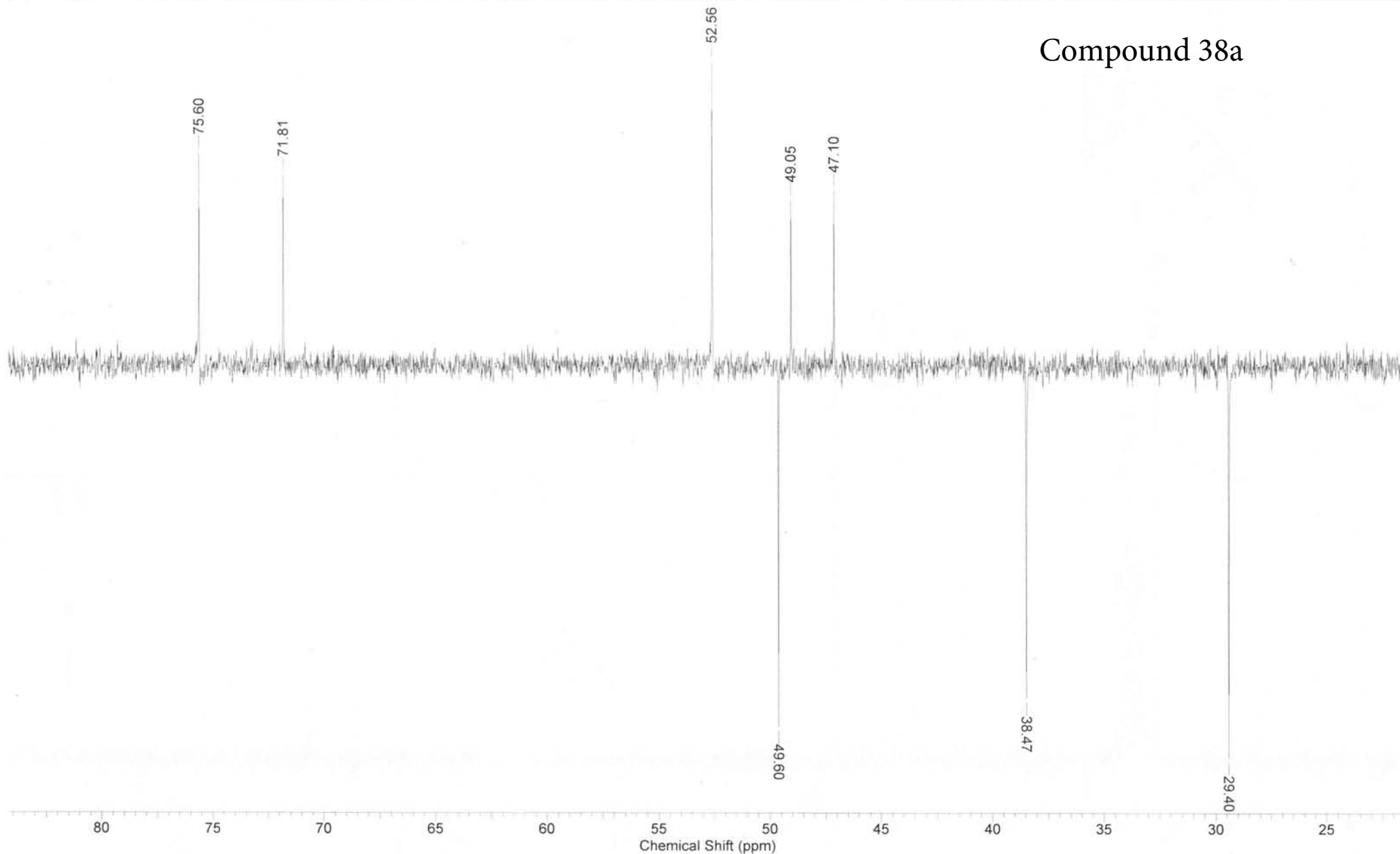


Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	14 Apr 2011 07:04:32	
File Name	D:\NMR\13.04.2011	C-13\rudn-130411-N4-c13dec\rudn-130411-N4-c13dec_001000fid			Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	384	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	32.000

Compound 38a

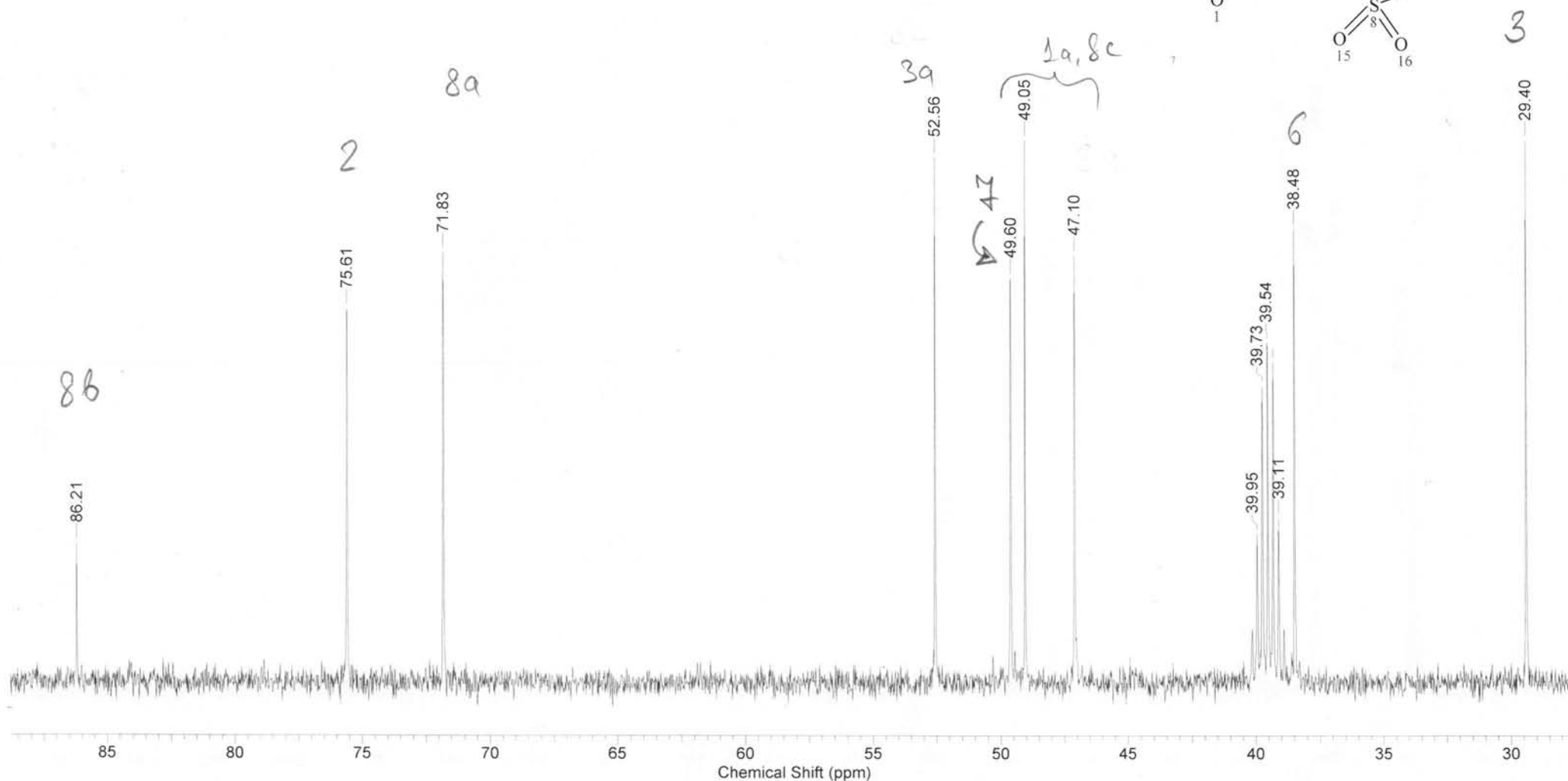
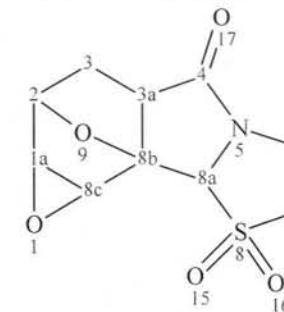


Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	14 Apr 2011 07:13:04	
File Name	D:\NMR\13.04.2011	C-13\rudn-130411-N4-dept135\rudn-130411-N4-dept135_001000fid			Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	241	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	32.000



Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	14 Apr 2011 07:04:32	
File Name	D:\NMR\13.04.2011	C-13\rudn-130411-N4-c13dec\rudn-130411-N4-c13dec_001000fid			Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	384	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	32.000

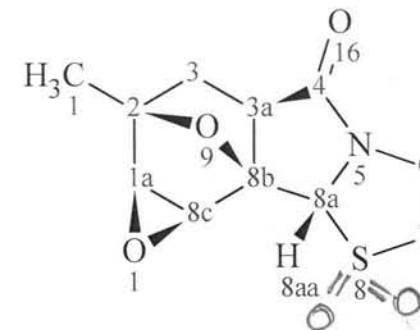
Compound 38a



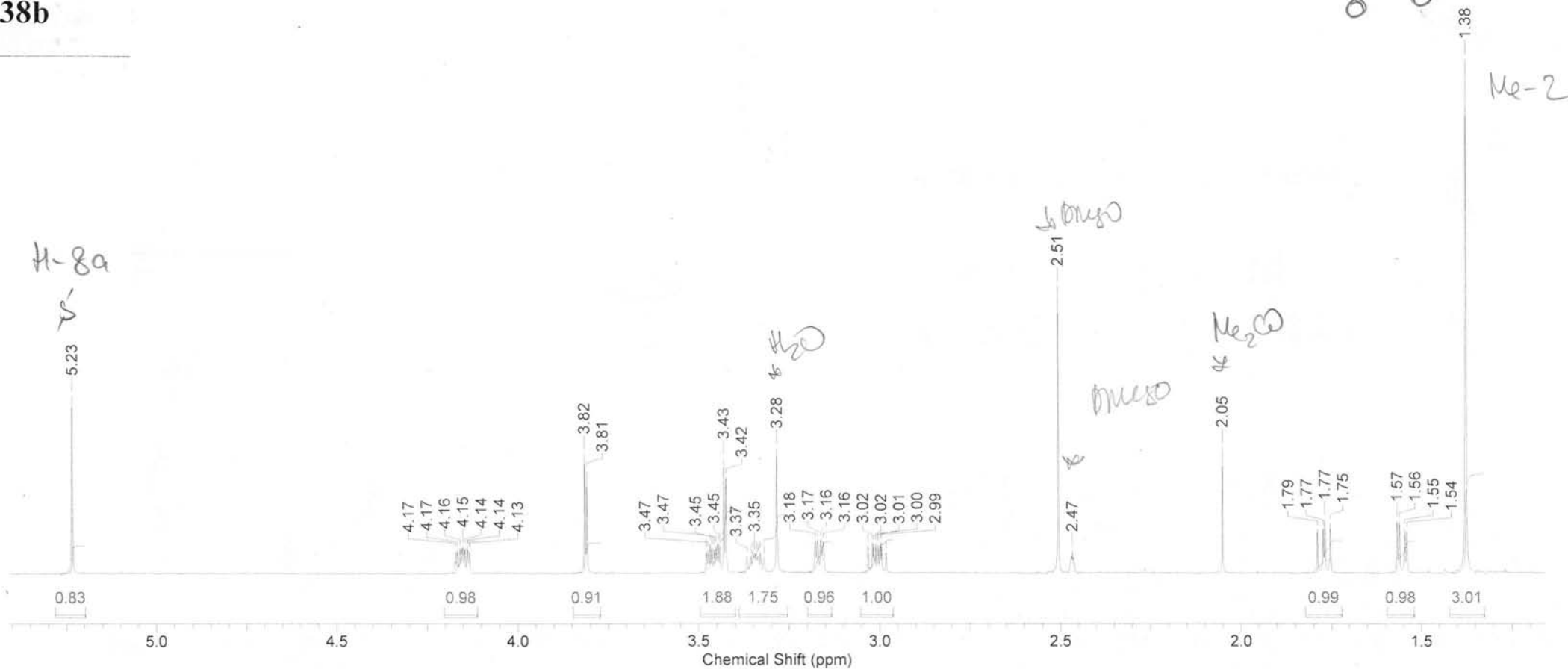
Formula $C_{11}H_{13}NO_3S$ FW 239.2908

Acquisition Time (sec)	1.8193	Comment	single_pulse	Date	24 May 2010 15:57:57	Date Stamp	24 May 2010 15:56:38
File Name	D:\NMR\11.05.10\1236-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	2
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	30.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3601.0339	Sweep Width (Hz)	9005.76
						Temperature (degree C)	25.000

Compound 38b



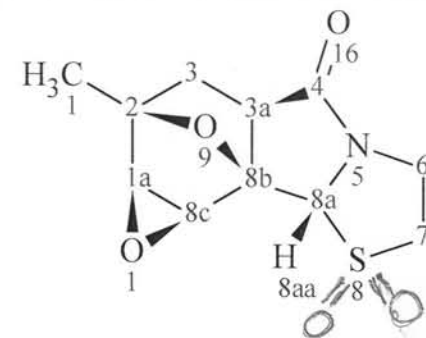
38b



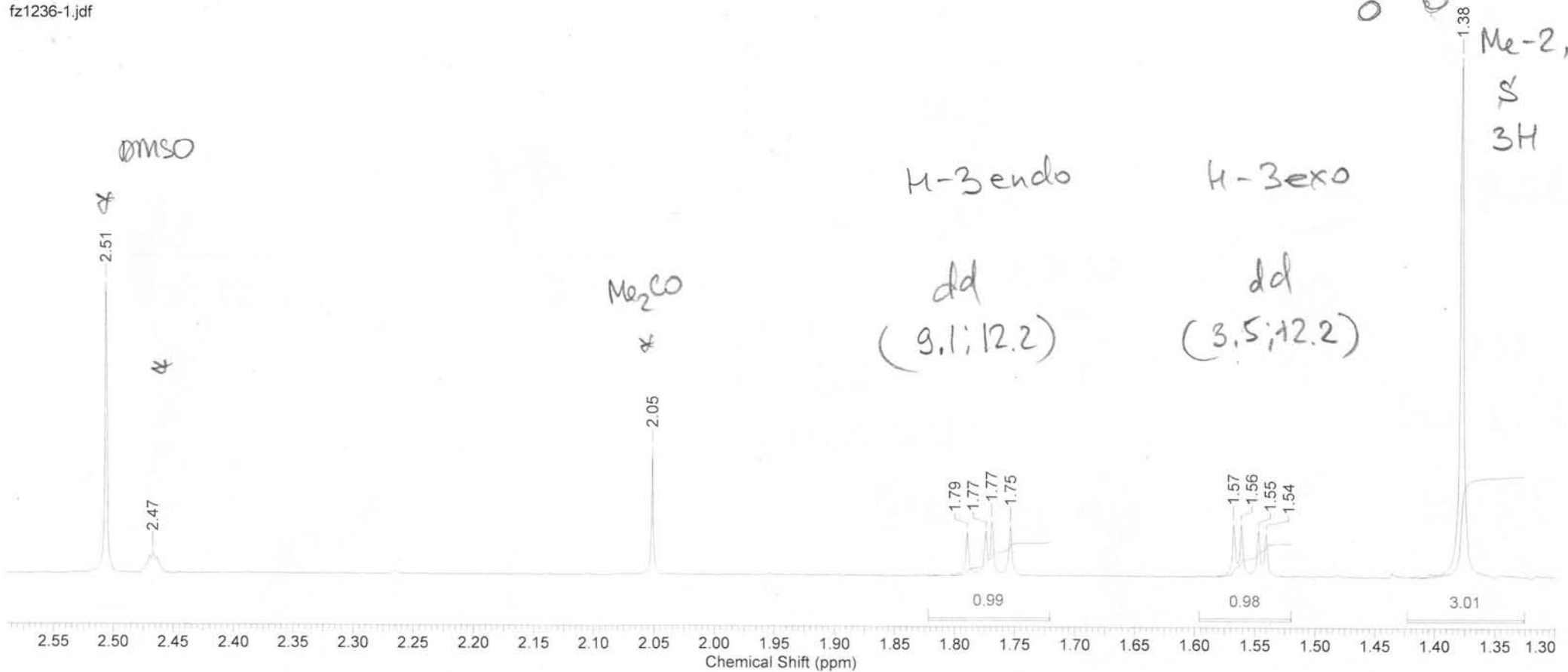
Formula $C_{11}H_{13}NO_3S$ FW 239.2908

Acquisition Time (sec)	1.8193	Comment	single_pulse	Date	24 May 2010 15:57:57	Date Stamp	24 May 2010 15:56:38
File Name	D:\NMR\11.05.10\1236-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	2
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	30.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3601.0339	Sweep Width (Hz)	9005.76
						Temperature (degree C)	25.000

Compound 38b



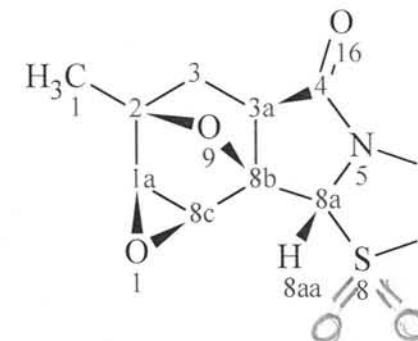
fz1236-1.jdf



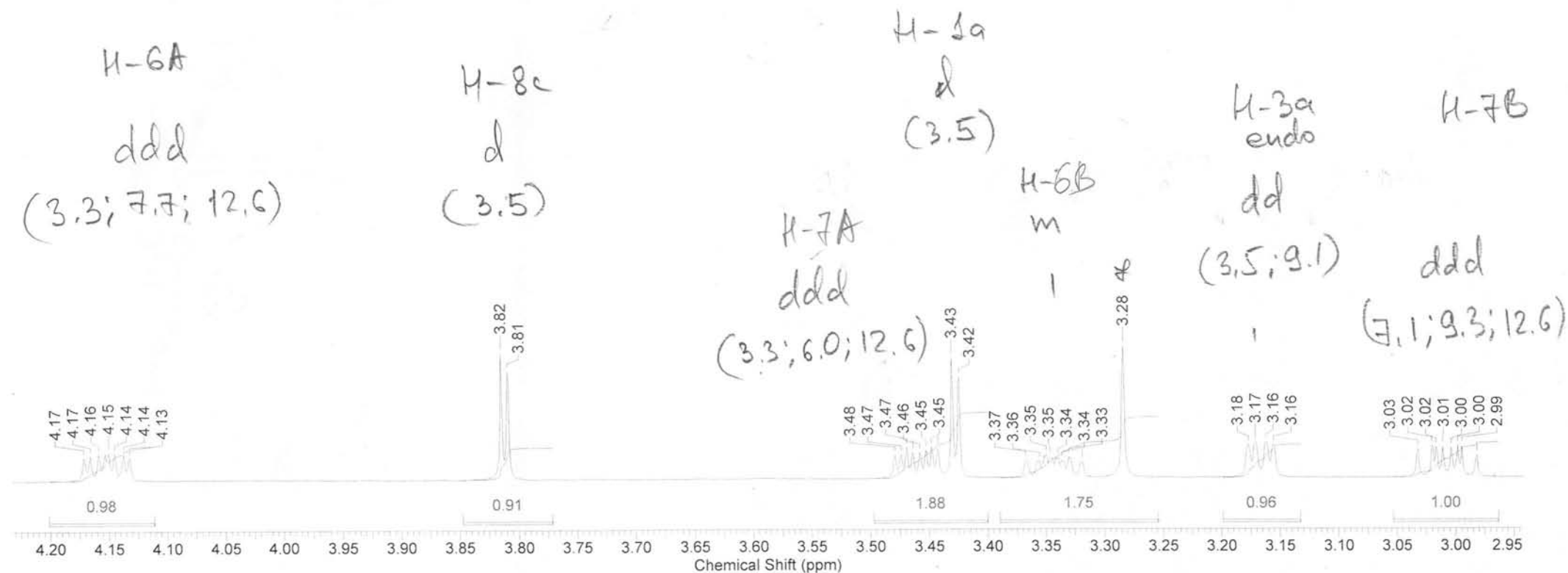
Formula C₁₁H₁₃NO₃S FW 239.2908

Acquisition Time (sec)	1.8193	Comment	single_pulse	Date	24 May 2010 15:57:57	Date Stamp	24 May 2010 15:56:38
File Name	D:\NMR\11.05.10\fz1236-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	2
Origin	ECA 600	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	30.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	3601.0339	Sweep Width (Hz)	9005.76
						Pulse Sequence	single_pulse.ex2
						Temperature (degree C)	25.000

Compound 38b



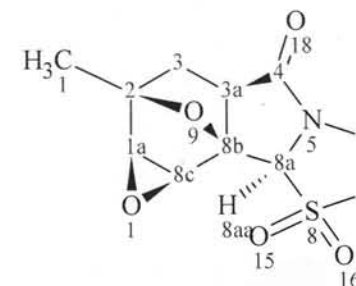
fz1236-1.jdf



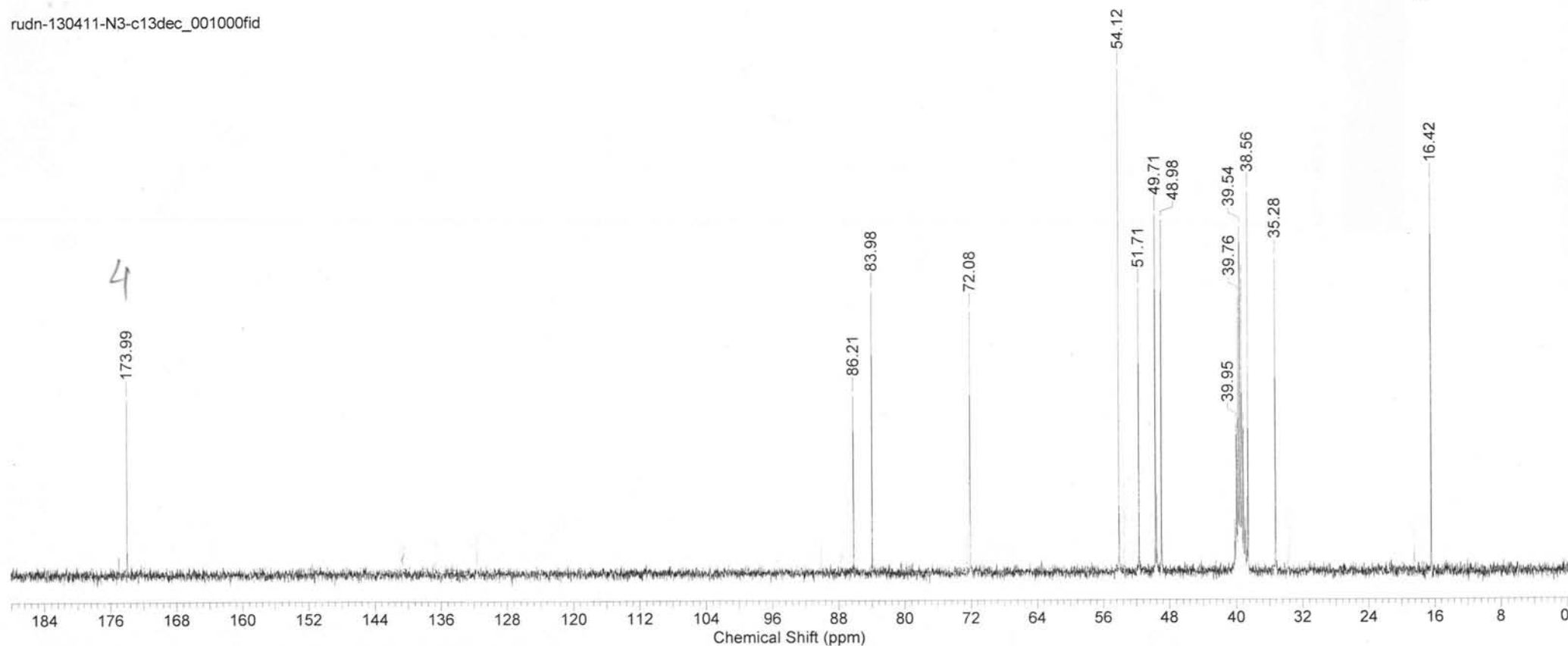
Formula C₁₁H₁₃NO₅S FW 271.2896

Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	13 Apr 2011 17:21:04	
Date Stamp	13 Apr 2011 17:21:04	File Name	D:\NMR\13\13.04.11 C-13\rudn-130411-N3-c13dec\rudn-130411-N3-c13dec_001000fid				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	305	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zgpg
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6	Spectrum Offset (Hz)	10548.5234
Sweep Width (Hz)	29409.97	Temperature (degree C)	32.000				

Compound 38b



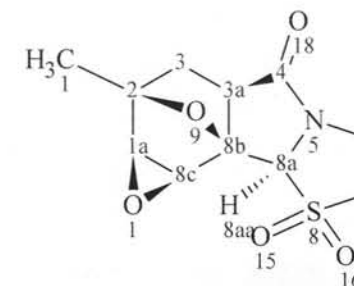
rudn-130411-N3-c13dec_001000fid



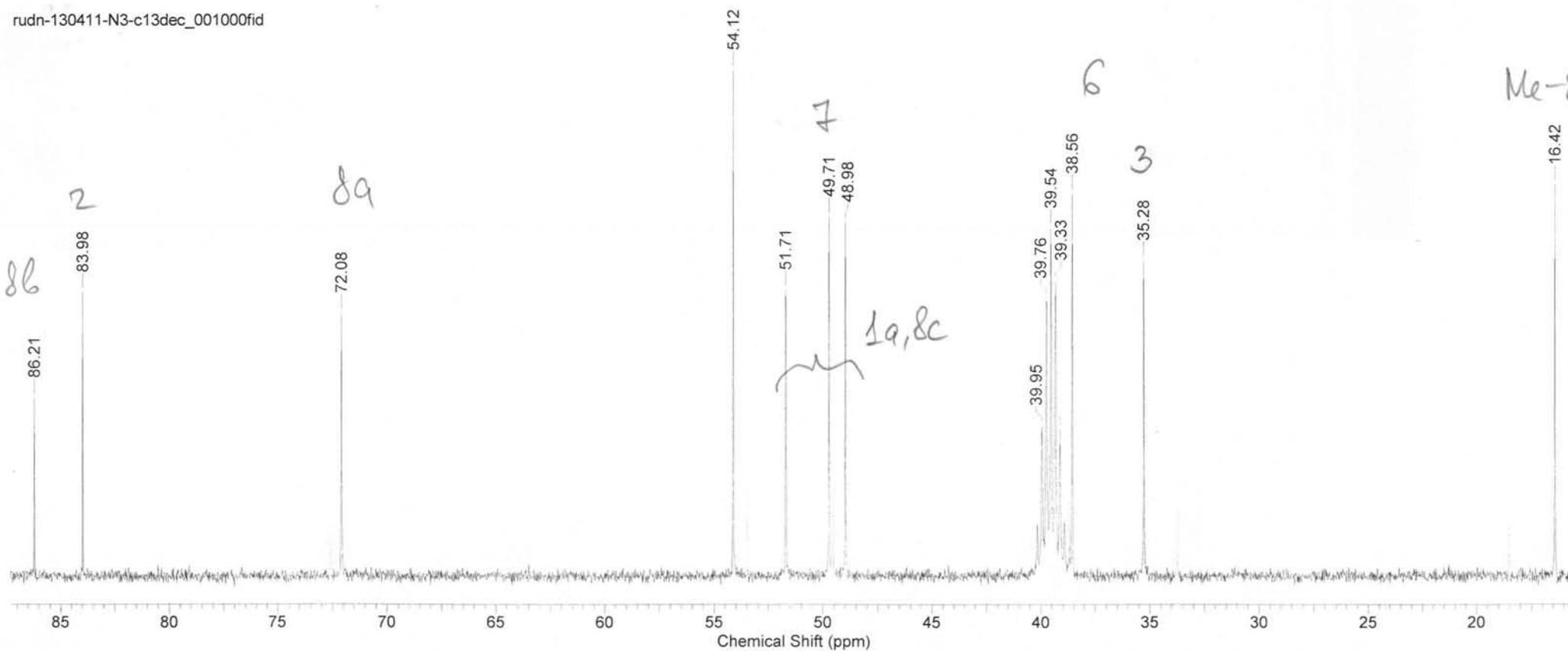
Formula C₁₁H₁₃NO₅S FW 271.2896

Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	13 Apr 2011 17:21:04
Date Stamp	13 Apr 2011 17:21:04	File Name	D:\NMR\C_13\13.04.11 C-13\rudn-130411-N3-c13dec\rudn-130411-N3-c13dec_001000fid		
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	305
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Pulse Sequence	zgpg
Sweep Width (Hz)	29409.97	Temperature (degree C)	32.000	Spectrum Offset (Hz)	10548.5234

Compound 38b

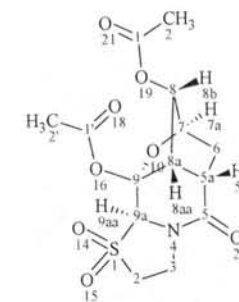


rudn-130411-N3-c13dec_001000fid

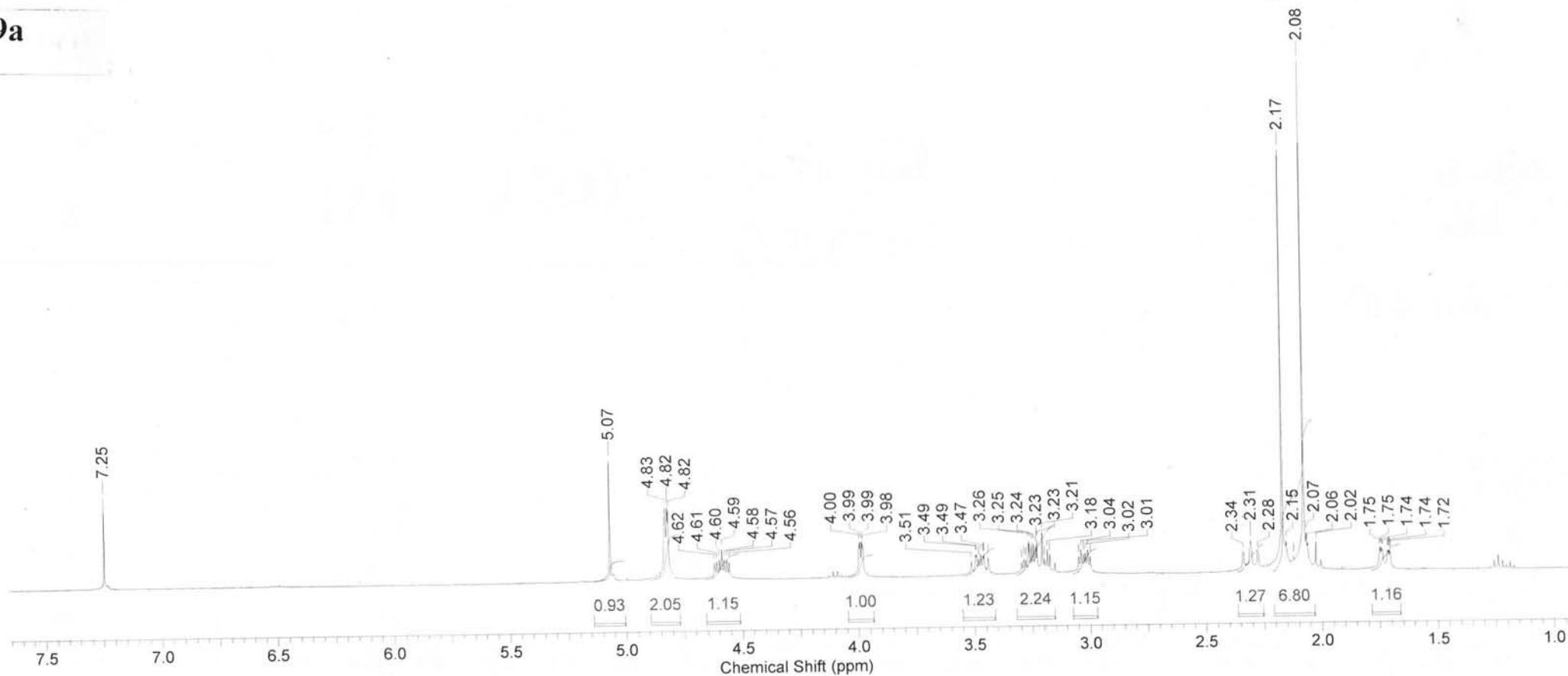


Formula C ₁₄ H ₁₇ NO ₈ S		FW 359.3517					Date Stamp	11 Mar 2011 00:14:31	
Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	10 Mar 2011 13:48:45				
File Name	D:\NMR\9.03.11\FZ1702-1.jdf			Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	10
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384	Pulse Sequence	single_pulse.ex2
Receiver Gain	38.00	Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2398.6931	Sweep Width (Hz)	7503.00
Temperature (degree C)	21.500								

Compound 39a



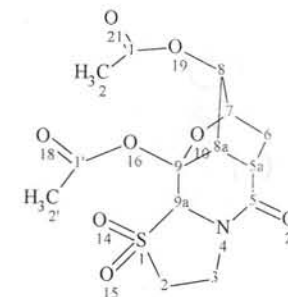
39a



Formula C₁₄H₁₇NO₈S FW 359.3517

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	10 Mar 2011 13:48:45	Date Stamp	11 Mar 2011 00:14:31
File Name	D:\NMR\9.03.11\FZ1702-1.jdf	Original Points Count	16384	Frequency (MHz)	399.78	Nucleus	1H
Origin	ECS 400	Solvent	CHLOROFORM-d	Owner	delta	Points Count	16384
Receiver Gain	38.00	Spectrum Offset (Hz)	2398.6931	Pulse Sequence	single_pulse.ex2	Sweep Width (Hz)	7503.00
Temperature (degree C)	21.500						

Compound 39a



FZ1702-1.jdf

H-9a

H-7

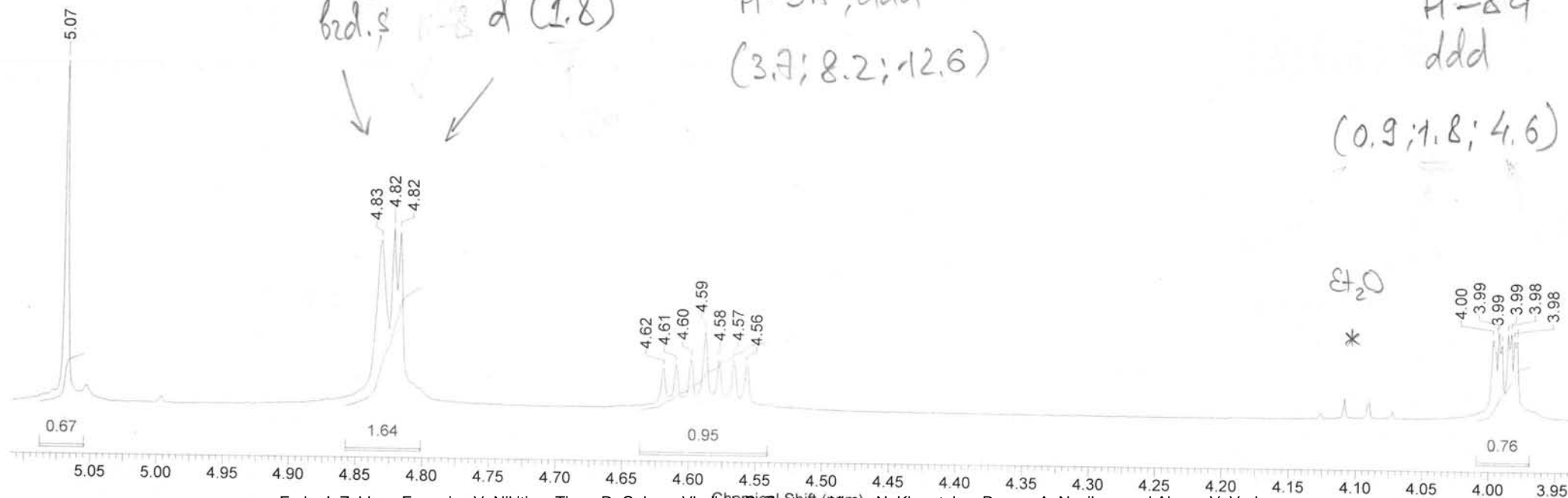
H-8

H-3A, ddd
(3.7; 8.2; 12.6)H-8a
ddd

(0.9; 1.8; 4.6)

Et₂O

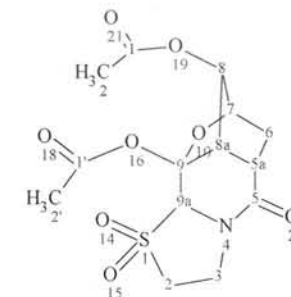
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Formula C₁₄H₁₇NO₈S FW 359.3517

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	10 Mar 2011 13:48:45	Date Stamp	11 Mar 2011 00:14:31
File Name	D:\NMR\9.03.11\FZ1702-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	10
Origin	ECS 400	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2398.6931	Sweep Width (Hz)	7503.00
Temperature (degree C)	21.500						

Compound 39a



FZ1702-1.jdf

H-3B
ddd

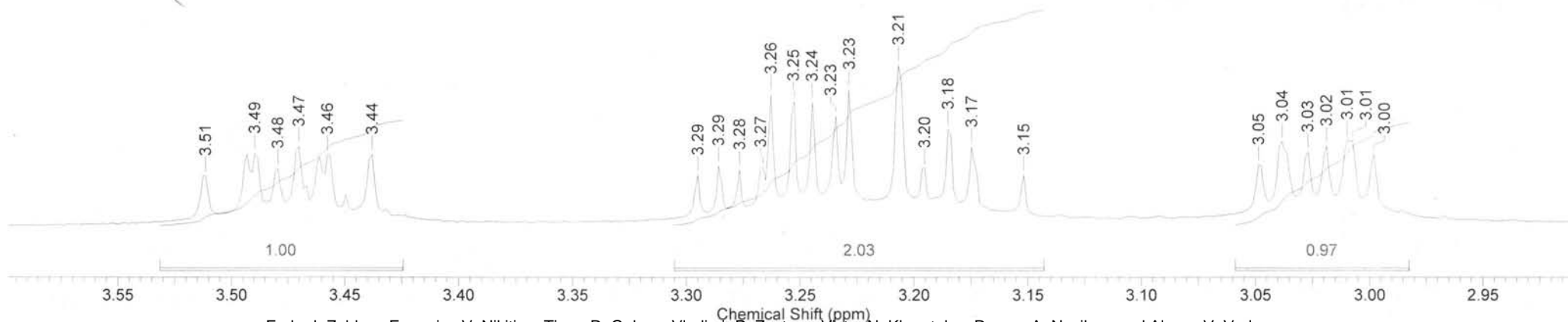
(7.3; 8.7; 12.6)

H-2, m, 2H

H-5a

ddd

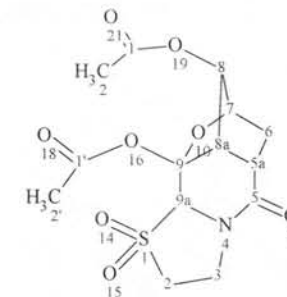
(3.5; 4.6; 11.5)



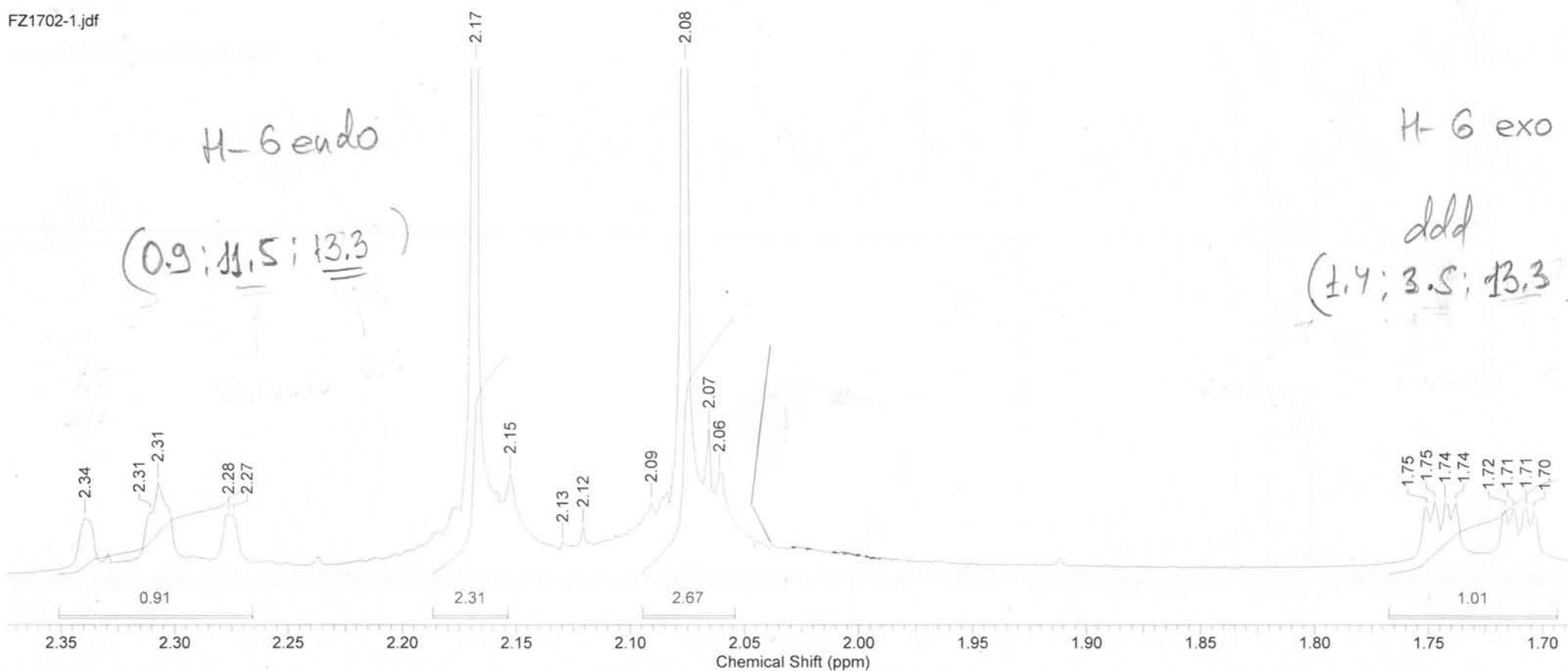
Formula $C_{14}H_{17}NO_8S$ FW 359.3517

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	10 Mar 2011 13:48:45	Date Stamp	11 Mar 2011 00:14:31
File Name	D:\NMR\9.03.11\FZ1702-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	10
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2398.6931	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	21.500			Sweep Width (Hz)	7503.00		

Compound 39a

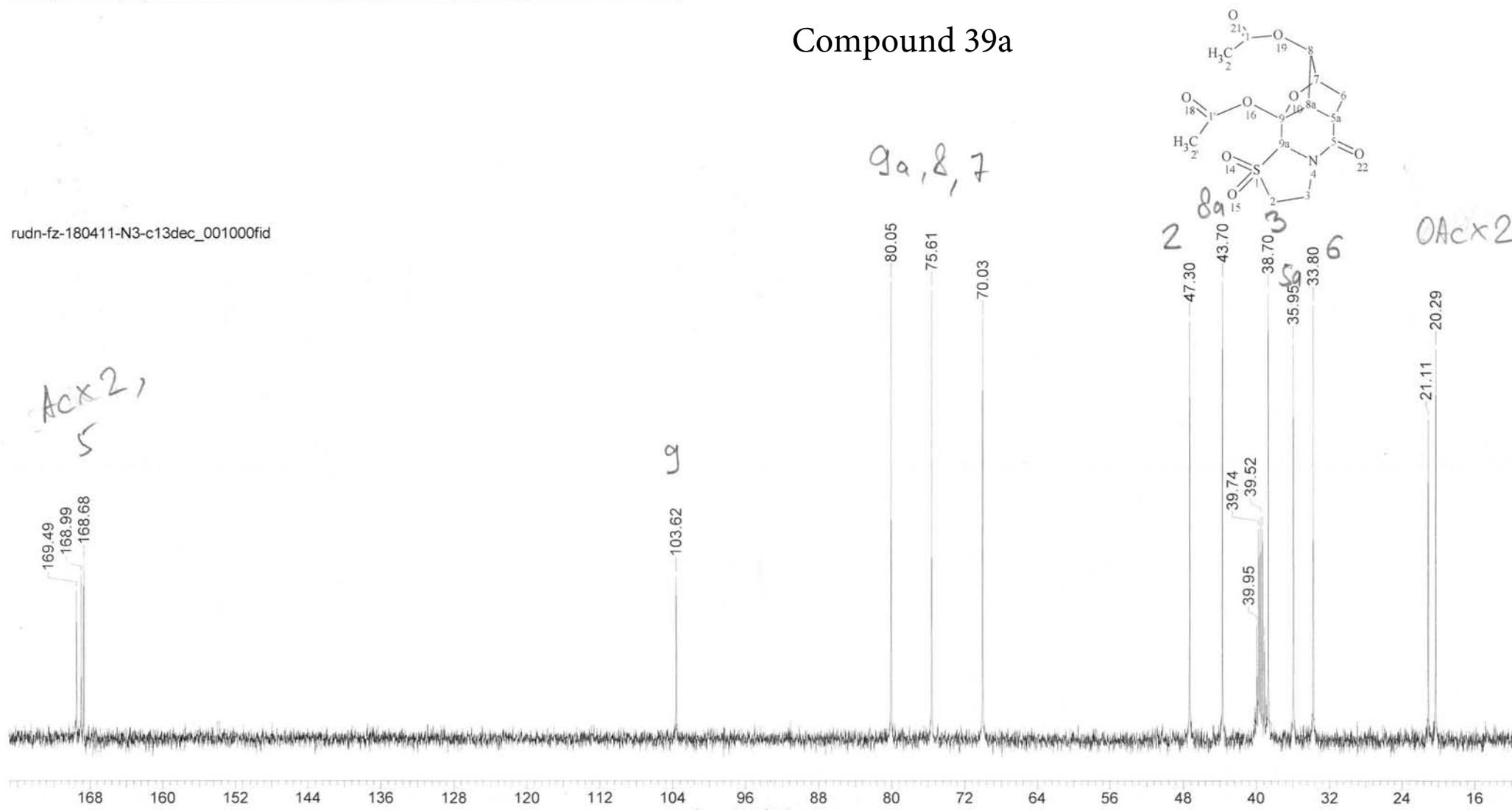


FZ1702-1.jdf



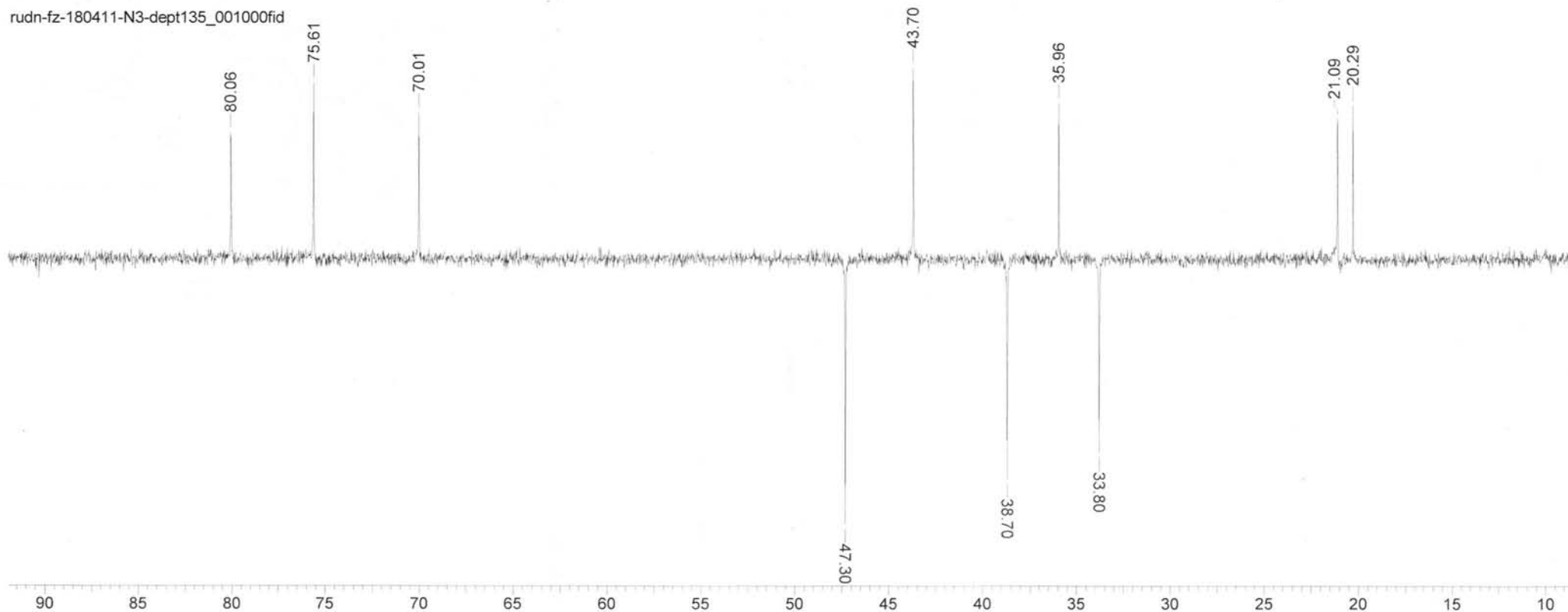
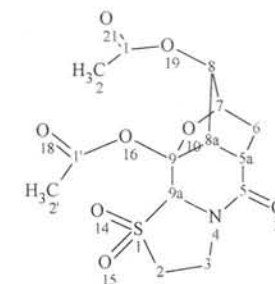
Formula	C ₁₄ H ₁₇ NO ₈ S	FW	359.3517
Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400
Date Stamp	18 Apr 2011 16:55:28	Date	18 Apr 2011 16:55:28
File Name	D:\NMR\4.04.2011 (Рома Димер Женя + Ира перегруп. с серой)\rudn-fz-180411-N3-c13dec\rudn-fz-180411-N3-c13dec_001000fid		
Frequency (MHz)	100.62	Nucleus	13C
Original Points Count	16384	Number of Transients	762
Receiver Gain	32768.00	Origin	spect
Sweep Width (Hz)	29409.97	Owner	root
		Points Count	16384
		Pulse Sequence	zgpgg
		Solvent	DMSO-d6
		Spectrum Offset (Hz)	10535.4922
		Temperature (degree C)	50.000

Compound 39a



Formula C ₁₄ H ₁₇ NO ₈ S	FW 359.3517			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 18 Apr 2011 17:12:32		
Date Stamp 18 Apr 2011 17:12:32				
File Name D:\NMR\4.04.2011 (Рома Димер Женя + Ира перегруп. с серой)\rudn-fz-180411-N3-dept135\rudn-fz-180411-N3-dept135_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 331	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence dept135	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent CHLOROFORM-d	Spectrum Offset (Hz) 9085.0840	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

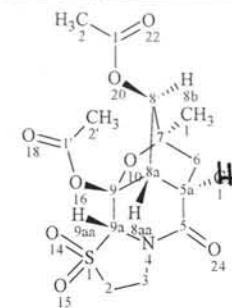
Compound 39a



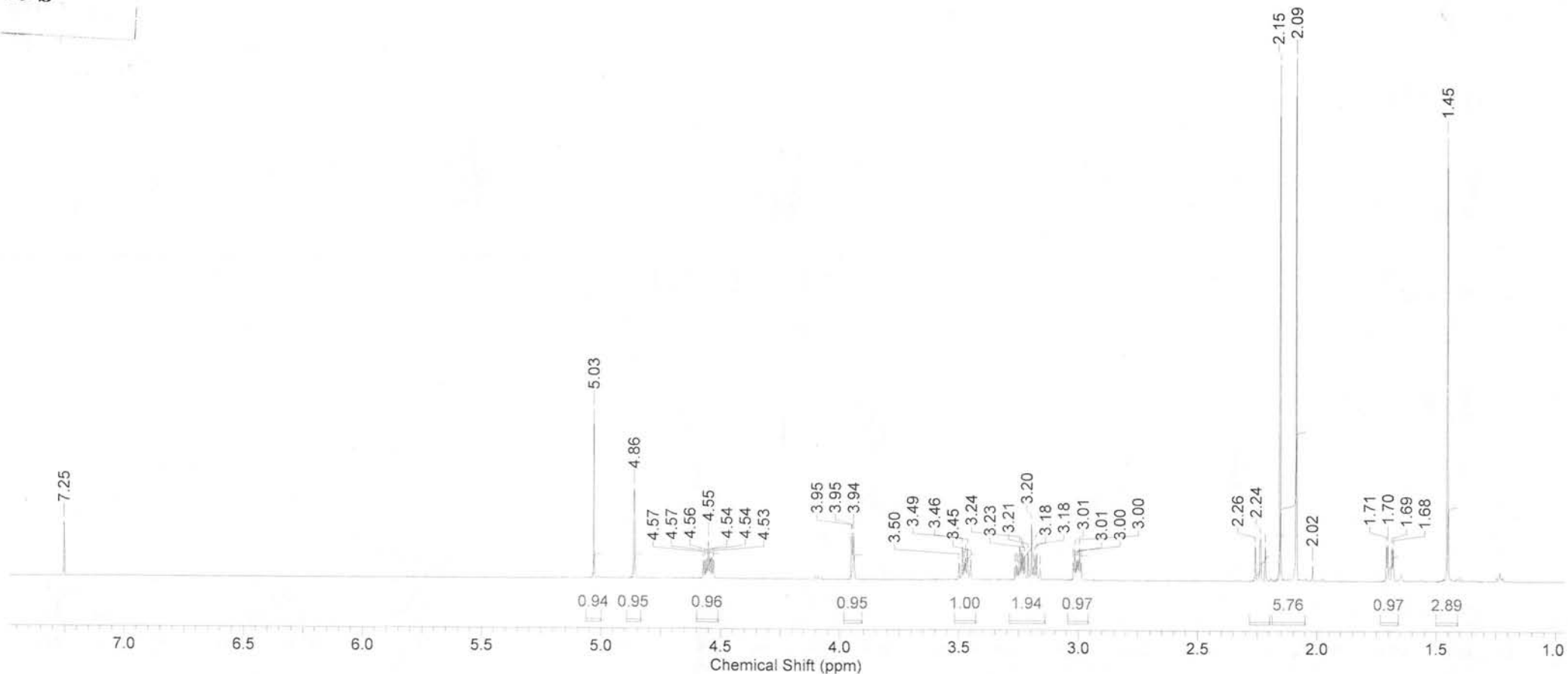
Formula C₁₆H₂₁NO₈S FW 387.4048

Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	07 Dec 2010 10:39:04	Date Stamp	07 Dec 2010 09:50:47
File Name	D:\NMR\06.12.10\FZ1519-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	10
Origin	ECA 600	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	46.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3601.0339	Sweep Width (Hz)	11261.26

Compound 39b



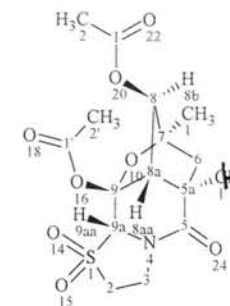
39b



Formula $C_{16}H_{21}NO_8S$ FW 387.4048

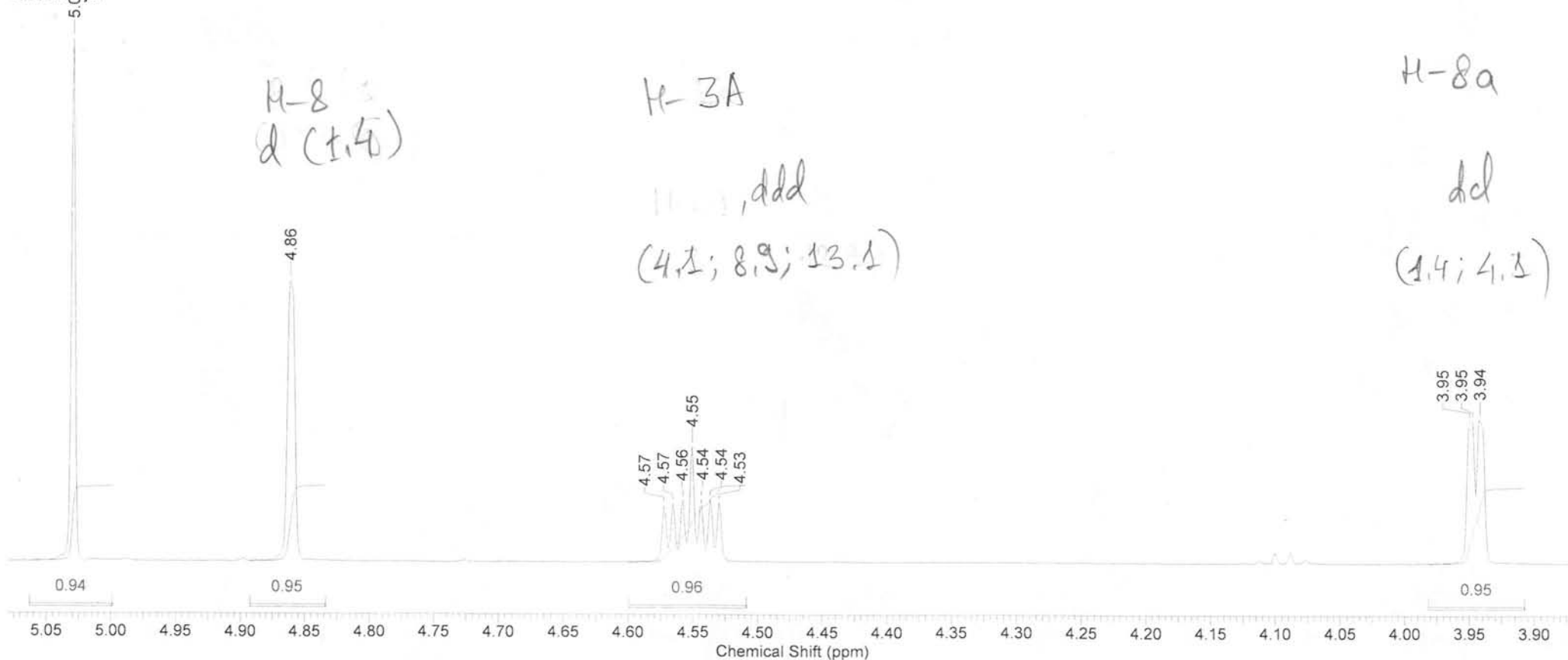
Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	07 Dec 2010 10:39:04	Date Stamp	07 Dec 2010 09:50:47
File Name	D:\NMR\06.12.10\FZ1519-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	10
Origin	ECA 600	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	46.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3601.0339	Sweep Width (Hz)	11261.26

Compound 39b



H-9a, s

FZ1519-1.jdf

H-8
d (1.4)

H-3A

ddd
(4.1; 8.9; 13.1)

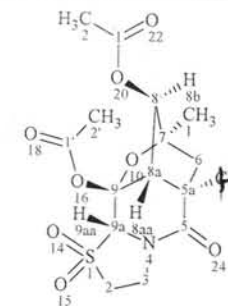
H-8a

dd
(1.4; 4.3)

Formula $C_{16}H_{21}NO_8S$ FW 387.4048

Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	07 Dec 2010 10:39:04	Date Stamp	07 Dec 2010 09:50:47
File Name	D:\NMR\06.12.10\FZ1519-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	10
Origin	ECA 600	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	46.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3601.0339	Sweep Width (Hz)	11261.26

Compound 39b



3.27 - 3.16

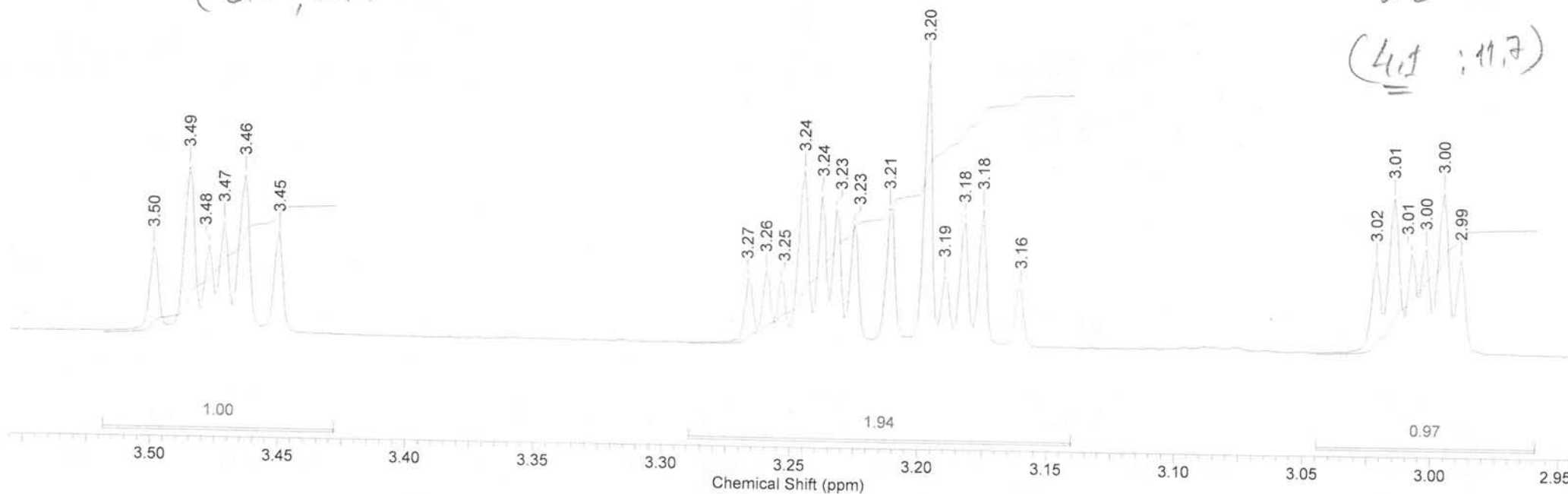
H-2
m, 2H

H-5a

dt

(4.1 ; 4.7)

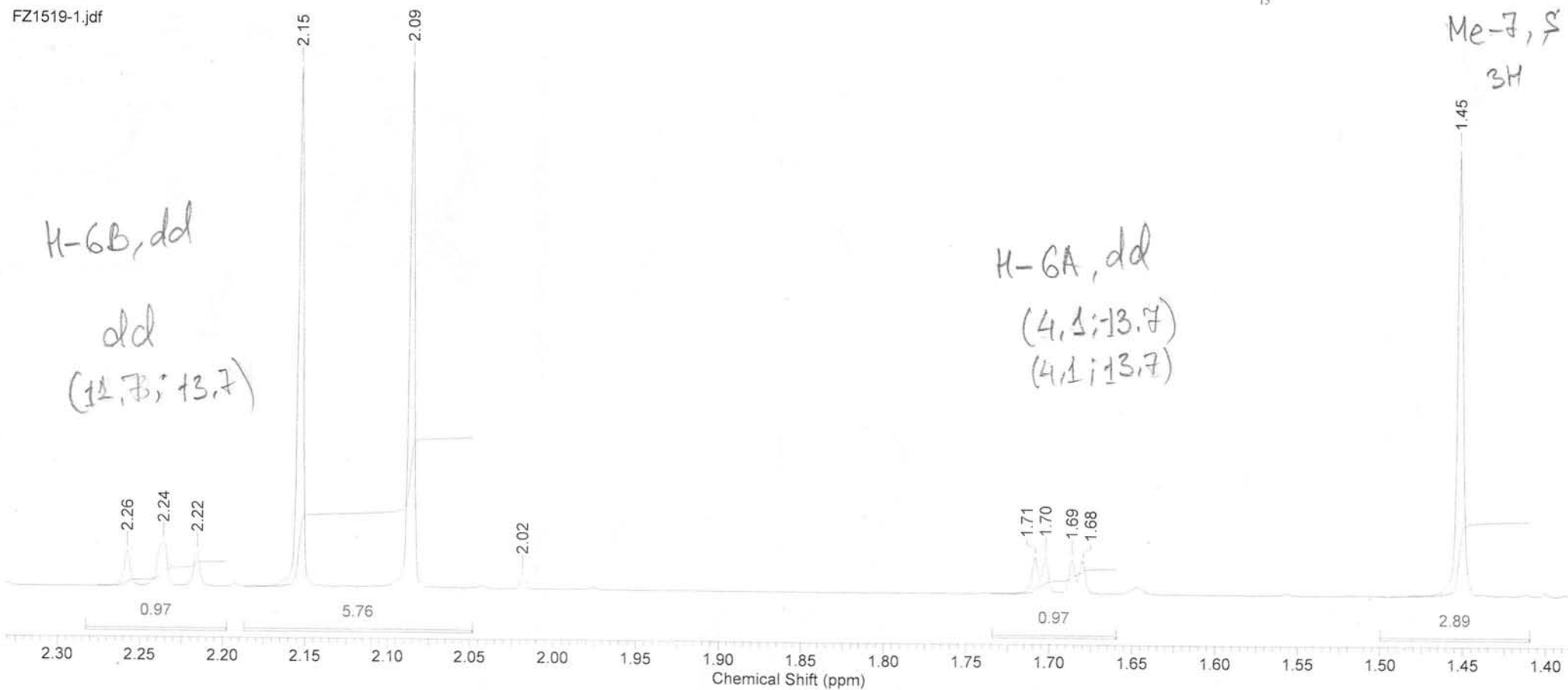
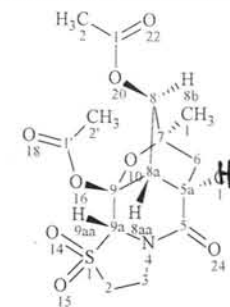
FZ1519-1.jdf

H-3B
dt
(8.3 ; 8.1)

Formula $C_{16}H_{21}NO_8S$ FW 387.4048

Acquisition Time (sec)	1.4549	Comment	single_pulse	Date	07 Dec 2010 10:39:04	Date Stamp	07 Dec 2010 09:50:47
File Name	D:\NMR\06.12.10\FZ1519-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	10
Origin	ECA 600	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	46.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3601.0339	Sweep Width (Hz)	11261.26

Compound 39b

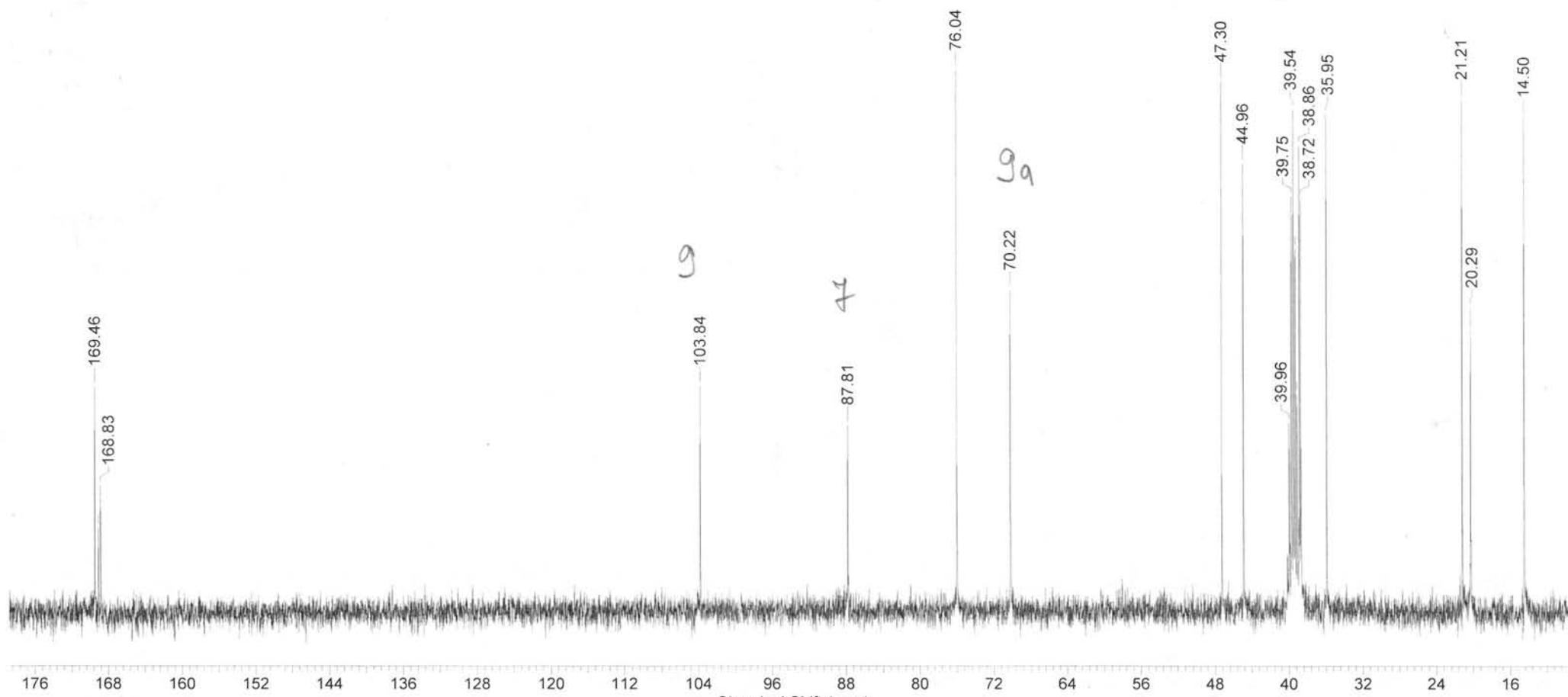
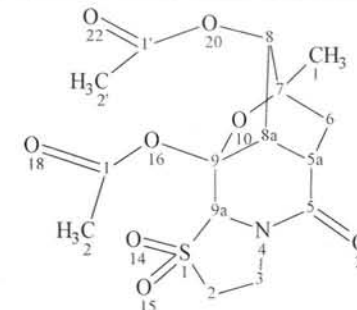


c¹³, DMSO

19 Apr 2011

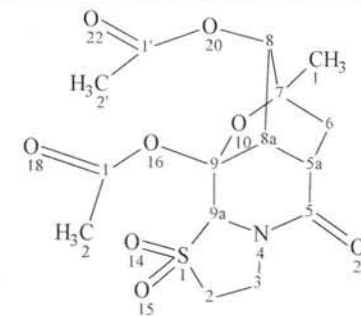
Acquisition Time (sec)	0.5571	Comment	Imported from UXNMR.		Date	18 Apr 2011 17:21:04	
File Name	C:\Users\Fedor\Desktop\4.04.2011 (Poma)\rudn-fz-180411-N4-c13dec\rudn-fz-180411-N4-c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	793	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	50.000

Compound 39b



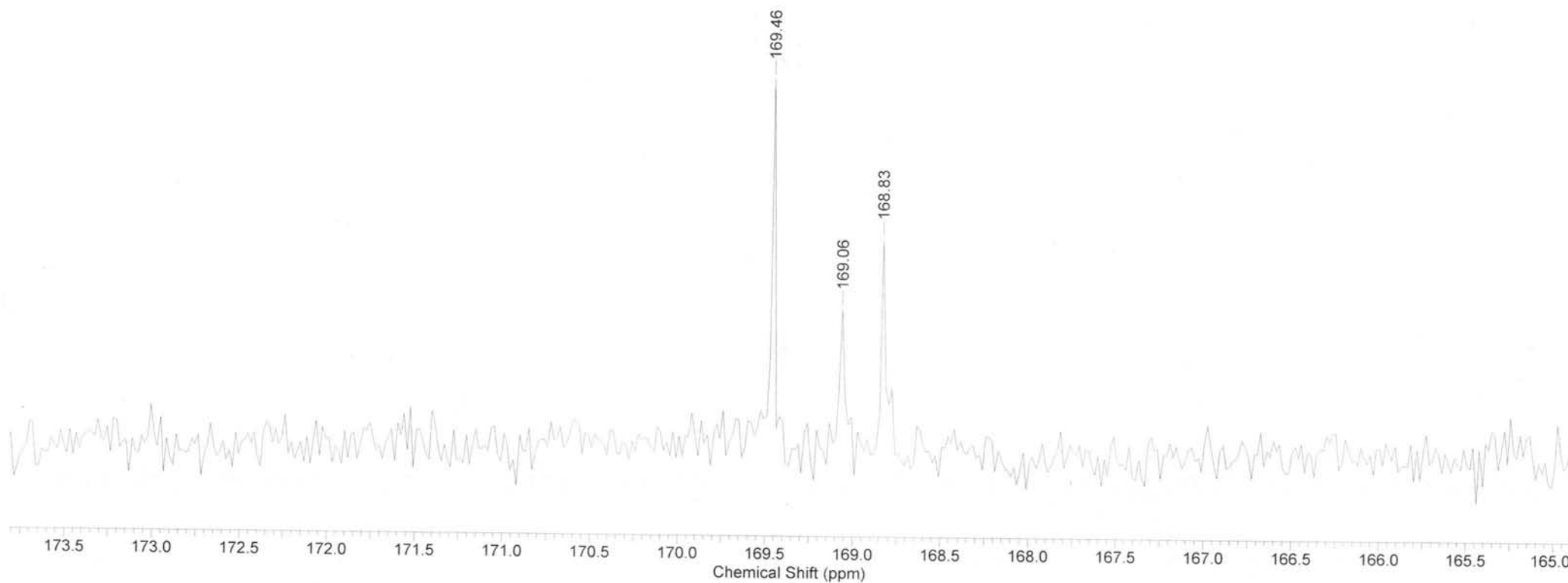
Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	18 Apr 2011 17:21:04
File Name	C:\Users\Fedor\Desktop\4.04.2011 (Poma)\rudn-fz-180411-N4-c13dec\rudn-fz-180411-N4-c13dec_001000fid			Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	793	Original Points Count	16384	
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	
				Temperature (degree C)	50.000	

Compound 39b



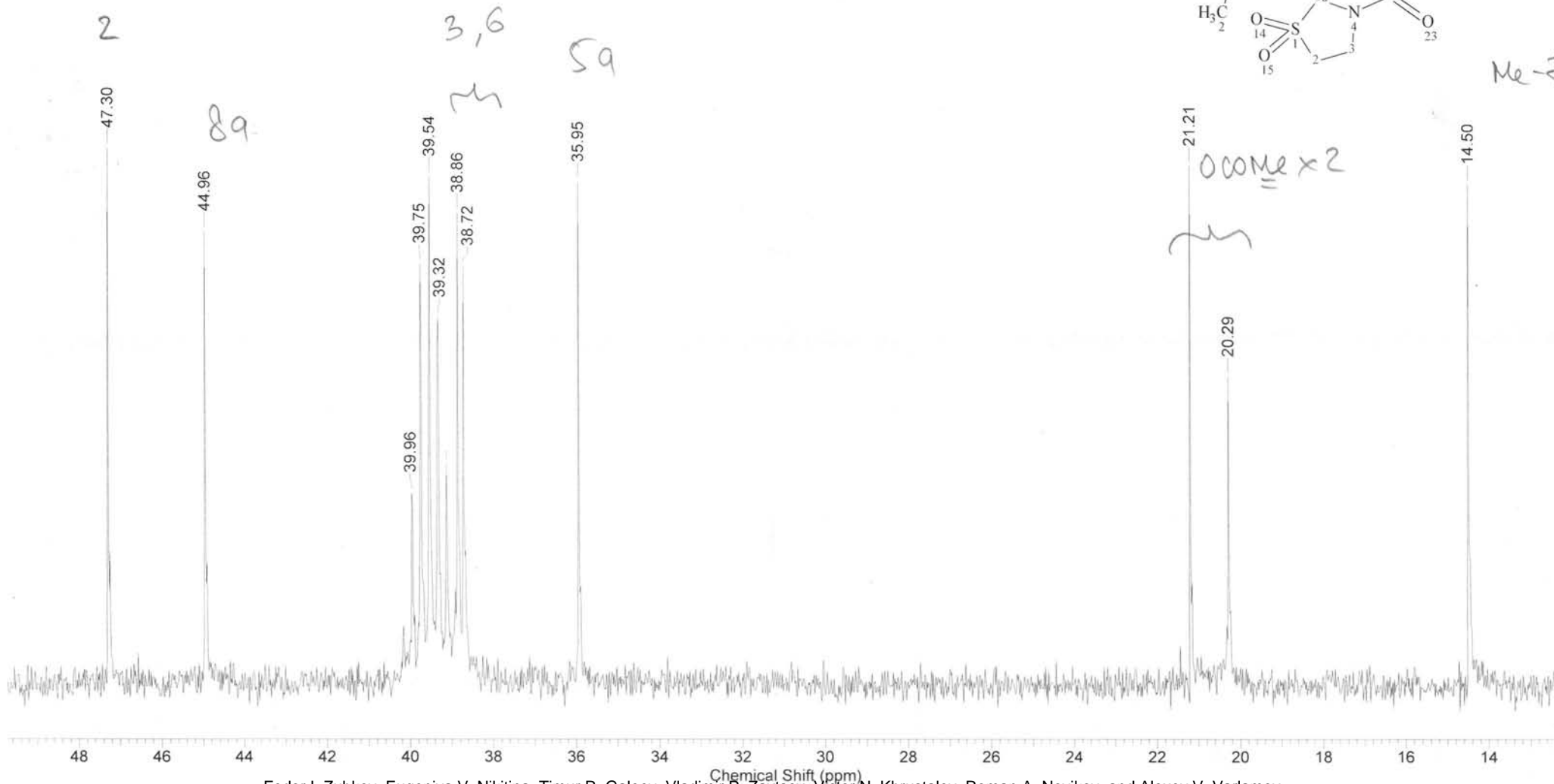
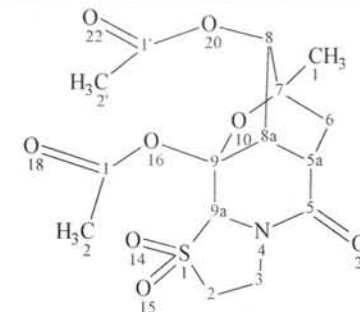
O=CMe x 2

5



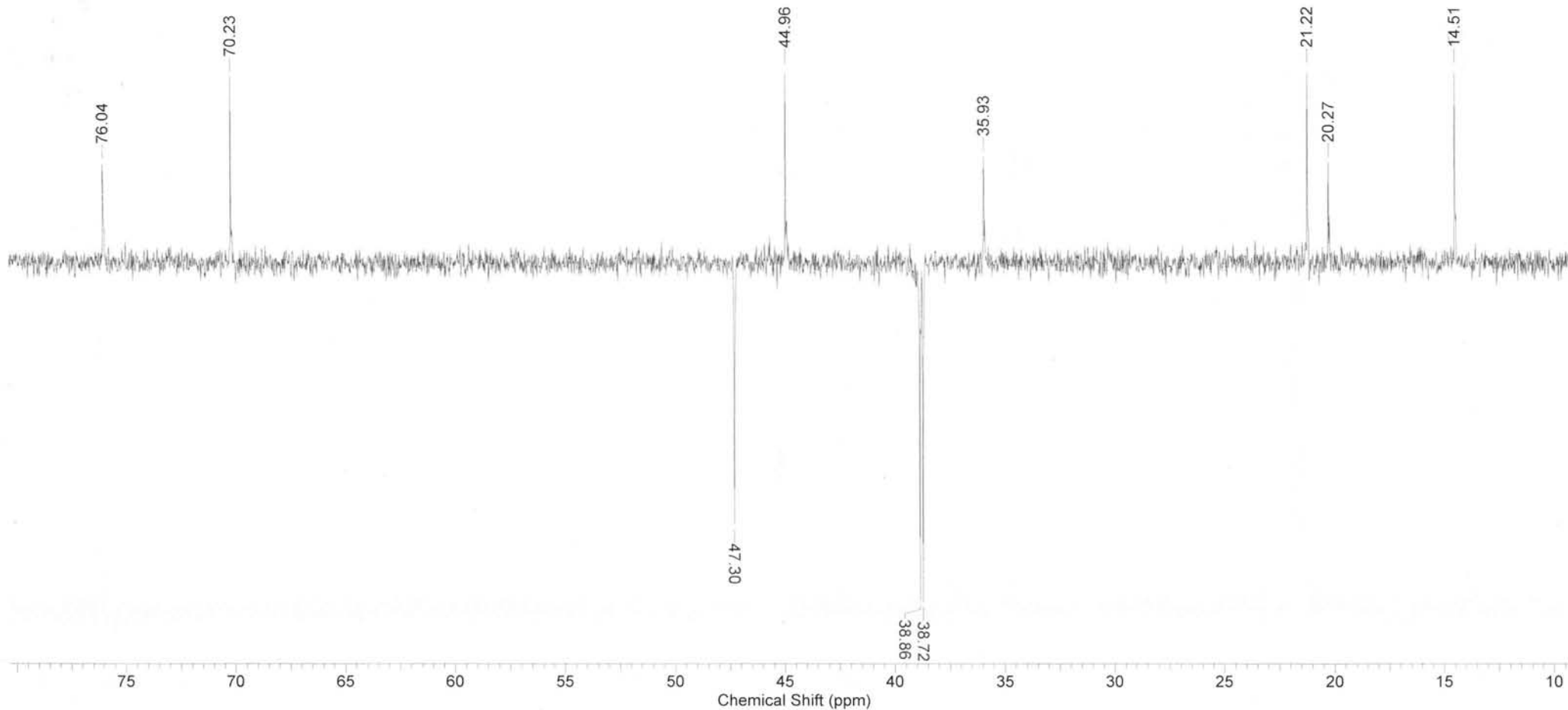
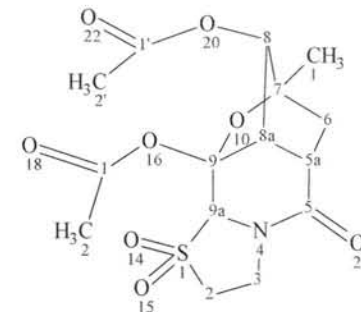
Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	18 Apr 2011 17:21:04	
File Name	C:\Users\Fedor\Desktop\4.04.2011 (Poma)\rudn-fz-180411-N4-c13dec\rudn-fz-180411-N4-c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	793	Original Points Count	16384	Points Count	16384
Pulse Sequence	zpgg	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	50.000

Compound 39b



Acquisition Time (sec)	0.5571	Comment	Imported from UXNMR.	Date	18 Apr 2011 17:38:08
File Name	C:\Users\Fedor\Desktop\4.04.2011 (Poma)\rudn-fz-180411-N4-dept135\rudn-fz-180411-N4-dept135_001000fid			Frequency (MHz)	100.62
Nucleus	13C	Number of Transients	532	Original Points Count	16384
Pulse Sequence	dept135	Solvent	CHLOROFORM-D	Sweep Width (Hz)	29411.77
				Points Count	16384
				Temperature (degree C)	50.000

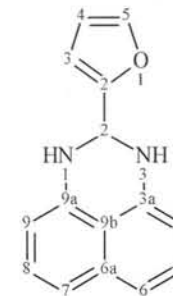
Compound 39b



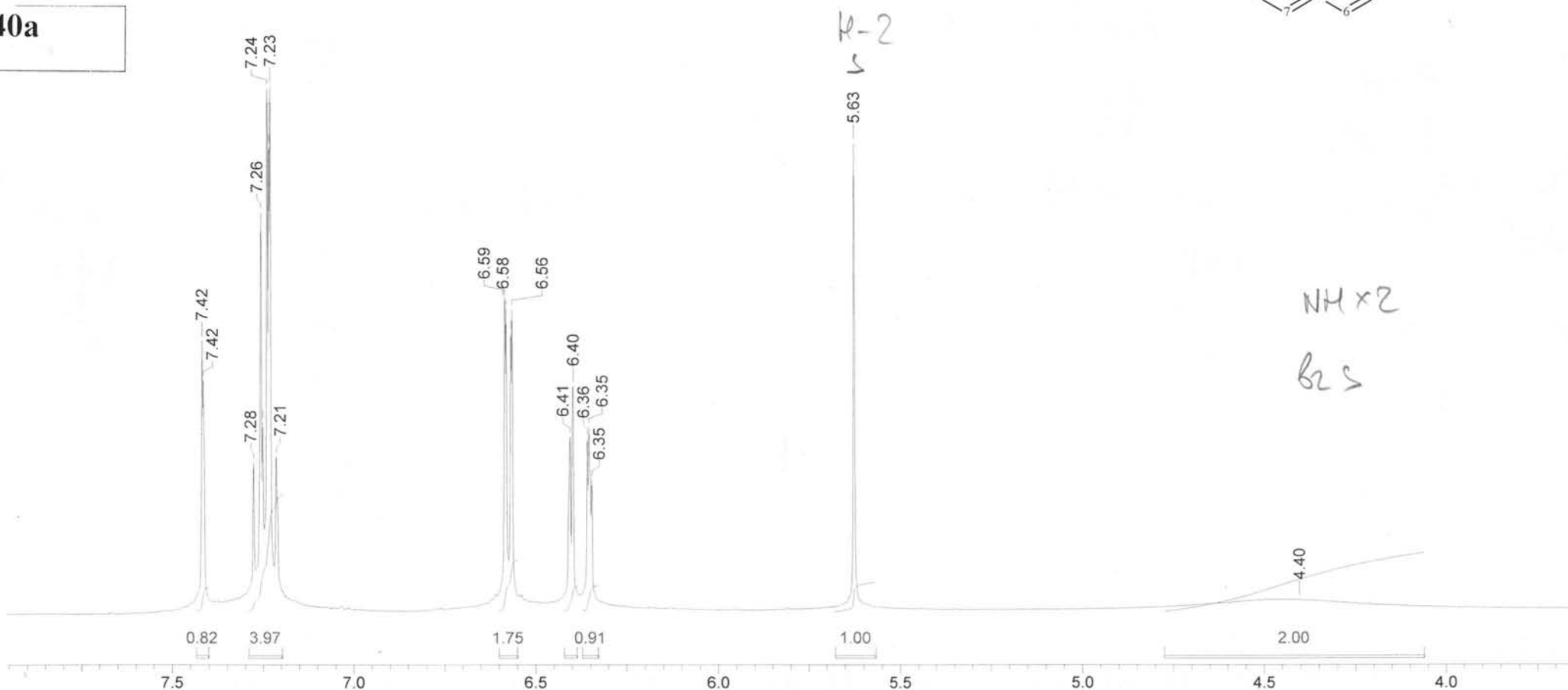
Formula	C ₁₅ H ₁₂ N ₂ O	FW	236.2686
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Acquisition Time (sec)	1.8193	Comment	single_pulse	Date	06 Oct 2011 09:01:49	Date Stamp	06 Oct 2011 12:50:43
File Name	D:\NMR\03.10.11\FZ1958-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8
Origin	ECS 400	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2398.6931	Sweep Width (Hz)	9005.76

Compound 40a



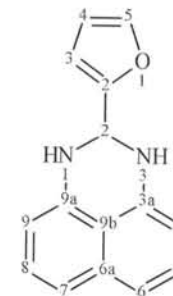
40a



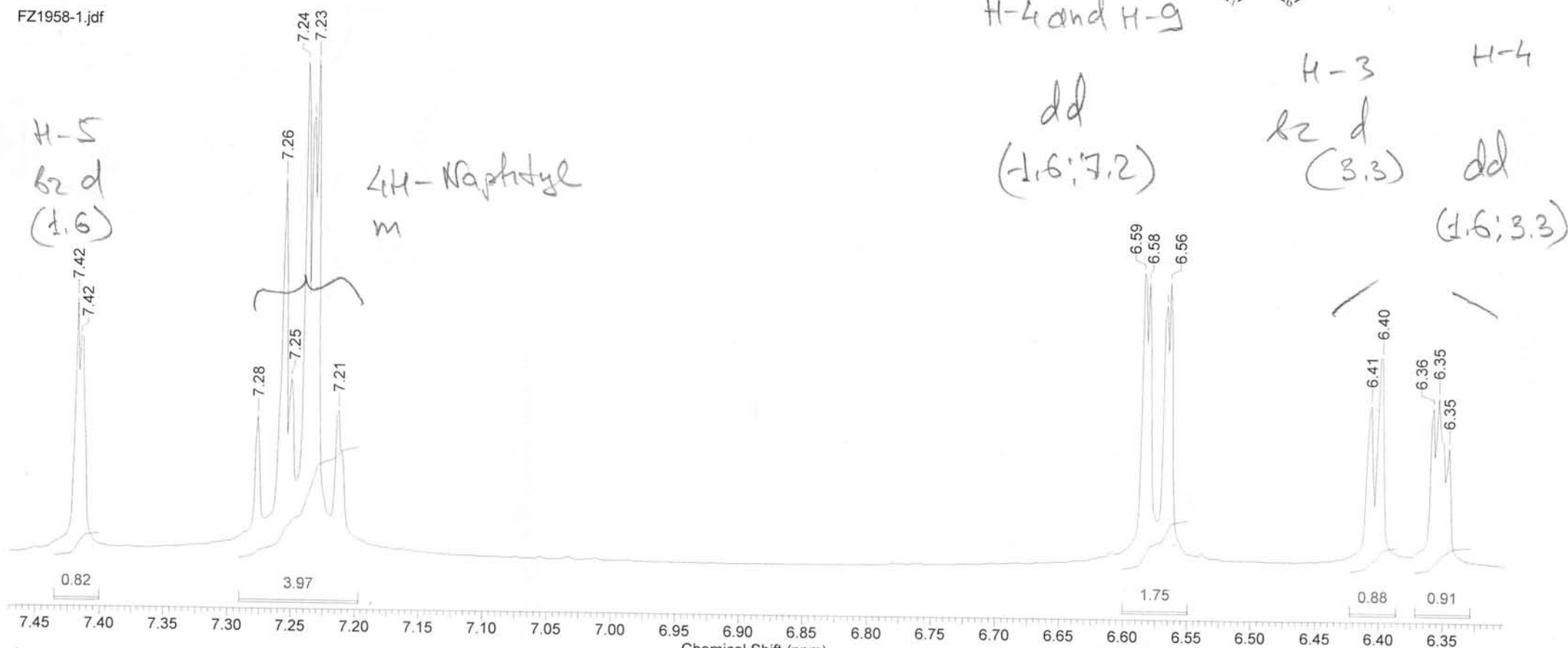
Formula	C ₁₅ H ₁₂ N ₂ O	FW	236.2686
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Acquisition Time (sec)	1.8193	Comment	single_pulse	Date	06 Oct 2011 09:01:49	Date Stamp	06 Oct 2011 12:50:43
File Name	D:\NMR\03.10.11\FZ1958-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2398.6931	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	9005.76

Compound 40a



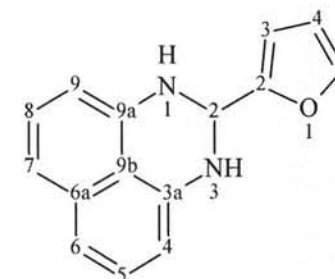
FZ1958-1.jdf



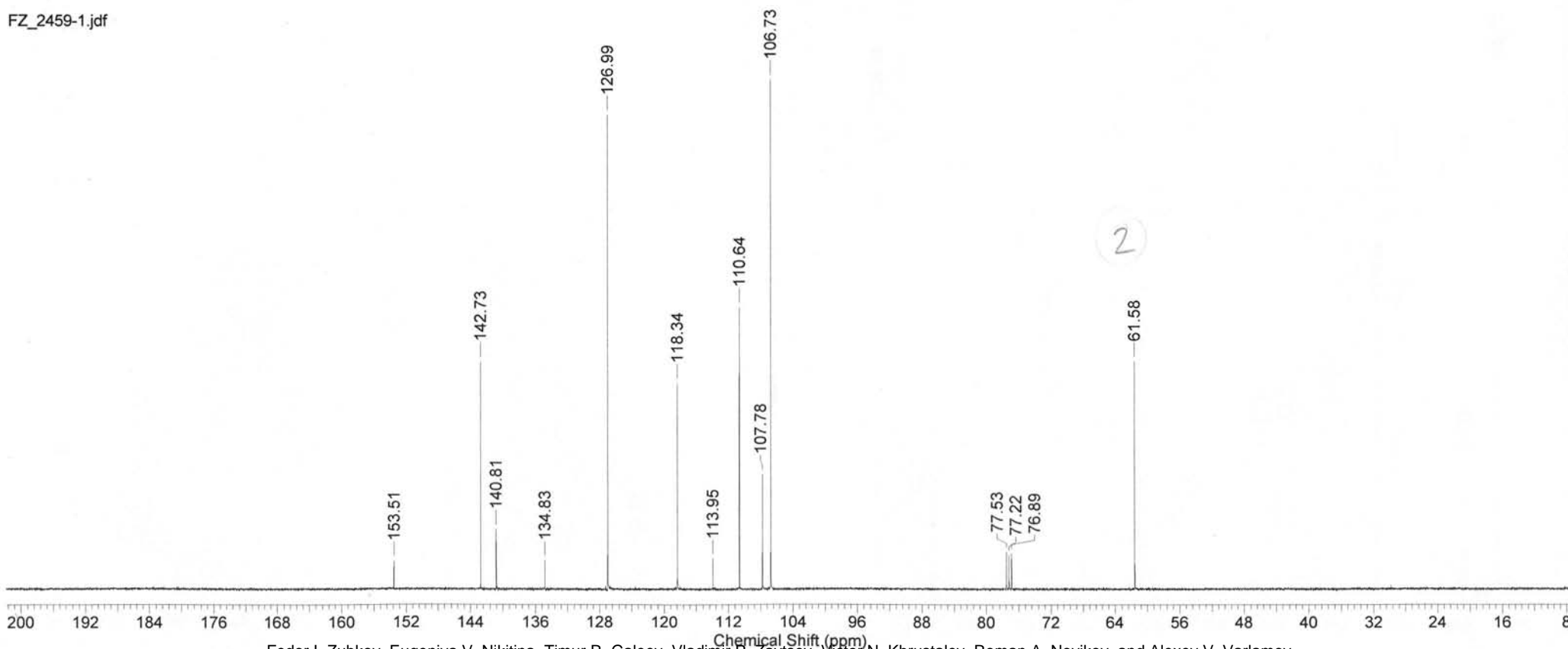
Formula	C ₁₅ H ₁₂ N ₂ O	FW	236.2686
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Acquisition Time (sec)	1.0433	Comment	single pulse decoupled gated NOE	Date	18 Jun 2012 11:51:51
Date Stamp	18 Jun 2012 15:41:34	File Name	C:\Users\Fedor\Desktop\13.06.12\FZ_2459-1.jdf		
Frequency (MHz)	100.53	Nucleus	13C	Number of Transients	241
Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	60.00	Solvent	CHLOROFORM-d	Pulse Sequence	single_pulse_dec
Sweep Width (Hz)	31407.04	Temperature (degree C)	23.200	Spectrum Offset (Hz)	10052.5303

Compound 40a



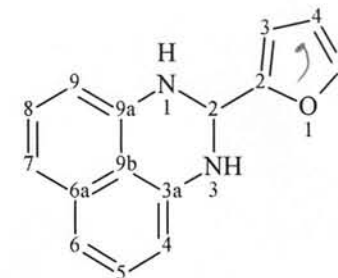
FZ_2459-1.jdf



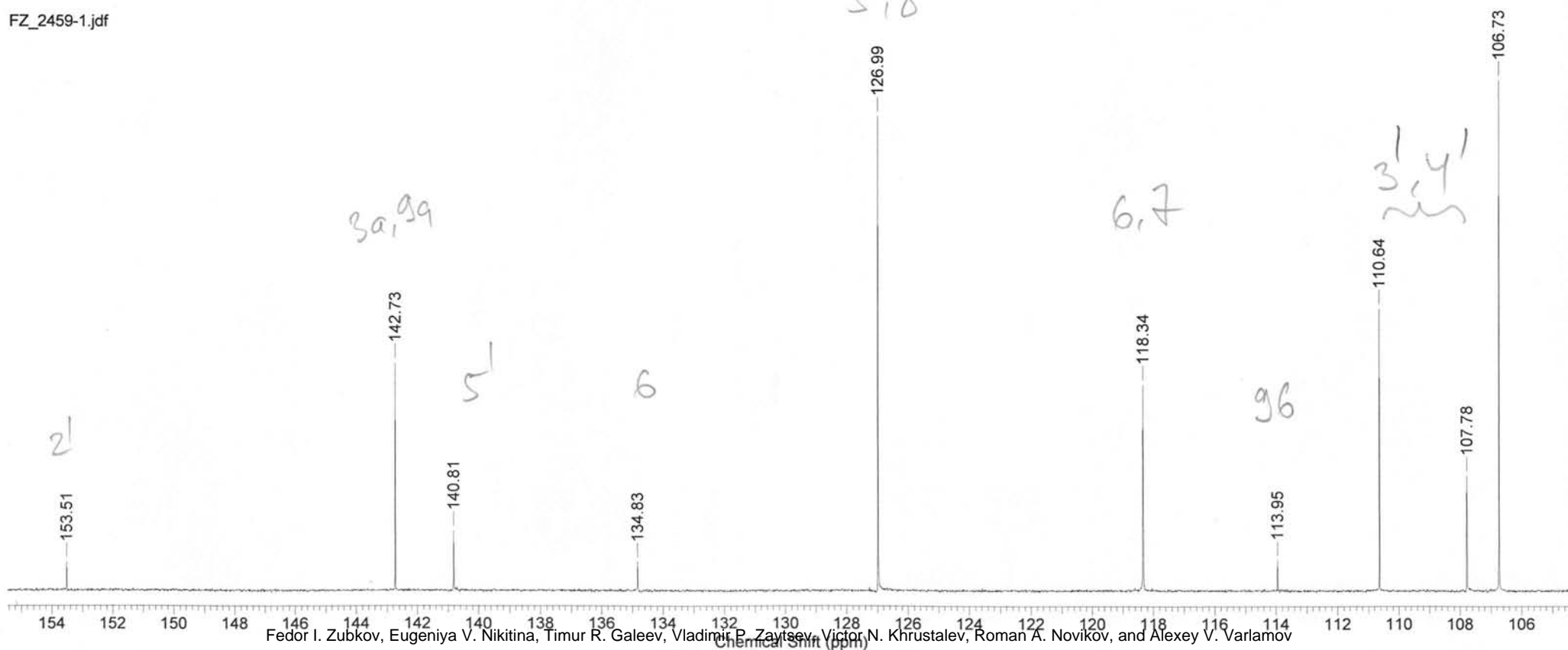
Formula	C ₁₅ H ₁₂ N ₂ O	FW	236.2686
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Acquisition Time (sec)	1.0433	Comment	single pulse decoupled gated NOE	Date	18 Jun 2012 11:51:51
Date Stamp	18 Jun 2012 15:41:34	File Name	C:\Users\Fedor\Desktop\13.06.12\FZ_2459-1.jdf		
Frequency (MHz)	100.53	Nucleus	13C	Number of Transients	241
Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	60.00	Solvent	CHLOROFORM-d	Pulse Sequence	single_pulse_dec
Sweep Width (Hz)	31407.04	Temperature (degree C)	23.200	Spectrum Offset (Hz)	10052.5303

Compound 40a



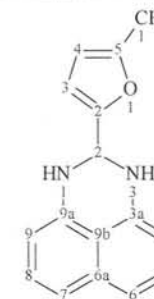
FZ_2459-1.jdf



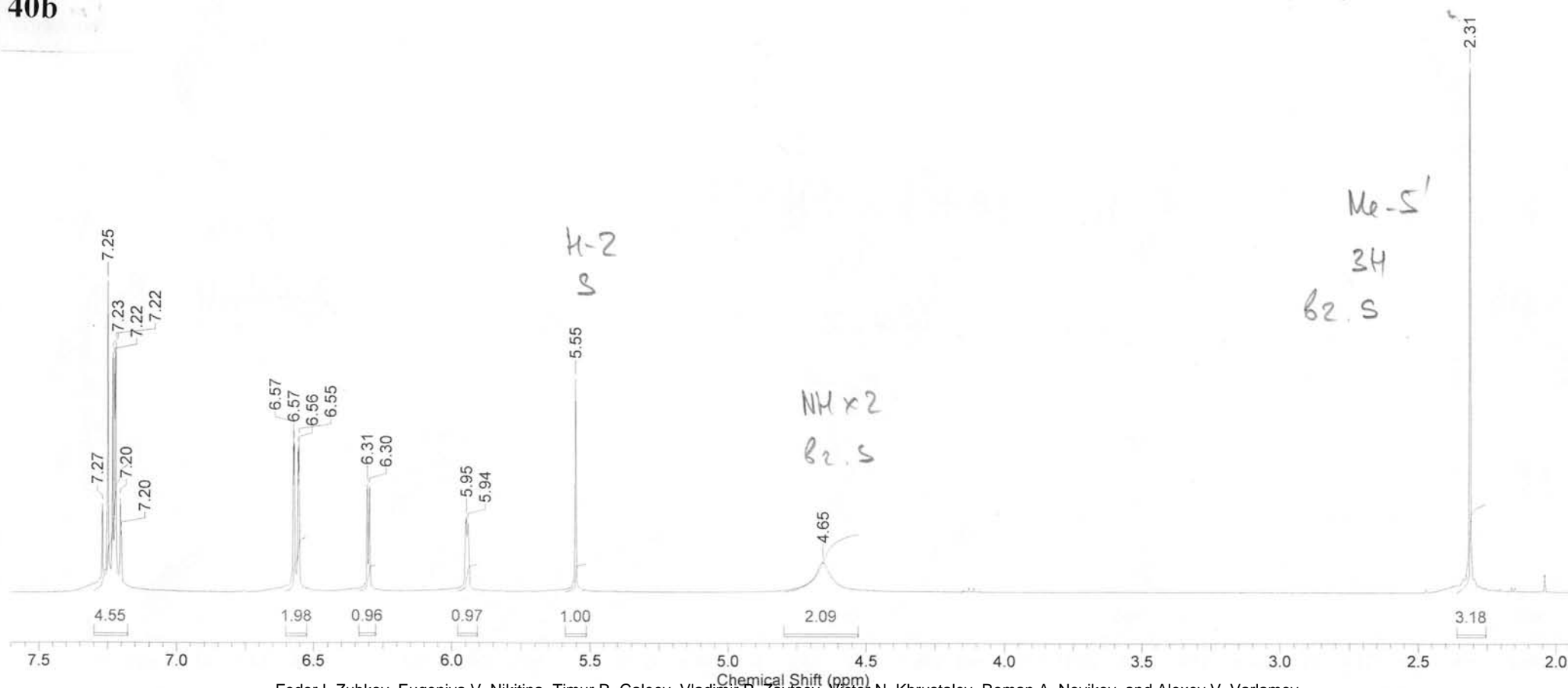
Formula	C ₁₆ H ₁₄ N ₂ O	FW	250.2952
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Acquisition Time (sec)	1.8193	Comment	single_pulse	Date	06 Oct 2011 08:11:57	Date Stamp	06 Oct 2011 12:00:52
File Name	D:\NMR\03.10.11\FZ1962-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8
Origin	ECS 400	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2398.6931	Sweep Width (Hz)	9005.76

Compound 40b



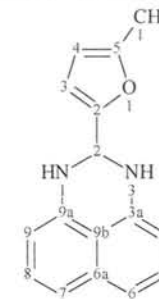
40b



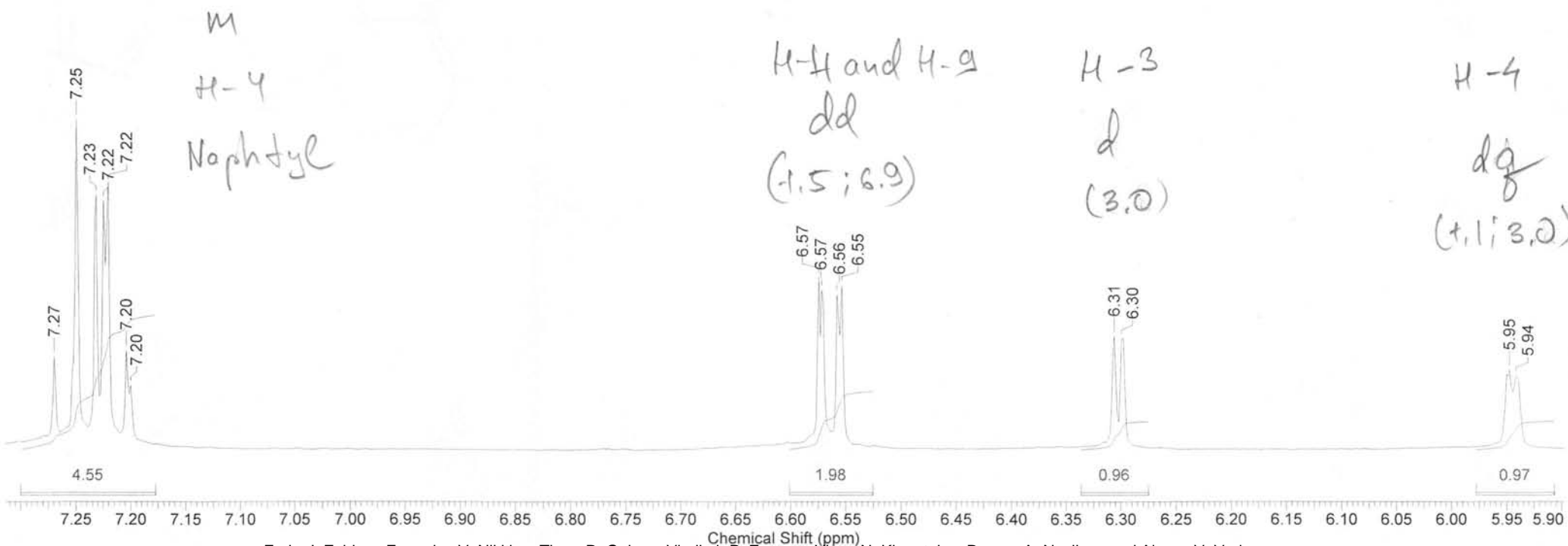
Formula C₁₆H₁₄N₂O FW 250.2952

Acquisition Time (sec)	1.8193	Comment	single_pulse	Date	06 Oct 2011 08:11:57	Date Stamp	06 Oct 2011 12:00:52
File Name	D:\NMR\03.10.11\FZ1962-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8
Origin	ECS 400	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2398.6931	Sweep Width (Hz)	9005.76

Compound 40b



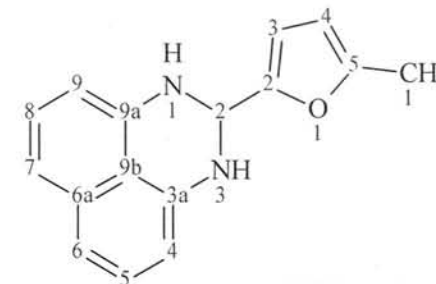
FZ1962-1.jdf



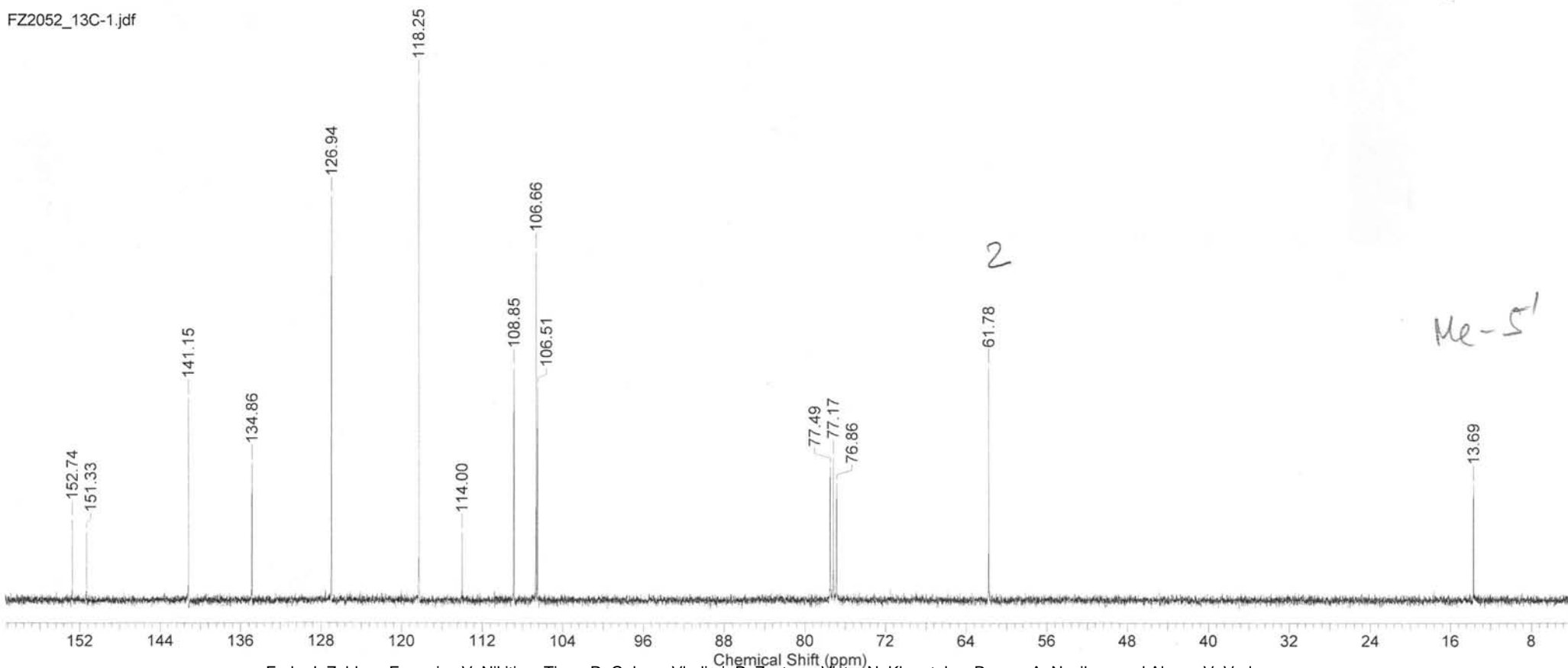
Formula	C ₁₆ H ₁₄ N ₂ O	FW	250.2952
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Acquisition Time (sec)	1.0433	Comment	single pulse decoupled gated NOE	Date	16 Nov 2011 13:50:02
Date Stamp	17 Nov 2011 00:13:11	File Name	D:\NMR\14.11.11\FZ2052_13C-1.jdf	Frequency (MHz)	100.53
Nucleus	13C	Number of Transients	82	Origin	ECS 400
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Solvent	CHLOROFORM-d	Receiver Gain	60.00	Owner	delta
		Spectrum Offset (Hz)	12063.0361	Sweep Width (Hz)	31407.04
				Temperature (degree C)	26.000

Compound 40b



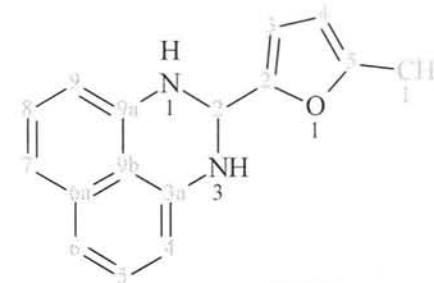
FZ2052_13C-1.jdf



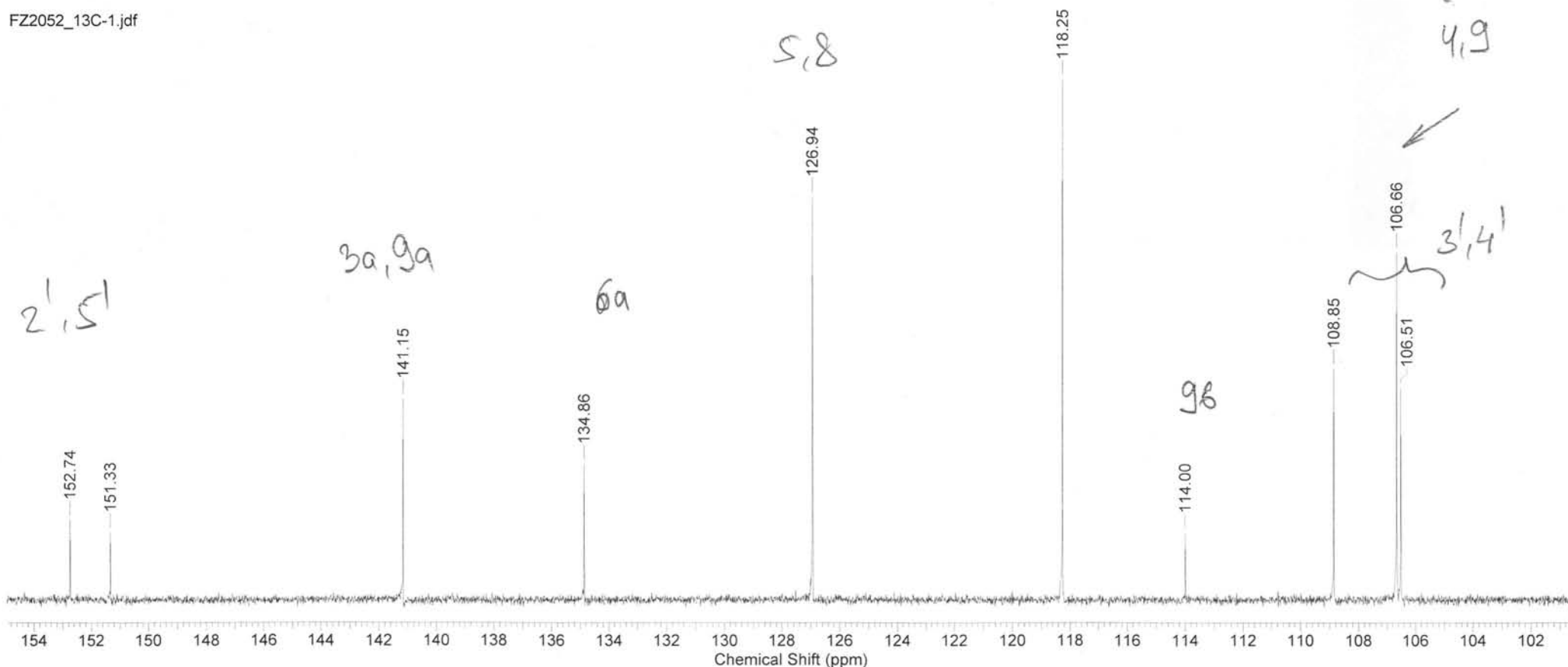
Formula	C ₁₆ H ₁₄ N ₂ O	FW	250.2952
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Acquisition Time (sec)	1.0433	Comment	single pulse decoupled gated NOE	Date	16 Nov 2011 13:50:02
Date Stamp	17 Nov 2011 00:13:11	File Name	D:\NMR\14.11.11\FZ2052_13C-1.jdf	Frequency (MHz)	100.53
Nucleus	13C	Number of Transients	82	Origin	ECS 400
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	12063.0361	Receiver Gain	60.00
		Sweep Width (Hz)	31407.04	Temperature (degree C)	26.000

Compound 40b

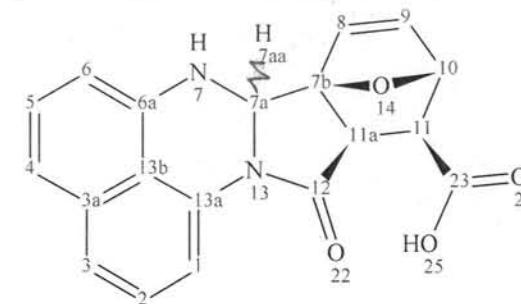


FZ2052_13C-1.jdf



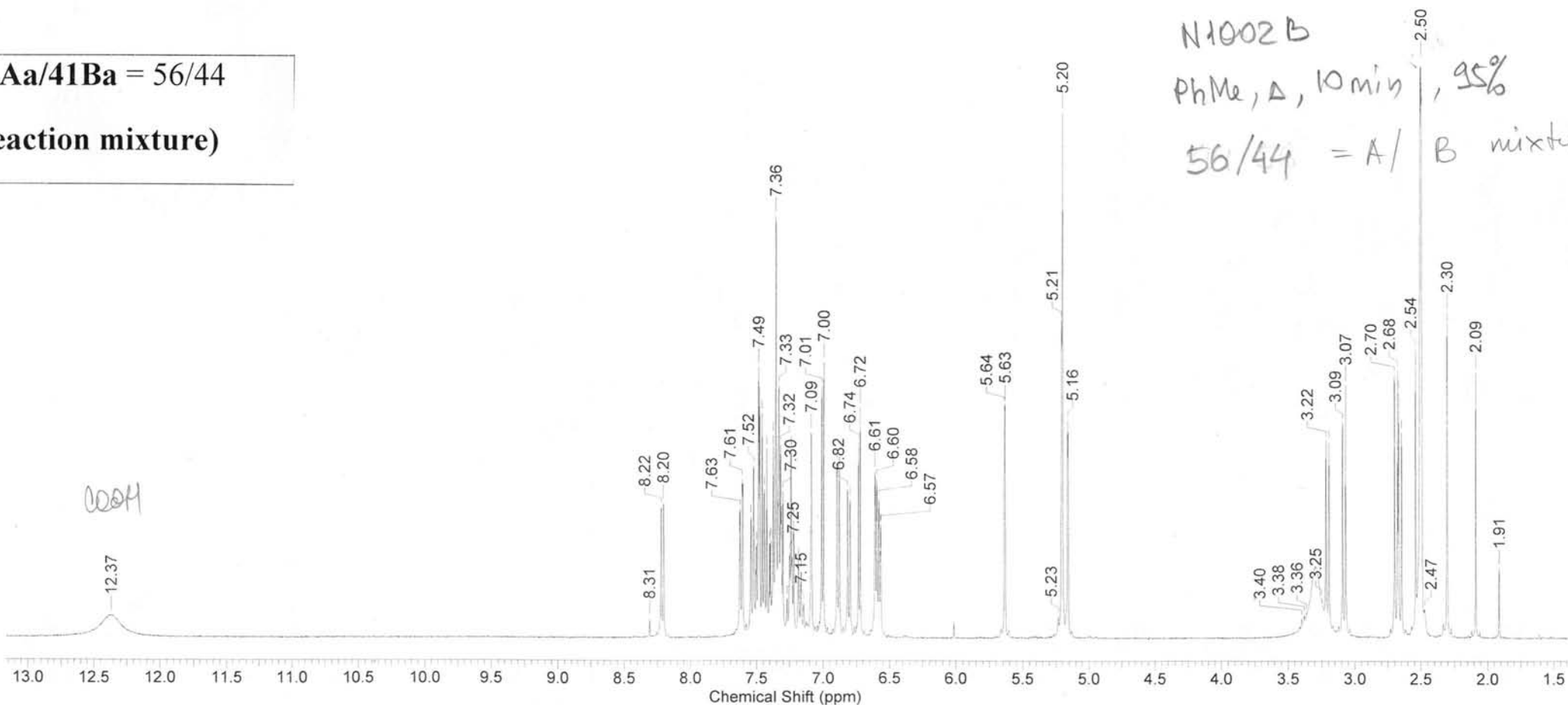
Acquisition Time (sec)	1.5729	Comment	Imported from UXNMR.		Date	14 Oct 2011 16:10:40	
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N3\rudn-141011-N3_001000fid			Frequency (MHz)	400.14		
Nucleus	1H	Number of Transients	32	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	10416.67	Temperature (degree C)	32.000

Compounds 41Aa/41Ba
reaction mixture



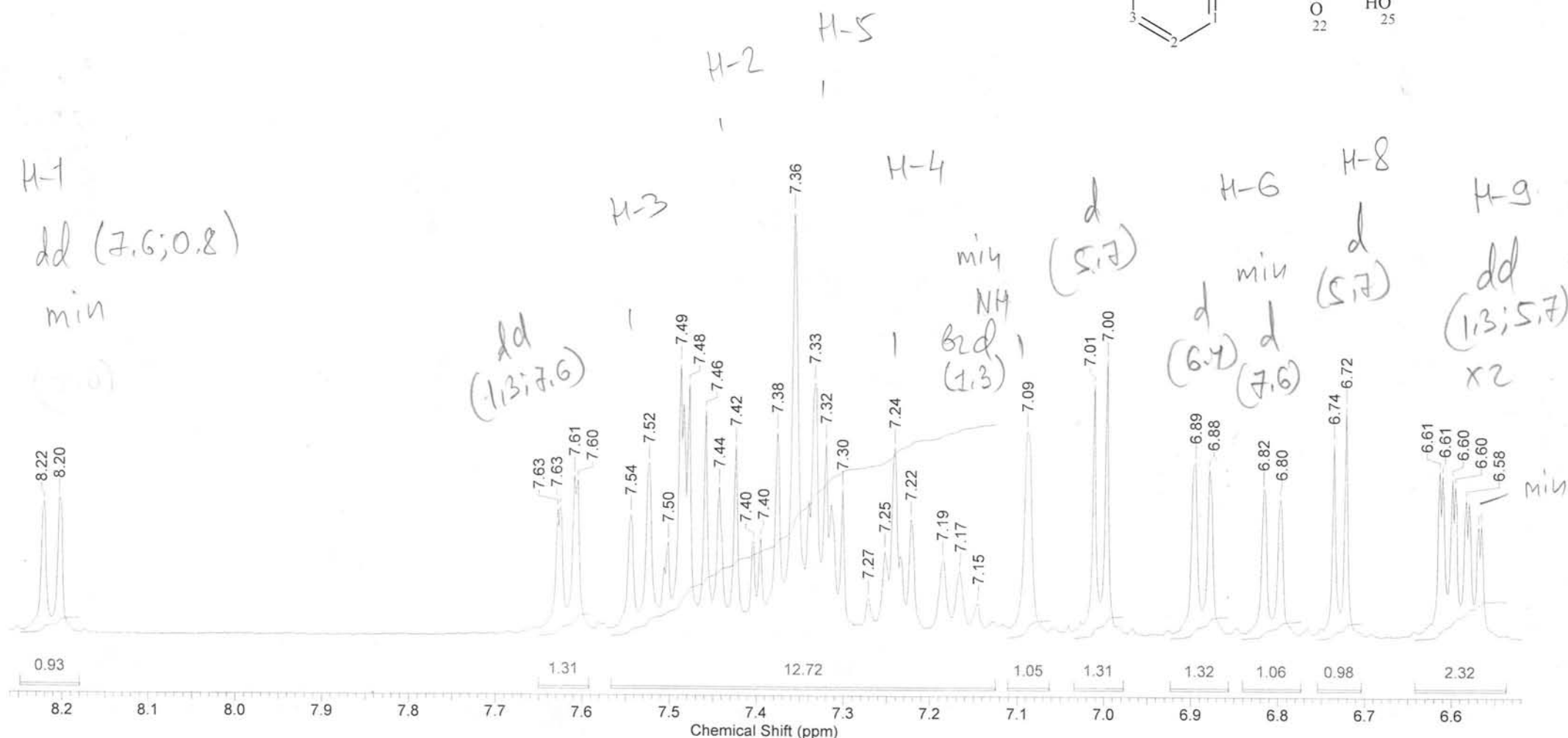
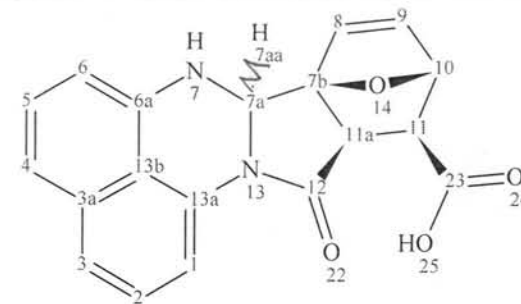
41Aa/41Ba = 56/44
(reaction mixture)

N1002 B
PhMe, Δ, 10 min, 95%
56/44 = A/B mixture

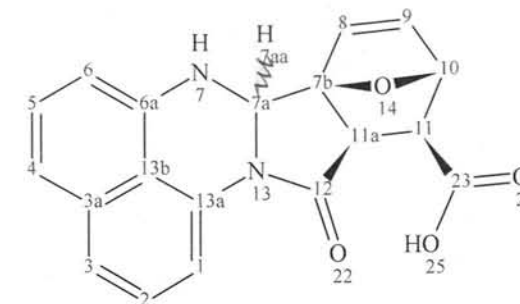


Acquisition Time (sec)	1.5729	Comment	Imported from UXMNR.		Date	14 Oct 2011 16:10:40	
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N3\rudn-141011-N3_001000fid				Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	32	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	10416.67	Temperature (degree C)	32.000

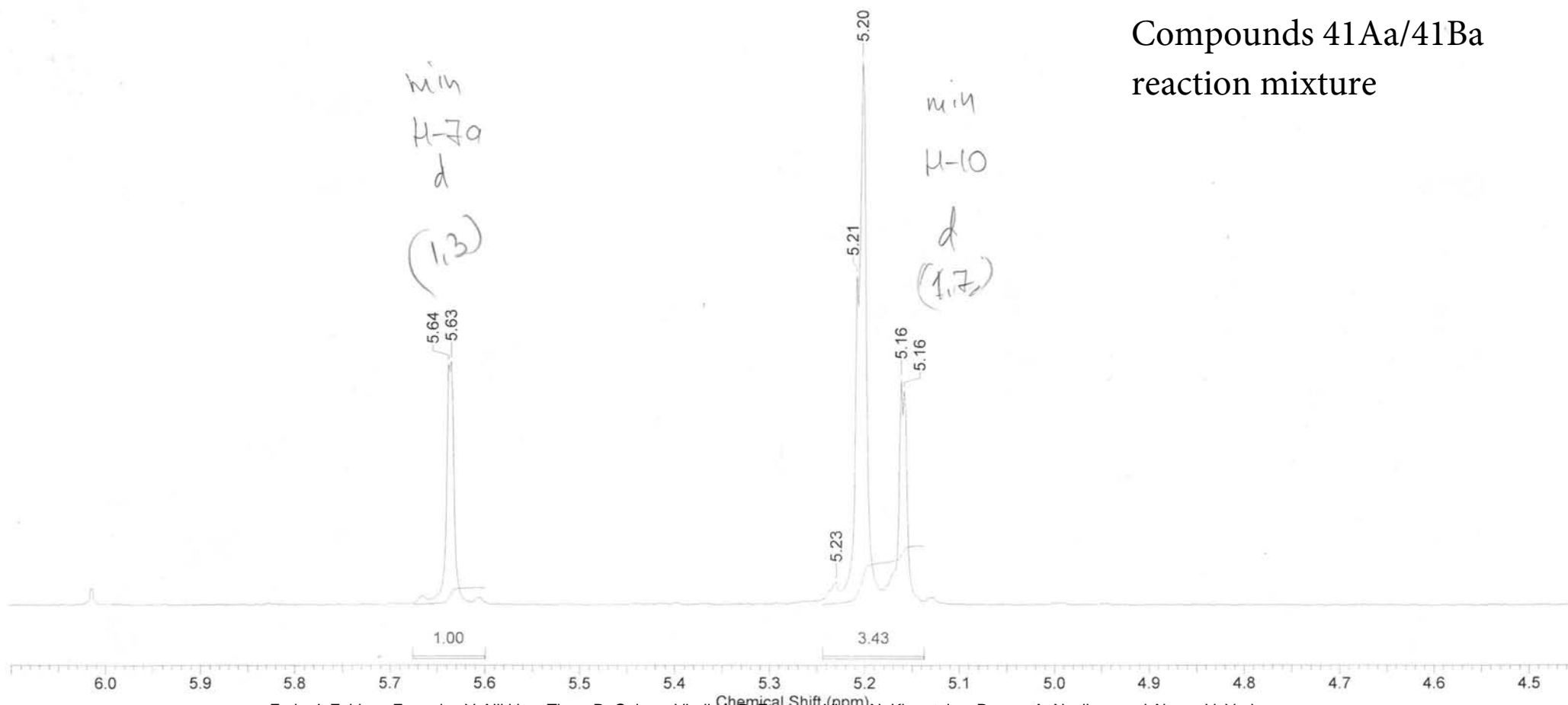
Compounds 41Aa/41Ba reaction mixture



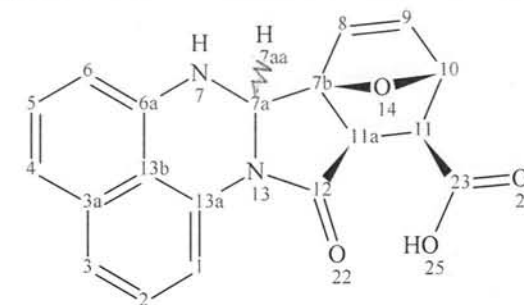
Acquisition Time (sec)	1.5729	Comment	Imported from UXNMR.		Date	14 Oct 2011 16:10:40	
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N3\rudn-141011-N3_001000fid				Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	32	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	10416.67	Temperature (degree C)	32.000



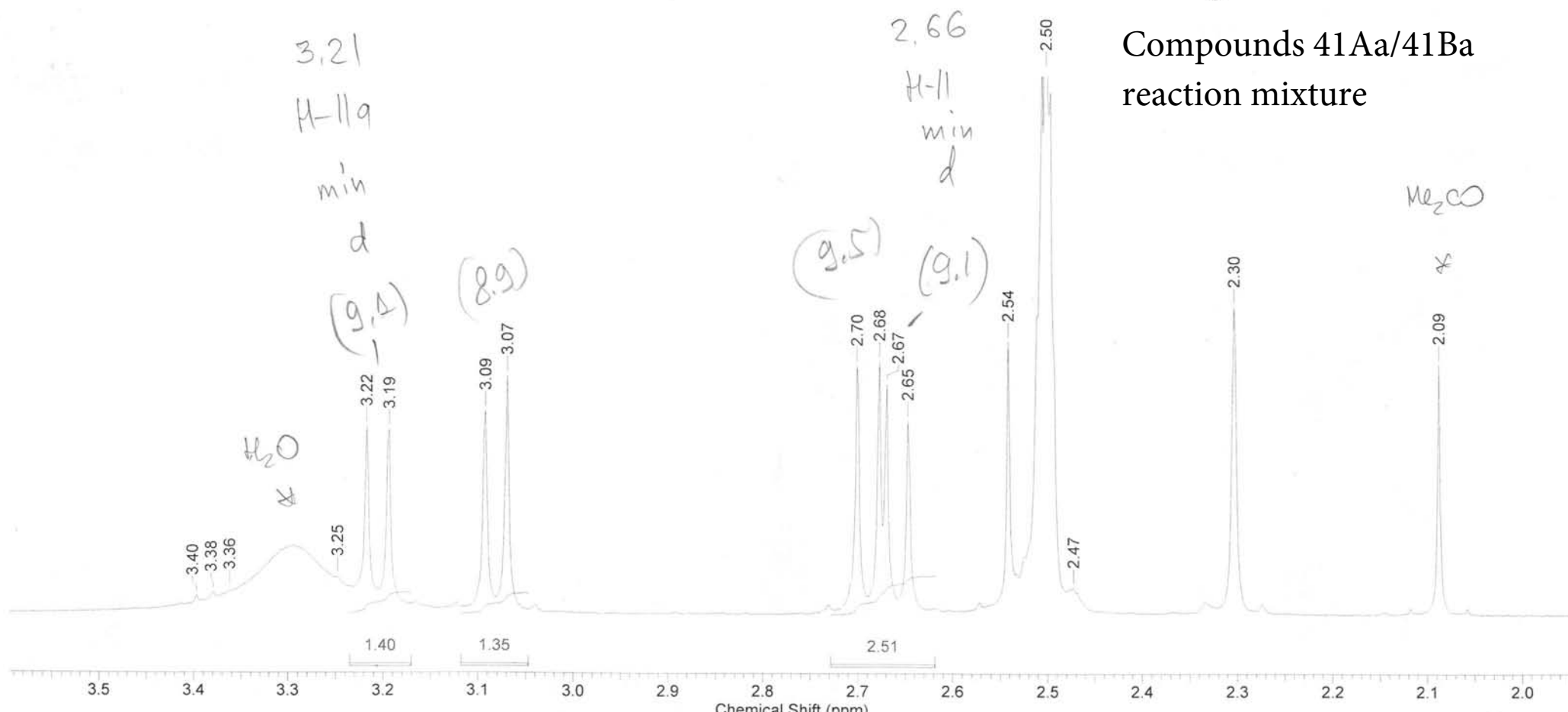
Compounds 41Aa/41Ba
reaction mixture



Acquisition Time (sec)	1.5729	Comment	Imported from UXMNR.		Date	14 Oct 2011 16:10:40	
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N3\rudn-141011-N3_001000fid				Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	32	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	10416.67	Temperature (degree C)	32.000



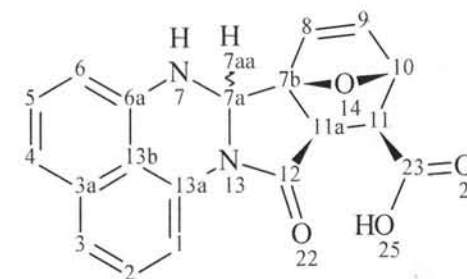
Compounds 41Aa/41Ba
reaction mixture



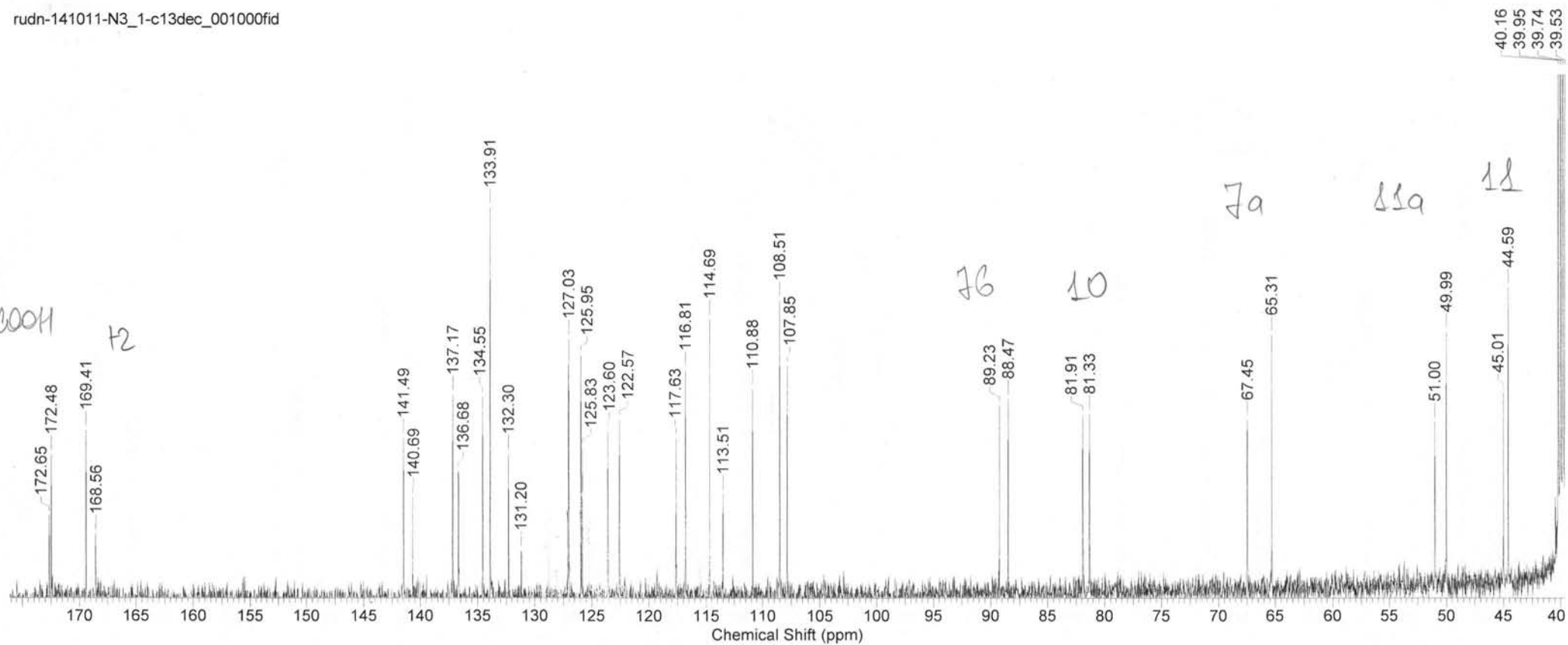
Formula C₁₉H₁₄N₂O₄ FW 334.3255

Acquisition Time (sec)	0.5243	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	26 Oct 2011 17:50:56
Date Stamp	26 Oct 2011 17:50:56	File Name	D:\NMR\14.10.11\rudn-141011-N3_1-c13dec\rudn-141011-N3_1-c13dec_001000fid		
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	10000
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	31250.00	Solvent	DMSO-d6
Sweep Width (Hz)	31248.09	Temperature (degree C)	27.000	Spectrum Offset (Hz)	10547.7090

Compounds 41Aa/41Ba
reaction mixture



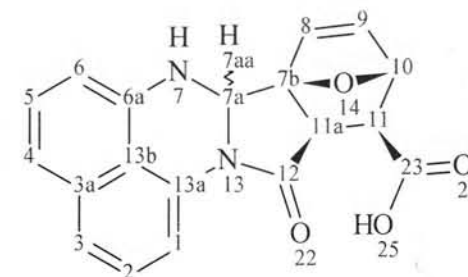
rudn-141011-N3_1-c13dec_001000fid



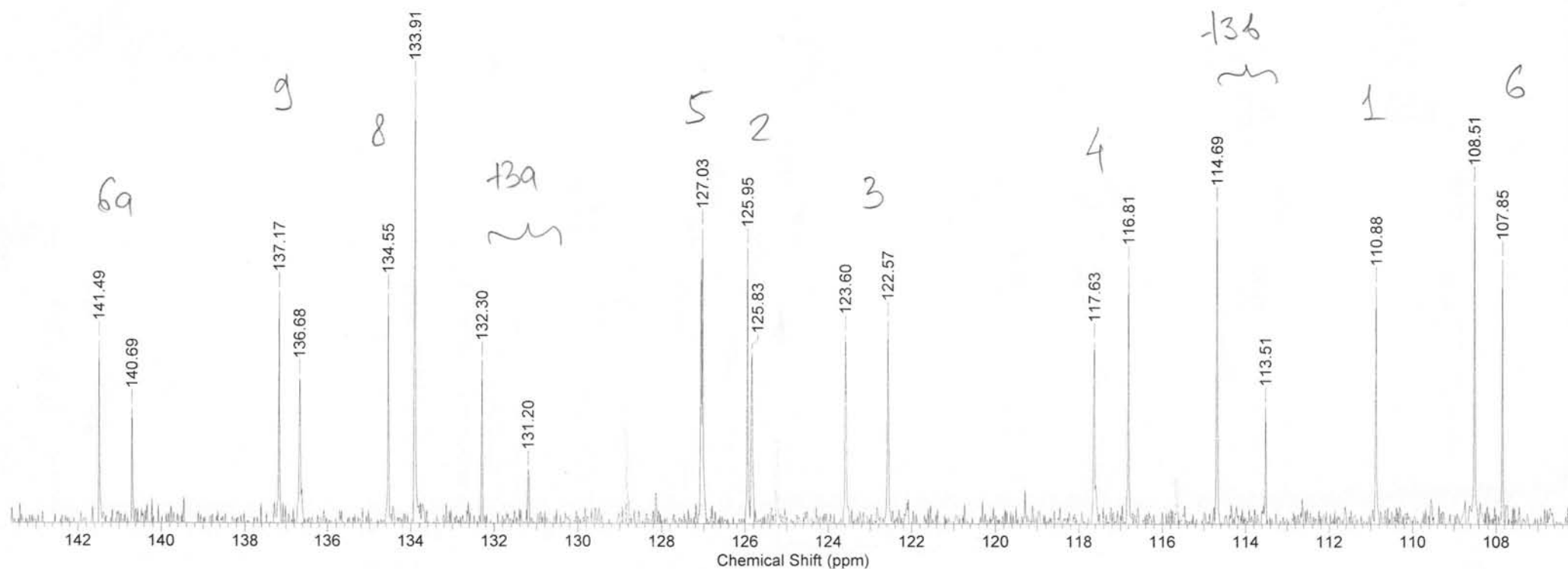
Formula $C_{19}H_{14}N_2O_4$ FW 334.3255

Acquisition Time (sec)	0.5243	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	26 Oct 2011 17:50:56
Date Stamp	26 Oct 2011 17:50:56	File Name	D:\NMR\14.10.11\rudn-141011-N3_1-c13dec\rudn-141011-N3_1-c13dec_001000fid	Number of Transients	10000
Frequency (MHz)	100.62	Nucleus	13C	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	31250.00	Pulse Sequence	zpgg
Sweep Width (Hz)	31248.09	Temperature (degree C)	27.000	Spectrum Offset (Hz)	10547.7090

Compounds 41Aa/41Ba
reaction mixture



rudn-141011-N3_1-c13dec_001000fid

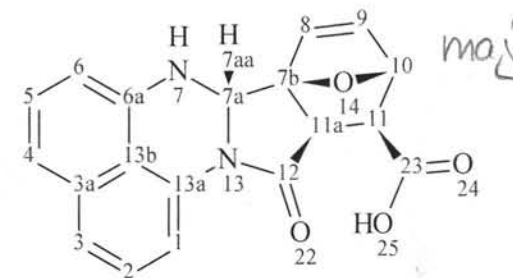


Formula $C_{19}H_{14}N_2O_4$ FW 334.3255

Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	24 Oct 2011 17:46:40
Date Stamp	24 Oct 2011 17:46:40	File Name	D:\NMR\14.10.11\rudn-141011-N1_2\rudn-141011-N1_2_001000fid		
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	40
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	1024.00	SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6
Sweep Width (Hz)	10416.03	Temperature (degree C)	32.000	Spectrum Offset (Hz)	2712.0542

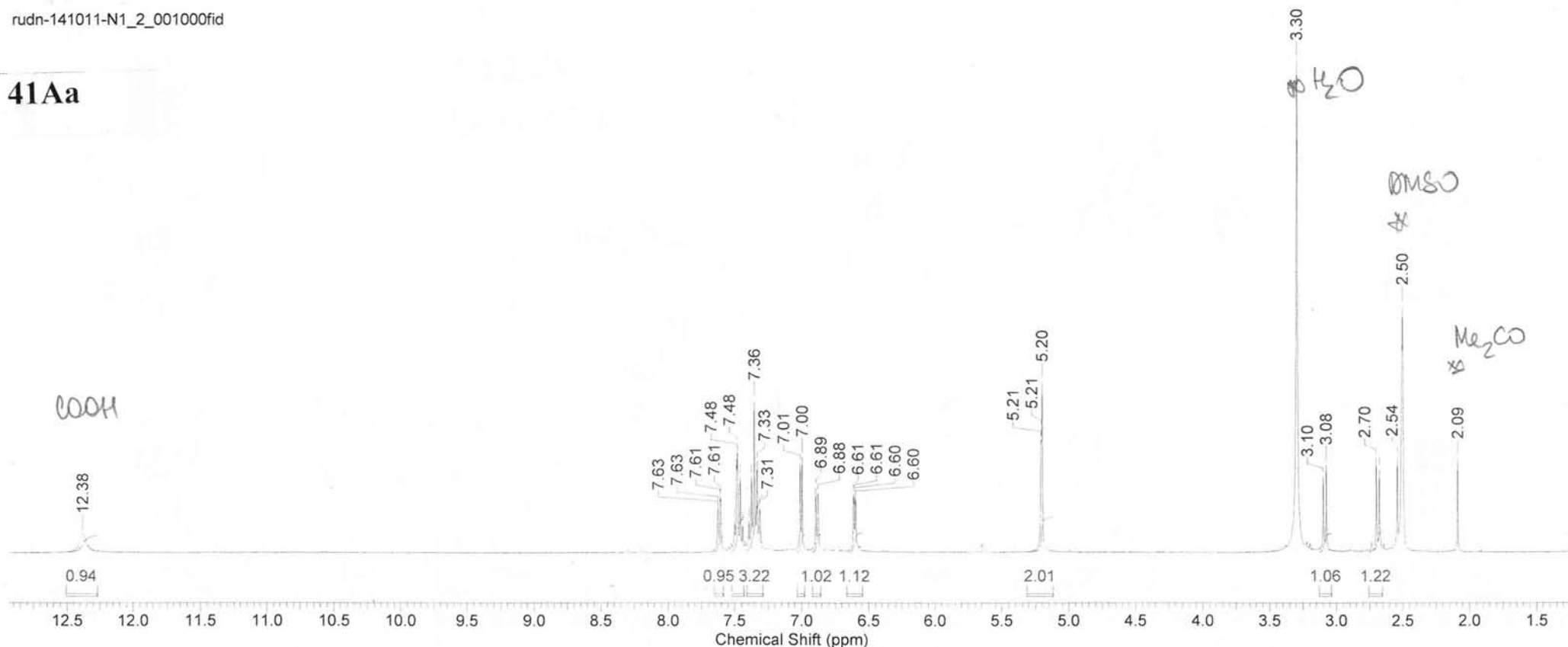
N1000A (CH₂Cl₂) 0,2g

Compound 41Aa



rudn-141011-N1_2_001000fid

41Aa

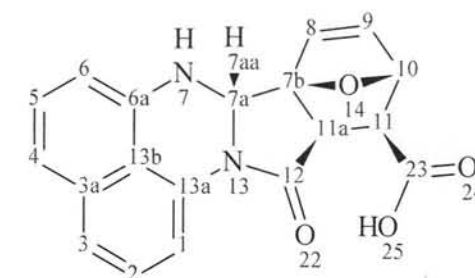


Formula C₁₉H₁₄N₂O₄ FW 334.3255

Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	24 Oct 2011 17:46:40	
Date Stamp	24 Oct 2011 17:46:40	File Name	D:\NMR\14.10.11\rudn-141011-N1_2\rudn-141011-N1_2_001000fid				
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	40	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zg
Receiver Gain	1024.00	SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542
Sweep Width (Hz)	10416.03	Temperature (degree C)	32.000				

H-1
7.49, dd
(7.1; 1.6)

H-2
7.46, dd
(7.1; 7.7)



Compound 41Aa

rudn-141011-N1_2_001000fid

H-5
7.38, dd
(7.7; 7.2)

H-3
dd
(7.7; 1.3)

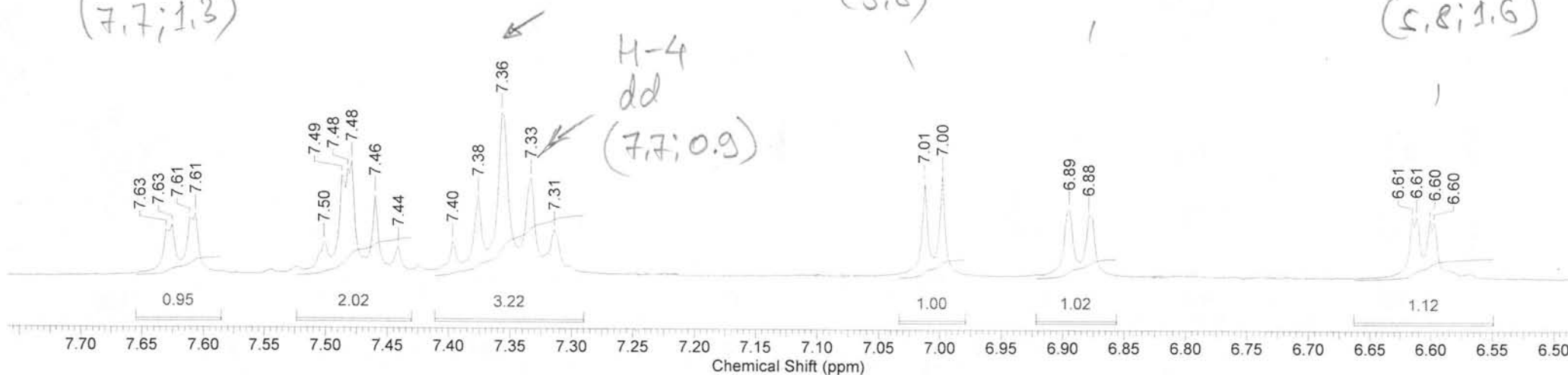
NH, br, s

H-8
d
(5.8)

H-6
dd
(7.2; 0.9)

H-9
dd
(5.8; 1.6)

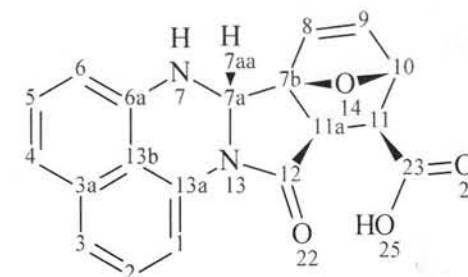
H-4
dd
(7.7; 0.9)



Formula C₁₉H₁₄N₂O₄ FW 334.3255

Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	24 Oct 2011 17:46:40
Date Stamp	24 Oct 2011 17:46:40	File Name	D:\NMR\14.10.11\rudn-141011-N1_2\rudn-141011-N1_2_001000fid	Origin	spect
Frequency (MHz)	400.14	Nucleus	1H	Points Count	16384
Original Points Count	16384	Owner	root	Pulse Sequence	zg
Receiver Gain	1024.00	SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6
Sweep Width (Hz)	10416.03	Temperature (degree C)	32.000	Spectrum Offset (Hz)	2712.0542

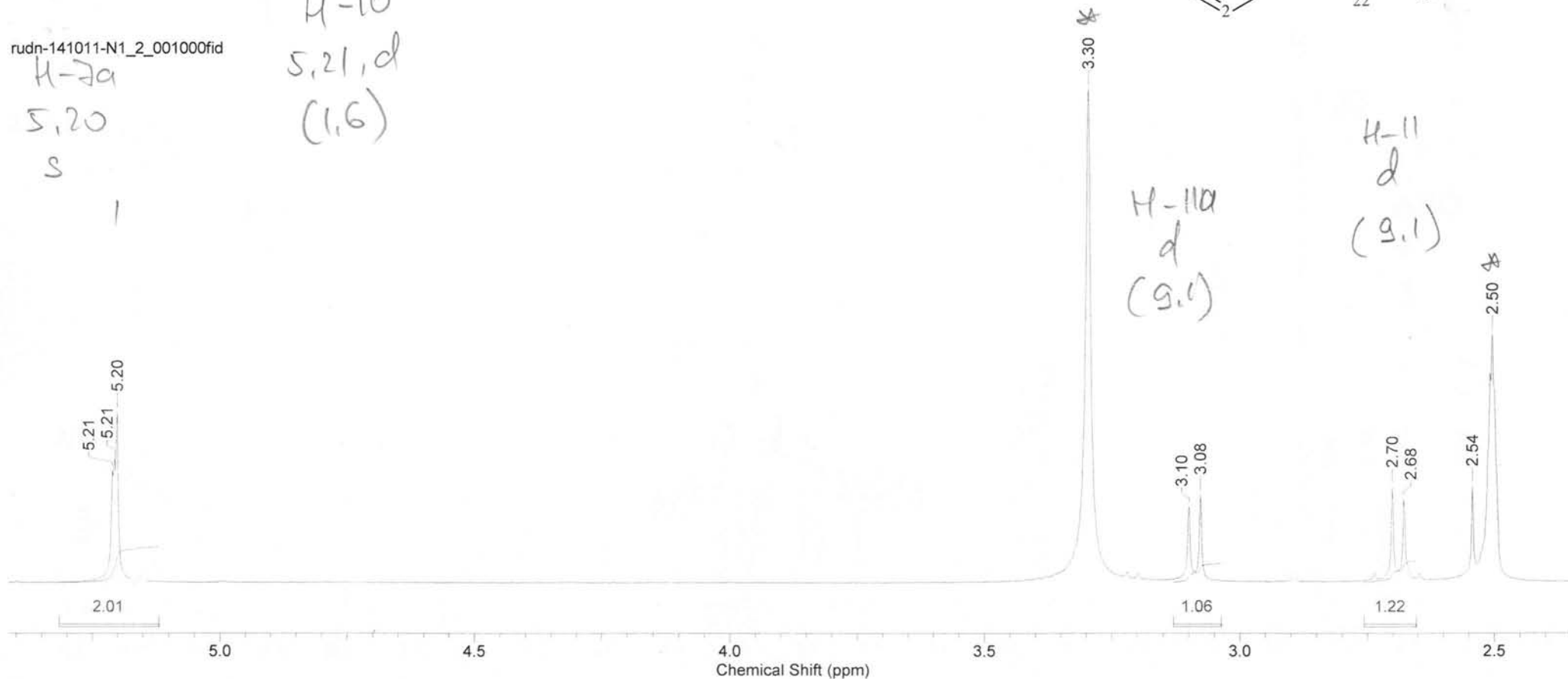
Compound 41Aa



rudn-141011-N1_2_001000fid

H-7a
5.20
s

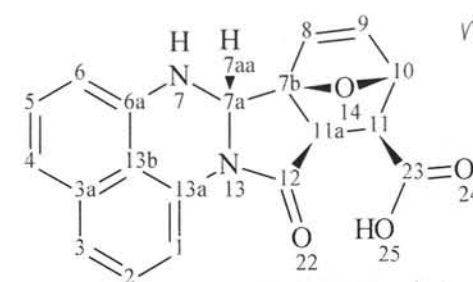
H-10
5.21, d
(1.6)



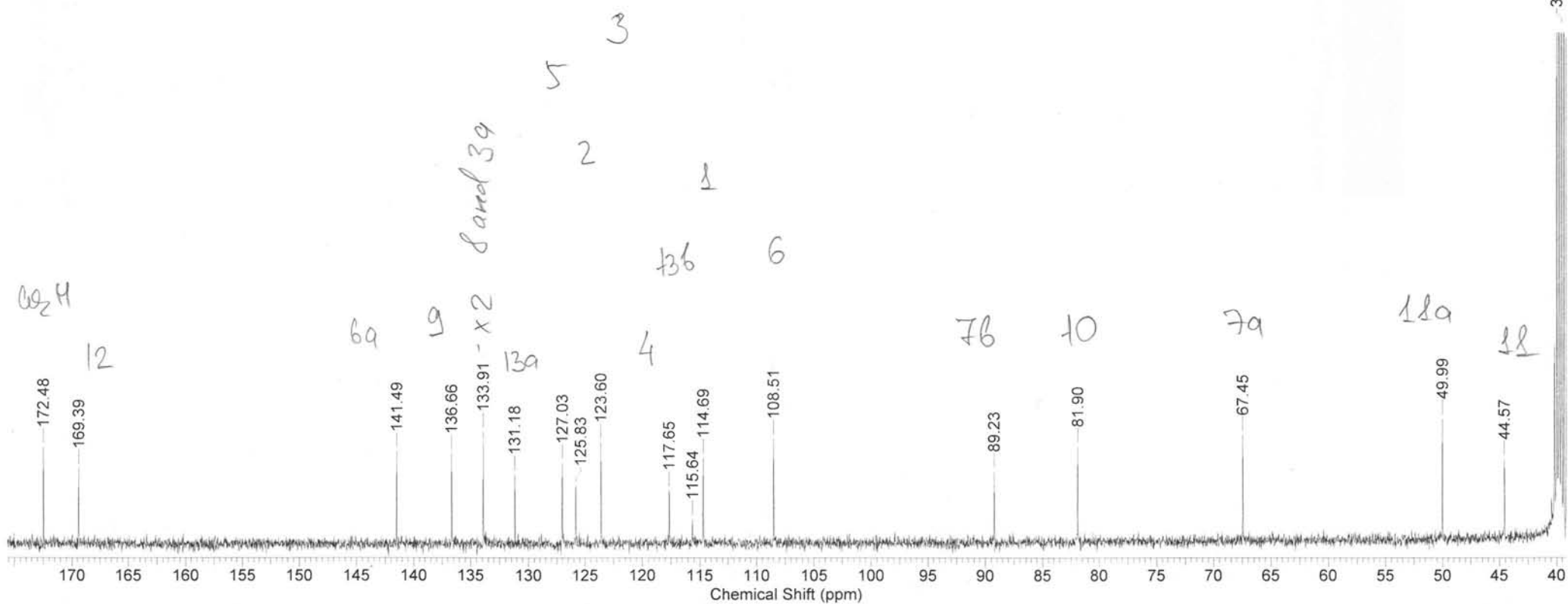
Formula $C_{19}H_{14}N_2O_4$ FW 334.3255

Acquisition Time (sec)	0.5243	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	24 Oct 2011 18:01:36	
Date Stamp	24 Oct 2011 18:01:36		File Name	D:\NMR\14.10.11\rudn-141011-N1_2-c13dec\rudn-141011-N1_2-c13dec_001000fid			
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	7000	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zgpg
Receiver Gain	32768.00	SW(cyclical) (Hz)	31250.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	10547.7090
Sweep Width (Hz)	31248.09	Temperature (degree C)	27.000				

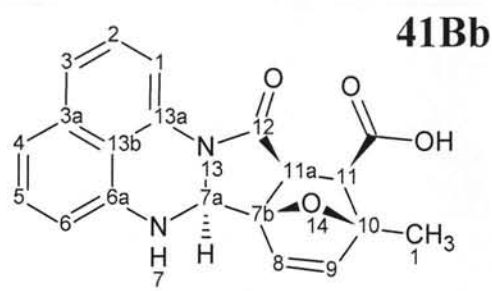
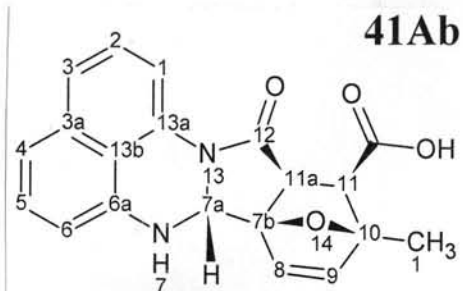
Compound 41Aa



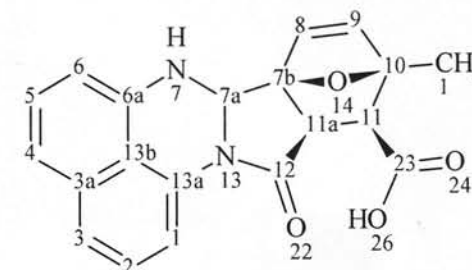
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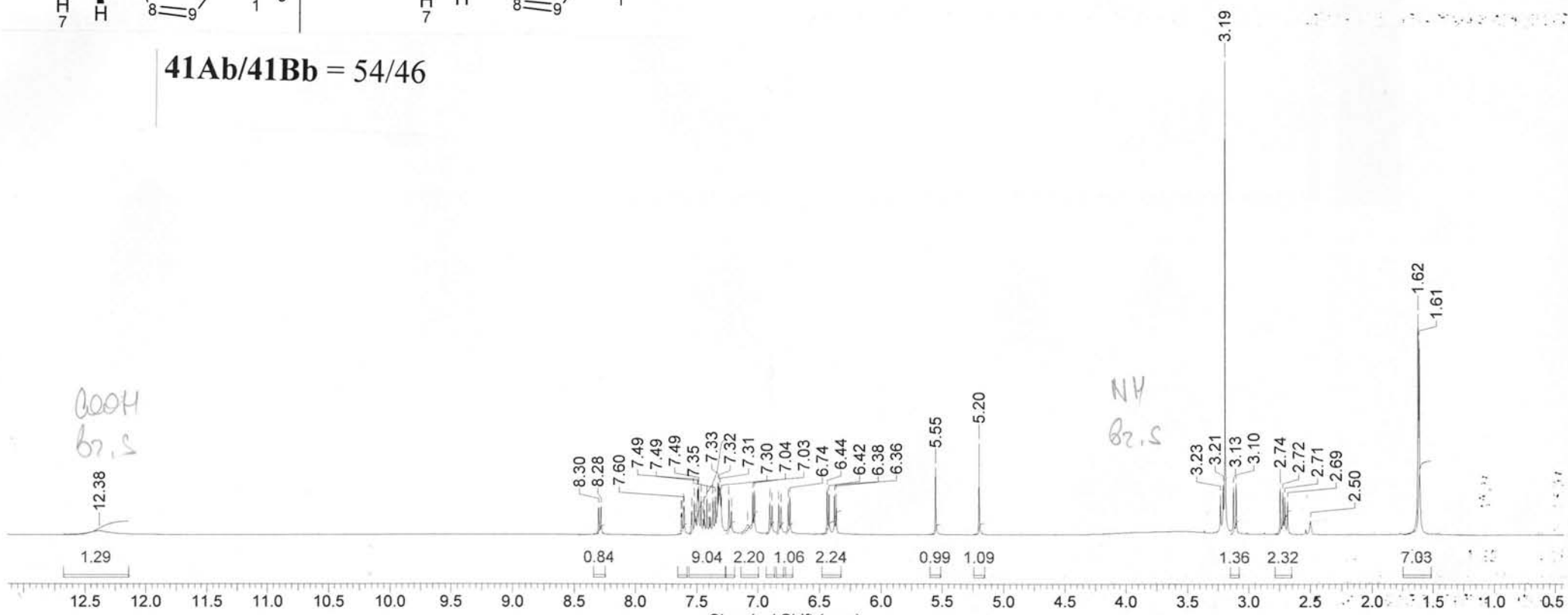
Formula C ₂₀ H ₁₆ N ₂ O ₄	FW 348.3520			
Acquisition Time (sec) 1.5729	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 21 Jun 2012 13:24:16		
Date Stamp 21 Jun 2012 13:24:16				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-41b\rudn-250512-41b_001000fid	Frequency (MHz) 400.14			
Nucleus 1H	Number of Transients 20	Origin spect	Original Points Count 16384	
Owner root	Points Count 16384	Pulse Sequence zg	Receiver Gain 128.00	
SW(cyclical) (Hz) 10416.67	Solvent DMSO-d6	Spectrum Offset (Hz) 2712.0542	Sweep Width (Hz) 10416.03	
Temperature (degree C) 32.000				



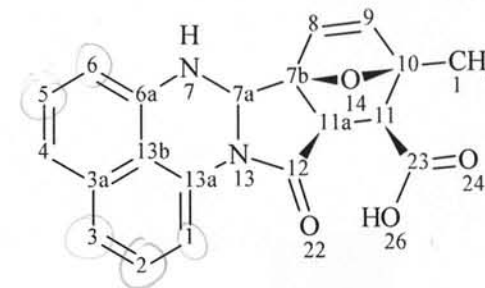
Compounds 41Ab/41Bb



41Ab/41Bb = 54/46

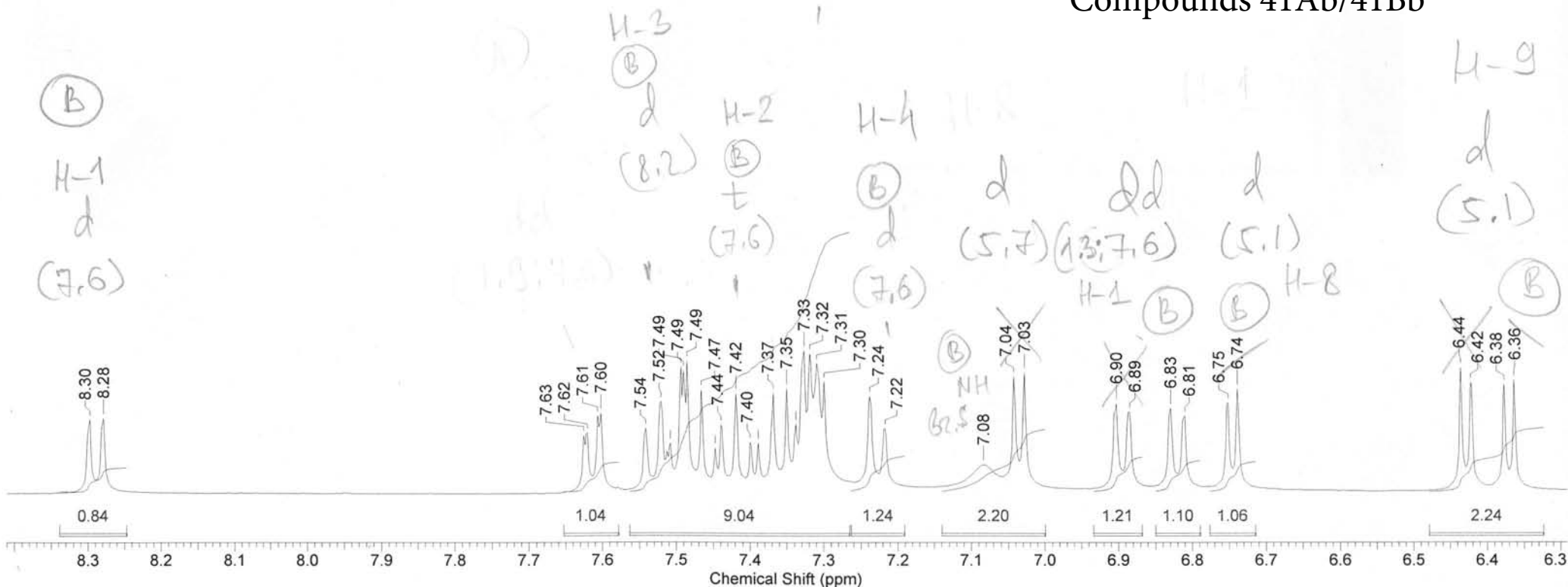


Formula C ₂₀ H ₁₆ N ₂ O ₄	FW 348.3520			
Acquisition Time (sec) 1.5729	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400			Date 21 Jun 2012 13:24:16
Date Stamp 21 Jun 2012 13:24:16				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-41b\rudn-250512-41b_001000fid			Frequency (MHz) 400.14	
Nucleus 1H	Number of Transients 20	Origin spect	Original Points Count 16384	
Owner root	Points Count 16384	Pulse Sequence zg	Receiver Gain 128.00	
SW(cyclical) (Hz) 10416.67	Solvent DMSO-d6	Spectrum Offset (Hz) 2712.0542	Sweep Width (Hz) 10416.03	
Temperature (degree C) 32.000				



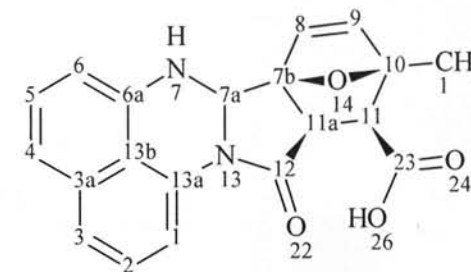
Compounds 41Ab/41Bb

rudn-250512-41b_001000fid

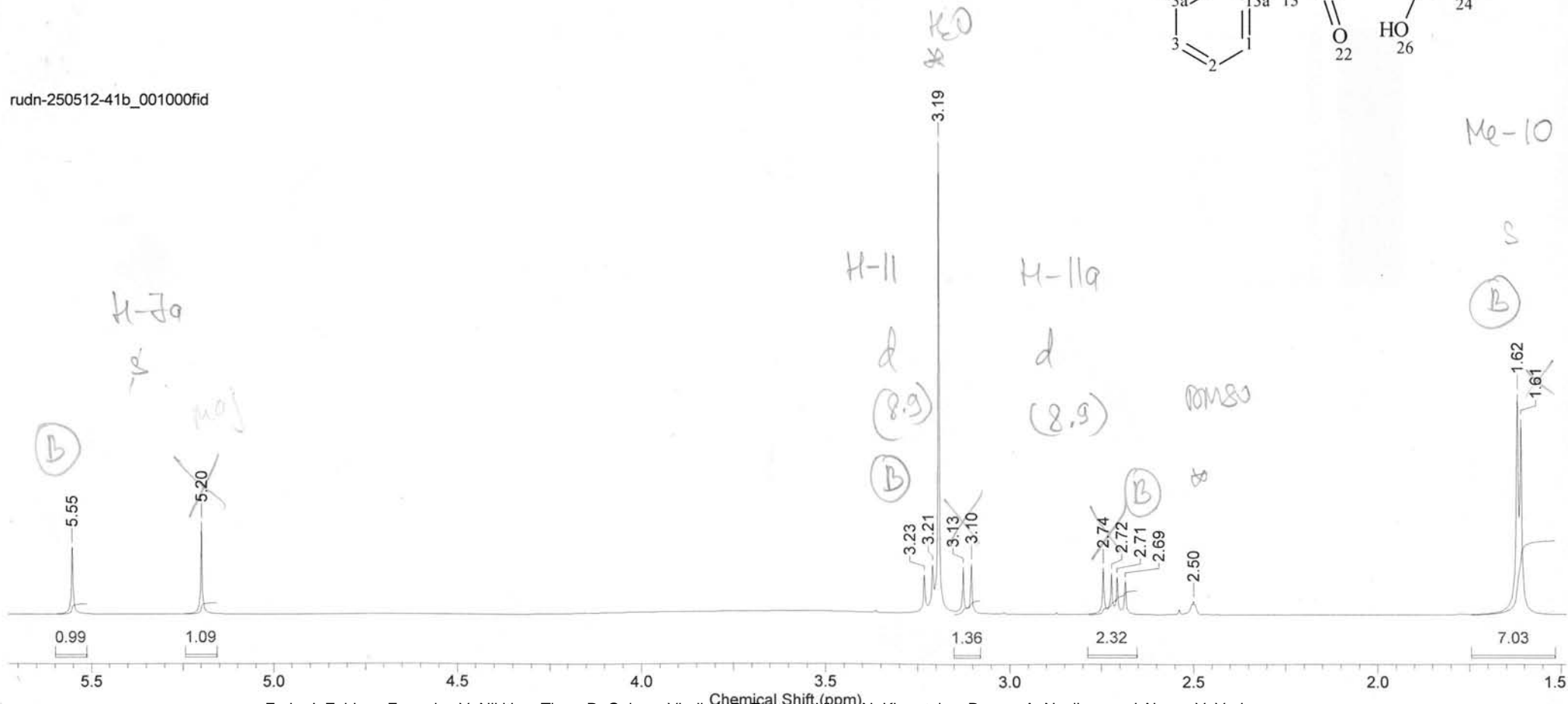


Formula C ₂₀ H ₁₆ N ₂ O ₄		FW 348.3520			
Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		
Date Stamp	21 Jun 2012 13:24:16		Date	21 Jun 2012 13:24:16	
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-41b\rudn-250512-41b_001000fid		Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	20	Origin	spect
Owner	root	Points Count	16384	Original Points Count	16384
SW(cyclical) (Hz)	10416.67	Pulse Sequence	zg	Receiver Gain	128.00
Temperature (degree C)	32.000	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542
				Sweep Width (Hz)	10416.03

Compounds 41Ab/41Bb

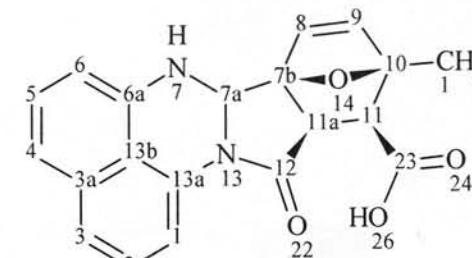
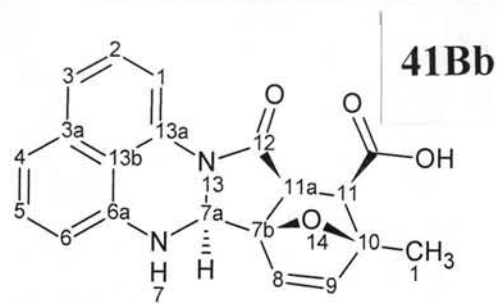
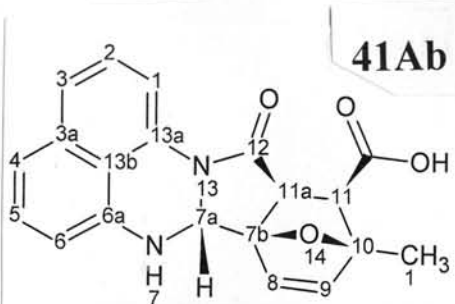


rudn-250512-41b_001000fid



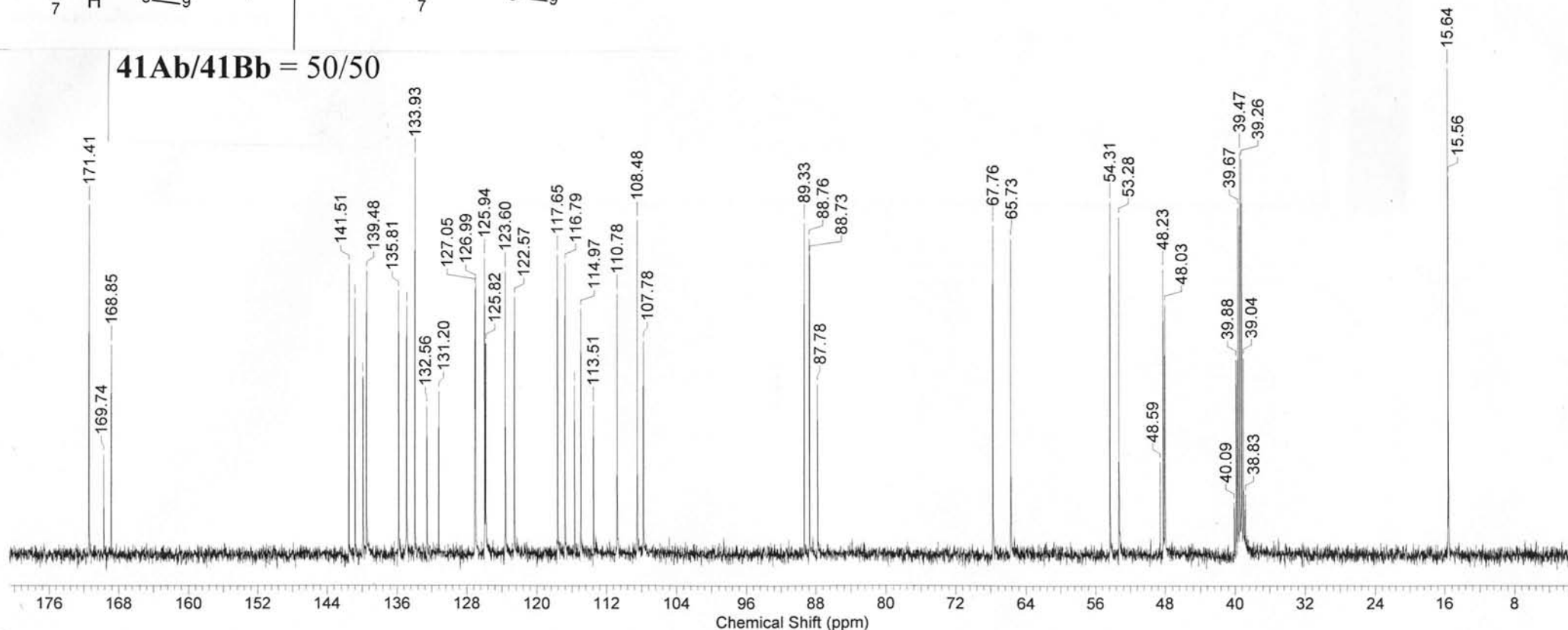
Formula	C ₂₀ H ₁₆ N ₂ O ₄	FW	348.3520
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	21 Jun 2012 13:24:16	
Date Stamp	21 Jun 2012 13:24:16						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-41b-c13dec\rudn-250512-41b-c13dec_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	1123	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zgpg
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6	Spectrum Offset (Hz)	10548.2051
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				



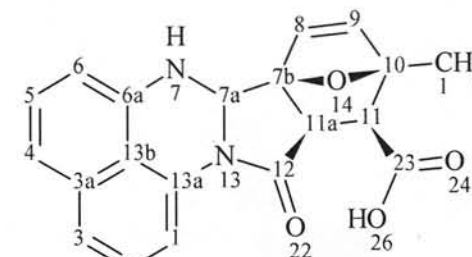
Compounds 41Ab/41Bb

41Ab/41Bb = 50/50

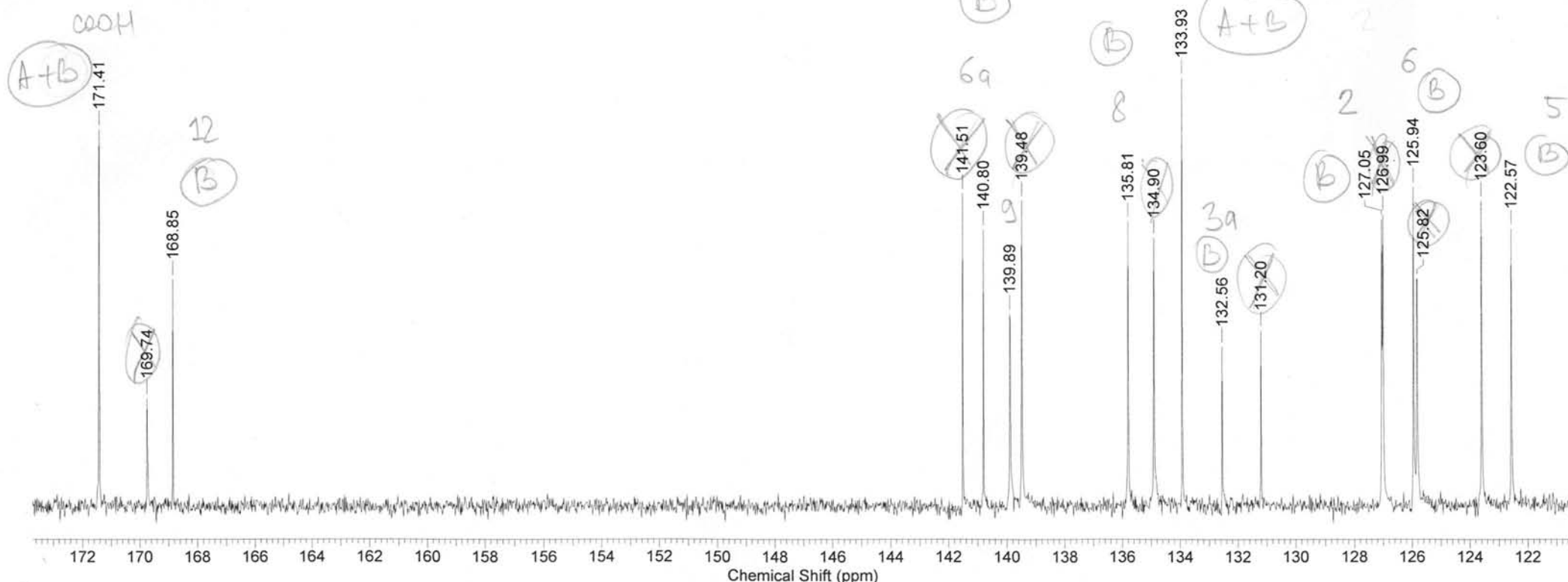


Formula C ₂₀ H ₁₆ N ₂ O ₄	FW 348.3520			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 21 Jun 2012 13:24:16		
Date Stamp 21 Jun 2012 13:24:16				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-41b-c13dec\rudn-250512-41b-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 1123	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10548.2051	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compounds 41Ab/41Bb

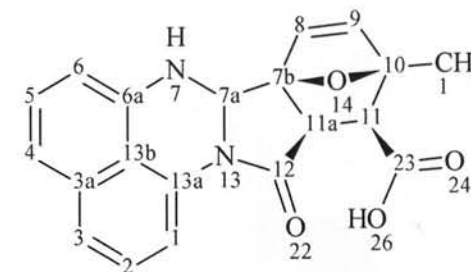


rudn-250512-41b-c13dec_001000fid

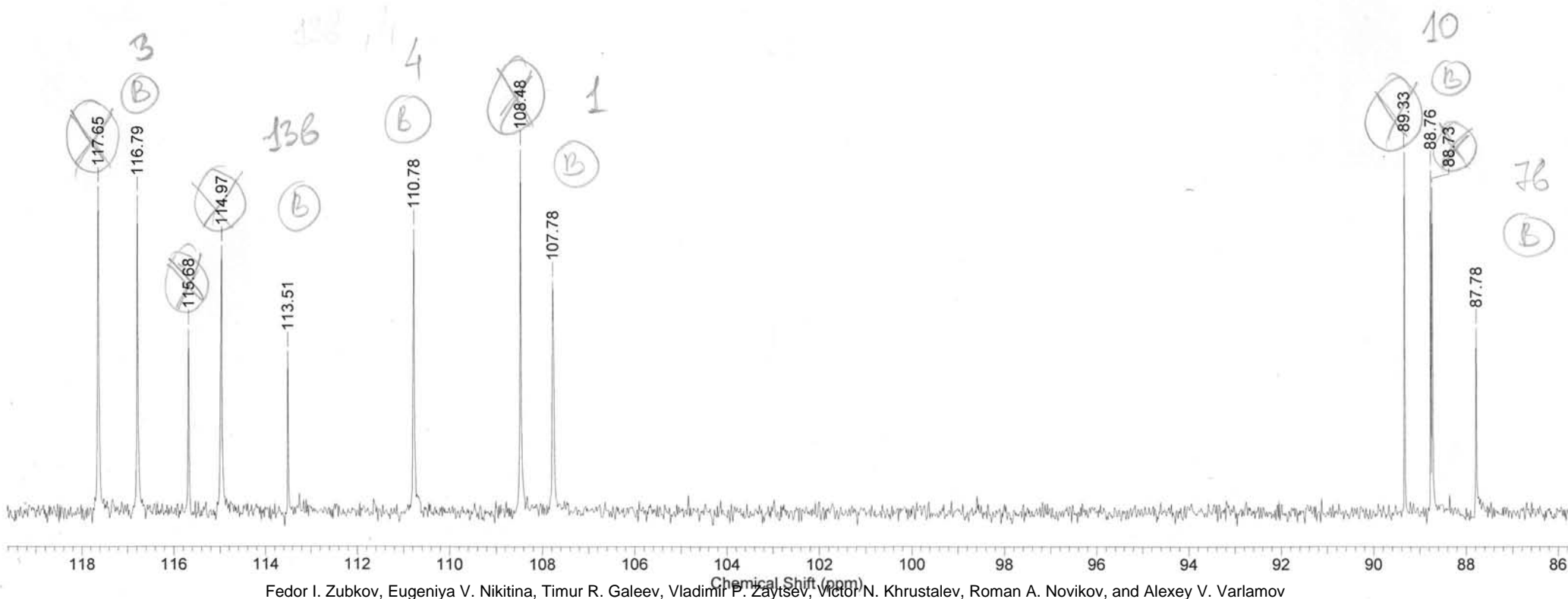


Formula C ₂₀ H ₁₆ N ₂ O ₄		FW 348.3520		
Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	
Date Stamp	21 Jun 2012 13:24:16		Date	21 Jun 2012 13:24:16
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-41b-c13dec\rudn-250512-41b-c13dec_001000fid			
Frequency (MHz)	100.62	Nucleus	13C	
Original Points Count	16384	Number of Transients	1123	
Receiver Gain	32768.00	Owner	root	
Sweep Width (Hz)	29409.97	Points Count	16384	
		SW(cyclical) (Hz)	29411.77	
		Solvent	DMSO-d6	
		Pulse Sequence	zgpg	
		Spectrum Offset (Hz)	10548.2051	
		Temperature (degree C)	27.000	

Compounds 41Ab/41Bb



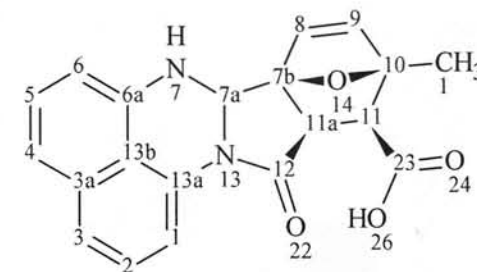
rudn-250512-41b-c13dec_001000fid



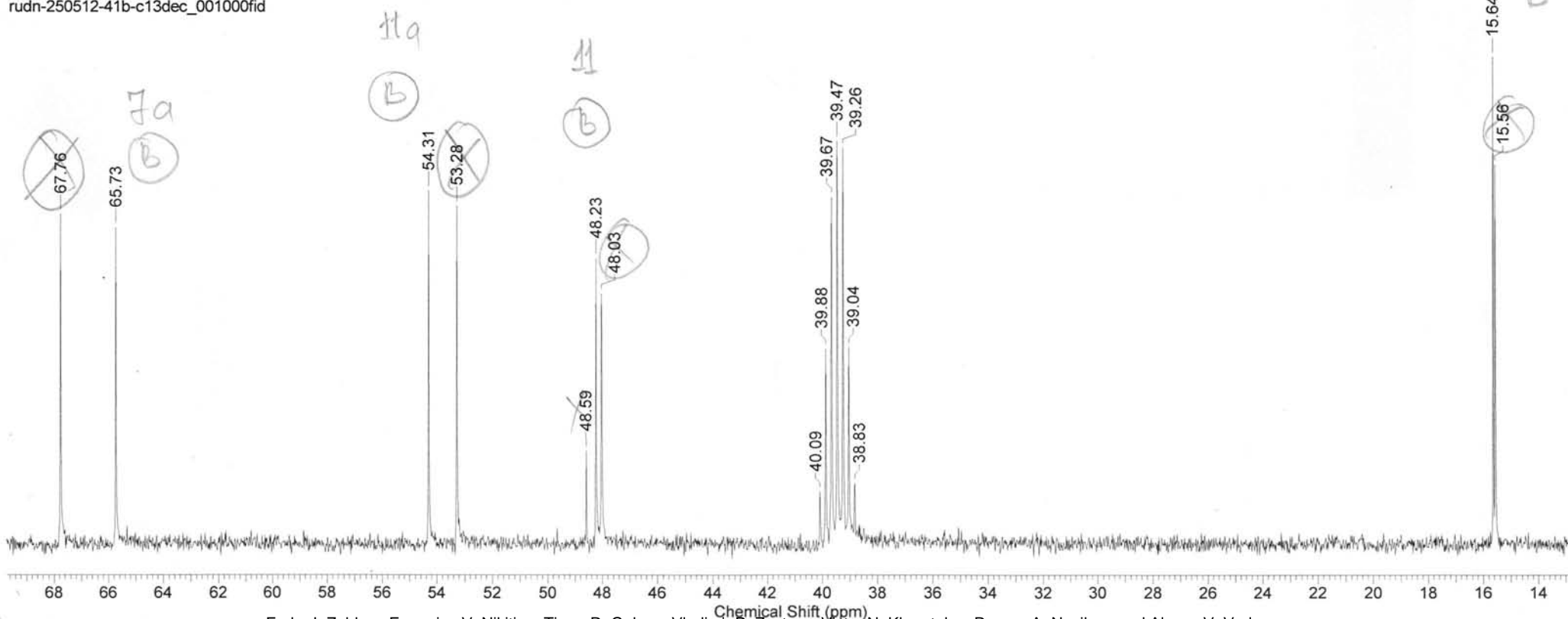
Formula	C ₂₀ H ₁₆ N ₂ O ₄	FW	348.3520
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	21 Jun 2012 13:24:16	
Date Stamp	21 Jun 2012 13:24:16						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-41b-c13dec\rudn-250512-41b-c13dec_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	1123	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zgpg
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6	Spectrum Offset (Hz)	10548.2051
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				

Compounds 41Ab/41Bb



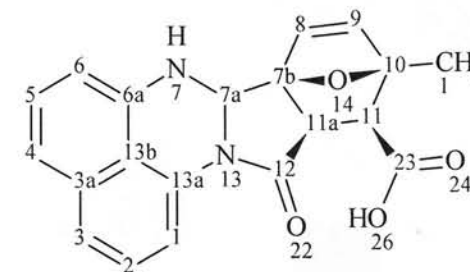
rudn-250512-41b-c13dec_001000fid



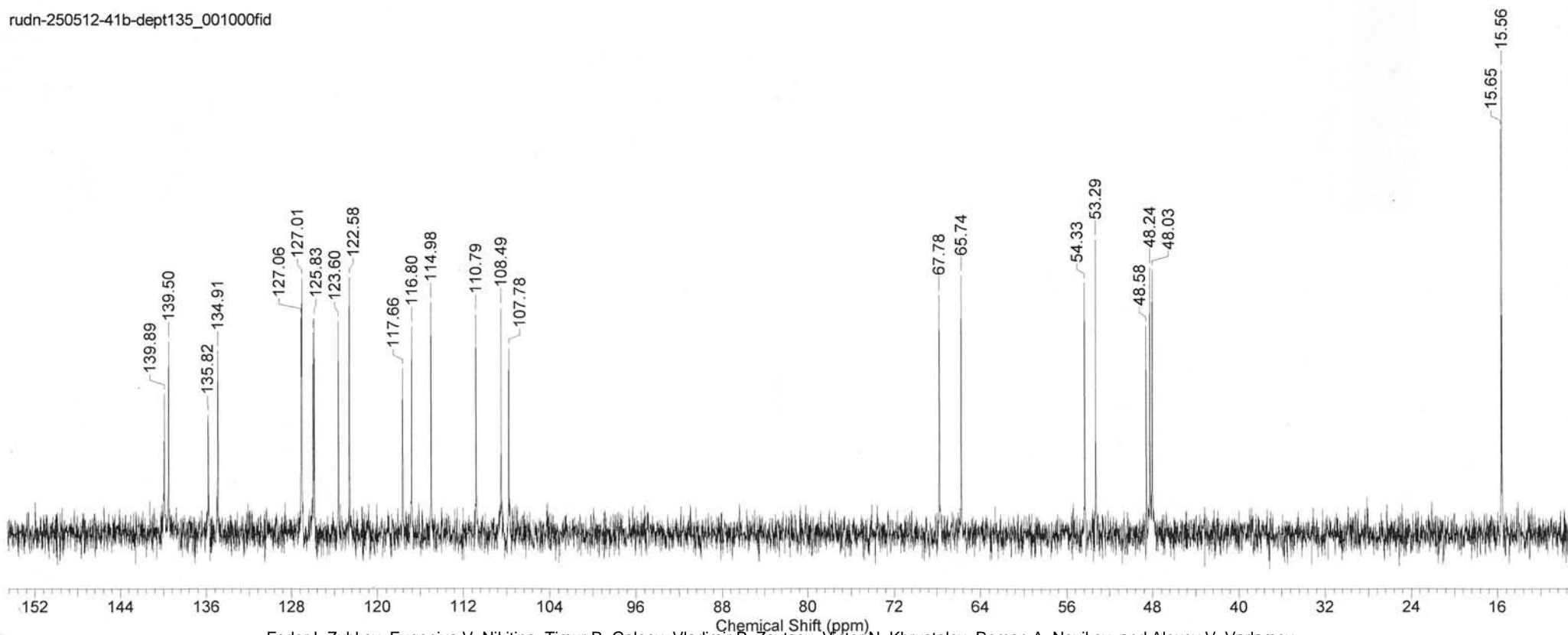
Formula	C ₂₀ H ₁₆ N ₂ O ₄	FW	348.3520
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	21 Jun 2012 13:47:44
Date Stamp	21 Jun 2012 13:47:44				
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-41b-dept135\rudn-250512-41b-dept135_001000fid				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	641
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000	Spectrum Offset (Hz)	9099.0557

Compounds 41Ab/41Bb

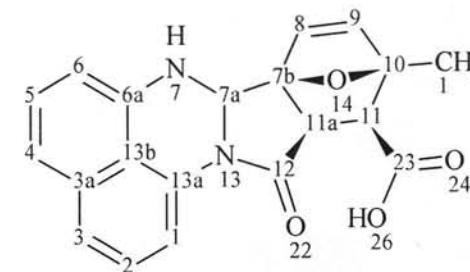


rudn-250512-41b-dept135_001000fid

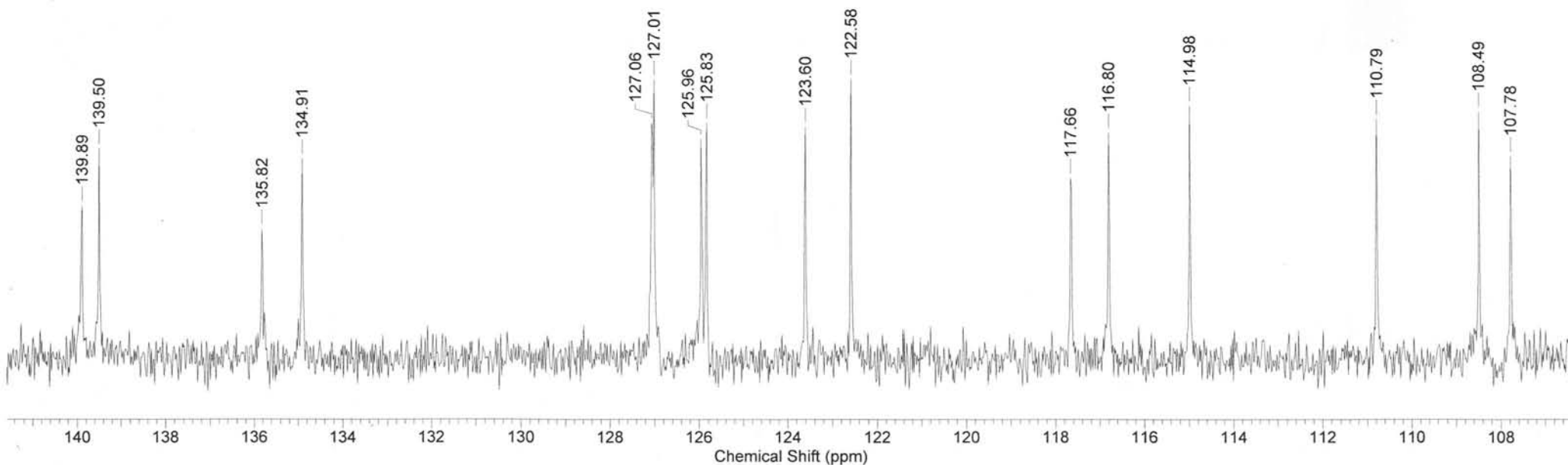


Formula C ₂₀ H ₁₆ N ₂ O ₄	FW 348.3520			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 21 Jun 2012 13:47:44		
Date Stamp 21 Jun 2012 13:47:44				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-41b-dept135\rudn-250512-41b-dept135_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 641	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence dept135	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 9099.0557	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compounds 41Ab/41Bb



rudn-250512-41b-dept135_001000fid

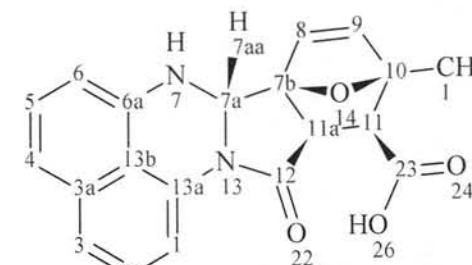


unpurified isomer

12.05.2012 19:43:05

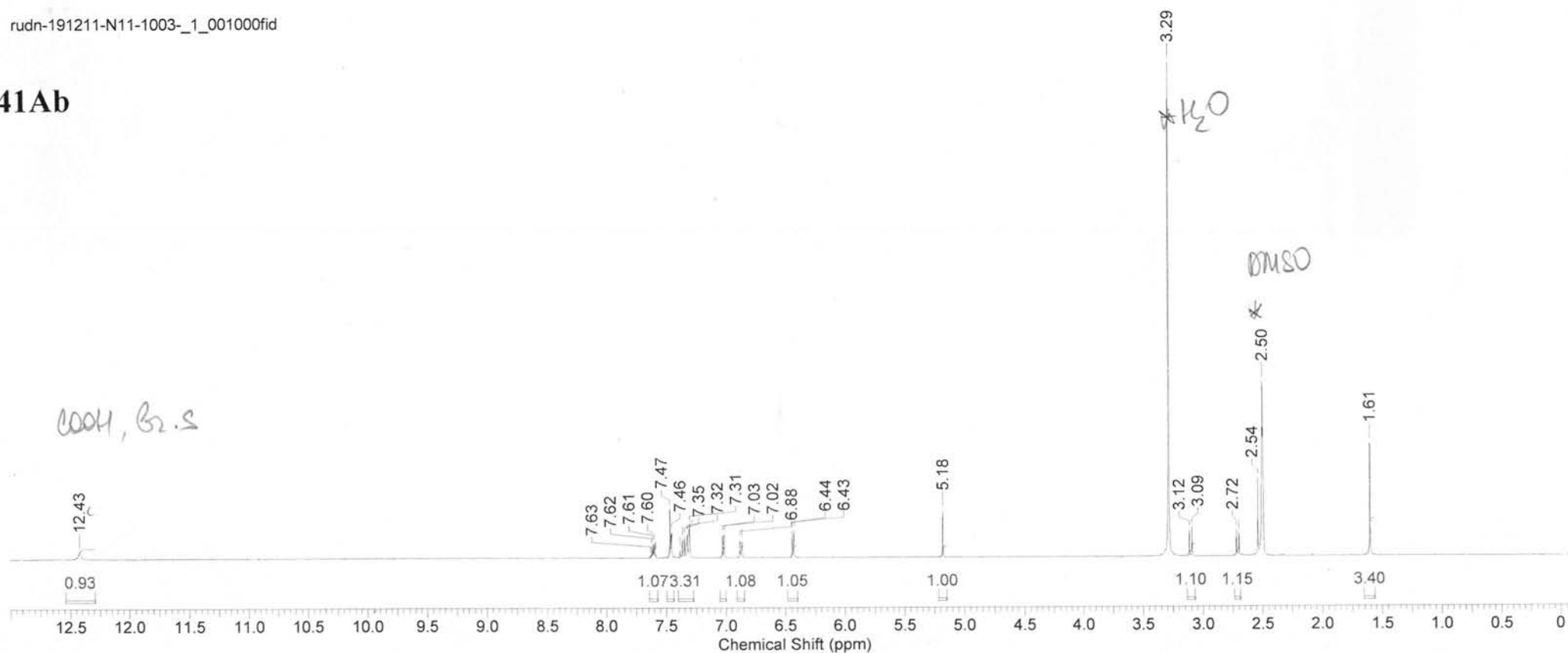
Formula C ₂₀ H ₁₆ N ₂ O ₄		FW 348.3520	
Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400
Date Stamp	30 Dec 2011 11:01:20	File Name	D:\NMR\19.12.11 (Рома)\rudn-191211-N11-1003-1\rudn-191211-N11-1003-1_001000fid
Frequency (MHz)	400.14	Nucleus	1H
Original Points Count	16384	Number of Transients	96
Receiver Gain	1024.00	Origin	spect
Sweep Width (Hz)	10416.03	Owner	root
		Points Count	16384
		Pulse Sequence	zg
		Solvent	DMSO-d6
		Spectrum Offset (Hz)	2712.0542
		Temperature (degree C)	32.000

Compound 41Ab



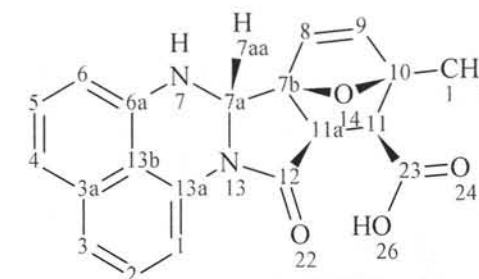
rudn-191211-N11-1003-1_001000fid

41Ab



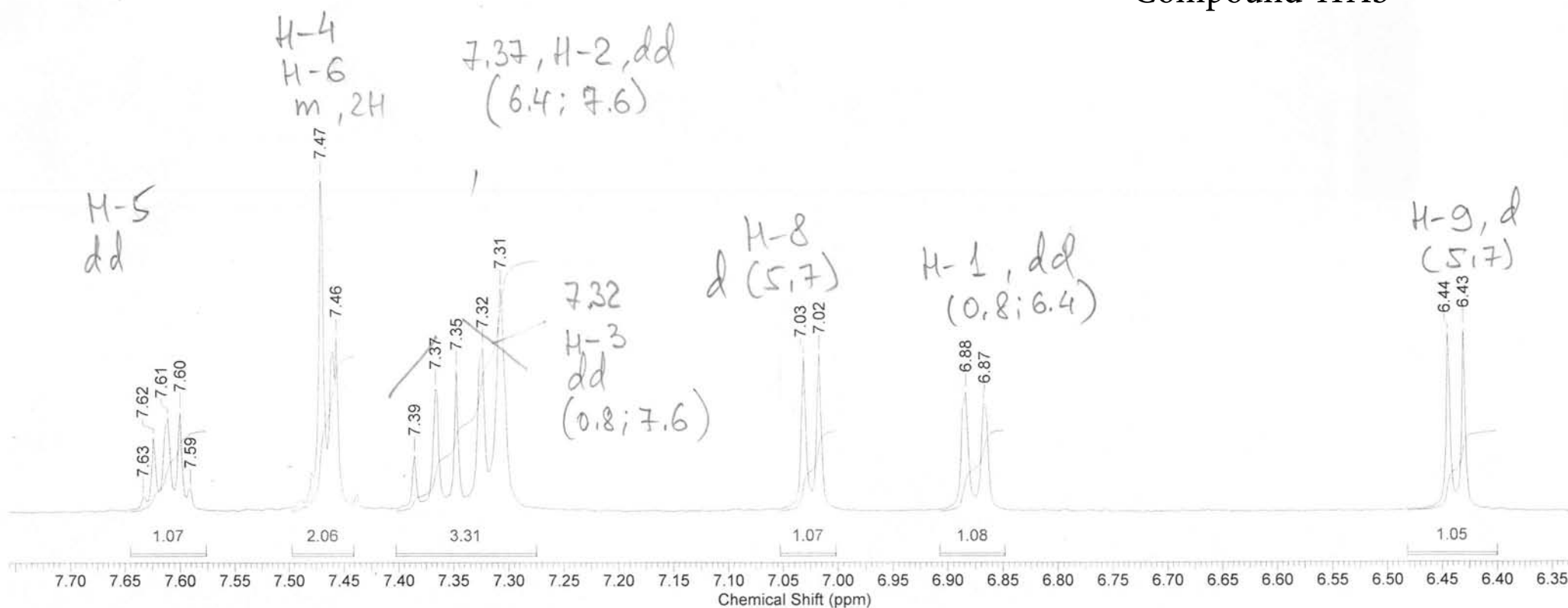
Formula C₂₀H₁₆N₂O₄ FW 348.3520

Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	30 Dec 2011 11:01:20
Date Stamp	30 Dec 2011 11:01:20	File Name	D:\NMR\19.12.11 (Роман)\rudn-191211-N11-1003-_1\rudn-191211-N11-1003-_1_001000fid		
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	96
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	1024.00	SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6
Sweep Width (Hz)	10416.03	Temperature (degree C)	32.000	Pulse Sequence	zg
				Spectrum Offset (Hz)	2712.0542



Compound 41Ab

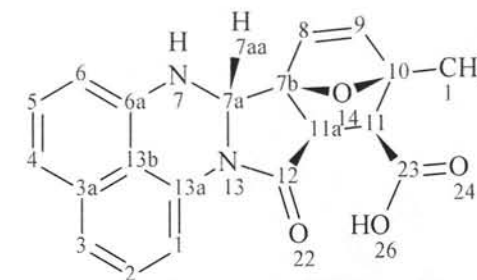
rudn-191211-N11-1003-_1_001000fid



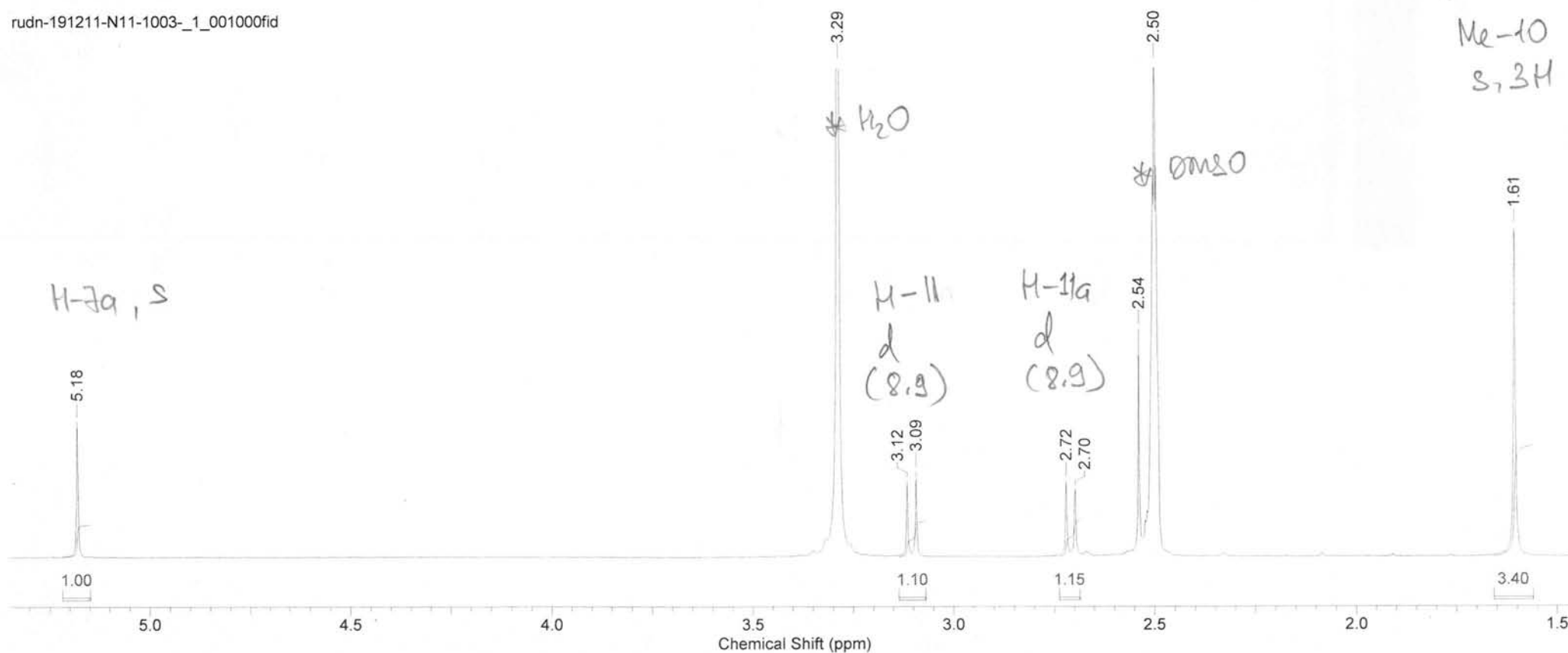
Formula $C_{20}H_{16}N_2O_4$ FW 348.3520

Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	30 Dec 2011 11:01:20
Date Stamp	30 Dec 2011 11:01:20	File Name	D:\NMR\19.12.11 (Роман)\rudn-191211-N11-1003-_1\rudn-191211-N11-1003-_1_001000fid		
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	96
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	1024.00	SW(cyclical) (Hz)	10416.67	Pulse Sequence	zg
Sweep Width (Hz)	10416.03	Temperature (degree C)	32.000	Spectrum Offset (Hz)	2712.0542

Compound 41Ab



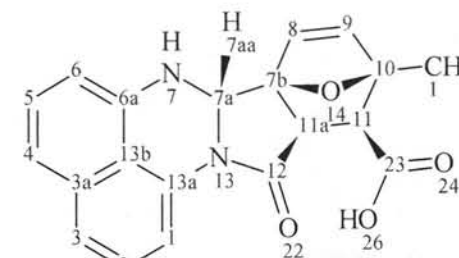
rudn-191211-N11-1003-_1_001000fid



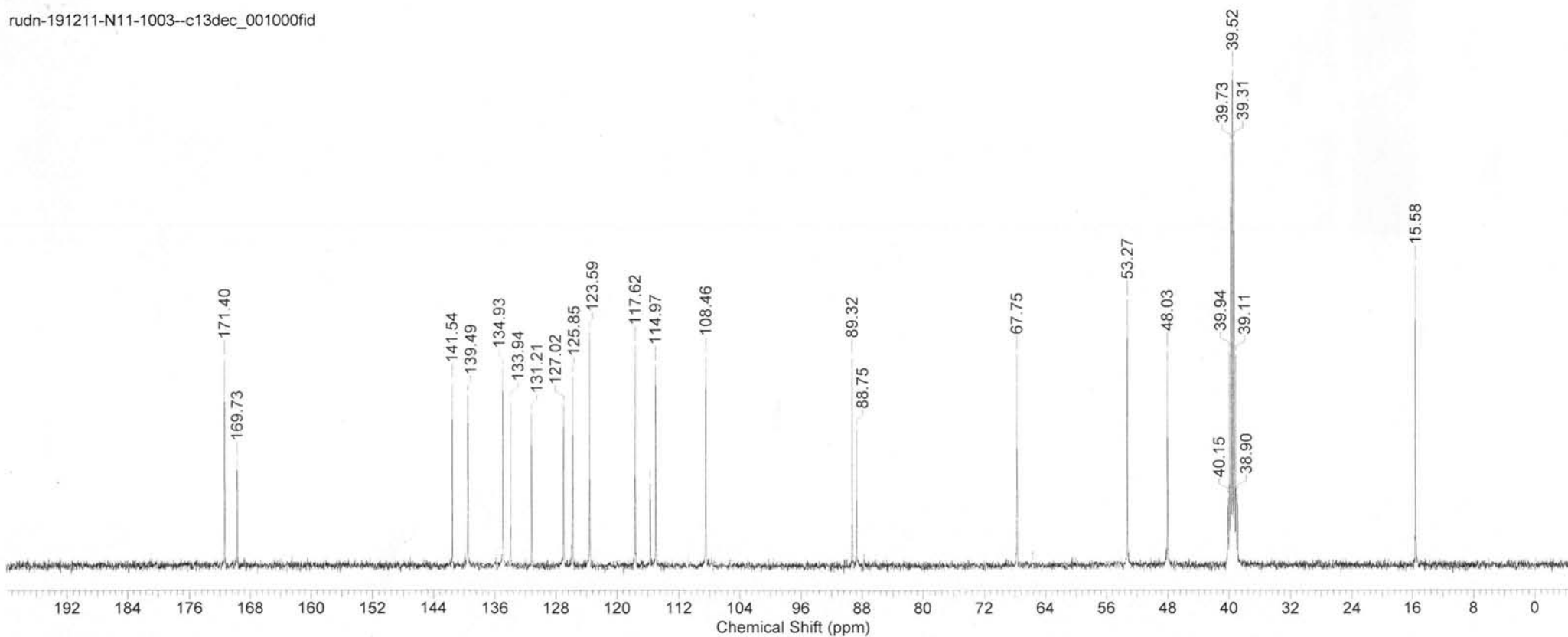
Formula C₂₀H₁₆N₂O₄ FW 348.3520

Acquisition Time (sec)	0.5243	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	29 Dec 2011 18:57:04
Date Stamp	29 Dec 2011 18:57:04				
File Name	D:\NMR\19.12.11 (Poma)\rudn-191211-N11-1003--c13dec\rudn-191211-N11-1003--c13dec_001000fid			Frequency (MHz)	100.62
Nucleus	13C	Number of Transients	7000	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zgpg
SW(cyclical) (Hz)	31250.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	9099.1699
Temperature (degree C)	27.000			Sweep Width (Hz)	31248.09

Compound 41Ab



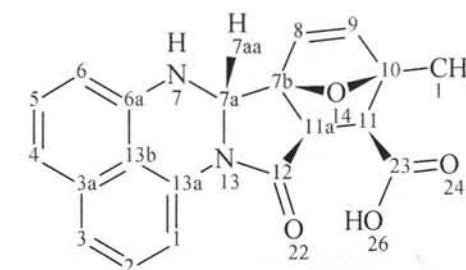
rudn-191211-N11-1003--c13dec_001000fid



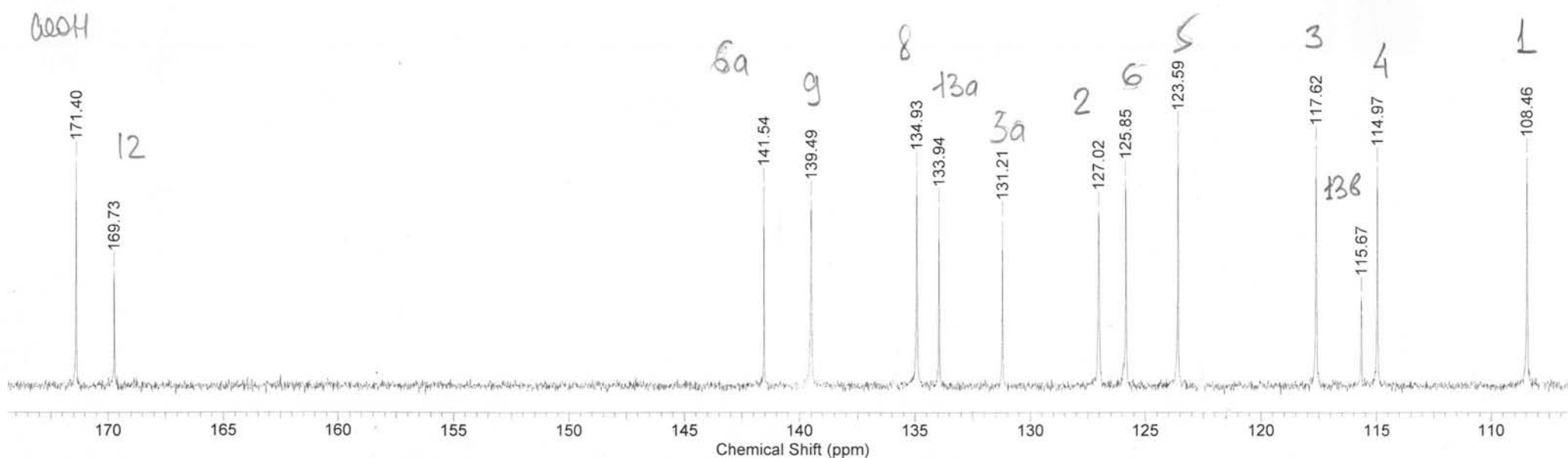
Formula $C_{20}H_{16}N_2O_4$ FW 348.3520

Acquisition Time (sec)	0.5243	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	29 Dec 2011 18:57:04
Date Stamp	29 Dec 2011 18:57:04				
File Name	D:\NMR\19.12.11 (Poma)\rudn-191211-N11-1003--c13dec\rudn-191211-N11-1003--c13dec_001000fid			Frequency (MHz)	100.62
Nucleus	13C	Number of Transients	7000	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zgpg
SW(cyclical) (Hz)	31250.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	9099.1699
Temperature (degree C)	27.000			Sweep Width (Hz)	31248.09

Compound 41Ab



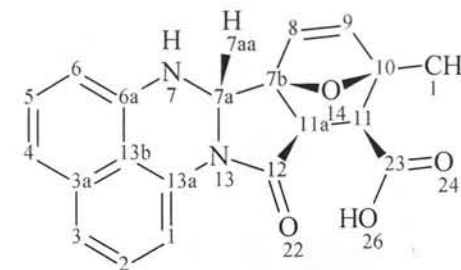
rudn-191211-N11-1003--c13dec_001000fid



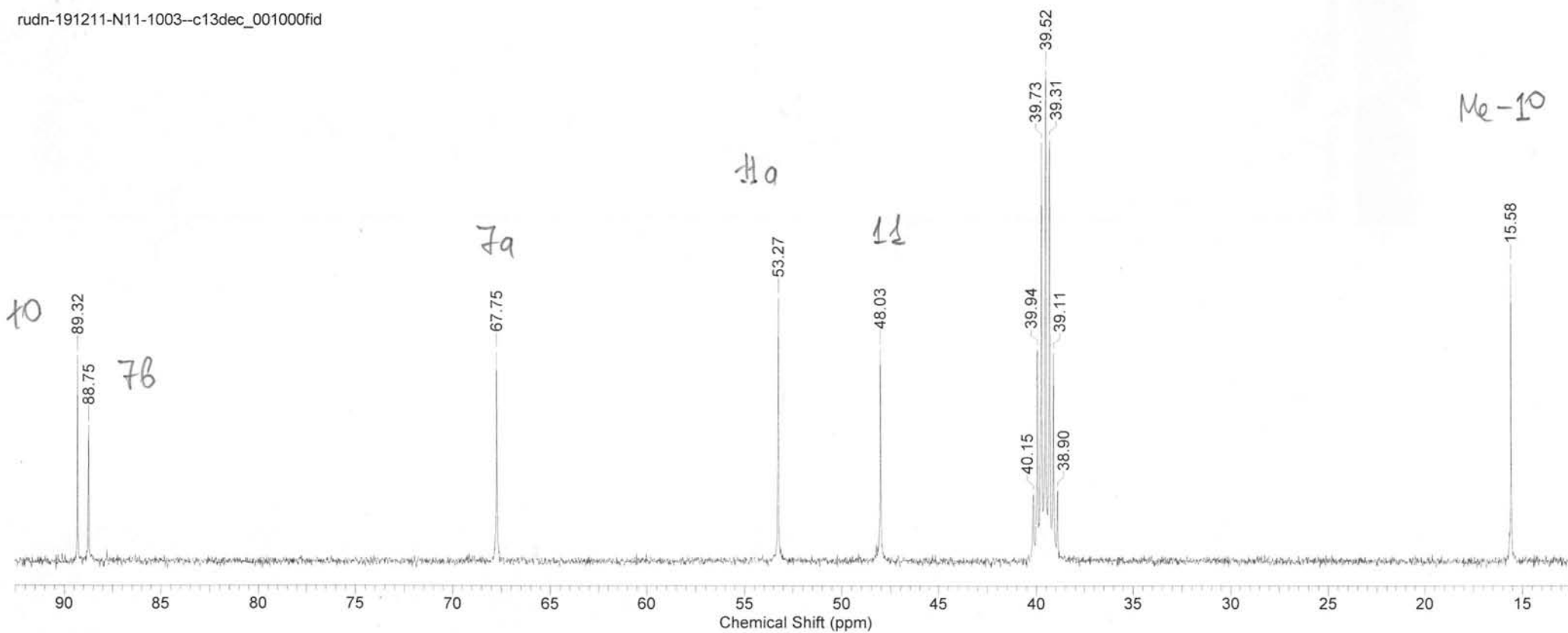
Formula	C ₂₀ H ₁₆ N ₂ O ₄	FW	348.3520
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Acquisition Time (sec)	0.5243	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	29 Dec 2011 18:57:04
Date Stamp	29 Dec 2011 18:57:04				
File Name	D:\NMR\19.12.11 (Poma)\rudn-191211-N11-1003--c13dec\rudn-191211-N11-1003--c13dec_001000fid			Frequency (MHz)	100.62
Nucleus	13C	Number of Transients	7000	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zgpg
SW(cyclical) (Hz)	31250.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	9099.1699
Temperature (degree C)	27.000			Sweep Width (Hz)	31248.09

Compound 41Ab



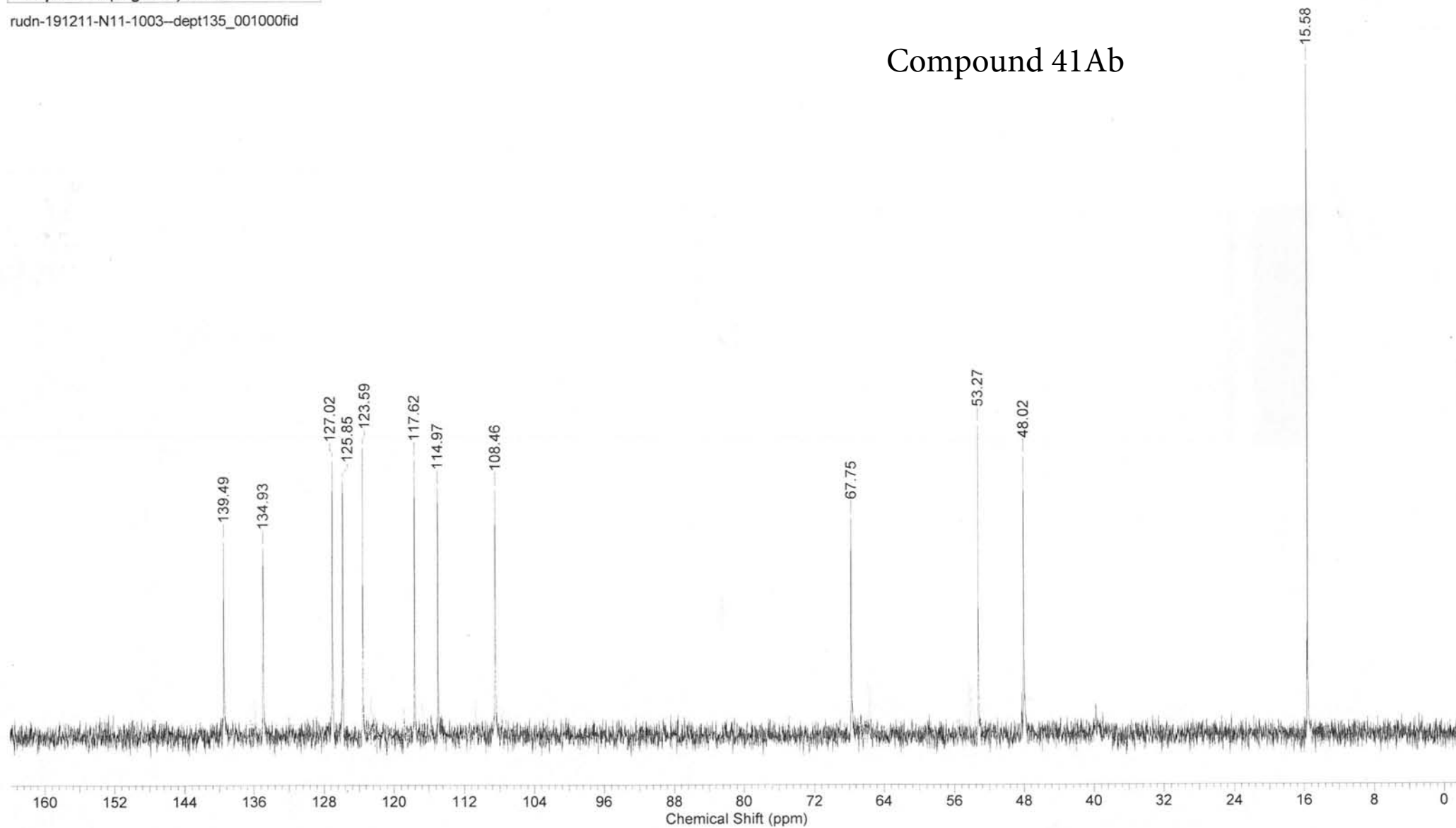
rudn-191211-N11-1003--c13dec_001000fid



Acquisition Time (sec)	0.5243	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	30 Dec 2011 00:08:32	
Date Stamp	30 Dec 2011 00:08:32						
File Name	D:\NMR\19.12.11 (Poma)\rudn-191211-N11-1003--dept135\rudn-191211-N11-1003--dept135_001000fid			Frequency (MHz)	100.62		
Nucleus	13C	Number of Transients	5000	Origin	spect	Original Points Count	16384
Owner	root	Points Count	16384	Pulse Sequence	dept135	Receiver Gain	32768.00
SW(cyclical) (Hz)	31250.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	9099.1699	Sweep Width (Hz)	31248.09
Temperature (degree C)	27.000						

rudn-191211-N11-1003--dept135_001000fid

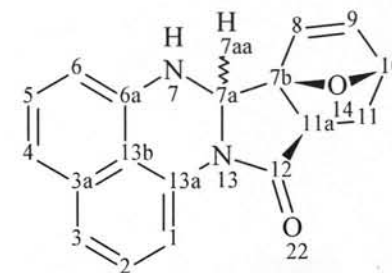
Compound 41Ab



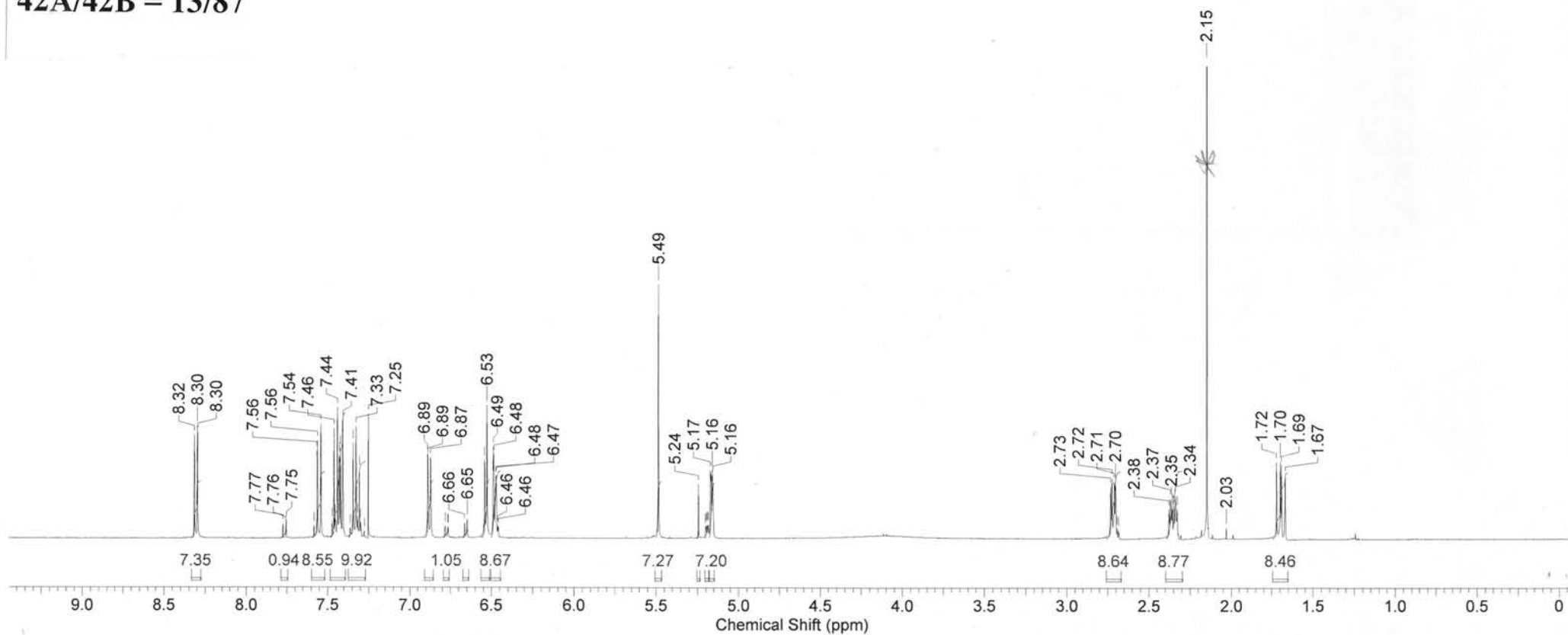
Formula	C ₁₈ H ₁₄ N ₂ O ₂	FW	290.3160
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Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	11 Jul 2012 13:37:04		
Date Stamp	11 Jul 2012 13:37:04						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-42-42_61\rudn-060712-42-42_61_001000fid						
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	20	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zg
Receiver Gain	512.00	SW(cyclical) (Hz)	10204.08	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2602.0486
Sweep Width (Hz)	10203.46	Temperature (degree C)	27.000				

Compounds 42A/42B

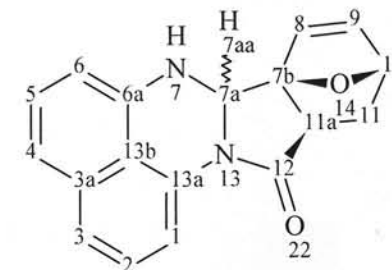


42A/42B = 13/87

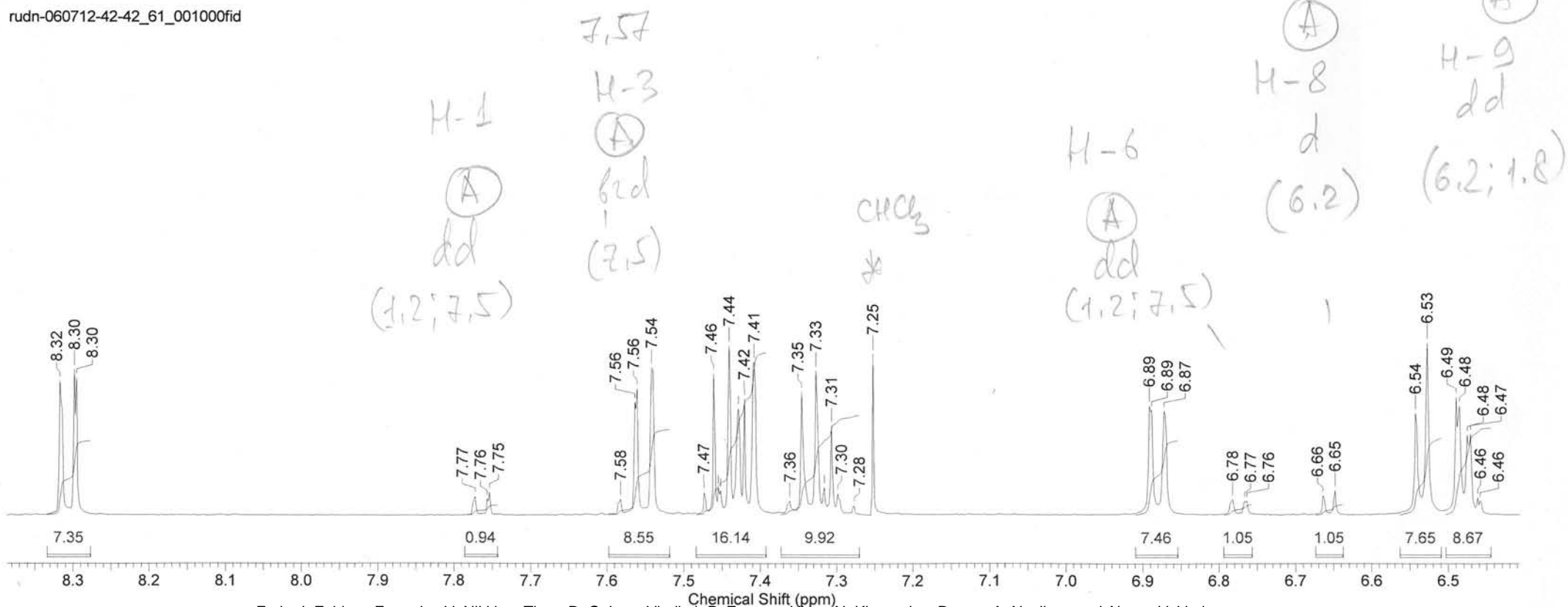


Formula	C ₁₈ H ₁₄ N ₂ O ₂	FW	290.3160
Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400
Date Stamp	11 Jul 2012 13:37:04	Date	11 Jul 2012 13:37:04
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-42-42_61\rudn-060712-42-42_61_001000fid		
Frequency (MHz)	400.14	Nucleus	1H
Original Points Count	16384	Number of Transients	20
Receiver Gain	512.00	Owner	root
Sweep Width (Hz)	10203.46	Points Count	16384
		Pulse Sequence	zg
		Solvent	CHLOROFORM-d
		Spectrum Offset (Hz)	2602.0486
		Temperature (degree C)	27.000

Compounds 42A/42B



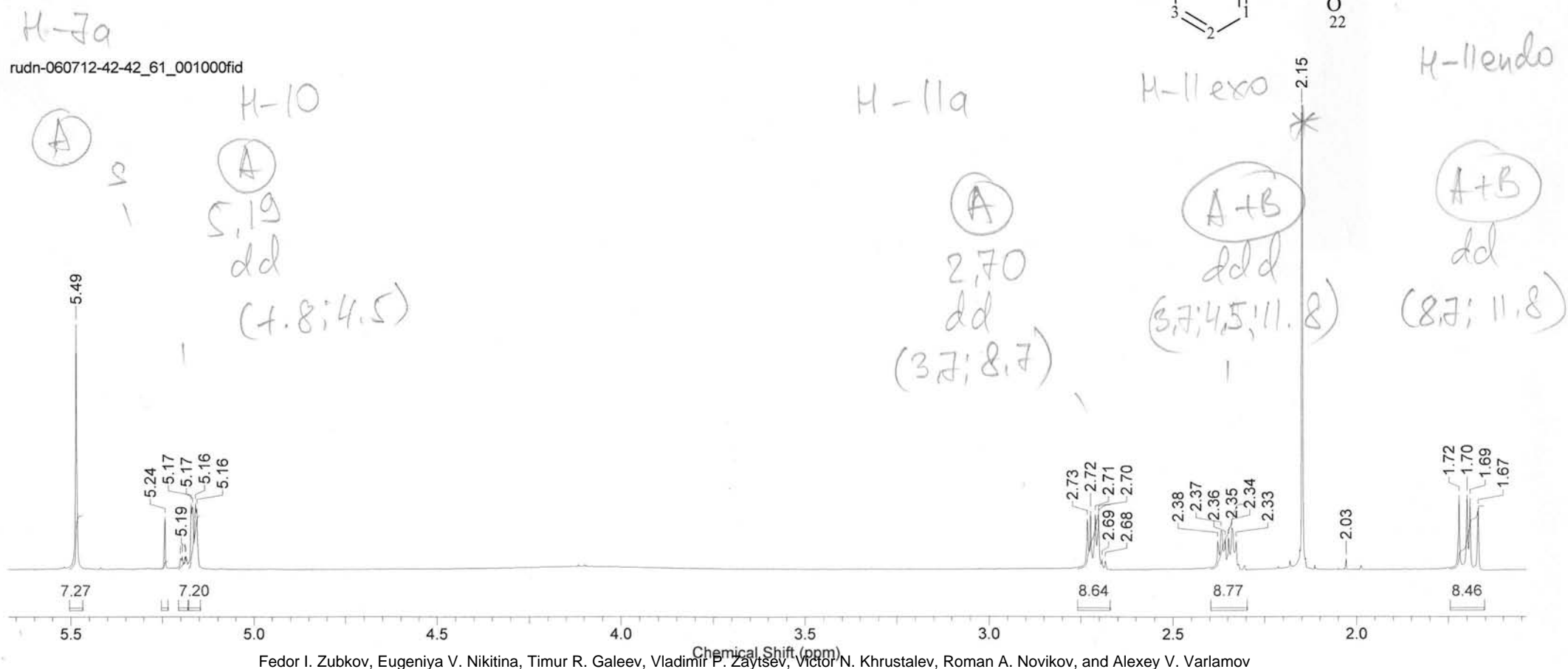
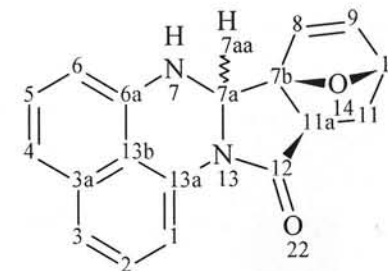
rudn-060712-42-42_61_001000fid



Formula	C ₁₈ H ₁₄ N ₂ O ₂	FW	290.3160
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Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	11 Jul 2012 13:37:04	
Date Stamp	11 Jul 2012 13:37:04						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-42-42_61\rudn-060712-42-42_61_001000fid						
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	20	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zg
Receiver Gain	512.00	SW(cyclical) (Hz)	10204.08	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2602.0486
Sweep Width (Hz)	10203.46	Temperature (degree C)	27.000				

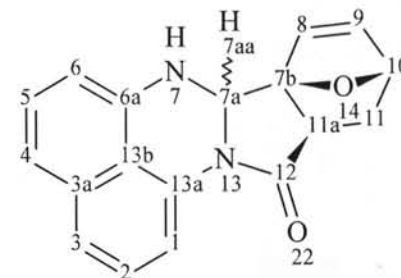
Compounds 42A/42B



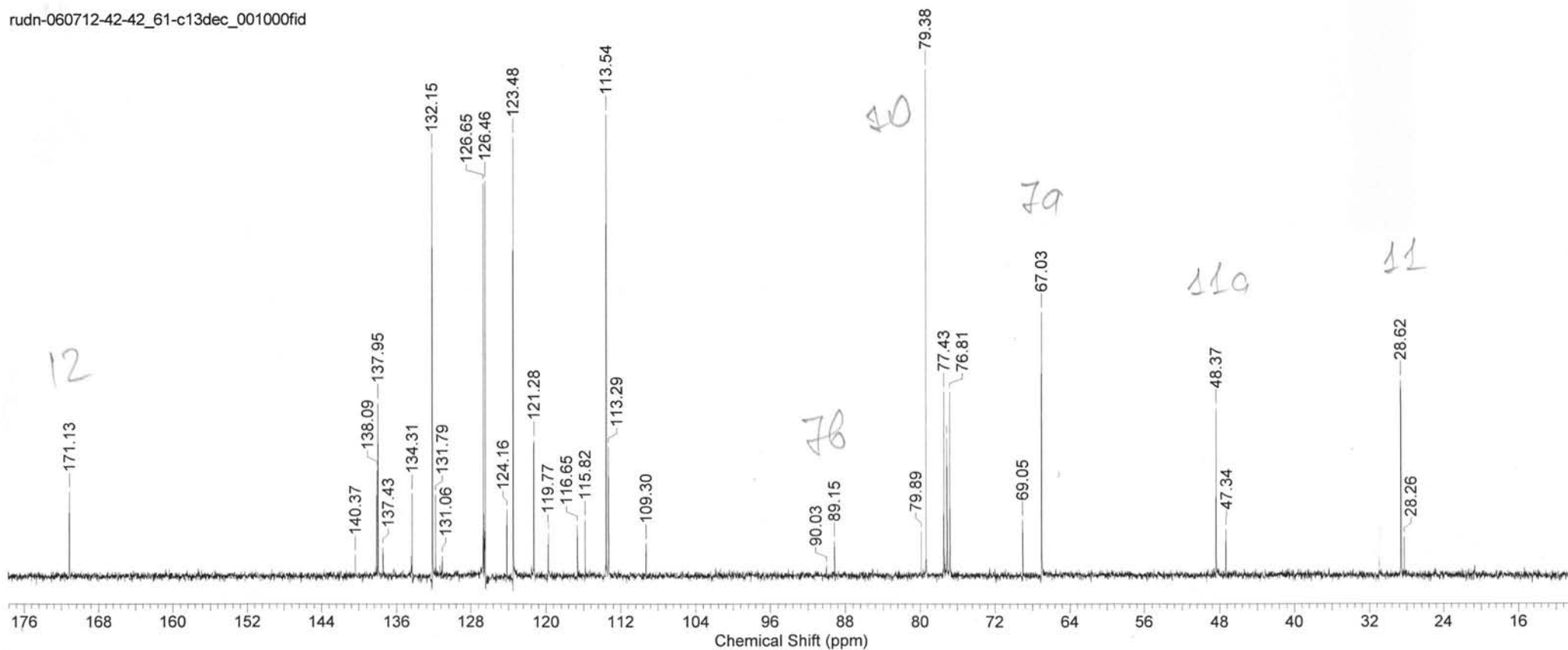
Formula	C ₁₈ H ₁₄ N ₂ O ₂	FW	290.3160
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	11 Jul 2012 13:37:04
Date Stamp	11 Jul 2012 13:37:04	File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-42-42_61-c13dec\rudn-060712-42-42_61-c13dec_001000fid		
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	1624
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	CHLOROFORM-d
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000	Spectrum Offset (Hz)	9632.4561

Compounds 42A/42B

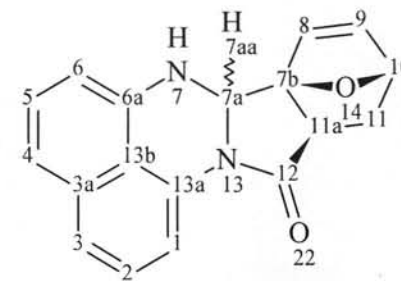


rudn-060712-42-42_61-c13dec_001000fid

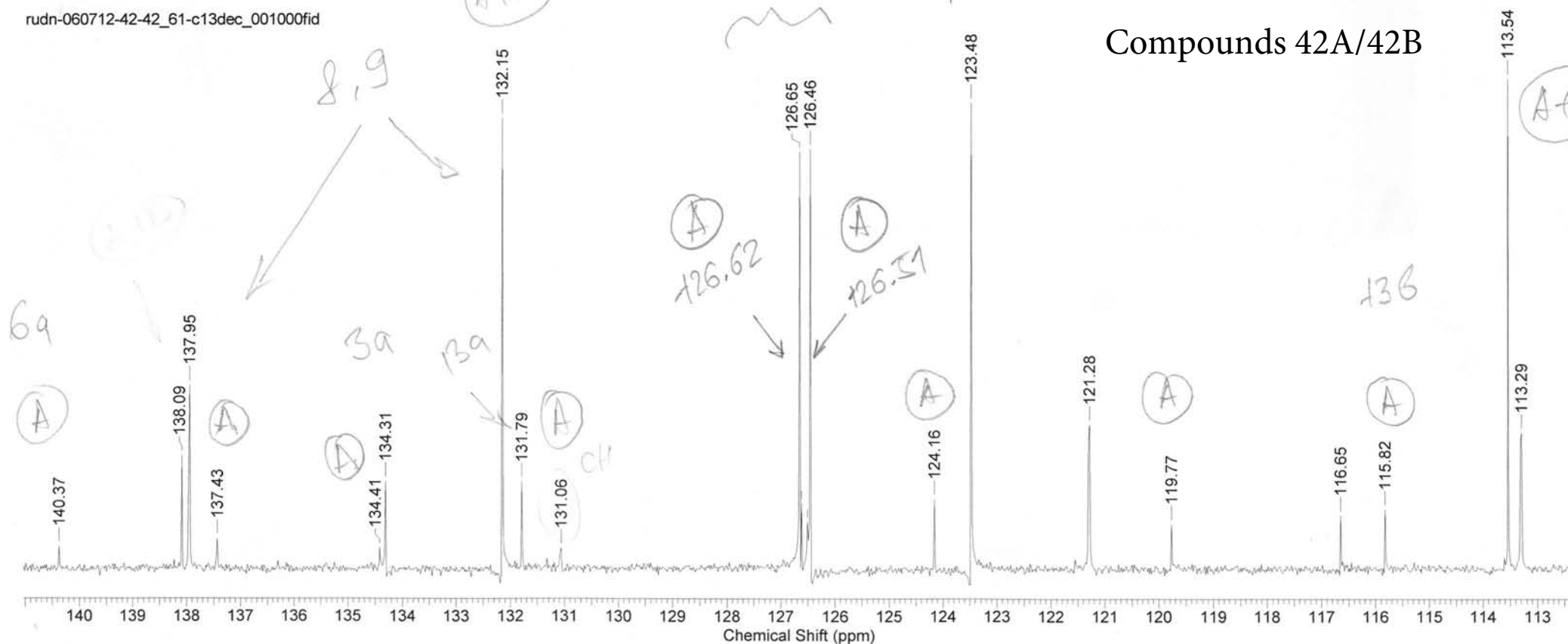


Formula	C ₁₈ H ₁₄ N ₂ O ₂	FW	290.3160
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	11 Jul 2012 13:37:04
Date Stamp	11 Jul 2012 13:37:04	File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-42-42_61-c13dec\rudn-060712-42-42_61-c13dec_001000fid		
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	1624
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	CHLOROFORM-d
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000	Spectrum Offset (Hz)	9632.4561



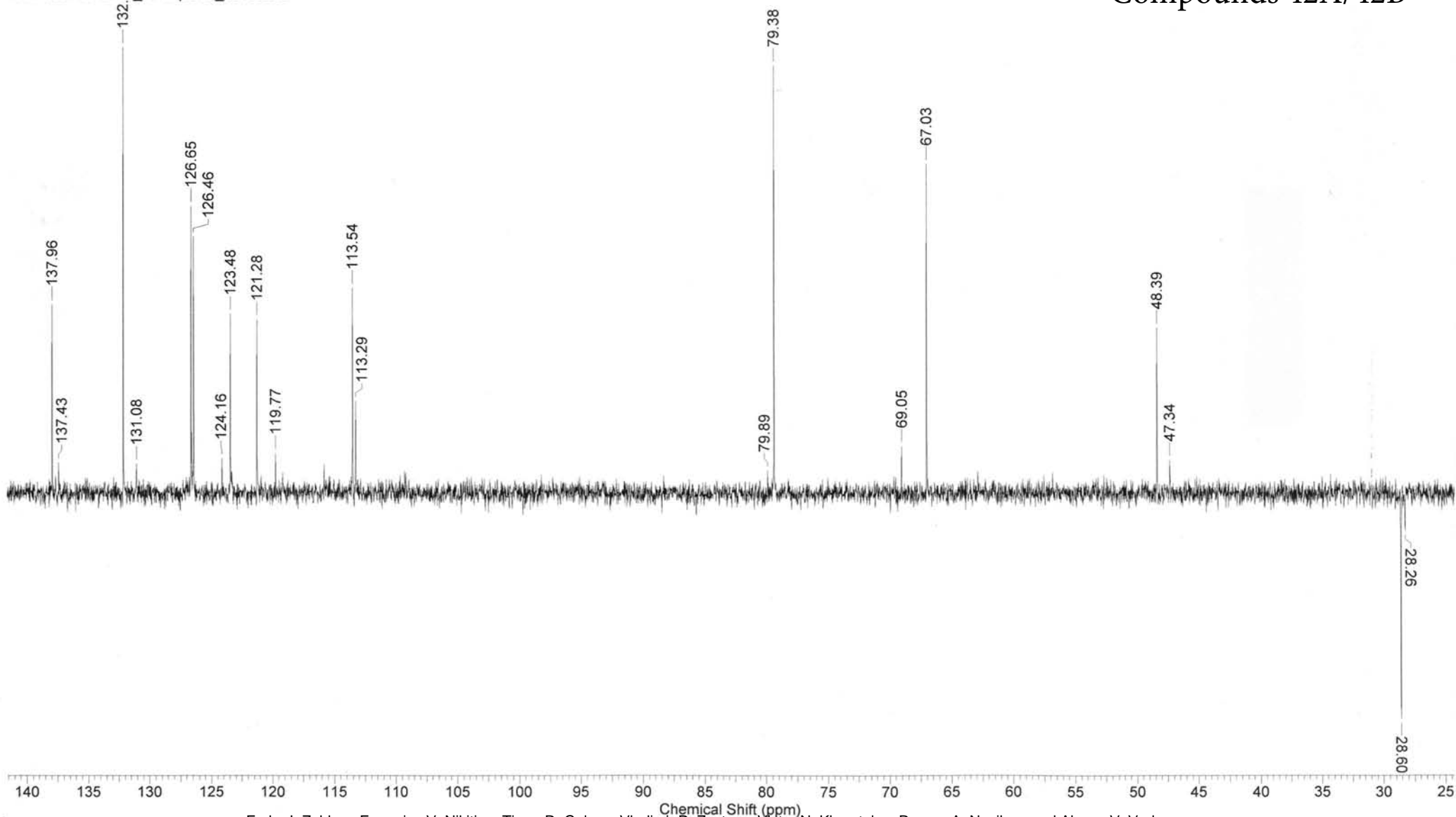
rudn-060712-42-42_61-c13dec_001000fid



Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	11 Jul 2012 14:28:16	
Date Stamp	11 Jul 2012 14:28:16	File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-42-42_61-dept135\rudn-060712-42-42_61-dept135_001000fid				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	948	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	dept135
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9632.4453
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				

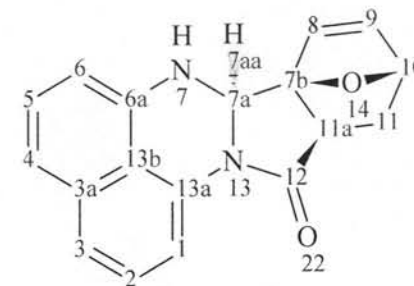
rudn-060712-42-42_61-dept135_001000fid

Compounds 42A/42B



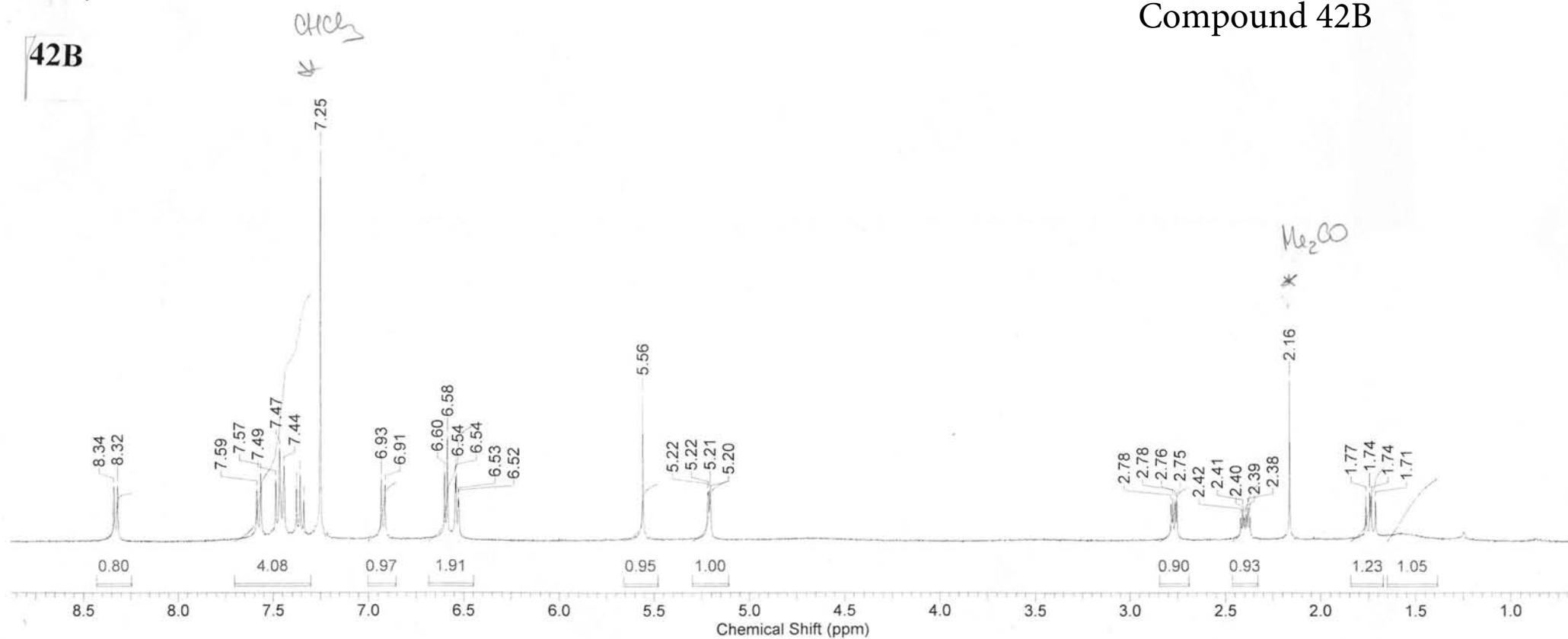
Formula C₁₈H₁₄N₂O₂ FW 290.3160

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	14 Dec 2011 10:20:06	Date Stamp	14 Dec 2011 14:54:45
File Name	D:\NMR\12.12.11\FZ2125-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8
Origin	ECS 400	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	46.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2398.6931	Sweep Width (Hz)	7503.00
Temperature (degree C)	23.100						



FZ2125-1.jdf

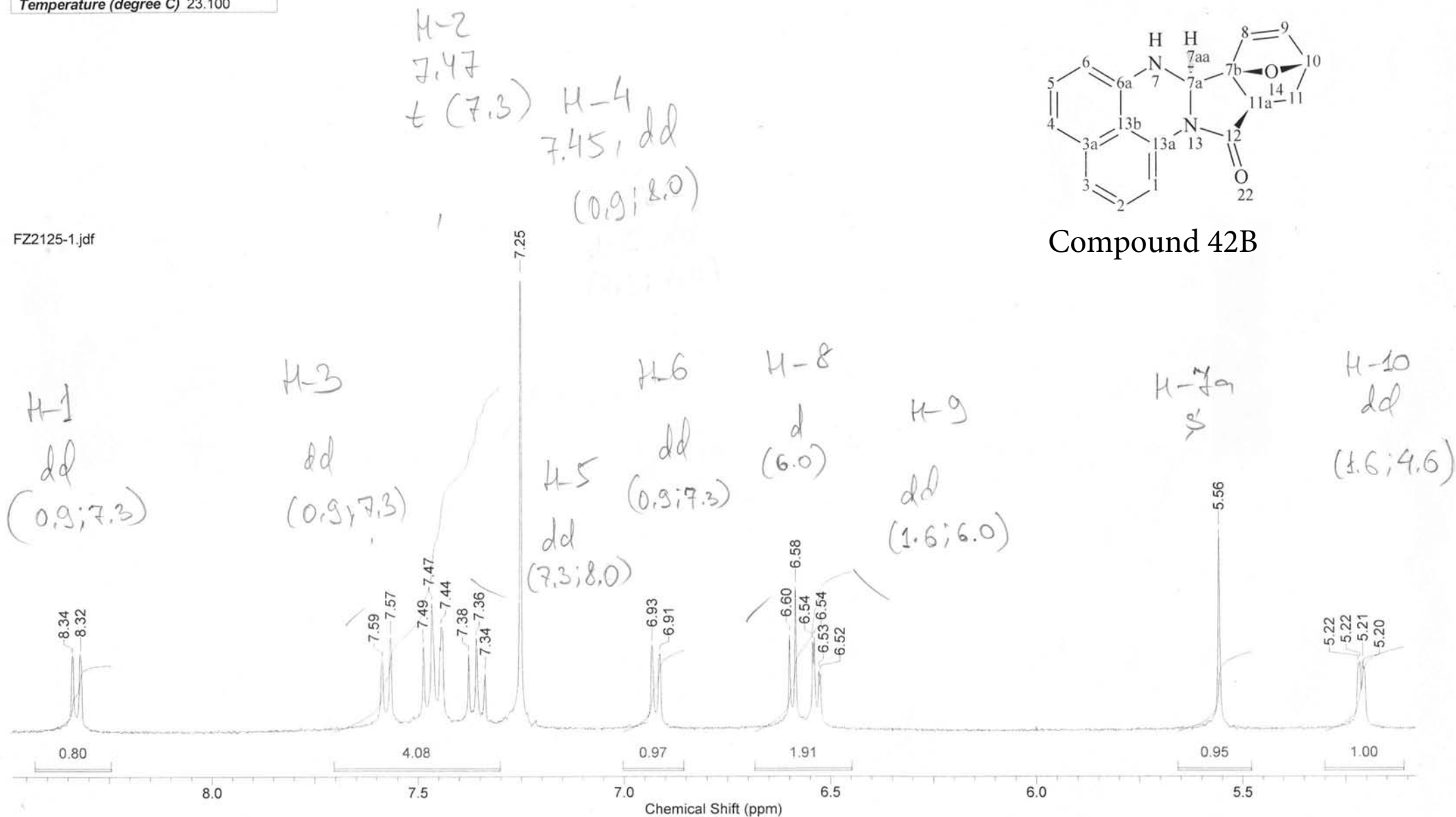
42B



Formula C₁₈H₁₄N₂O₂ FW 290.3160

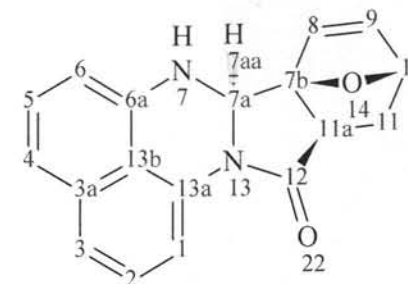
Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	14 Dec 2011 10:20:06	Date Stamp	14 Dec 2011 14:54:45
File Name	D:\NMR\12.12.11\FZ2125-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	46.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2398.6931	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	23.100			Sweep Width (Hz)	7503.00		

FZ2125-1.jdf



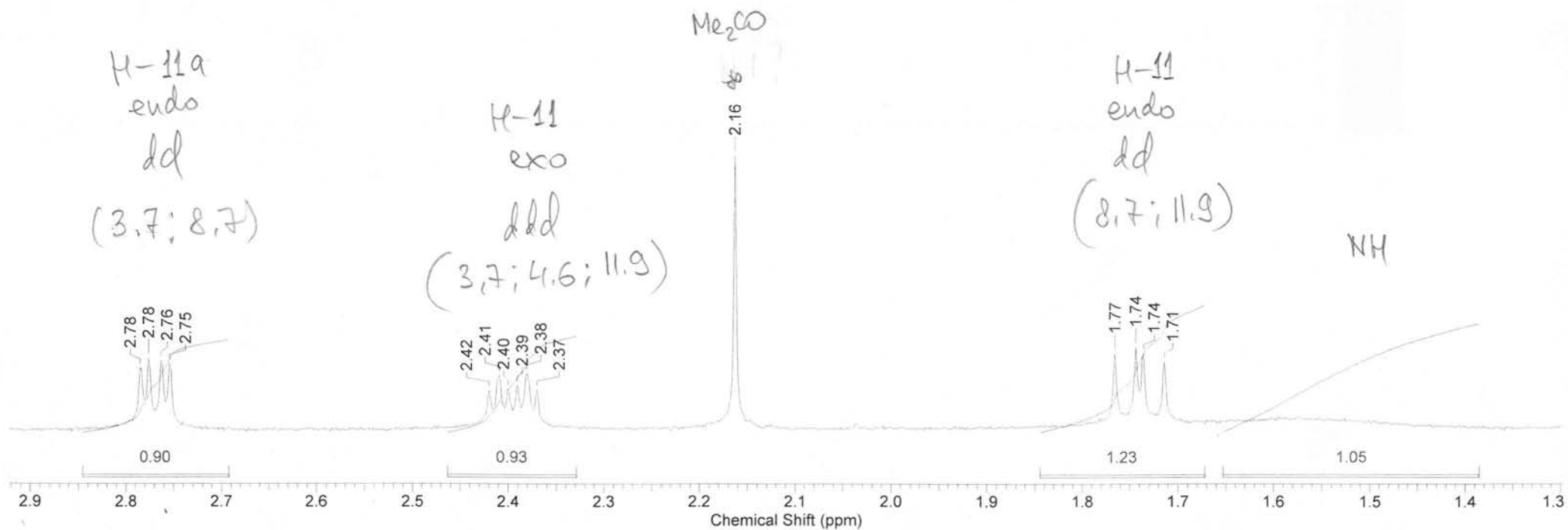
Formula C₁₈H₁₄N₂O₂ FW 290.3160

Acquisition Time (sec)	2.1837	Comment	single_pulse	Date	14 Dec 2011 10:20:06	Date Stamp	14 Dec 2011 14:54:45
File Name	D:\NMR\12.12.11\FZ2125-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8
Origin	ECS 400	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	46.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2398.6931	Sweep Width (Hz)	7503.00
Temperature (degree C)	23.100						



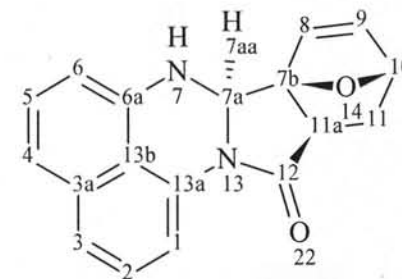
Compound 42B

FZ2125-1.jdf



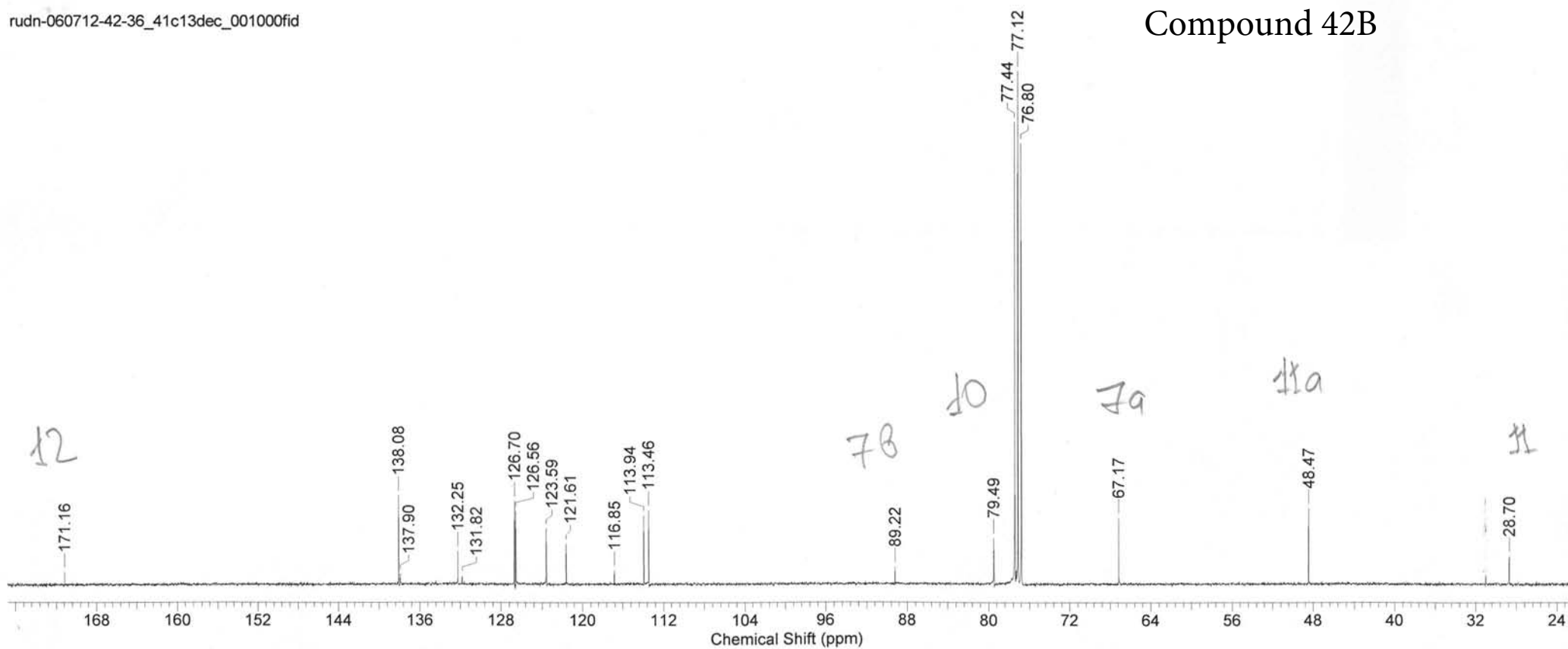
Formula	C ₁₈ H ₁₄ N ₂ O ₂	FW	290.3160
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	11 Jul 2012 21:54:08
Date Stamp	11 Jul 2012 21:54:08	File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-42-36_41c13dec\rudn-060712-42-36_41c13dec_001000fid		
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	34633
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	CHLOROFORM-d
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000	Spectrum Offset (Hz)	9638.7344



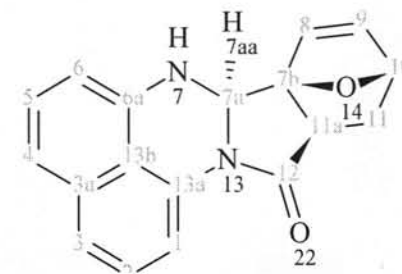
Compound 42B

rudn-060712-42-36_41c13dec_001000fid



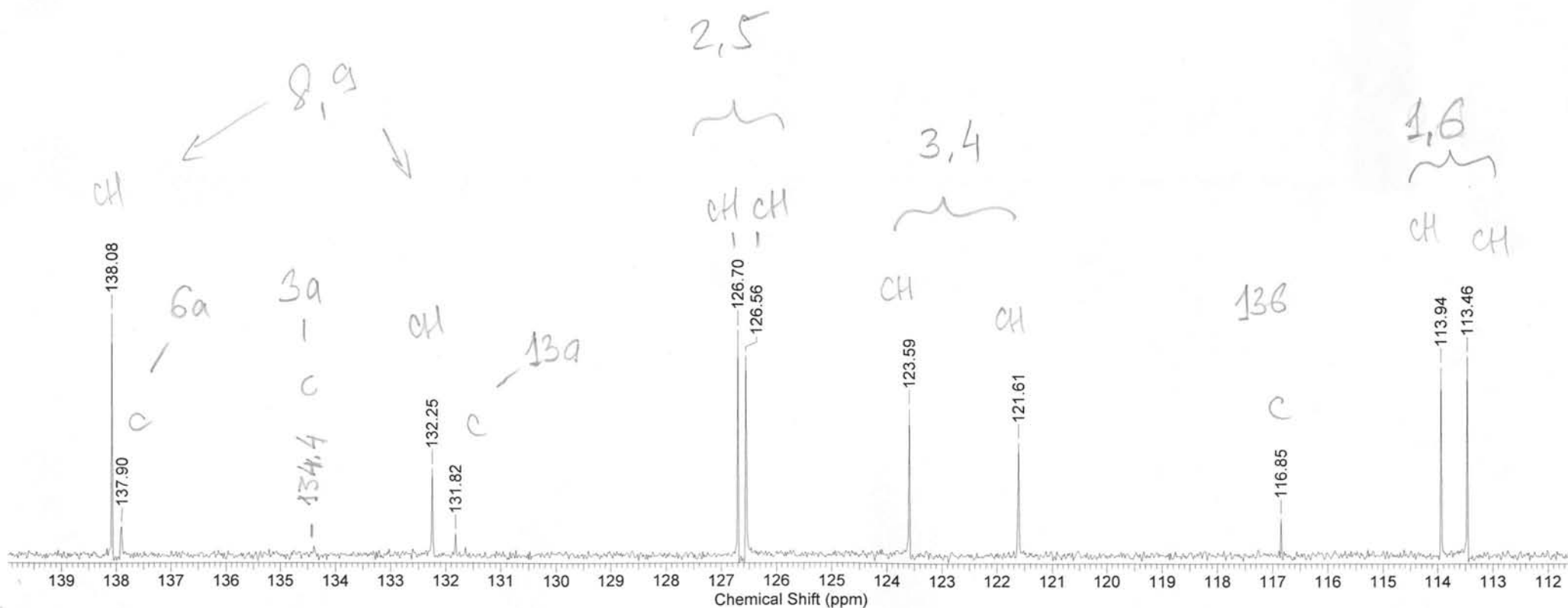
Formula	C ₁₈ H ₁₄ N ₂ O ₂	FW	290.3160
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	11 Jul 2012 21:54:08
Date Stamp	11 Jul 2012 21:54:08	File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-42-36_41c13dec\rudn-060712-42-36_41c13dec_001000fid		
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	34633
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	CHLOROFORM-d
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000	Spectrum Offset (Hz)	9638.7344



Compound 42B

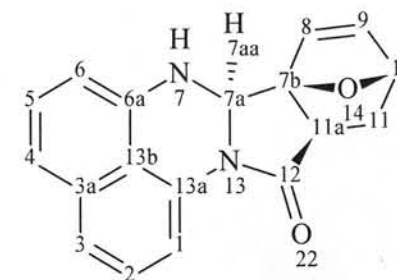
rudn-060712-42-36_41c13dec_001000fid



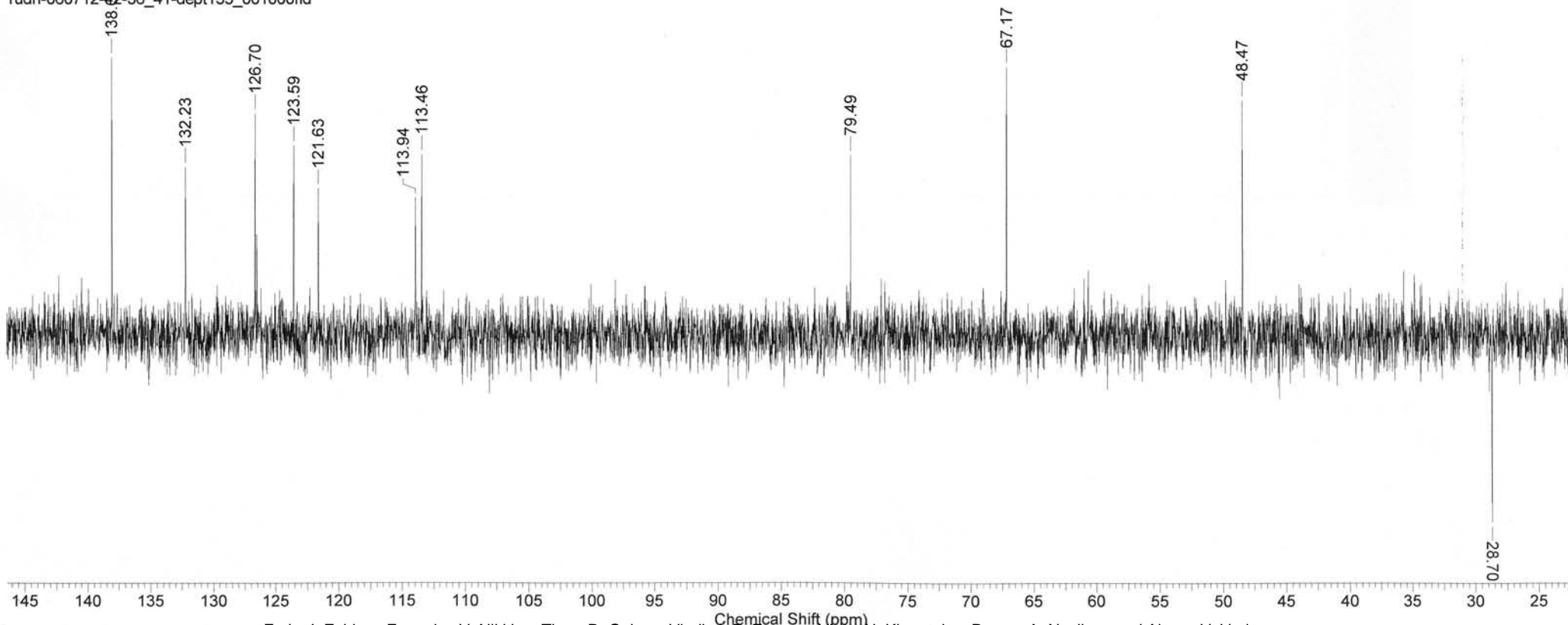
Formula	C ₁₈ H ₁₄ N ₂ O ₂	FW	290.3160
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	11 Jul 2012 18:18:40
Date Stamp	11 Jul 2012 18:18:40	File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-060712-42-36_41-dept135\rudn-060712-42-36_41-dept135_001000fid		
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	9000
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	CHLOROFORM-d
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000	Spectrum Offset (Hz)	9638.7344

Compound 42B

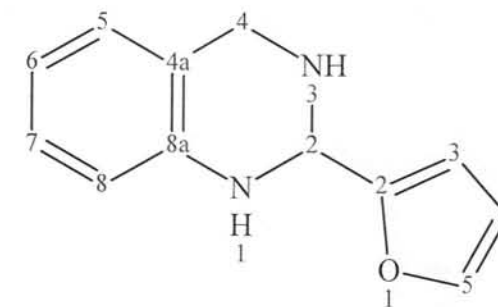


rudn-060712-42-36_41-dept135_001000fid

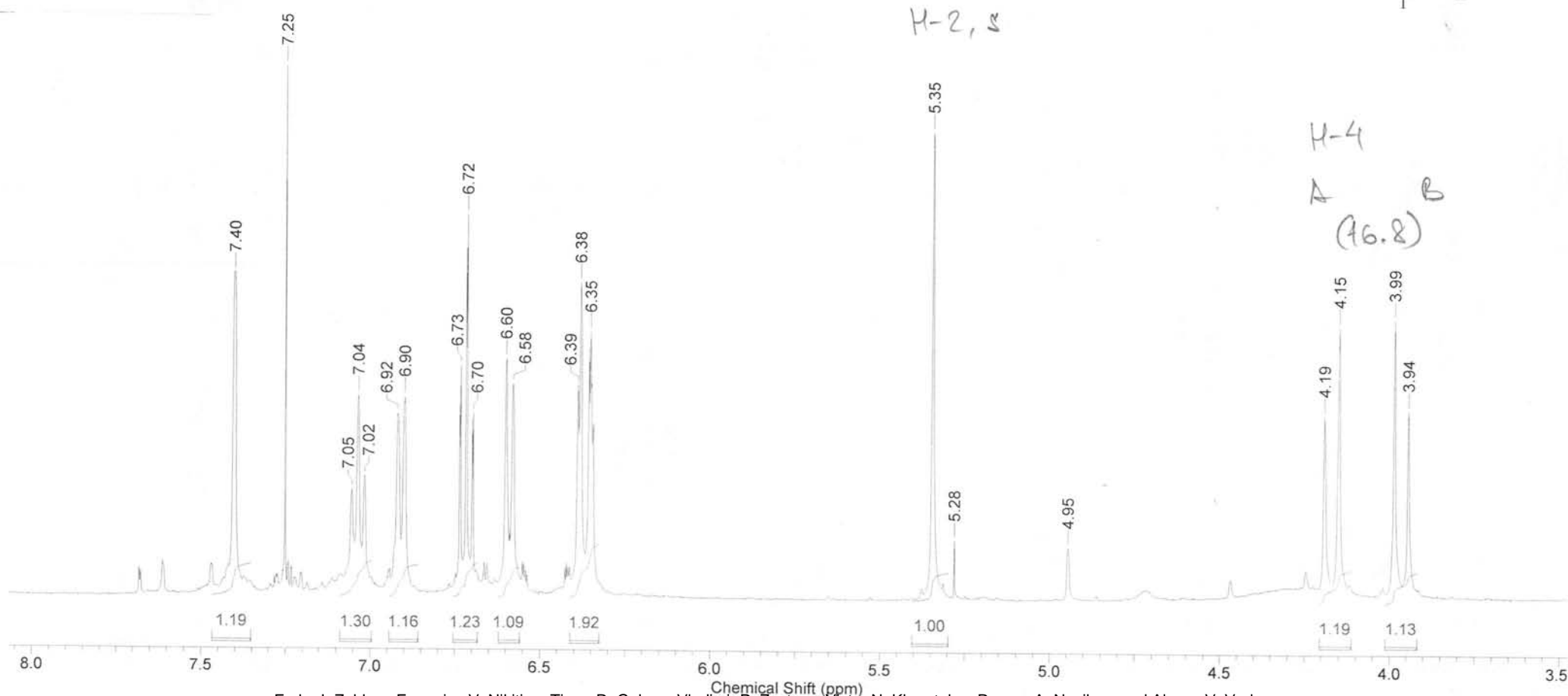


Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.		Date	23 Aug 2011 10:31:28	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-190811-N14\rudn-190811-N14_001000fid				Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	16	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	CHLOROFORM-D		Sweep Width (Hz)	10204.08	
Temperature (degree C)	27.000						

Compound 43a
reaction mixture

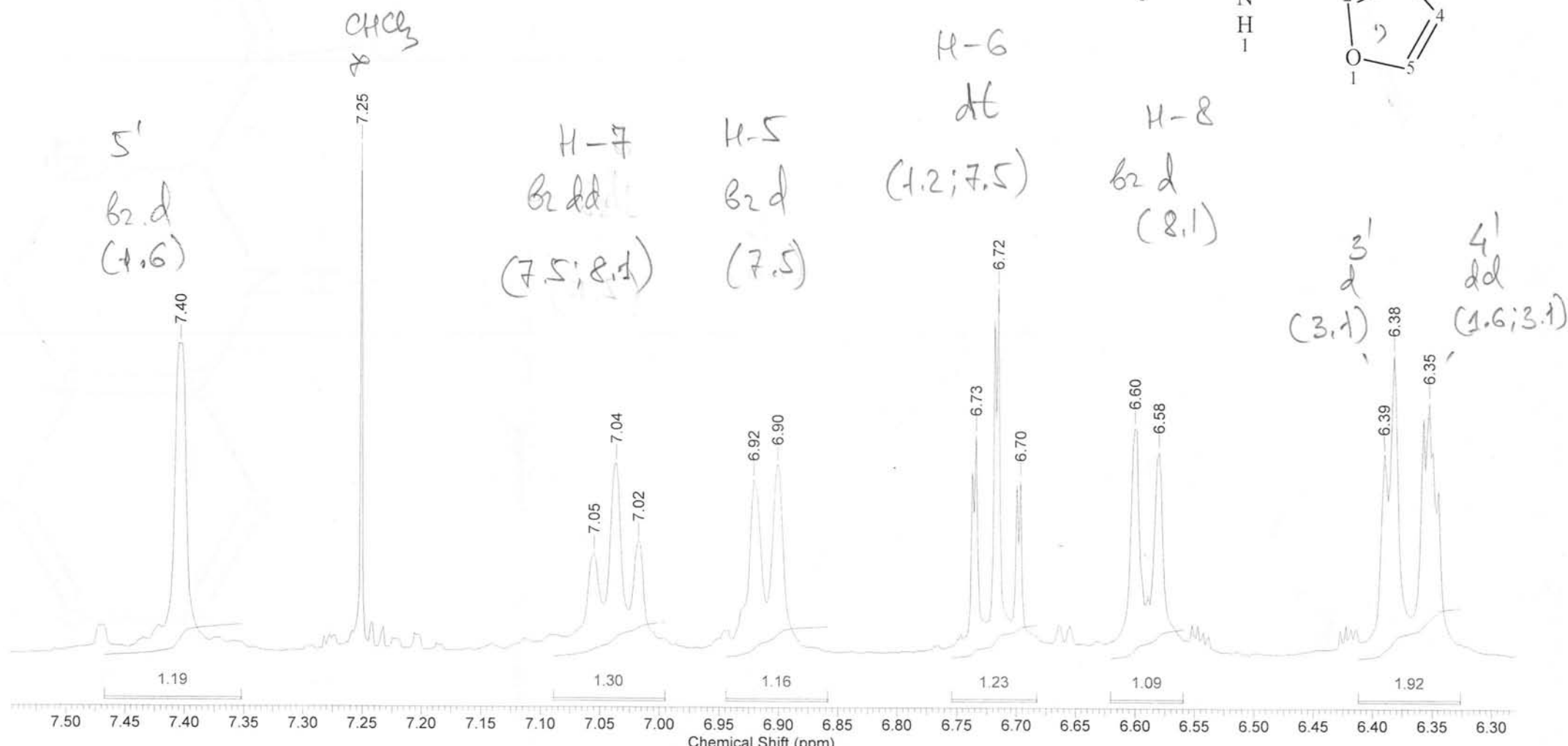
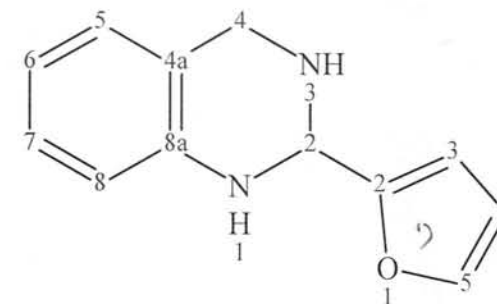


43a (reaction
mixture)



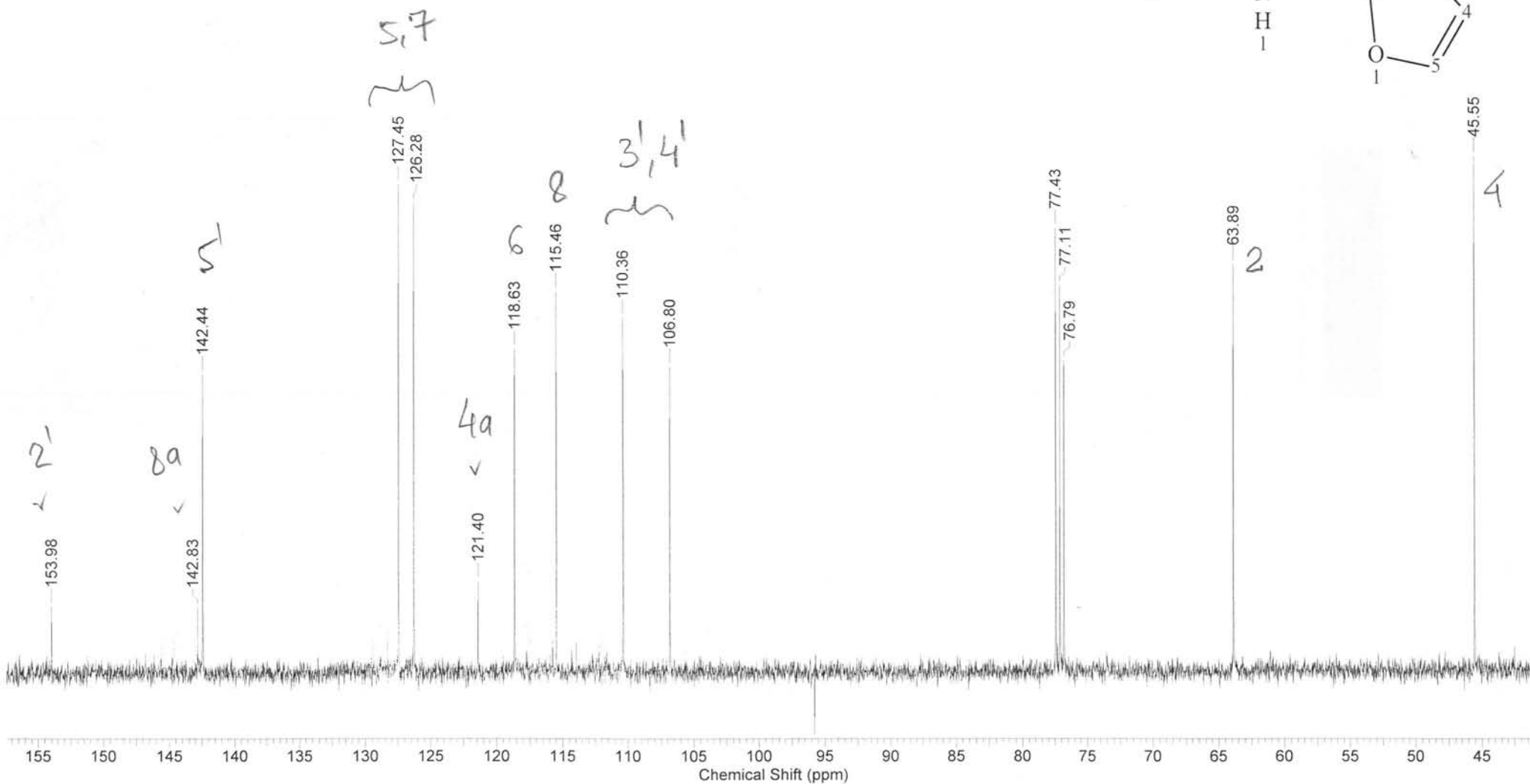
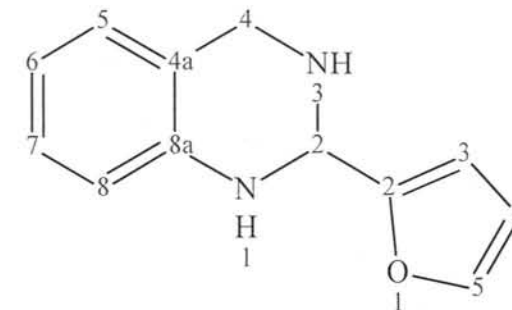
Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.		Date	23 Aug 2011 10:31:28	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-190811-N14\rudn-190811-N14_001000fid			Frequency (MHz)	400.14		
Nucleus	1H	Number of Transients	16	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	CHLOROFORM-D		Sweep Width (Hz)	10204.08	
Temperature (degree C)	27.000						

Compound 43a reaction mixture



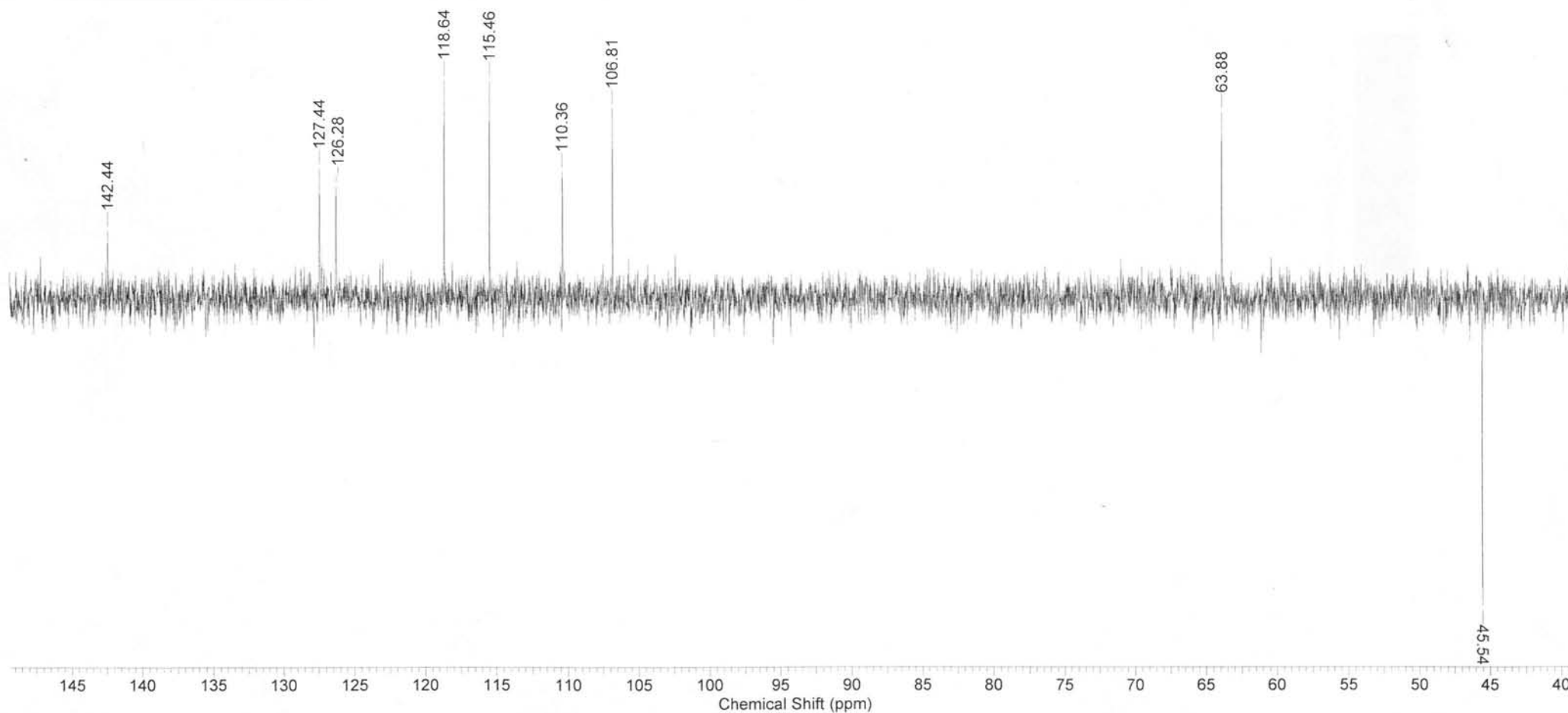
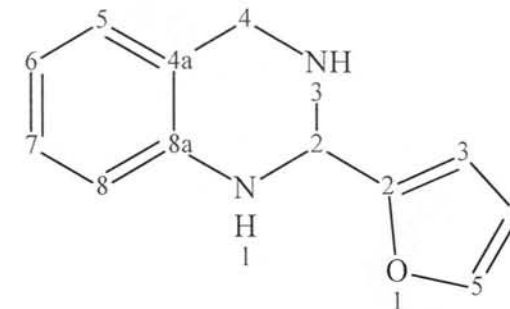
Acquisition Time (sec)	0.5898	Comment	Imported from UXNMR.		Date	23 Aug 2011 16:21:20	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-190811-N14-c13dec\rudn-190811-N14-c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	1933	Original Points Count	16384	Points Count	16384
Pulse Sequence	zpgg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	27777.78	Temperature (degree C)	27.000

Compound 43a reaction mixture



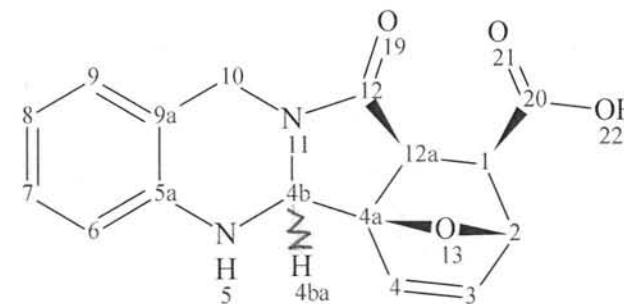
Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	23 Aug 2011 16:57:36	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-190811-N14-dept135\rudn-190811-N14-dept135_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	1908	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	CHLOROFORM-D	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compound 43a
reaction mixture



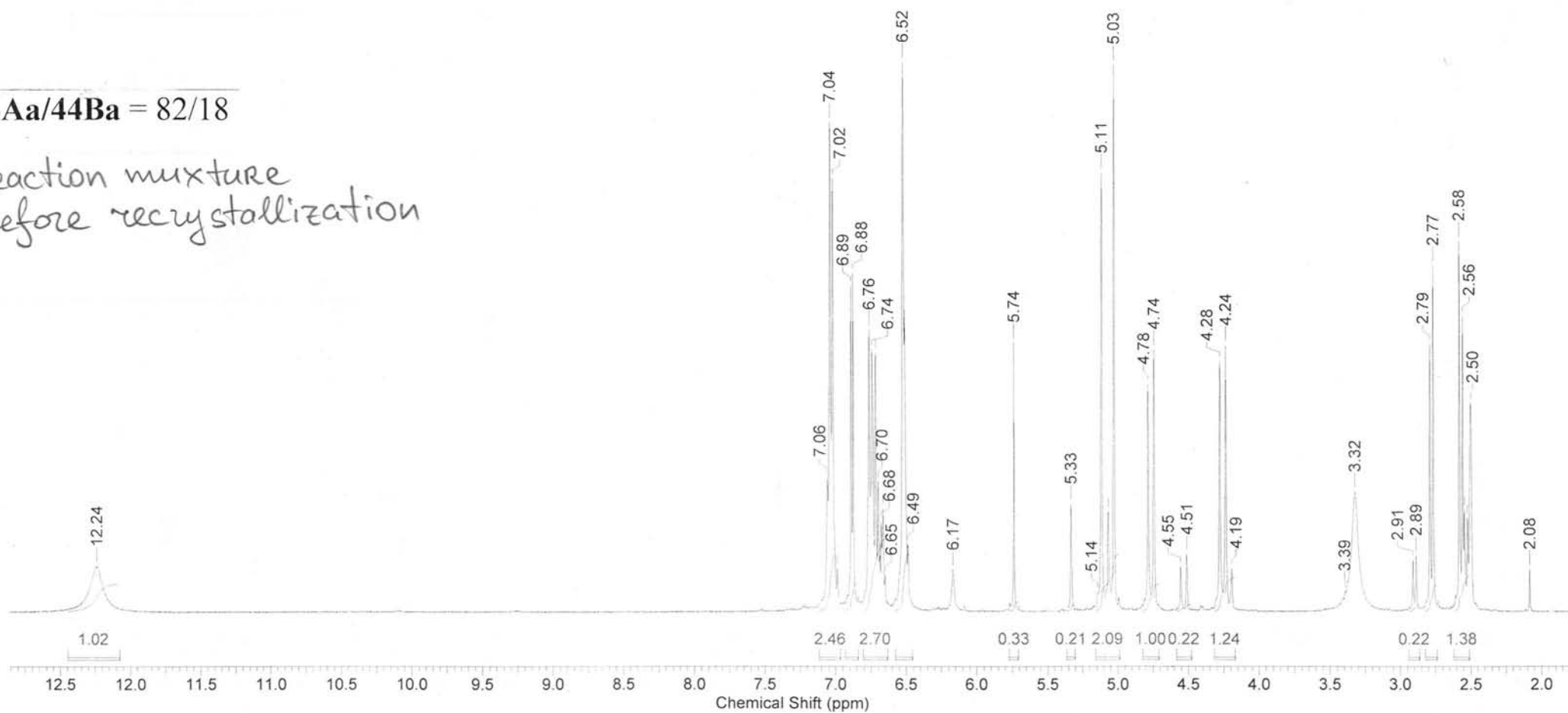
Acquisition Time (sec)	1.5729	Comment	Imported from UXNMR.		Date	23 Aug 2011 09:14:40	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-120811-N3\rudn-120811-N3_001000fid				Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	16	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	10416.67	Temperature (degree C)	32.000

Compounds 44Aa/44Ba
reaction mixture
before recrystallization



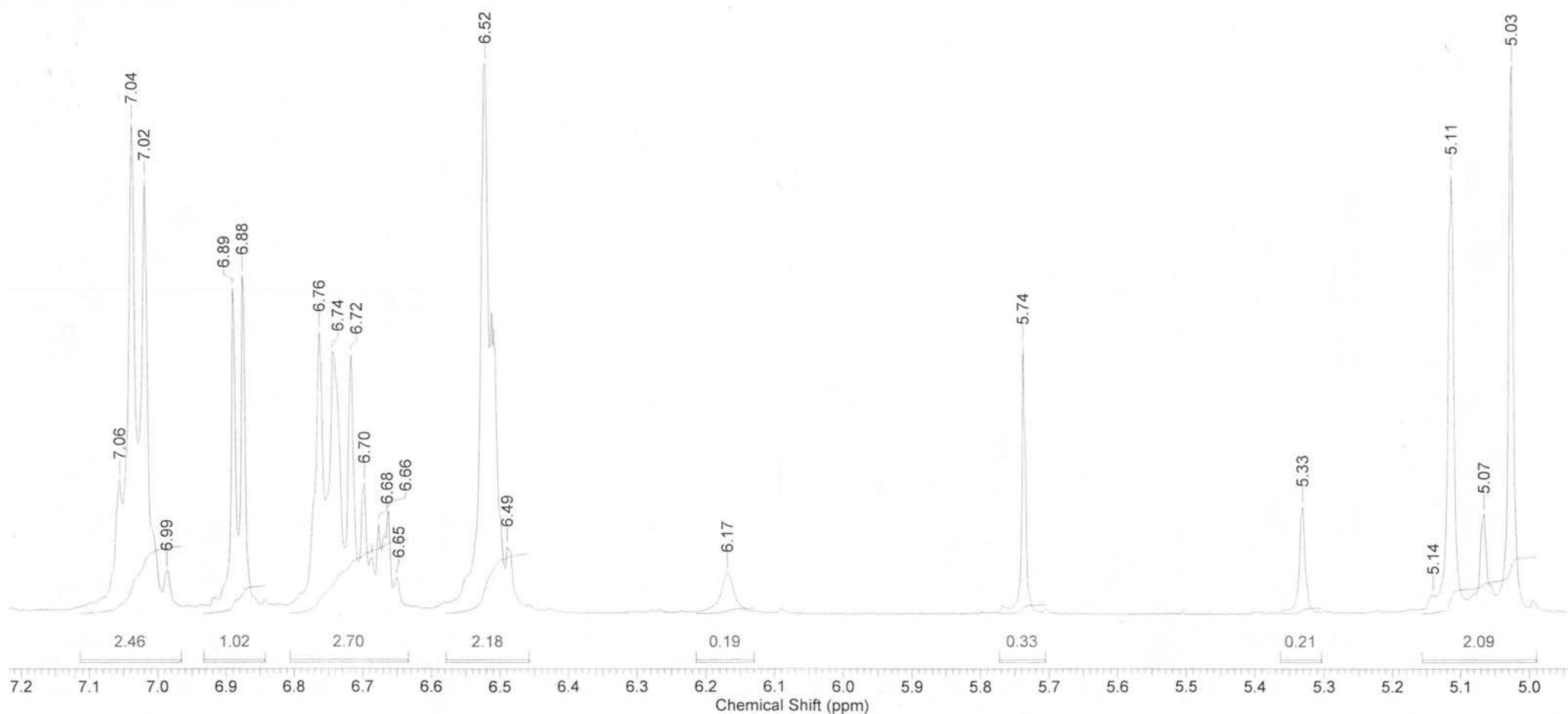
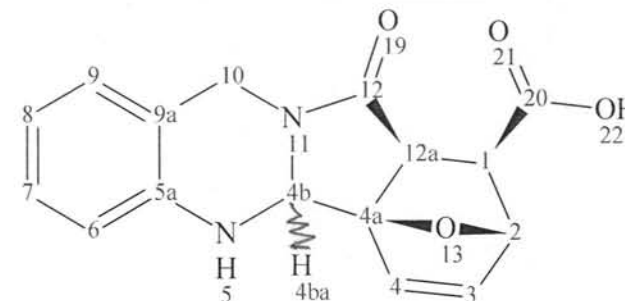
44Aa/44Ba = 82/18

reaction mixture
before recrystallization



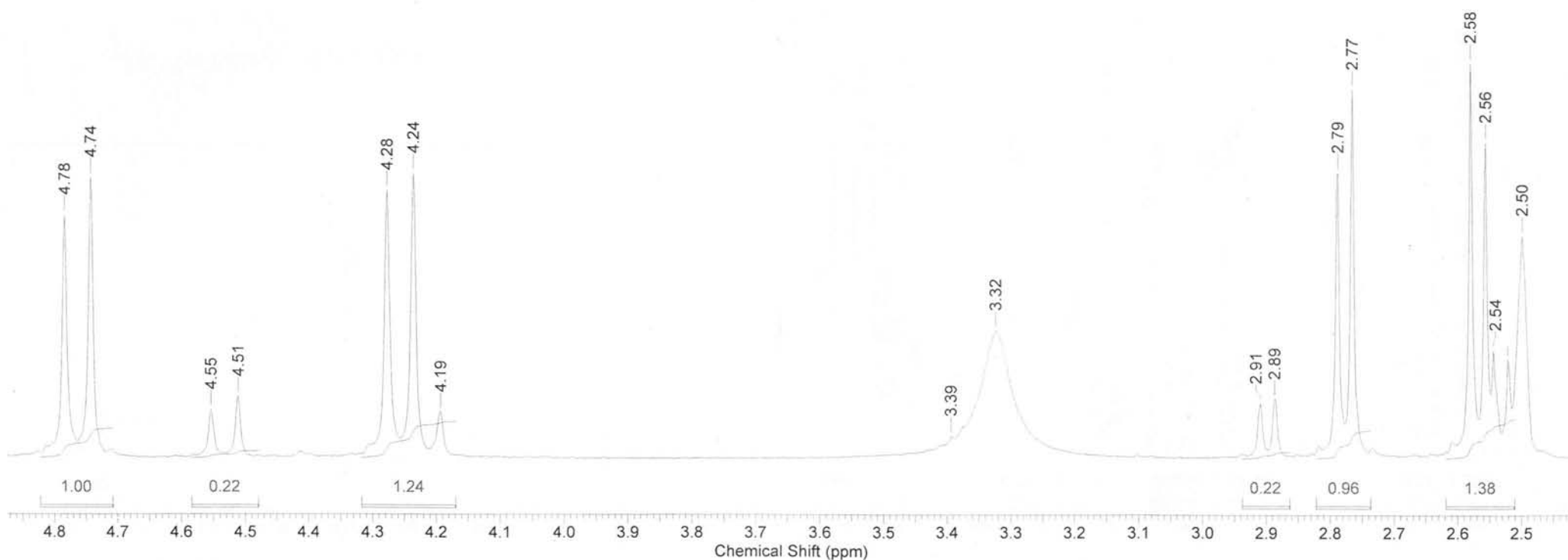
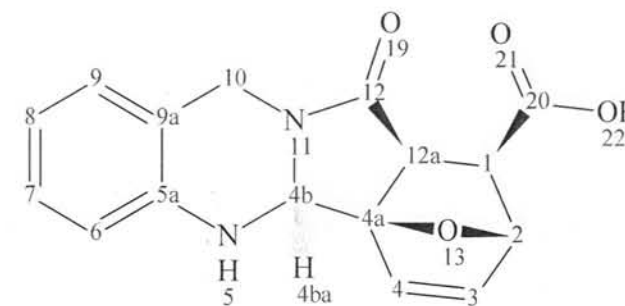
Acquisition Time (sec)	1.5729	Comment	Imported from UXNMR.		Date	23 Aug 2011 09:14:40	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-120811-N3\rudn-120811-N3_001000fid				Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	16	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	10416.67	Temperature (degree C)	32.000

Compounds 44Aa/44Ba
reaction mixture
before recrystallization



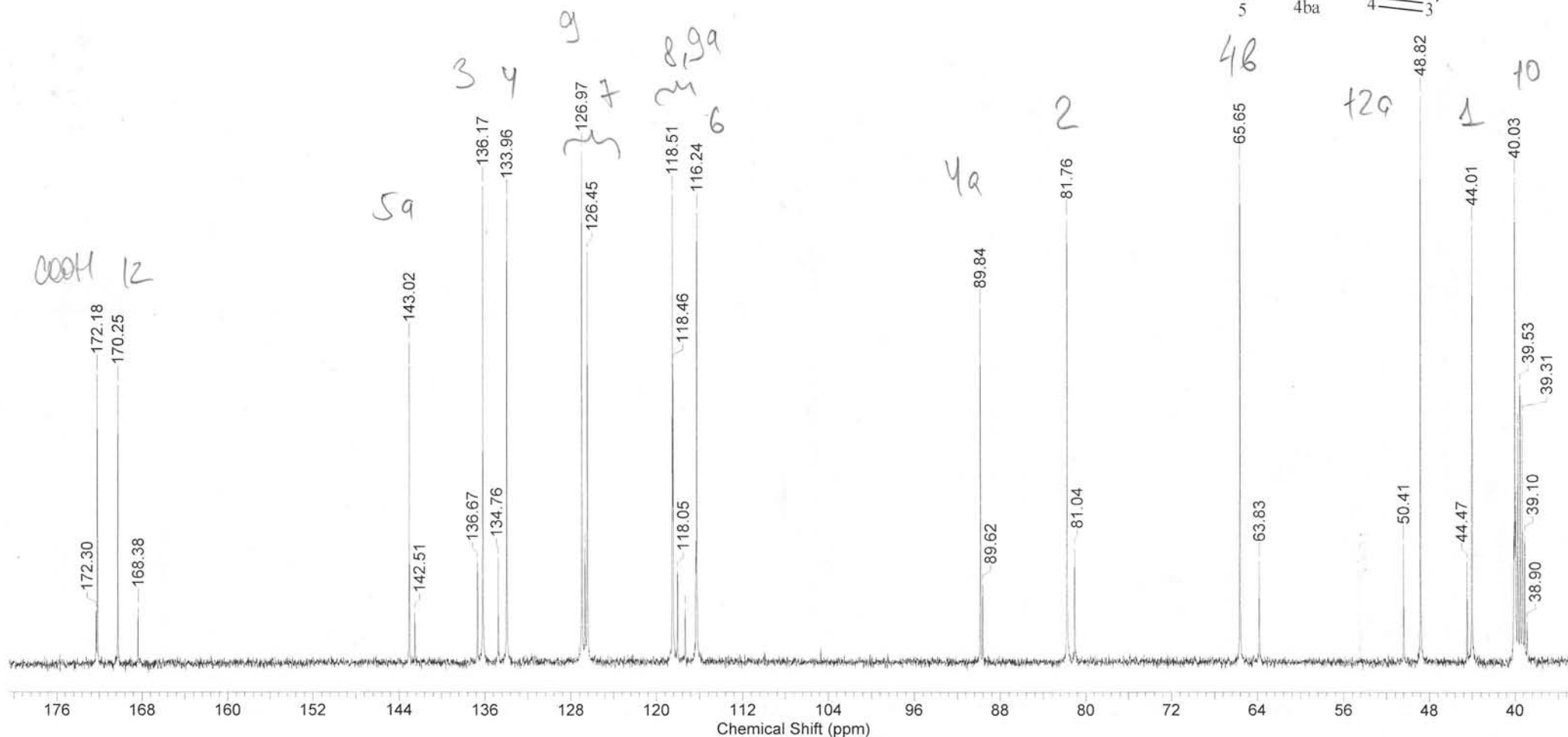
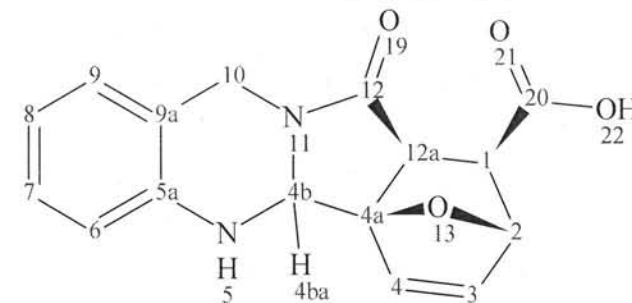
Acquisition Time (sec)	1.5729	Comment	Imported from UXNMR.		Date	23 Aug 2011 09:14:40	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-120811-N3\rudn-120811-N3_001000fid			Frequency (MHz)	400.14		
Nucleus	1H	Number of Transients	16	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	10416.67	Temperature (degree C)	32.000

Compounds 44Aa/44Ba
reaction mixture
before recrystallization



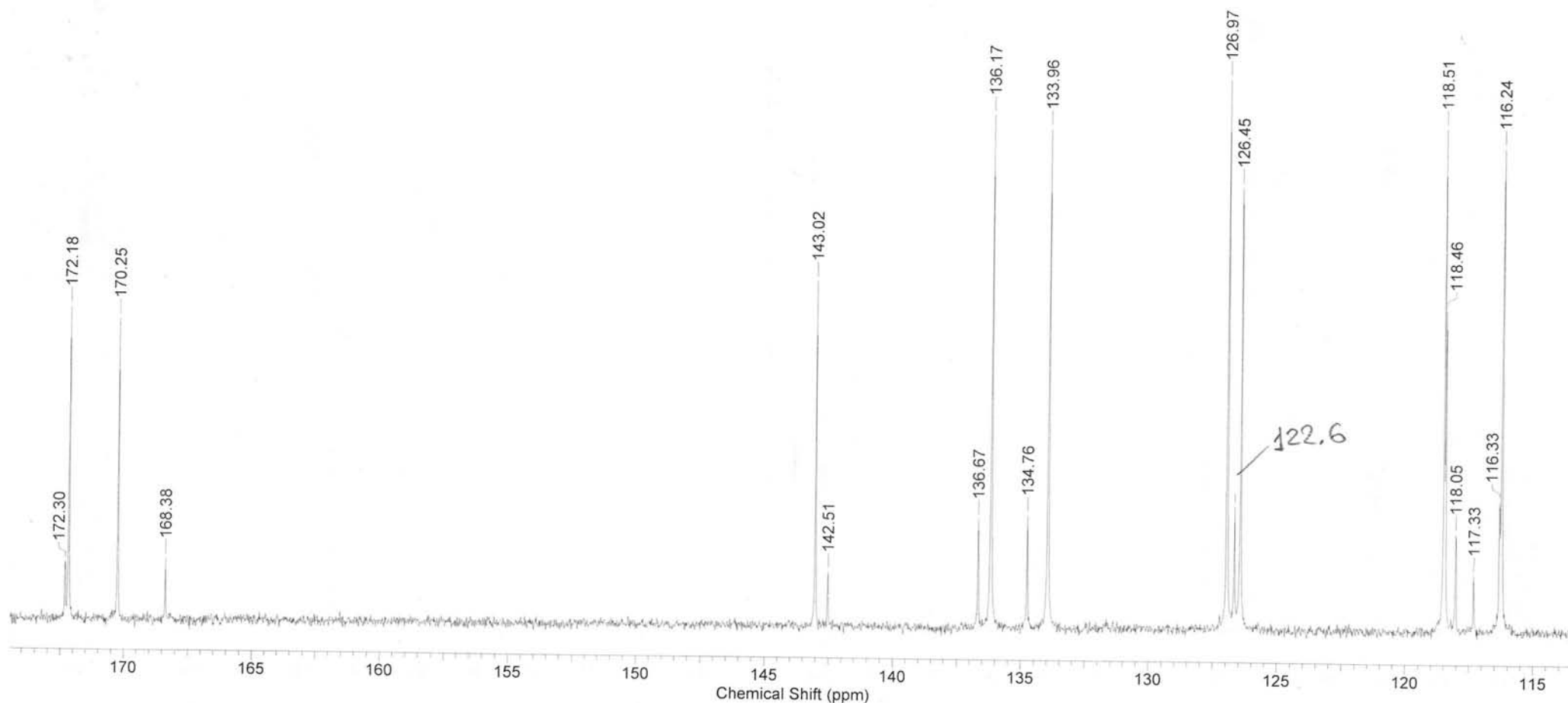
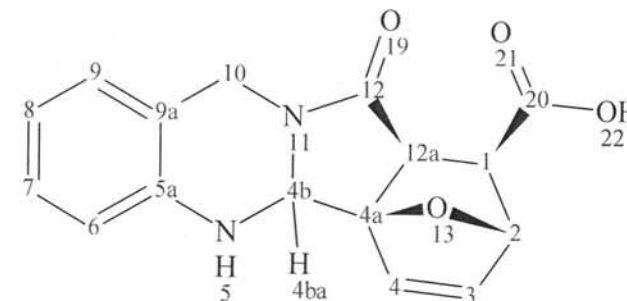
Acquisition Time (sec)	0.5571	Comment	Imported from UXNMR.		Date	24 Aug 2011 14:41:04	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-120811-N3-c13dec\rudn-120811-N3-c13dec_002000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	1957	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compounds 44Aa/44Ba
reaction mixture
before recrystallization



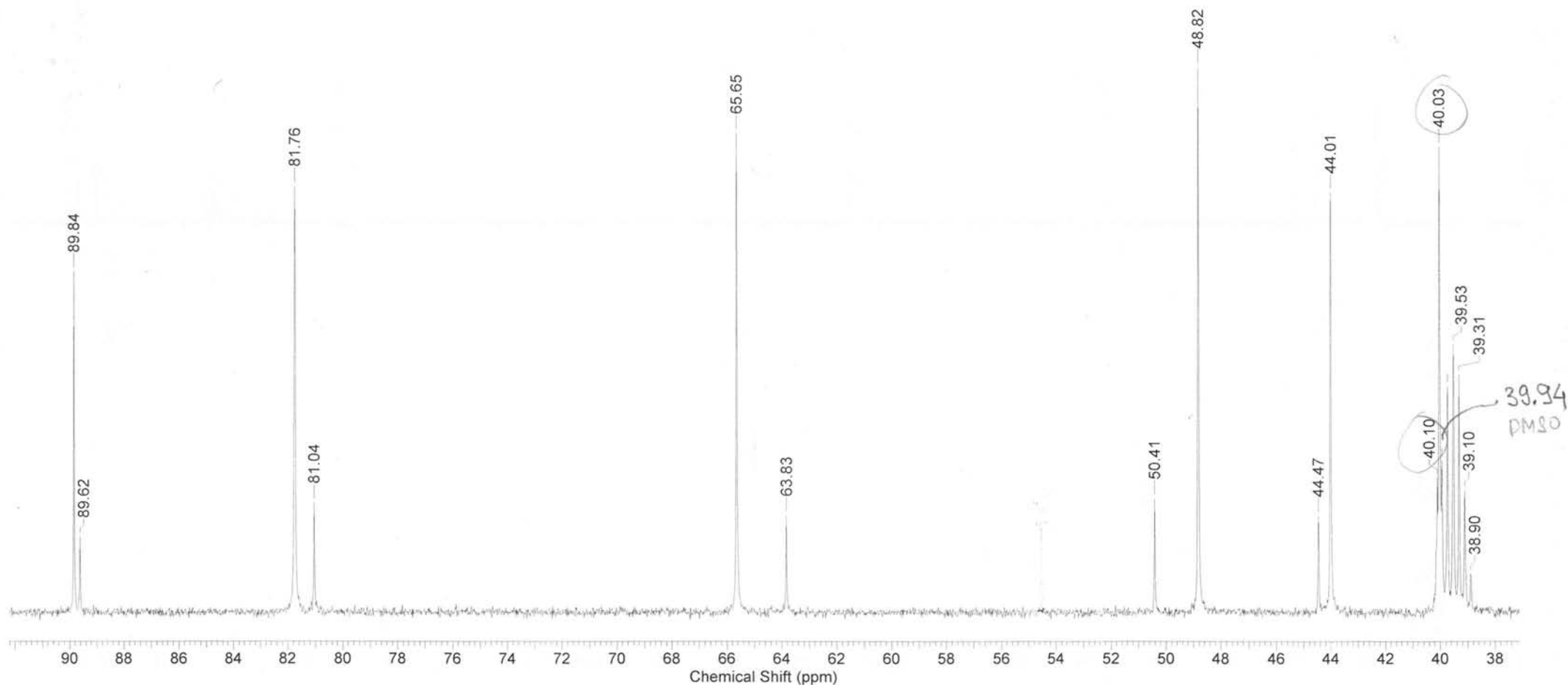
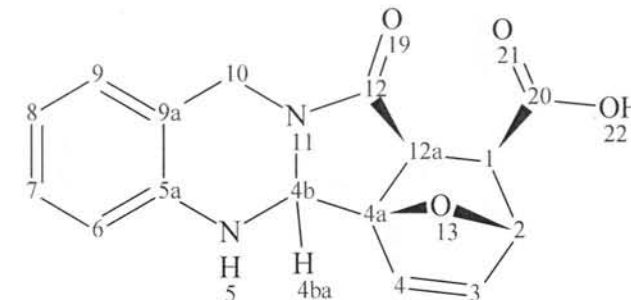
Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	24 Aug 2011 14:41:04	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-120811-N3-c13dec\rudn-120811-N3-c13dec_002000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	1957	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compounds 44Aa/44Ba
reaction mixture
before recrystallization

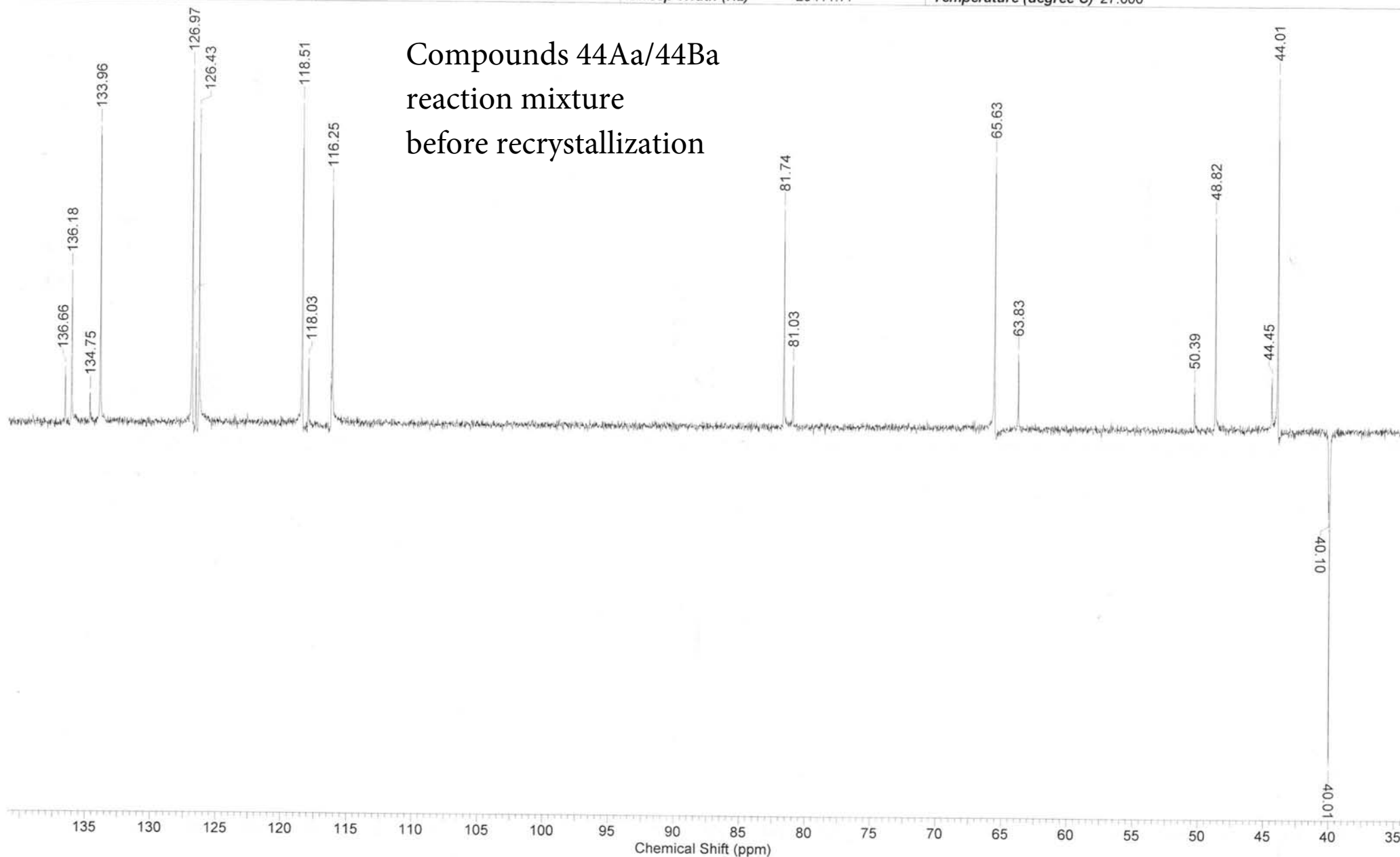


Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	24 Aug 2011 14:41:04	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-120811-N3-c13dec\rudn-120811-N3-c13dec_002000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	1957	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

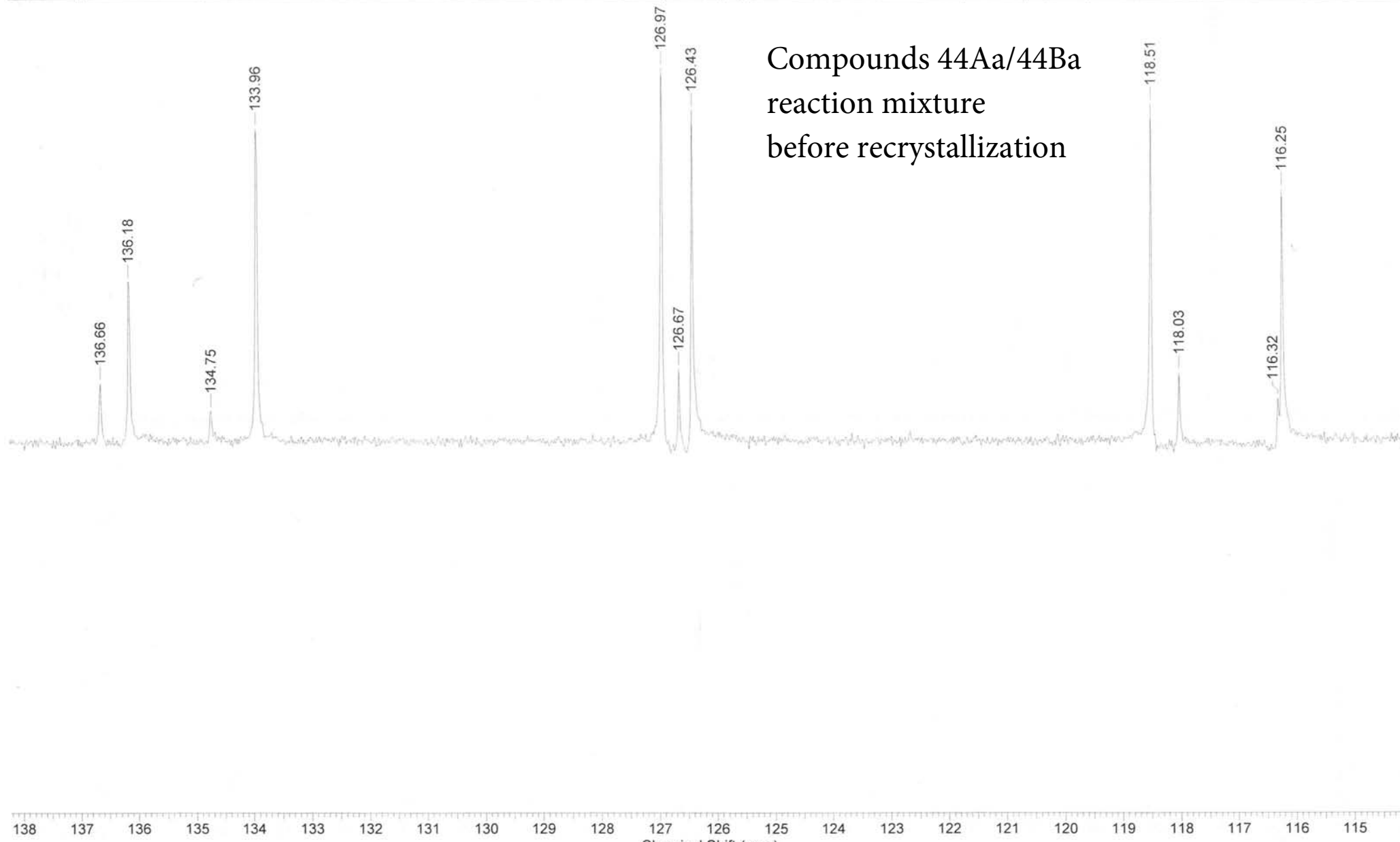
Compounds 44Aa/44Ba
reaction mixture
before recrystallization



Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	24 Aug 2011 15:25:52	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-120811-N3-dept135\rudn-120811-N3-dept135_002000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	901	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

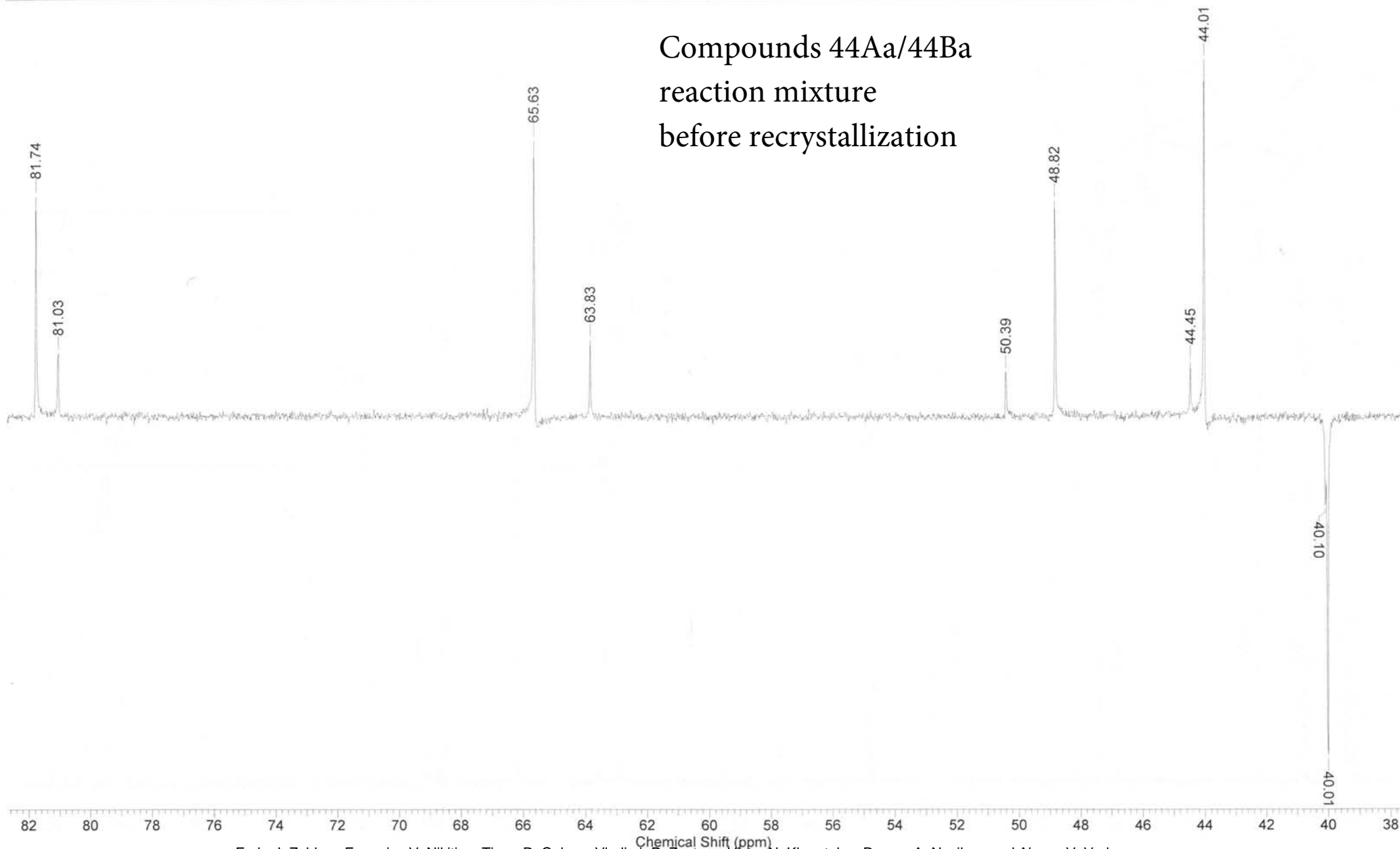


Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	24 Aug 2011 15:25:52	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-120811-N3-dept135\rudn-120811-N3-dept135_002000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	901	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000



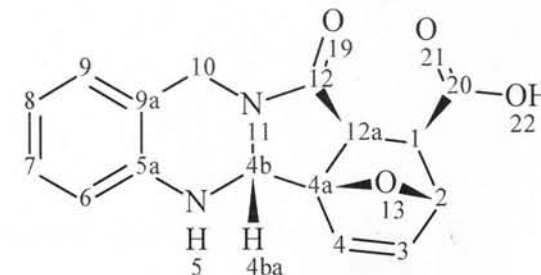
Acquisition Time (sec)	0.5571	Comment	Imported from UXNMR.		Date	24 Aug 2011 15:25:52	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-120811-N3-dept135\rudn-120811-N3-dept135_002000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	901	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compounds 44Aa/44Ba
reaction mixture
before recrystallization



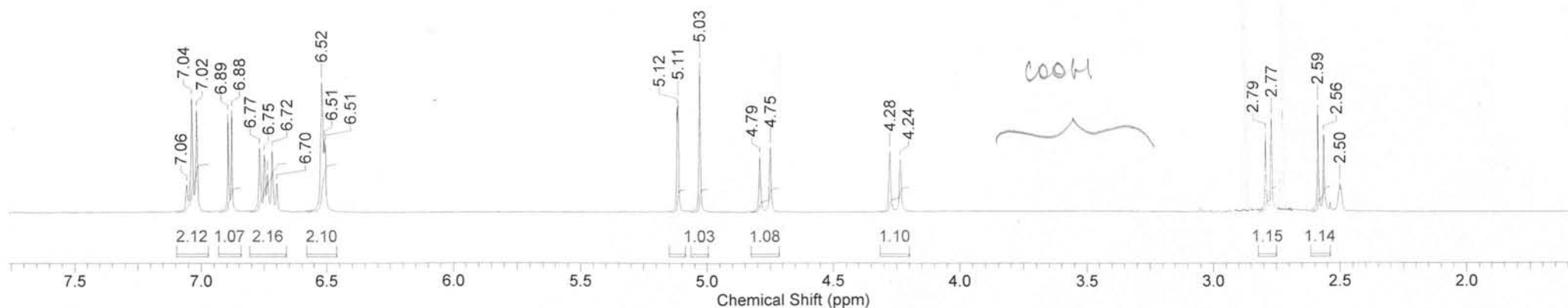
Formula C ₁₆ H ₁₄ N ₂ O ₄	FW 298.2934			
Acquisition Time (sec) 1.5729	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 28 May 2012 16:49:04		
Date Stamp 28 May 2012 16:49:04				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250212-44Aa\rudn-250212-44Aa_002000fid	Frequency (MHz) 400.14			
Nucleus 1H	Number of Transients 4	Origin spect	Original Points Count 16384	
Owner root	Points Count 16384	Pulse Sequence zg	Receiver Gain 128.00	
SW(cyclical) (Hz) 10416.67	Solvent DMSO-d6	Spectrum Offset (Hz) 2712.0542	Sweep Width (Hz) 10416.03	
Temperature (degree C) 32.000				

Compound 44Aa



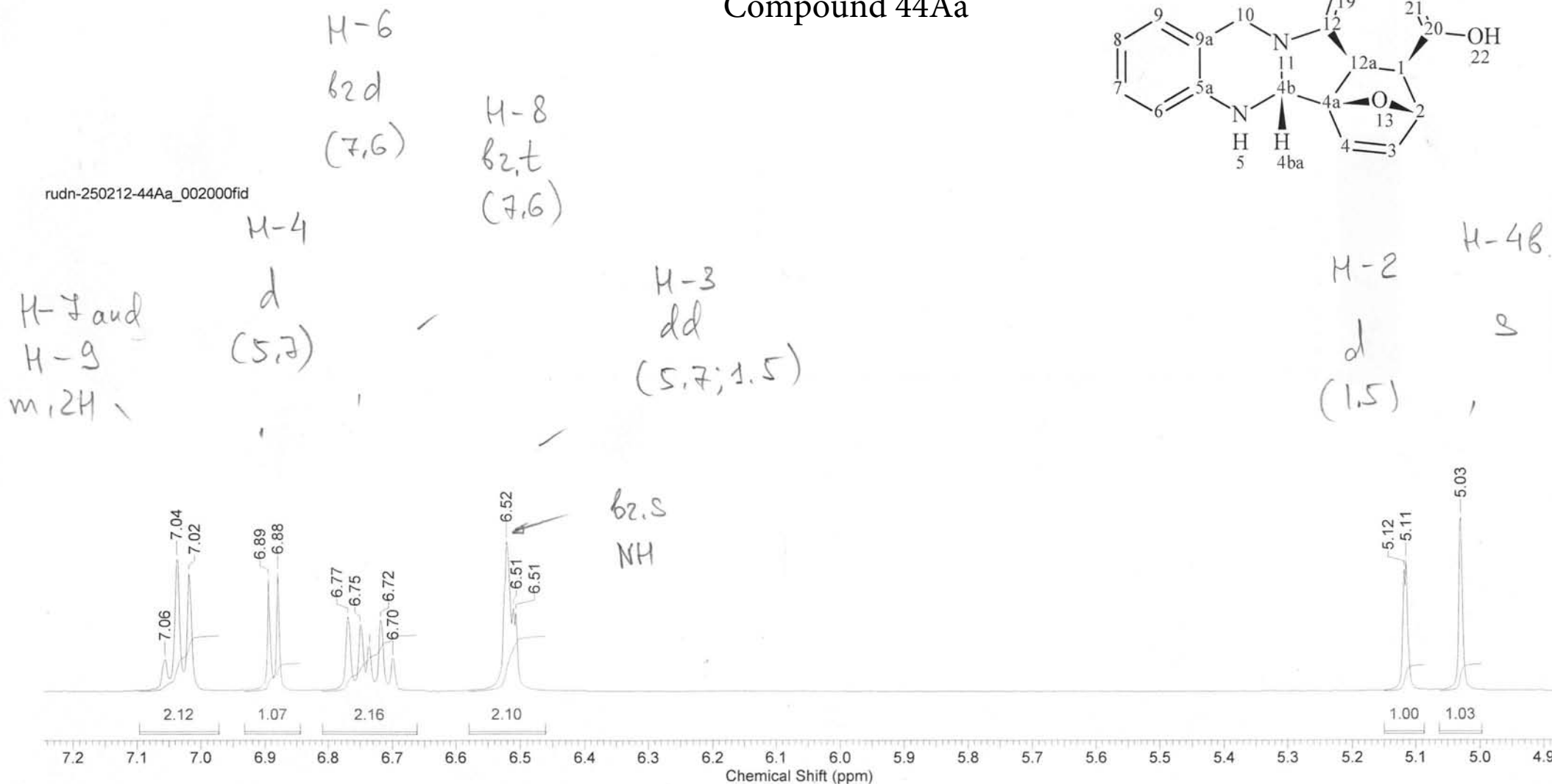
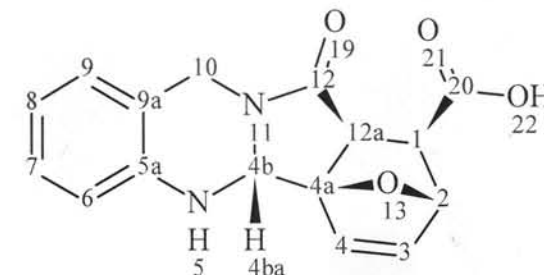
rudn-250212-44Aa_002000fid

44Aa



Formula C ₁₆ H ₁₄ N ₂ O ₄	FW 298.2934				
Acquisition Time (sec) 1.5729	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 28 May 2012 16:49:04			
Date Stamp 28 May 2012 16:49:04				Frequency (MHz) 400.14	Original Points Count 16384
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250212-44Aa\rudn-250212-44Aa_002000fid	Number of Transients 4	Origin spect	Pulse Sequence zg	Receiver Gain 128.00	Sweep Width (Hz) 10416.03
Nucleus 1H	Points Count 16384	Solvent DMSO-d6	Spectrum Offset (Hz) 2712.0542		
Owner root				Temperature (degree C) 32.000	

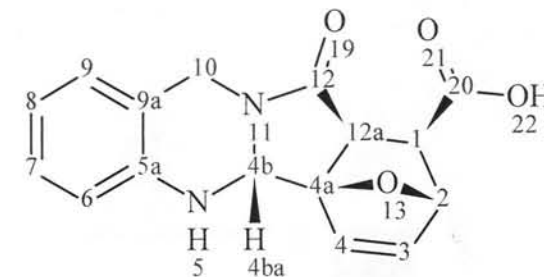
Compound 44Aa



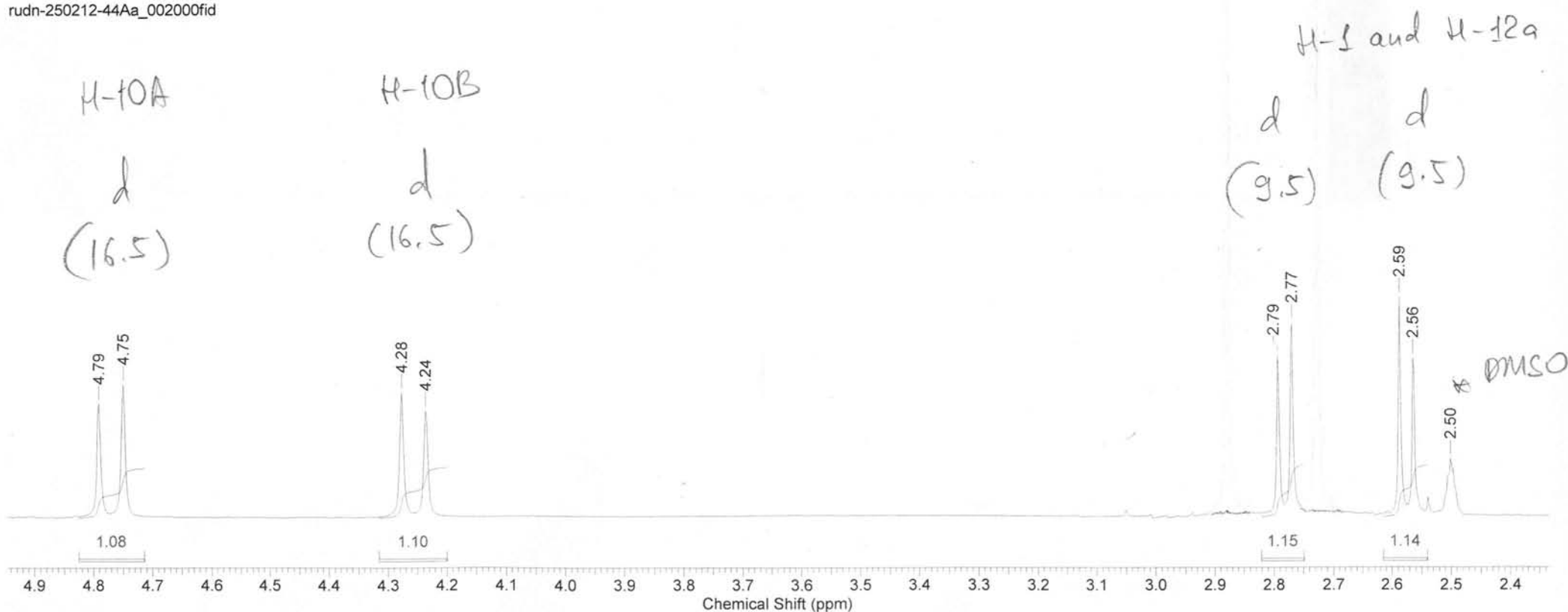
Formula C₁₆H₁₄N₂O₄ FW 298.2934

Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	28 May 2012 16:49:04
Date Stamp	28 May 2012 16:49:04				
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250212-44Aa\rudn-250212-44Aa_002000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	4	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zg
SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542
Temperature (degree C)	32.000			Sweep Width (Hz)	10416.03

Compound 44Aa



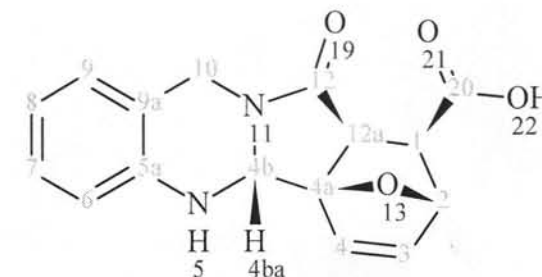
rudn-250212-44Aa_002000fid



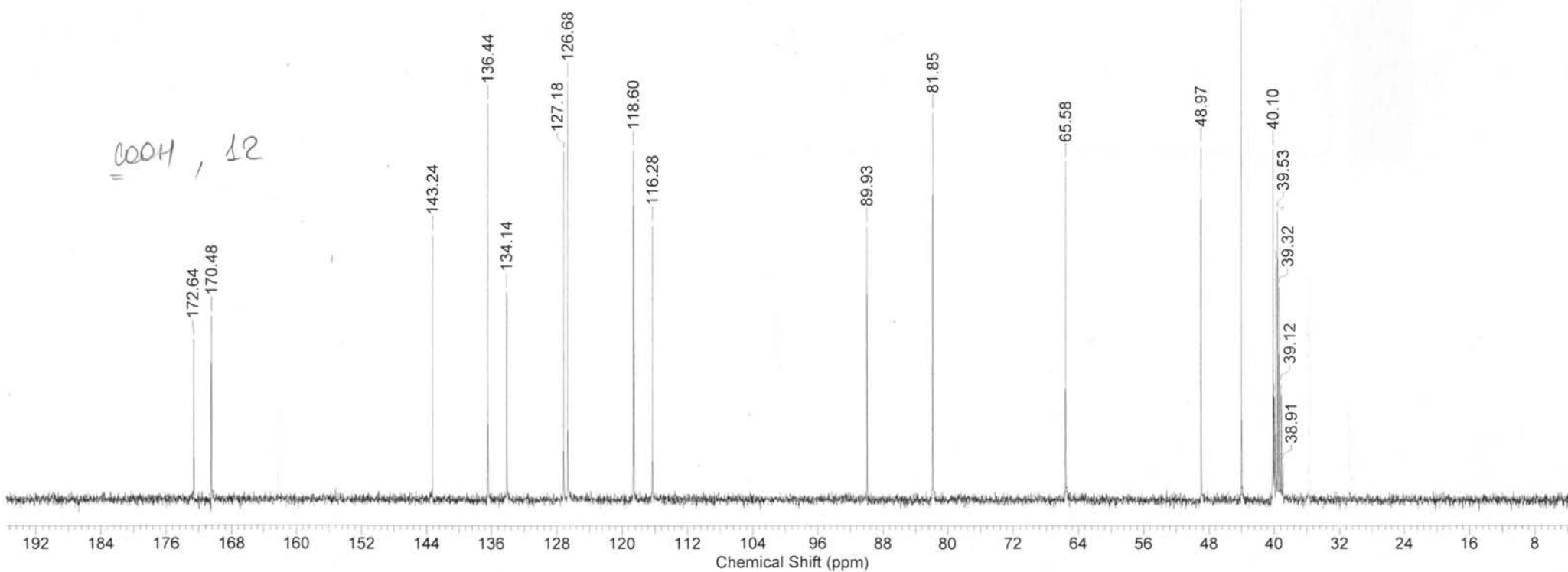
Formula C₁₆H₁₄N₂O₄ FW 298.2934

Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	28 May 2012 16:51:12
Date Stamp	28 May 2012 16:51:12				
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-44Aa-c13dec\rudn-250512-44Aa-c13dec_001000fid				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	730
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000	Spectrum Offset (Hz)	10554.3594

Compound 44Aa

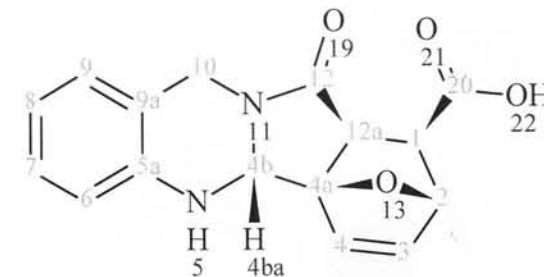


rudn-250512-44Aa-c13dec_001000fid

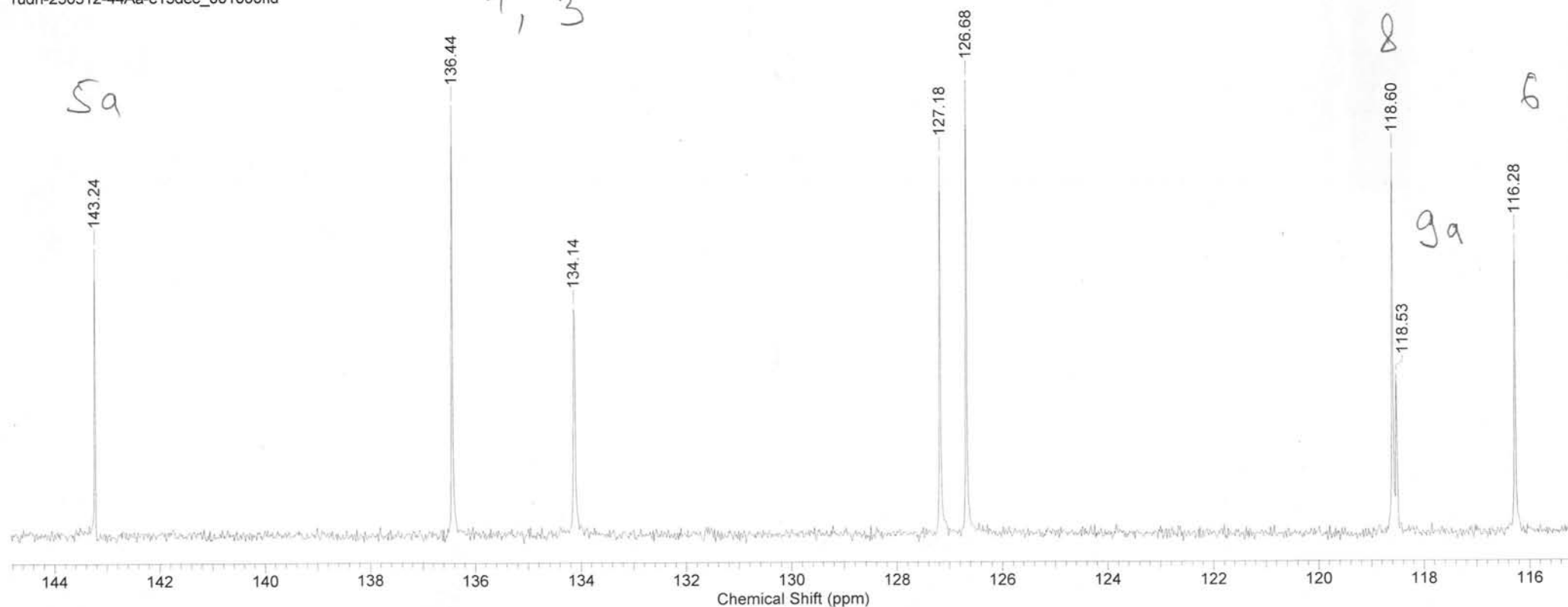


Formula C ₁₆ H ₁₄ N ₂ O ₄	FW 298.2934			
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400	Date 28 May 2012 16:51:12		
Date Stamp 28 May 2012 16:51:12				
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-44Aa-c13dec\rudn-250512-44Aa-c13dec_001000fid				
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 730	Origin spect	
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg	
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10554.3594	
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000			

Compound 44Aa



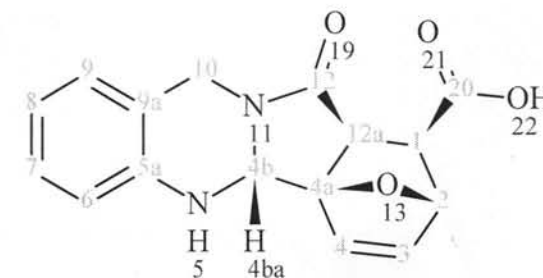
rudn-250512-44Aa-c13dec_001000fid



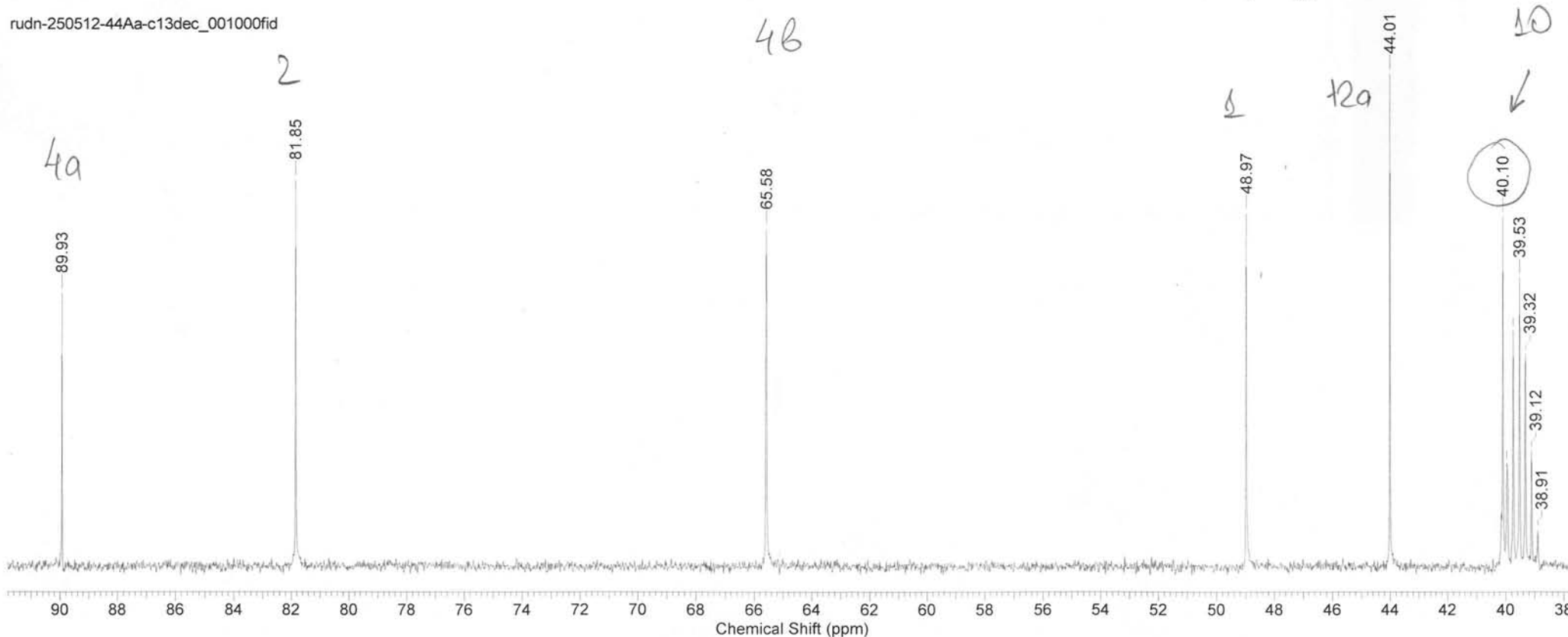
Formula C₁₆H₁₄N₂O₄ FW 298.2934

Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	28 May 2012 16:51:12	
Date Stamp	28 May 2012 16:51:12						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-44Aa-c13dec\rudn-250512-44Aa-c13dec_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	730	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zgpg
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6	Spectrum Offset (Hz)	10554.3594
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				

Compound 44Aa



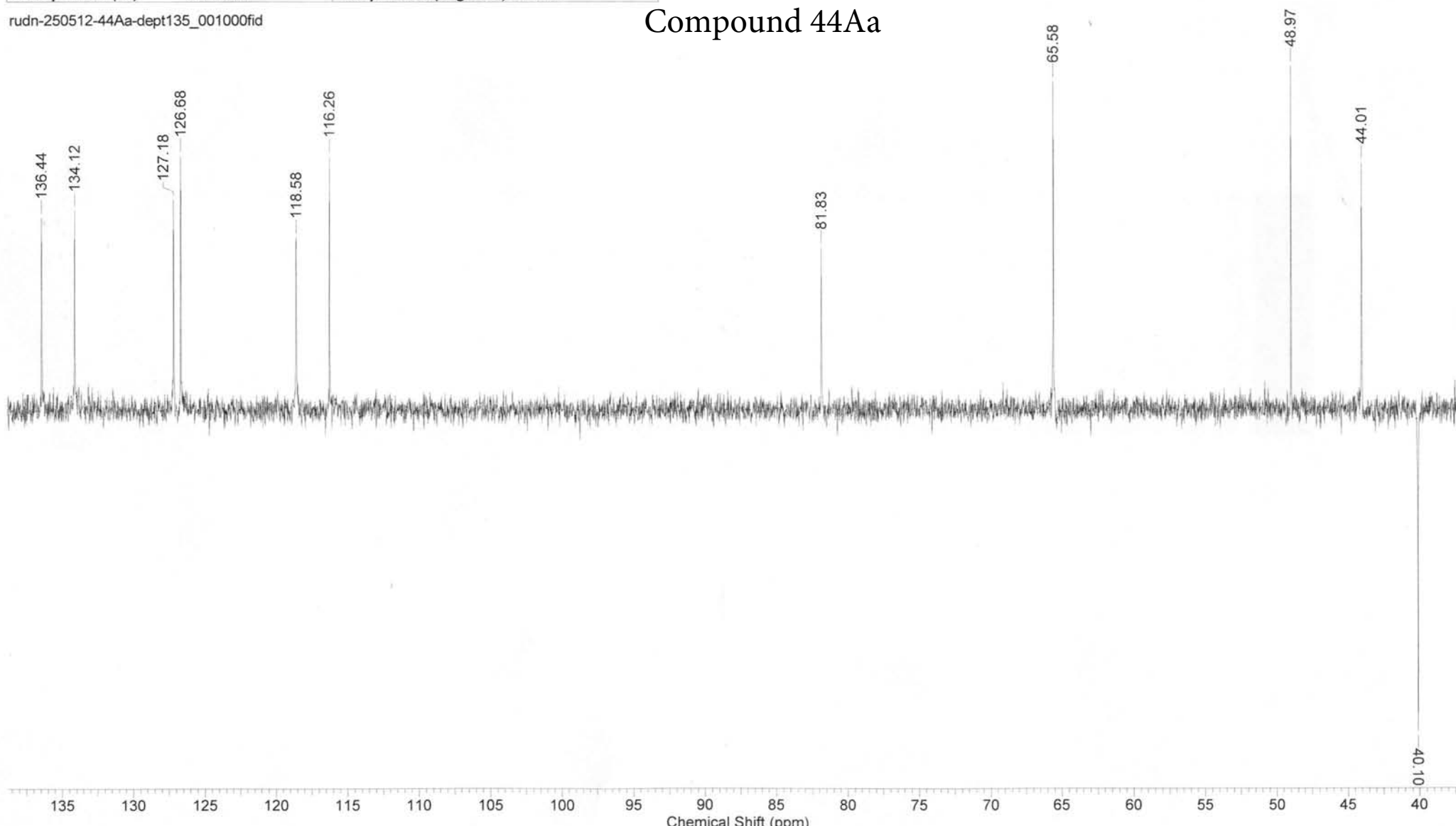
rudn-250512-44Aa-c13dec_001000fid



Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	28 May 2012 17:04:00	
Date Stamp	28 May 2012 17:04:00						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-44Aa-dept135\rudn-250512-44Aa-dept135_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	342	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	dept135
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6	Spectrum Offset (Hz)	9103.9404
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				

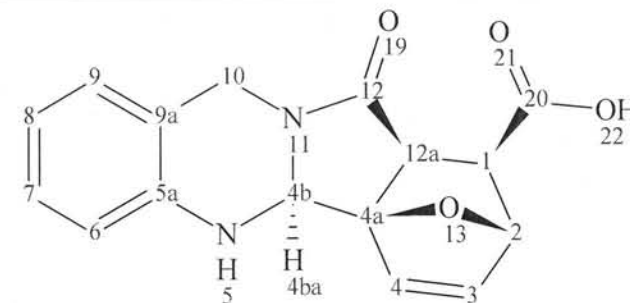
rudn-250512-44Aa-dept135_001000fid

Compound 44Aa

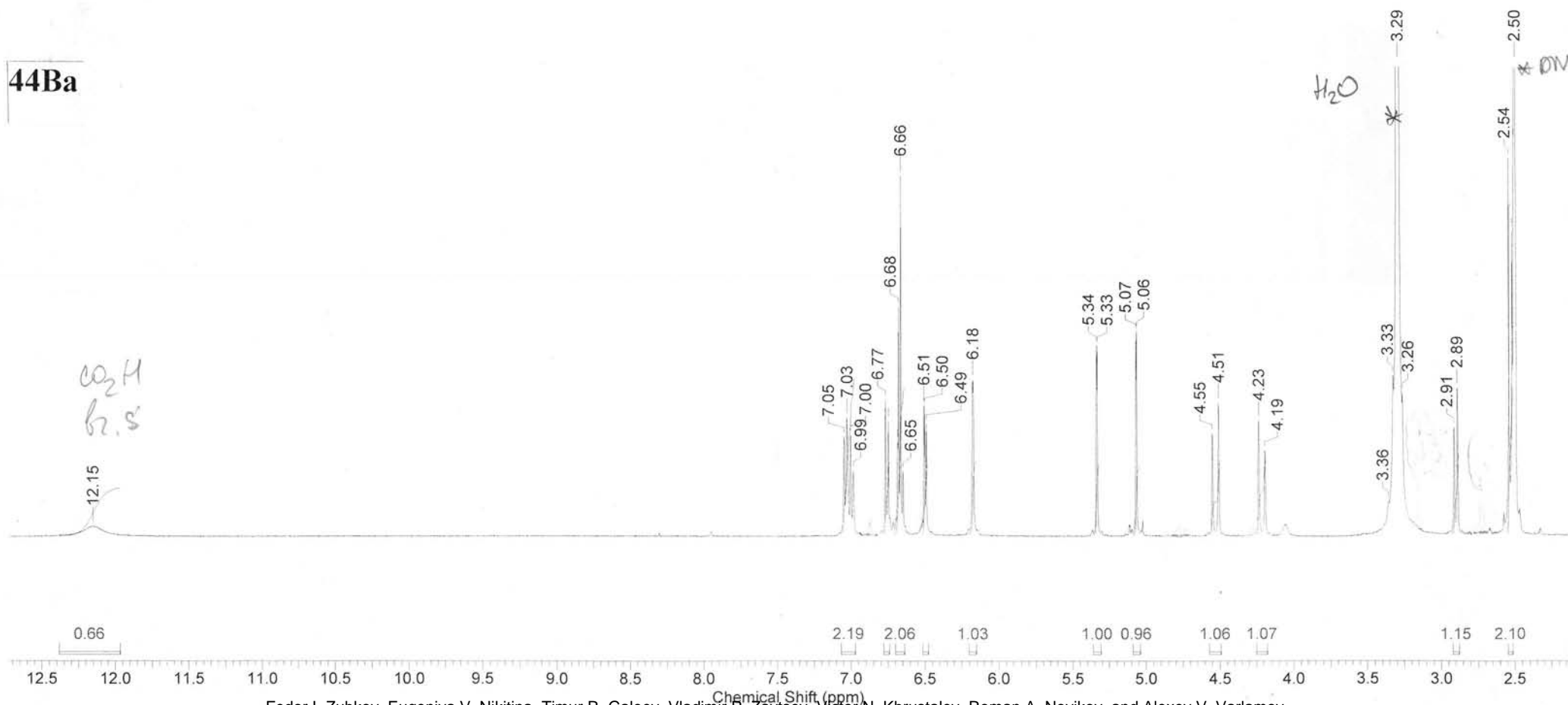


Acquisition Time (sec)	1.5729	Comment	Imported from UXNMR.		Date	26 Aug 2011 08:10:40	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-120811-N4-2\rudn-120811-N4-2_001000fid				Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	72	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	10416.67	Temperature (degree C)	32.000

Compound 44Ba



44Ba

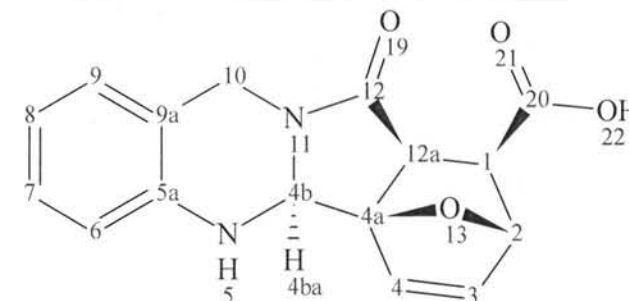


Acquisition Time (sec)	1.5729	Comment	Imported from UXMNR.		Date	26 Aug 2011 08:10:40	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-120811-N4-2\rudn-120811-N4-2_001000fid			Frequency (MHz)	400.14		
Nucleus	1H	Number of Transients	72	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	10416.67	Temperature (degree C)	32.000

H-8, 6.66, dt
(7.5; 4.0) (s)

H-4, 6.67, d (5.7)

Compound 44Ba



H-7, 7.00, dt
(7.5; 1.3)

H-9, 7.07, dd
(7.5; 1.3)

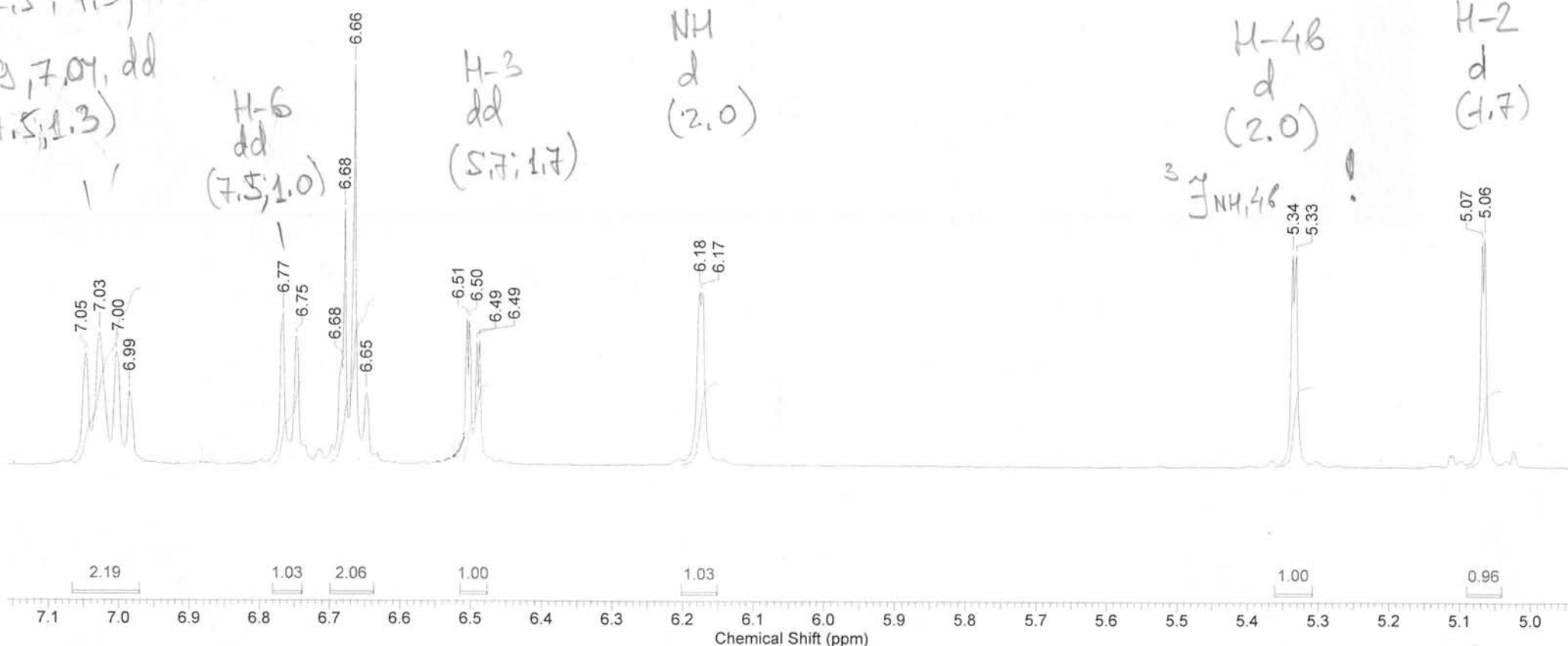
H-6
dd
(7.5; 1.0)

H-3
dd
(5.7; 1.7)

NH
d
(2.0)

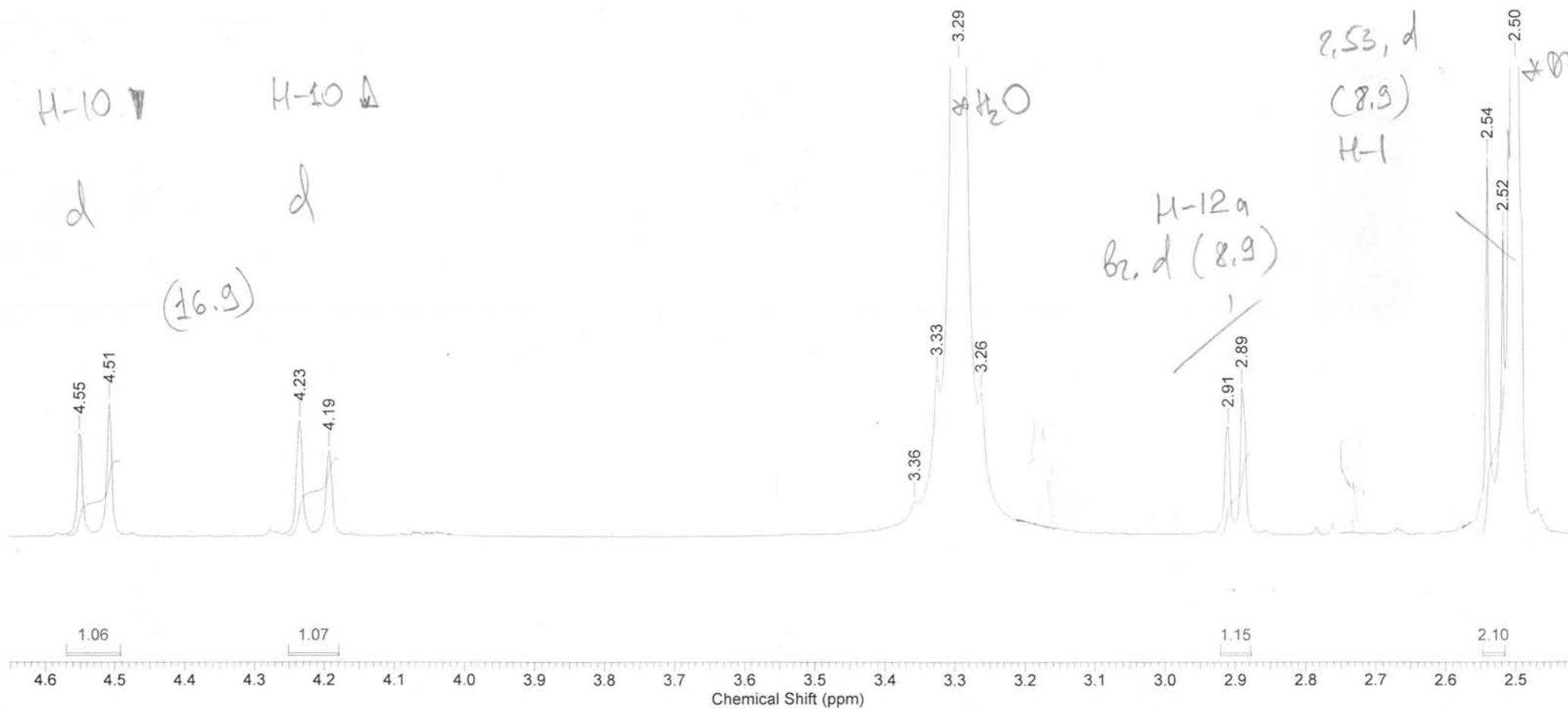
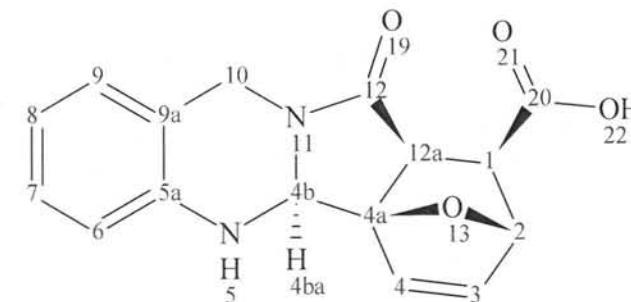
H-4b
d
(2.0)

H-2
d
(4.7)



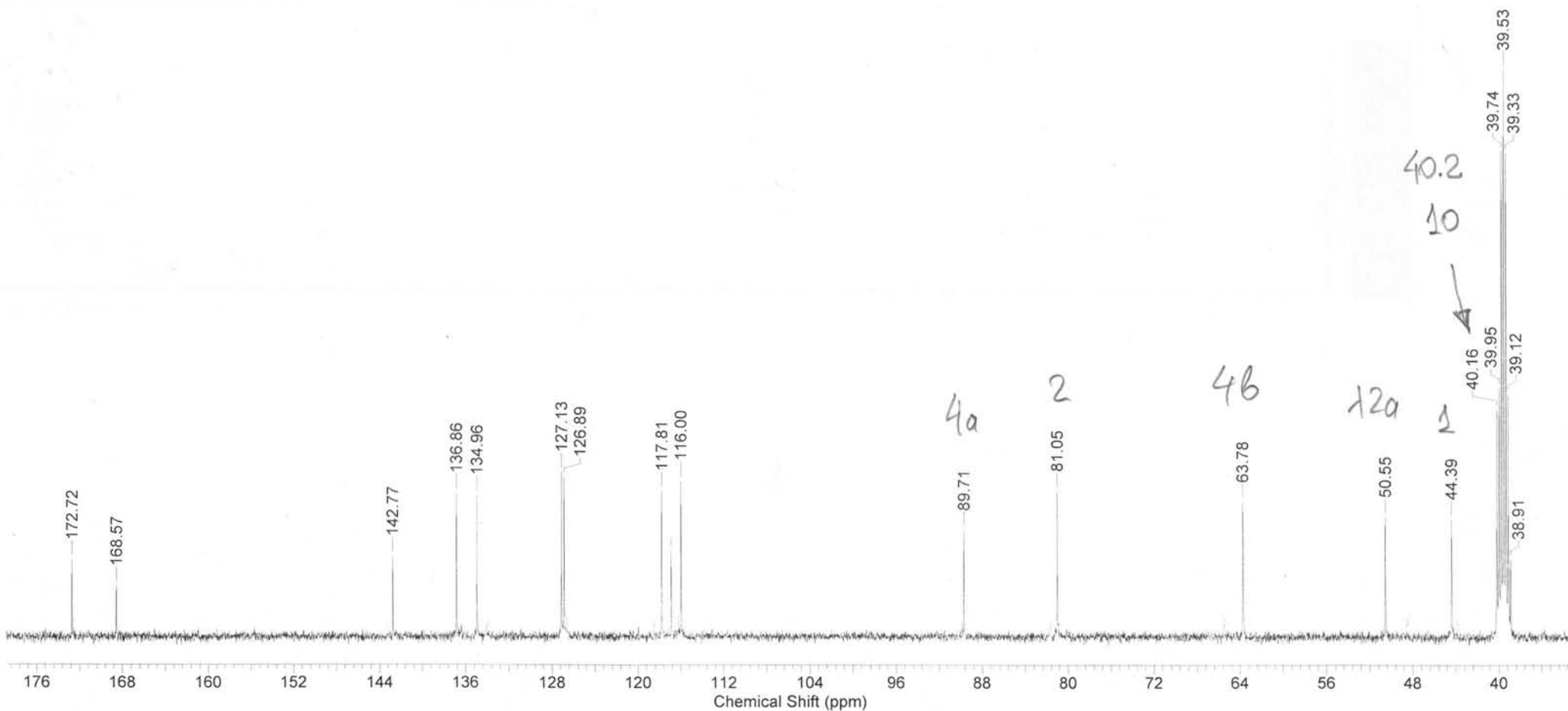
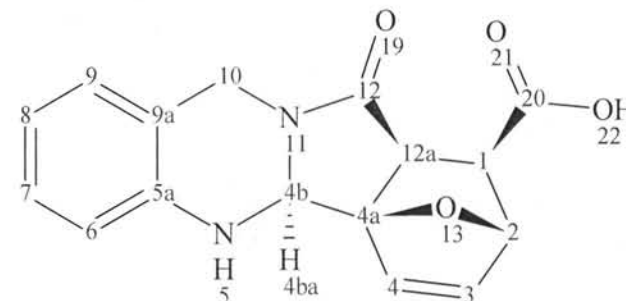
Acquisition Time (sec)	1.5729	Comment	Imported from UXMNR.		Date	26 Aug 2011 08:10:40	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-120811-N4-2\rudn-120811-N4-2_001000fid				Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	72	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	10416.67	Temperature (degree C)	32.000

Compound 44Ba



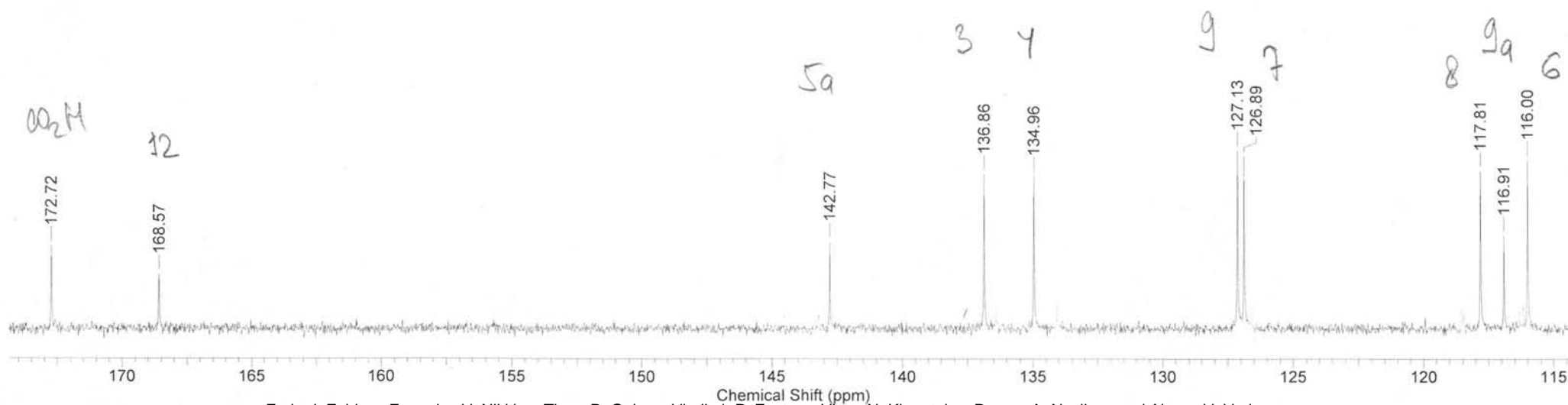
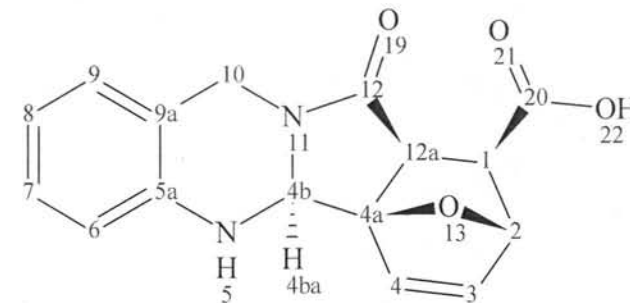
Acquisition Time (sec)	0.5243	Comment	Imported from UXMNR.		Date	25 Aug 2011 18:01:36	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-120811-N4-c13dec\rudn-120811-N4-c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	4000	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	31250.00	Temperature (degree C)	27.000

Compound 44Ba



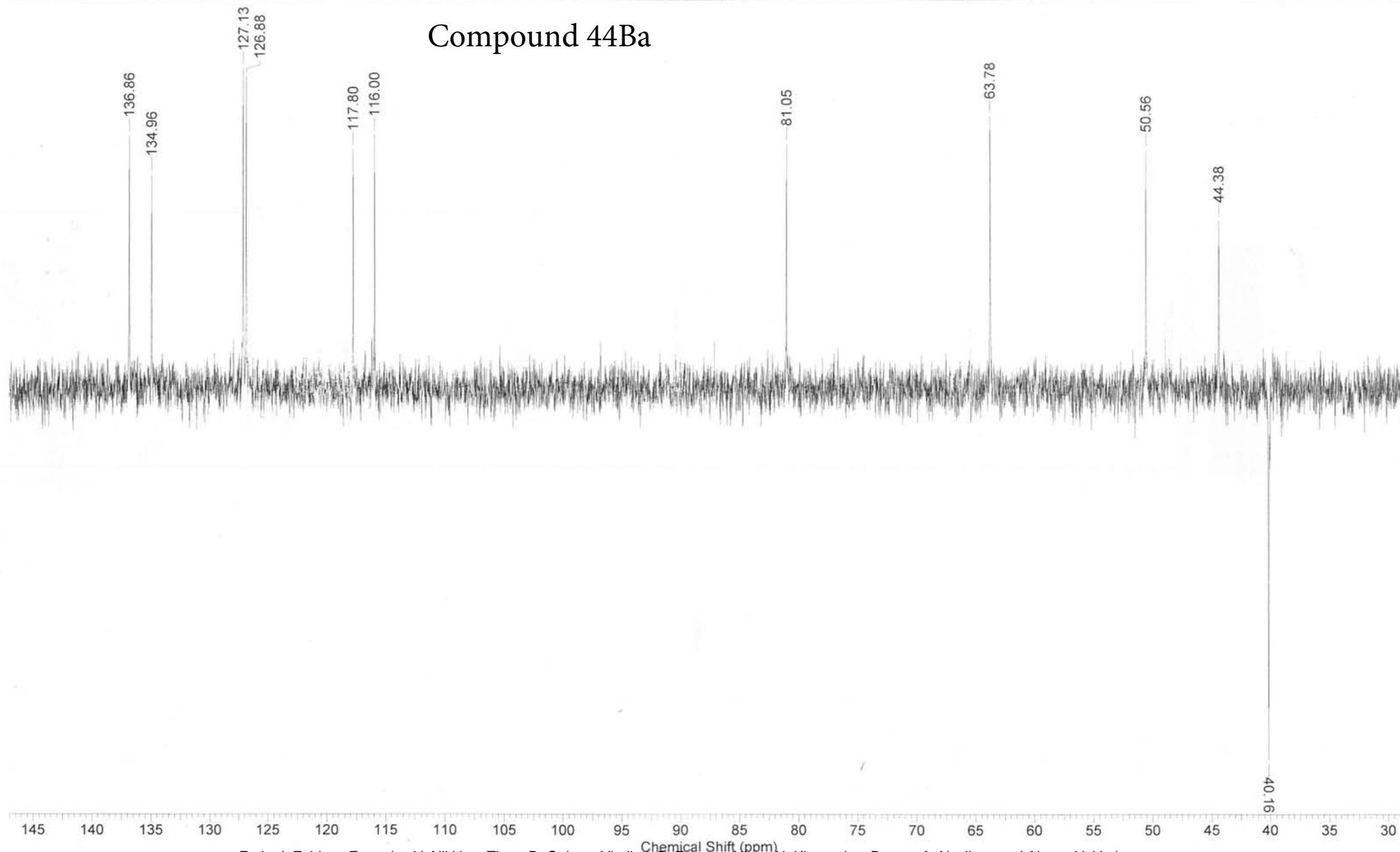
Acquisition Time (sec)	0.5243	Comment	Imported from UXMNR.		Date	25 Aug 2011 18:01:36	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-120811-N4-c13dec\rudn-120811-N4-c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	4000	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	31250.00	Temperature (degree C)	27.000

Compound 44Ba



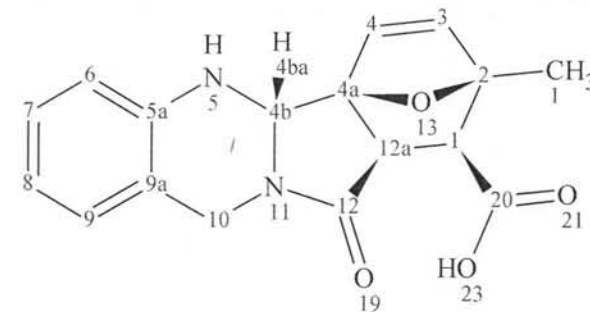
Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	25 Aug 2011 21:28:32	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-120811-N4-dept135\rudn-120811-N4-dept135_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	4000	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compound 44Ba

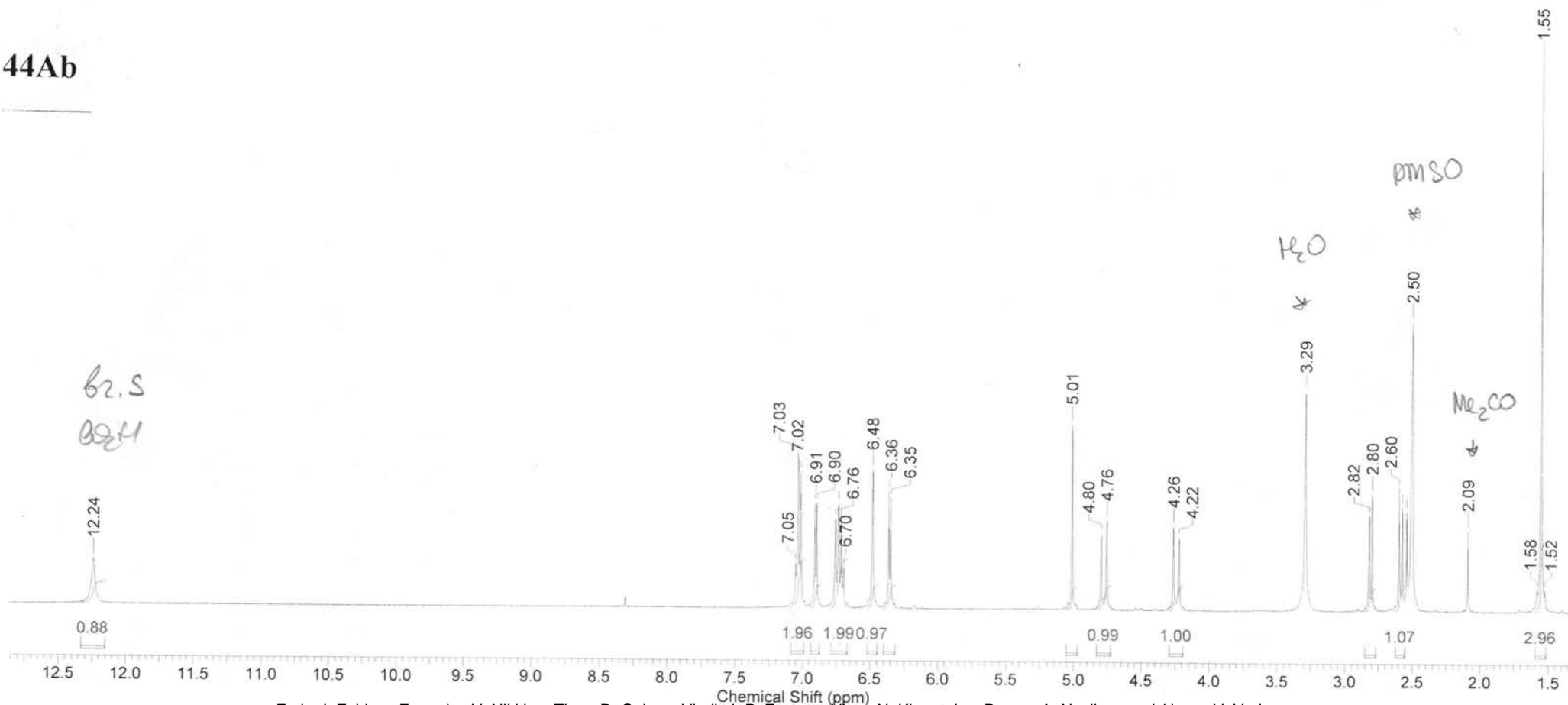


Acquisition Time (sec)	1.5729	Comment	Imported from UXMNR.		Date	14 Oct 2011 16:23:28	
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N5\rudn-141011-N5_001000fid			Frequency (MHz)	400.14		
Nucleus	1H	Number of Transients	32	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	10416.67	Temperature (degree C)	32.000

Compound 44Ab

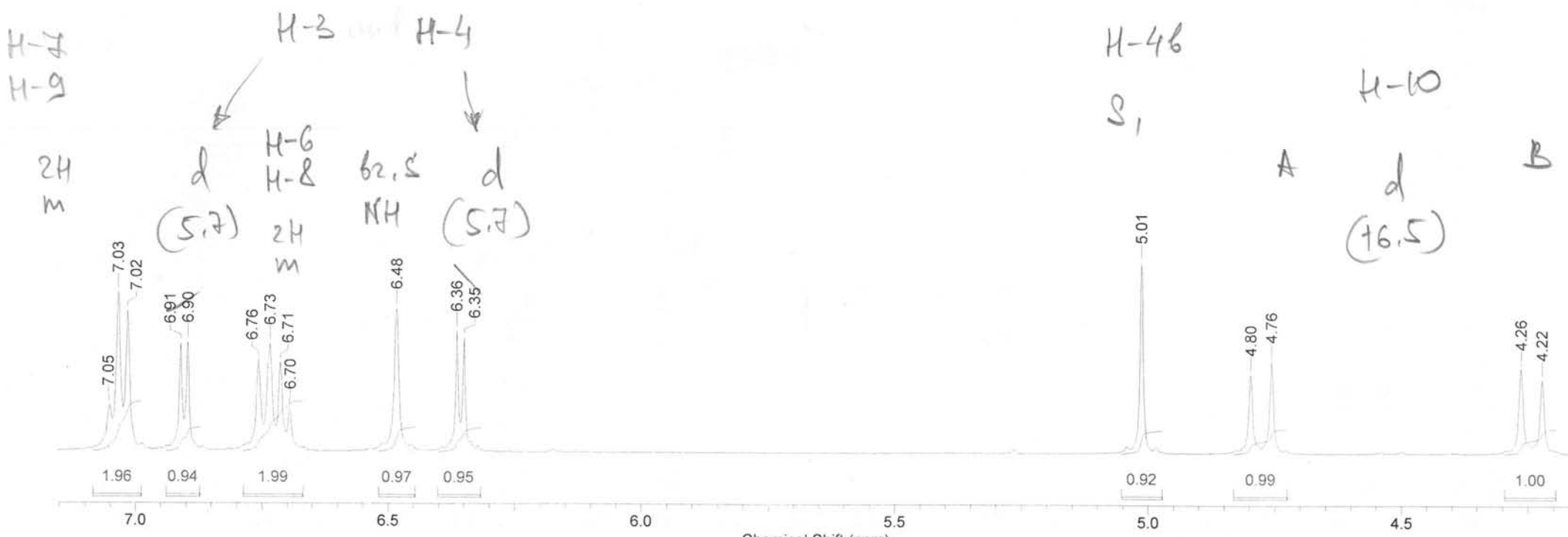
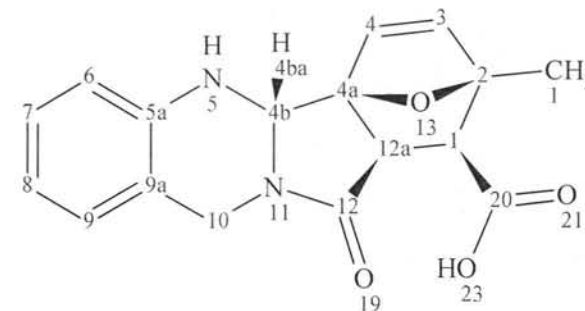


44Ab



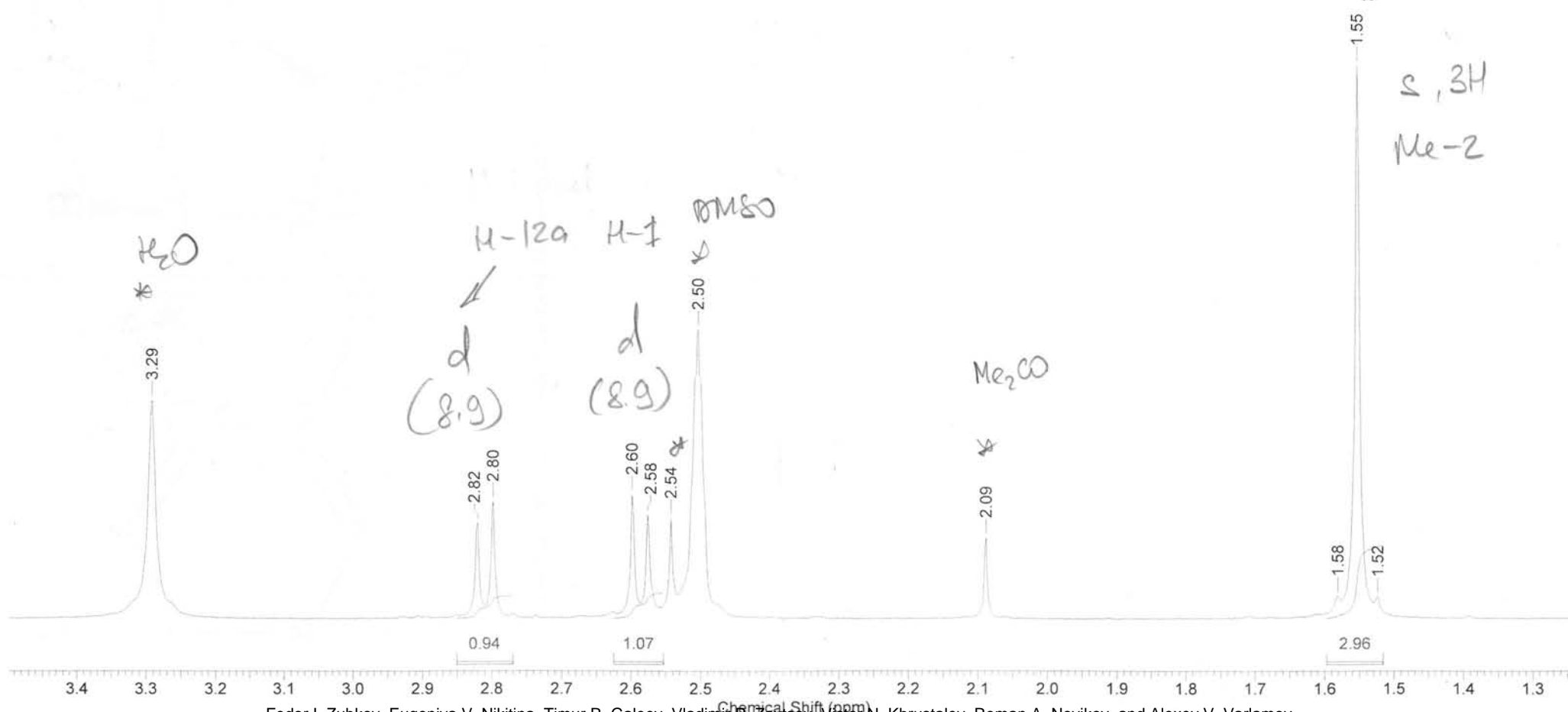
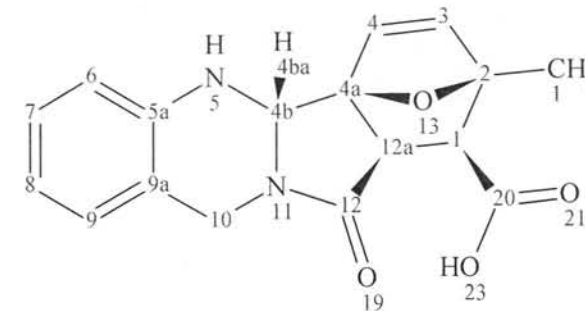
Acquisition Time (sec)	1.5729	Comment	Imported from UXNMR.		Date	14 Oct 2011 16:23:28	
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N5\rudn-141011-N5_001000fid				Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	32	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	10416.67	Temperature (degree C)	32.000

Compound 44Ab



Acquisition Time (sec)	1.5729	Comment	Imported from UXNMR.		Date	14 Oct 2011 16:23:28	
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N5\rudn-141011-N5_001000fid				Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	32	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	10416.67	Temperature (degree C)	32.000

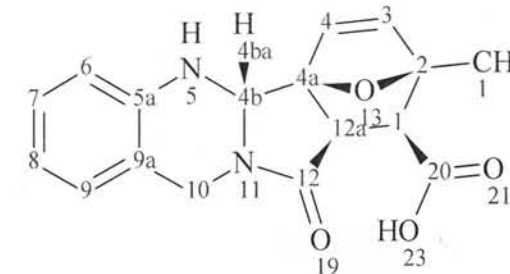
Compound 44Ab



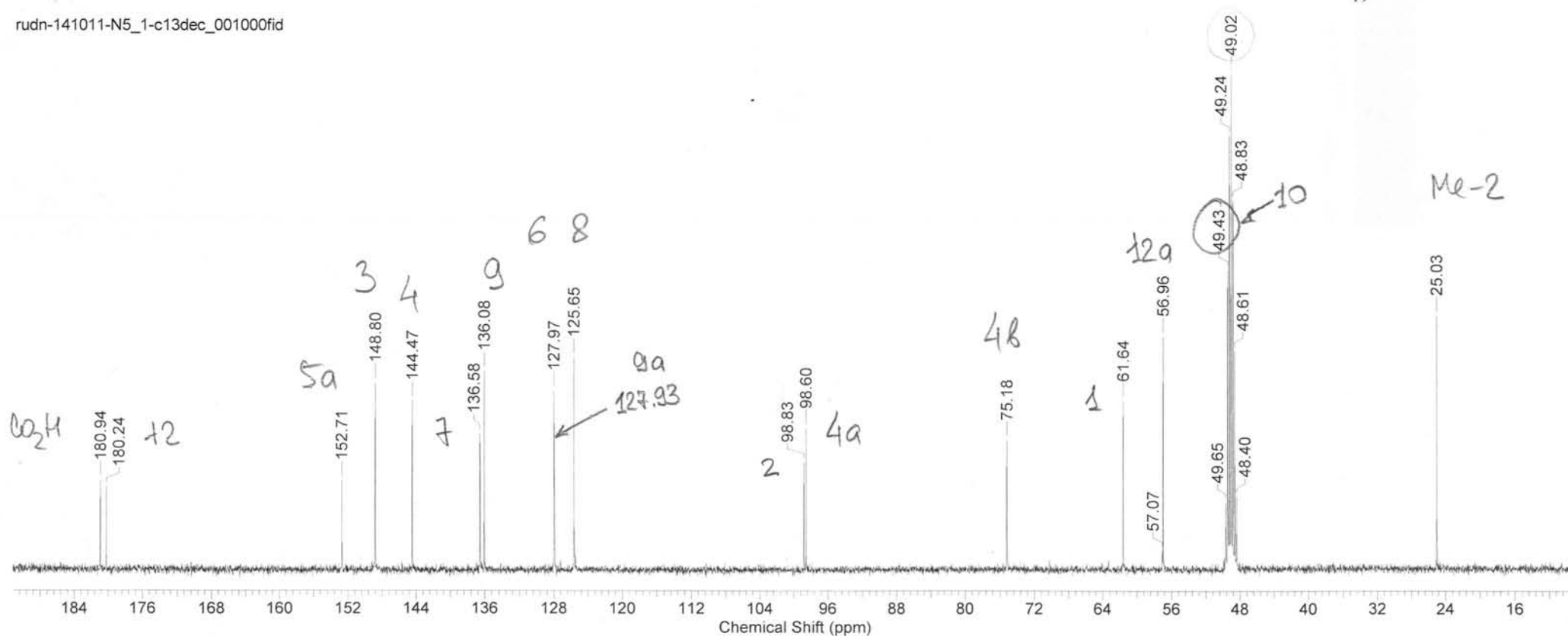
Formula $C_{17}H_{16}N_2O_4$ FW 312.3199

Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	21 Oct 2011 08:08:32
Date Stamp	21 Oct 2011 08:08:32				
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N5_1-c13dec\rudn-141011-N5_1-c13dec_001000fid			Frequency (MHz)	100.62
Nucleus	13C	Number of Transients	6000	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zgpg
SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6	Spectrum Offset (Hz)	10053.6455
Temperature (degree C)	27.000			Sweep Width (Hz)	29409.97

Compound 44Ab

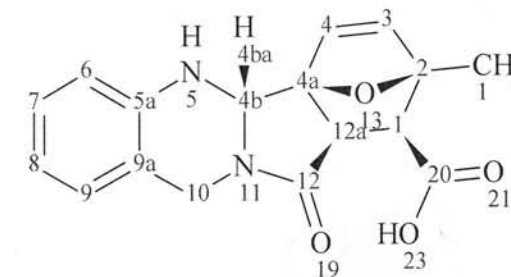


rudn-141011-N5_1-c13dec_001000fid

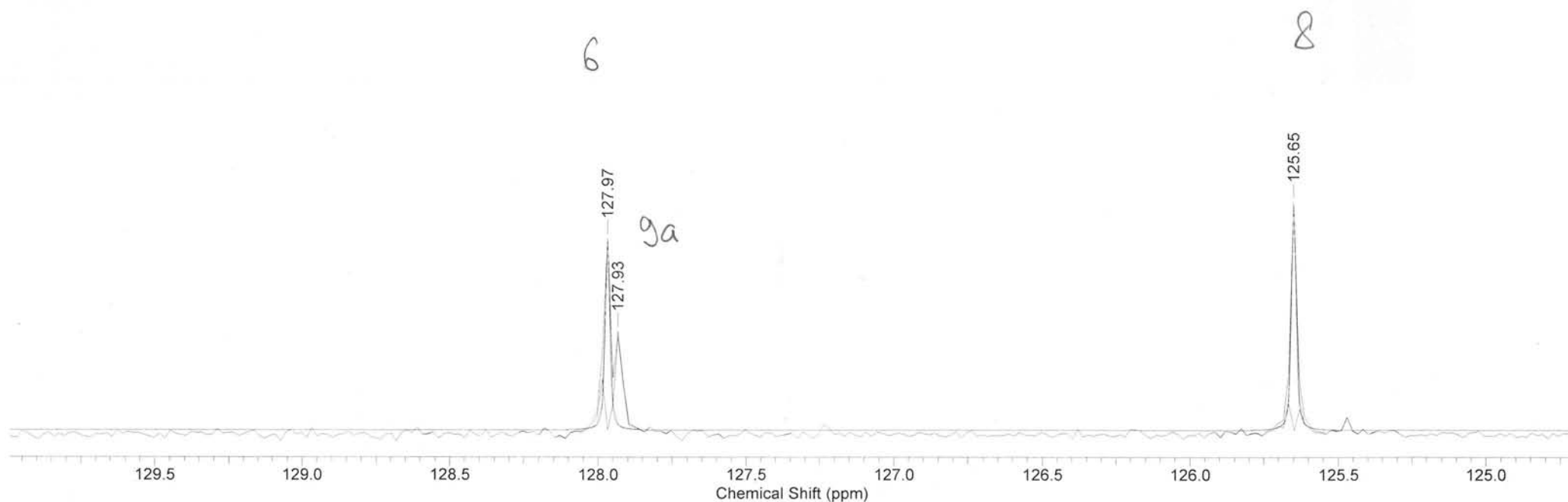


Formula C ₁₇ H ₁₆ N ₂ O ₄		FW 312.3199			
Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		
Date Stamp	21 Oct 2011 08:08:32		Date	21 Oct 2011 08:08:32	
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N5_1-c13dec\rudn-141011-N5_1-c13dec_001000fid		Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	6000	Origin	spect
Owner	root	Points Count	16384	Original Points Count	16384
SW(cyclical) (Hz)	29411.77	Pulse Sequence	zgpg	Receiver Gain	32768.00
Temperature (degree C)	27.000	Solvent	DMSO-d6	Spectrum Offset (Hz)	10053.6455
				Sweep Width (Hz)	29409.97

Compound 44Ab



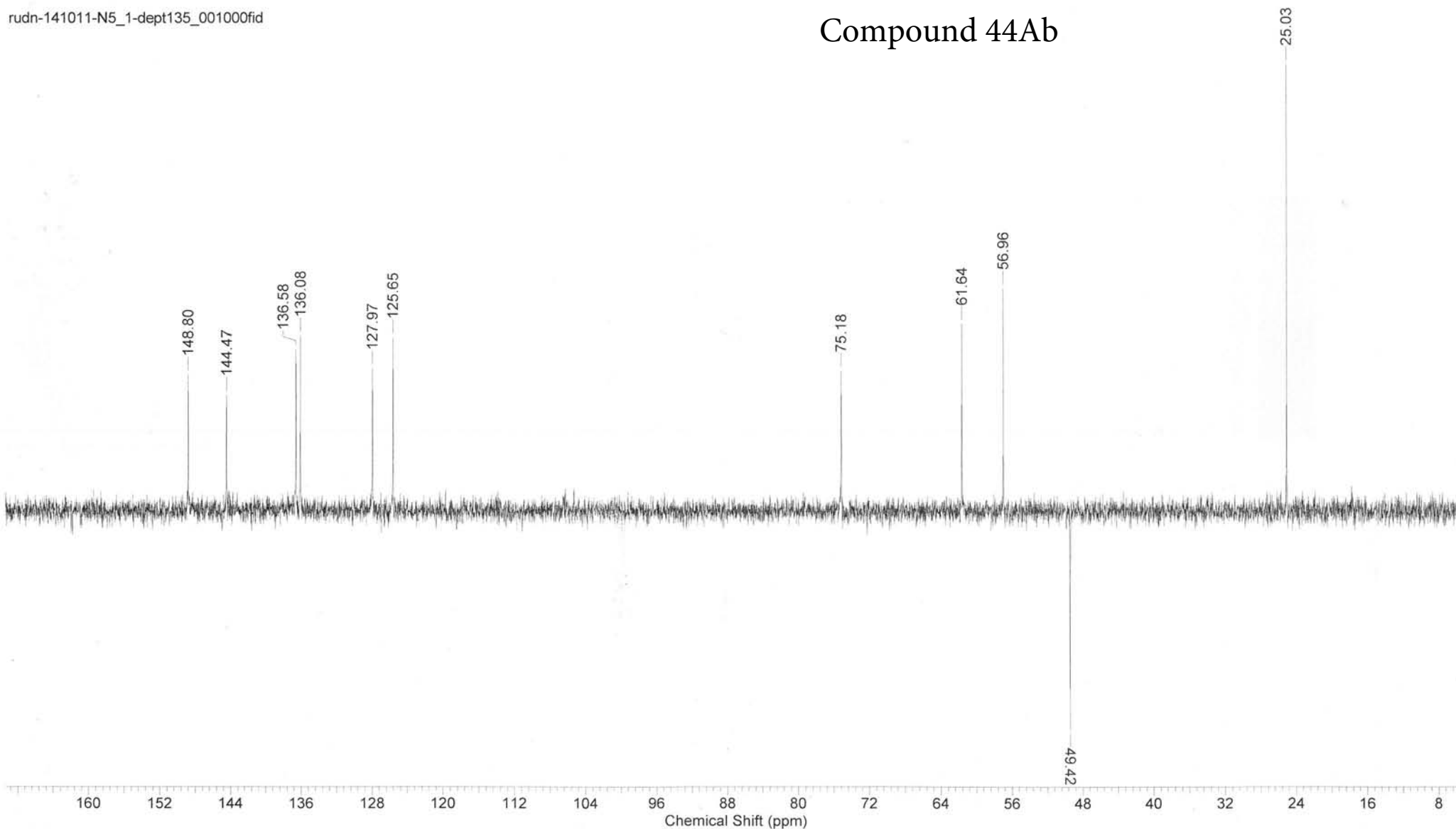
rudn-141011-N5_1-c13dec_001000fid



Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	21 Oct 2011 11:29:04	
Date Stamp	21 Oct 2011 11:29:04						
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N5_1-dept135\rudn-141011-N5_1-dept135_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	5000	Origin	spect	Original Points Count	16384
Owner	root	Points Count	16384	Pulse Sequence	dept135	Receiver Gain	32768.00
SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6	Spectrum Offset (Hz)	10053.6455	Sweep Width (Hz)	29409.97
Temperature (degree C)	27.000						

rudn-141011-N5_1-dept135_001000fid

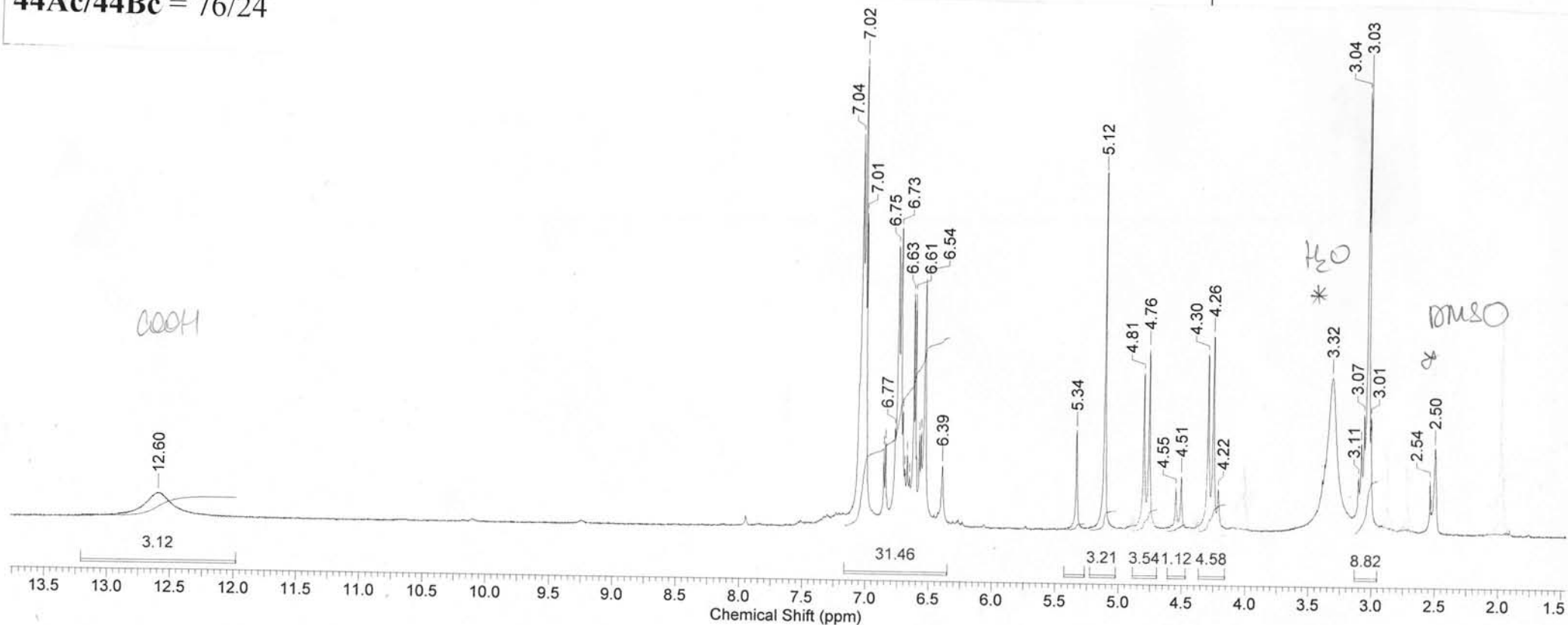
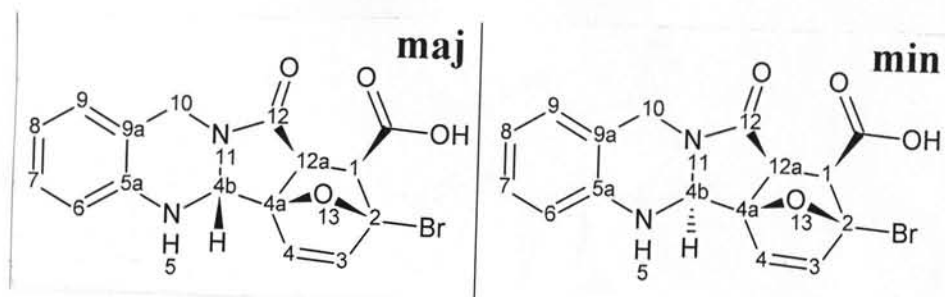
Compound 44Ab



Formula C ₁₆ H ₁₃ BrN ₂ O ₄		FW 377.1894	
Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400
Date Stamp	05 Jun 2012 17:36:00	Date	05 Jun 2012 17:36:00
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-44Ac-44Bc_1\rudn-250512-44Ac-44Bc_1_001000fid		
Frequency (MHz)	400.14	Nucleus	1H
Original Points Count	16384	Owner	root
Receiver Gain	128.00	SW(cyclical) (Hz)	10416.67
Sweep Width (Hz)	10416.03	Temperature (degree C)	32.000
		Number of Transients	12
		Points Count	16384
		Solvent	DMSO-d6
		Origin	spect
		Pulse Sequence	zg
		Spectrum Offset (Hz)	2712.0542

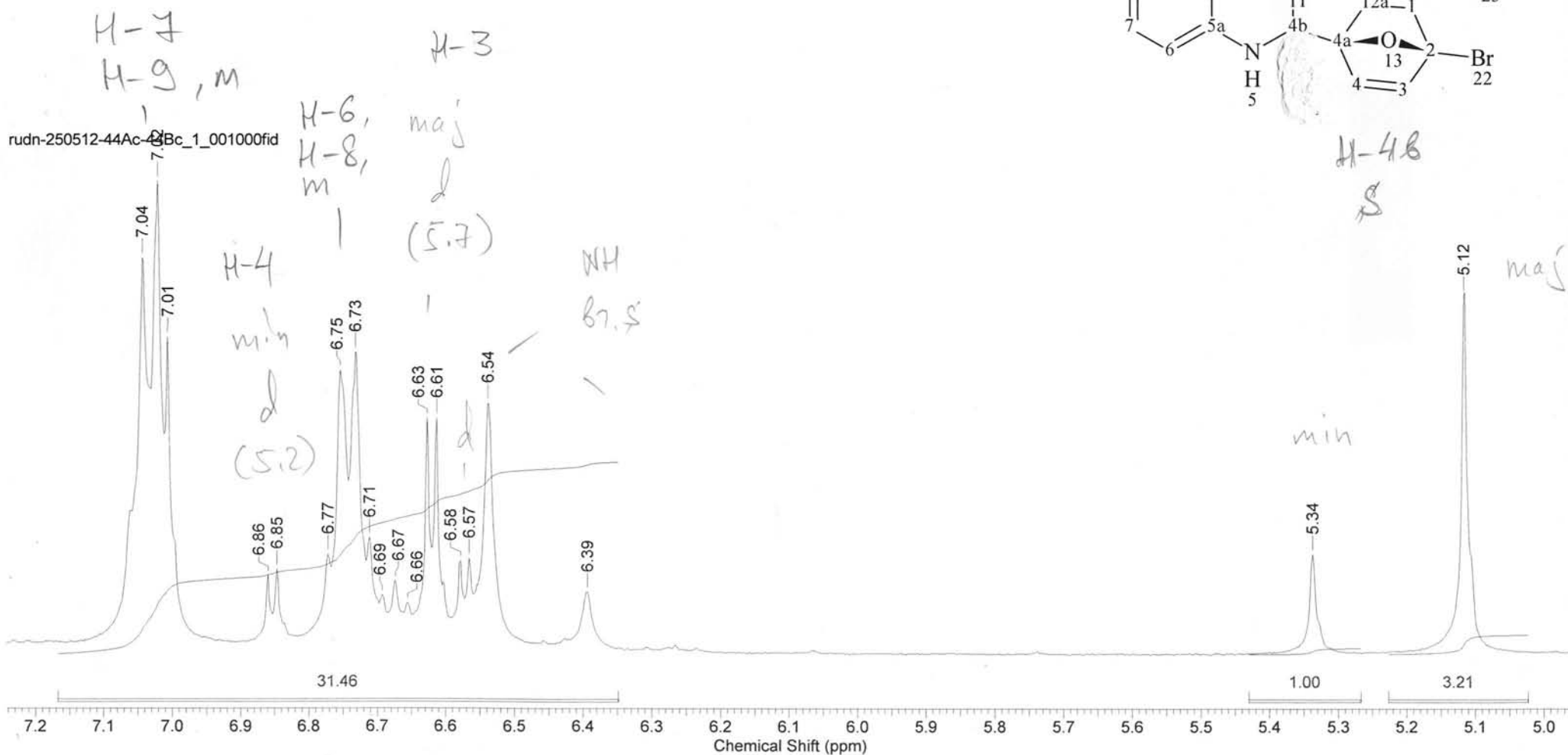
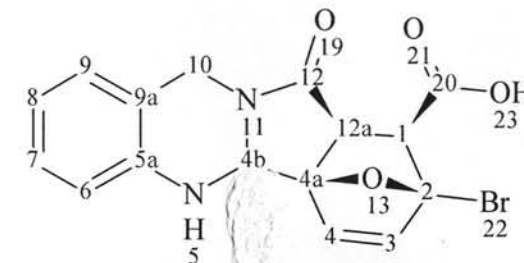
Compounds 44Ac/44Bc

44Ac/44Bc = 76/24



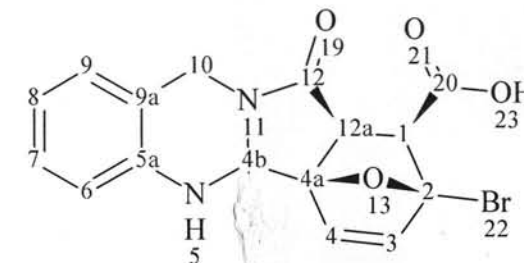
Formula C ₁₆ H ₁₃ BrN ₂ O ₄		FW 377.1894	
Acquisition Time (sec) 1.5729	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400		Date 05 Jun 2012 17:36:00
Date Stamp 05 Jun 2012 17:36:00			
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-44Ac-44Bc_1\rudn-250512-44Ac-44Bc_1_001000fid			
Frequency (MHz) 400.14	Nucleus 1H	Number of Transients 12	Origin spect
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zg
Receiver Gain 128.00	SW(cyclical) (Hz) 10416.67	Solvent DMSO-d6	Spectrum Offset (Hz) 2712.0542
Sweep Width (Hz) 10416.03	Temperature (degree C) 32.000		

Compounds 44Ac/44Bc

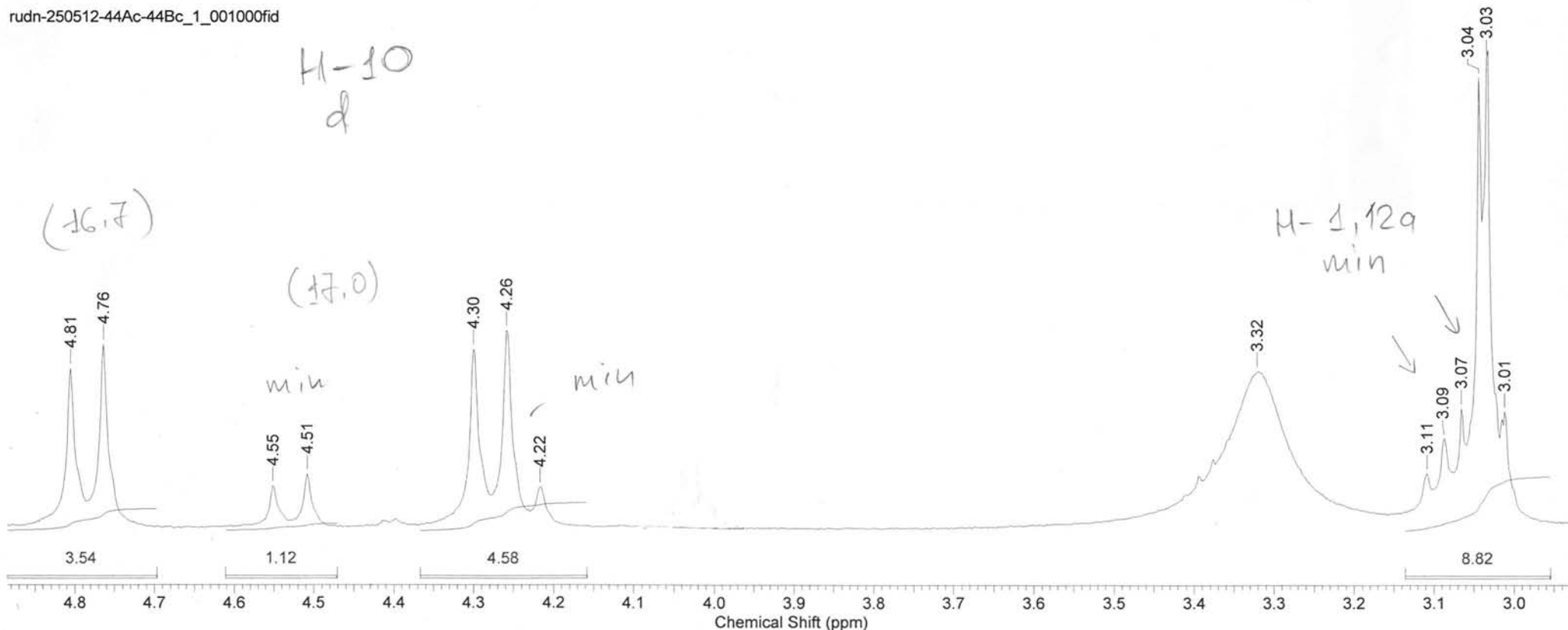


Formula C ₁₆ H ₁₃ BrN ₂ O ₄		FW 377.1894	
Acquisition Time (sec) 1.5729	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400		Date 05 Jun 2012 17:36:00
Date Stamp 05 Jun 2012 17:36:00			
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-44Ac-44Bc_1\rudn-250512-44Ac-44Bc_1_001000fid			
Frequency (MHz) 400.14	Nucleus 1H	Number of Transients 12	Origin spect
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zg
Receiver Gain 128.00	SW(cyclical) (Hz) 10416.67	Solvent DMSO-d6	Spectrum Offset (Hz) 2712.0542
Sweep Width (Hz) 10416.03	Temperature (degree C) 32.000		

Compounds 44Ac/44Bc

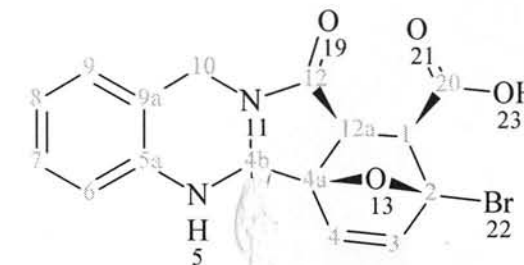


rudn-250512-44Ac-44Bc_1_001000fid

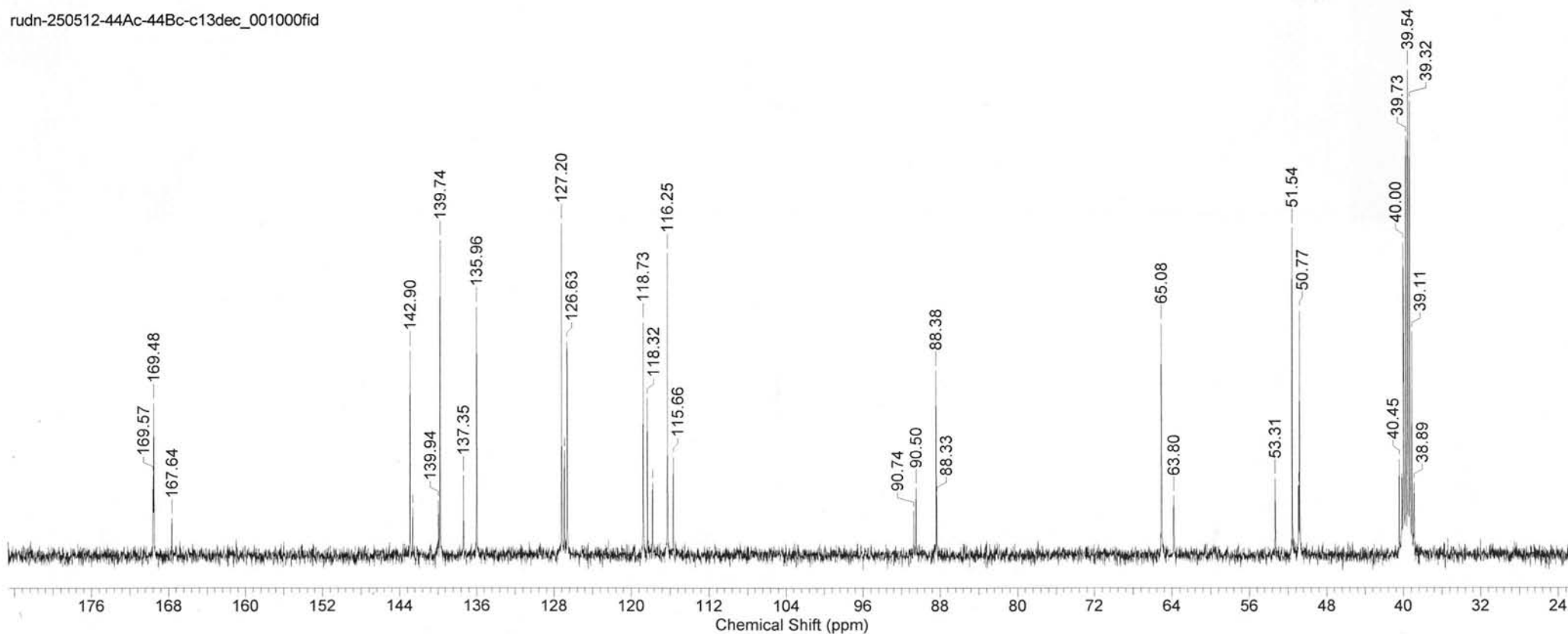


Formula C ₁₆ H ₁₃ BrN ₂ O ₄		FW 377.1894	
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400		Date 05 Jun 2012 16:25:36
Date Stamp 05 Jun 2012 16:25:36			
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-44Ac-44Bc-c13dec\rudn-250512-44Ac-44Bc-c13dec_001000fid			
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 3812	Origin spect
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10549.4092
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000		

Compounds 44Ac/44Bc

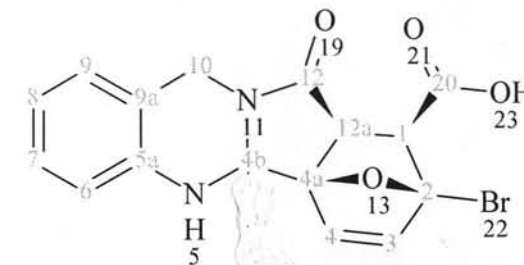


rudn-250512-44Ac-44Bc-c13dec_001000fid

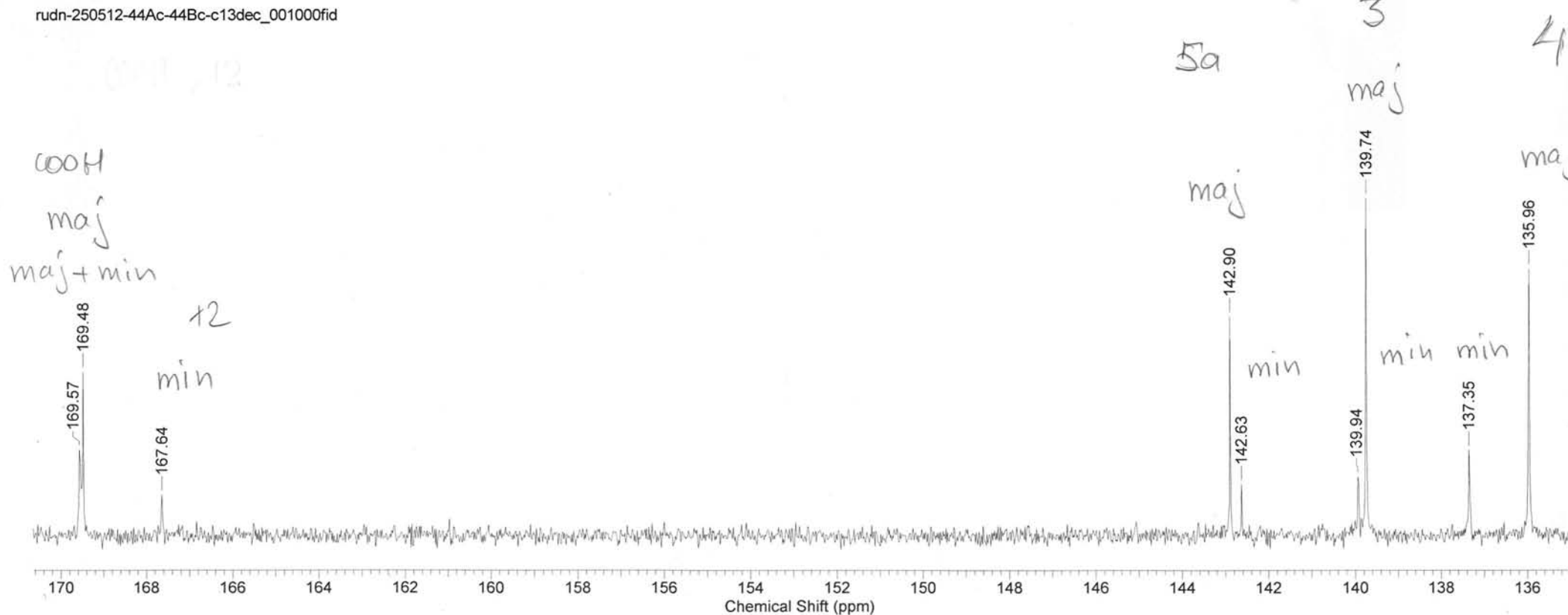


Formula C ₁₆ H ₁₃ BrN ₂ O ₄		FW 377.1894	
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400		Date 05 Jun 2012 16:25:36
Date Stamp 05 Jun 2012 16:25:36			
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-44Ac-44Bc-c13dec\rudn-250512-44Ac-44Bc-c13dec_001000fid			
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 3812	Origin spect
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10549.4092
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000		

Compounds 44Ac/44Bc

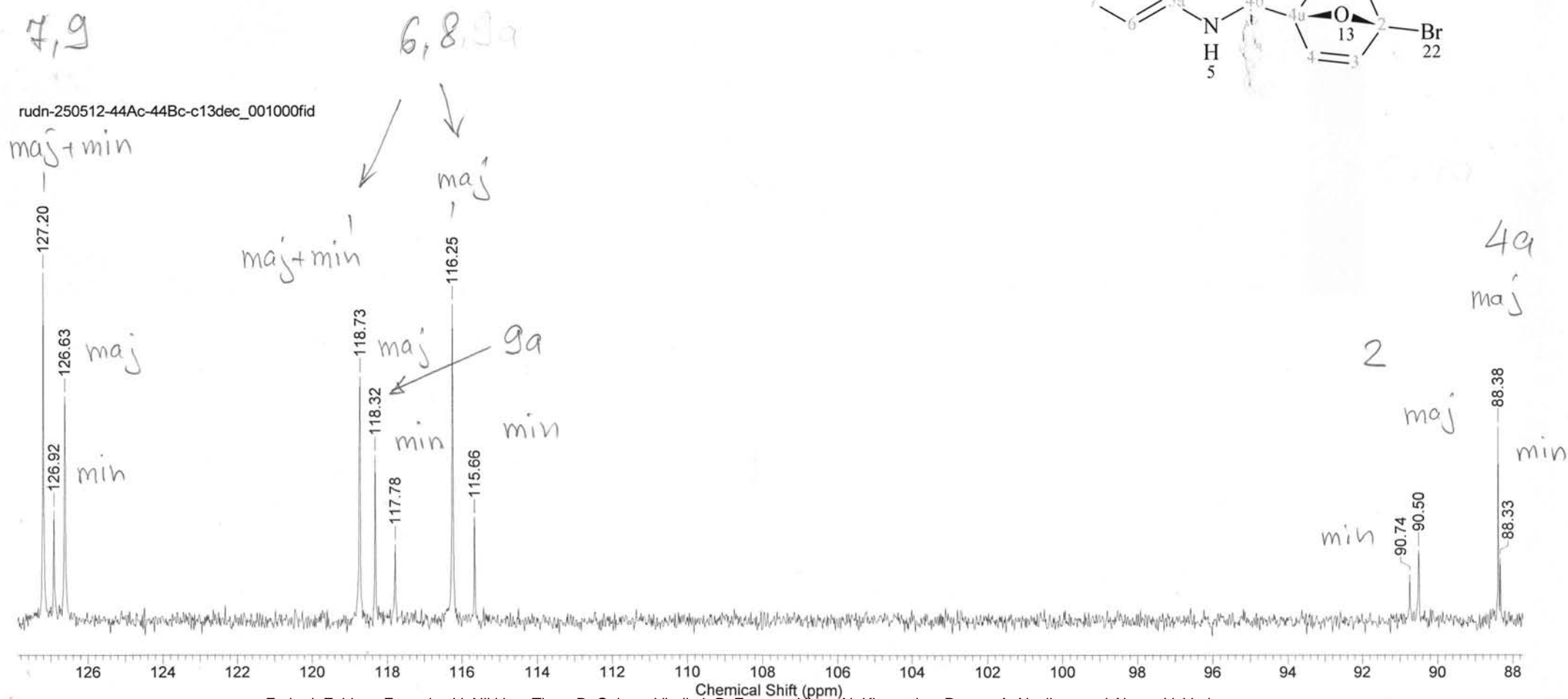
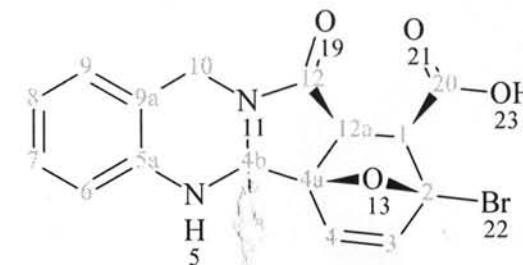


rudn-250512-44Ac-44Bc-c13dec_001000fid



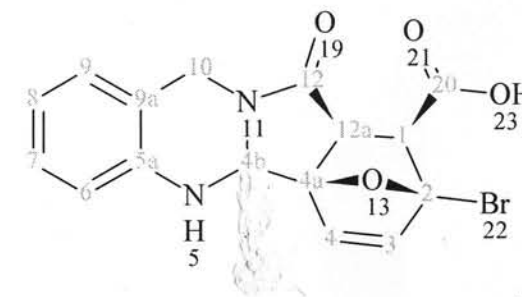
Formula C ₁₆ H ₁₃ BrN ₂ O ₄		FW 377.1894					
Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	05 Jun 2012 16:25:36		
Date Stamp	05 Jun 2012 16:25:36						
File Name	C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-44Ac-44Bc-c13dec\rudn-250512-44Ac-44Bc-c13dec_001000fid						
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	3812	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zgpg
Receiver Gain	32768.00	SW(cyclical) (Hz)	29411.77	Solvent	DMSO-d6	Spectrum Offset (Hz)	10549.4092
Sweep Width (Hz)	29409.97	Temperature (degree C)	27.000				

Compounds 44Ac/44Bc



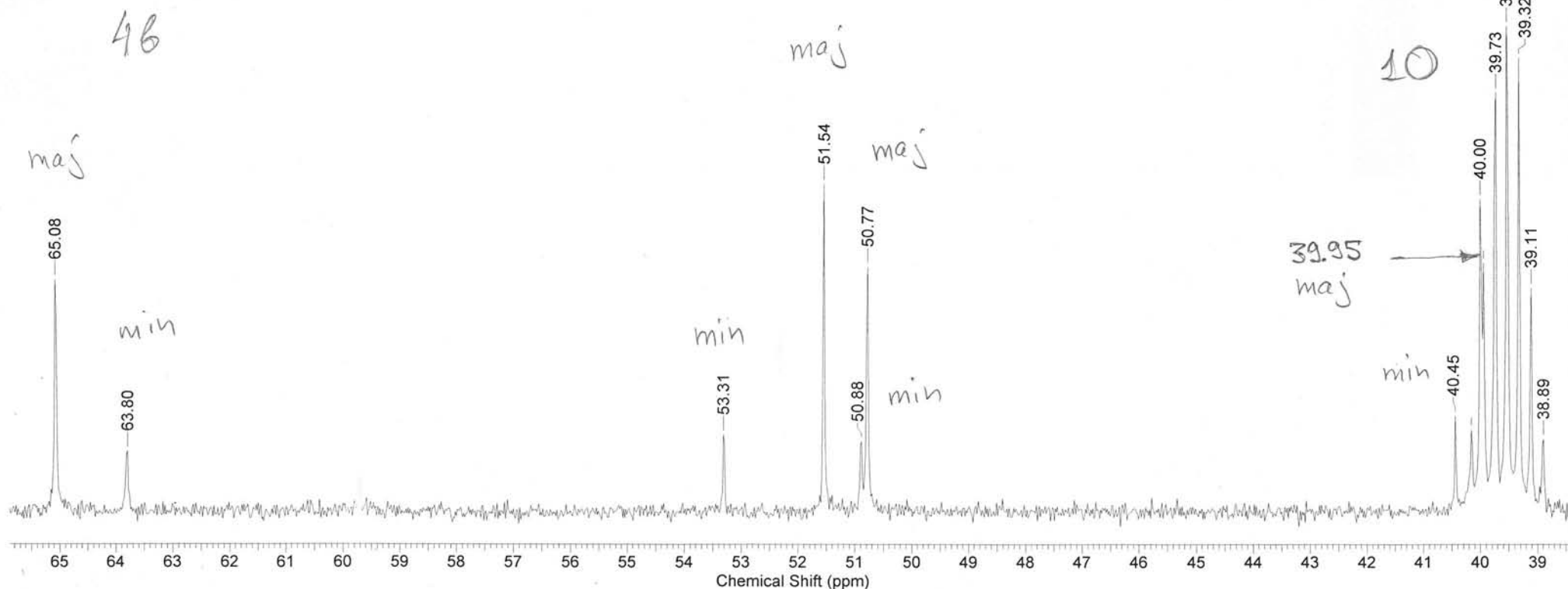
Formula C ₁₆ H ₁₃ BrN ₂ O ₄		FW 377.1894	
Acquisition Time (sec) 0.5571	Comment 5 mm QNP 1H/15N/13C/31P Z3379/0400		Date 05 Jun 2012 16:25:36
Date Stamp 05 Jun 2012 16:25:36			
File Name C:\Users\Fedor\Desktop\C13 Рома Для Статьи в JOC 25.05.12\rudn-250512-44Ac-44Bc-c13dec\rudn-250512-44Ac-44Bc-c13dec_001000fid			
Frequency (MHz) 100.62	Nucleus 13C	Number of Transients 3812	Origin spect
Original Points Count 16384	Owner root	Points Count 16384	Pulse Sequence zgpg
Receiver Gain 32768.00	SW(cyclical) (Hz) 29411.77	Solvent DMSO-d6	Spectrum Offset (Hz) 10549.4092
Sweep Width (Hz) 29409.97	Temperature (degree C) 27.000		

Compounds 44Ac/44Bc



1, 12a

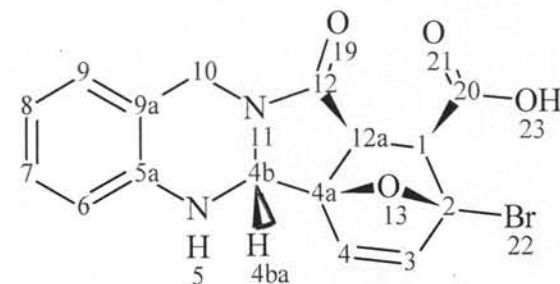
rudn-250512-44Ac-44Bc-c13dec_001000fid



Formula $C_{16}H_{13}BrN_2O_4$ FW 377.1894

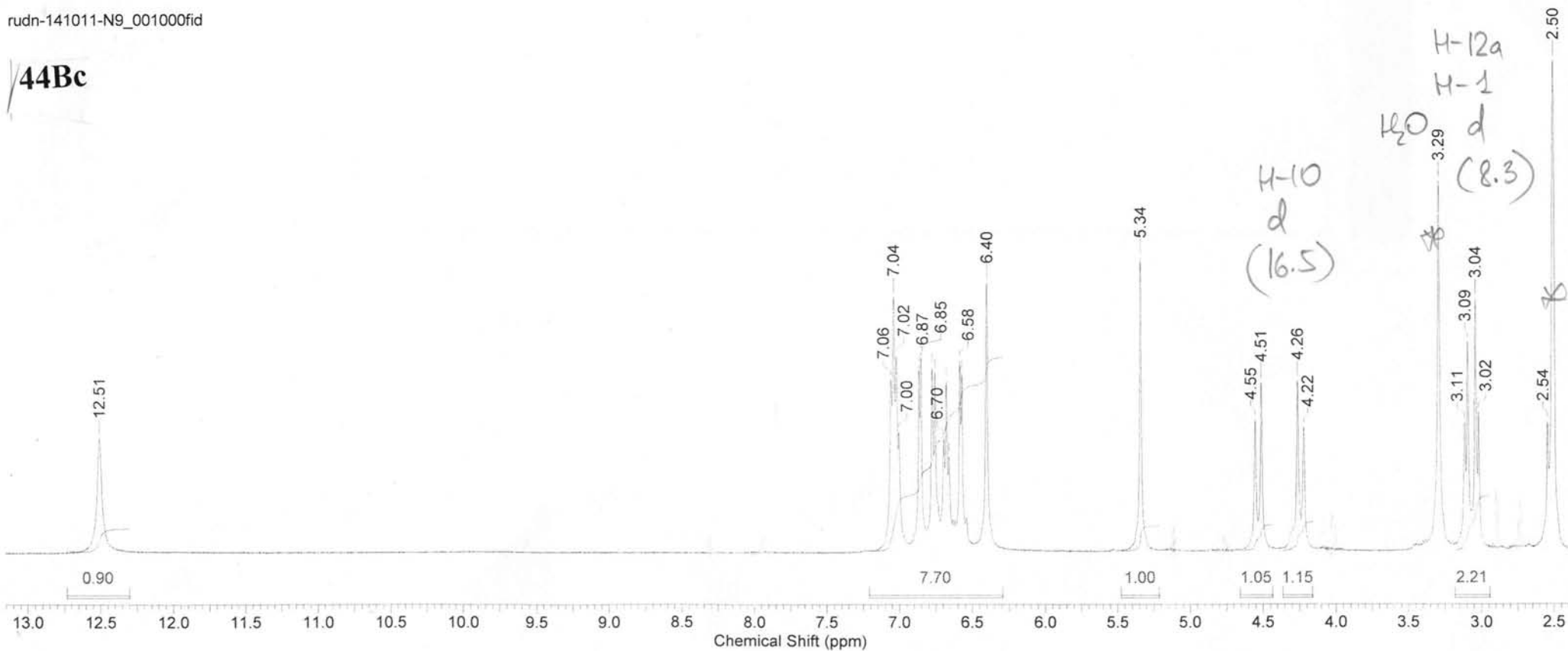
Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	14 Oct 2011 16:40:32
Date Stamp	14 Oct 2011 16:40:32	File Name	D:\NMR\14.10.11 (Рома)\rudn-141011-N9\rudn-141011-N9_001000fid	Origin	spect
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	48
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	512.00	SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6
Sweep Width (Hz)	10416.03	Temperature (degree C)	32.000	Spectrum Offset (Hz)	2712.0542

Compound 44Bc



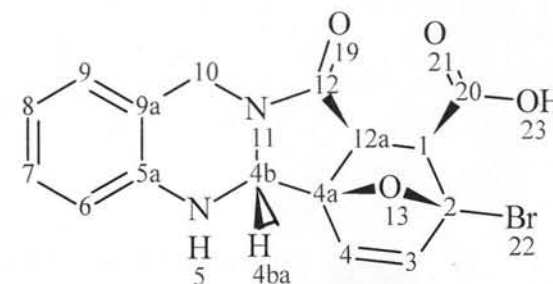
rudn-141011-N9_001000fid

44Bc



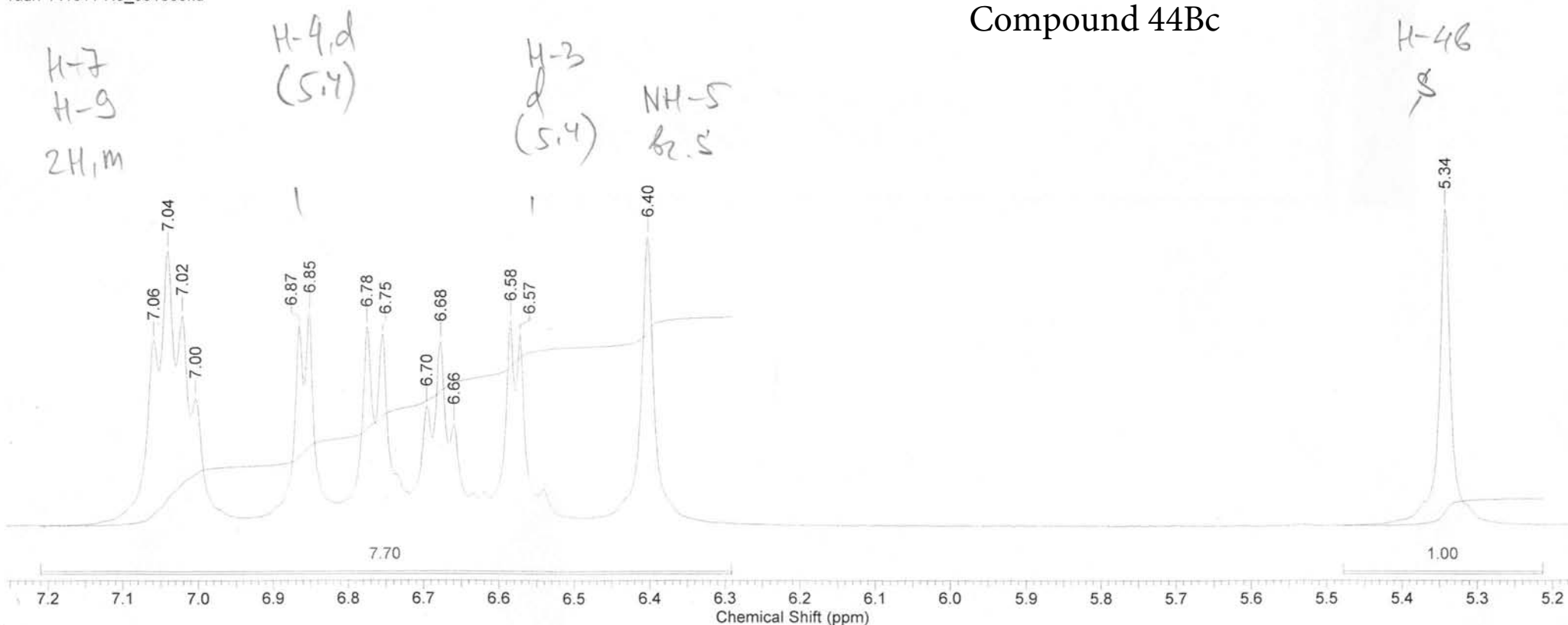
Formula C₁₆H₁₃BrN₂O₄ FW 377.1894

Acquisition Time (sec)	1.5729	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	14 Oct 2011 16:40:32	
Date Stamp	14 Oct 2011 16:40:32	File Name	D:\NMR\14.10.11 (Poma)\rudn-141011-N9\rudn-141011-N9_001000fid				
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	48	Origin	spect
Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence	zg
Receiver Gain	512.00	SW(cyclical) (Hz)	10416.67	Solvent	DMSO-d6	Spectrum Offset (Hz)	2712.0542
Sweep Width (Hz)	10416.03	Temperature (degree C)	32.000				



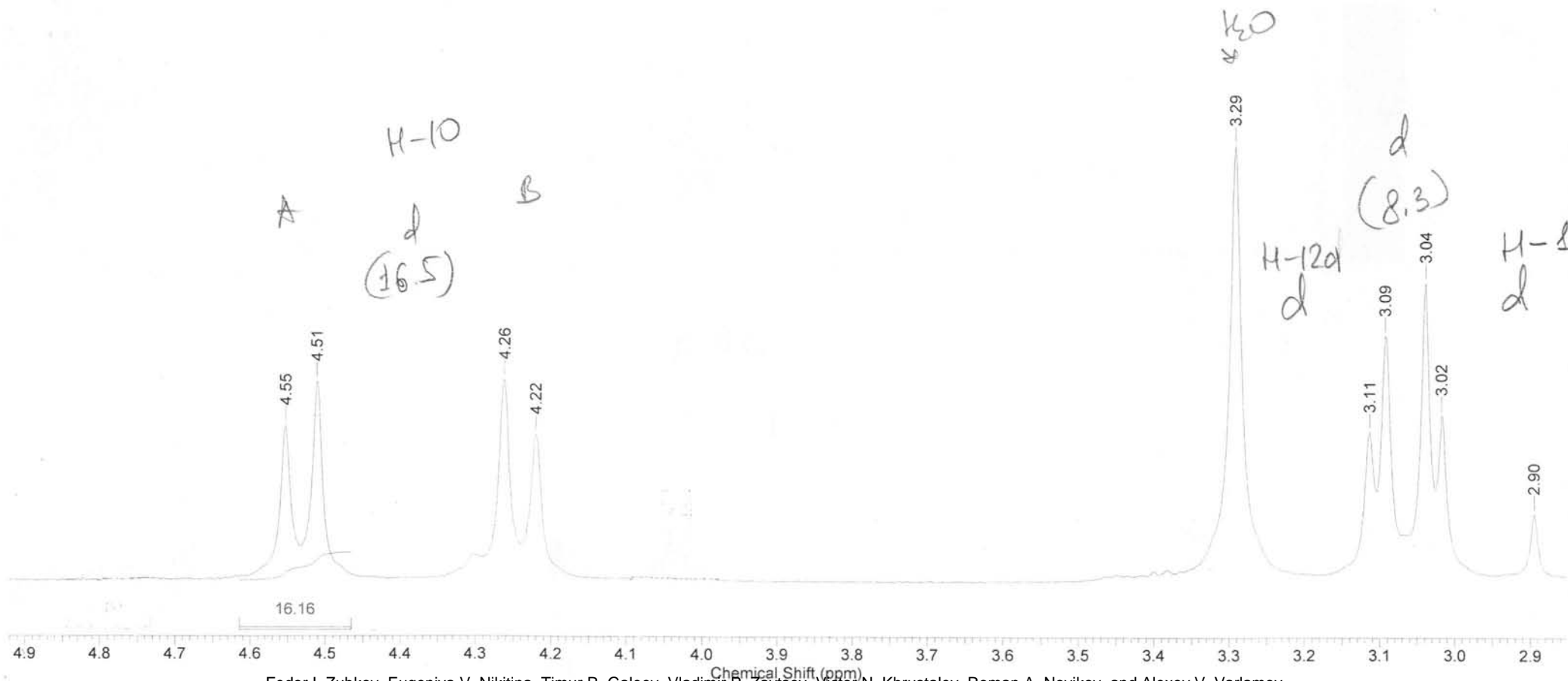
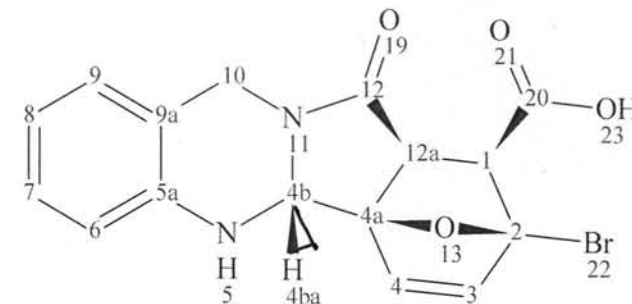
rudn-141011-N9_001000fid

Compound 44Bc



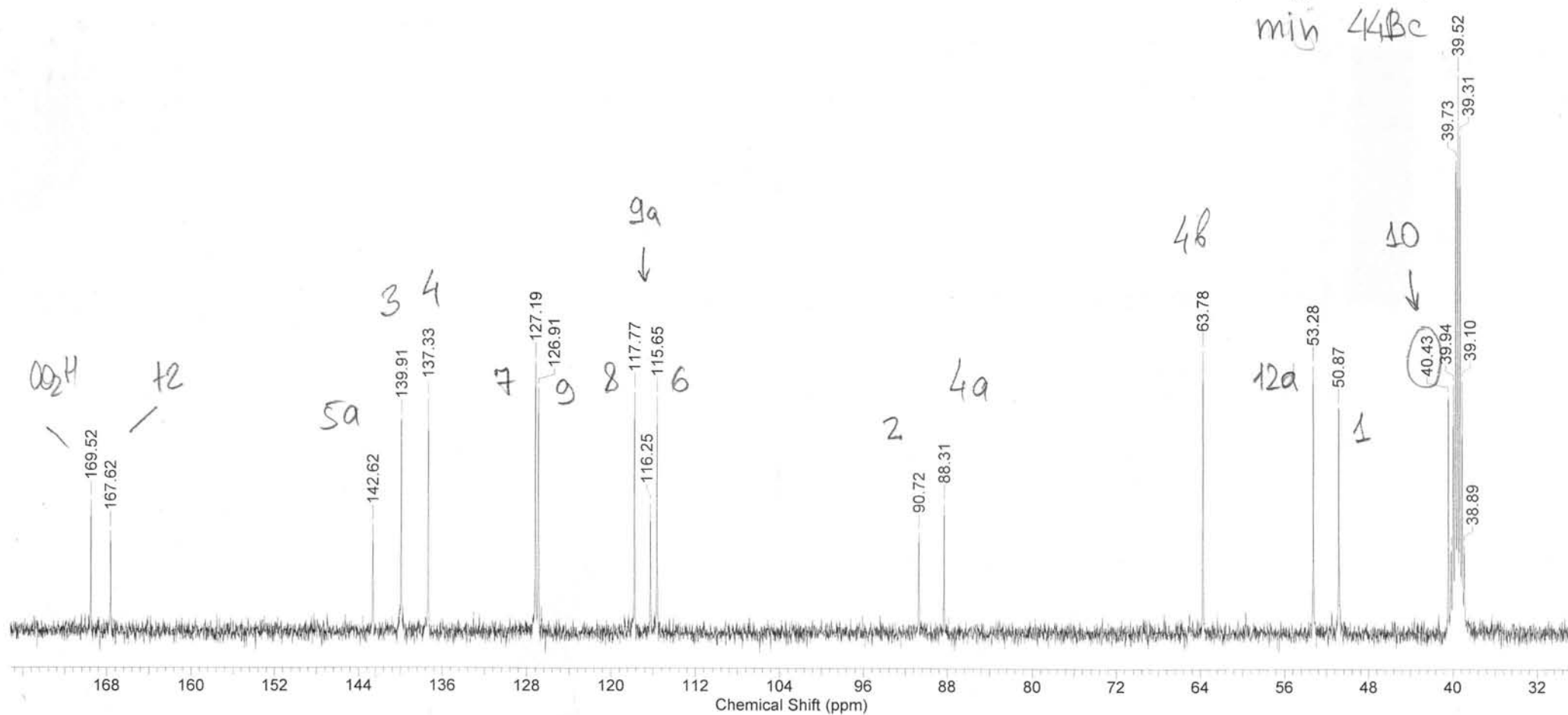
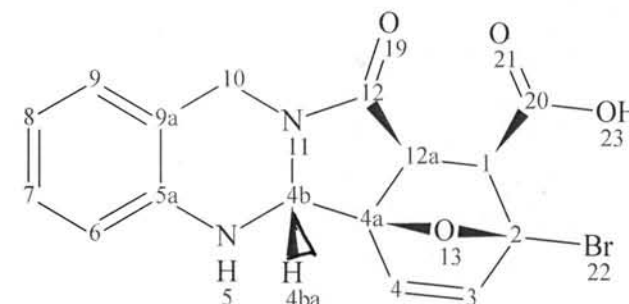
Acquisition Time (sec)	1.5729	Comment	Imported from UXNMR.		Date	14 Oct 2011 16:40:32	
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N9\rudn-141011-N9_001000fid				Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	48	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	10416.67	Temperature (degree C)	32.000

Compound 44Bc



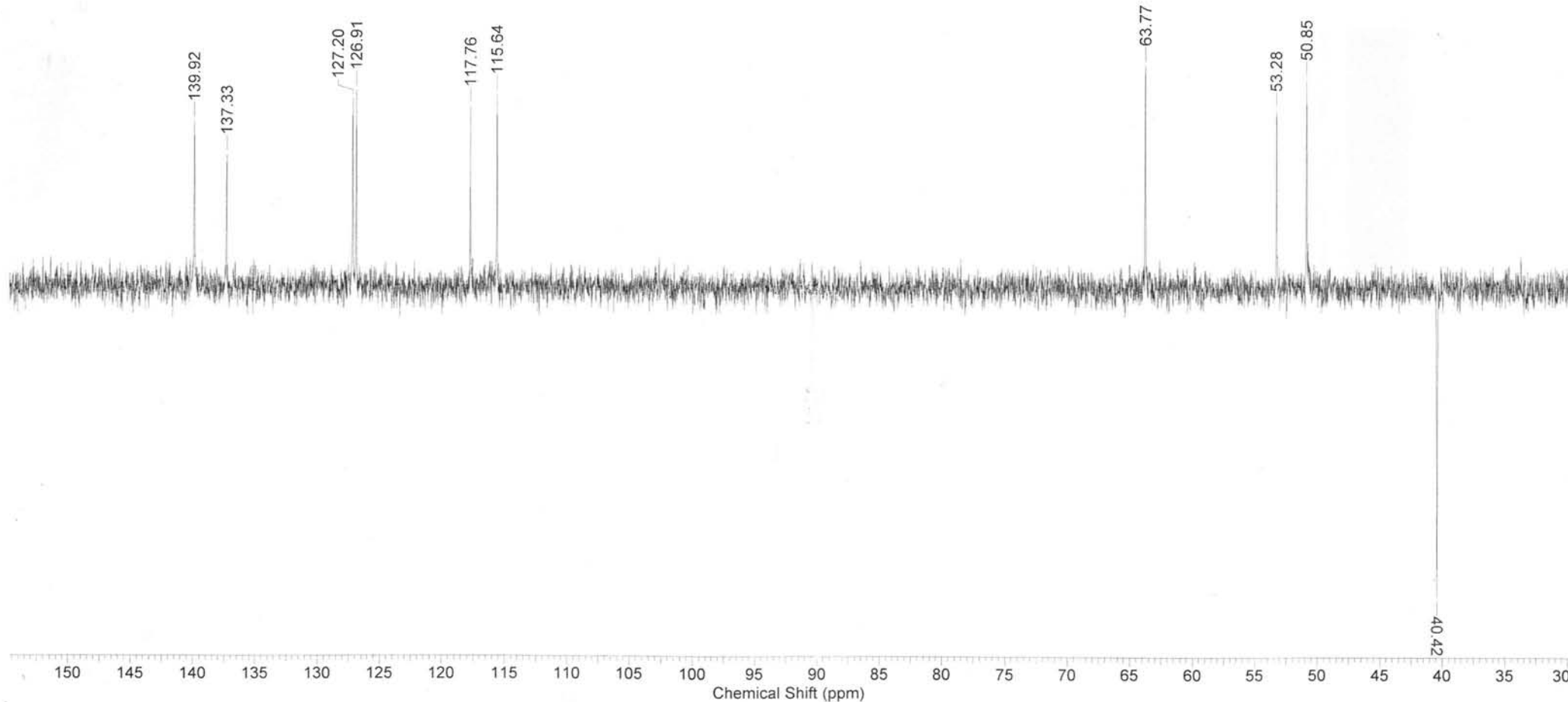
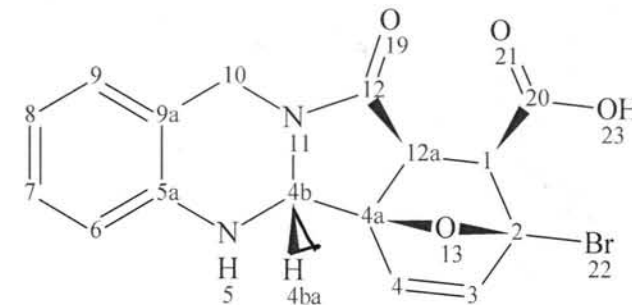
Acquisition Time (sec)	0.5243	Comment	Imported from UXMNR.		Date	26 Oct 2011 11:18:24	
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N9_1-c13dec\rudn-141011-N9_1-c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	4000	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	DMSO-D6	Sweep Width (Hz)	31250.00	Temperature (degree C)	27.000

Compound 44Bc



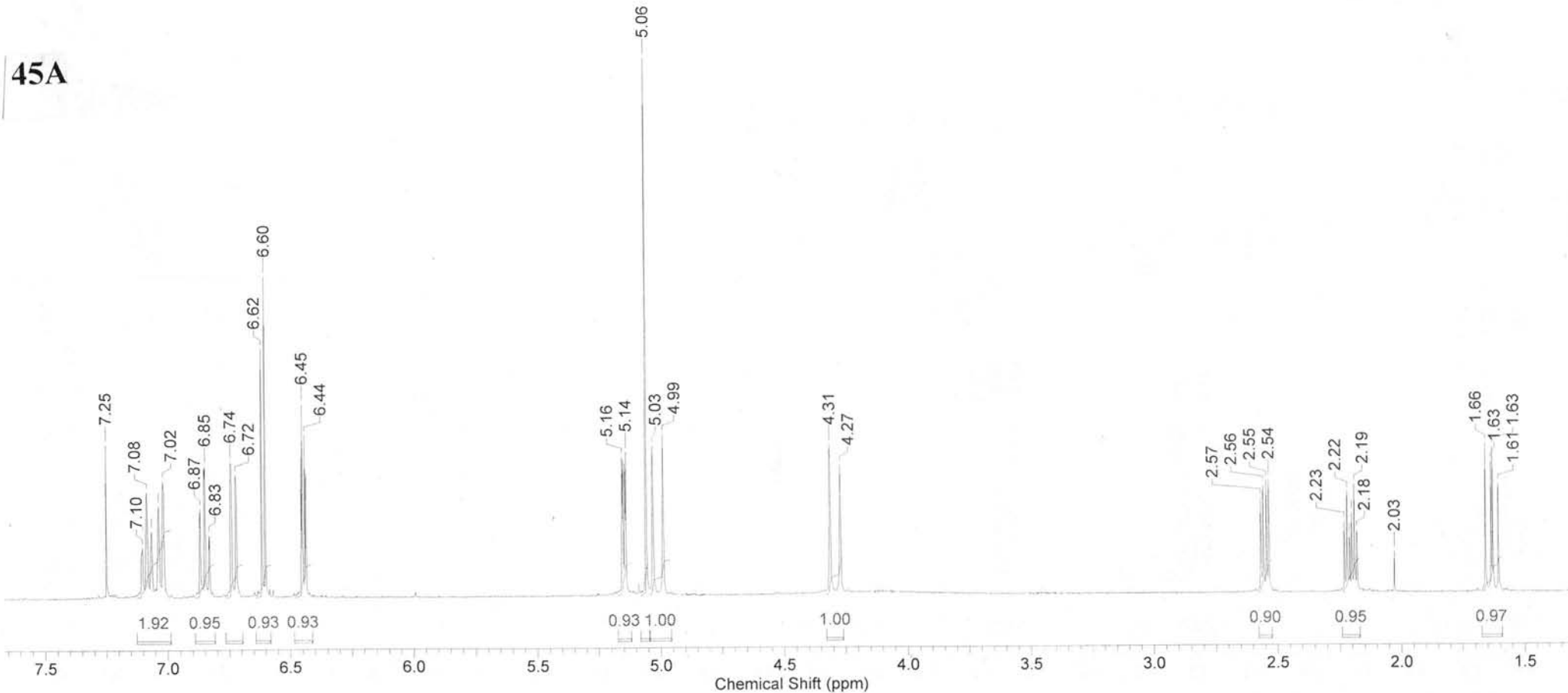
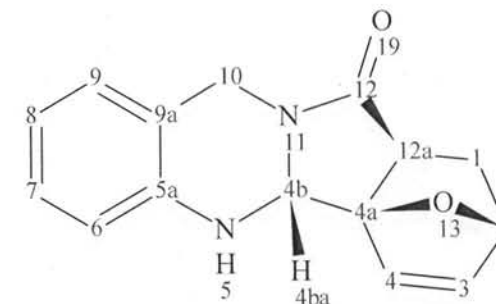
Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	26 Oct 2011 13:22:08	
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N9_1-dept135\rudn-141011-N9_1-dept135_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	3000	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	DMSO-D6	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compound 44Bc



Acquisition Time (sec)	1.6056	Comment	Imported from UXNMR.		Date	23 Aug 2011 10:01:36	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-190811-N11\rudn-190811-N11_001000fid				Frequency (MHz)	400.14	
Nucleus	¹ H	Number of Transients	24	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	CHLOROFORM-D		Sweep Width (Hz)	10204.08	
Temperature (degree C)	27.000						

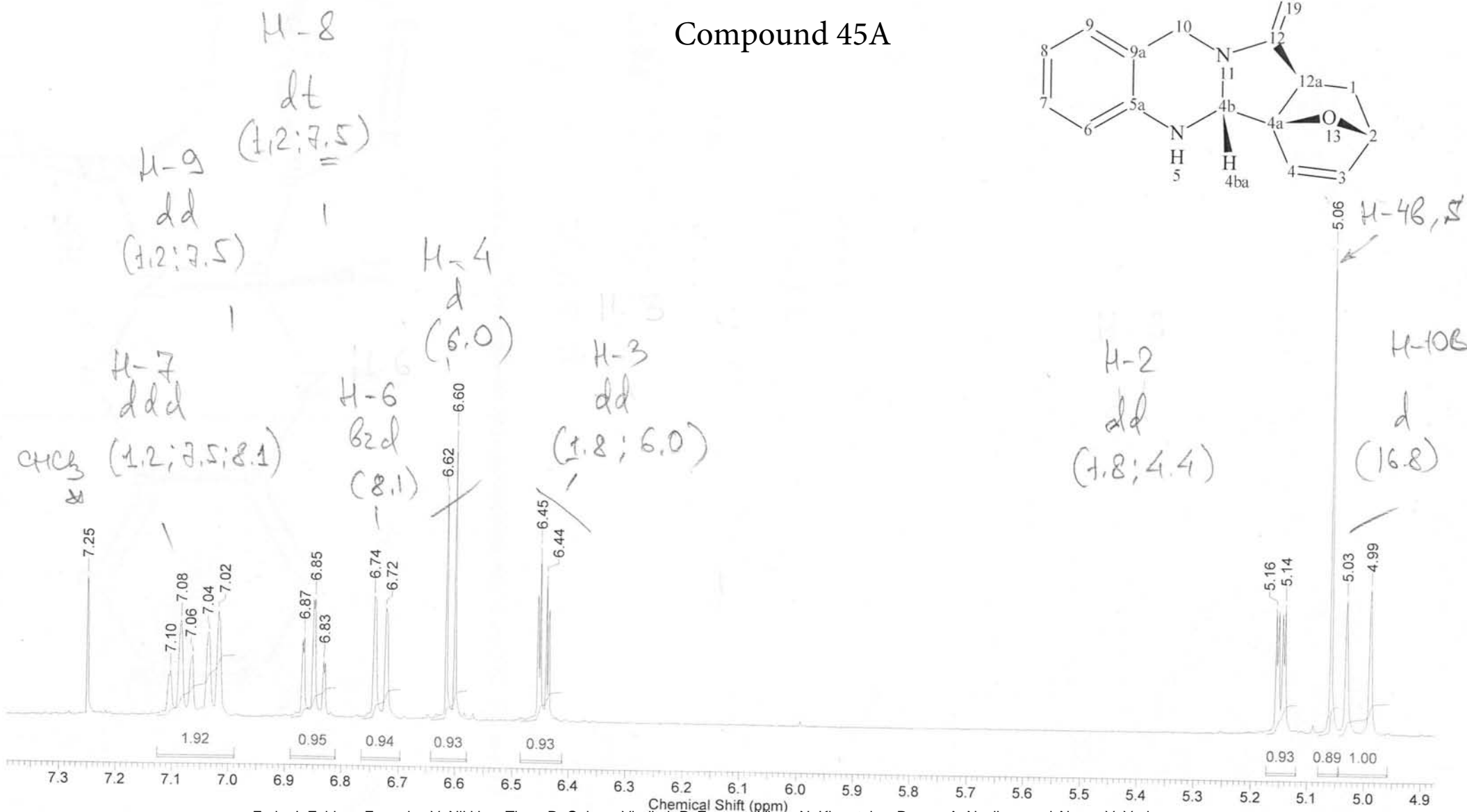
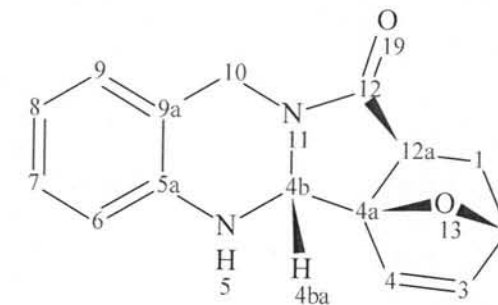
Compound 45A



23 Aug 2011

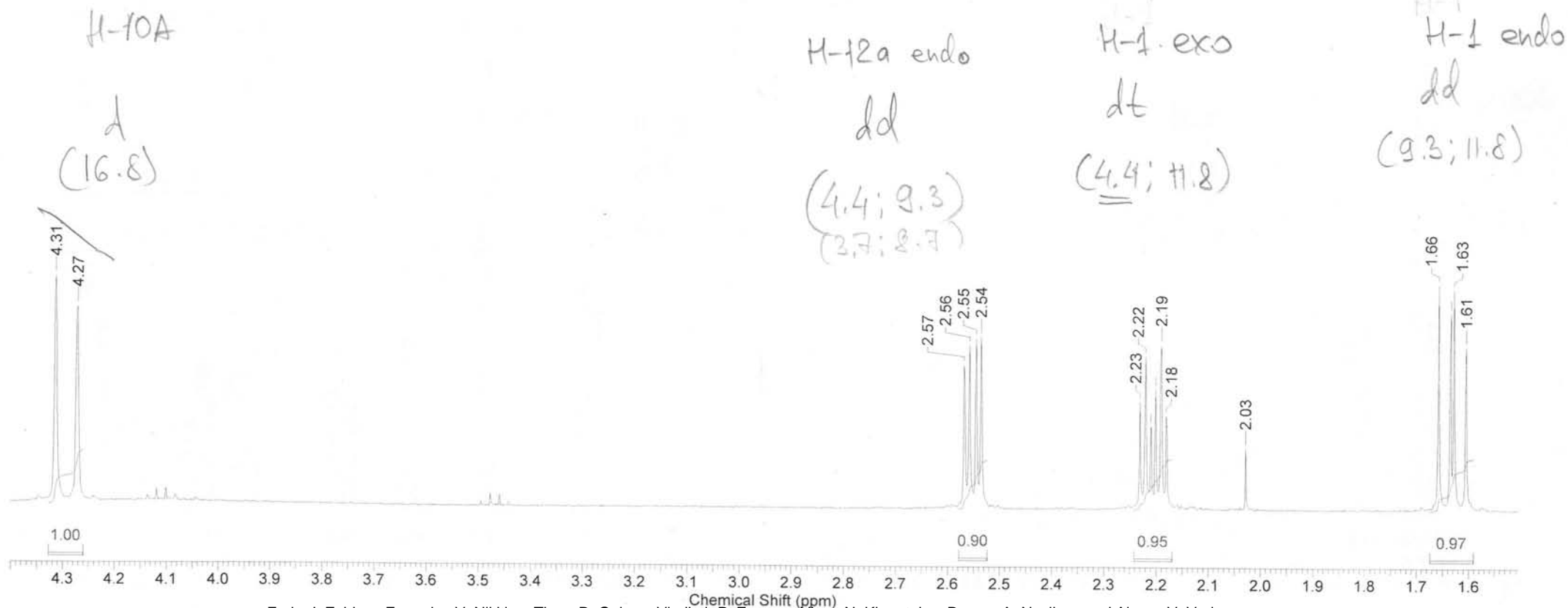
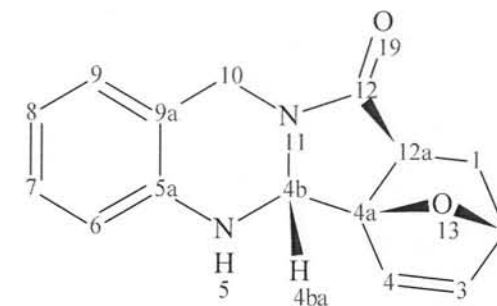
Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.		Date	23 Aug 2011 10:01:36	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-190811-N11\rudn-190811-N11_001000fid			Frequency (MHz)	400.14		
Nucleus	1H	Number of Transients	24	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	CHLOROFORM-D		Sweep Width (Hz)	10204.08	
Temperature (degree C)	27.000						

Compound 45A



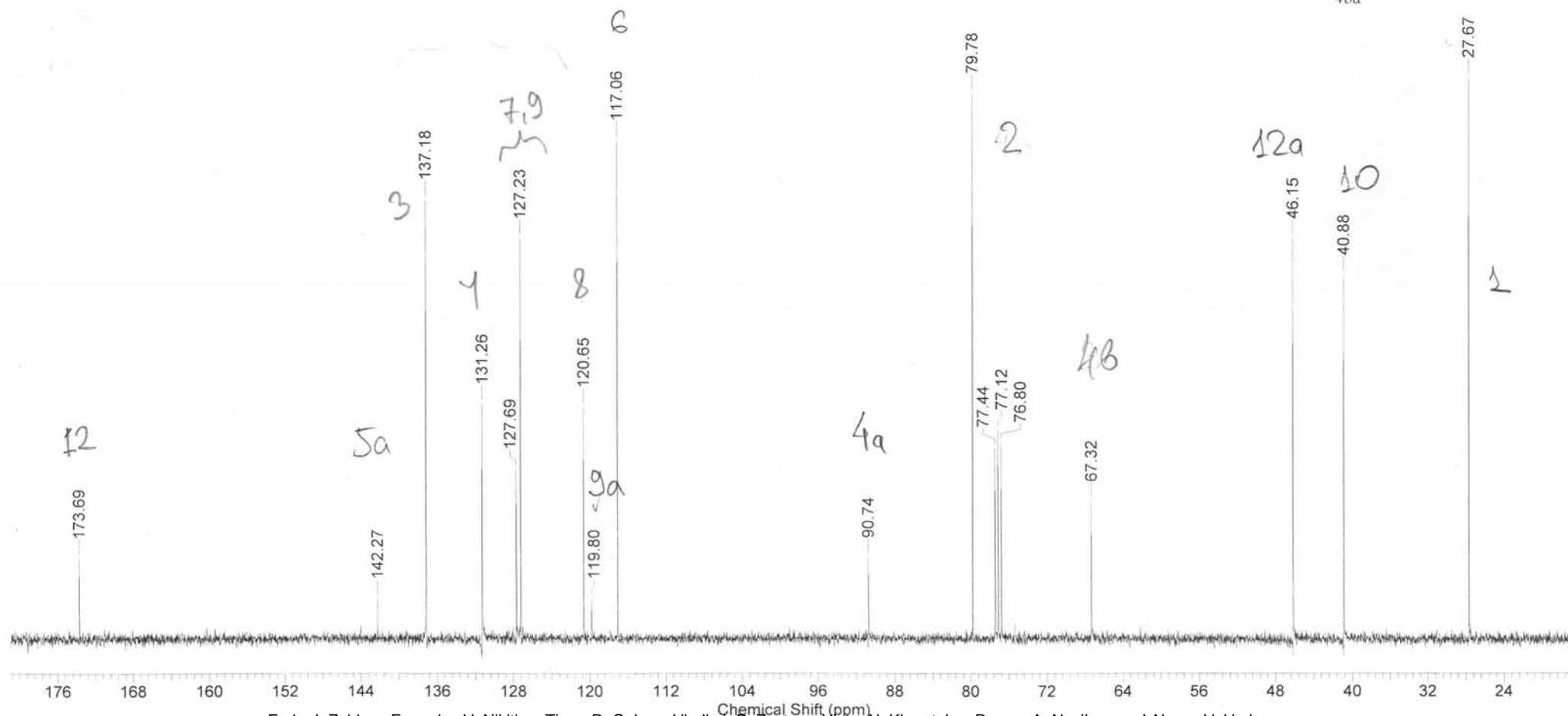
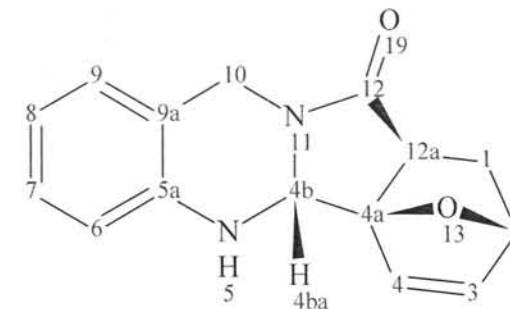
Acquisition Time (sec)	1.6056	Comment	Imported from UXNMR.		Date	23 Aug 2011 10:01:36	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-190811-N11\rudn-190811-N11_001000fid				Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	24	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	CHLOROFORM-D		Sweep Width (Hz)	10204.08	
Temperature (degree C)	27.000						

Compound 45A



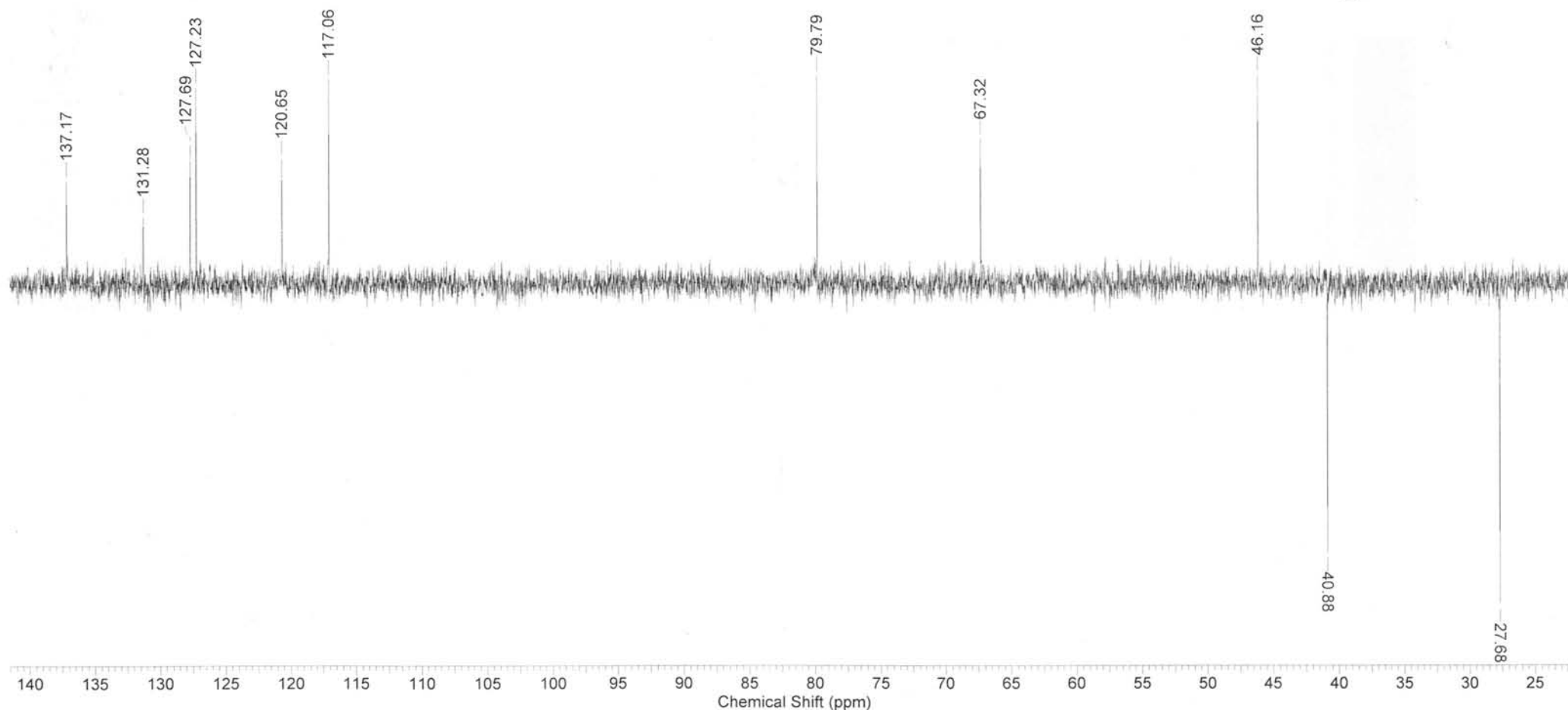
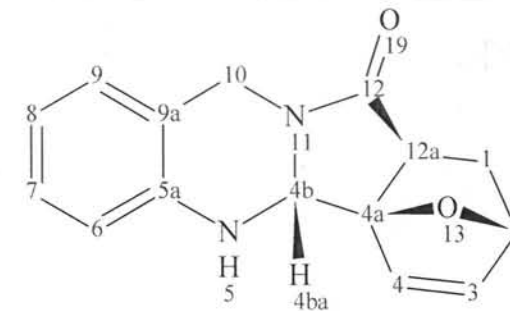
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File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-190811-N11-c13dec\rudn-190811-N11-c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	1740	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	27777.78	Temperature (degree C)	27.000

Compound 45A



Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	23 Aug 2011 15:55:44	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-190811-N11-dept135\rudn-190811-N11-dept135_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	1231	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	CHLOROFORM-D	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compound 45A



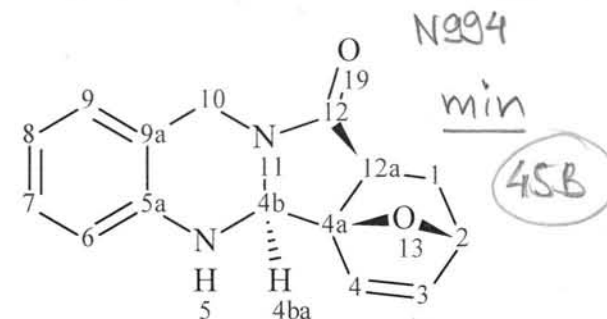
Baba N 397 opp-chem 16-21

28.11.2011 20:01:54

Formula C₁₅H₁₄N₂O₂ FW 254.2839

Acquisition Time (sec)	1.8193	Comment	single_pulse	Date	23 Nov 2011 11:52:55	Date Stamp	23 Nov 2011 16:28:34
File Name	D:\NMR\21.11.11\FZ2064-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2398.6931	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	27.700			Sweep Width (Hz)	9005.76		

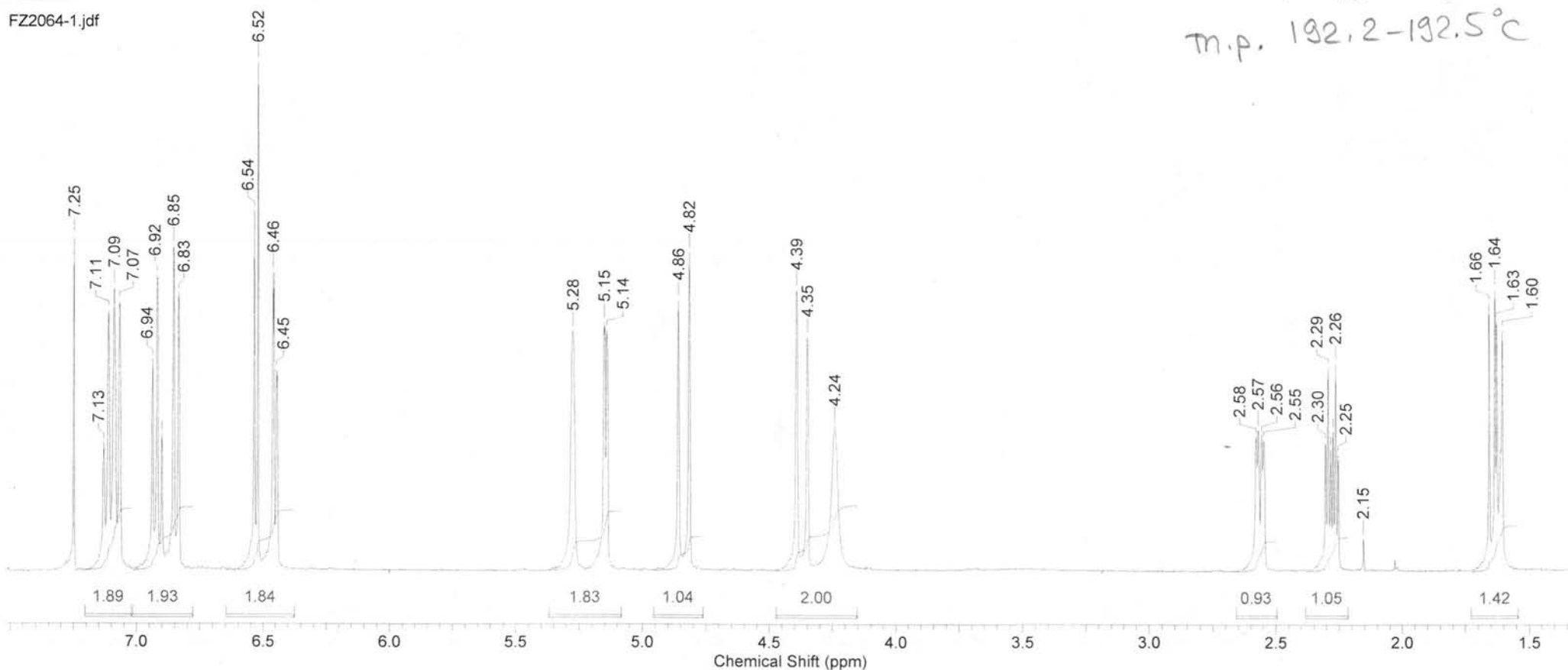
Compound 45B



m.p. 192.2-192.5 °C

45B

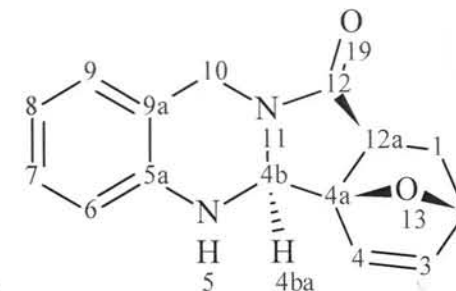
FZ2064-1.jdf



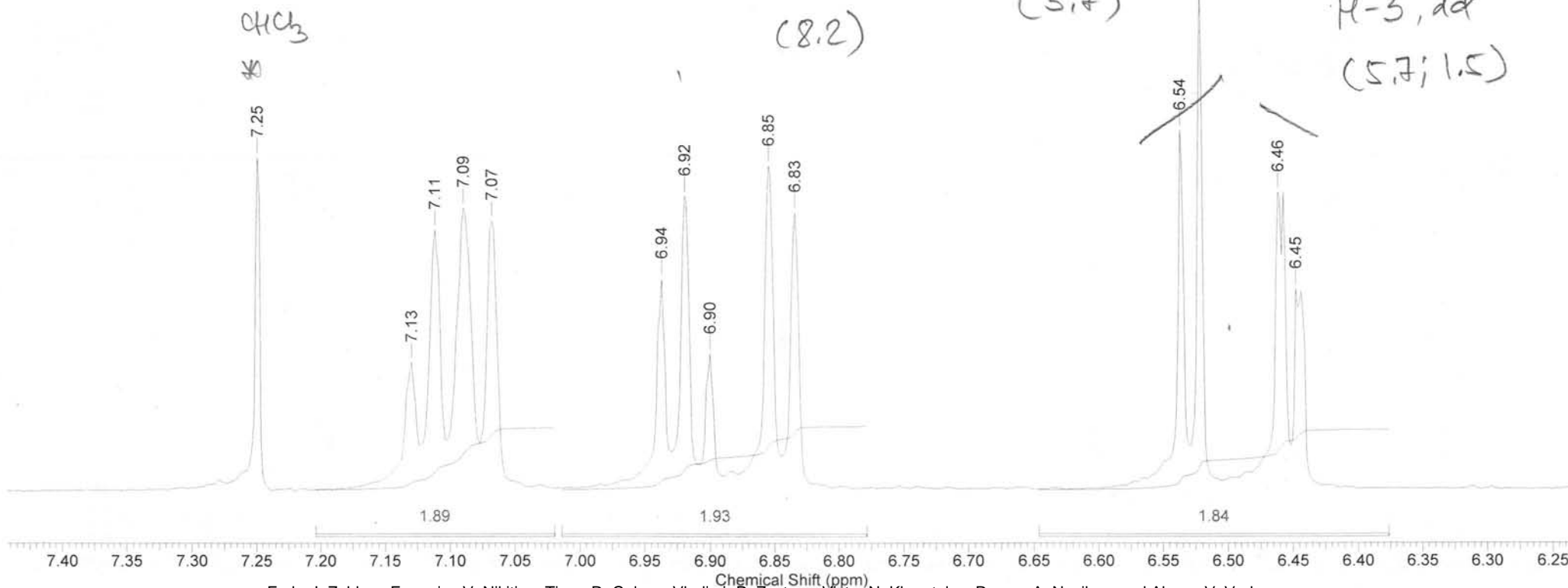
Formula C₁₅H₁₄N₂O₂ FW 254.2839

Acquisition Time (sec)	1.8193	Comment	single_pulse	Date	23 Nov 2011 11:52:55	Date Stamp	23 Nov 2011 16:28:34
File Name	D:\NMR\21.11.11\FZ2064-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8
Origin	ECS 400	Original Points Count	16384	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2398.6931	Sweep Width (Hz)	9005.76
Temperature (degree C)	27.700						

Compound 45B



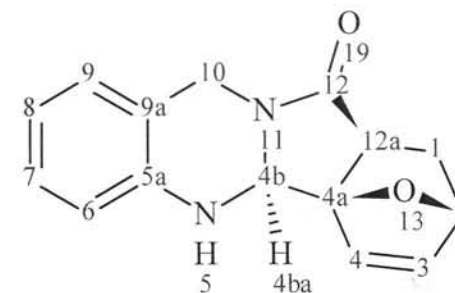
FZ2064-1.jdf



Formula $C_{15}H_{14}N_2O_2$ FW 254.2839

Acquisition Time (sec)	1.8193	Comment	single_pulse	Date	23 Nov 2011 11:52:55	Date Stamp	23 Nov 2011 16:28:34
File Name	D:\NMR\21.11.11\FZ2064-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2398.6931	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	27.700					Sweep Width (Hz)	9005.76

Compound 45B



FZ2064-1.jdf

H-4b
bz s

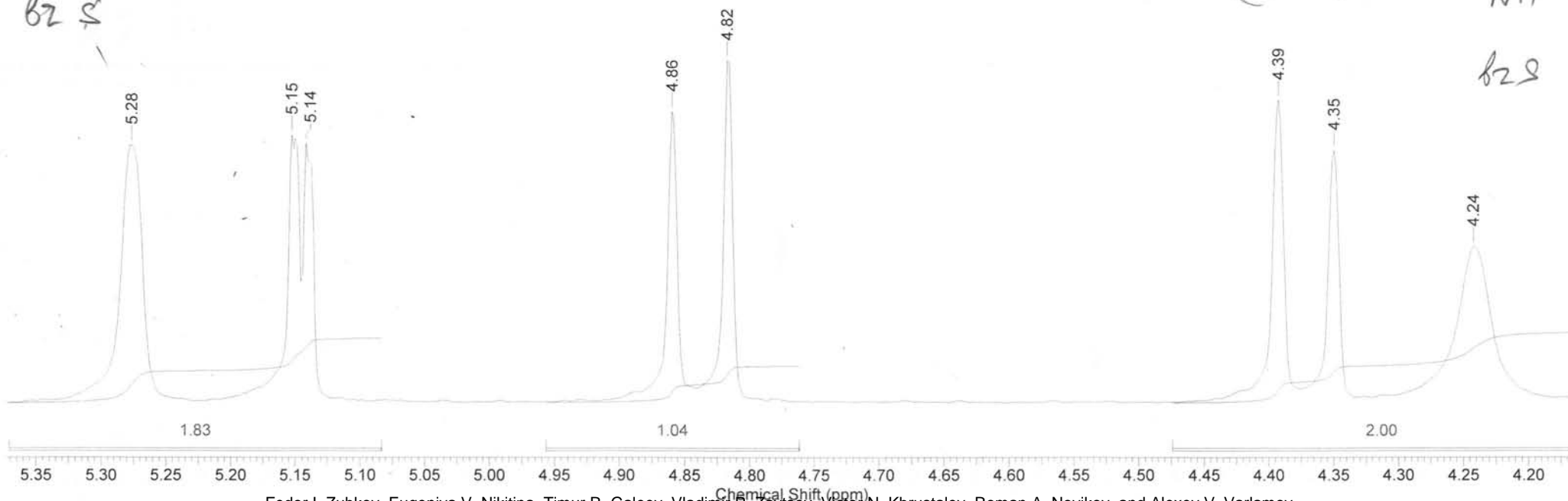
H-2
dd
(1.5; 4.4)

H-10a
d
(7.0)

H-10b
d
(7.0)

NH

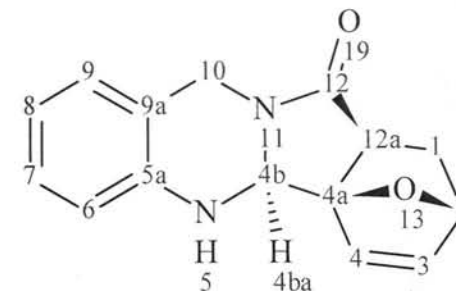
bz s



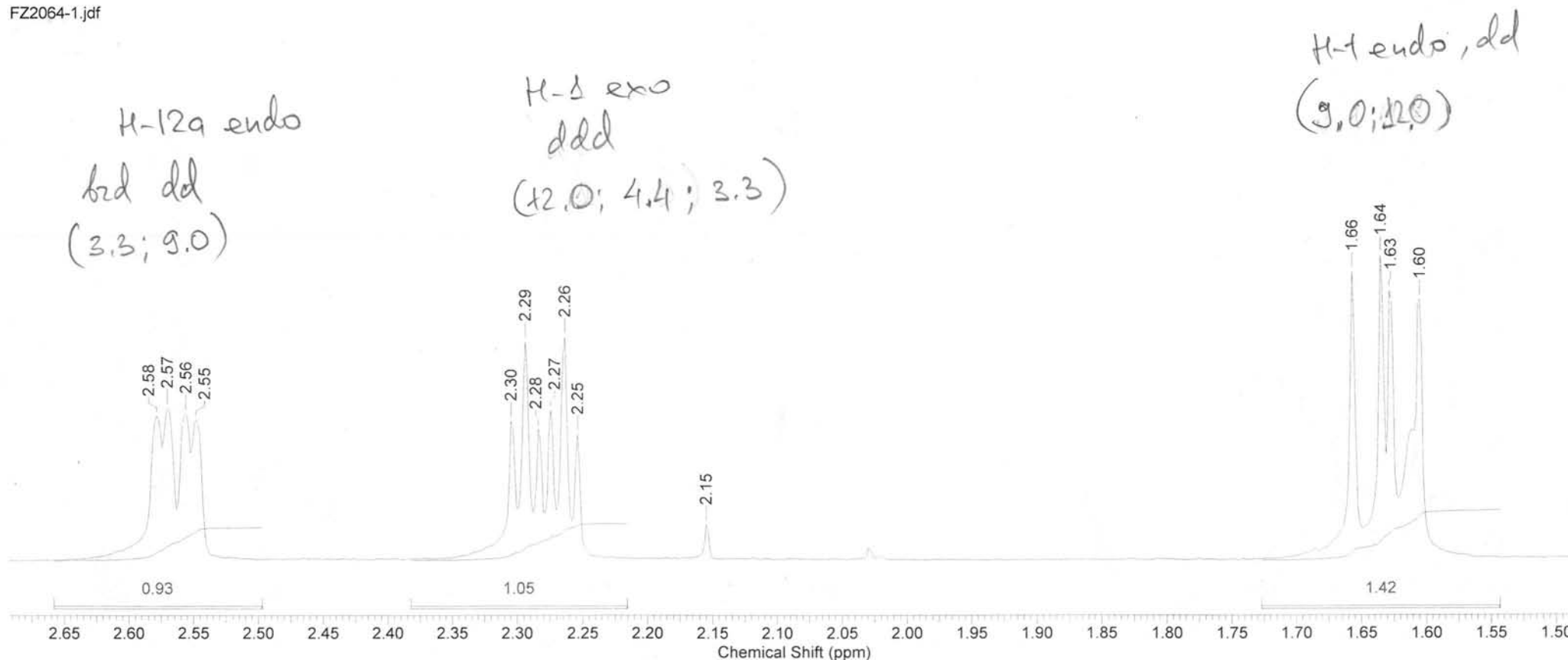
Formula C₁₅H₁₄N₂O₂ FW 254.2839

Acquisition Time (sec)	1.8193	Comment	single_pulse	Date	23 Nov 2011 11:52:55	Date Stamp	23 Nov 2011 16:28:34
File Name	D:\NMR\21.11.11\FZ2064-1.jdf	Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8
Origin	ECS 400	Original Points Count	16384	Owner	delta	Points Count	16384
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2398.6931	Pulse Sequence	single_pulse.ex2
Temperature (degree C)	27.700					Sweep Width (Hz)	9005.76

Compound 45B



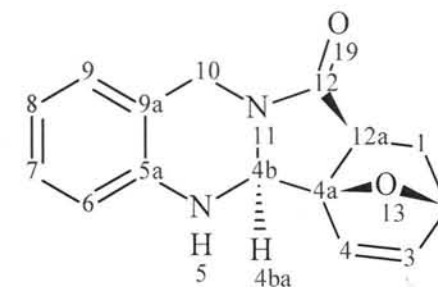
FZ2064-1.jdf



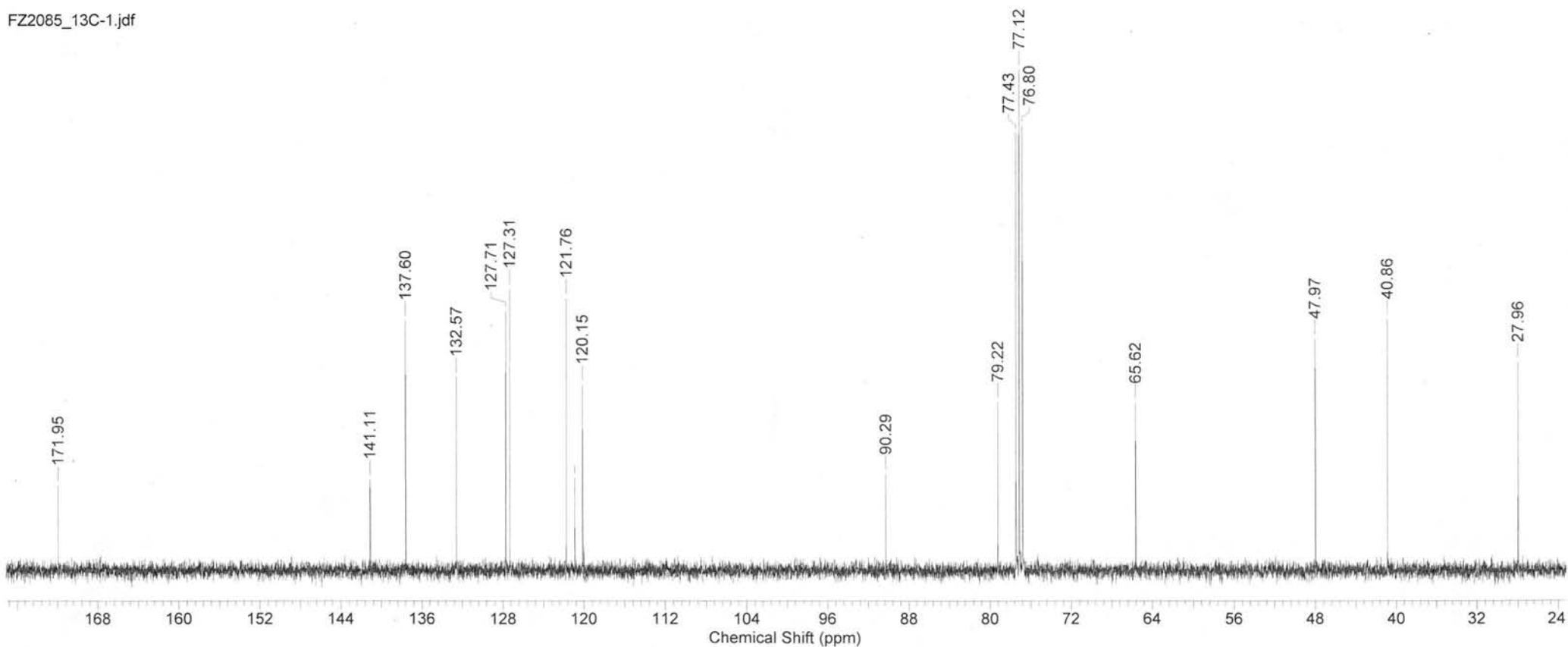
Formula $C_{15}H_{14}N_2O_2$ FW 254.2839

Acquisition Time (sec)	1.0433	Comment	single pulse decoupled gated NOE	Date	30 Nov 2011 10:48:13
Date Stamp	30 Nov 2011 15:24:08	File Name	D:\NMR\28.11.11\FZ2085_13C-1.jdf		
Frequency (MHz)	100.53	Nucleus	13C	Number of Transients	162
Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	60.00	Solvent	CHLOROFORM-d	Pulse Sequence	single_pulse_dec
Sweep Width (Hz)	31407.04	Temperature (degree C)	26.100	Spectrum Offset (Hz)	12063.0361

Compound 45B



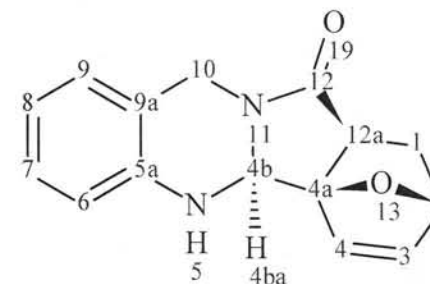
FZ2085_13C-1.jdf



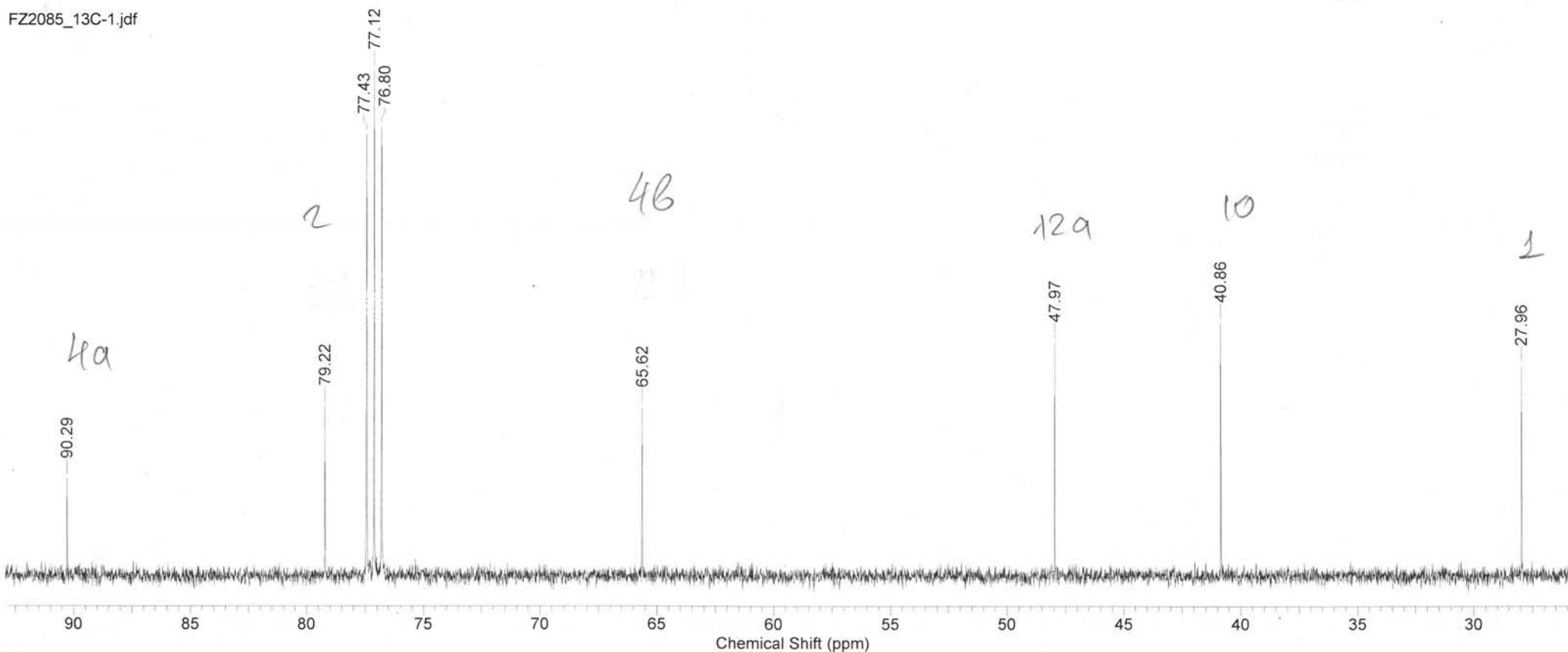
Formula C₁₅H₁₄N₂O₂ FW 254.2839

Acquisition Time (sec)	1.0433	Comment	single pulse decoupled gated NOE		Date	30 Nov 2011 10:48:13	
Date Stamp	30 Nov 2011 15:24:08	File Name	D:\NMR\28.11.11\FZ2085_13C-1.jdf				
Frequency (MHz)	100.53	Nucleus	13C	Number of Transients	162	Origin	ECS 400
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single_pulse_dec
Receiver Gain	60.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	12063.0361		
Sweep Width (Hz)	31407.04	Temperature (degree C)	26.100				

Compound 45B



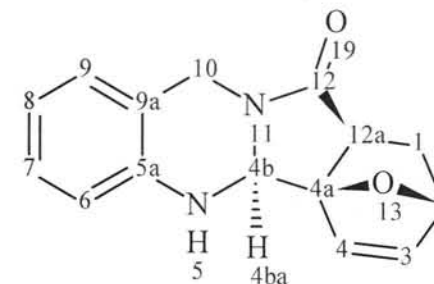
FZ2085_13C-1.jdf



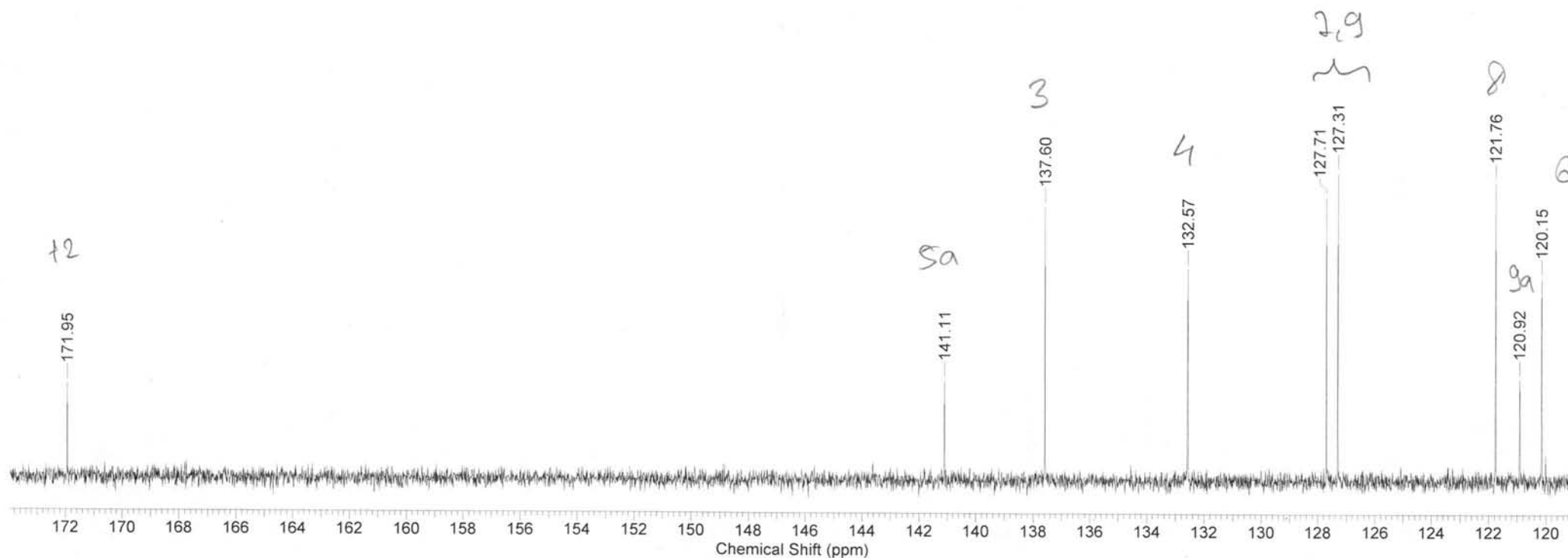
Formula C₁₅H₁₄N₂O₂ FW 254.2839

Acquisition Time (sec)	1.0433	Comment	single pulse decoupled gated NOE	Date	30 Nov 2011 10:48:13
Date Stamp	30 Nov 2011 15:24:08	File Name	D:\NMR\28.11.11\FZ2085_13C-1.jdf		
Frequency (MHz)	100.53	Nucleus	13C	Number of Transients	162
Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	60.00	Solvent	CHLOROFORM-d	Pulse Sequence	single_pulse_dec
Sweep Width (Hz)	31407.04	Temperature (degree C)	26.100	Spectrum Offset (Hz)	12063.0361

Compound 45B

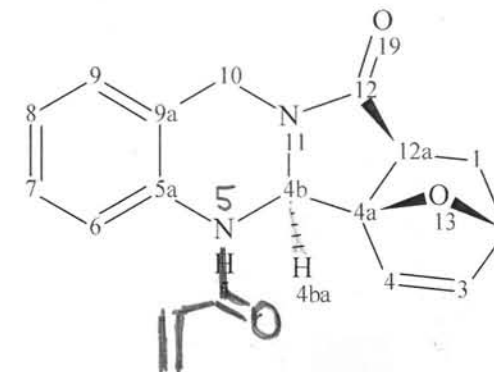


FZ2085_13C-1.jdf

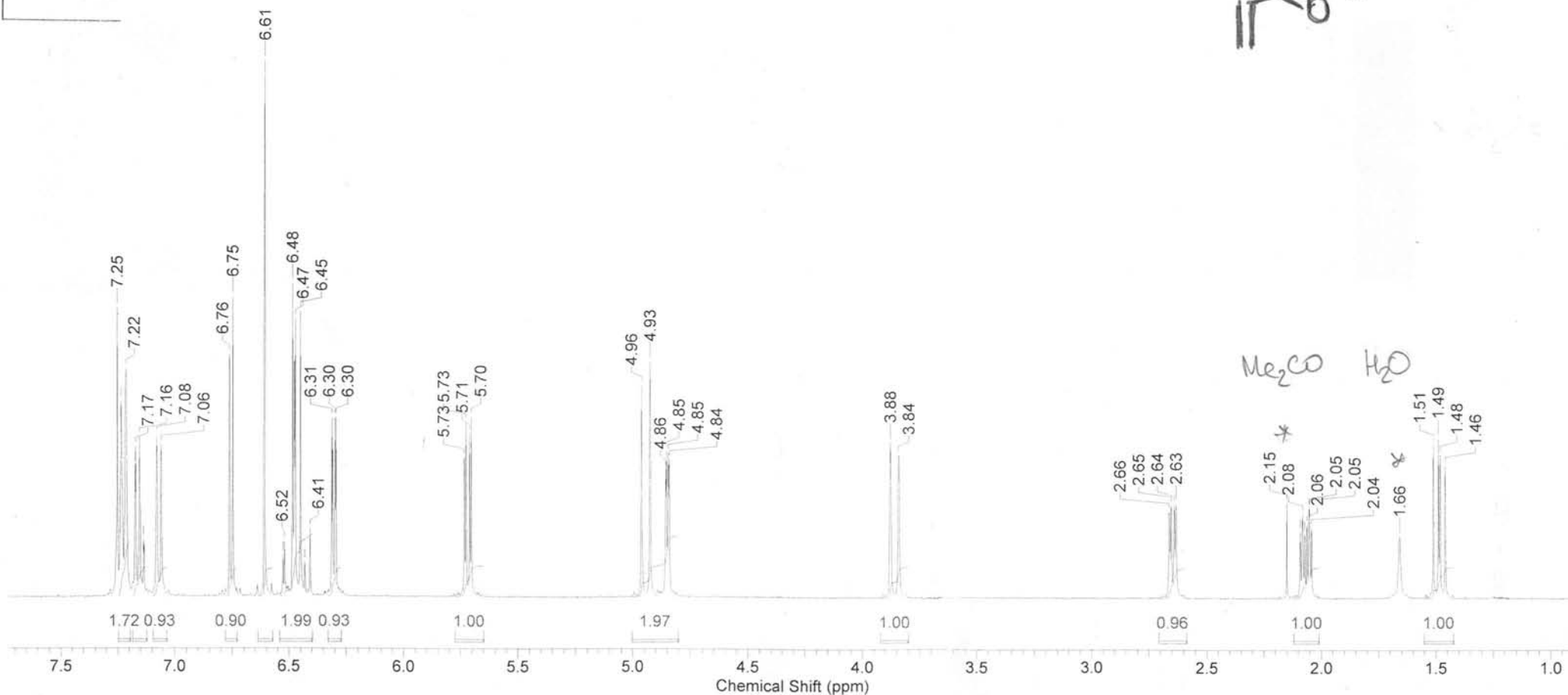


Acquisition Time (sec)	1.6056	Comment	Imported from UXNMR.	Date	14 Oct 2011 16:59:44
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N10\rudn-141011-N10_001000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	20	Original Points Count	16384
Pulse Sequence	zg	Solvent	CHLOROFORM-D	Points Count	16384
Temperature (degree C)	27.000			Sweep Width (Hz)	10204.08

Compound 46

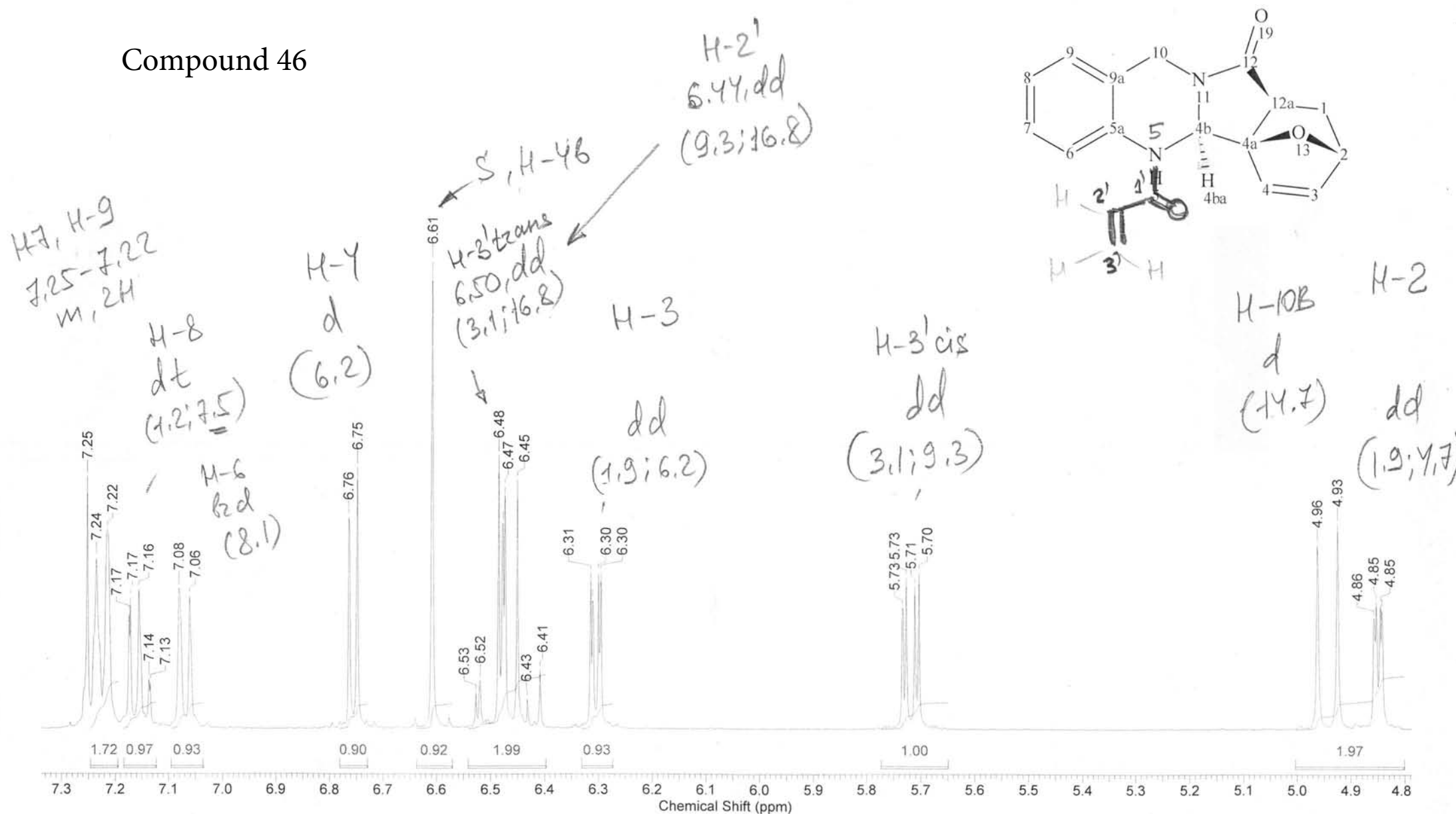


46



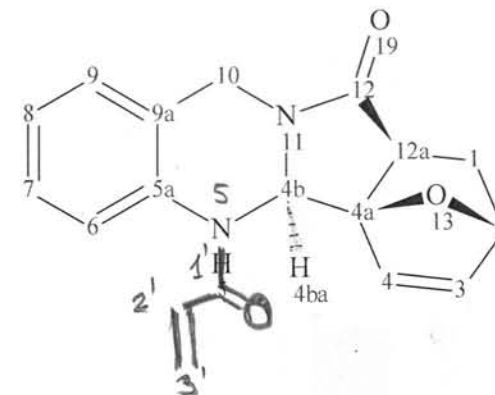
Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.	Date	14 Oct 2011 16:59:44
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N10\rudn-141011-N10_001000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	20	Original Points Count	16384
Pulse Sequence	zg	Solvent	CHLOROFORM-D	Points Count	16384
Temperature (degree C)	27.000			Sweep Width (Hz)	10204.08

Compound 46



Acquisition Time (sec)	1.6056	Comment	Imported from UXMNR.		Date	14 Oct 2011 16:59:44	
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N10\rudn-141011-N10_001000fid			Frequency (MHz)	400.14		
Nucleus	1H	Number of Transients	20	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	CHLOROFORM-D		Sweep Width (Hz)	10204.08	
Temperature (degree C)	27.000						

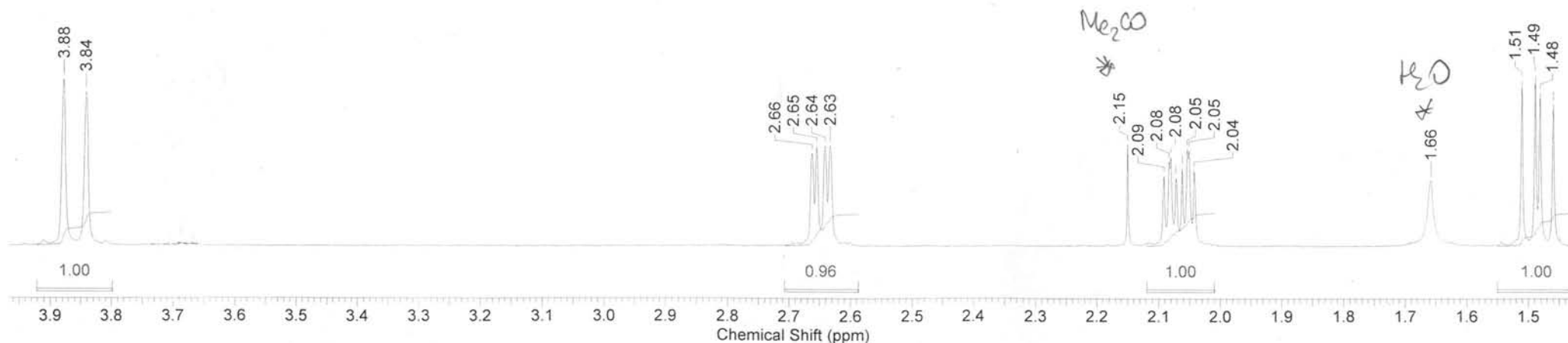
Compound 46



H-12a, endo

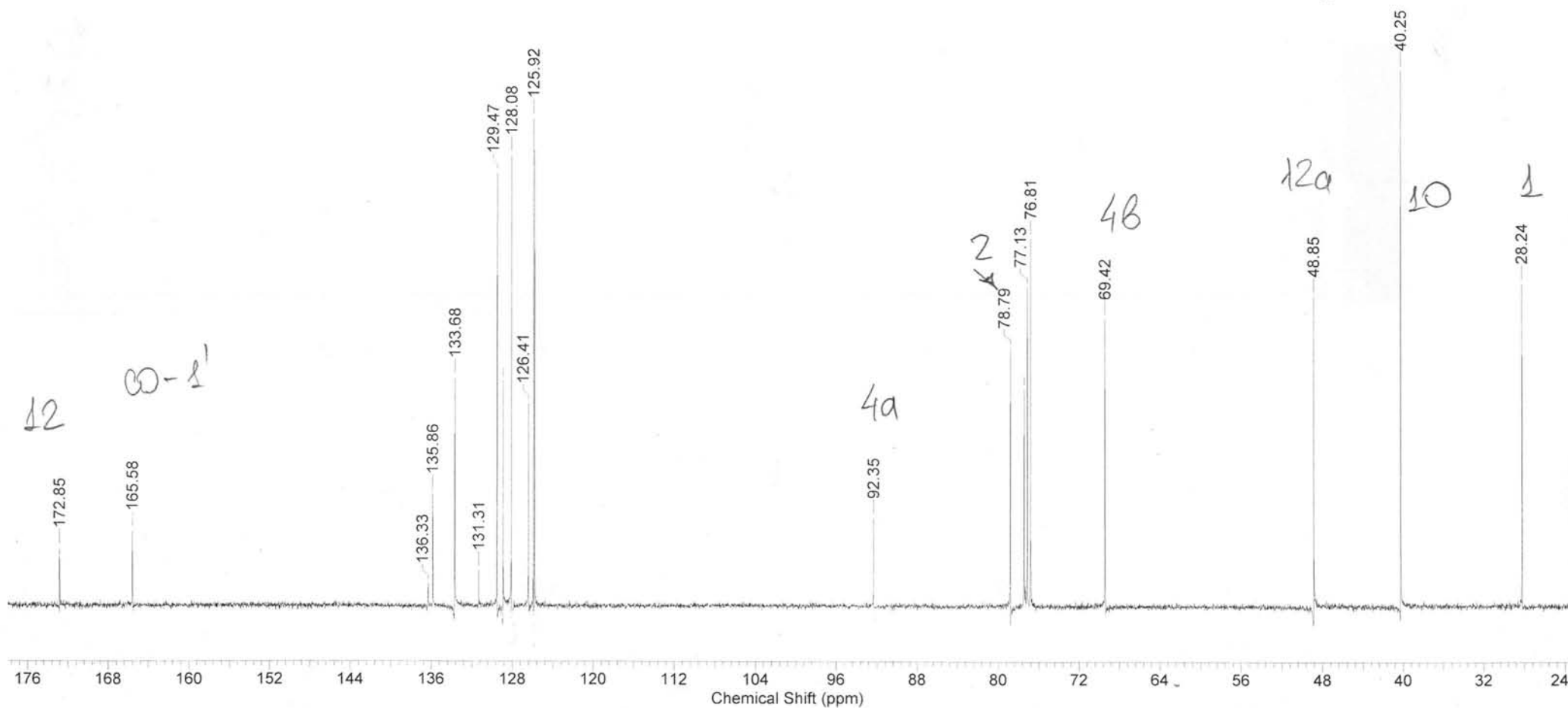
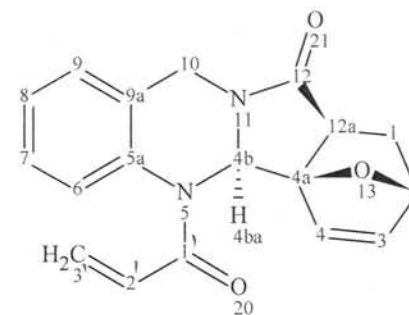
H-1, exo

H-1, endo

10A
d
(14.7)dd
(3.1; 8.7)ddd
(3.1; 4.4; 11.8)dd
(8.7; 11.8)

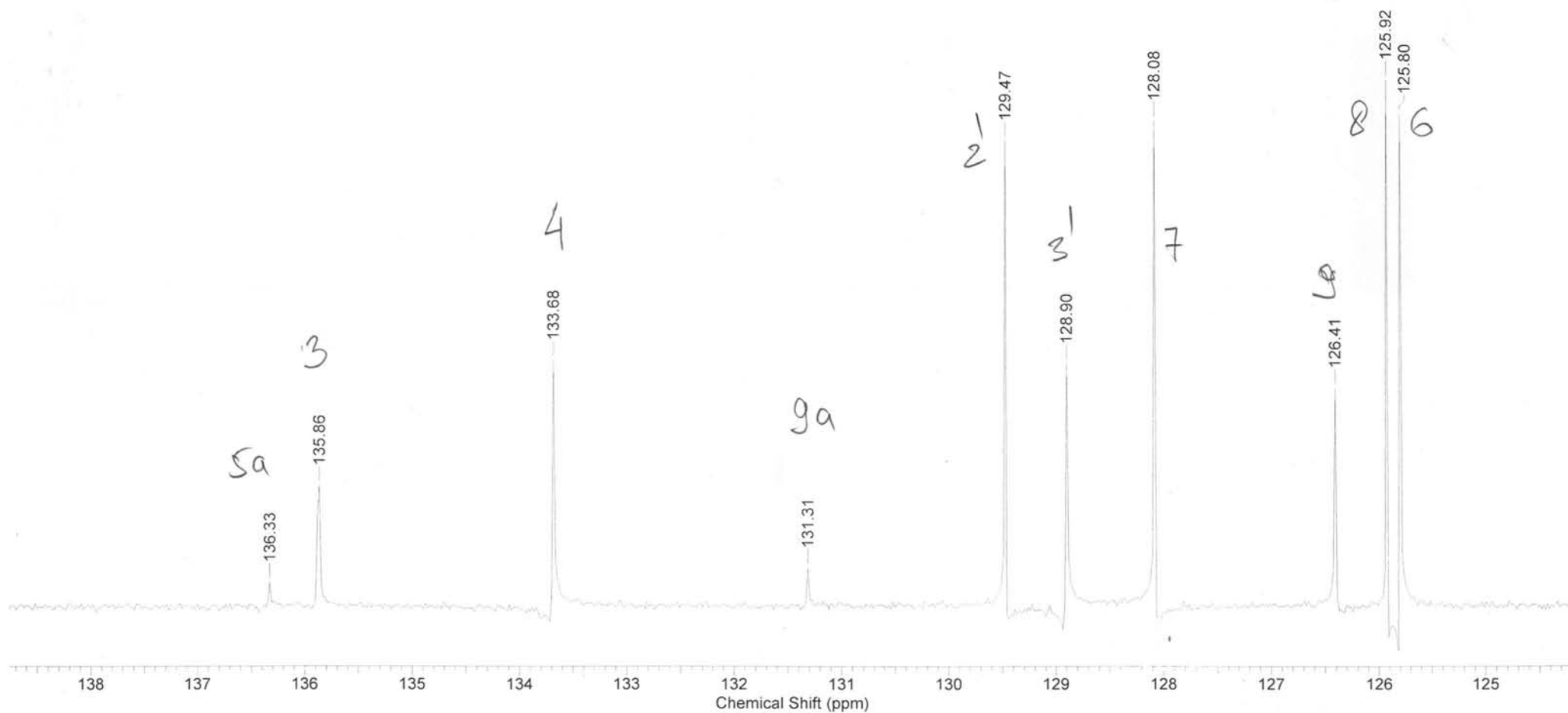
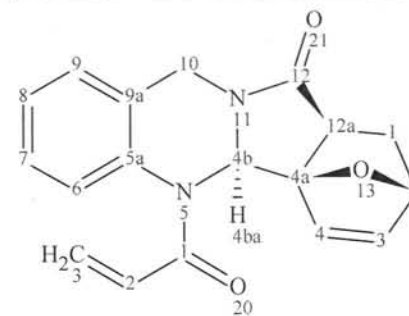
Acquisition Time (sec)	0.5571	Comment	Imported from UXNMR.		Date	20 Oct 2011 18:05:52	
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N10-c13dec\rudn-141011-N10-c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	5000	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compound 46



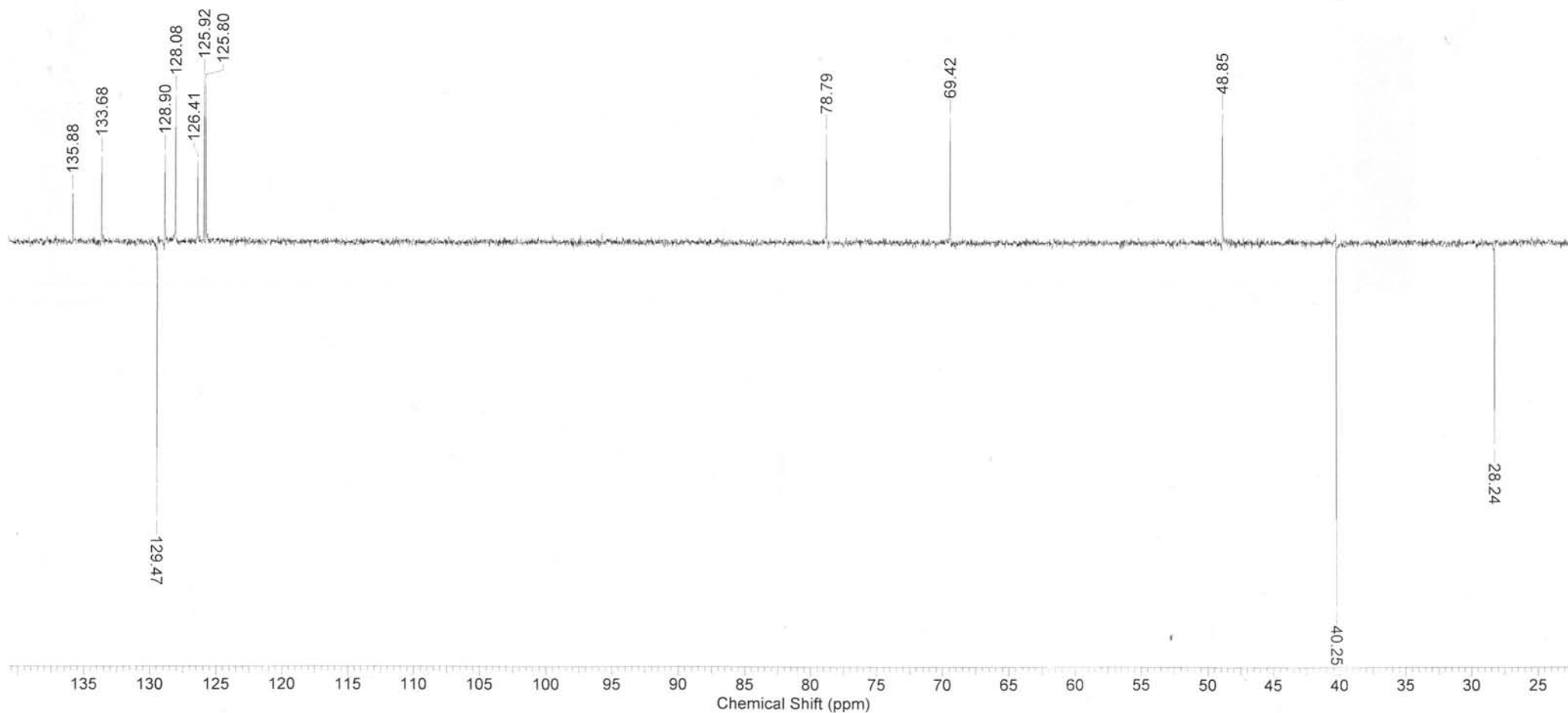
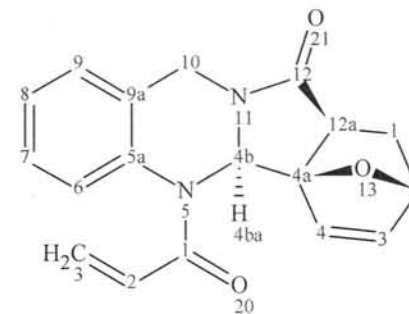
Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	20 Oct 2011 18:05:52	
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N10-c13dec\rudn-141011-N10-c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	5000	Original Points Count	16384	Points Count	16384
Pulse Sequence	zpgg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compound 46



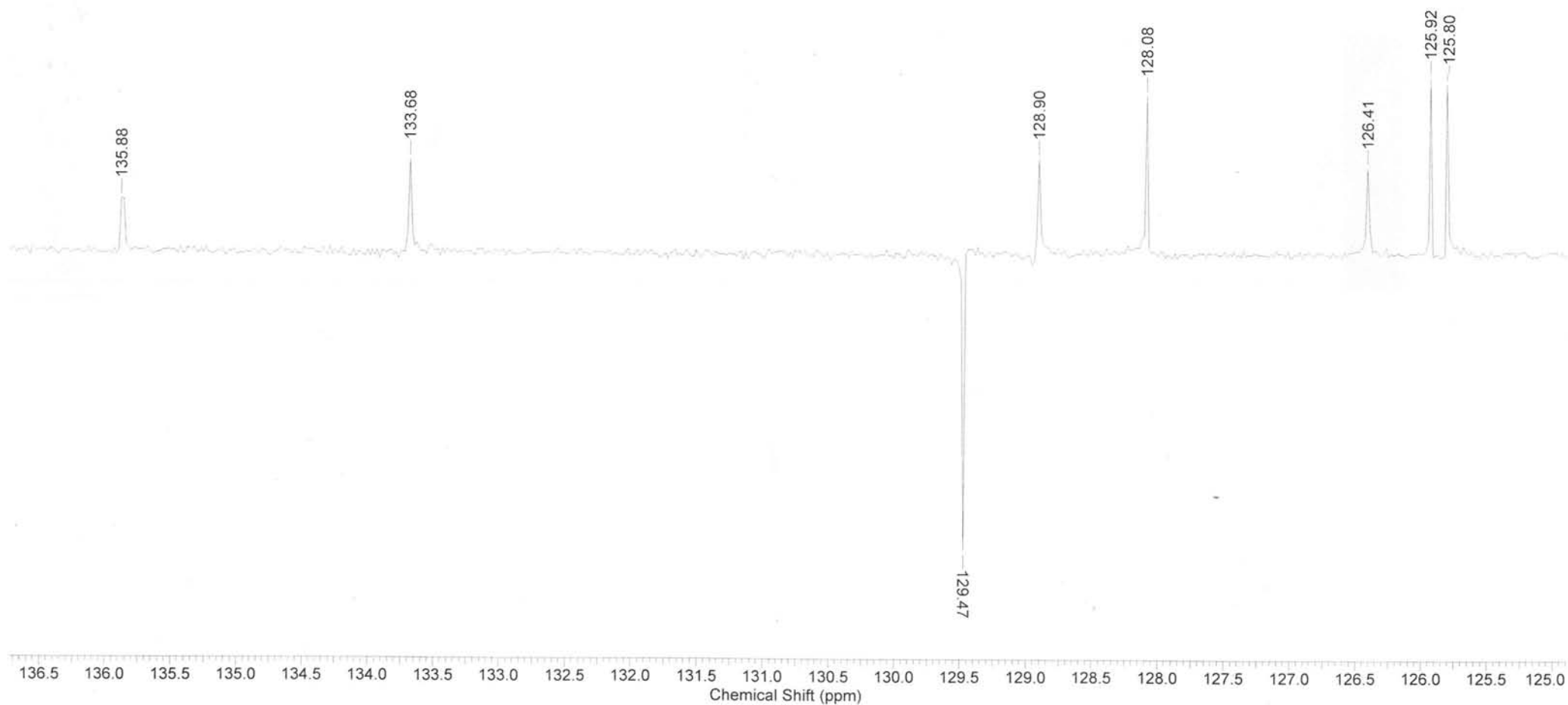
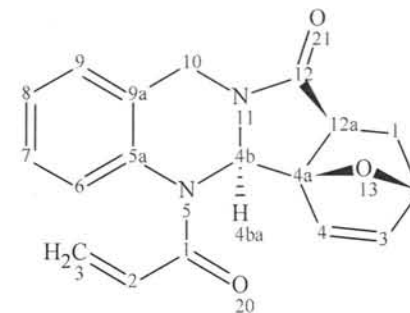
Acquisition Time (sec)	0.5571	Comment	Imported from UXNMR.		Date	20 Oct 2011 22:02:40	
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N10-dept135\rudn-141011-N10-dept135_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	4000	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	CHLOROFORM-D	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compound 46

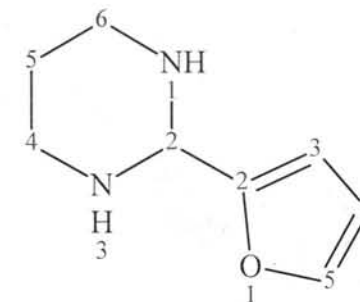


Acquisition Time (sec)	0.5571	Comment	Imported from UXMNR.		Date	20 Oct 2011 22:02:40	
File Name	C:\Users\Fedor\Desktop\14.10.11\rudn-141011-N10-dept135\rudn-141011-N10-dept135_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	4000	Original Points Count	16384	Points Count	16384
Pulse Sequence	dept135	Solvent	CHLOROFORM-D	Sweep Width (Hz)	29411.77	Temperature (degree C)	27.000

Compound 46



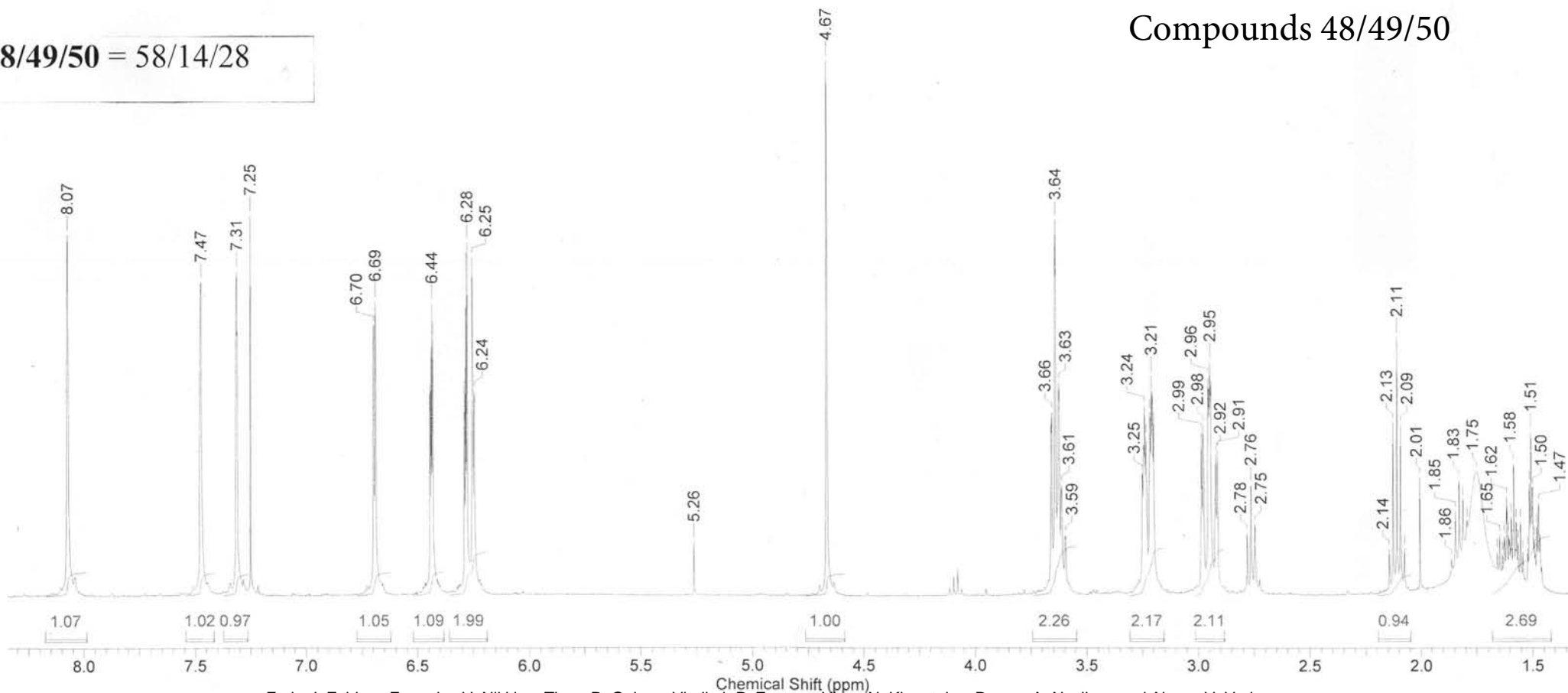
Acquisition Time (sec)	1.6056	Comment	Imported from UXNMR.	Date	23 Aug 2011 10:35:44
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-190811-N15\rudn-190811-N15_001000fid			Frequency (MHz)	400.14
Nucleus	1H	Number of Transients	20	Original Points Count	16384
Pulse Sequence	zg	Solvent	CHLOROFORM-D	Points Count	16384
Temperature (degree C)	27.000			Sweep Width (Hz)	10204.08



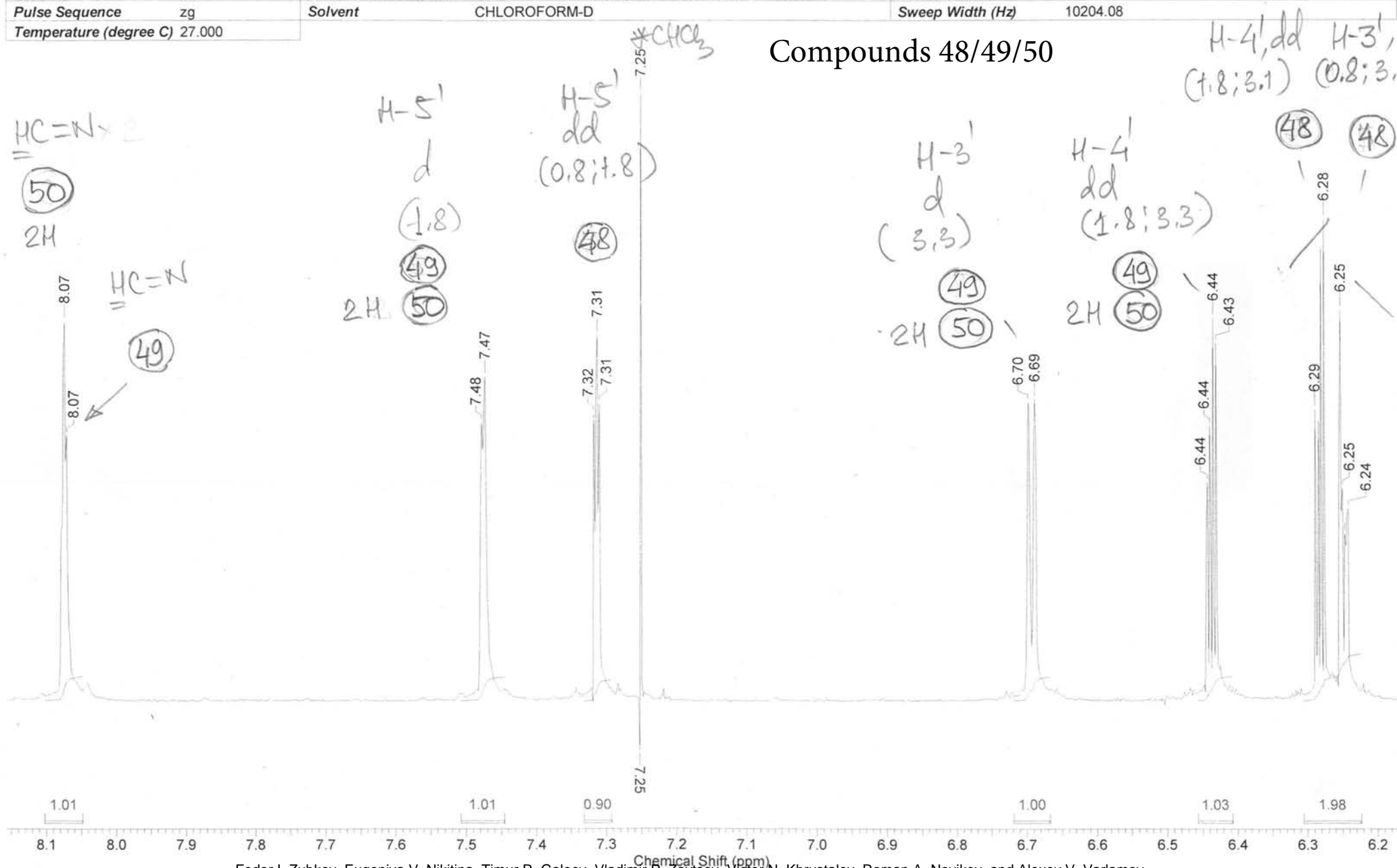
48
H-2, 3

Compounds 48/49/50

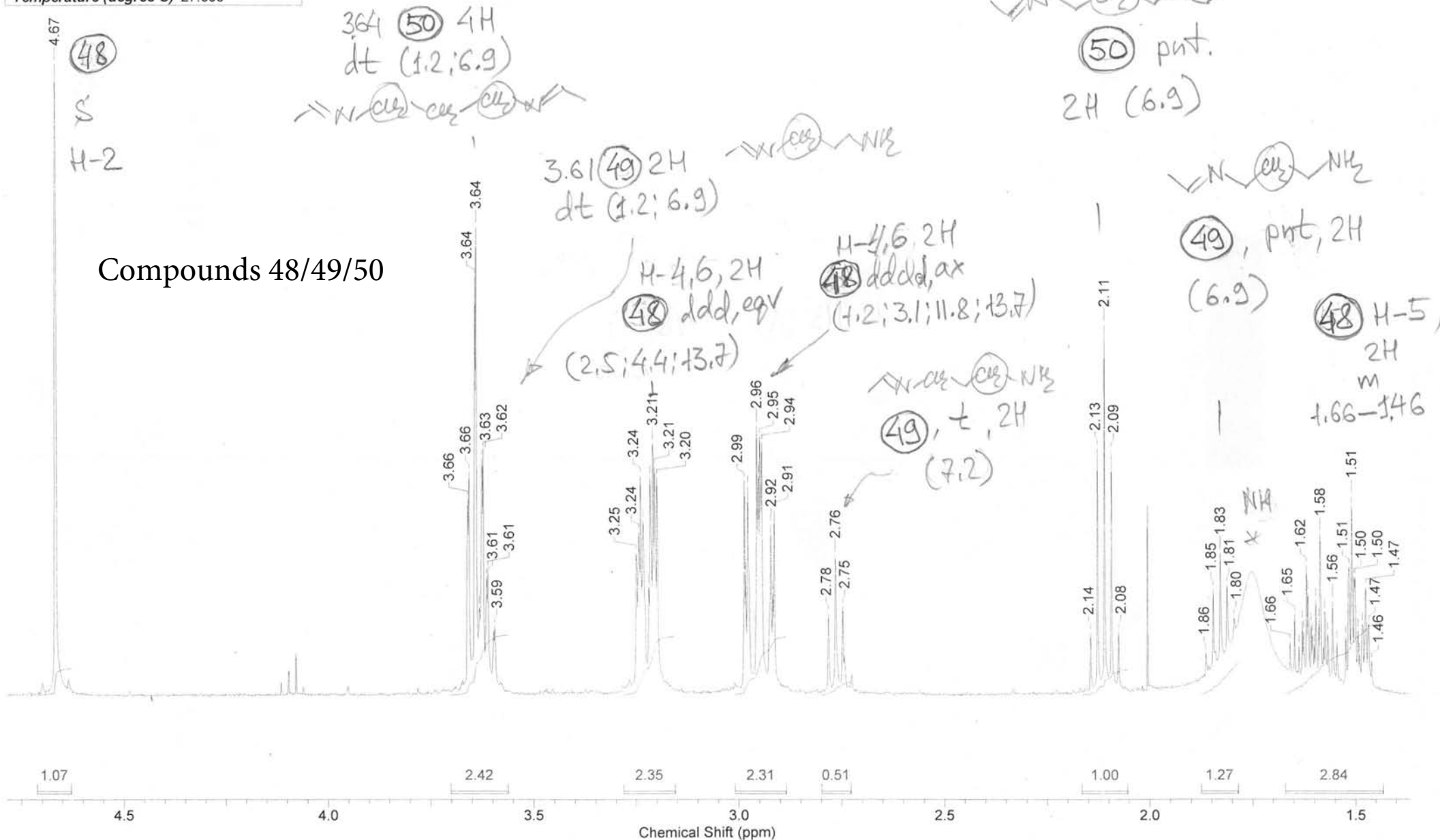
48/49/50 = 58/14/28



Acquisition Time (sec)	1.6056	Comment	Imported from UXNMR.	Date	23 Aug 2011 10:35:44
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-190811-N15\rudn-190811-N15_001000fid	Number of Transients	20	Frequency (MHz)	400.14
Nucleus	¹ H	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	10204.08
Temperature (degree C)	27.000				

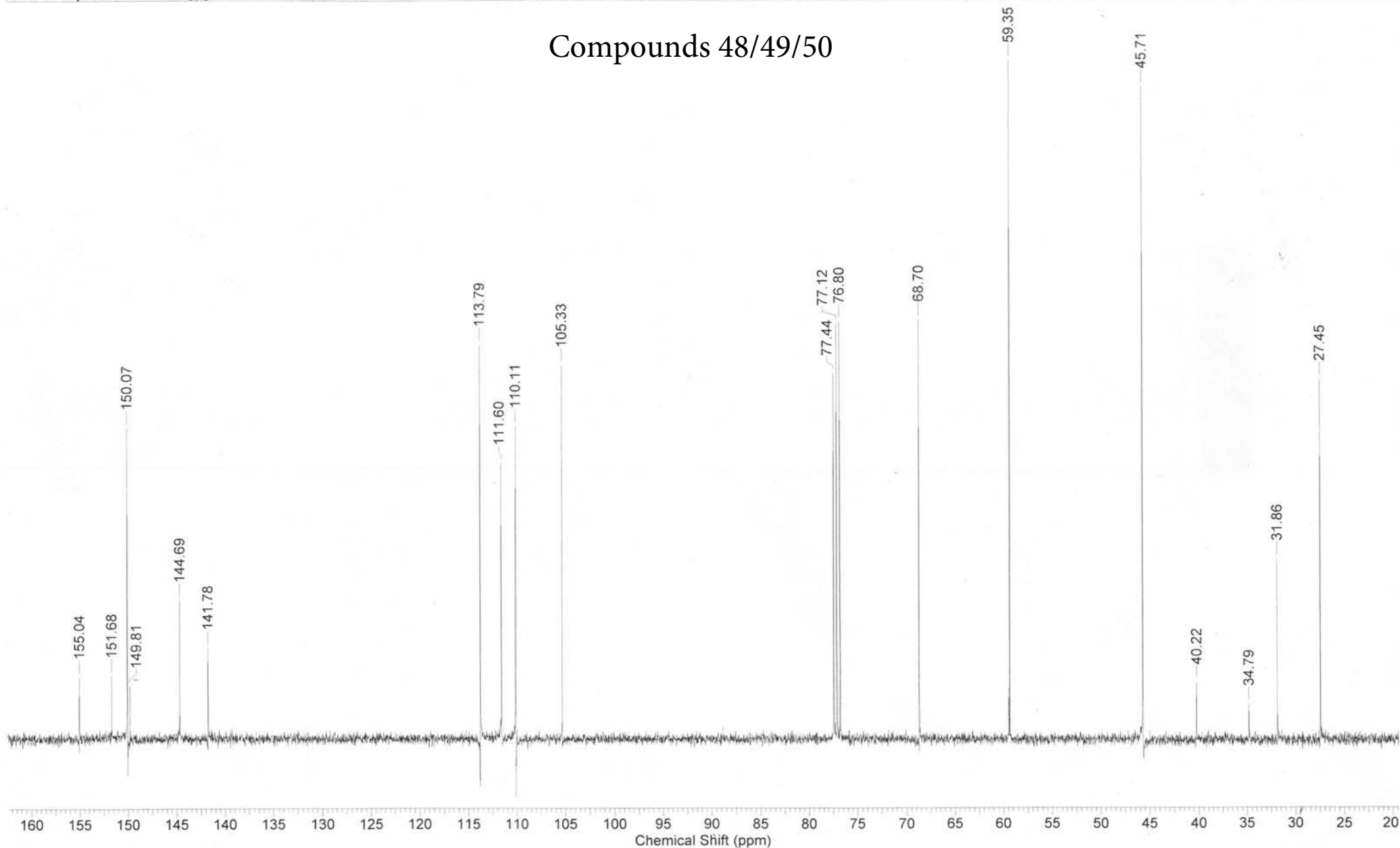


Acquisition Time (sec)	1.6056	Comment	Imported from UXNMR.		Date	23 Aug 2011 10:35:44	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-190811-N15\rudn-190811-N15_001000fid				Frequency (MHz)	400.14	
Nucleus	1H	Number of Transients	20	Original Points Count	16384	Points Count	16384
Pulse Sequence	zg	Solvent	CHLOROFORM-D		Sweep Width (Hz)	10204.08	
Temperature (degree C)	27.000						



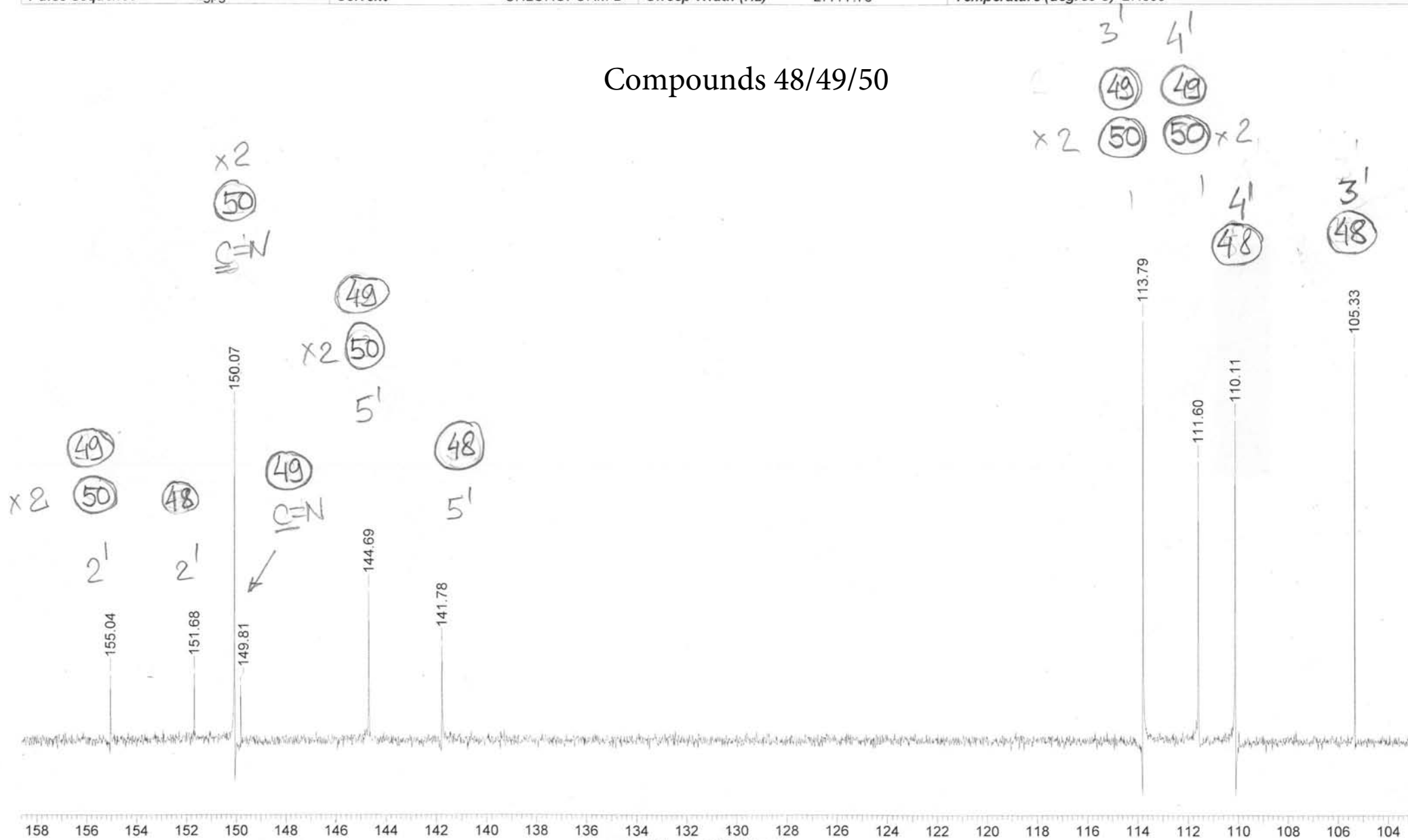
Acquisition Time (sec)	0.5898	Comment	Imported from UXMNR.		Date	24 Aug 2011 08:12:48	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-190811-N15-c13dec\rudn-190811-N15-c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	3099	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	27777.78	Temperature (degree C)	27.000

Compounds 48/49/50

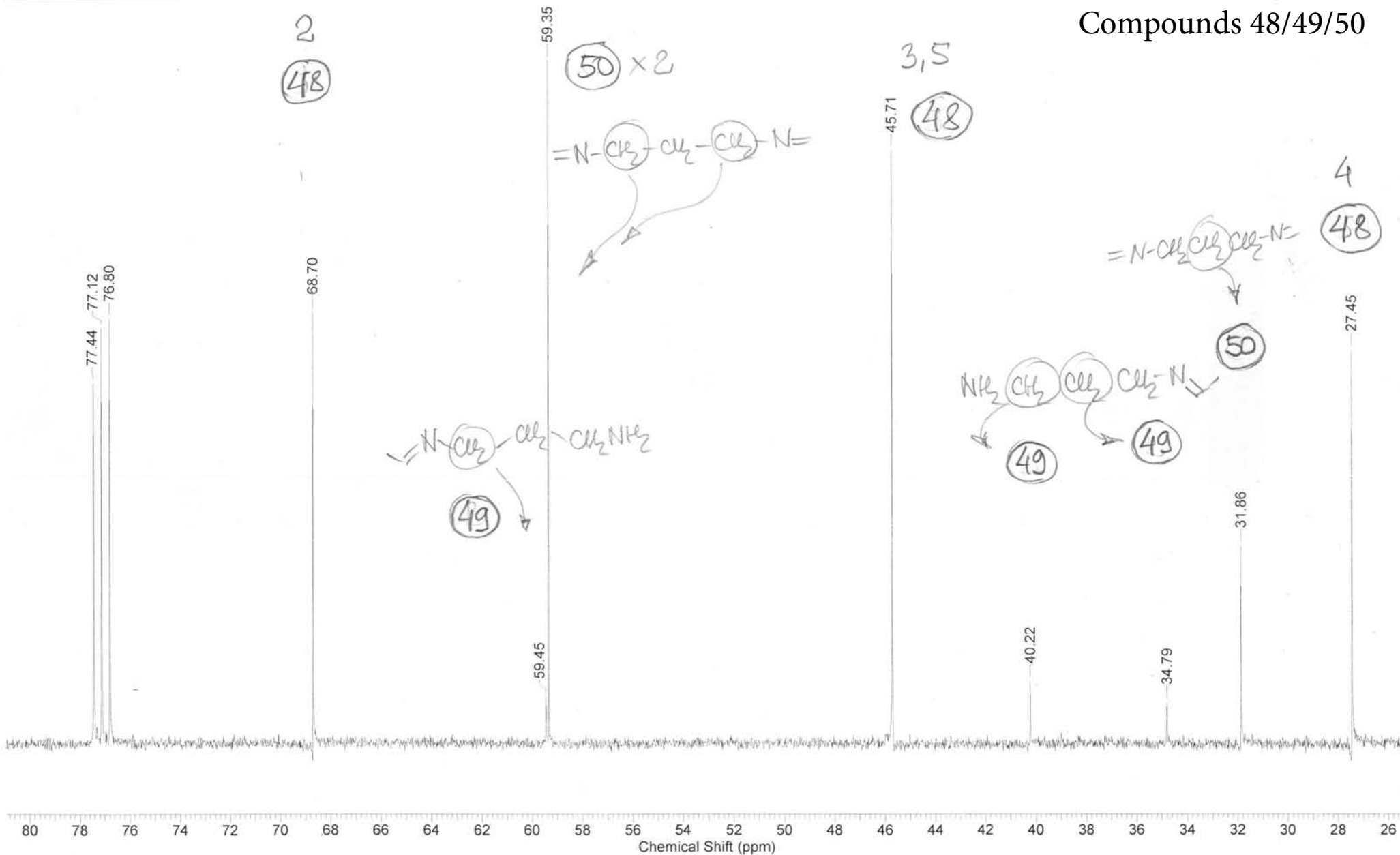


Acquisition Time (sec)	0.5898	Comment	Imported from UXMNR.		Date	24 Aug 2011 08:12:48	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-190811-N15-c13dec\rudn-190811-N15-c13dec_001000fid			Frequency (MHz)	100.62		
Nucleus	13C	Number of Transients	3099	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	27777.78	Temperature (degree C)	27.000

Compounds 48/49/50



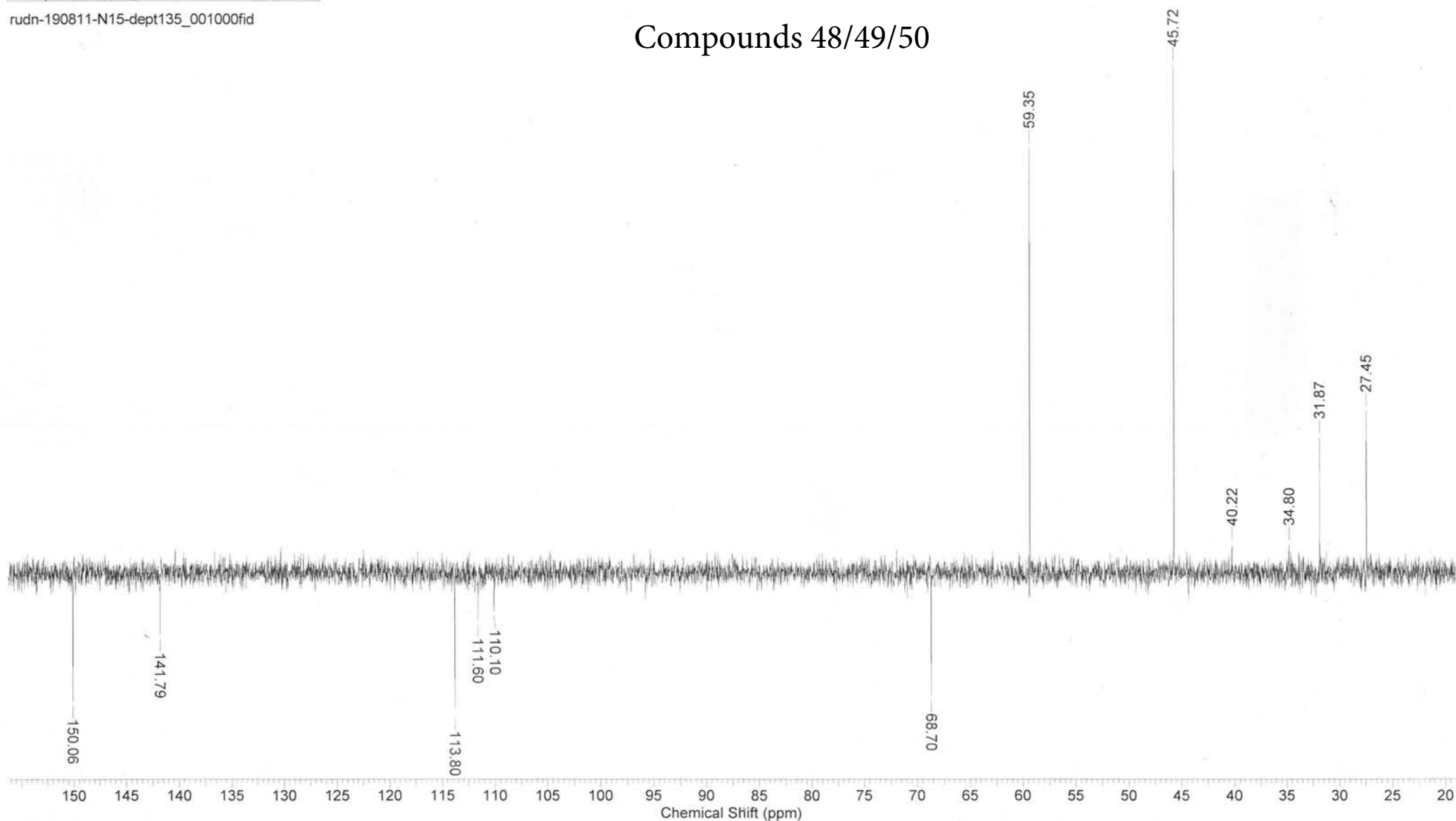
Acquisition Time (sec)	0.5898	Comment	Imported from UXMNR.		Date	24 Aug 2011 08:12:48	
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-190811-N15-c13dec\rudn-190811-N15-c13dec_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	3099	Original Points Count	16384	Points Count	16384
Pulse Sequence	zgpg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	27777.78	Temperature (degree C)	27.000



Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400		Date	24 Aug 2011 09:14:40	
Date Stamp	24 Aug 2011 09:14:40						
File Name	C:\Users\Fedor\Desktop\12.08.11\rudn-190811-N15-dept135\rudn-190811-N15-dept135_001000fid			Frequency (MHz)	100.62		
Nucleus	13C	Number of Transients	2007	Origin	spect	Original Points Count	16384
Owner	root	Points Count	16384	Pulse Sequence	dept135	Receiver Gain	32768.00
SW(cyclical) (Hz)	29411.77	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9636.4912	Sweep Width (Hz)	29409.97
Temperature (degree C)	27.000						

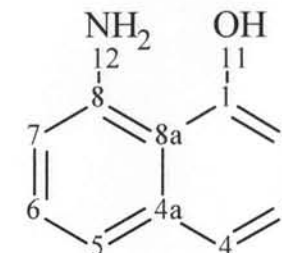
rudn-190811-N15-dept135_001000fid

Compounds 48/49/50

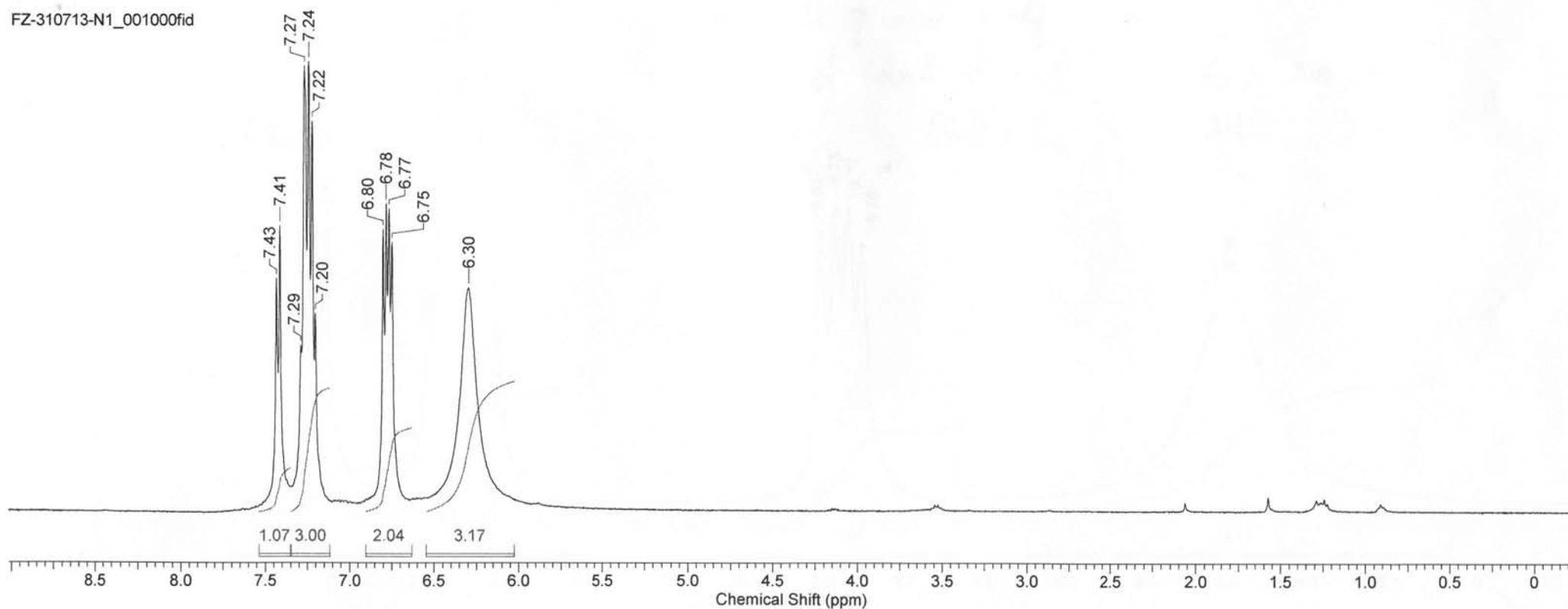


Formula	C ₁₀ H ₉ NO	FW	159.1846
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Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	31 Jul 2013 14:56:00
Date Stamp	31 Jul 2013 14:56:00	File Name	C:\Users\asus\Desktop\Рома лето 2013\nmrlastsamples\FZ-310713-N1\FZ-310713-N1_001000fid		
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	8
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	256.00	SW(cyclical) (Hz)	10204.08	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2602.0486	Sweep Width (Hz)	10203.46	Temperature (degree C)	27.000



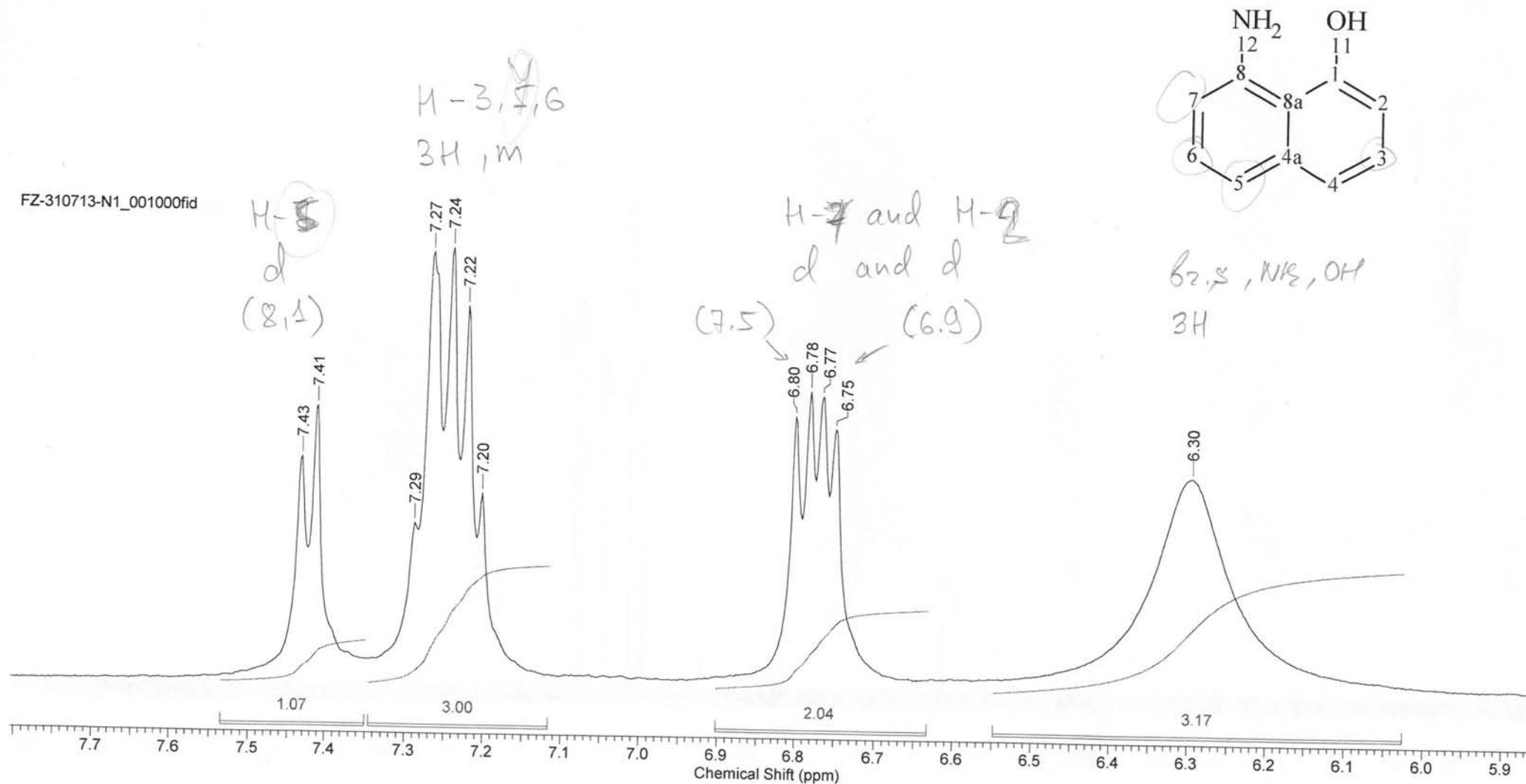
FZ-310713-N1_001000fid



C:\Users\asus\Desktop\Рома лето 2013\nmrlastsamples\FZ-310713-N1\FZ-310713-N1_001000fid

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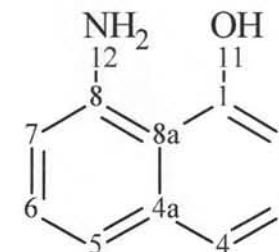
Formula	C ₁₀ H ₉ NO	FW	159.1846		
Acquisition Time (sec)	1.6056	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	31 Jul 2013 14:56:00
Date Stamp	31 Jul 2013 14:56:00	File Name	C:\Users\lasus\Desktop\Рома нето 2013\nmrlastsamples\FZ-310713-N1\FZ-310713-N1_001000fid		
Frequency (MHz)	400.14	Nucleus	1H	Number of Transients	8
Original Points Count	16384	Owner	root	Points Count	16384
Receiver Gain	256.00	SW(cyclical) (Hz)	10204.08	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2602.0486	Sweep Width (Hz)	10203.46	Temperature (degree C)	27.000
				Origin	spect
				Pulse Sequence	zg



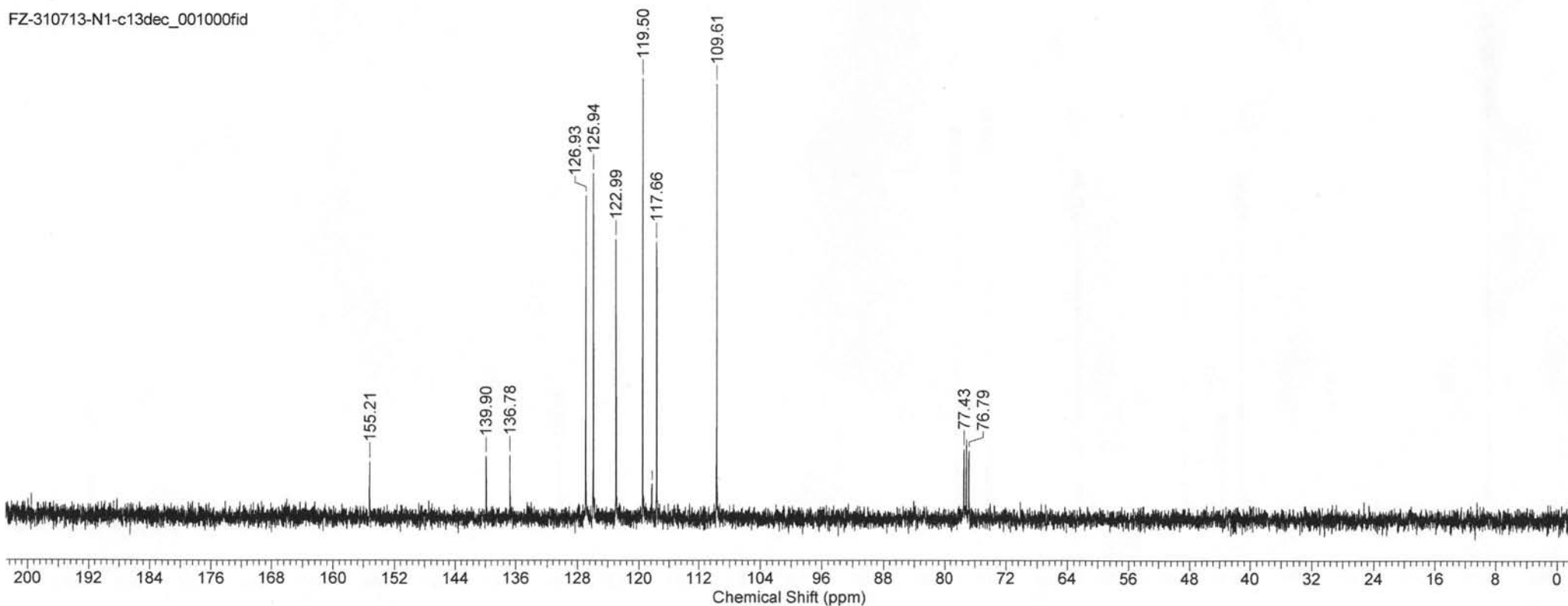
C:\Users\lasus\Desktop\Рома нето 2013\nmrlastsamples\FZ-310713-N1\FZ-310713-N1_001000fid

Formula	C ₁₀ H ₉ NO	FW	159.1846
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	31 Jul 2013 15:02:24
Date Stamp	31 Jul 2013 15:02:24				
File Name	C:\Users\lasus\Desktop\Рома лето 2013\nmr\lastsamples\FZ-310713-N1-c13dec\FZ-310713-N1-c13dec_001000fid			Frequency (MHz)	100.62
Nucleus	13C	Number of Transients	318	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zgpg
SW(cyclical) (Hz)	29411.77	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9630.2021
Temperature (degree C)	27.000			Sweep Width (Hz)	29409.97



FZ-310713-N1-c13dec_001000fid



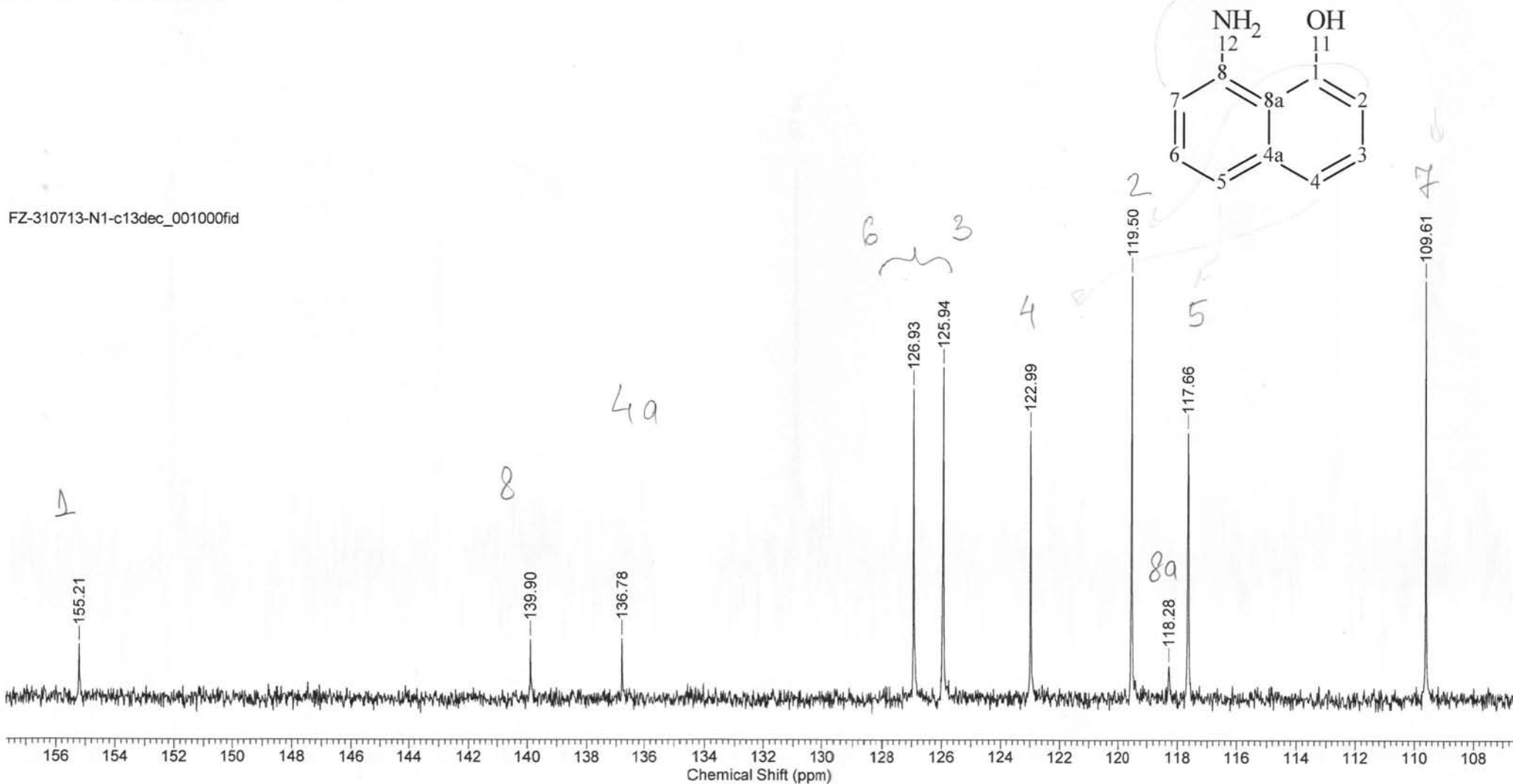
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Formula	C ₁₀ H ₉ NO	FW	159.1846
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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C/31P Z3379/0400	Date	31 Jul 2013 15:02:24
Date Stamp	31 Jul 2013 15:02:24				
File Name	C:\Users\asus\Desktop\Пома лето 2013\nmrlastsamples\FZ-310713-N1-c13dec\FZ-310713-N1-c13dec_001000fid			Frequency (MHz)	100.62
Nucleus	13C	Number of Transients	318	Origin	spect
Owner	root	Points Count	16384	Pulse Sequence	zgpg
SW(cyclical) (Hz)	29411.77	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9630.2021
Temperature (degree C)	27.000			Sweep Width (Hz)	29409.97

FZ-310713-N1-c13dec_001000fid

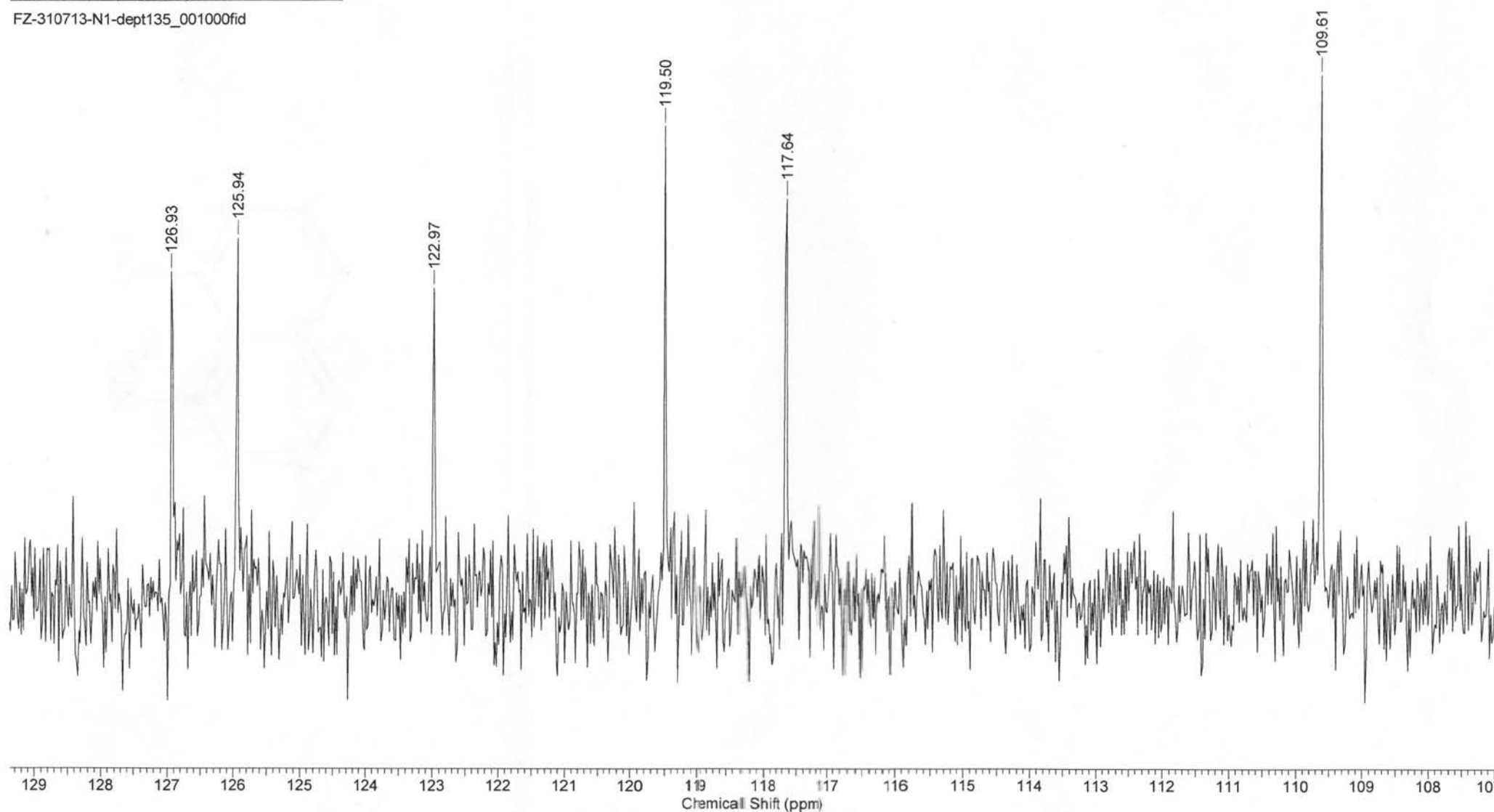


C:\Users\asus\Desktop\Пома лето 2013\nmrlastsamples\FZ-310713-N1-c13dec\FZ-310713-N1-c13dec_001000fid

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Acquisition Time (sec)	0.5571	Comment	5 mm QNP 1H/15N/13C31P Z3379/0400		Date	31 Jul 2013 15:04:32	
Date Stamp	31 Jul 2013 15:04:32						
File Name	C:\Users\asus\Desktop\Рома лето 2013\nmr\lastsamples\FZ-310713-N1-dept135\FZ-310713-N1-dept135_001000fid				Frequency (MHz)	100.62	
Nucleus	13C	Number of Transients	355	Origin	spect	Original Points Count	16384
Owner	root	Points Count	16384	Pulse Sequence	dept135	Receiver Gain	32768.00
SW(cyclical) (Hz)	29411.77	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9630.2119	Sweep Width (Hz)	29409.97
Temperature (degree C)	27.000						

FZ-310713-N1-dept135_001000fid



C:\Users\asus\Desktop\Рома лето 2013\nmr\lastsamples\FZ-310713-N1-dept135\FZ-310713-N1-dept135_001000fid

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