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Graphical Abstract

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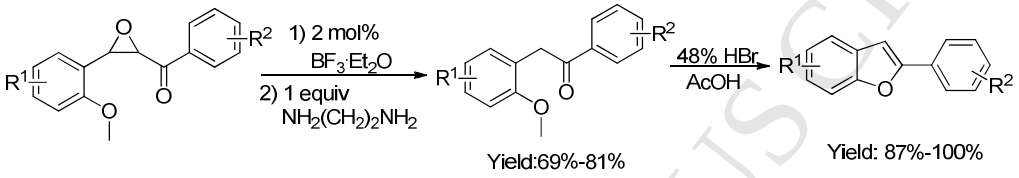
Libo Ruan, Min Shi, Shiwei Mao, Lifang Yu, Fan Yang, Jie Tang
Institute of Drug Discovery and Development, Shanghai Engineering Research Center of Molecular Therapeutics and New Drug Development, East China Normal University, 3663 North Zhongshan Road, Shanghai, China



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An efficient approach to construct 2-arylbenzo[*b*]furans from 2-methoxychalcone epoxides

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Institute of Drug Discovery and Development, Shanghai Engineering Research Center of Molecular Therapeutics and New Drug Development, East China Normal University, Shanghai 200062, China

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ABSTRACT

An efficient and practical method for construction of 2-arylbenzo[*b*]furans from 2-methoxychalcone epoxides has been reported. Catalyzed by 2mol% of $BF_3{\cdot}Et_2O$, 2-methoxychalcone epoxides went through the Meerwein rearrangement, followed by deformylation in one-pot to successfully afforded 2-methoxydeoxybenzoins. Afterwards, 2-arylbenzo[*b*]furans were obtained in high yields (87%-100%) via intermolecular cyclodehydration of 2-methoxydeoxybenzoins with 48% HBr. By utilization of this approach, the natural product stemofuran A and the key intermediate of eupomatenoid 6 have been synthesized conveniently.

1. Introduction

2-Arylbenzo[*b*]furans widely exist in natural products,[1] and many compounds including 2-arylbenzo[*b*]furan structural unit were found to possess attractive pharmacological activities, such as antitumor,[2] antiviral,[3] antioxidative,[4] and antifungal properties.[5] Their broad range of biological activities and significant pharmacological potentials have resulted in the development of many methods for their synthesis.[6] The palladium-catalyzed cross-coupling cyclization reaction from alkynes and *o*-halophenols was found to be efficient.[7] Other approaches for the synthesis of benzo[*b*]furans include cyclization of vinylic phenols through McMurry coupling reaction,[8] [3,3]-sigmatropic rearrangement of oxime ethers,[9] palladium-catalyzed enolate arylation.[10]

The relative ease of preparation chalcone epoxides makes them promising starting materials for preparation of a variety of heterocyclic compounds. Our group is interested in extent the application scope of these versatile molecules. Previously, we successfully used chalcone epoxides as a synthetic precursor for the preparation of 3-aryl quinolines.[11] Herein, we reported a new practical synthetic route for the preparation of 2-arylbenzo[*b*]furans from 2-methoxychalcone epoxides.

2. Results and discussion

Asokan et al. observed that β–ketoaldehydes could react with 1,2-diaminoethane in THF to yield deoxybenzoins.[12] However, only 4-substitute substrates were tested. We considered that if the 2-alkyloxysubstituted chalcone epoxides were used in these reactions, 2-methoxydeoxybenzoins should be obtained conveniently, which could be further transformed to the corresponding 2-arylbenzo[*b*]furans via cyclodehydration.

We firstly focused on the optimization of the reaction conditions with 2,3-epoxy-3-(2-metoxy-phenyl)-1-phenylpropan-1-one (**1a)** as a model substrate (Table 1). Meerwein rearrange-

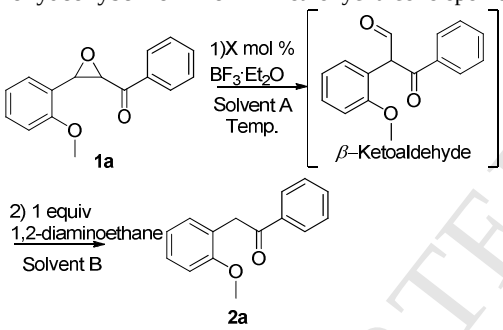
* Corresponding author. Tel.: +86-21-62232764; E-mail: fyang@chem.ecnu.edu.cn

* Corresponding author. Tel.: +86-21-62232100; E-mail: jtang@chem.ecnu.edu.cn

ment of chalcone epoxides to form β–ketoaldehydes has been known for a long time,[13] and 2 equiv[13] or 1 equiv[12] of $BF_3{\cdot}Et_2O$ was used in the reaction. From the viewpoint of catalytic mechanism, we attempted to carry out the reaction with catalytic amount of $BF_3{\cdot}Et_2O$, and the results showed that the reduction of the amount of $BF_3{\cdot}Et_2O$ from 100 mol% to 2 mol% did not affect the yield (Table 1, entries 2-5). When the catalyst was further reduced to 0.5 mol% the yield of the product dropped to 21% due to an incomplete rearrangement reaction (Table 1, entry 6). Therefore, 2 mol% of $BF_3{\cdot}Et_2O$ was chosen as the optimal catalyst amount for the following rearrangement reactions. Change of the organic solvent of the rearrangement reaction indicated that the solvent played a paramount role in terms of rates and chemical yields, and DCM was still the best choice. The reaction finished in 5 min at 25 °C (Table 1, entry 5). The reactions were sluggish and gave lower yields in PhMe, MeCN, or THF due to the incomplete rearrangement (Table 1, entries 7-9). The influence of temperature on the rearrangement reaction was also preliminarily tested, and lower yield was obtained when decrease the temperature was decreased from 25 °C to 0 °C (Table 1, entry 10).

In addition, we found that the deformylation reaction of 2-methoxy-β–ketoaldehyde could also be carried out in DCM instead of THF (Table 1, entry 11). Therefore the procedure was further simplified by successively performing the deformylation after the rearrangement of chalcone epoxides, and the two-step reaction proceeded in one-pot to afford the desired product **2a** in good yield.

Table 1. Optimization of reaction conditions for synthesis of 2-methoxydeoxybenzoin from 2-methoxychalcone epoxide

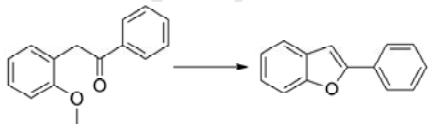


Entry[a]	$BF_3{\cdot}Et_2O$	Solvent A	Solvent B	Temp (°C)	Yield (%)[b]
1	100 mol%	DCM	THF	25	72
2	50 mol%	DCM	THF	25	71
3	10 mol%	DCM	THF	25	72
4	5 mol%	DCM	THF	25	77
5	2 mol%	DCM	THF	25	75
6	0.5 mol%	DCM[c]	THF	25	21[c]
7	2 mol%	Toluene	THF	25	64
8	2 mol%	MeCN	THF	25	32
9	2 mol%	THF	THF	25	56
10	2 mol%	DCM[c]	THF	0	57
11	2 mol%	DCM	DCM	25	72

[a] Raction conditions: 1 mmol of chalcone epoxides, 5 mL of solvent A, after the rearrangement reaction was complete, the solvent A was removed in vacuo, then added 5 mL solvent B , 1 equiv of 1,2-diaminoethane.
[b] Isolated yields.
[c] Reaction conducted for 4 h.

To construct 2-arylbenzo[*b*]furan **3a**, **2a** was selected as a model substrate to examine its behavior under different demethylation conditions (Table 2). There are very few reports about the cyclodehydration of 2-alkyloxydeoxybenzoin to afford benzo[*b*]furans, which was only carried out the reaction with BCl_3 at -78 °C,[14a] or with $AlBr_3$ in benzene.[14c] To our delight, treatment of **2a** with 48% HBr in AcOH, deoxybenzoin **2a** could be demethylated, and subsequently cyclodehydrated to give the desired benzo[*b*]furan **3a** in quatitative yield (Table 2, entry 5). Treatment of **2a** with BBr_3 in CH_2Cl_2 at 0°C gave **3a** in 43% yield due to side reaction (Table 2, entrie 1), and only trace of **3a** was detected when $AlCl_3$/Py or LiCl was used(Table 2, entries 2, 6). Although HI and TMSI/KI were competent reagents for this reaction (Table 2, entries 3, 4), from the standpoint of overall cost and for large scale reactions, 48% HBr was chosen as the demethylation reagent in the following reaction.

Table 2. Optimization of reaction conditions for conversion of 2-methoxydeoxybenzoins to benzo[*b*]furan[a]



2a 3a

Entry	Demethylation reagents	Solvent	Time	Temp (°C)	Yield (%)[b]
1	BBr_3	DCM	0.5 h	0 °	43
2	$AlCl_3$/Py	DCM	6 h	rt	trace
3	HI	H_2O	6 h	reflux	92
4	TMSI/KI	MeCN	6 h	reflux	88
5	48 % HBr	AcOH	6 h	reflux	100
6	LiCl	DMF	12 h	110	trace

[a] Reaction conditions: 1 mmol of **2a,** 4 equivalents of demethylation reagents, the progress of the reaction was monitored by TLC.
[b] Isolated yields.

In order to examine the scope of this construction method for 2-arylbenzo[*b*]furans, a variety of 2-arylbenzo[*b*]furans were prepared through this two-step one-pot synthetic strategy, and the results were shown in Table 3. The variation of R_1 and R_2 groups had little influence on the reaction yields, and moderate to good overall yields were observed (Table 3, entries 1-11) regardless of the steric (*ortho*, *meta* and *para* positions) and electronic properties (both electronic rich and deficient). Importantly, heteroaromatic chalcone epoxide **1i** was a suitable substrate, giving the desired product **3i** in 87% yield (Table 3, entry 9). It is worth noting that the obtained halide products such as bromide and iodide are very useful intermediates which could be further functionalized to give avariety of derivatives (Table 3, entries 4-7, 10, 11).

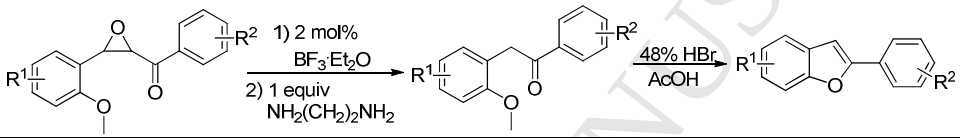
To expand the utilization of the method, we attempted to construct a useful natural product stemofuran A and the key intermediate of natural product eupomatenoid 6, 4-(5-bromo-3-methylbenzofuran-2-yl)phenol (**4m)**. Stemofuran A was isolated from a methanolic extract of *Stemona collinsae* root which was reported to have potential antifungal activity.[2c] Stemofuran A has been synthesized by several groups using different approaches.[9,14a,14b] 4-(5-Bromo-3-methylbenzofuran2-yl)phenol (**4m)** is an important synthetic intermediate used in the production of eupomatenoid 6,[9] which was first isolated in 1969 from the bark of *Eupomatia laurina R.* with a broad range of biological activities.[14c-14e] **4m** was prepared by *Naito* and co-workers

starting from oxime ethers through [3,3]-sigmatropic rearrangement reaction with 53% overall yield (4 steps).[9]

As illustrated in Scheme 1, stemofuran A was achieved with an overall yield of 71% began with 2-methoxychalcone epoxide (**1l**) which was treated with 2 mol% of $BF_3{\cdot}Et_2O$ and then deformylated to afford the desired compound (**2l)** in 76% yield. **2l** underwent demethylation and cyclodehydration reactions in the presence of 48% HBr in acetic acid to give stemofuran A in excellent yield (94%). The spectral data of **3l** are identical with those reported in the literature.[14b] Similarly, 4-(5-bromo-3-methylbenzofuran2-yl)-phenol (**4m)** was synthesized in 64% overall yield. The readily available 2-methoxychalcone epoxide (**1m)** was converted into the corresponding deoxybenzoin (**2m)** by the sequence of Meerwein rearrangement, deformylation in 71% yield. The reaction of **2m** with methyl iodide in the presence of potassium *tert*-butoxide in THF gave the compound **3m** in 100% yield. Compound **3m** was then treated with 48% HBr in acetic acid under reflux to give 4-(5-bromo-3-methylbenzofuran2-yl)-phenol (**4m)** in 90% yield. The procedure for synthesis of stemofuran A and **4m** is practical and convenient, and all the substrates and reagents are cheap and commercially available.

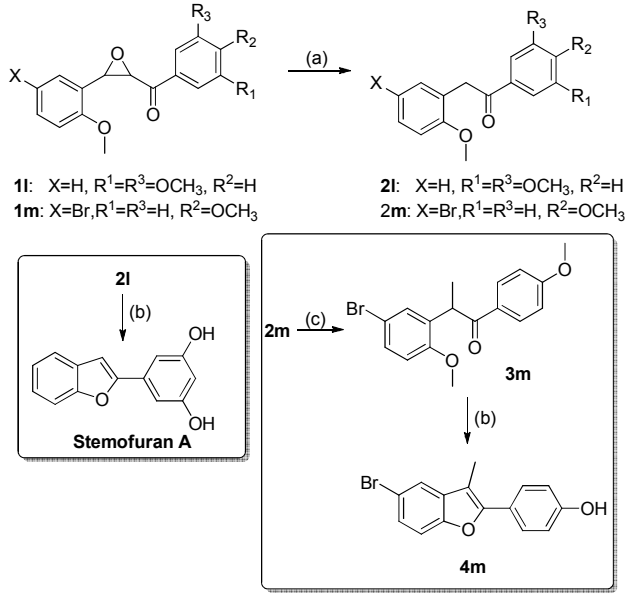
According to our experimental results and the reported literature,[13,14] a plausible reaction mechanism is proposed as shown in Scheme 2, which includes: i) The chalcone epoxides A undergoes smooth Meinwald rearrangement reaction with $BF_3{\cdot}Et_2O$ to give β–ketoaldehyde B. ii) Reaction of β–Ketoaldehyde B with 1,2-diaminoethane gives the intermediate C, which is possibly converted to intermediate D. The intermediate D undergoes a [3,3]-sigmatropic rearrangement type rearrangement produces the corresponding deoxybenzoin E. iii) Deoxybenzoin E is demethylated to form 2-(2-hydroxyphenyl)-1-phenylethanone F, which is cyclized to give the intermediate **G,** subsequent dehydrated of intermediate **G** form the desired 2-arylbenzo[*b*]furan.

Table 3. Synthesis of 2-arylbenzo[*b*]furan from 2-methoxychalcone epoxide.

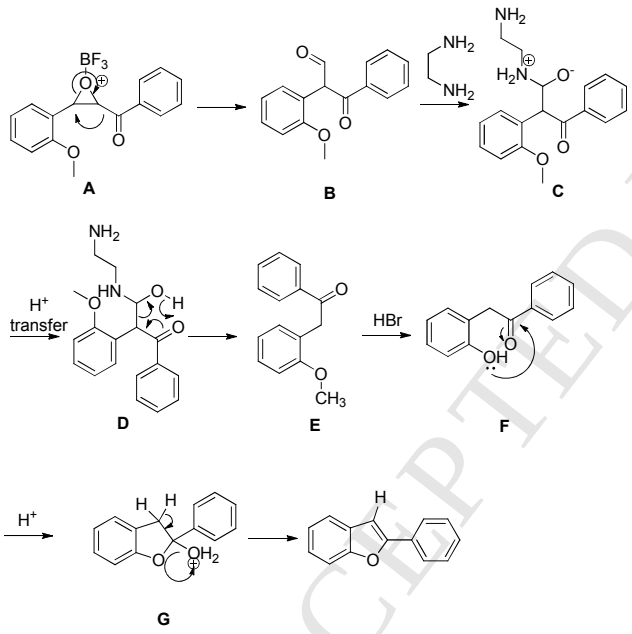


Entry	R_1	R_2	Starting material	Deoxybenzoins	Yield (%)	Benzofurans	Yield (%)[a]
1	H	H	**1a**	**2a**	72	**3a**	100
2	H	4-OCH_3	**1b**	**2b**	73	**3b**	98
3	H	3-OCH_3	**1c**	**2c**	78	**3c**	95
4	H	2-Br	**1d**	**2d**	76	**3d**	100
5	H	3-Br	**1e**	**2e**	74	**3e**	96
6	H	4-Br	**1f**	**2f**	69	**3f**	98
7	H	4-I	**1g**	**2g**	77	**3g**	96
8	H	4-Me	**1h**	**2h**	74	**3h**	100
9	H	2-thiophyl	**1i**	**2i**	81	**3i**	87
10	Br	H	**1j**	**2j**	71	**3j**	93
11	Br	4-OCH_3	**1k**	**2k**	75	**3k**	92

[a] Isolated yields.



Scheme 1. Synthesis of stemofuran A and 4-(5-bromo-3-methylbenzofuran-2-yl)phenol. Reagents and conditions: (a) 1) 2 mol% $BF_3{\cdot}Et_2O$, DCM, 5min; 2) 1,2-diaminoethane, 5min (76% yield for **2l**; 71% yield for **2m**); (b) 48% HBr-AcOH, reflux, 8h (94% yield for stemofuran A; 90% yield for **4m**); (c) *t*-BuOK, CH_3I, THF, 0°C, 2h (100% yield for **3m**).



Scheme 2. Possible reaction pathway

3. Conclusions

In conclusion, we developed a facile synthetic strategy for the synthesis of 2-arylbenzo[*b*]furan using commercially available, suitably functionalized 2-methoxychalcone epoxides. Catalyzed by 2 mol% of $BF_3{\cdot}Et_2O$, 2-methoxychalcone epoxides went through the Meerwein rearrangement, followed by deformylation in one-pot to successfully afforded 2-methoxydeoxybenzoins. Afterwards, 2-arylbenzo[b]furan were obtained in high yields (87%-100%) by intramolecular cyclodehydration of 2-methoxydeoxybenzoin with 48% HBr. The effectiveness of the protocol was demonstrated by the synthesis of stemofuran A and the key intermediate of eupomatenoid 6, 4-(5-bromo-3-methylbenzofuran2-yl)-phenol. The present method has several advantages including that the reagents used are readily available, the protocols are simple to carry out and not involving metal catalysts. This methodology will be a valuable addition to the existing methods in the field of 2-arylbenzo[*b*]furan synthesis.

4. Experimental

4.1. General methods

All reagents were purchased from commercial sources and used without treatment. ^1H and ^{13}C NMR spectra were recorded at 400 and 100 MHz, respectively, using TMS as the internal standard. HRMS were recorded on a Bruker micrOTOF II spectrometer (ESI ionization).

4.2. General Procedure for Synthesis of 2-methoxydeoxybenzoins

To a solution of 2 mmol of the chalcone epoxide in CH_2Cl_2 (10 mL) was added 2 mol% of $BF_3{\cdot}Et_2O$ at 25 °C. The mixture was stirred for 5 min, then 1, 2-diaminoethane (120 mg, 2 mmol) was added in one portion. The reaction mixture was stirred at 25 °C until TLC indicated complete (about 5 min). The mixture was poured into ice water. The organic phase was separated and the water phase was extracted with dichloromethane for three times (3×10 mL). The combined organic phases were dried over anhydrous Na_2SO_4. Removal of the solvent *in vacuo*, and the residue was column chromatographed over silica gel to give pure deoxybenzoins.

4.2.1. 2-(2-Methoxyphenyl)-1-phenylethanone (***2a***). The title compound was prepared according to the general procedure. The product was obtained as white solid (324 mg, 72% yield, mp 59-61 °C; [Lit. 60-61 °C][15]); ^1H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, J = 7.3 Hz, 2H), 7.53 (d, J = 7.3 Hz, 1H), 7.48-7.42 (m, 2H), 7.28-7.22 (m, 1H), 7.17 (d, J = 7.3 Hz, 1 H), 6.95-6.86 (m, 2H), 4.27 (s, 2H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.9, 157.1, 136.9, 132.8, 130.9, 128.4 (2C), 128.3 (2C), 128.3, 123.6, 120.5, 110.5, 55.3, 39.9.

4.2.2. 2-(2-Methoxyphenyl)-1-(4-methoxyphenyl)ethanone (***2b***). The title compound was prepared according to the general procedure. The product was obtained as yellow solid (373 mg, 73% yield, mp 88–90 °C; [Lit. 89.5 °C][16]); ^1H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 8.8 Hz, 2H), 7.27-7.19 (m, 1H), 7.17 (d, J = 7.3 Hz, 1H), 6.94-6.85 (m, 4H), 4.22 (s, 2H), 3.84 (s, 3H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.6, 163.4, 157.2, 131.0, 130.7 (2C), 130.1, 128.3, 124.1, 120.7, 113.7 (2C), 110.6, 55.4, 55.3, 39.6.

4.2.3. 2-(2-Methoxyphenyl)-1-(3-methoxyphenyl)ethanone (***2c***) The title compound was prepared according to the general procedure. The product was obtained as a colourless oil (400 mg, 78% yield); ^1H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, J = 7.5 Hz, 1H), 7.55 (s, 1H), 7.33 (t, J = 8.0 Hz, 1H), 7.26-7.20 (m, 1H), 7.16 (d, J = 7.0 Hz, 1H), 7.09-7.04 (m, 1H), 6.93-6.83 (m, 2H), 4.24 (s, 2H), 3.80 (s, 3H), 3.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.6, 159.6, 157.0, 138.2, 130.8, 129.4, 128.2, 123.6, 120.9, 120.5, 119.2, 112.6, 110.4, 55.2, 55.2, 39.9.

4.2.4. 1-(2-Bromophenyl)-2-(2-methoxyphenyl)ethanone (***2d***). The title compound was prepared according to the general procedure. The product was obtained as colorless oil (463 mg, 76% yield); ^1H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, J = 8.0 Hz, 1H), 7.41 (dd, J = 1.5, 7.5 Hz, 1H), 7.34-7.29 (m, 1H), 7.27-7.20 (m, 3H), 6.92 (t, J = 7.5 Hz, 1H), 6.83 (d, J = 8.0 Hz, 1H), 4.20 (s, 2H), 3.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.7, 157.3, 141.8, 133.5, 131.4, 131.2, 128.7, 128.6, 127.1, 123.1, 120.6, 118.7, 110.4, 55.3, 44.4.

4.2.5. 1-(3-Bromophenyl)-2-(2-methoxyphenyl)ethanone (***2e***). The title compound was prepared according to the general procedure. The product was obtained as white solid (451 mg, 74% yield, mp 78 -79 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (s, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.33-7.21 (m, 2H), 7.16 (d, *J* = 7.0 Hz, 1H), 6.94-6.85 (m, 2H), 4.22 (s, 2H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.5, 157.0, 138.6, 135.6, 131.5, 130.9, 130.0, 128.5, 126.9, 123.1, 122.7, 120.6, 110.6, 55.3, 39.9. HRMS (ESI) calcd for $C_{15}H_{13}BrO_2Na$ $[M+Na]^+$ 326.9997, found 326.9984.

4.2.6. 1-(4-Bromophenyl)-2-(2-methoxyphenyl)ethanone (***2f***). The title compound was prepared according to the general procedure. The product was obtained as white solid (421 mg, 69% yield, mp 90 -91 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.5 Hz, 2H), 7.57 (d, *J* = 8.5 Hz, 2H), 7.28-7.21 (m, 1H), 7.16 (d, *J* = 7.3 Hz, 1H), 6.95-6.84 (m, 2H), 4.22 (s, 2H), 3.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.1, 157.1, 135.7, 131.8, 131.0 (2C), 130.0 (2C), 128.6, 128.0, 123.4, 120.7, 110.6, 55.4, 40.0. HRMS (ESI) calcd for $C_{15}H_{13}BrO_2Na$ $[M+Na]^+$ 326.9997, found found 326.9984.

4.2.7 1-(4-Iodophenyl)-2-(2-methoxyphenyl)ethanone (***2g***). The title compound was prepared according to the general procedure. The product was obtained as white solid (542 mg, 77% yield, mp 118-120 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82-7.78 (m, 2H), 7.74-7.71 (m, 2H), 7.28-7.22 (m, 1H), 7.15 (d, *J* = 7.3 Hz, 1H), 6.94-6.85 (m, 2H), 4.21 (s, 2H), 3.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.3, 157.0, 137.8(2C), 136.2, 130.9, 129.8(2C), 128.5, 123.3, 120.7, 110.6, 100.7, 55.3, 39.9. HRMS (ESI) calcd for $C_{15}H_{13}IO_2Na$ $[M+Na]^+$ 374.9858, found 374.9841.

4.2.8. 2-(2-Methoxyphenyl)-1-(p-tolyl)ethanone (***2h***). The title compound was prepared according to the general procedure. The product was obtained as white solid (355 mg, 74% yield, mp 44-45 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.0 Hz, 2H), 7.27-7.12 (m, 4H), 6.93-6.82 (m, 2H), 4.23 (s, 2H), 3.75 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.6, 157.3, 143.6, 134.6, 131.0, 129.2 (2C), 128.6 (2C), 128.3, 124.0, 120.7, 110.6, 55.4, 39.9, 21.7. HRMS (ESI) calcd for $C_{16}H_{16}O_2Na$ $[M+Na]^+$ 263.1048, found 263.1039.

4.2.9. 2-(2-Methoxyphenyl)-1-(thiophen-2-yl)ethanone (***2i***). The title compound was prepared according to the general procedure. The product was obtained as white solid (376 mg, 81% yield, mp 75-76 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 3.8 Hz, 1H), 7.57 (d, *J* = 5.0 Hz, 1H), 7.27-7.19 (m, 2H), 7.08 (t, *J* = 4.4 Hz, 1H), 6.94-6.84 (m, 2H), 4.19 (s, 2H), 3.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.7, 157.1, 144.1, 133.3, 132.2, 130.9, 128.4, 127.9, 123.3, 120.6, 110.6, 55.3, 40.5. HRMS (ESI) calcd for $C_{13}H_{12}O_2SNa$ $[M+Na]^+$ 255.0456, found 255.0445.

4.2.10. 2-(5-Bromo-2-methoxyphenyl)-1-phenylethanone (***2j***). The title compound was prepared according to the general procedure. The product was obtained as white solid (433 mg, 71% yield, mp 68-69 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 7.3 Hz, 2H), 7.59-7.53 (m, 1H), 7.50-7.43 (m, 1H), 7.34 (dd, *J* = 2.3, 8.5 Hz, 1H), 7.28 (d, *J* = 2.3 Hz, 1H), 6.74 (d, *J* = 8.5 Hz, 1H), 4.23 (s, 2H), 3.74 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.0, 156.4, 136.7, 133.7, 133.1, 131.0, 128.5 (2C), 128.3 (2C), 125.9, 112.7, 112.2, 55.6, 39.6. HRMS (ESI) calcd for $C_{15}H_{13}BrO_2Na$$[M+Na]^+$ 326.9997, found 326.9984.

4.2.11. 2-(5-Bromo-2-methoxyphenyl)-1-(4-methoxyphenyl)-ethanone (***2k***). The title compound was prepared according to the genera procedure. The product was obtained as white solid (500 mg, 75% yield, mp 117-118 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-7.96 (m, 2H), 7.36-7.27 (m, 2H), 6.93 (d, *J* = 8.5 Hz, 2H), 6.74 (d, *J* = 8.5 Hz, 1H), 4.18 (s, 2H), 3.86 (s, 3H), 3.75 (s, 3H); ^{13}C NMR (100 MHz , $CDCl_3$) δ 195.6, 163.5, 156.4, 133.6, 130.9, 130.6 (2C), 129.8, 126.3, 113.7 (2C), 112.7, 112.2, 55.6, 55.4, 39.2. HRMS (ESI) calcd for $C_{16}H_{15}BrO_3Na$ $[M+Na]^+$ 357.0102, found 357.0110.

4.3. ***General Procedure for Synthesis of 2-benzo[b]furan.***

To a stirred solution of **2a-2k** (1 mmol) in 48% HBr (4 mL) was added AcOH (5 mL) and the mixture was heated to reflux. The reaction was stirred until TLC indicated complete (about 8h). The reaction mixture was cooled to room temperature, AcOH was removed under reduced pressure and the aqueous part was extracted with extracted with EtOAc (2 × 100 mL), washed with brine, dried (Na_2SO_4), and concentrated to obtain corresponding pure benzo[*b*]furans. Pure products of ***3a***, ***3b***, ***3c***, ***3d***, ***3e***, ***3f***, and ***3h*** were obtained by simple extraction. The yields of ***3g***, ***3i***, ***3j***, ***3k***, were determined after silica gel column chromatography (petroleum ether / EtOAc).

4.3.1. 2-Phenylbenzofuran (***3a***). The title compound was prepared according to the general procedure. The product was obtained as white solid (194 mg, 100% yield, mp 117-119 °C; [Lit. 119 °C][17]); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.0 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.43-7.36 (m, 2H), 7.34-7.15 (m, 3H), 6.96 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.9, 154.9, 130.4, 129.2, 128.7 (2C), 128.5, 124.9 (2C), 124.2, 122.9, 120.9, 111.1, 101.3.

4.3.2. 4-(Benzofuran-2-yl)phenol (***3b***). The title compound was prepared according to the general procedure. The product was obtained as white solid (206 mg, 98% yield, mp 194-195 °C; [Lit. 194-195 °C][18]); ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.90 (s, 1H), 7.76 (d, *J* = 8.5 Hz, 2H), 7.58 (t, *J* = 6.8 Hz, 2H), 7.24 (quin, *J* = 7.1 Hz, 2H), 7.14 (s, 1 H), 6.92 (d, *J* = 8.5 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.3, 155.9, 153.9, 129.2, 126.4 (2C), 123.7, 123.0, 120.9, 120.6, 115.9 (2C), 110.8, 99.3.

4.3.3. 3-(Benzofuran-2-yl)phenol (***3c***). The title compound was prepared according to the general procedure. The product was obtained as white solid (252 mg, 95% yield, mp 131-133 °C; [Lit.131-132 °C][19]); ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.71 (s, 1H), 7.63 (dd, *J* = 7.8, 12.3 Hz, 2H), 7.39-7.23 (m, 6H), 6.82 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 157.8, 155.3, 154.1, 130.9, 130.2, 128.8, 124.5, 123.2, 121.1, 116.0, 115.7, 111.2, 111.1, 101.9.

4.3.4. 2-(2-Bromophenyl)benzofuran (***3d***). The title compound was prepared according to the general procedure. The product was obtained as colorless liquid (271 mg, 100% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (dd, *J* = 1.0, 8.0 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 8.0 Hz, 1H), 7.54-7.49 (m, 2H), 7.37 (t, *J* = 8.0 Hz, 1H), 7.30 (t, *J* = 8.0 Hz, 1H), 7.26-7.20 (m, 1H), 7.18-7.12 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.2, 153.1, 134.2, 131.0, 129.7, 129.3, 128.8, 127.4, 124.8, 122.9, 121.4, 120.7, 111.1, 107.0.

4.3.5. 2-(3-Bromophenyl)benzofuran (***3e***). The title compound was prepared according to the general procedure. The product was obtained as white solid (261 mg, 96% yield, mp 84-85 °C; [Lit. 85 °C][20]); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.96 (m, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.56 (d, *J* = 7.3 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.46-7.42 (m, 1H), 7.32-7.19 (m, 3H), 6.99 (s, 1H); ^{13}C NMR (100 MHz ,$CDCl_3$) δ 154.9, 154.1, 132.4, 131.3, 130.3, 128.9, 127.8, 124.7, 123.4, 123.1, 122.9, 121.1, 111.2, 102.4.

4.3.5. 2-(4-Bromophenyl)benzofuran (***3f***). The title compound was prepared according to the general procedure. The product was obtained as white solid (265 mg, 98% yield, mp 149-150 °C; [Lit. 149-150 °C][21]); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.5 Hz, 2H), 7.59-7.53 (m, 3H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.32-7.26 (m, 1H), 7.25-7.20 (m, 1H), 7.00 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.9, 154.8, 131.9 (2C), 129.4, 129.0, 126.3 (2C), 124.6, 123.1, 122.5, 121.0, 111.2, 101.8.

4.3.7. 2-(4-Iodophenyl)benzofuran (***3g***). The title compound was prepared according to the general procedure. The product was obtained as white solid (361 mg, 96% yield, mp 180-181 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.3 Hz, 2H), 7.57 (d, *J* = 8.3 Hz, 3H), 7.50 (d, *J* = 8.3 Hz, 1H), 7.32-7.26 (m, 1H), 7.25-7.20 (m, 1H), 7.01 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.9, 154.8, 137.9 (2C), 129.9, 129.0, 126.4 (2C), 124.6, 123.1, 121.0, 111.2, 101.9, 94.1. HRMS (ESI) calcd for $C_{14}H_{10}IO$ $[M+H]^+$ 320.9776, found 320.9761.

4.3.8. 2-(*p*-Tolyl)benzofuran (***3h***). The title compound was prepared according to the general procedure. The product was obtained as white solid (208 mg, 100% yield, mp 125-126 °C; [Lit. 127-128.5 °C][22]); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.0 Hz, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.29-7.18 (m, 4H), 6.94 (s, 1H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.2, 154.8, 138.6, 129.5 (2C), 129.3, 127.7, 124.9 (2C), 124.0, 122.8, 120.7, 111.1, 100.5, 21.4.

4.3.9. 2-(Thiophen-2-yl)benzofuran (***3i***). The title compound was prepared according to the general procedure. The product was obtained as white solid (174 mg, 87% yield, mp 92-94 °C; [Lit. 94.1-95.1 °C][22]); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.3 Hz, 1H), 7.51-7.45 (m, 2H), 7.32 (d, *J* = 4.8 Hz, 1H), 7.29-7.18 (m, 2H), 7.08 (t, *J* = 4.3 Hz, 1H), 6.85 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.6, 151.3, 133.3, 129.1, 127.8, 125.8, 124.6, 124.3, 123.1, 120.7, 111.0, 101.1.

4.3.10. 5-Bromo-2-phenylbenzofuran (***3j***). The title compound was prepared according to the general procedure. The product was obtained as white solid (255 mg, 93% yield, mp 156-158 °C; [Lit.156-157 °C][23]); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.5 Hz, 2H), 7.68 (s, 1H), 7.47-7.41 (m, 2H), 7.40-7.33 (m, 3H), 6.93 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.2, 153.6, 131.2, 129.9 (2C), 129.0, 128.8, 127.1, 125.0, 123.5, 116.0, 112.6, 100.6.

4.3.11. 4-(5-Bromobenzofuran-2-yl)phenol (***3k***). The title compound was prepared according to the general procedure. The product was obtained as white solid (266 mg, 92% yield, mp 220-222 °C; [Lit. 221-223 °C][24]); ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.93 (br. s, 1H), 7.77 (d, *J* = 2.0 Hz, 1H), 7.74 (d, *J* = 8.5 Hz, 2H), 7.54 (d, *J* = 8.5 Hz, 1H), 7.37 (dd, *J* = 2.0, 8.5 Hz, 1H), 7.13 (s, 1H), 6.90 (d, *J* = 8.5 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.7, 157.4, 152.8, 131.5, 126.6 (2C), 126.2, 122.9, 120.3, 115.9 (2C), 115.3, 112.8, 98.8.

4.4. Total synthesis of Stemofuran A.

4.4.1. 1-(3,5-Dimethoxyphenyl)-2-(2-methoxyphenyl)ethanone (***2l***). The title compound was prepared according to the general procedure. The product was obtained as colorless liquid (435 mg, 76% yield, mp106-107 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 (s, 1 H), 7.20-7.15 (m, *J* = 2.3 Hz, 2H), 6.94-6.86 (m, 2H), 6.64-6.62 (m, 1H), 4.23 (s, 2H), 3.80 (s, 6H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.6, 160.7 (2C), 157.0, 138.8, 130.9, 128.3, 123.6, 120.6, 110.5, 106.2 (2C), 105.3, 55.5(2C), 55.3, 40.0. HRMS (ESI) calcd for $C_{17}H_{18}O_4Na$ $[M+Na]^+$ 309.1103, found 309.1089.

4.4.2. *Stemofuran A*. The title compound was prepared according to the general procedure. The product was obtained as white solid (212 mg, 94% yield, mp 181-182 °C [Lit. 182-183 °C][9]); ^{1}H NMR (400 MHz, Acetone-d_6) δ 8.43 (s, 2 H), 7.63 (dd, *J* = 0.8, 8.3 Hz, 1 H), 7.54 (dd, *J* = 0.8, 8.3 Hz, 1 H), 7.30 (ddd, *J* = 1.4, 7.2, 8.3 Hz, 1 H), 7.24 (ddd, *J* = 1.4, 7.2, 8.3 Hz, 1 H), 7.16 (d, *J* = 1.0 Hz, 1 H), 6.94 (d, *J* = 2.0 Hz, 2 H), 6.42 (t, *J* = 2.0 Hz, 1 H); ^{13}C NMR (100 MHz, Acetone-d_6) δ 160.2(2C), 157.2, 155.9, 133.4, 130.5, 125.6, 124.2, 122.2, 112.1, 104.7(2C), 104.5, 102.7.

4.5. Synthesis of 4-(5-bromo-3-methylbenzofuran-2-yl)phenol

4.5.1. 2-(5-Bromo-2-methoxyphenyl)-1-(4-methoxyphenyl)-ethanone (***2m***). The title compound was prepared according to the general procedure. The product was obtained as white solid (476 mg, 75% yield, mp 117-118 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-7.96 (m, 2H), 7.36-7.27 (m, 2H), 6.93 (d, *J* = 8.5 Hz, 2H), 6.74 (d, *J* = 8.5 Hz, 1H), 4.18 (s, 2H), 3.86 (s, 3H), 3.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.6, 163.5, 156.4, 133.6, 130.9, 130.6 (2C), 129.8, 126.3, 113.7 (2C), 112.7, 112.2, 55.6, 55.4, 39.2. HRMS (ESI) calcd for $C_{16}H_{15}BrO_3Na$ $[M+Na]^+$ 357.0102, found 357.0110.

4.5.2. 2-(5-Bromo-2-methoxyphenyl)-1-(4-methoxyphenyl)-pro-pan-1-one (***3m***). To a suspension of potassium *tert*-butoxide (161 mg, 1.44 mmol) in tetrahydrofuran (THF) was added a solution of deoxybenzoin (2m) (400 mg, 1.2 mmol) in THF dropwise at 0 °C. Iodomethane (170 mg, 1.44 mmol) solution in THF (2 mL) was added gradually. The reaction was then allowed to warm to 25 °C. After 2 h of stirring at 25 °C, the reaction mixture was slowly quenched with 2 N HCl and diluted with ethyl acetate. **3m** were obtained by simple extraction (colourless oil, 416 mg, 100% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-7.90 (m, 2H), 7.28-7.22 (m, 2H), 6.89-6.82 (m, 2H), 6.72 (d, *J* = 9.3 Hz, 1H), 5.01 (d, *J* = 6.8 Hz, 1H), 3.83 (s, 3H), 3.80 (s, 3H), 1.42 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 163.2, 154.9, 132.6, 130.8 (2C), 130.7 (2C), 130.5, 113.6, 113.3, 112.4, 55.7, 55.3, 39.5, 17.6; HRMS (ESI) calcd for $C_{17}H_{17}BrO_3Na$ $[M+Na]^+$ 371.0259, found 371.0244.

4.5.3. 4-(5-Bromo-3-methylbenzofuran-2-yl)phenol (***4m***). The title compound was prepared according to the general procedure. The product was obtained as white solid (272 mg, 90% yield, mp155-156°C; [Lit. 157-159 °C][9]); ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.02 (s, 1H), 7.93 (d, *J* = 1.5 Hz, 1H), 7.76 (d, *J* = 8.5 Hz, 2H), 7.63 (d, *J* = 8.5 Hz, 1H), 7.52 (dd, *J* = 1.5, 8.5 Hz, 1H), 7.07 (d, *J* = 8.5 Hz, 2H), 3.49 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.0, 152.1, 151.6, 133.2, 128.1 (2C), 126.3, 121.7, 121.0, 115.8, 114.9 (2C), 112.5, 108.5, 8.9.

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Supplementary Material

Supplementary data associated with this article can be found in online version

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Supporting Information

An efficient approach to construct 2-arylbenzo[*b*]furans from 2-methoxychalcone epoxides

Libo Ruan, Min Shi, Shiwei Mao, Lifang Yu, Fan Yang*, Jie Tang*

Institute of Drug Discovery and Development, Shanghai Engineering Research Center of Molecular Therapeutics and New Drug Development, East China Normal University, Shanghai 200062, China

Contents

* Corresponding author. Tel.: +86-21-62232764; E-mail: fyang@chem.ecnu.edu.cn; jtang@chem.ecnu.edu.cn

13/8/2013 PM 2:20:29

Acquisition Time (sec)	3.9846	***Comment***				***Date***	10 May 2013 19:03:28		
Date Stamp	10 May 2013 19:03:28			***File Name***	E:\ \ \ &MAss\RLB-Fu-30\1\fid			***Frequency (MHz)***	400.13
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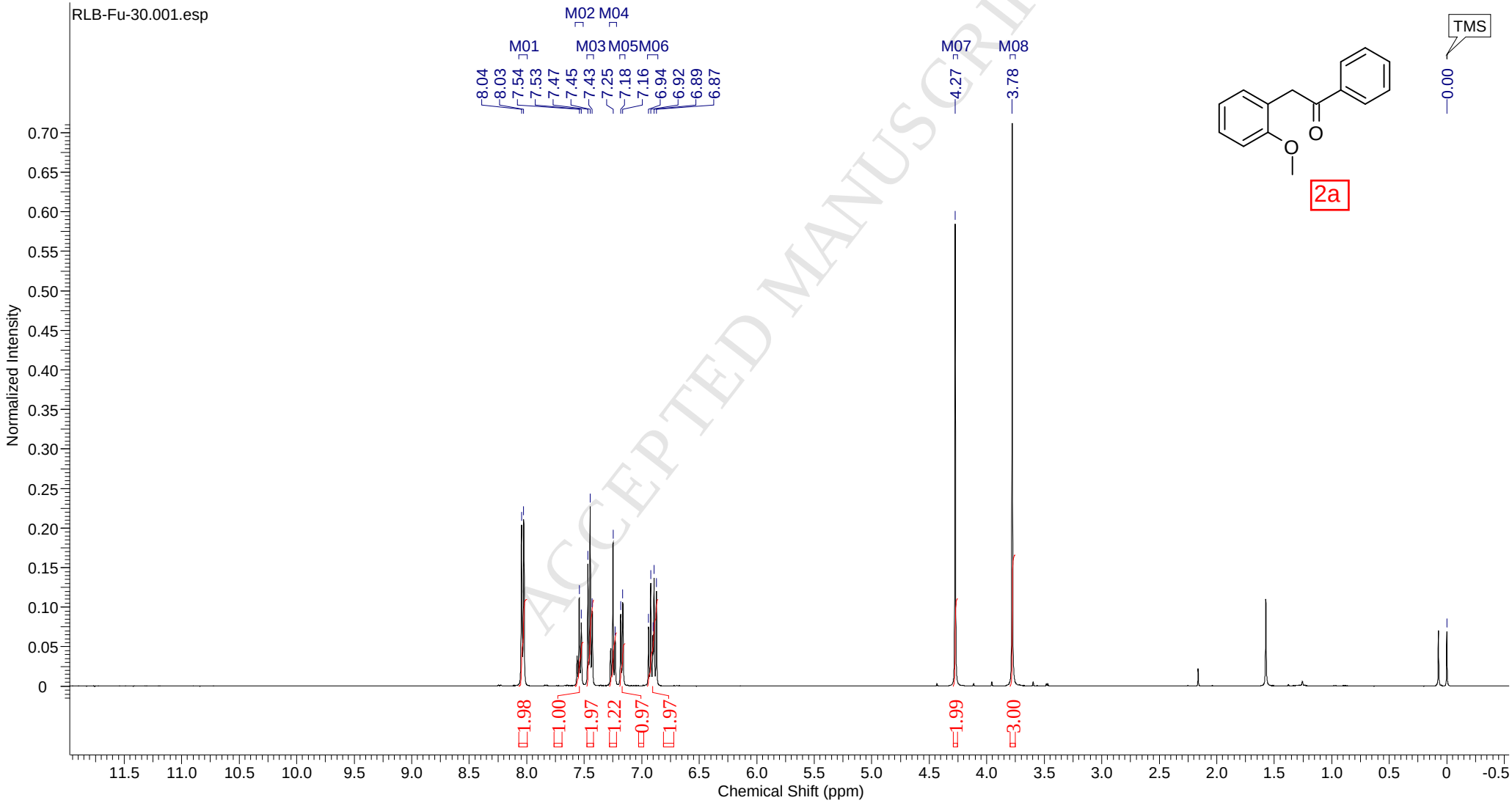
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	69.91	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	2457.3428	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	26.275		

^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 8.04 (d, *J* = 7.3 Hz, 2 H), 7.53 (d, *J* = 7.3 Hz, 1 H), 7.48 - 7.42 (m, 2 H), 7.28 - 7.22 (m, 1 H), 7.17 (d, *J* = 7.3 Hz, 1 H), 6.95 - 6.86 (m, 2 H), 4.27 (s, 2 H), 3.78 (s, 3 H)



13/8/2013 PM 3:13:06

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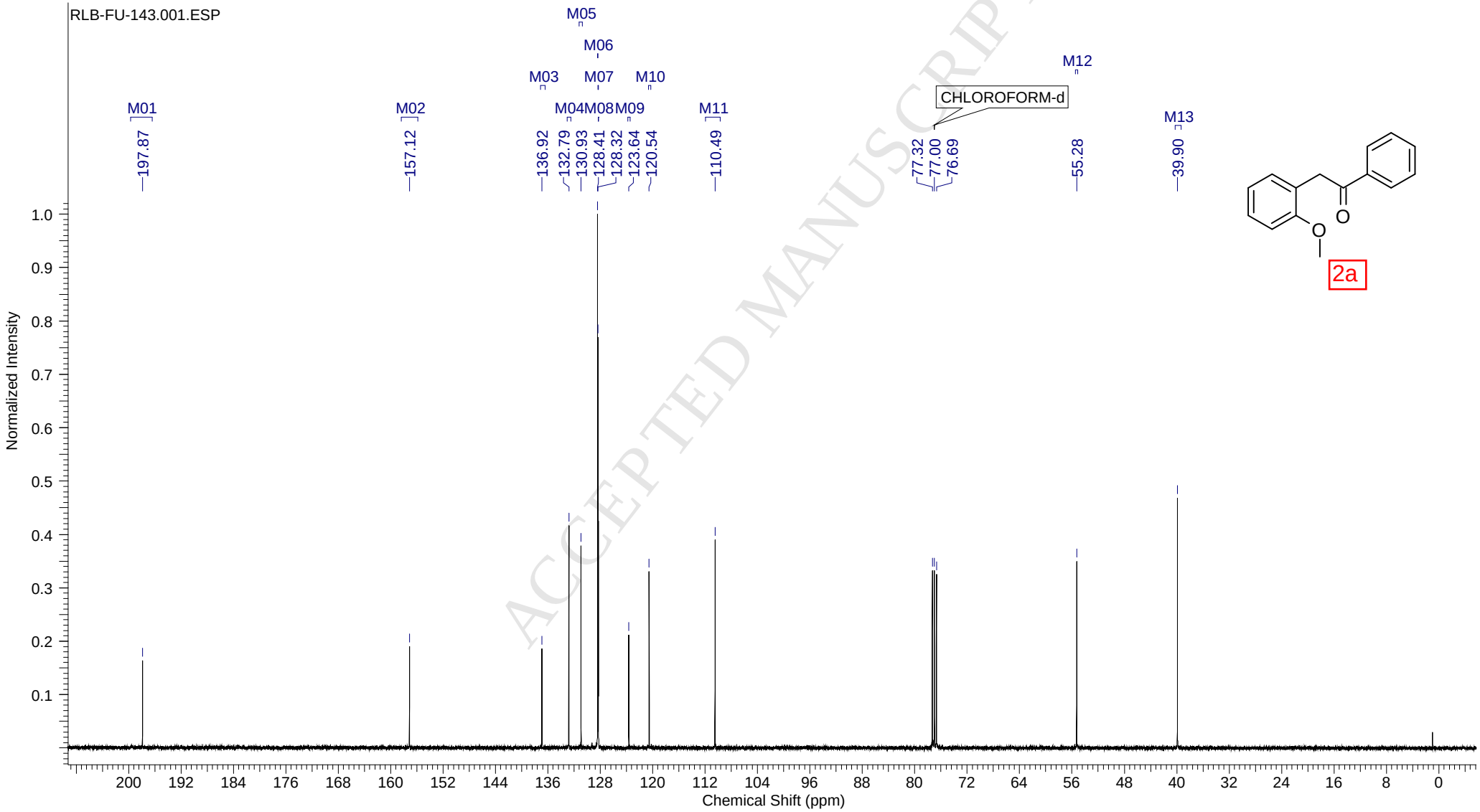
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10046.6465	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	25.484		

^{13}C NMR (100MHz ,CHLOROFORM-d) δ = 197.9, 157.1, 136.9, 132.8, 130.9, 128.4, 128.3, 128.3, 123.6, 120.5, 110.5, 55.3, 39.9



31/5/2013 PM 8:14:10

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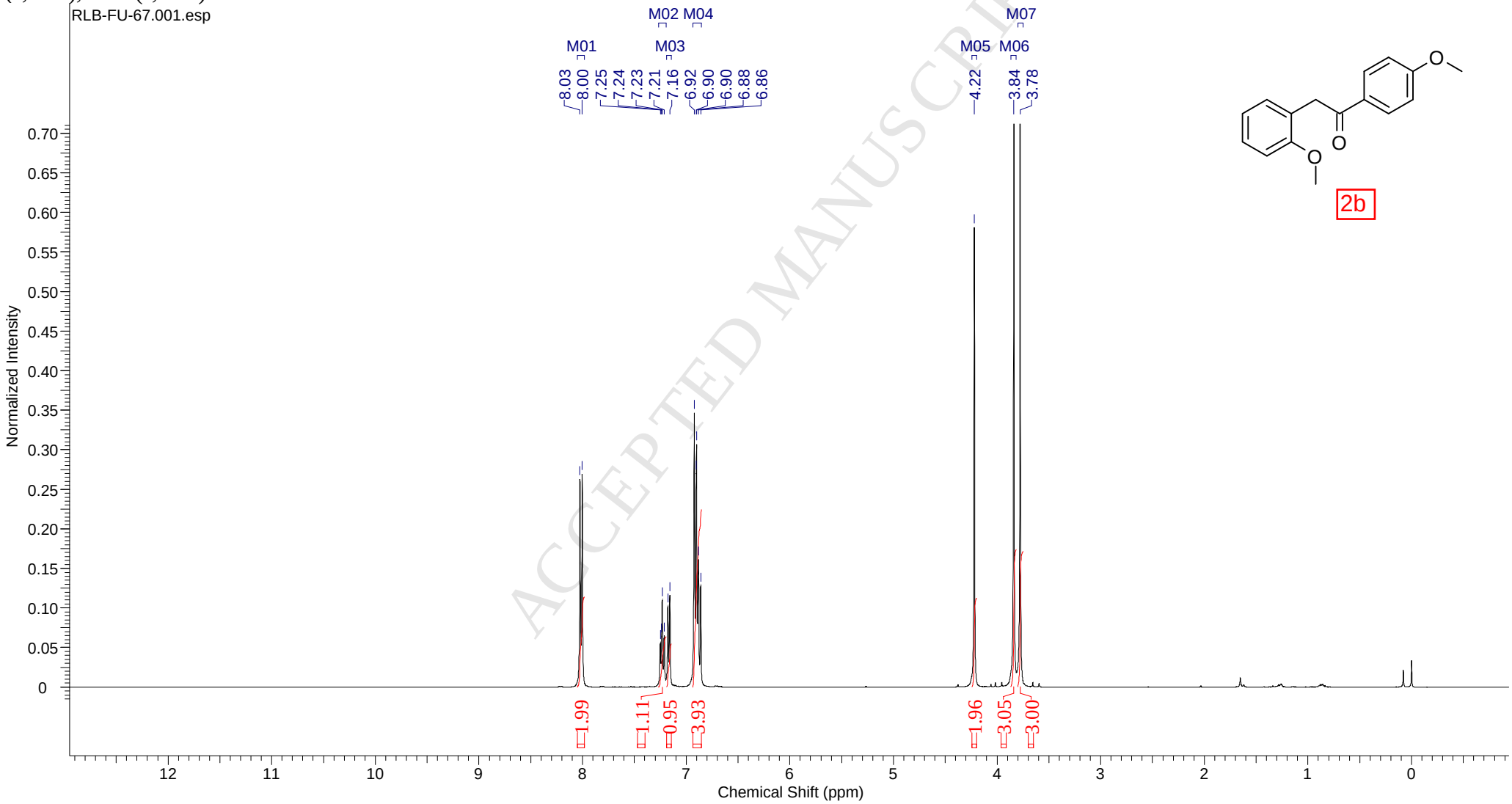
Spectrum Offset (Hz)	2453.4751	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	25.629		

^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 8.01 (d, *J* = 8.8 Hz, 2 H), 7.27 - 7.19 (m, 1 H), 7.17 (d, *J* = 7.3 Hz, 1 H), 6.94 - 6.85 (m, 4 H), 4.22 (s, 2 H), 3.84 (s, 3 H), 3.78 (s, 3 H)



15/8/2013 PM 10:55:30

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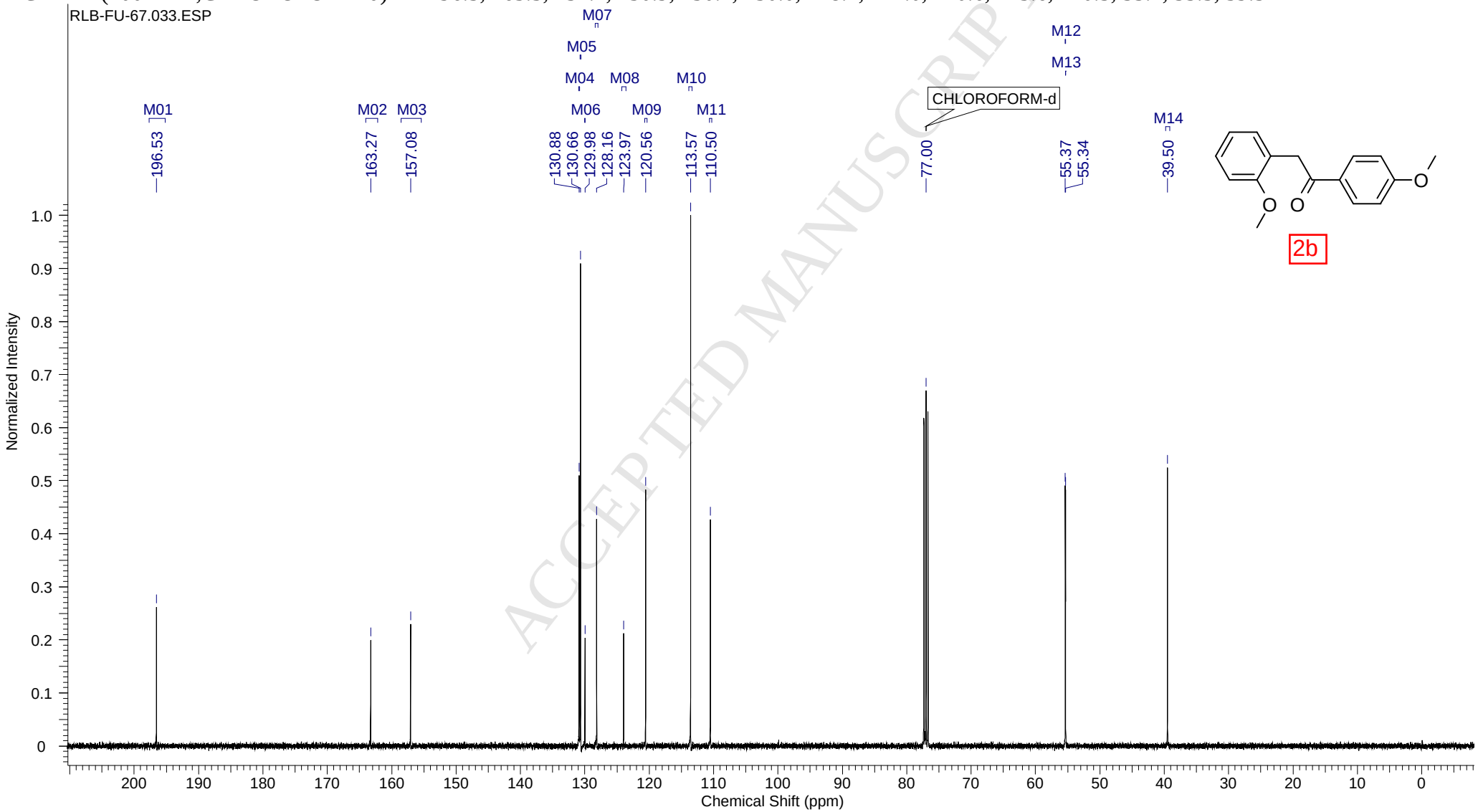
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10051.0400	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	25.577		

^{13}C NMR (100MHz ,CHLOROFORM-d) δ = 196.5, 163.3, 157.1, 130.9, 130.7, 130.0, 128.2, 124.0, 120.6, 113.6, 110.5, 55.4, 55.3, 39.5



5/6/2013 PM 8:33:44

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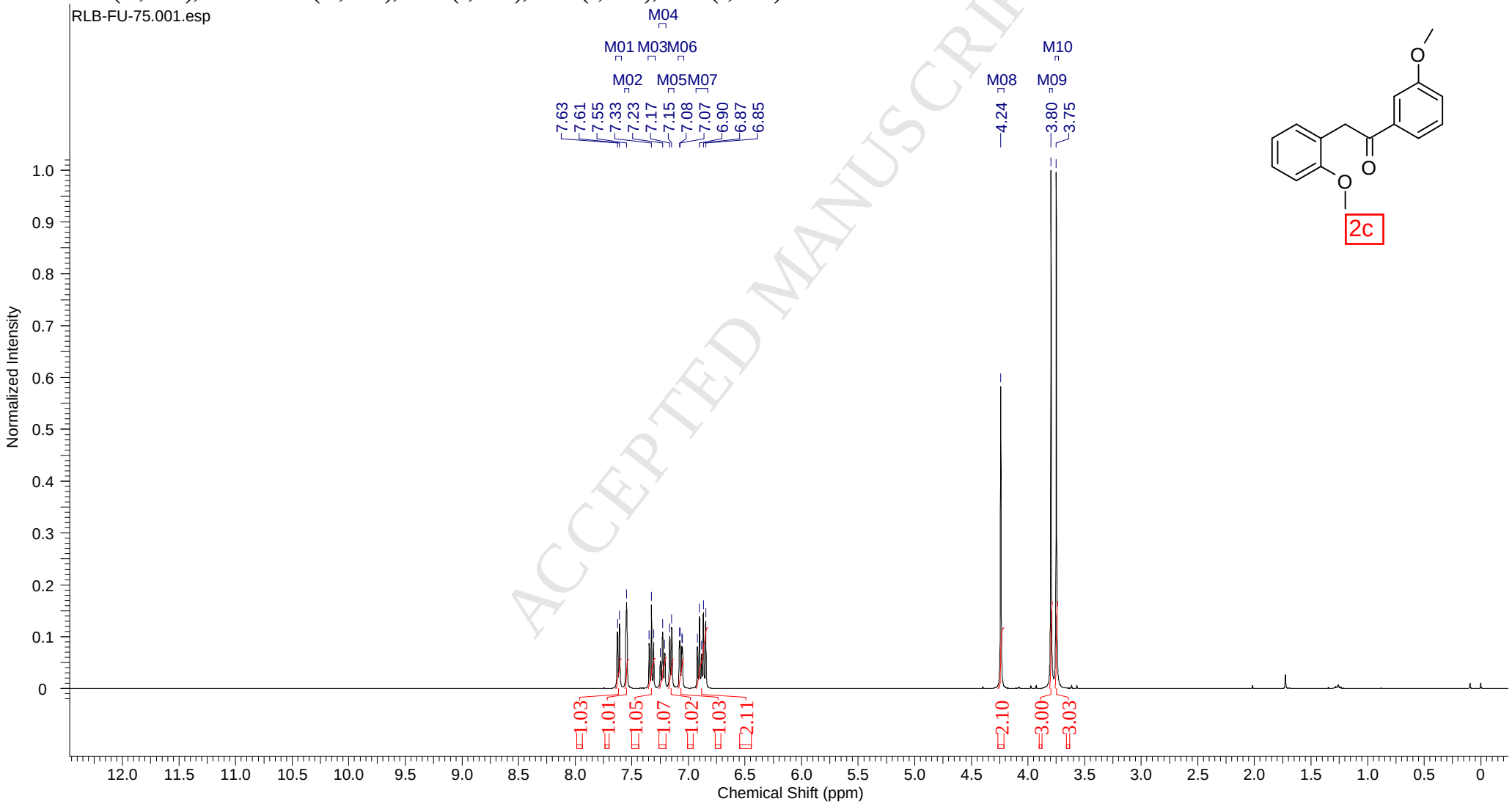
Receiver Gain	19.91	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2442.7522
Spectrum Type	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	25.472				

^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 7.62 (d, *J* = 7.5 Hz, 1 H), 7.55 (s, 1 H), 7.33 (t, *J* = 8.0 Hz, 1 H), 7.26 - 7.20 (m, 1 H), 7.16 (d, *J* = 7.0 Hz, 1 H), 7.09 - 7.04 (m, 1 H), 6.93 - 6.83 (m, 2 H), 4.24 (s, 2 H), 3.80 (s, 3 H), 3.75 (s, 3 H)



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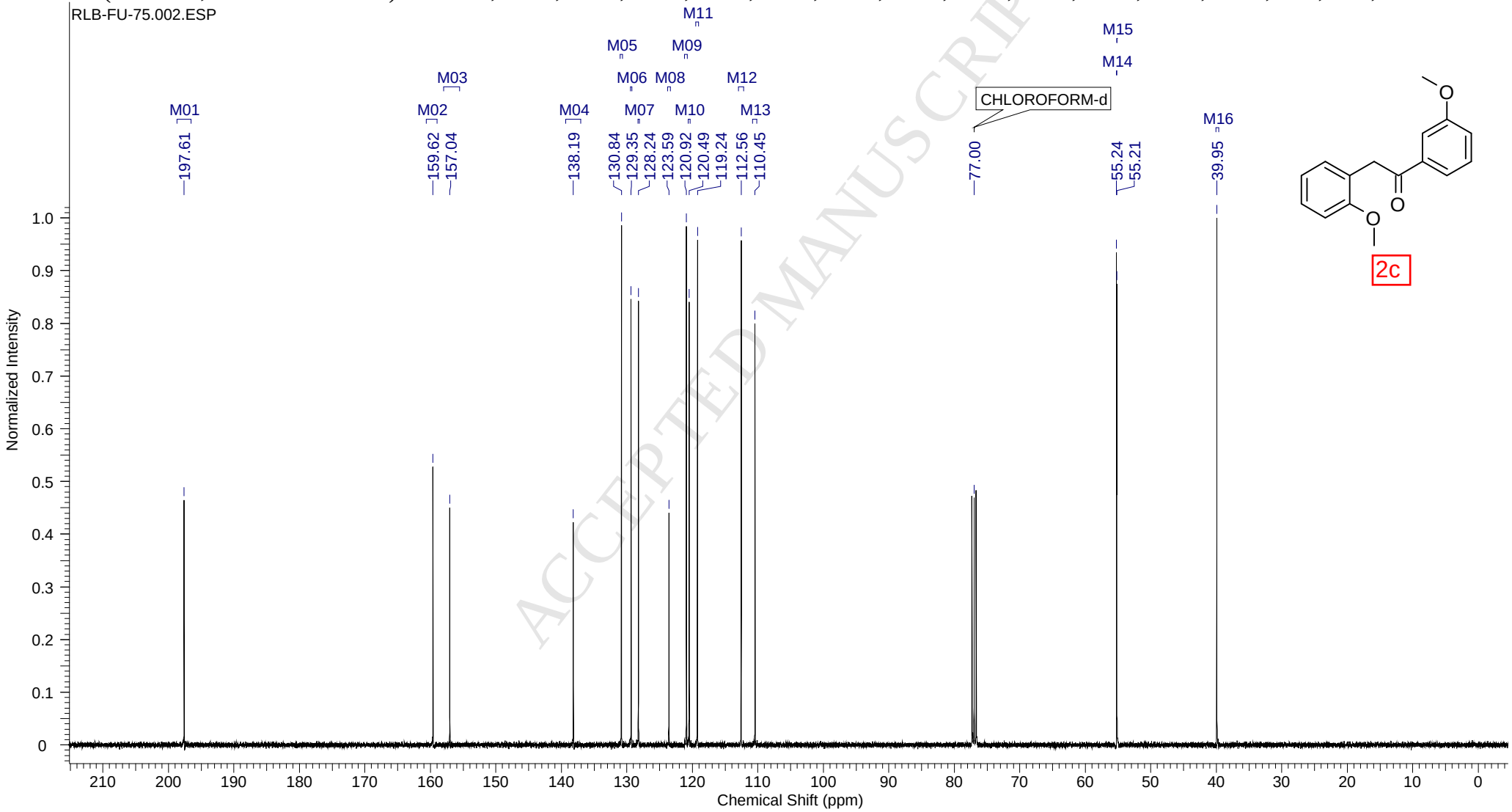
Receiver Gain	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10041.5039
Spectrum Type	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	25.777				

^{13}C NMR (100MHz ,CHLOROFORM-d) δ = 197.6, 159.6, 157.0, 138.2, 130.8, 129.4, 128.2, 123.6, 120.9, 120.5, 119.2, 112.6, 110.4, 55.2, 55.2, 39.9



4/6/2013 PM 8:19:42

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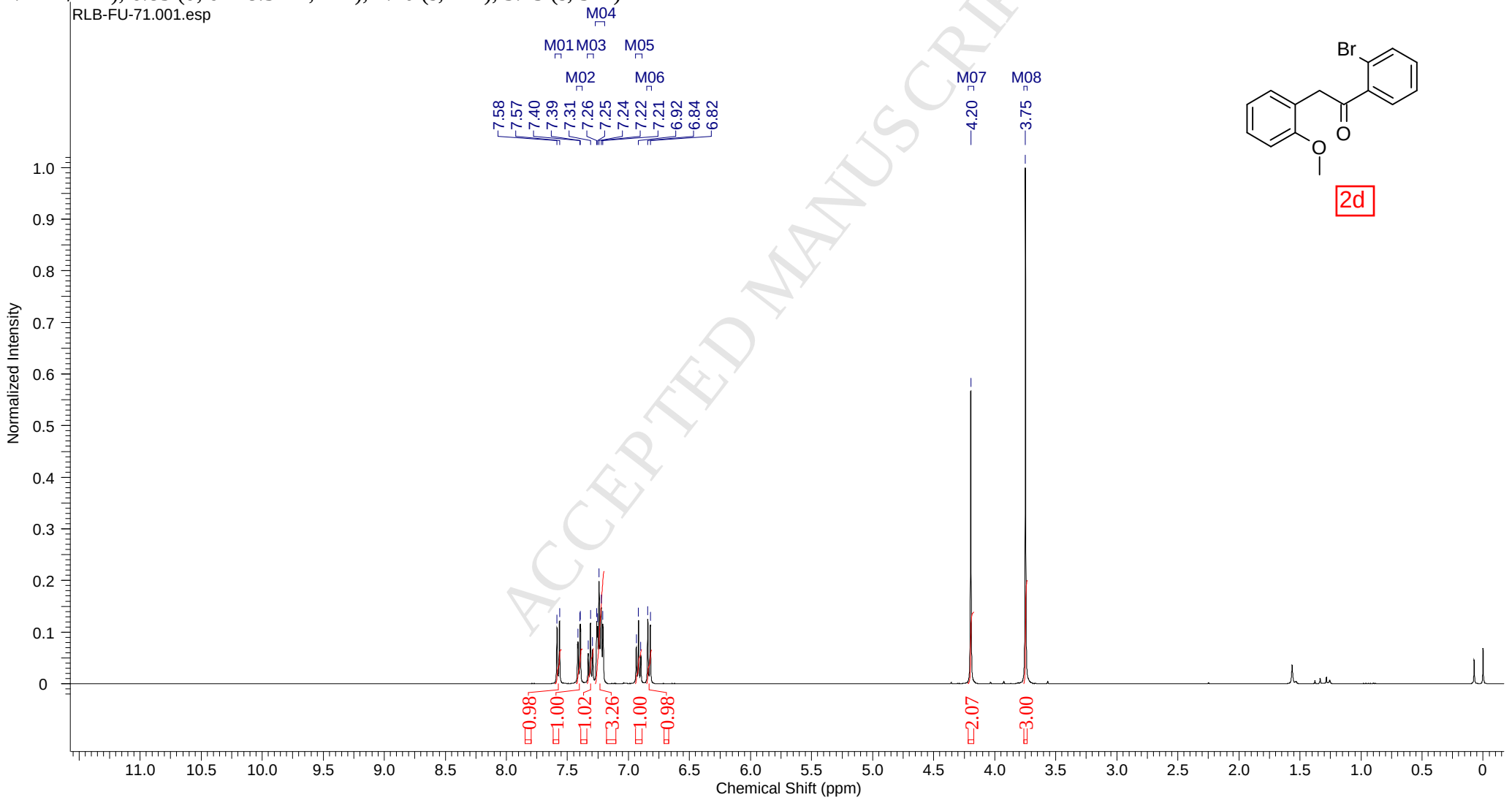
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	69.91	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2458.1841
Spectrum Type	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	25.225				

^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 7.57 (d, *J* = 7.8 Hz, 1 H), 7.41 (dd, *J* = 1.5, 7.5 Hz, 1 H), 7.34 - 7.29 (m, 1 H), 7.27 - 7.20 (m, 3 H), 6.92 (t, *J* = 7.4 Hz, 1 H), 6.83 (d, *J* = 8.3 Hz, 1 H), 4.20 (s, 2 H), 3.75 (s, 3 H)



5/6/2013 PM 2:50:36

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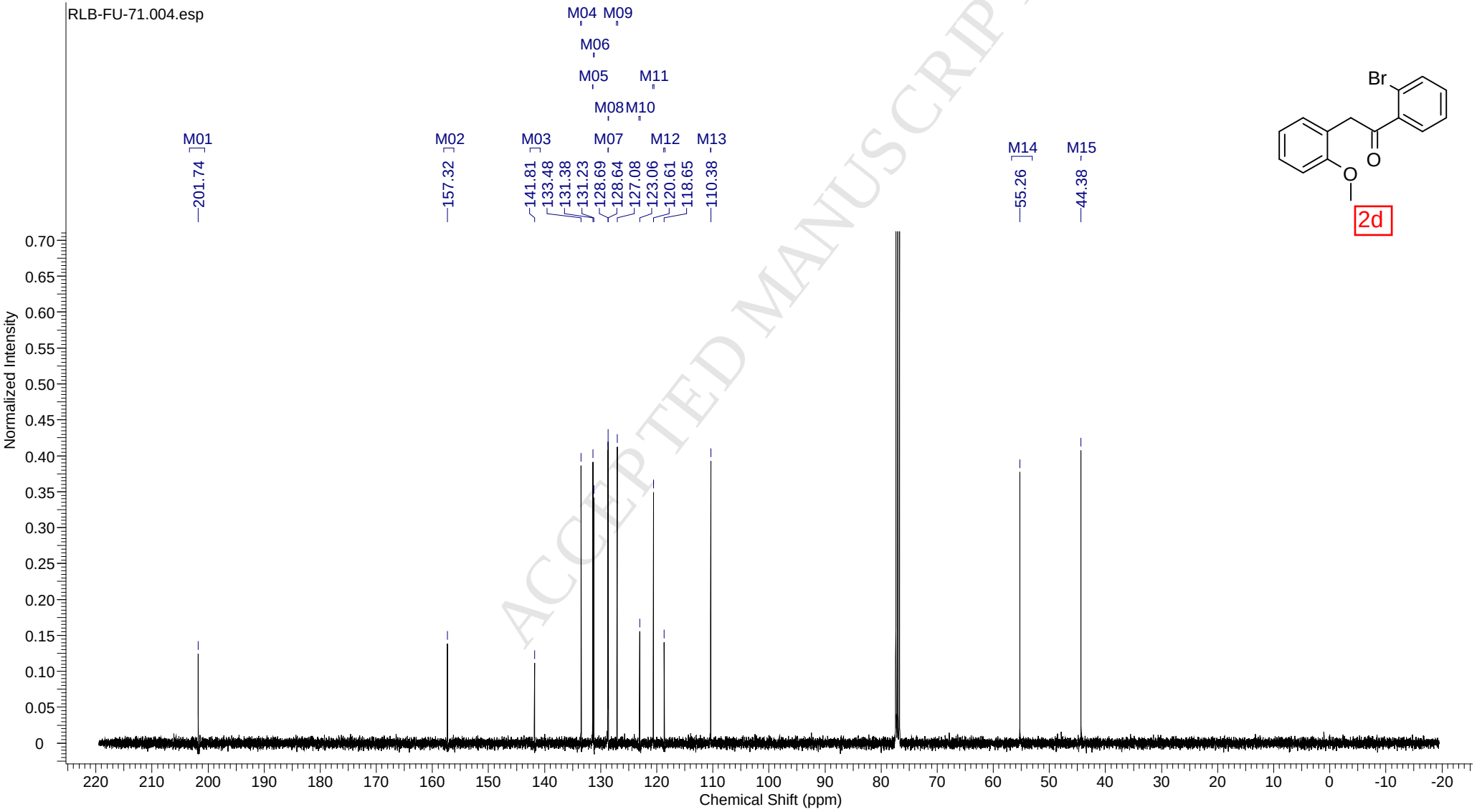
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10060.3320	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	25.885		

^{13}C NMR (101MHz ,CHLOROFORM-d) δ = 201.7, 157.3, 141.8, 133.5, 131.4, 131.2, 128.7, 128.6, 127.1, 123.1, 120.6, 118.7, 110.4, 55.3, 44.4



18/6/2013 PM 12:44:41

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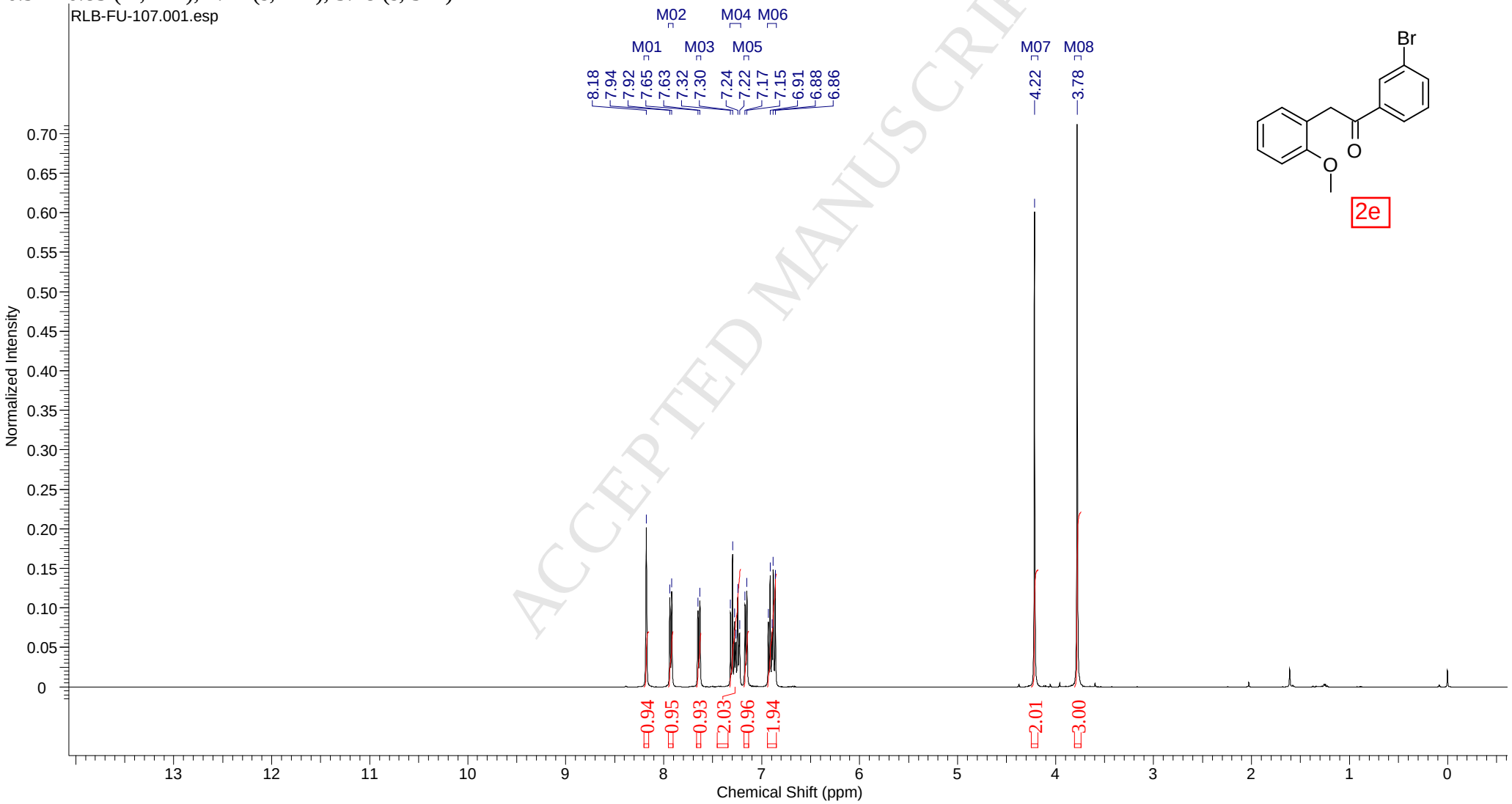
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	31.69	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	2450.4307	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	28.086		

^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 8.18 (s, 1 H), 7.93 (d, *J* = 8.0 Hz, 1 H), 7.64 (d, *J* = 8.0 Hz, 1 H), 7.33 - 7.21 (m, 2 H), 7.16 (d, *J* = 7.0 Hz, 1 H), 6.94 - 6.85 (m, 2 H), 4.22 (s, 2 H), 3.78 (s, 3 H)



13/8/2013 PM 3:51:43

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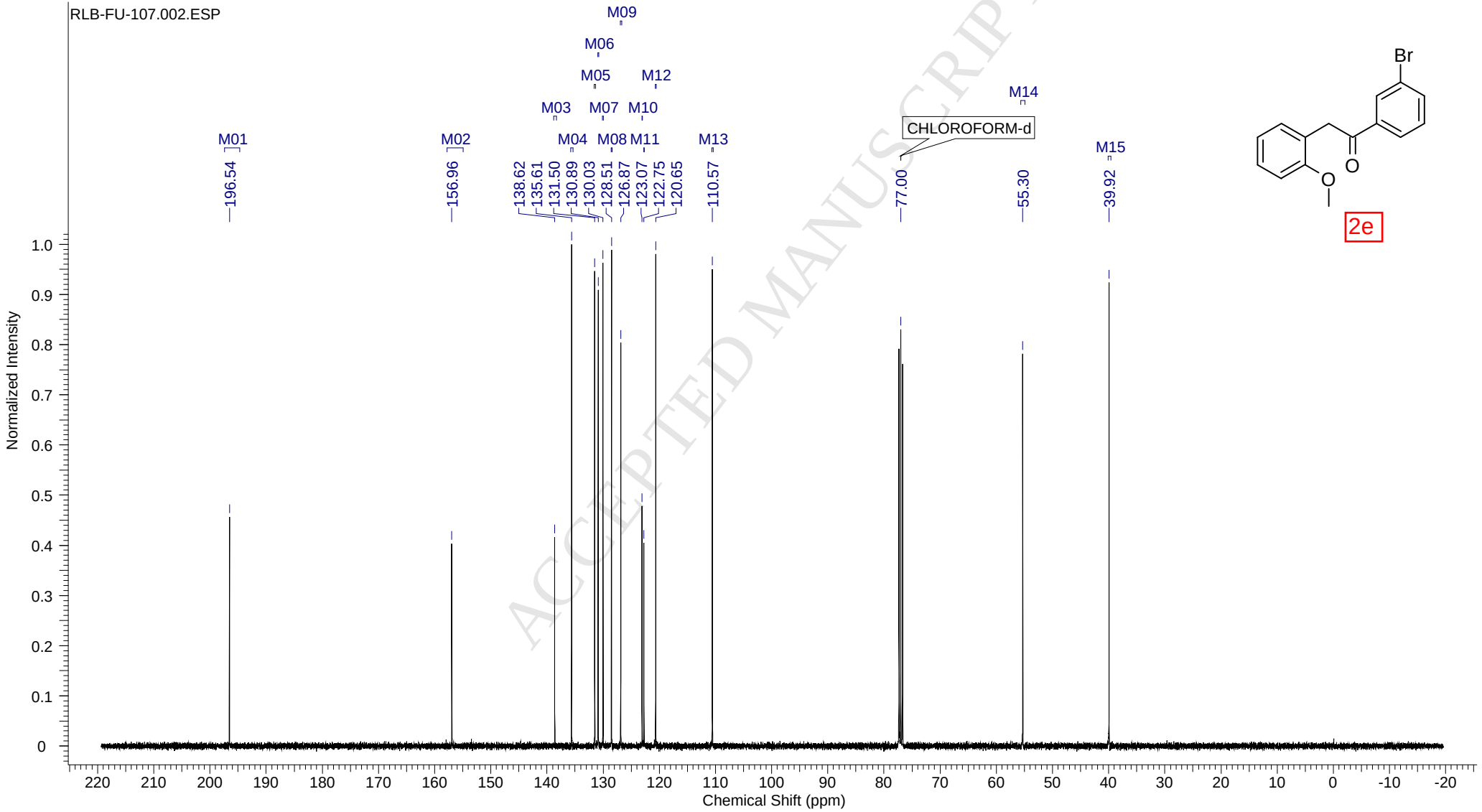
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10049.5732	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	28.437		

^{13}C NMR (100MHz ,CHLOROFORM-d) δ = 196.5, 157.0, 138.6, 135.6, 131.5, 130.9, 130.0, 128.5, 126.9, 123.1, 122.7, 120.6, 110.6, 55.3, 39.9



31/5/2013 PM 8:05:25

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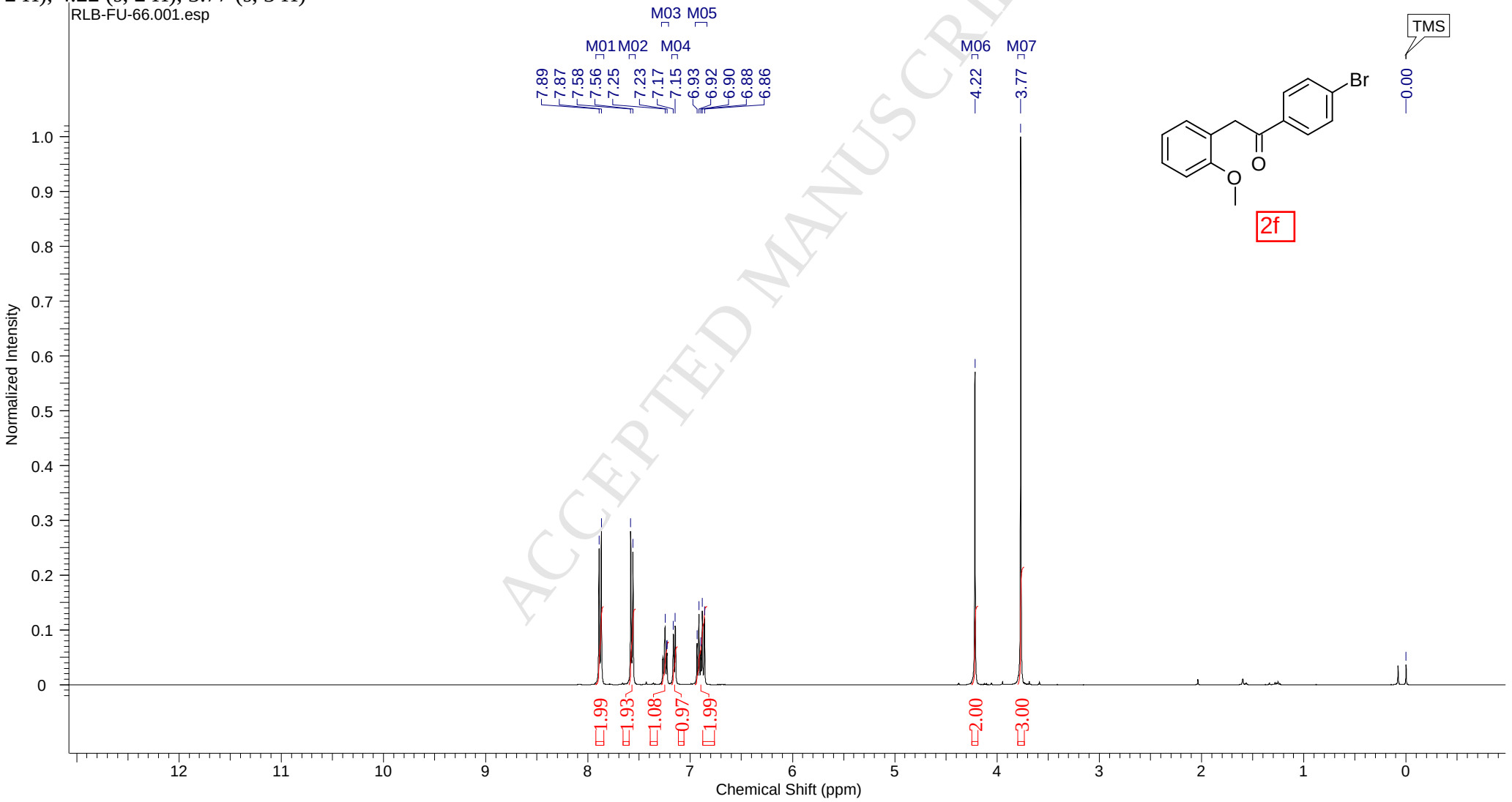
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	31.69	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	2454.5820	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	25.629		

^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 7.88 (d, *J* = 8.5 Hz, 2 H), 7.57 (d, *J* = 8.5 Hz, 2 H), 7.28 - 7.21 (m, 1 H), 7.16 (d, *J* = 7.3 Hz, 1 H), 6.95 - 6.84 (m, 2 H), 4.22 (s, 2 H), 3.77 (s, 3 H)



31/5/2013 PM 8:10:17

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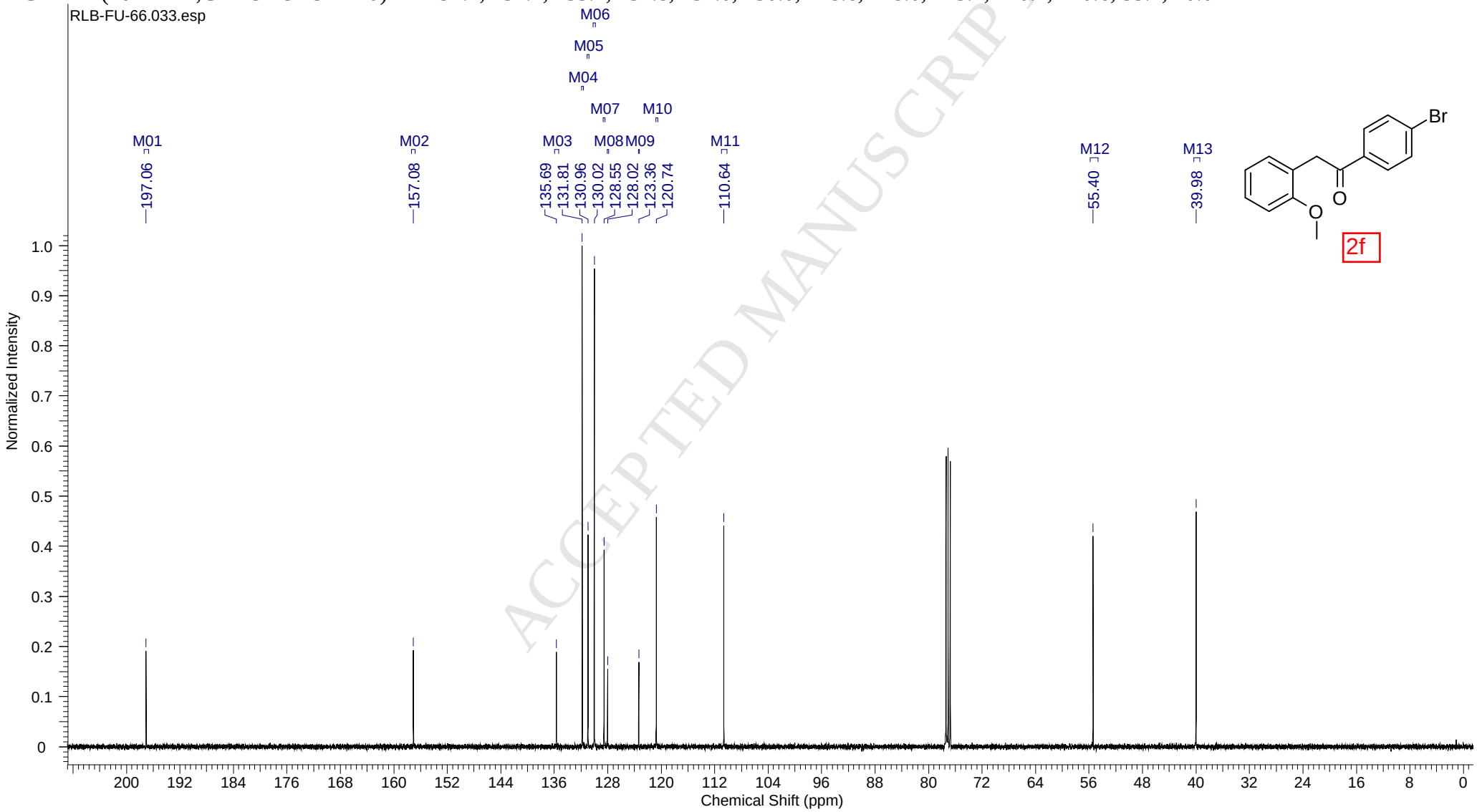
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10060.3320	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	25.428		

^{13}C NMR (101MHz ,CHLOROFORM-d) δ = 197.1, 157.1, 135.7, 131.8, 131.0, 130.0, 128.6, 128.0, 123.4, 120.7, 110.6, 55.4, 40.0



13/10/2013 PM 12:11:43

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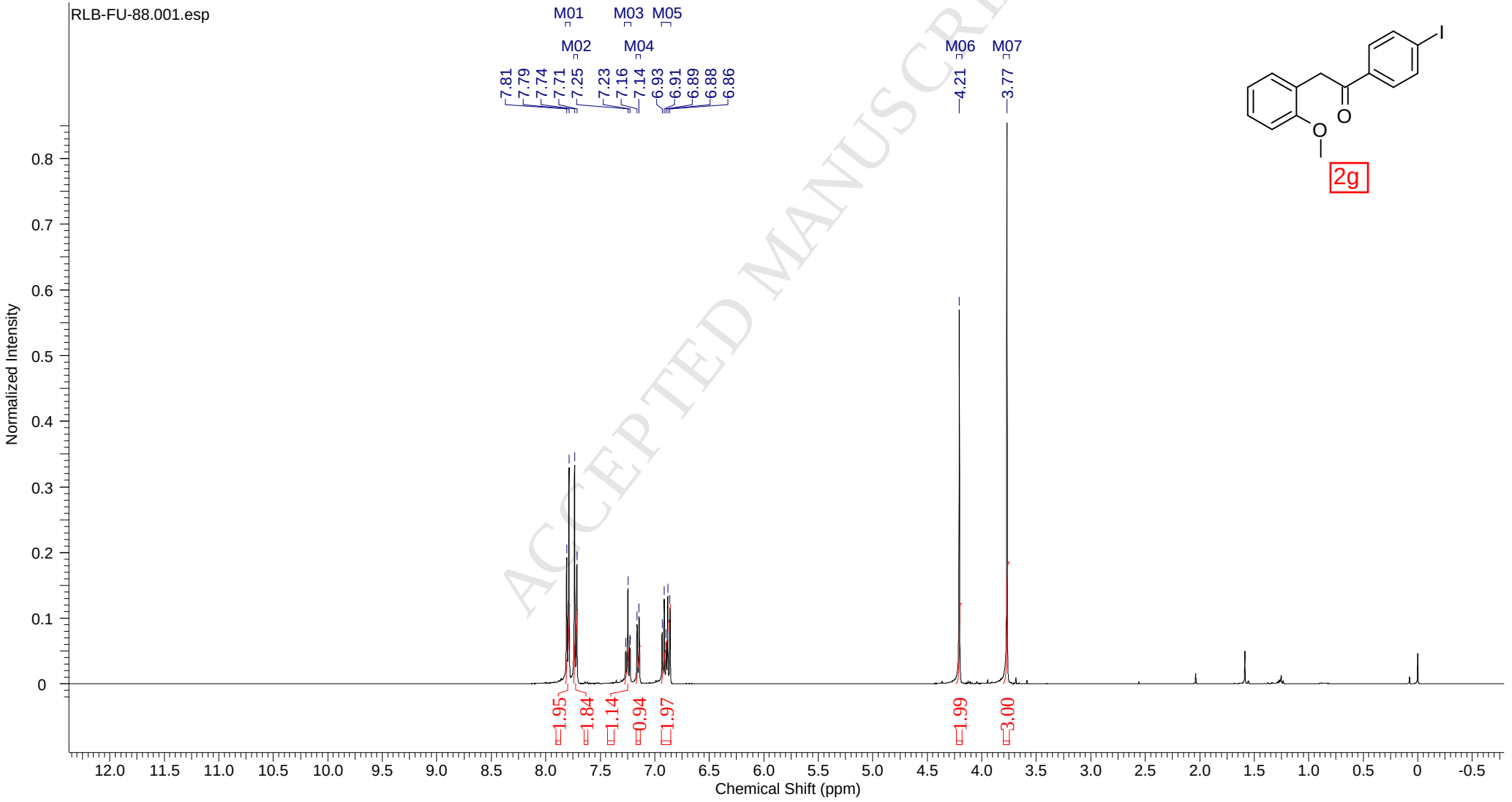
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	56.68	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	2456.0754	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	26.845		

^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 7.82 - 7.78 (m, 2 H), 7.74 - 7.71 (m, 2 H), 7.28 - 7.22 (m, 1 H), 7.15 (d, *J* = 7.3 Hz, 1 H), 6.94 - 6.85 (m, 2 H), 4.21 (s, 2 H), 3.77 (s, 3 H)



13/10/2013 PM 12:24:49

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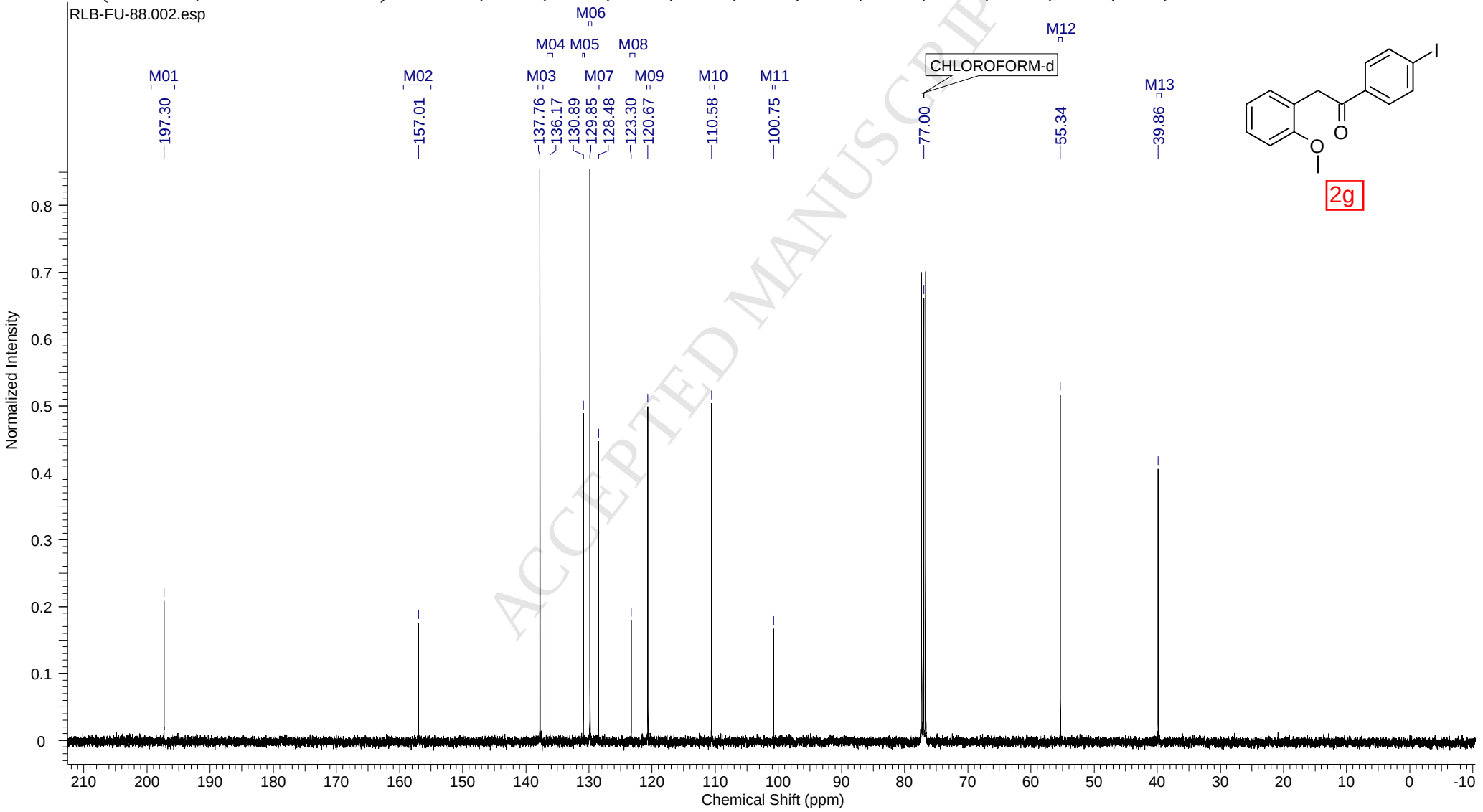
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10053.9746	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	27.227		

^{13}C NMR (101MHz ,CHLOROFORM-d) δ = 197.3, 157.0, 137.8, 136.2, 130.9, 129.8, 128.5, 123.3, 120.7, 110.6, 100.7, 55.3, 39.9



27/6/2013 PM 4:31:11

Acquisition Time (sec)	3.9846	***Comment***		***Date***	21 Jun 2013 12:28:48			***Date Stamp***	21 Jun 2013 12:28:48
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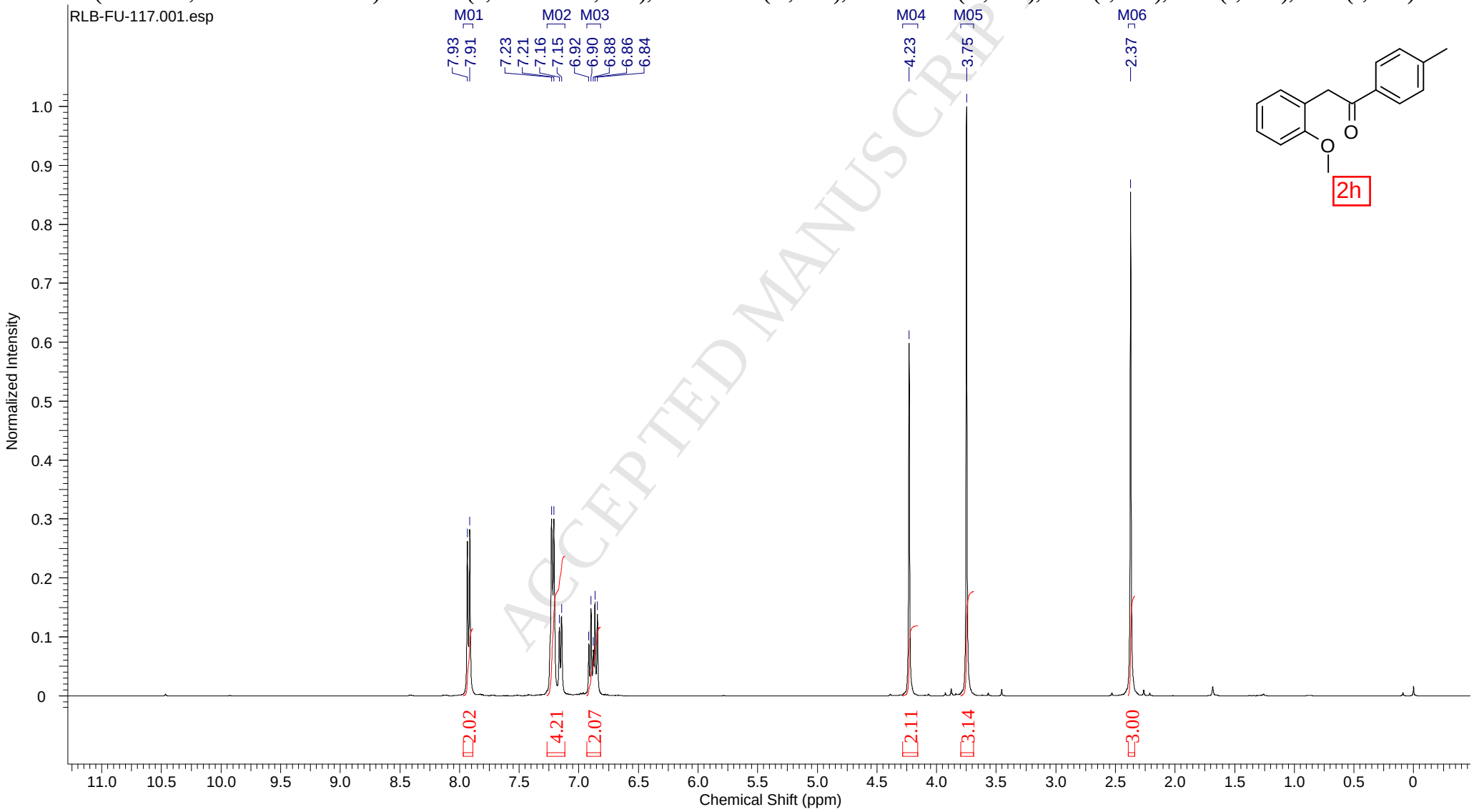
Receiver Gain	19.91	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2441.5037
Spectrum Type	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	26.608				

^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 7.92 (d, *J* = 8.0 Hz, 2 H), 7.27 - 7.12 (m, 4 H), 6.93 - 6.82 (m, 2 H), 4.23 (s, 2 H), 3.75 (s, 3 H), 2.37 (s, 3 H)



27/6/2013 PM 4:34:40

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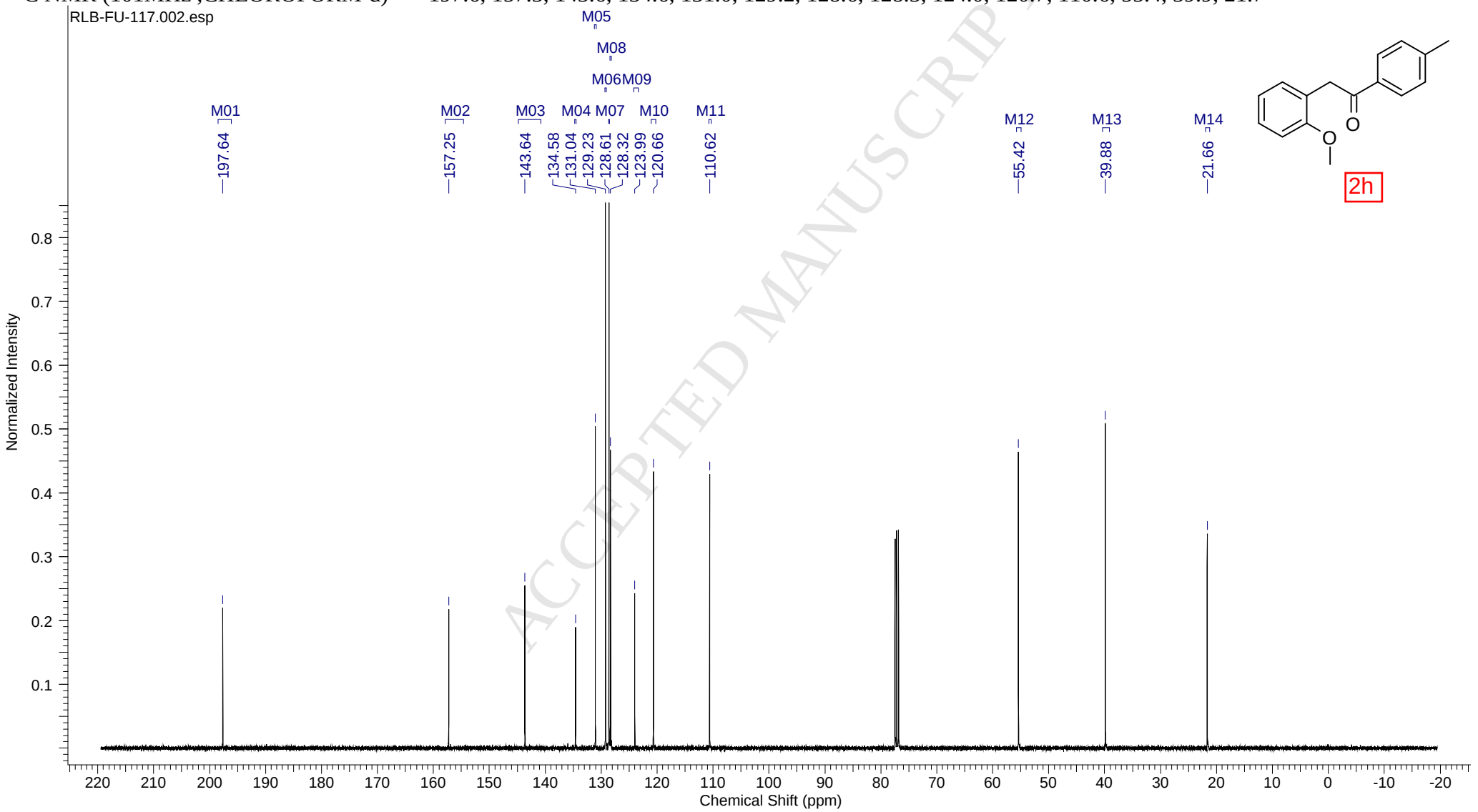
Spectrum Offset (Hz)	10060.3320	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	27.067		

^{13}C NMR (101MHz ,CHLOROFORM-d) δ = 197.6, 157.3, 143.6, 134.6, 131.0, 129.2, 128.6, 128.3, 124.0, 120.7, 110.6, 55.4, 39.9, 21.7



30/6/2013 PM 8:15:06

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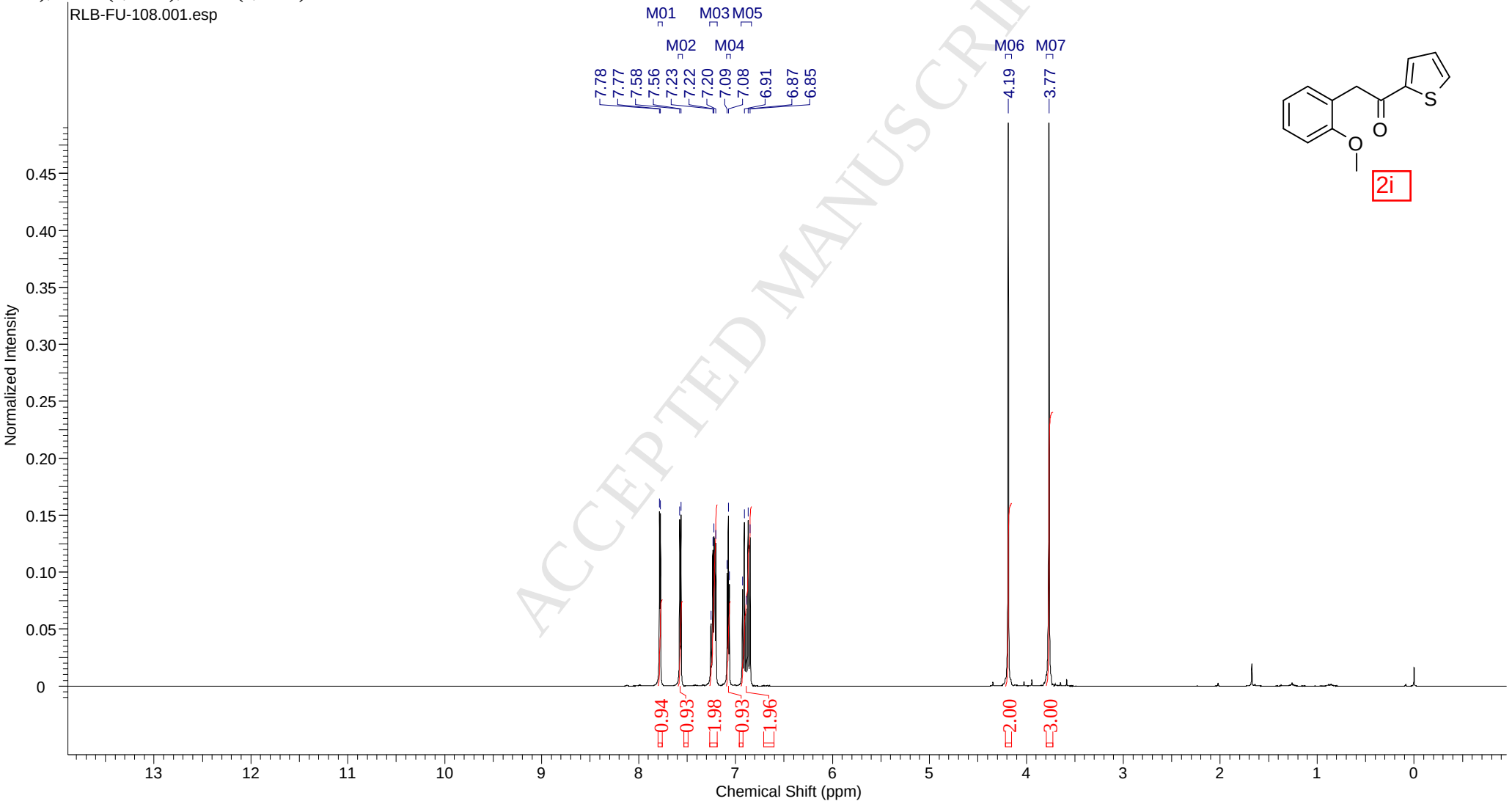
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	31.69	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	2447.8533	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	28.648		

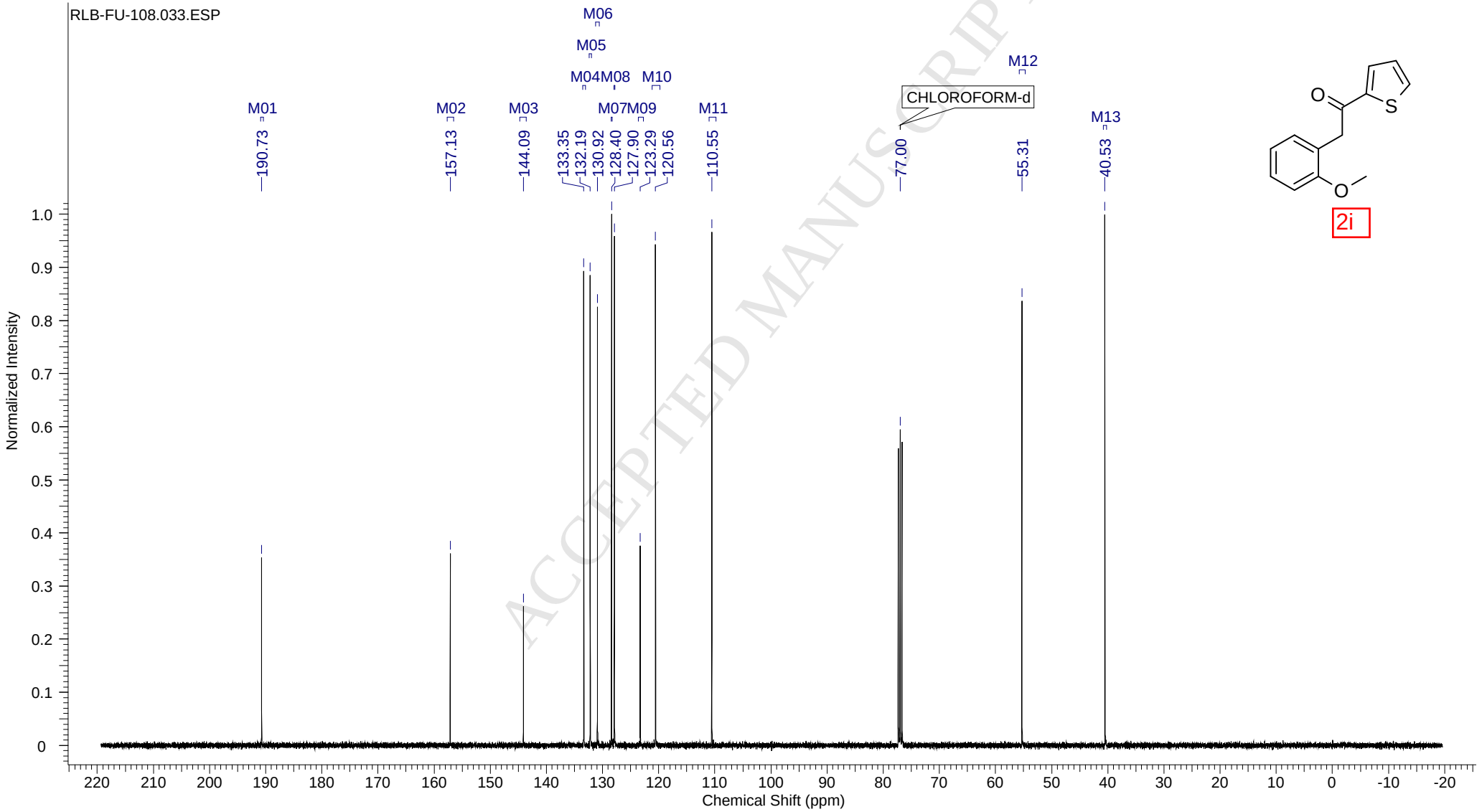
^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 7.78 (d, *J* = 3.8 Hz, 1 H), 7.57 (d, *J* = 5.0 Hz, 1 H), 7.27 - 7.19 (m, 2 H), 7.08 (t, *J* = 4.4 Hz, 1 H), 6.94 - 6.84 (m, 2 H), 4.19 (s, 2 H), 3.77 (s, 3 H)



13/8/2013 PM 4:21:15

Acquisition Time (sec)	1.3631	***Comment***		***Date***	18 Jun 2013 17:27:28				
Date Stamp	18 Jun 2013 17:27:28			***File Name***	E:\ \ \ &MAss\RLB-FU-108\33\fid			***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	256	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10045.9043	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	29.508		

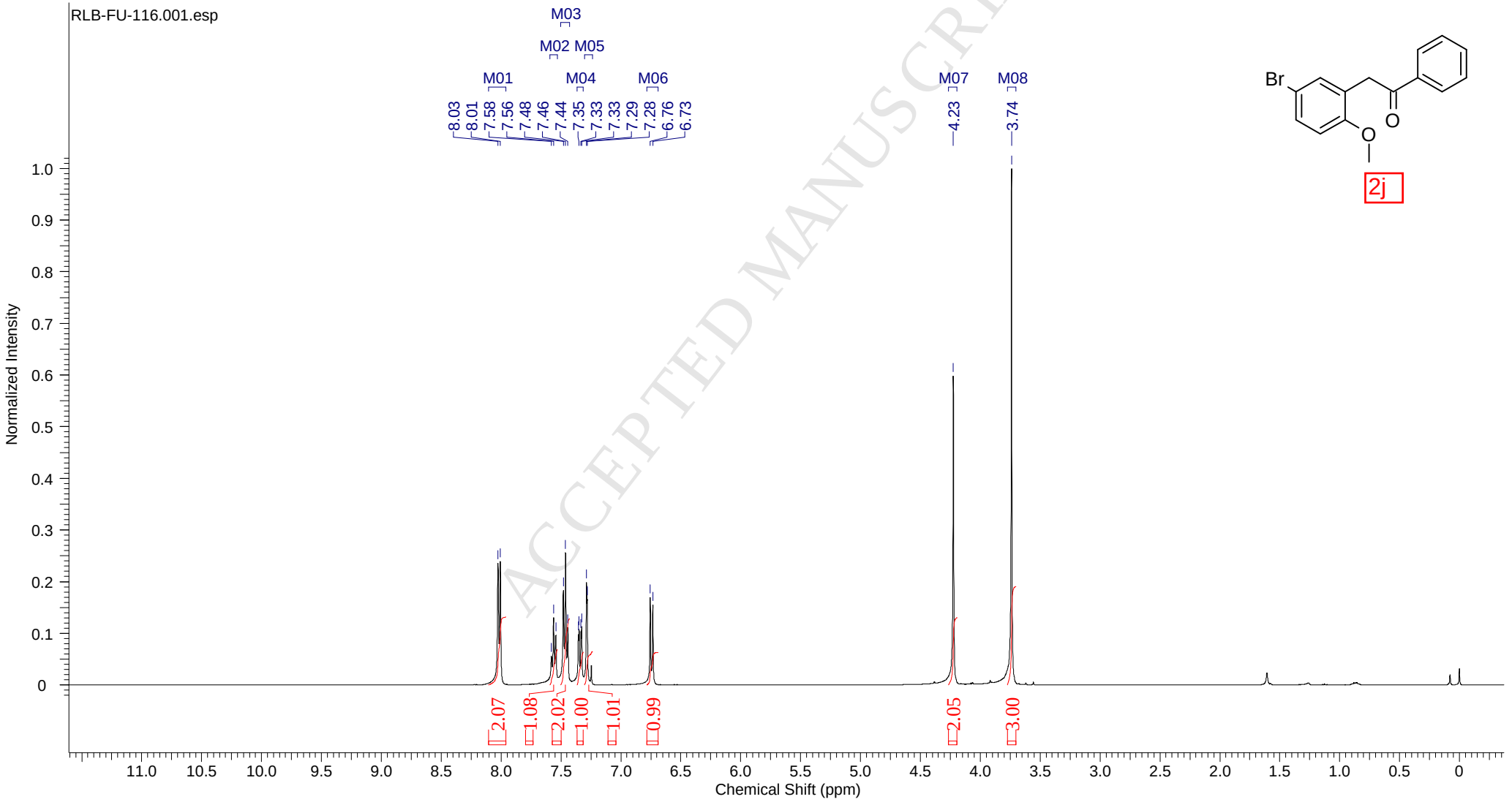
^{13}C NMR (100MHz ,CHLOROFORM-d) δ = 190.7, 157.1, 144.1, 133.3, 132.2, 130.9, 128.4, 127.9, 123.3, 120.6, 110.6, 55.3, 40.5



27/6/2013 PM 4:41:02

Acquisition Time (sec)	3.9846	***Comment***				***Date***	21 Jun 2013 11:01:20		
Date Stamp	21 Jun 2013 11:01:20			***File Name***	E:\ \ \ &MAss\RLB-FU-116\1\fid			***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	31.69	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	2456.5317	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	26.568		

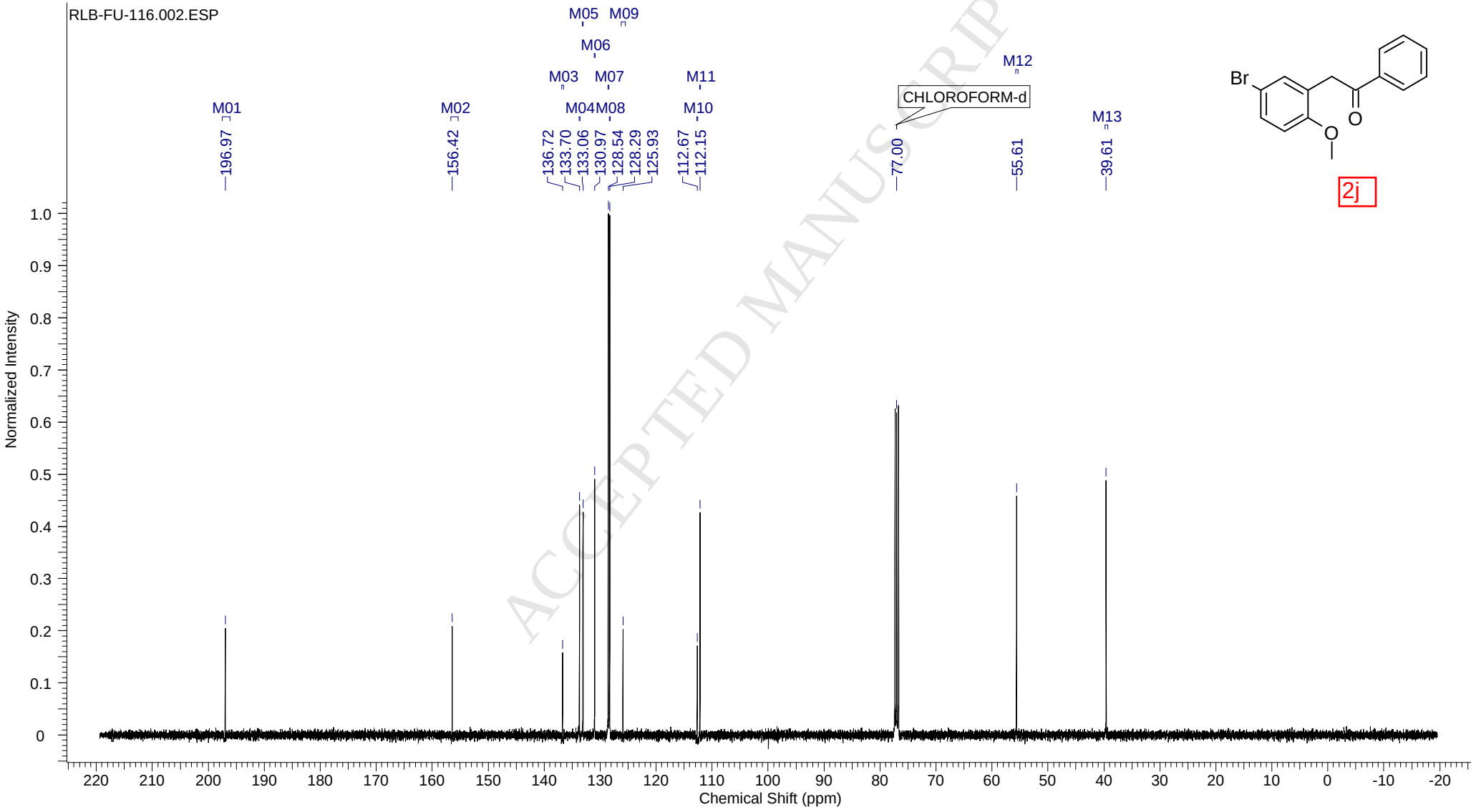
^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 8.02 (d, *J* = 7.3 Hz, 2 H), 7.59 - 7.53 (m, 1 H), 7.50 - 7.43 (m, 1 H), 7.34 (dd, *J* = 2.3, 8.5 Hz, 1 H), 7.28 (d, *J* = 2.3 Hz, 1 H), 6.74 (d, *J* = 8.5 Hz, 1 H), 4.23 (s, 2 H), 3.74 (s, 3 H)



13/8/2013 PM 4:27:58

Acquisition Time (sec)	1.3631	***Comment***		***Date***	21 Jun 2013 11:07:44				
Date Stamp	21 Jun 2013 11:07:44			***File Name***	E:\ \ \ &MAss\RLB-FU-116\2\fid			***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	125	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10052.5078	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	26.944		

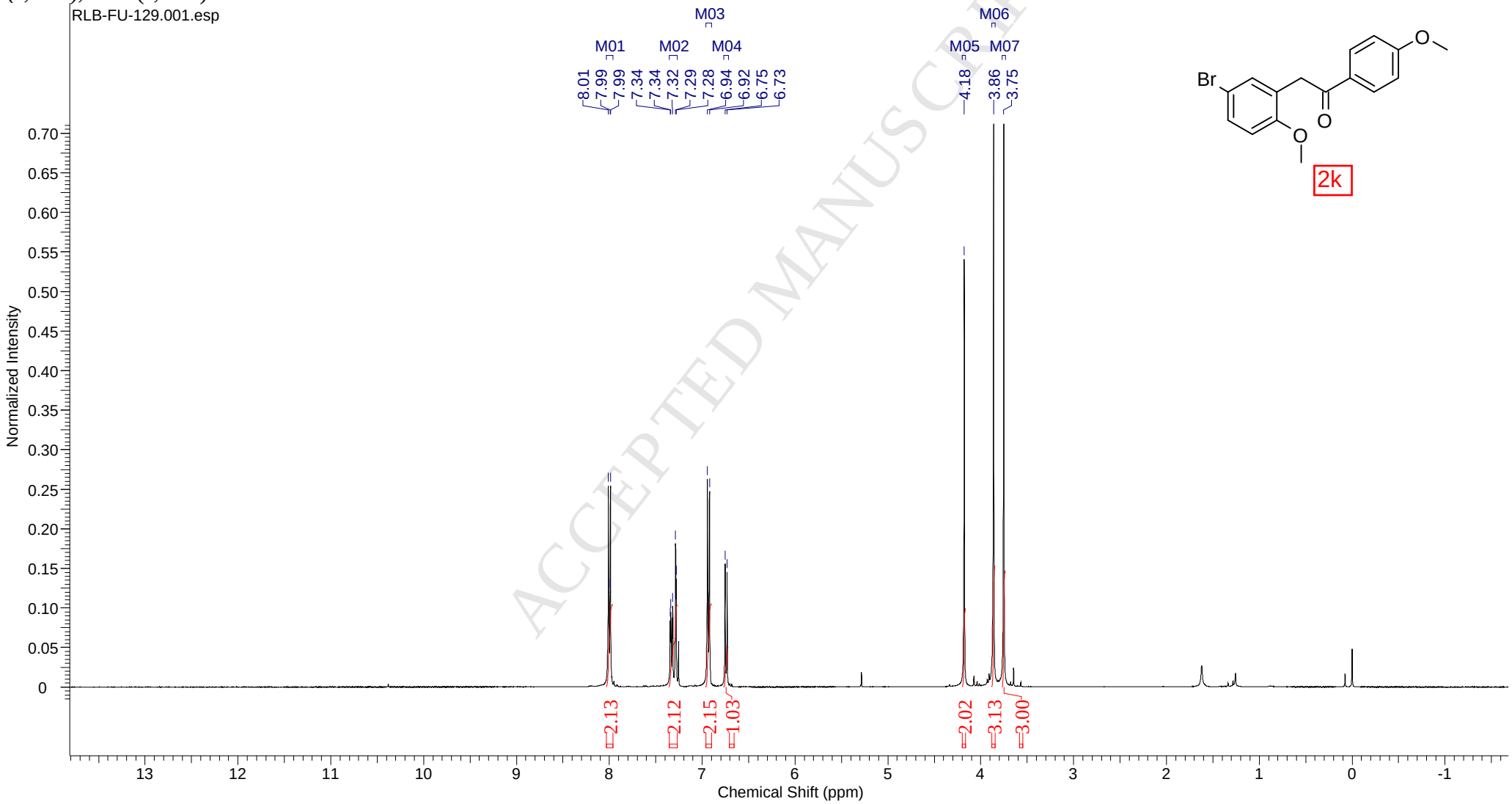
^{13}C NMR (100MHz ,CHLOROFORM-d) δ = 197.0, 156.4, 136.7, 133.7, 133.1, 131.0, 128.5, 128.3, 125.9, 112.7, 112.2, 55.6, 39.6



2/7/2013 PM 1:38:46

Acquisition Time (sec)	3.9846	***Comment***		***Date***	02 Jul 2013 12:16:00			***Date Stamp***	02 Jul 2013 12:16:00
File Name	E:\ \ \ &MAss\RLB-FU-129\1\fid			***Frequency (MHz)***	400.13	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	31.69	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2459.5967
Spectrum Type	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	27.387				

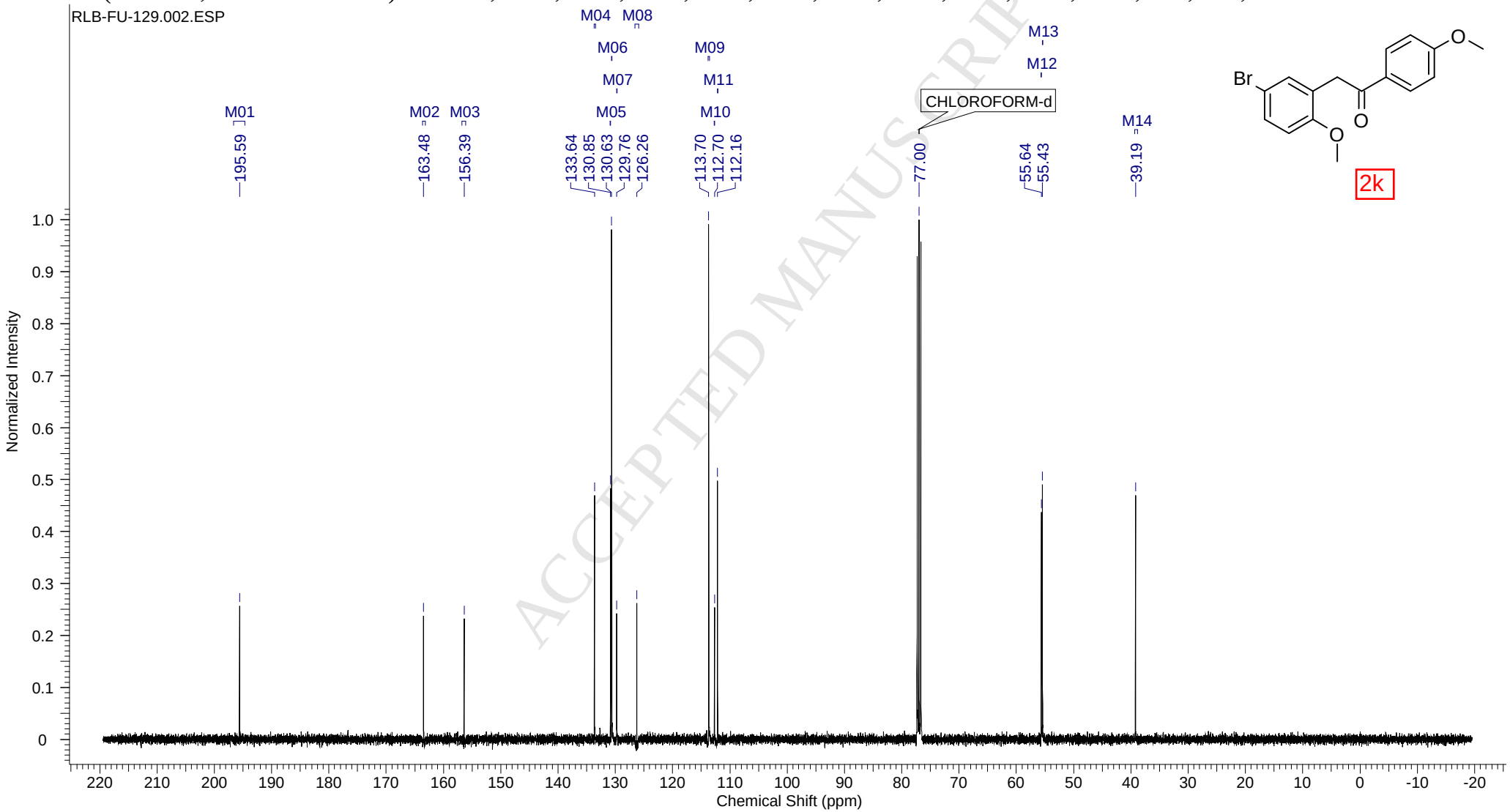
^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 8.03 - 7.96 (m, 2 H), 7.36 - 7.27 (m, 2 H), 6.93 (d, J = 8.5 Hz, 2 H), 6.74 (d, J = 8.5 Hz, 1 H), 4.18 (s, 2 H), 3.86 (s, 3 H), 3.75 (s, 3 H)



13/8/2013 PM 4:43:28

Acquisition Time (sec)	1.3631	***Comment***		***Date***	02 Jul 2013 12:33:04			***Date Stamp***	02 Jul 2013 12:33:04
File Name	E:\ \ \ &MAss\RLB-FU-129\2\fid			***Frequency (MHz)***	100.61	***Nucleus***	13C	***Number of Transients***	256
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10054.7080
Spectrum Type	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	27.699				

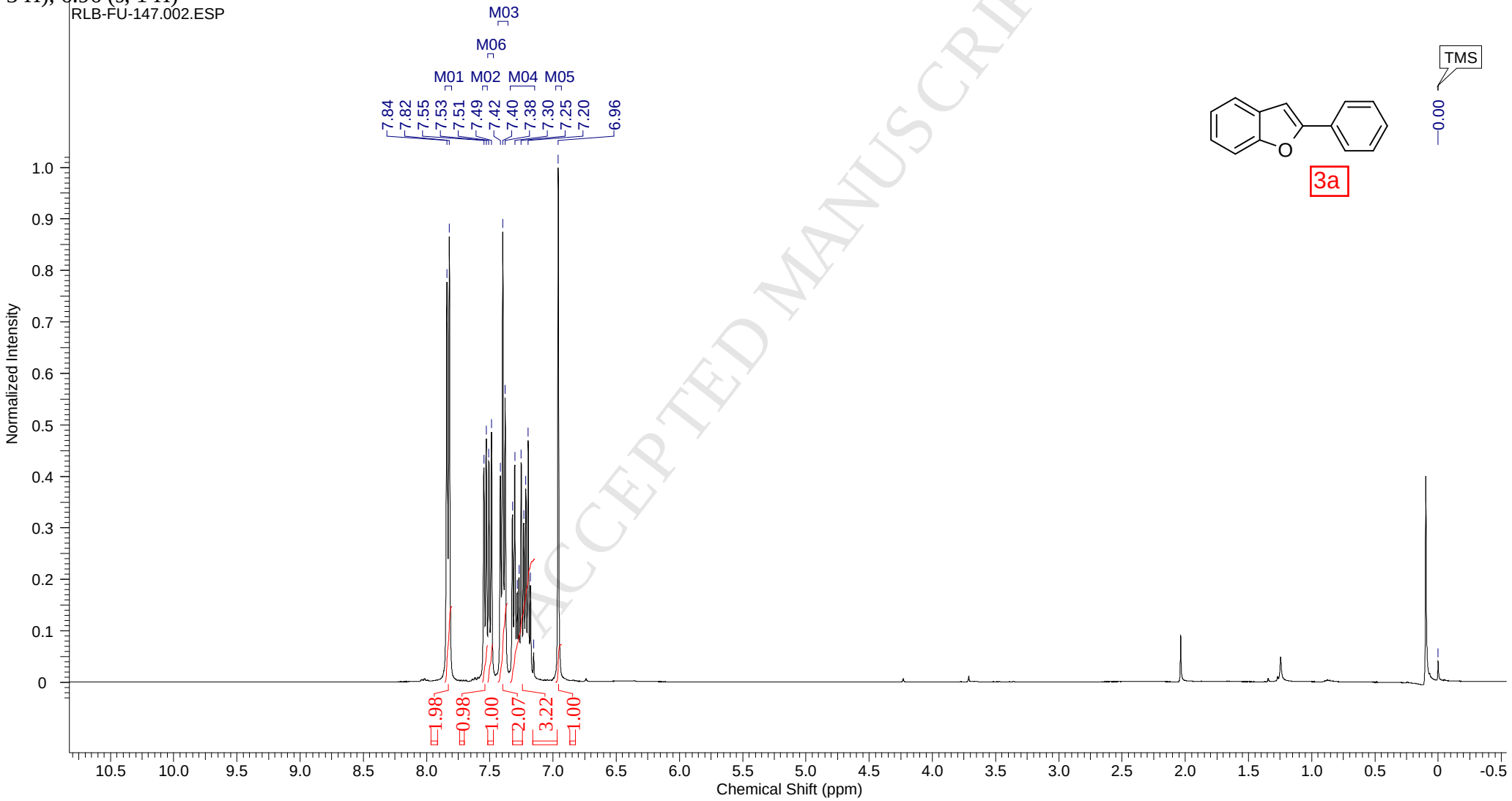
^{13}C NMR (100MHz ,CHLOROFORM-d) δ = 195.6, 163.5, 156.4, 133.6, 130.9, 130.6, 129.8, 126.3, 113.7, 112.7, 112.2, 55.6, 55.4, 39.2



14/8/2013 PM 3:55:10

Acquisition Time (sec)	3.9846	***Comment***		***Date***	14 Aug 2013 10:52:48			***Date Stamp***	14 Aug 2013 10:52:48
File Name	E:\ \ \ &MAss\RLB-FU-147\2\fid			***Frequency (MHz)***	400.13	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	22.51	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2419.4468
Spectrum Type	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	26.996				

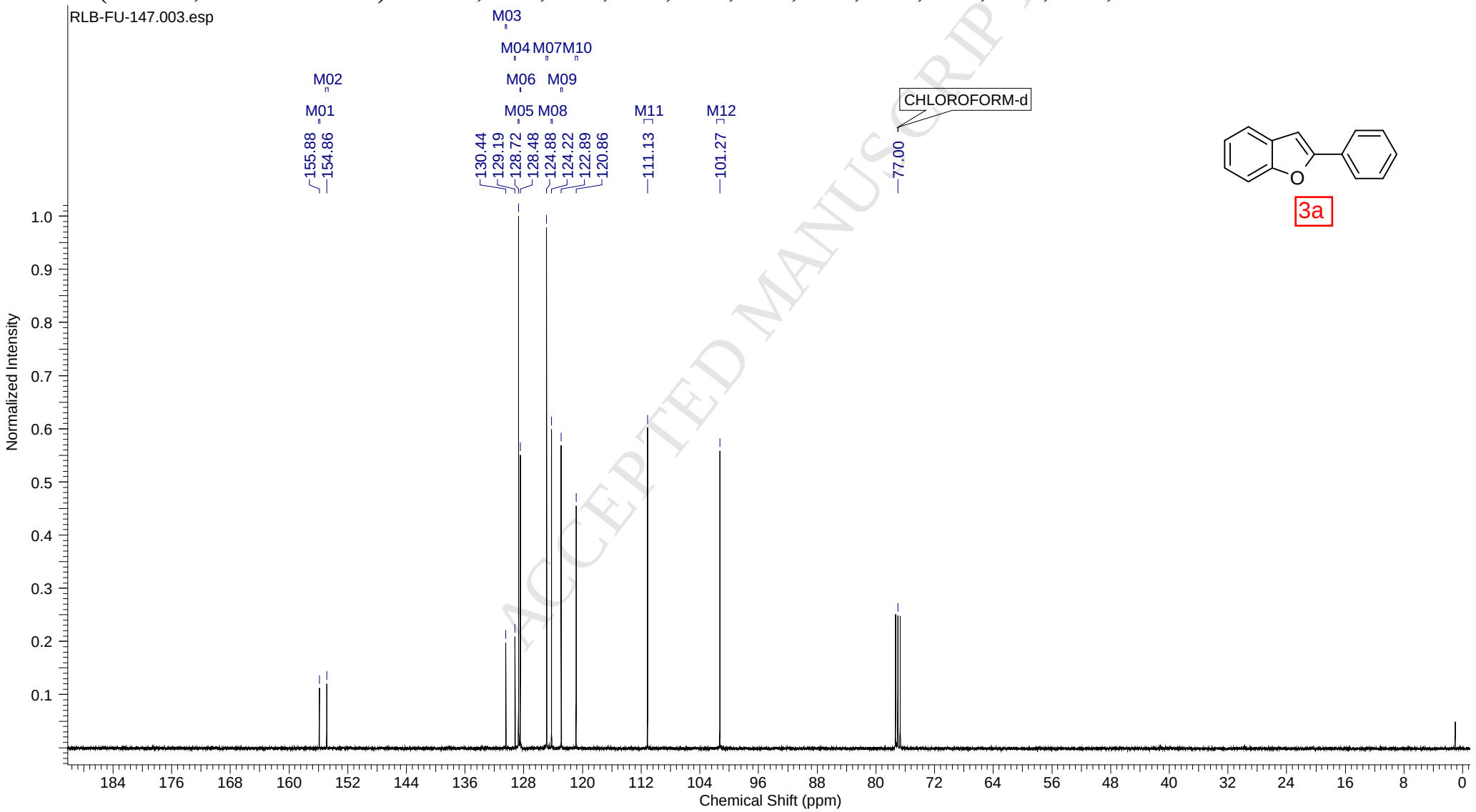
^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 7.83 (d, *J* = 8.0 Hz, 2 H), 7.54 (d, *J* = 8.0 Hz, 1 H), 7.50 (d, *J* = 8.0 Hz, 1 H), 7.43 - 7.36 (m, 2 H), 7.34 - 7.15 (m, 3 H), 6.96 (s, 1 H)



14/8/2013 PM 3:42:38

Acquisition Time (sec)	1.3631	***Comment***		***Date***	14 Aug 2013 11:07:44				
Date Stamp	14 Aug 2013 11:07:44			***File Name***	E:\ \ \ &MAss\RLB-FU-147\3\fid			***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	256	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10045.9131	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	26.999		

^{13}C NMR (100MHz ,CHLOROFORM-d) δ = 155.9, 154.9, 130.4, 129.2, 128.7, 128.5, 124.9, 124.2, 122.9, 120.9, 111.1, 101.3

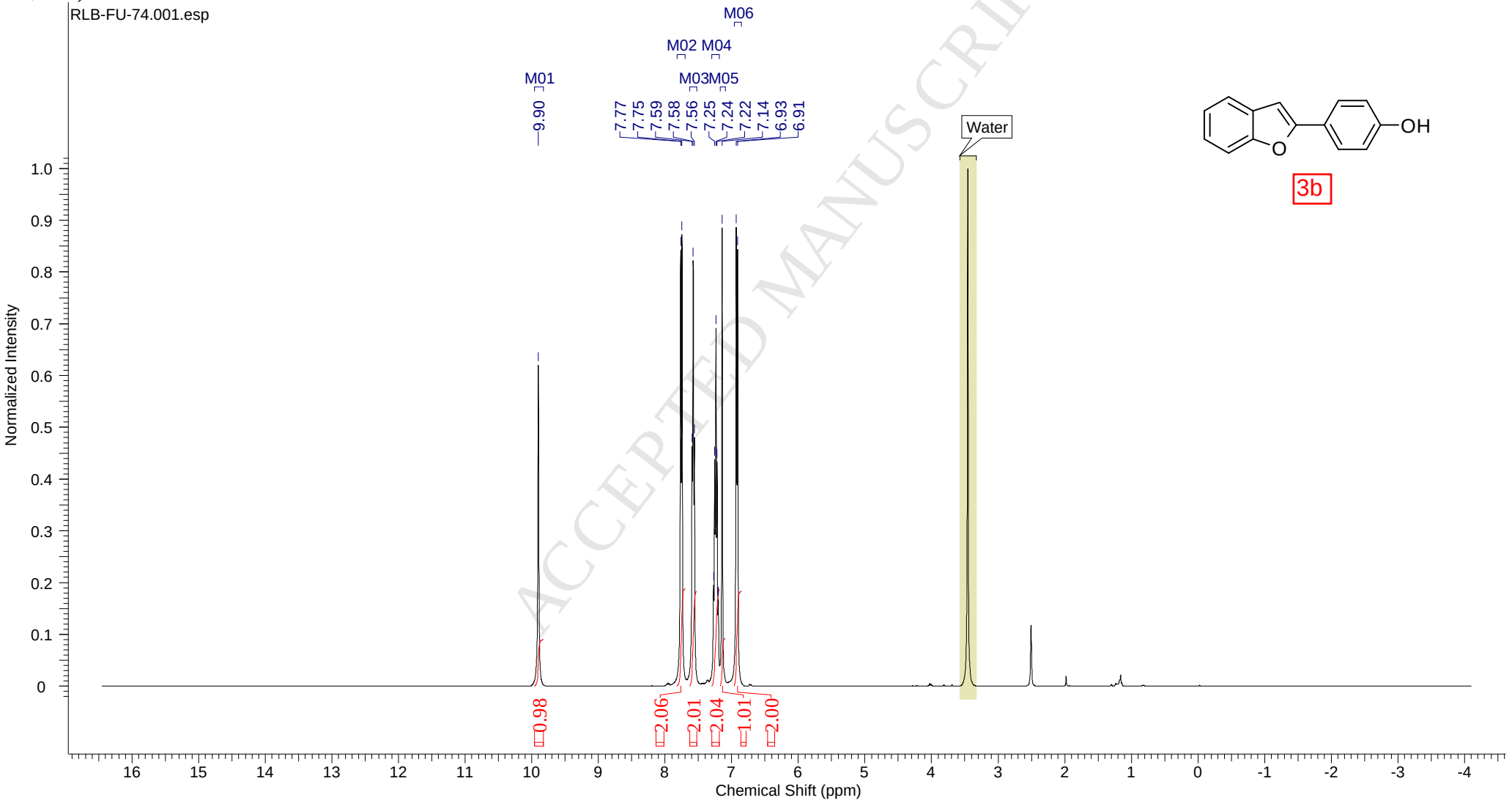


3a

5/6/2013 PM 5:57:17

Acquisition Time (sec)	3.9846	***Comment***		***Date***	05 Jun 2013 12:28:48			***Date Stamp***	05 Jun 2013 12:28:48
File Name	E:\ \ \ &MAss\RLB-FU-74\1\fid			***Frequency (MHz)***	400.13	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	31.69	***SW(cyclical) (Hz)***	8223.68	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9683	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8223.43	***Temperature (degree C)***	25.760						

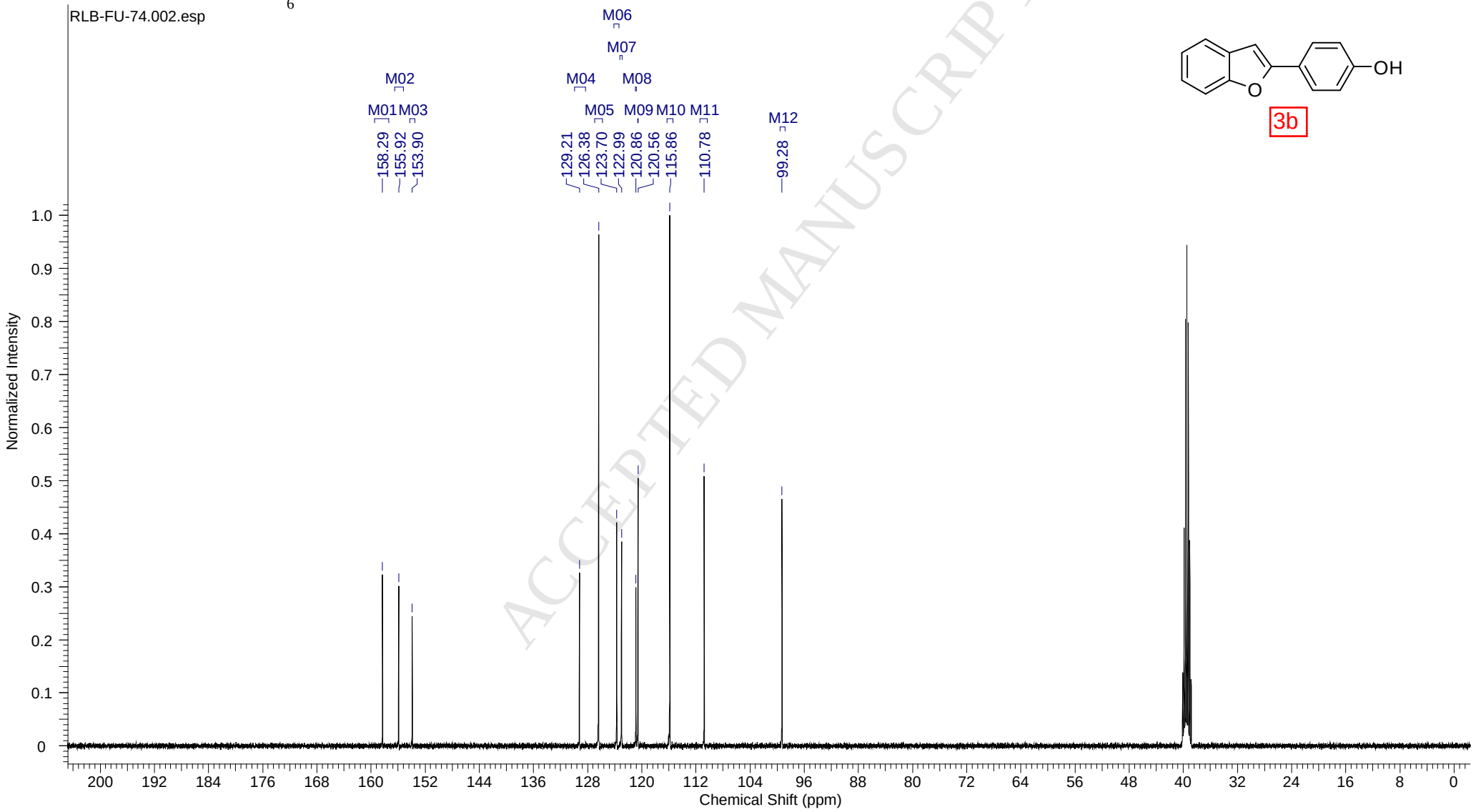
^{1}H NMR (400MHz ,DMSO-d$_6$) δ = 9.90 (s, 1 H), 7.76 (d, J = 8.5 Hz, 2 H), 7.58 (t, J = 6.8 Hz, 2 H), 7.24 (quin, J = 7.1 Hz, 2 H), 7.14 (s, 1 H), 6.92 (d, J = 8.5 Hz, 2 H)



5/6/2013 PM 6:00:40

Acquisition Time (sec)	1.3631	***Comment***		***Date***	05 Jun 2013 12:26:40			***Date Stamp***	05 Jun 2013 12:26:40
File Name	E:\ \ \ &MAss\RLB-FU-74\2\fid			***Frequency (MHz)***	100.61	***Nucleus***	13C	***Number of Transients***	256
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	10010.0264	***Spectrum Type***	STANDARD
Sweep Width (Hz)	24037.73	***Temperature (degree C)***	26.004						

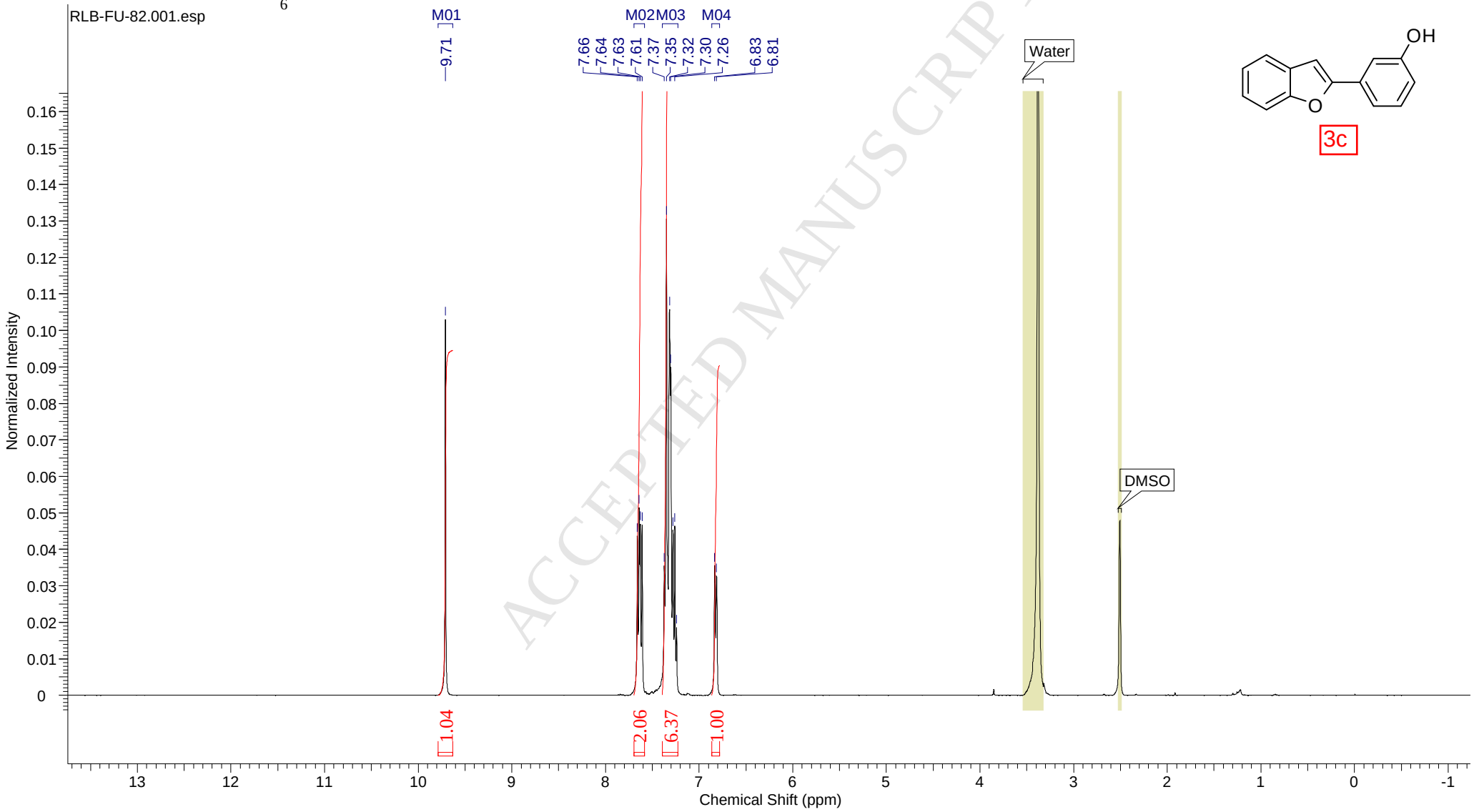
^{13}C NMR (101MHz ,DMSO-d$_6$) δ = 158.3, 155.9, 153.9, 129.2, 126.4, 123.7, 123.0, 120.9, 120.6, 115.9, 110.8, 99.3



13/8/2013 PM 6:04:39

Acquisition Time (sec)	3.9846	***Comment***		***Date***	07 Jun 2013 10:59:12			***Date Stamp***	07 Jun 2013 10:59:12
File Name	E:\ \ \ &MAss\RLB-FU-82\1\fid			***Frequency (MHz)***	400.13	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	56.68	***SW(cyclical) (Hz)***	8223.68	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9683	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8223.43	***Temperature (degree C)***	26.059						

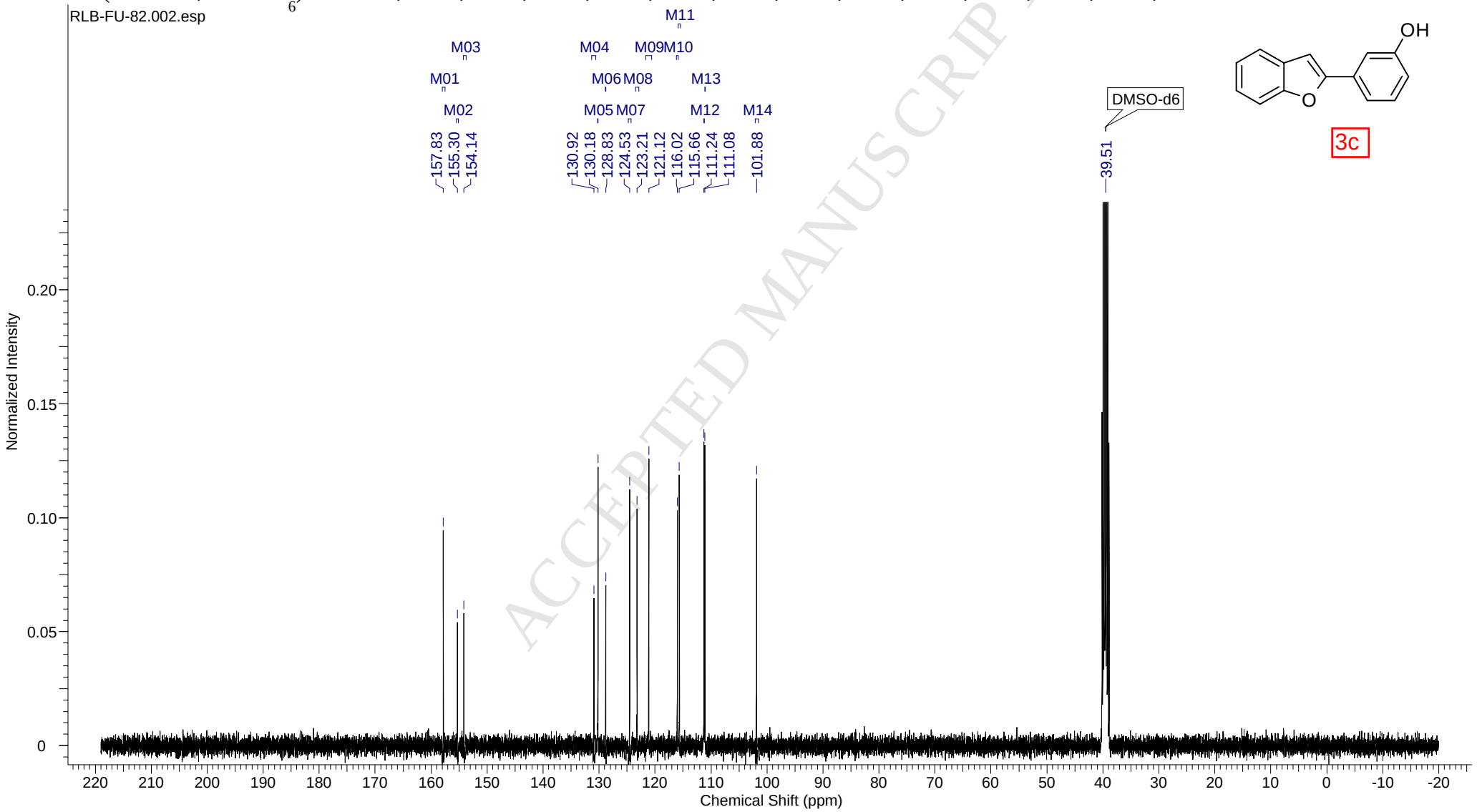
^{1}H NMR (400MHz ,DMSO-d$_6$) δ = 9.71 (s, 1 H), 7.63 (dd, *J* = 7.8, 12.3 Hz, 2 H), 7.39 - 7.23 (m, 6 H), 6.82 (d, *J* = 7.8 Hz, 1 H)



13/8/2013 PM 6:14:32

Acquisition Time (sec)	1.3631	***Comment***		***Date***	07 Jun 2013 11:14:08			***Date Stamp***	07 Jun 2013 11:14:08
File Name	E:\ \ \ &MAss\RLB-FU-82\2\fid			***Frequency (MHz)***	100.61	***Nucleus***	13C	***Number of Transients***	256
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	10013.8037	***Spectrum Type***	STANDARD
Sweep Width (Hz)	24037.73	***Temperature (degree C)***	26.439						

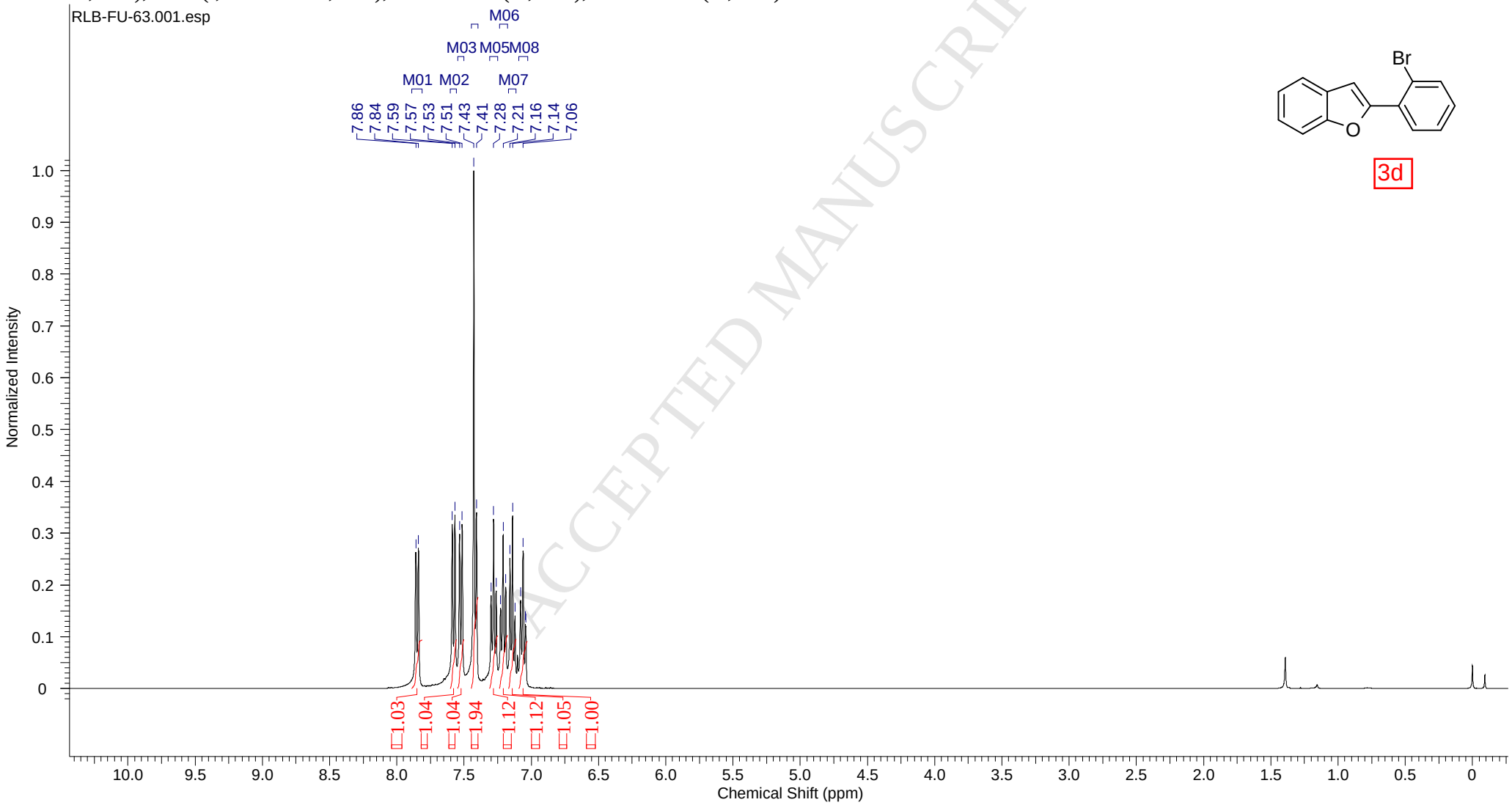
^{13}C NMR (100MHz ,DMSO-d$_6$) δ = 157.8, 155.3, 154.1, 130.9, 130.2, 128.8, 124.5, 123.2, 121.1, 116.0, 115.7, 111.2, 111.1, 101.9



30/5/2013 PM 10:18:55

Acquisition Time (sec)	3.9846	***Comment***				***Date***	30 May 2013 15:47:12		
Date Stamp	30 May 2013 15:47:12			***File Name***	E:\ \ \ &MAss\RLB-FU-63\1\fid			***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	31.69	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	2398.6504	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	25.620		

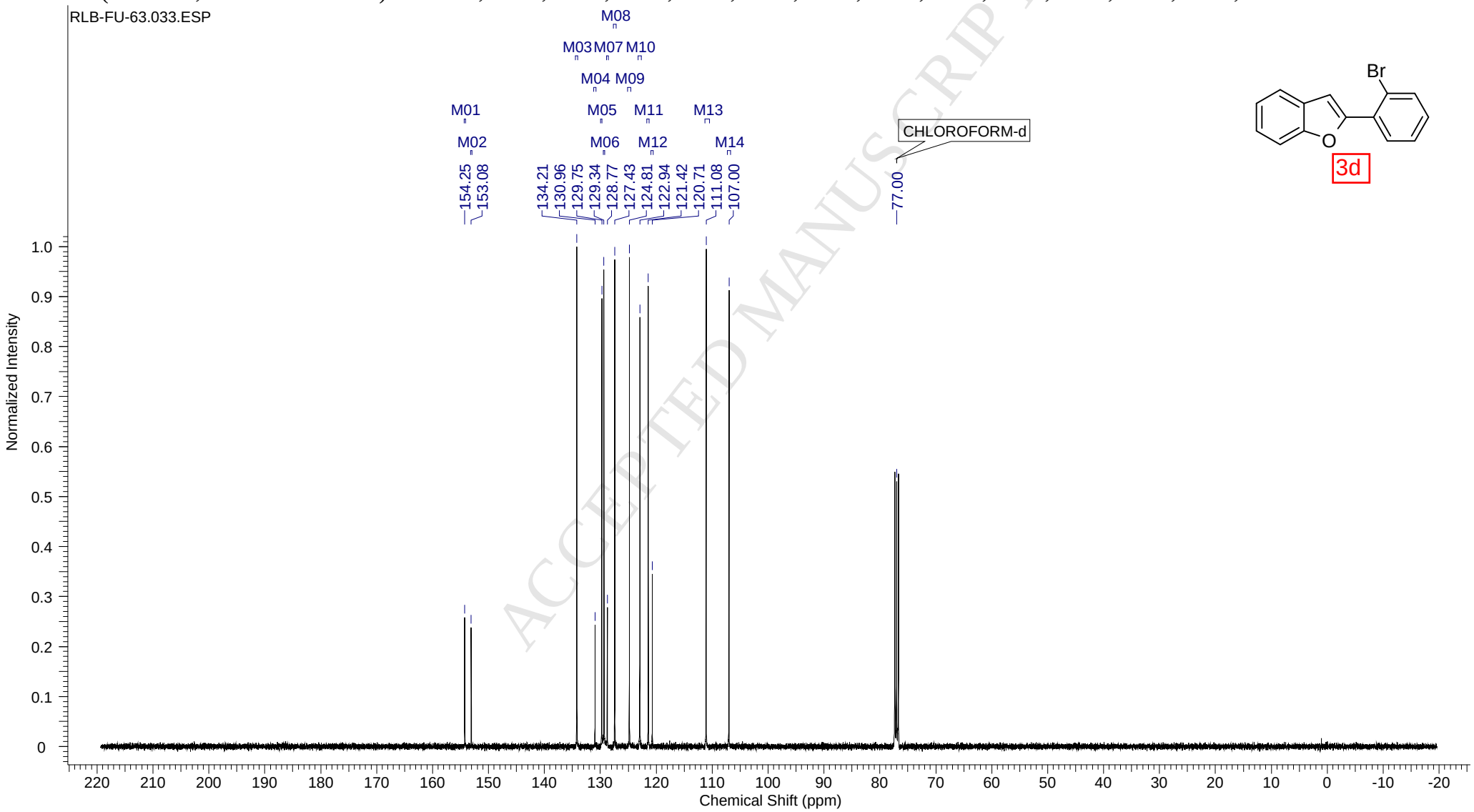
^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 7.85 (dd, *J* = 1.0, 7.8 Hz, 1 H), 7.58 (d, *J* = 8.0 Hz, 1 H), 7.52 (d, *J* = 7.5 Hz, 1 H), 7.45 - 7.40 (m, 2 H), 7.28 (t, *J* = 7.7 Hz, 1 H), 7.21 (t, *J* = 7.7 Hz, 1 H), 7.17 - 7.11 (m, 1 H), 7.09 - 7.03 (m, 1 H)



13/8/2013 PM 6:28:48

Acquisition Time (sec)	1.3631	***Comment***				***Date***	30 May 2013 16:59:44		
Date Stamp	30 May 2013 16:59:44			***File Name***	E:\ \ \ &MAss\RLB-FU-63\33\fid			***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	256	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10048.8389	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	26.252		

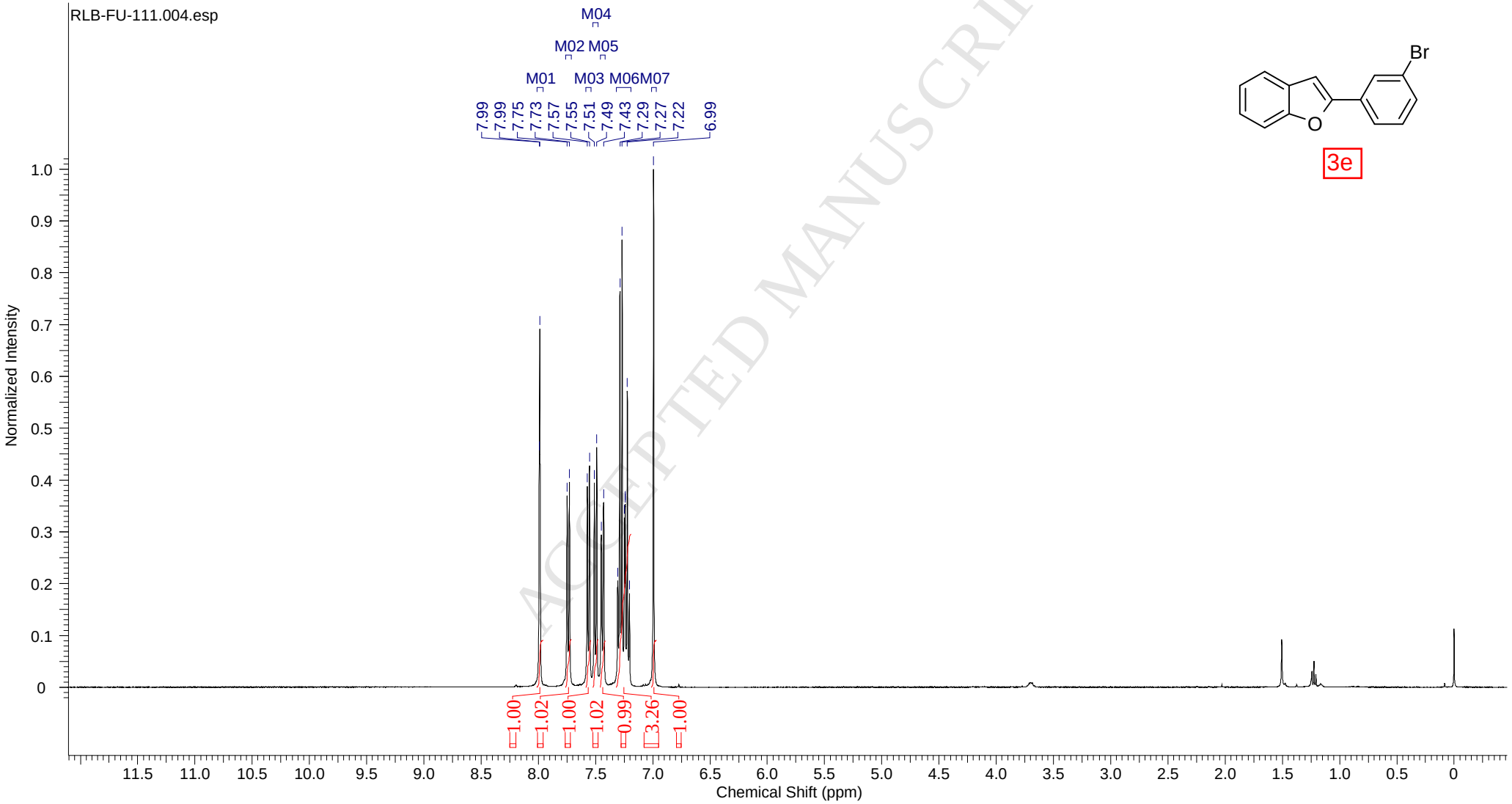
^{13}C NMR (100MHz ,CHLOROFORM-d) δ = 154.2, 153.1, 134.2, 131.0, 129.7, 129.3, 128.8, 127.4, 124.8, 122.9, 121.4, 120.7, 111.1, 107.0



29/6/2013 PM 8:23:58

Acquisition Time (sec)	3.9846	***Comment***		***Date***	20 Jun 2013 12:24:32			***Date Stamp***	20 Jun 2013 12:24:32
File Name	E:\ \ \ &MAss\RLB-FU-111\4\fid			***Frequency (MHz)***	400.13	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	50.23	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2446.5452
Spectrum Type	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	28.623				

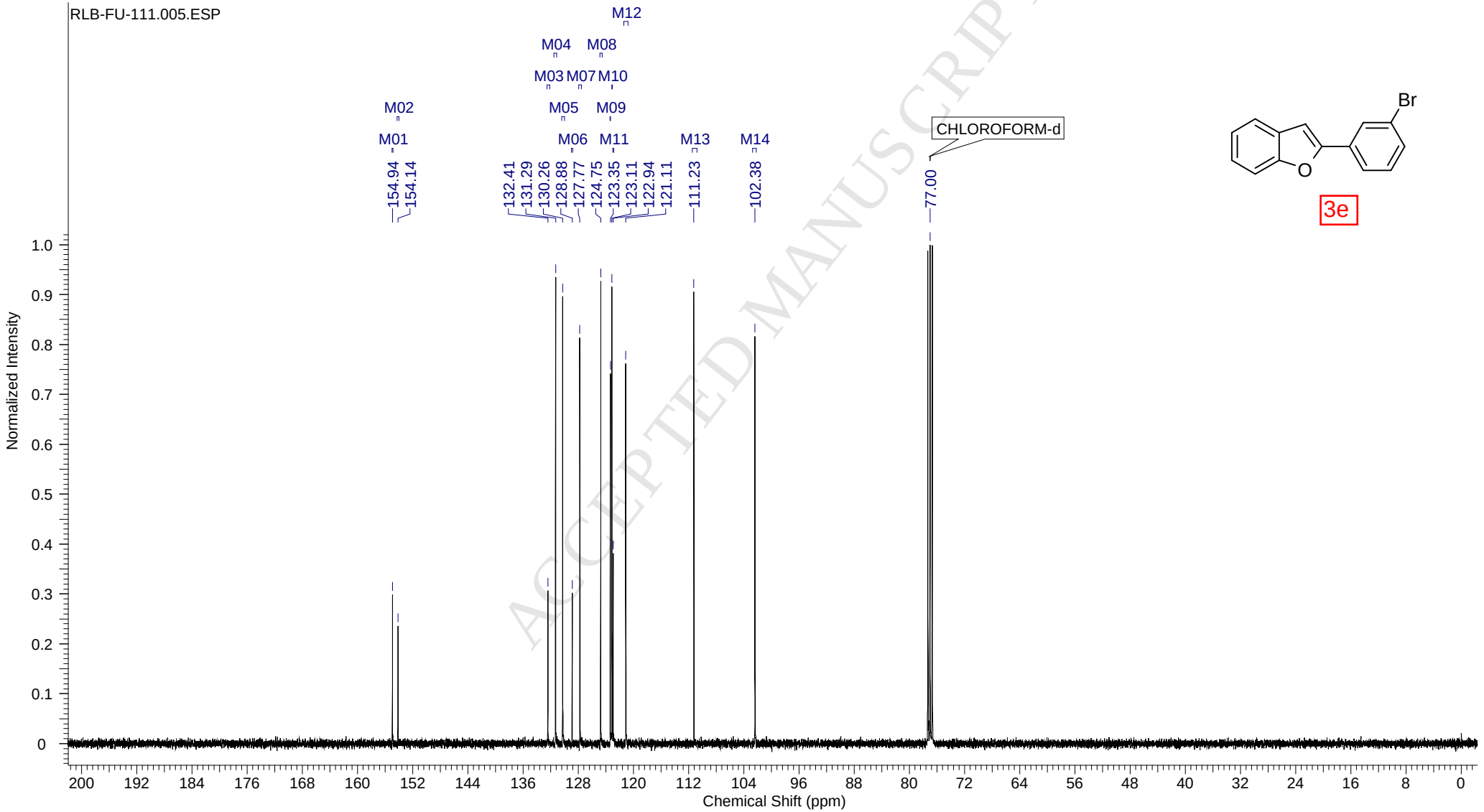
^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 8.01 - 7.96 (m, 1 H), 7.74 (d, *J* = 8.0 Hz, 1 H), 7.56 (d, *J* = 7.3 Hz, 1 H), 7.50 (d, *J* = 8.0 Hz, 1 H), 7.46 - 7.42 (m, 1 H), 7.32 - 7.19 (m, 3 H), 6.99 (s, 1 H)



13/8/2013 PM 6:35:01

Acquisition Time (sec)	1.3631	***Comment***		***Date***	20 Jun 2013 12:41:36				
Date Stamp	20 Jun 2013 12:41:36			***File Name***	E:\ \ \ &MAss\RLB-FU-111\5\fid			***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	256	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10053.9746	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	28.897		

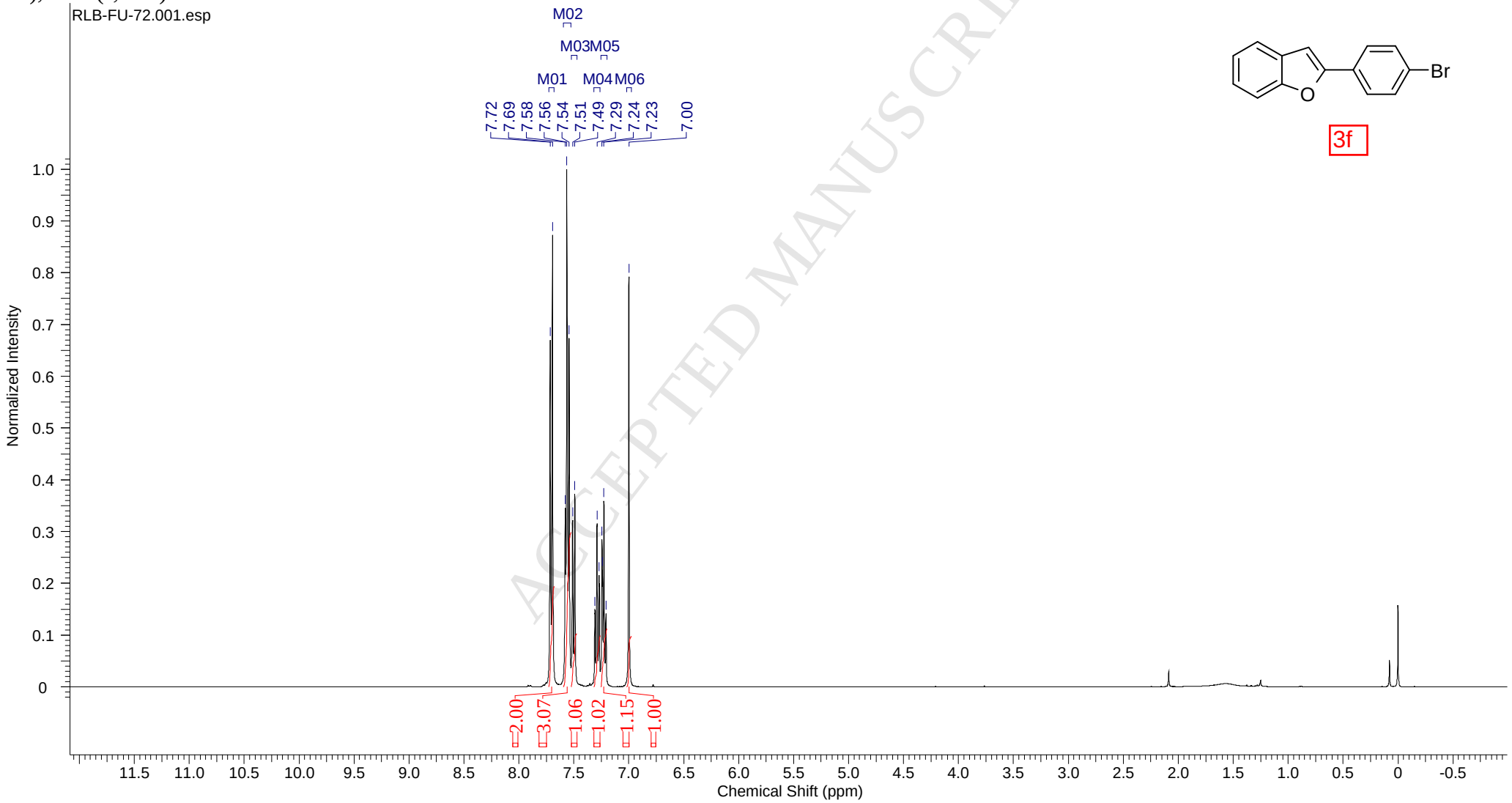
^{13}C NMR (101MHz ,CHLOROFORM-d) δ = 154.9, 154.1, 132.4, 131.3, 130.3, 128.9, 127.8, 124.7, 123.4, 123.1, 122.9, 121.1, 111.2, 102.4



4/6/2013 PM 8:23:06

Acquisition Time (sec)	3.9846	***Comment***		***Date***	04 Jun 2013 10:57:04			***Date Stamp***	04 Jun 2013 10:57:04
File Name	E:\ \ \ &MAss\RLB-FU-72\1\fid			***Frequency (MHz)***	400.13	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	69.91	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2452.9624
Spectrum Type	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	25.244				

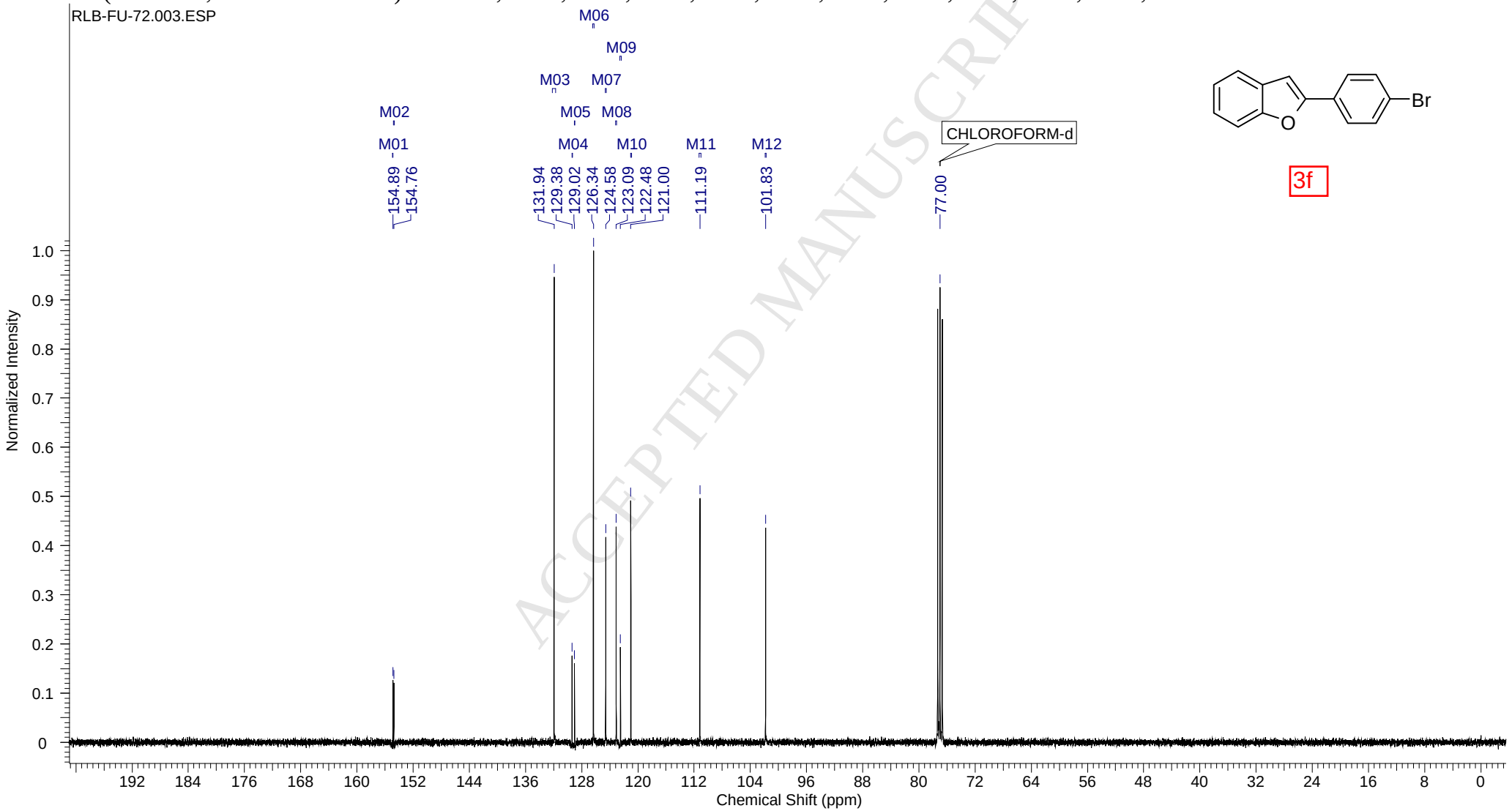
^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 7.71 (d, *J* = 8.5 Hz, 2 H), 7.59 - 7.53 (m, 3 H), 7.50 (d, *J* = 8.0 Hz, 1 H), 7.32 - 7.26 (m, 1 H), 7.25 - 7.20 (m, 1 H), 7.00 (s, 1 H)



13/8/2013 PM 6:41:44

Acquisition Time (sec)	1.3631	***Comment***		***Date***	04 Jun 2013 12:56:32			***Date Stamp***	04 Jun 2013 12:56:32
File Name	C:\Users\libo_ruan\Desktop\RLB-FU-72\3\fid			***Frequency (MHz)***	100.61	***Nucleus***	13C	***Number of Transients***	256
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10055.4414
Spectrum Type	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	25.783				

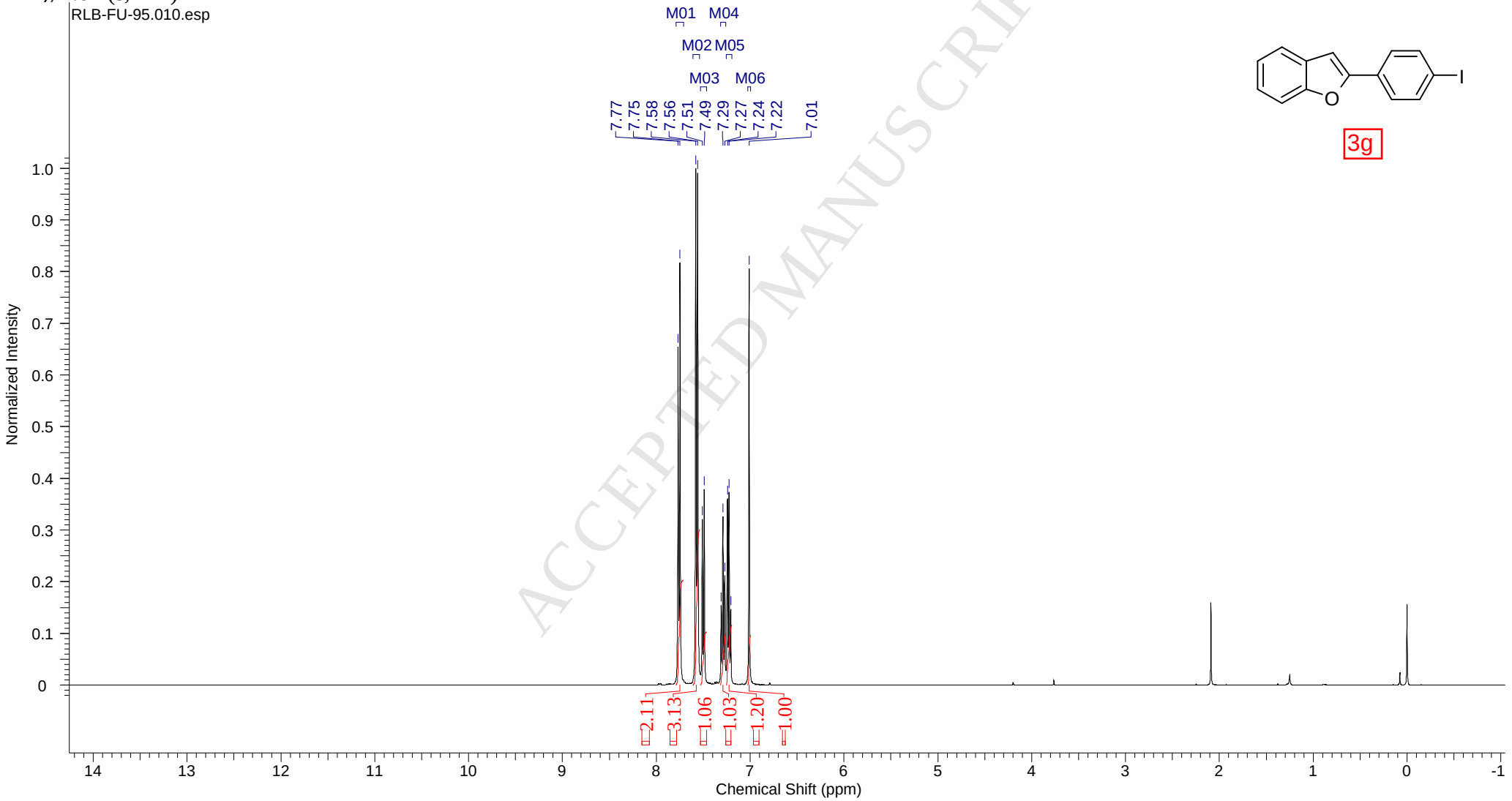
^{13}C NMR (100 MHz ,CHLOROFORM-d) δ = 154.9, 154.8, 131.9, 129.4, 129.0, 126.3, 124.6, 123.1, 122.5, 121.0, 111.2, 101.8



14/6/2013 PM 9:06:38

Acquisition Time (sec)	3.9846	***Comment***		***Date***	11 Jun 2013 15:23:44			***Date Stamp***	11 Jun 2013 15:23:44
File Name	E:\ \ \ &MAss\RLB-FU-95\10\fid			***Frequency (MHz)***	400.13	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	76.85	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2453.5591
Spectrum Type	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	25.022				

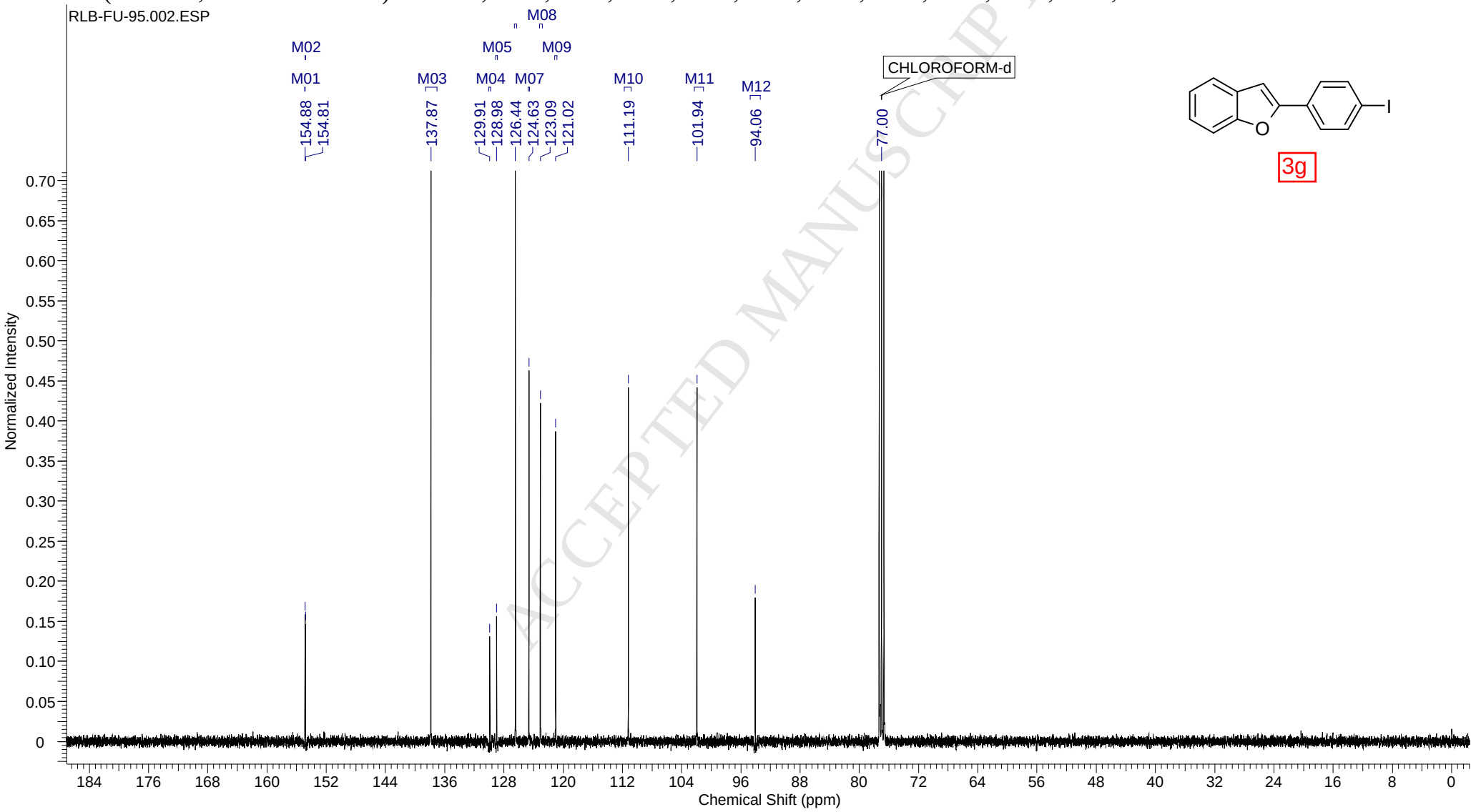
^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 7.76 (d, *J* = 8.3 Hz, 2 H), 7.57 (d, *J* = 8.3 Hz, 3 H), 7.50 (d, *J* = 8.3 Hz, 1 H), 7.32 - 7.26 (m, 1 H), 7.25 - 7.20 (m, 1 H), 7.01 (s, 1 H)



13/8/2013 PM 6:49:41

Acquisition Time (sec)	1.3631	***Comment***		***Date***	11 Jun 2013 15:40:48				
Date Stamp	11 Jun 2013 15:40:48			***File Name***	E:\ \ \ &MAss\RLB-FU-95\2\fid			***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	256	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10054.7080	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	25.402		

^{13}C NMR (100MHz ,CHLOROFORM-d) δ = 154.9, 154.8, 137.9, 129.9, 129.0, 126.4, 124.6, 123.1, 121.0, 111.2, 101.9, 94.1

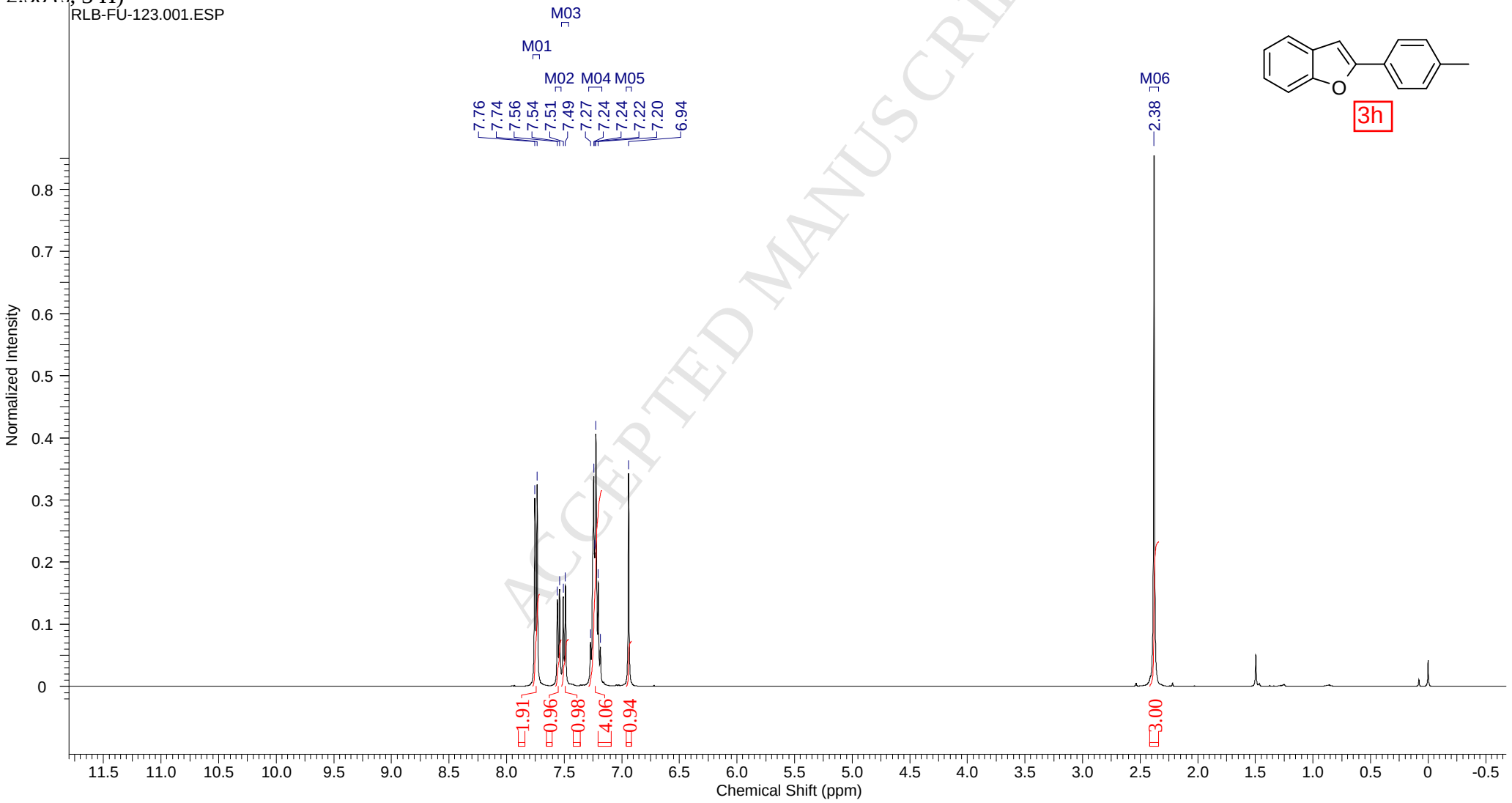


3g

13/10/2013 PM 1:01:50

Acquisition Time (sec)	3.9846	***Comment***				***Date***	26 Jun 2013 11:09:52		
Date Stamp	26 Jun 2013 11:09:52			***File Name***	E:\ \ \ &MAss\RLB-FU-123\1\fid			***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	56.68	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	2444.1321	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	25.595		

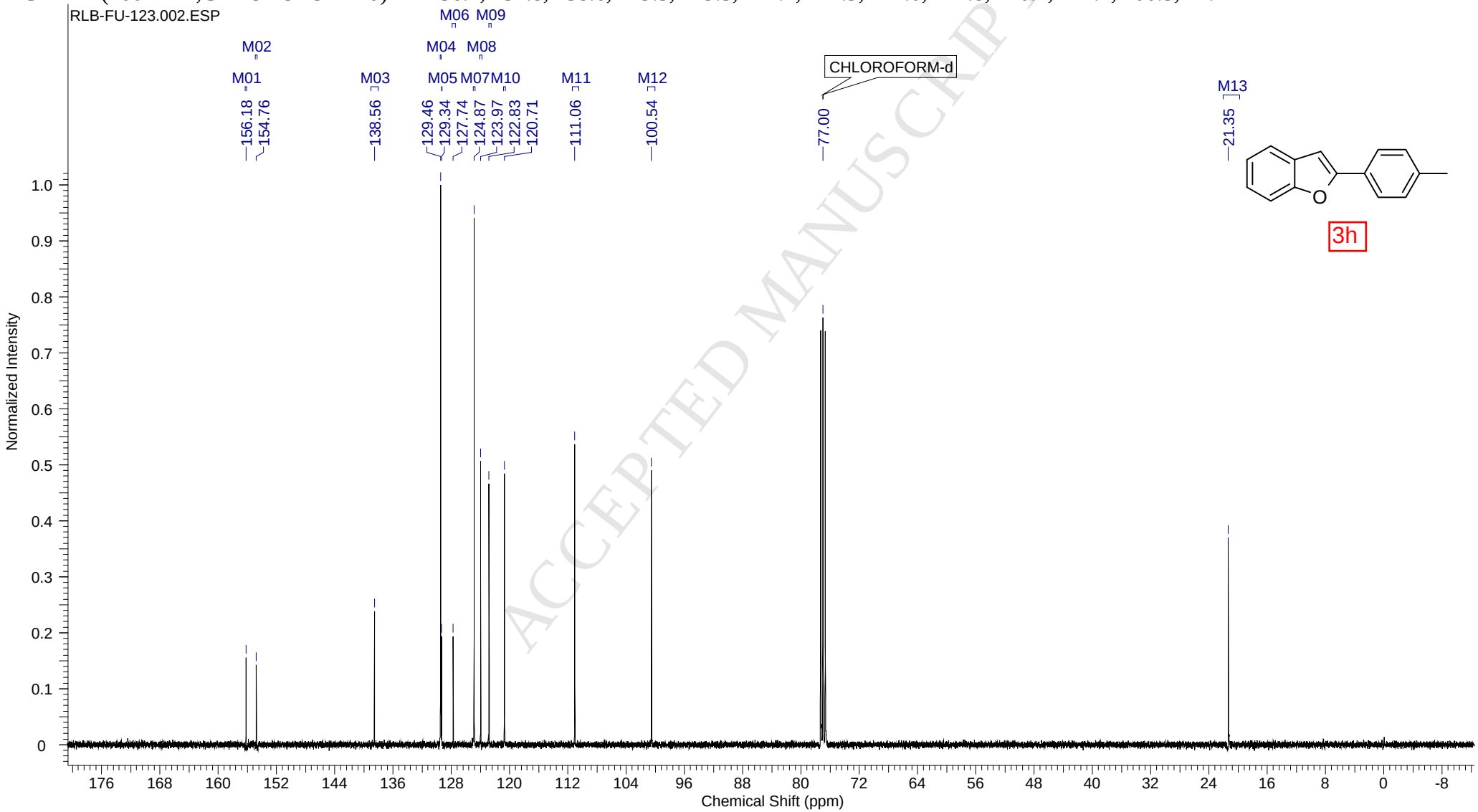
^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 7.75 (d, *J* = 8.0 Hz, 2 H), 7.55 (d, *J* = 8.0 Hz, 1 H), 7.50 (d, *J* = 8.0 Hz, 1 H), 7.29 - 7.18 (m, 4 H), 6.94 (s, 1 H), 2.38 (s, 3 H)



13/8/2013 PM 7:01:10

Acquisition Time (sec)	1.3631	***Comment***		***Date***	26 Jun 2013 11:24:48				
Date Stamp	26 Jun 2013 11:24:48			***File Name***	E:\ \ \ &MAss\RLB-FU-123\2\fid			***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	256	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10053.9746	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	25.941		

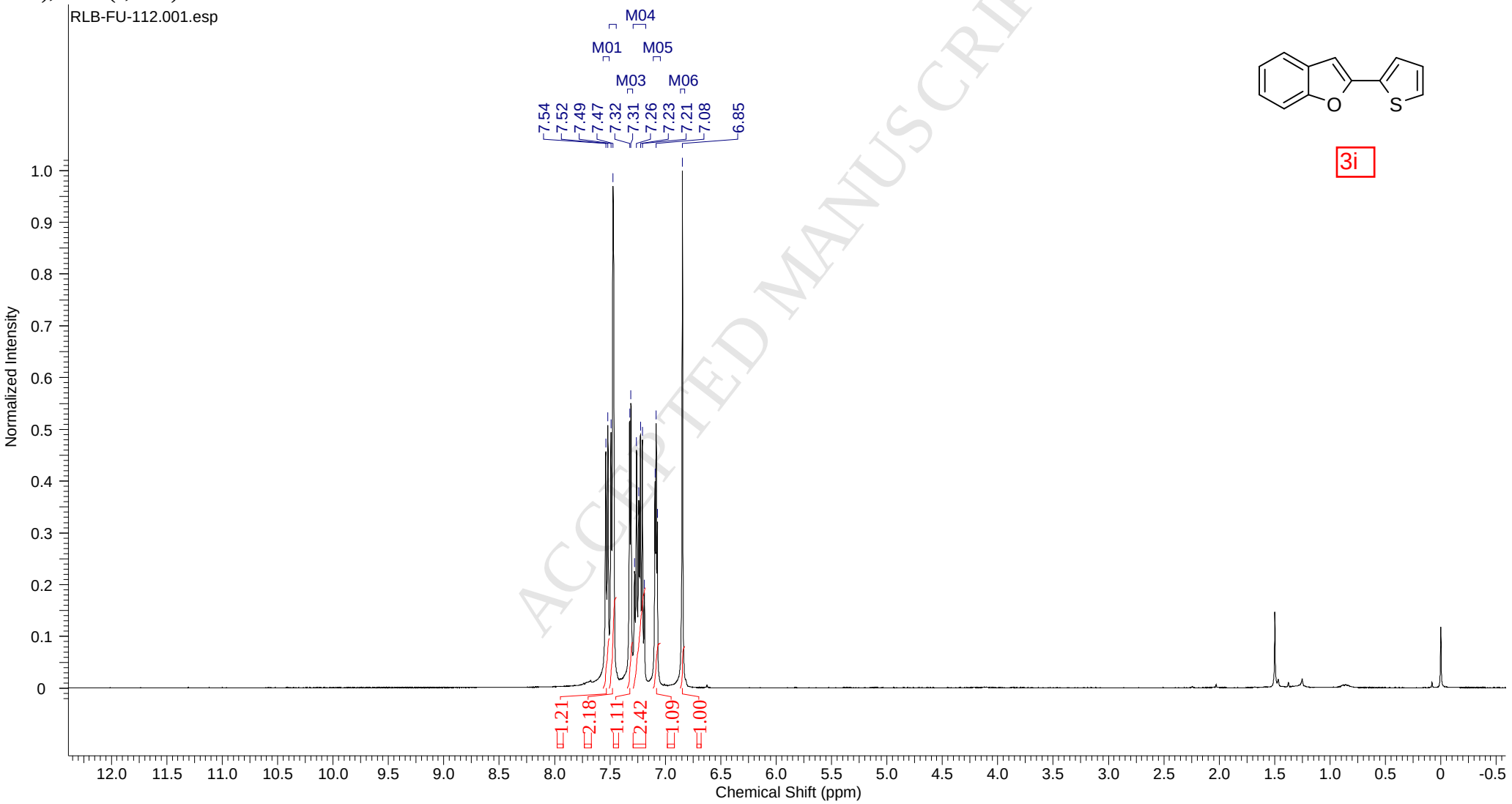
^{13}C NMR (100MHz ,CHLOROFORM-d) δ = 156.2, 154.8, 138.6, 129.5, 129.3, 127.7, 124.9, 124.0, 122.8, 120.7, 111.1, 100.5, 21.4



29/6/2013 PM 8:17:47

Acquisition Time (sec)	3.9846	***Comment***				***Date***	19 Jun 2013 12:33:04		
Date Stamp	19 Jun 2013 12:33:04			***File Name***	E:\ \ \ &MAss\RLB-FU-112\1\fid			***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	56.68	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	2447.2175	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	28.856		

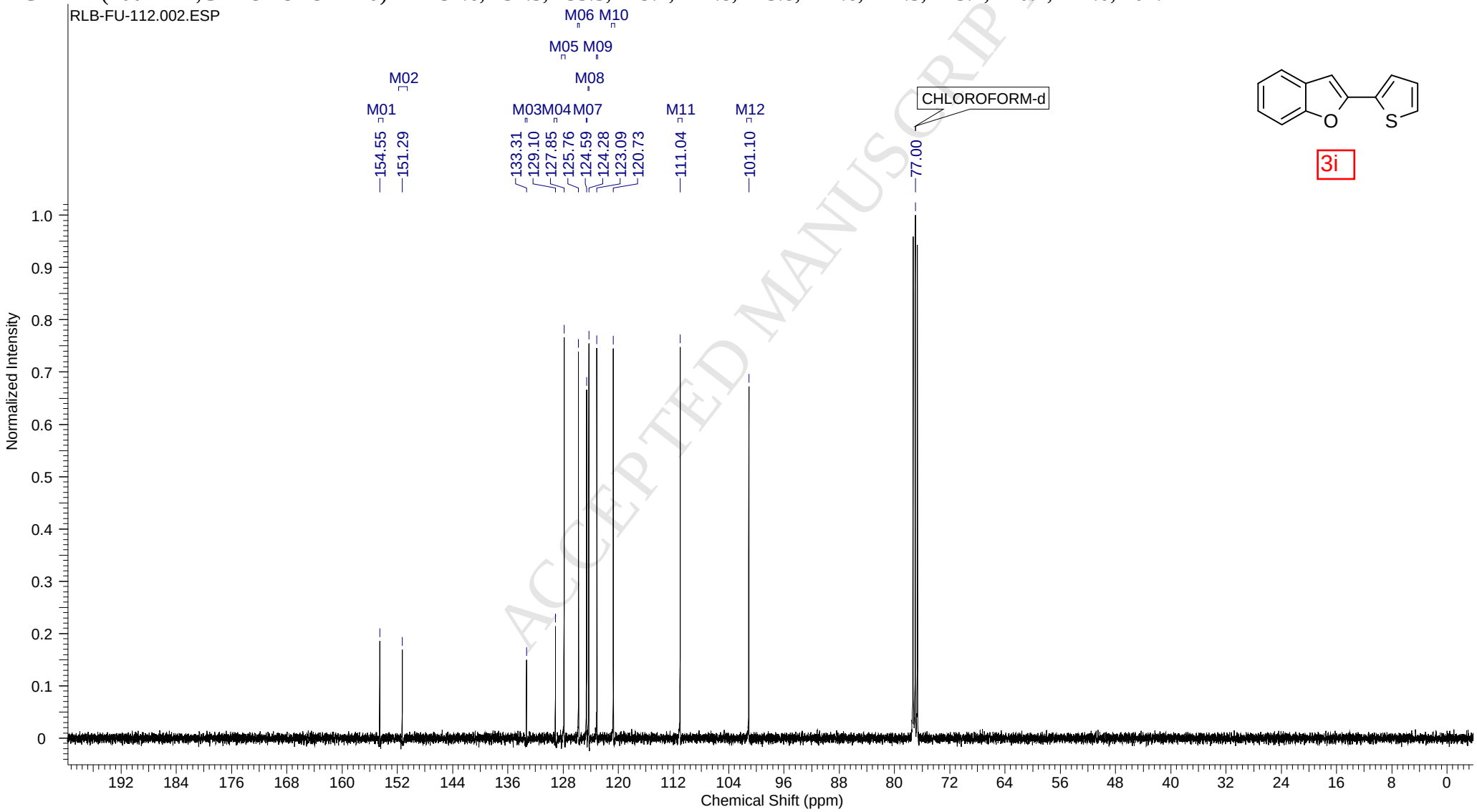
^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 7.53 (d, *J* = 7.3 Hz, 1 H), 7.51 - 7.45 (m, 2 H), 7.32 (d, *J* = 4.8 Hz, 1 H), 7.29 - 7.18 (m, 2 H), 7.08 (t, *J* = 4.3 Hz, 1 H), 6.85 (s, 1 H)



13/8/2013 PM 7:05:52

Acquisition Time (sec)	1.3631	***Comment***		***Date***	19 Jun 2013 12:48:00				
Date Stamp	19 Jun 2013 12:48:00			***File Name***	E:\ \ \ &MAss\RLB-FU-112\2\fid			***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	256	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10054.7080	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	29.088		

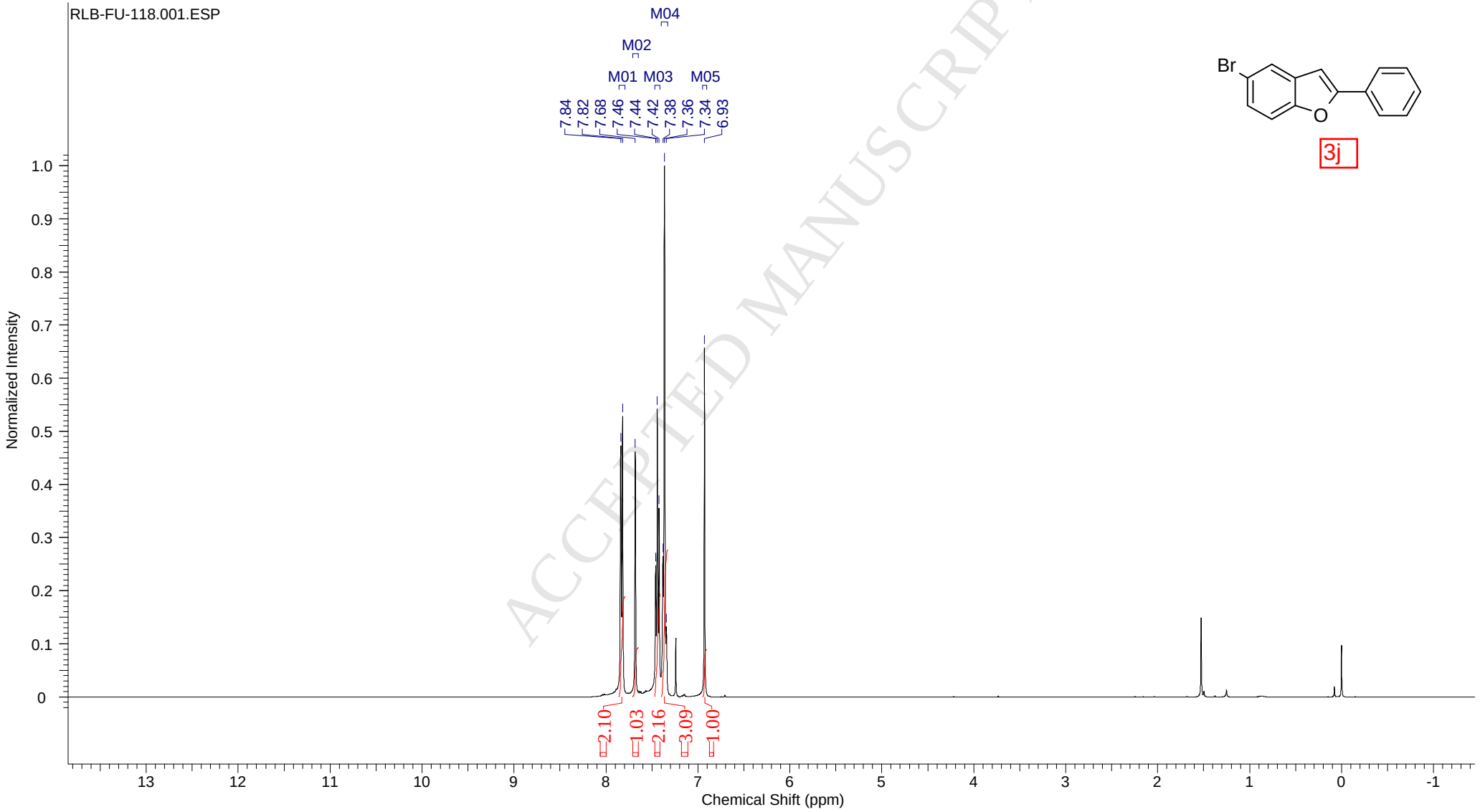
^{13}C NMR (100MHz ,CHLOROFORM-d) δ = 154.6, 151.3, 133.3, 129.1, 127.8, 125.8, 124.6, 124.3, 123.1, 120.7, 111.0, 101.1



13/8/2013 PM 7:26:10

Acquisition Time (sec)	3.9846	***Comment***				***Date***	22 Jun 2013 09:55:12		
Date Stamp	22 Jun 2013 09:55:12			***File Name***	E:\ \ \ &MAss\RLB-FU-118\1\fid			***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	76.85	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	2453.7554	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	26.169		

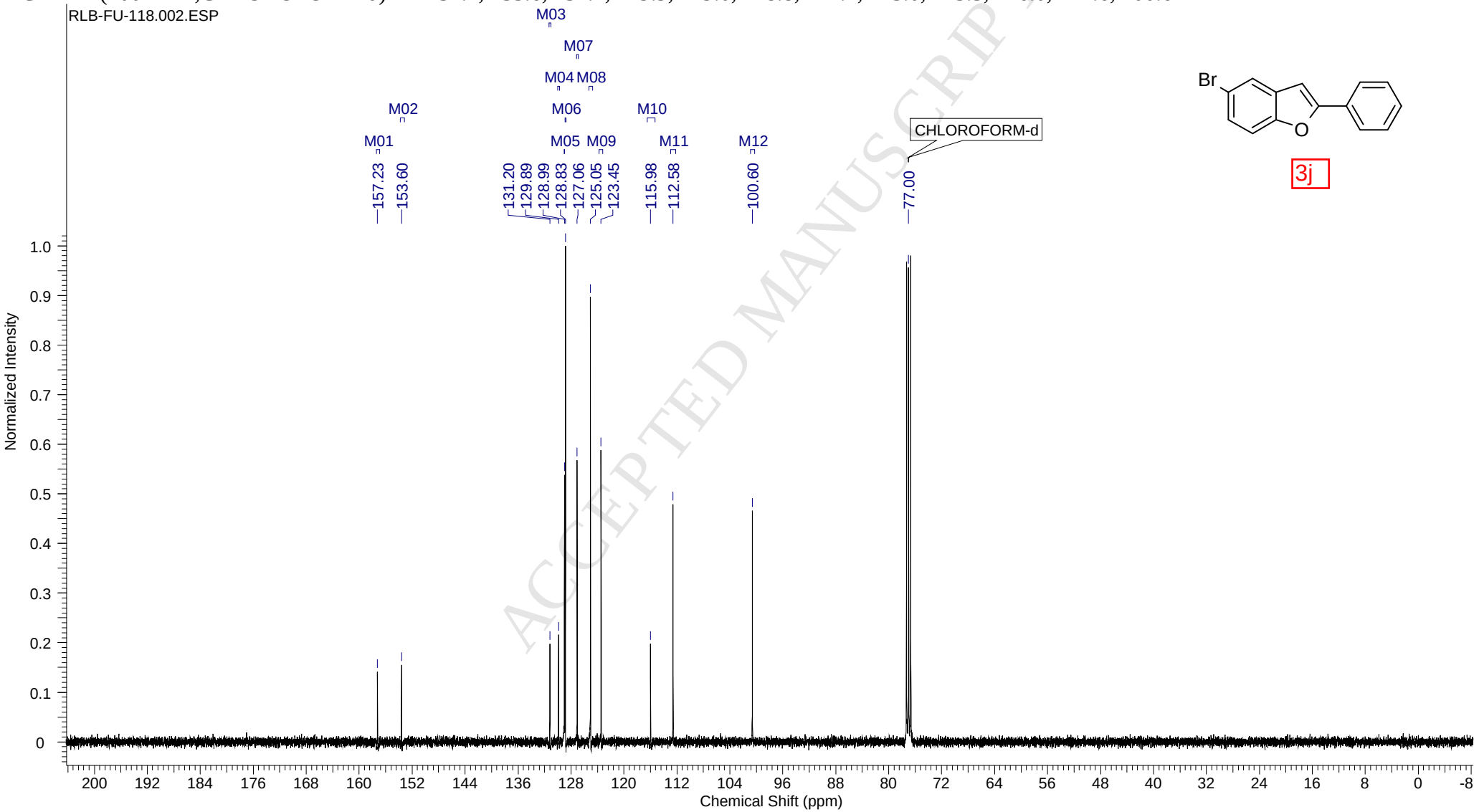
^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 7.83 (d, *J* = 7.5 Hz, 2 H), 7.68 (s, 1 H), 7.47 - 7.41 (m, 2 H), 7.40 - 7.33 (m, 3 H), 6.93 (s, 1 H)



13/8/2013 PM 7:20:24

Acquisition Time (sec)	1.3631	***Comment***		***Date***	22 Jun 2013 10:12:16				
Date Stamp	22 Jun 2013 10:12:16			***File Name***	E:\ \ \ &MAss\RLB-FU-118\2\fid			***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	256	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10056.1758	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	26.628		

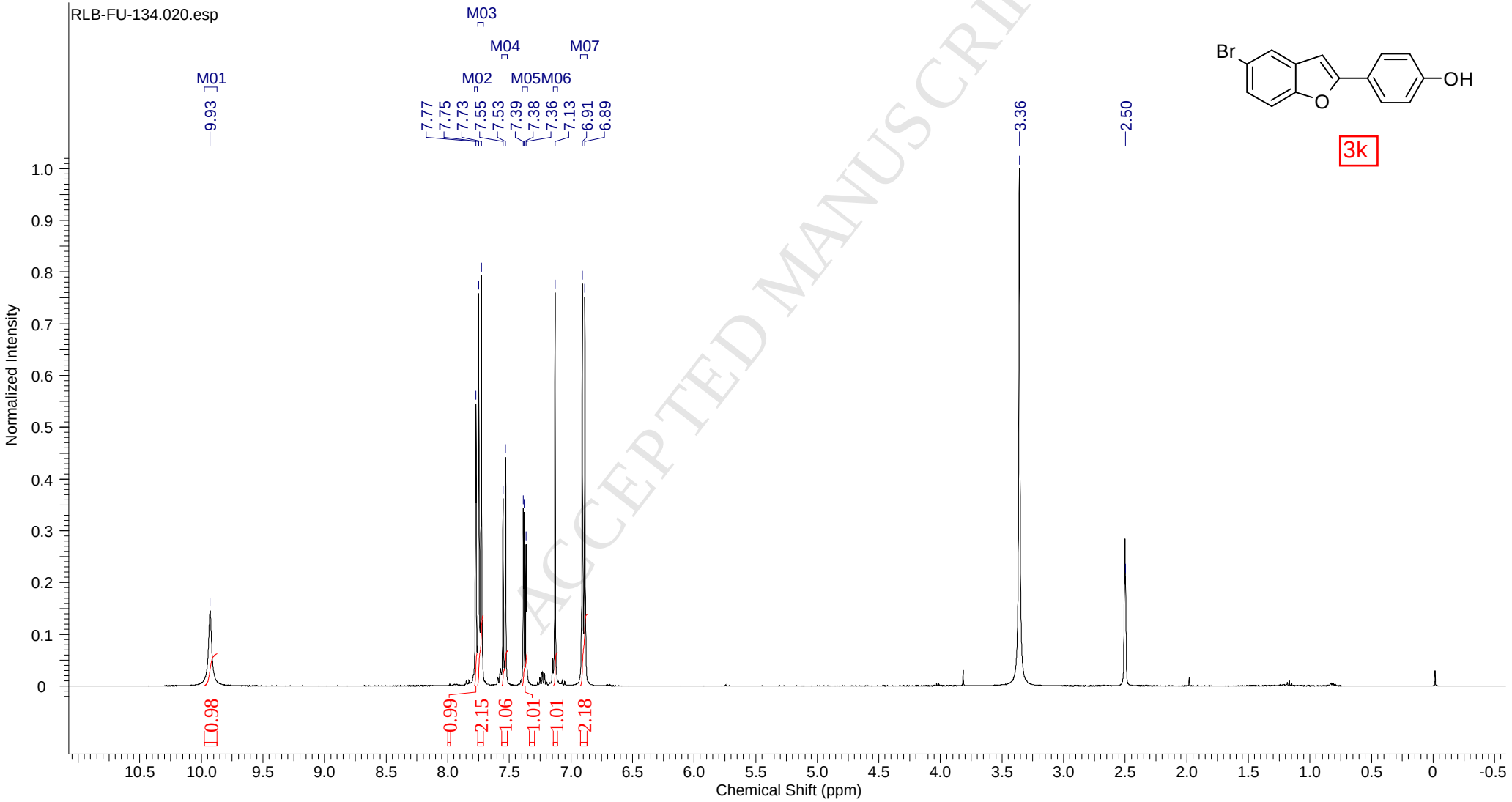
^{13}C NMR (100MHz ,CHLOROFORM-d) δ = 157.2, 153.6, 131.2, 129.9, 129.0, 128.8, 127.1, 125.0, 123.5, 116.0, 112.6, 100.6



13/8/2013 PM 7:41:30

Acquisition Time (sec)	3.9846	***Comment***				***Date***	08 Jul 2013 09:12:32		
Date Stamp	08 Jul 2013 09:12:32			***File Name***	E:\ \ \ &MAss\RLB-FU-134\20\fid			***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	62.90	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	567.9283	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	28.422		

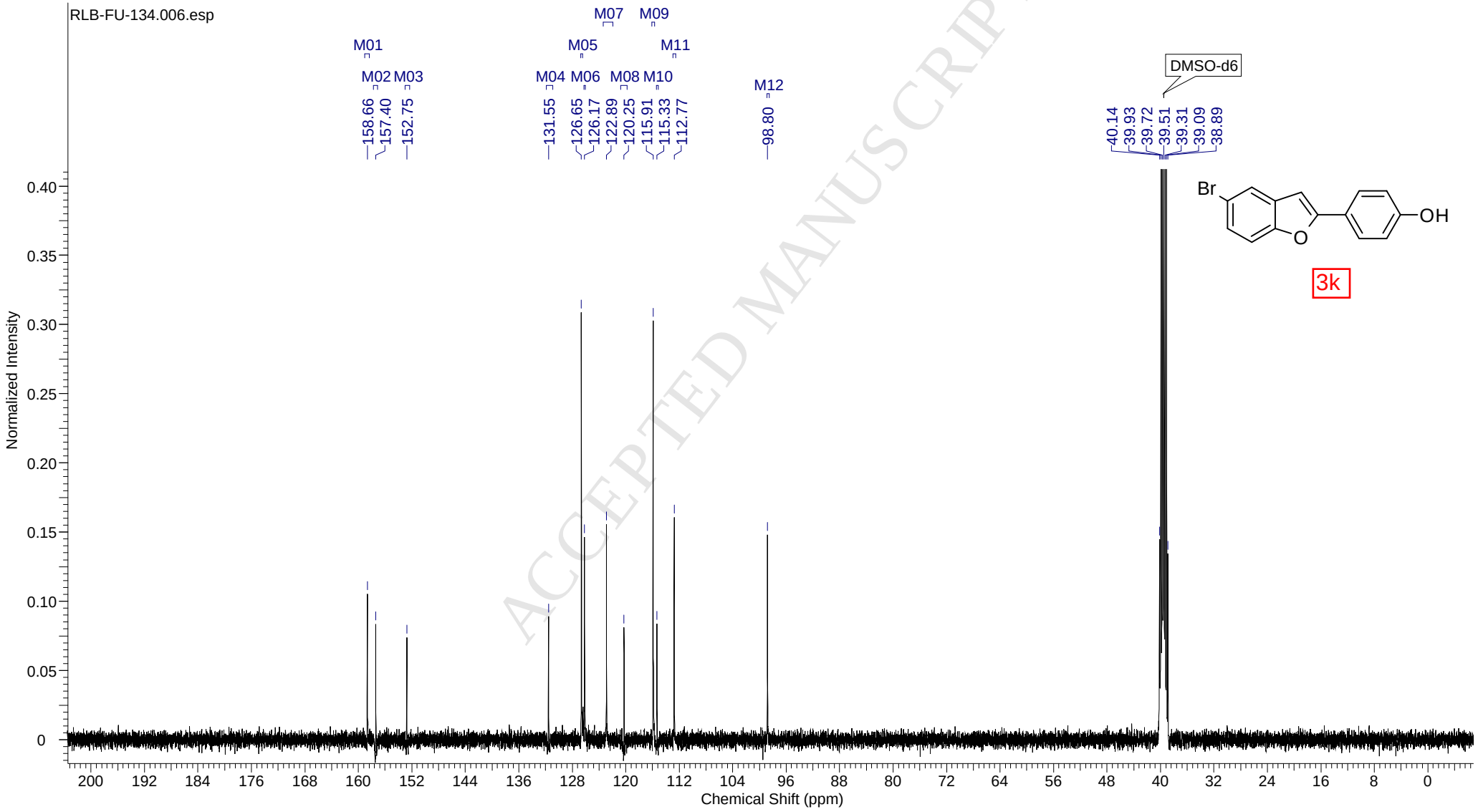
^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 9.93 (br. s., 1 H), 7.77 (d, *J* = 2.0 Hz, 1 H), 7.74 (d, *J* = 8.5 Hz, 2 H), 7.54 (d, *J* = 8.5 Hz, 1 H), 7.37 (dd, *J* = 2.0, 8.5 Hz, 1 H), 7.13 (s, 1 H), 6.90 (d, *J* = 8.5 Hz, 2 H)



13/8/2013 PM 7:45:39

Acquisition Time (sec)	1.3631	***Comment***		***Date***	06 Jul 2013 15:21:36			***Date Stamp***	06 Jul 2013 15:21:36
File Name	E:\ \ \ &MAss\RLB-FU-134\6\fid			***Frequency (MHz)***	100.61	***Nucleus***	13C	***Number of Transients***	256
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	10010.8701	***Spectrum Type***	STANDARD
Sweep Width (Hz)	24037.73	***Temperature (degree C)***	28.319						

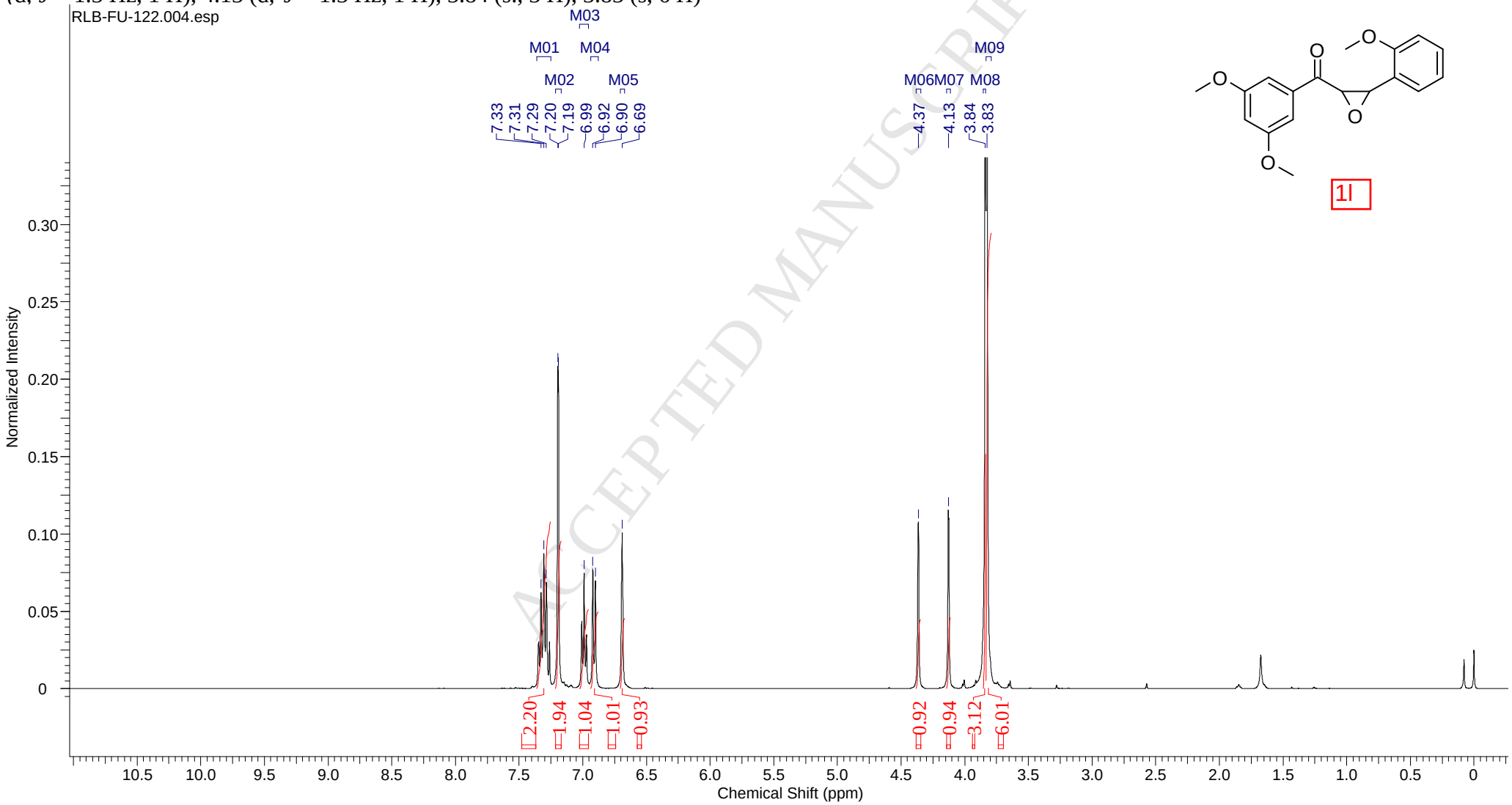
^{13}C NMR (100MHz ,DMSO-d_6) δ = 158.7, 157.4, 152.8, 131.5, 126.6, 126.2, 122.9, 120.3, 115.9, 115.3, 112.8, 98.8



27/6/2013 PM 3:19:57

Acquisition Time (sec)	3.9846	***Comment***		***Date***	26 Jun 2013 12:28:48			***Date Stamp***	26 Jun 2013 12:28:48
File Name	E:\ \ \ &MAss\RLB-FU-122\4\fid			***Frequency (MHz)***	400.13	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	50.23	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2462.2373
Spectrum Type	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	25.584				

^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 7.36 - 7.25 (m, 2 H), 7.19 (d, *J* = 2.0 Hz, 2 H), 7.02 - 6.96 (m, 1 H), 6.91 (d, *J* = 8.3 Hz, 1 H), 6.69 (s, 1 H), 4.37 (d, *J* = 1.3 Hz, 1 H), 4.13 (d, *J* = 1.3 Hz, 1 H), 3.84 (s., 3 H), 3.83 (s, 6 H)

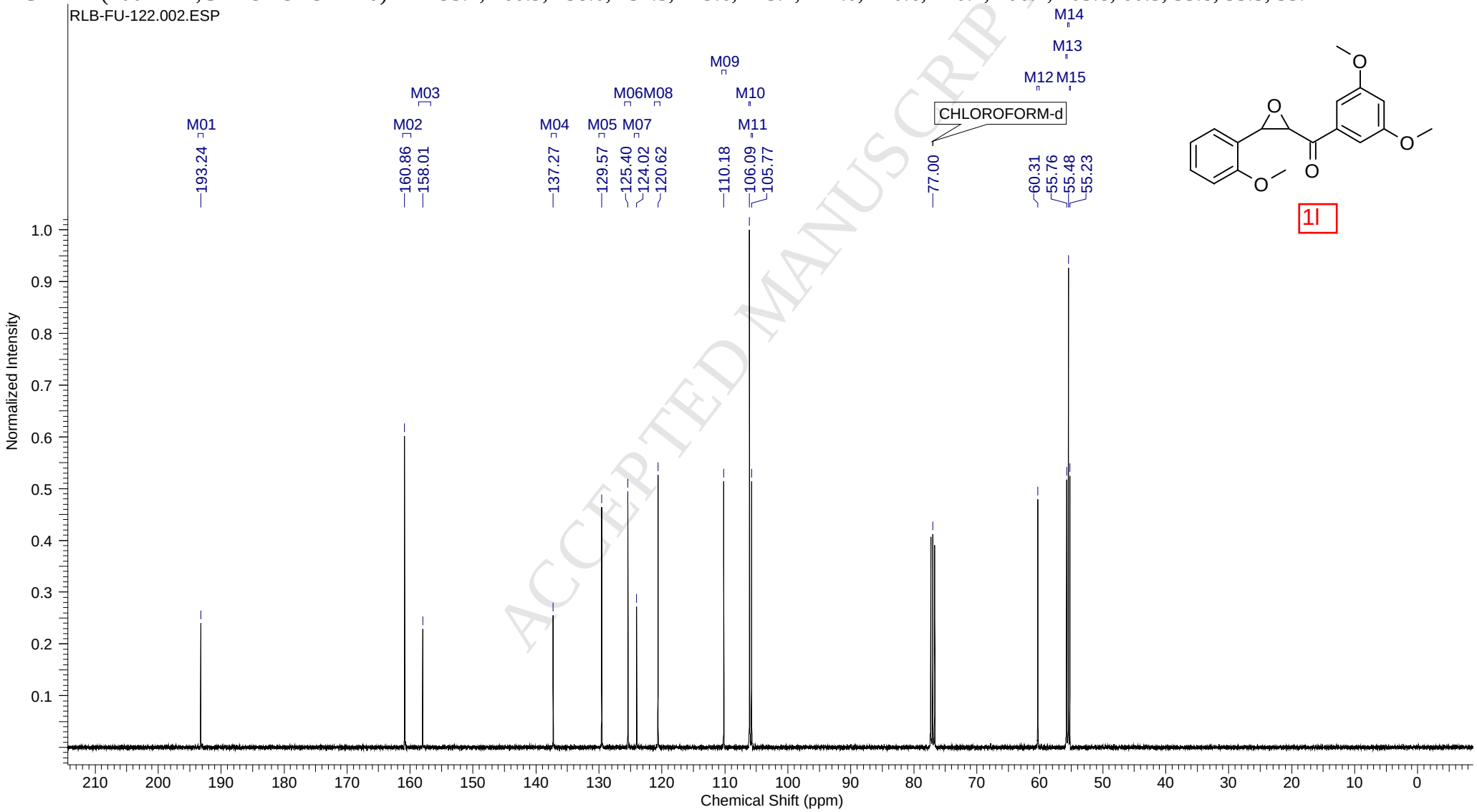


1l

14/8/2013 PM 12:05:42

Acquisition Time (sec)	1.3631	***Comment***		***Date***	26 Jun 2013 11:03:28				
Date Stamp	26 Jun 2013 11:03:28			***File Name***	E:\ \ \ &MAss\RLB-FU-122\2\fid			***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	256	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10045.1719	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	25.916		

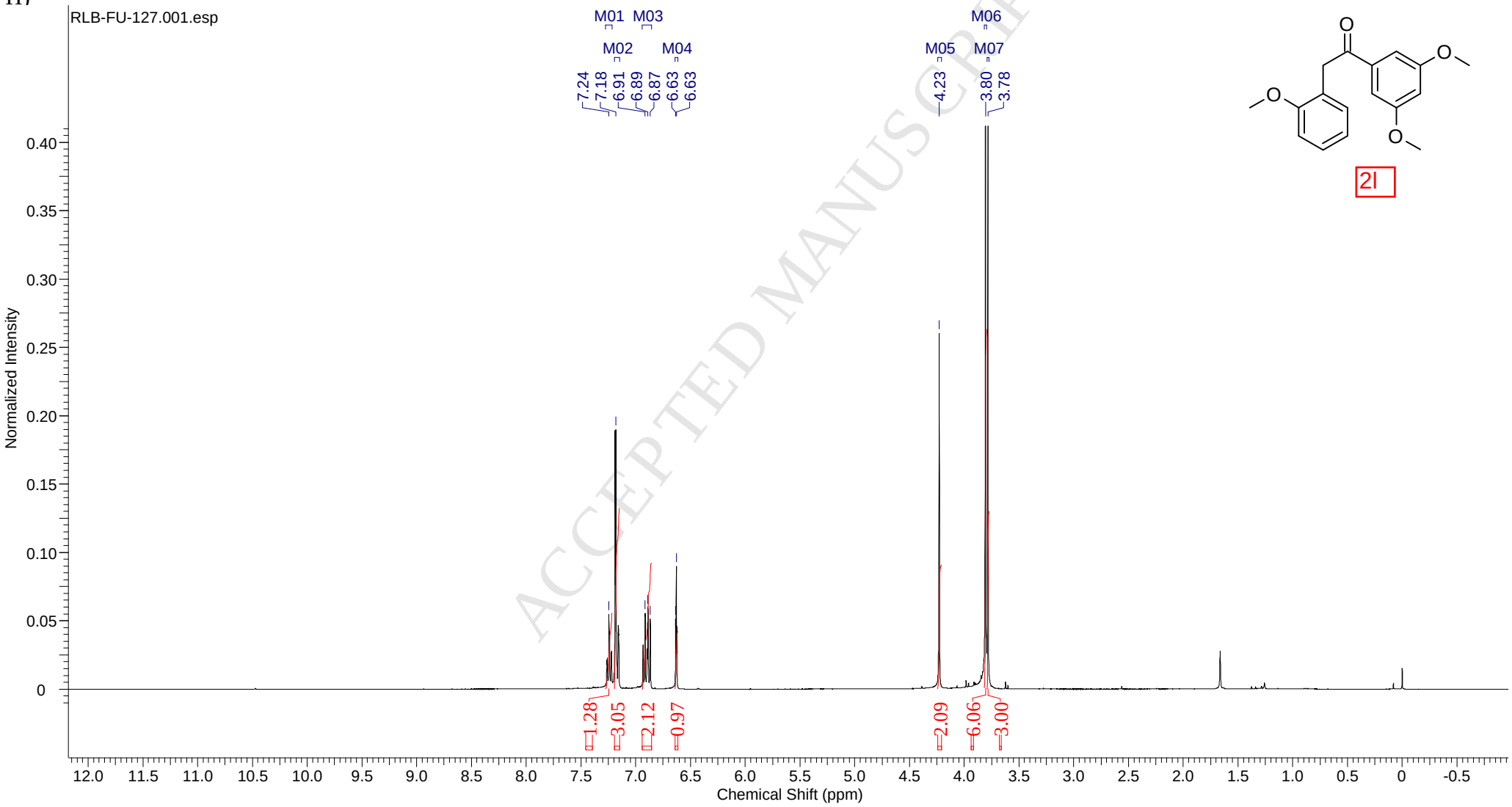
^{13}C NMR (100MHz ,CHLOROFORM-d) δ = 193.2, 160.9, 158.0, 137.3, 129.6, 125.4, 124.0, 120.6, 110.2, 106.1, 105.8, 60.3, 55.8, 55.5, 55.2



29/6/2013 PM 4:08:47

Acquisition Time (sec)	3.9846	***Comment***		***Date***	29 Jun 2013 13:02:56			***Date Stamp***	29 Jun 2013 13:02:56
File Name	E:\ \ \ &MAss\RLB-FU-127\1\fid			***Frequency (MHz)***	400.13	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	31.69	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2455.7114
Spectrum Type	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	25.415				

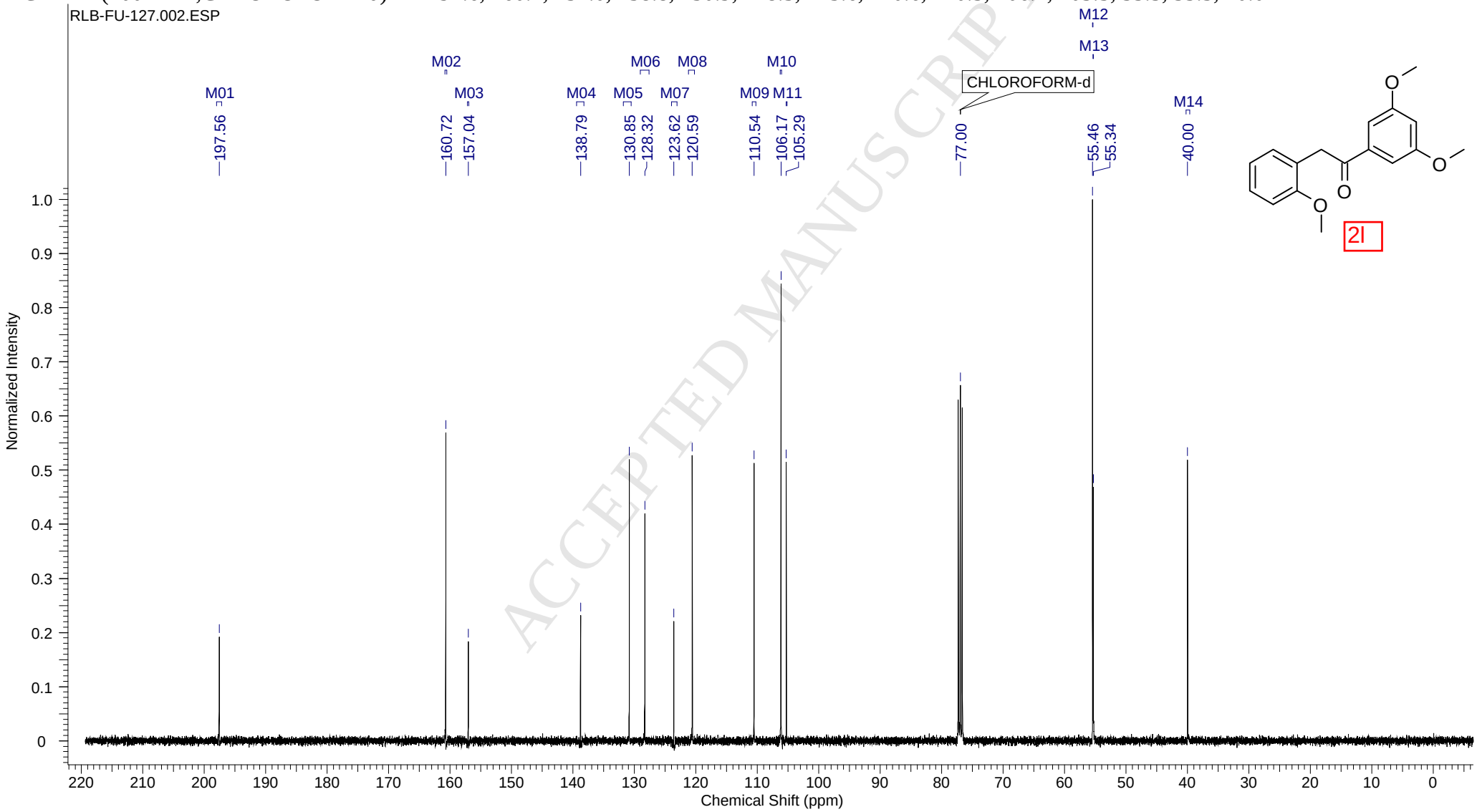
^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 7.24 (s, 1 H), 7.20-7.15 (m, 3 H), 6.94 - 6.86 (m, 2 H), 6.64 - 6.62 (m, 1 H), 4.23 (s, 2 H), 3.80 (s, 6 H), 3.78 (s, 3 H)



14/8/2013 PM 2:29:05

Acquisition Time (sec)	1.3631	***Comment***		***Date***	29 Jun 2013 13:13:36				
Date Stamp	29 Jun 2013 13:13:36			***File Name***	E:\ \ \ &MAss\RLB-FU-127\2\fid			***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	149	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10051.7734	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	25.732		

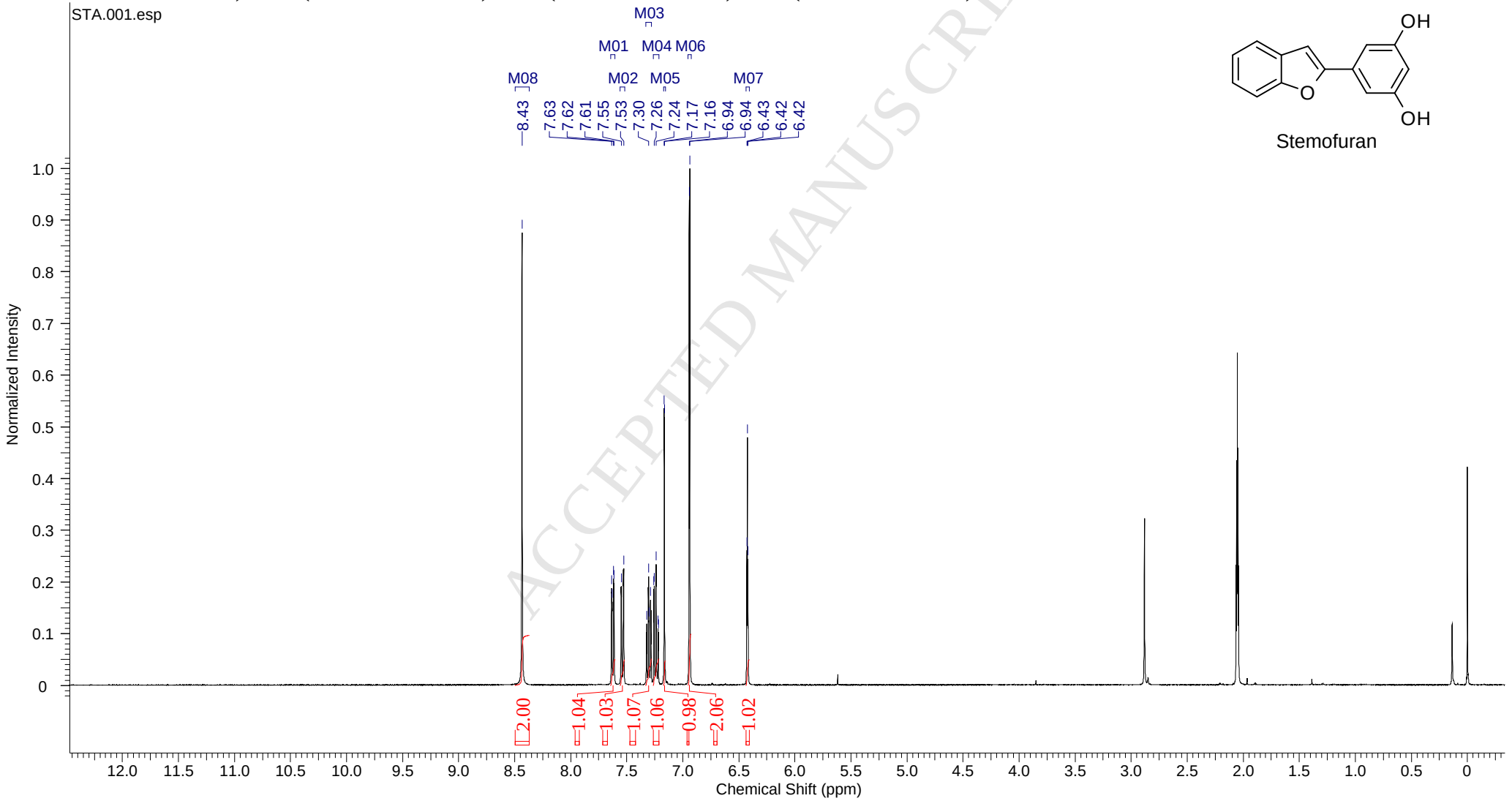
^{13}C NMR (100MHz ,CHLOROFORM-d) δ = 197.6, 160.7, 157.0, 138.8, 130.9, 128.3, 123.6, 120.6, 110.5, 106.2, 105.3, 55.5, 55.3, 40.0



14/10/2013 PM 7:42:27

Acquisition Time (sec)	3.9846	***Comment***				***Date***	14 Oct 2013 18:10:08		
Date Stamp	14 Oct 2013 18:10:08			***File Name***	C:\Users\libo_ruan\Desktop\STA\1\fid			***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	95.68	***SW(cyclical) (Hz)***	8223.68	***Solvent***	Acetone
Spectrum Offset (Hz)	2465.1306	***Spectrum Type***	STANDARD			***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	27.009

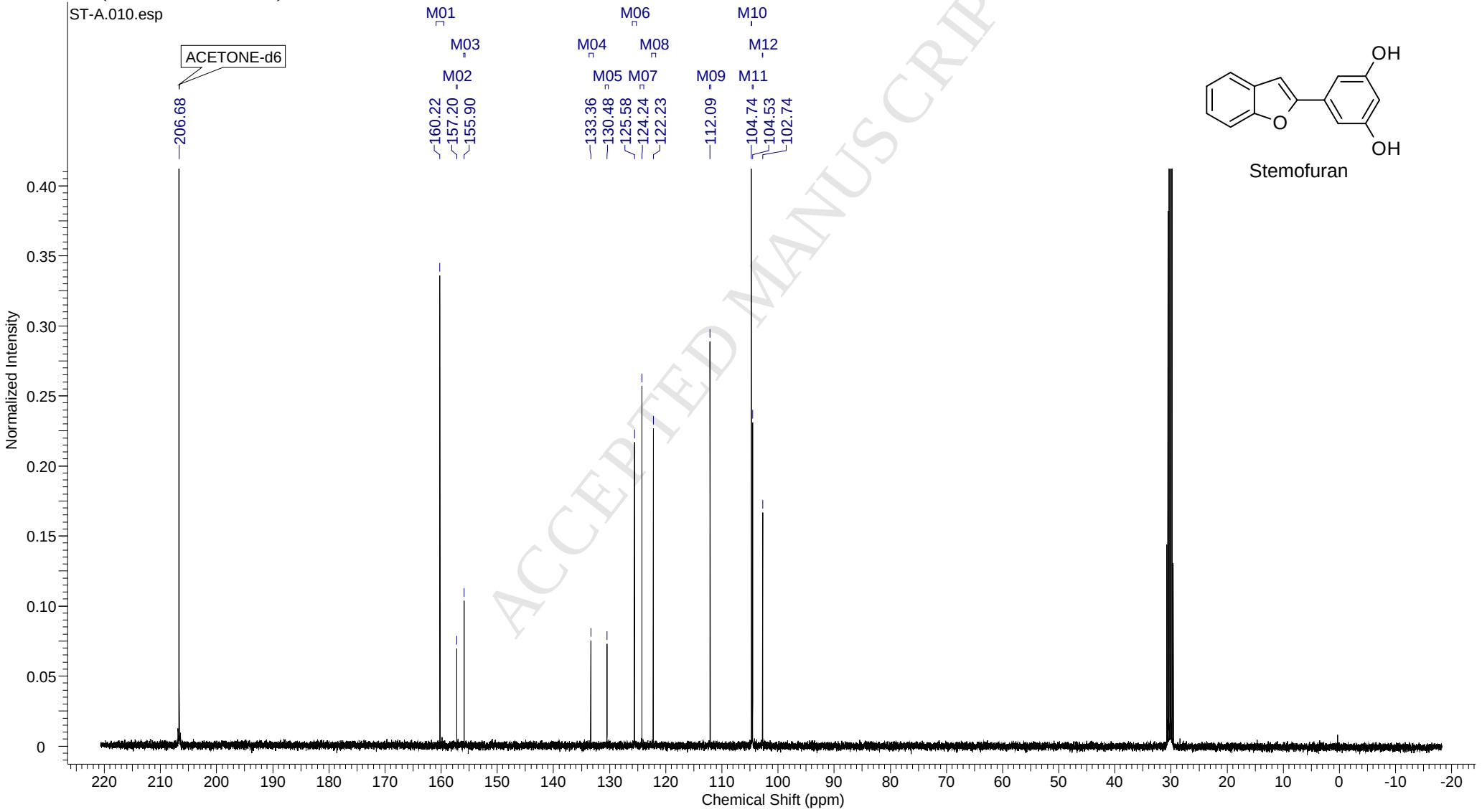
^{1}H NMR (400MHz ,Acetone) δ = 8.43 (s, 2 H), 7.63 (dd, *J* = 0.8, 8.3 Hz, 1 H), 7.54 (dd, *J* = 0.8, 8.3 Hz, 1 H), 7.30 (ddd, *J* = 1.4, 7.2, 8.3 Hz, 1 H), 7.24 (ddd, *J* = 1.4, 7.2, 8.3 Hz, 1 H), 7.16 (d, *J* = 1.0 Hz, 1 H), 6.94 (d, *J* = 2.0 Hz, 2 H), 6.42 (t, *J* = 2.0 Hz, 1 H)



14/10/2013 PM 8:21:23

Acquisition Time (sec)	1.3631	***Comment***		***Date***	14 Oct 2013 18:44:16			***Date Stamp***	14 Oct 2013 18:44:16
File Name	C:\Users\libo_ruan\Desktop\STA\ST-A\10\fid			***Frequency (MHz)***	100.61	***Nucleus***	13C	***Number of Transients***	256
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	Acetone	***Spectrum Offset (Hz)***	10182.0664	***Spectrum Type***	STANDARD
Sweep Width (Hz)	24037.73	***Temperature (degree C)***	26.990						

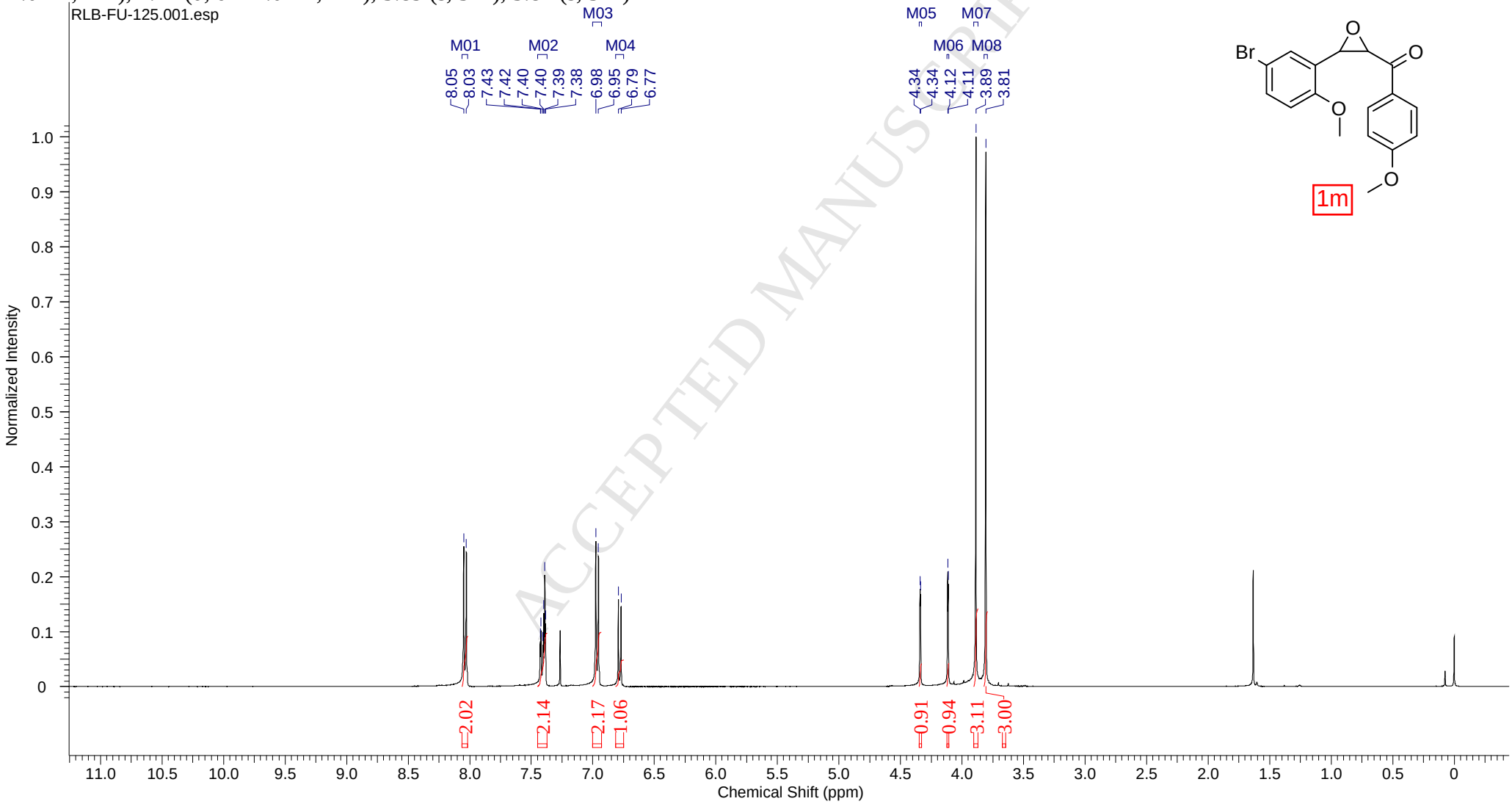
^{13}C NMR (101MHz ,Acetone) δ = 160.2, 157.2, 155.9, 133.4, 130.5, 125.6, 124.2, 122.2, 112.1, 104.7, 104.5, 102.7



29/6/2013 PM 3:36:31

Acquisition Time (sec)	3.9846	***Comment***				***Date***	29 Jun 2013 09:48:48		
Date Stamp	29 Jun 2013 09:48:48			***File Name***	E:\ \ \ &MAss\RLB-FU-125\1\fid			***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	76.85	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	2463.6064	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	24.793		

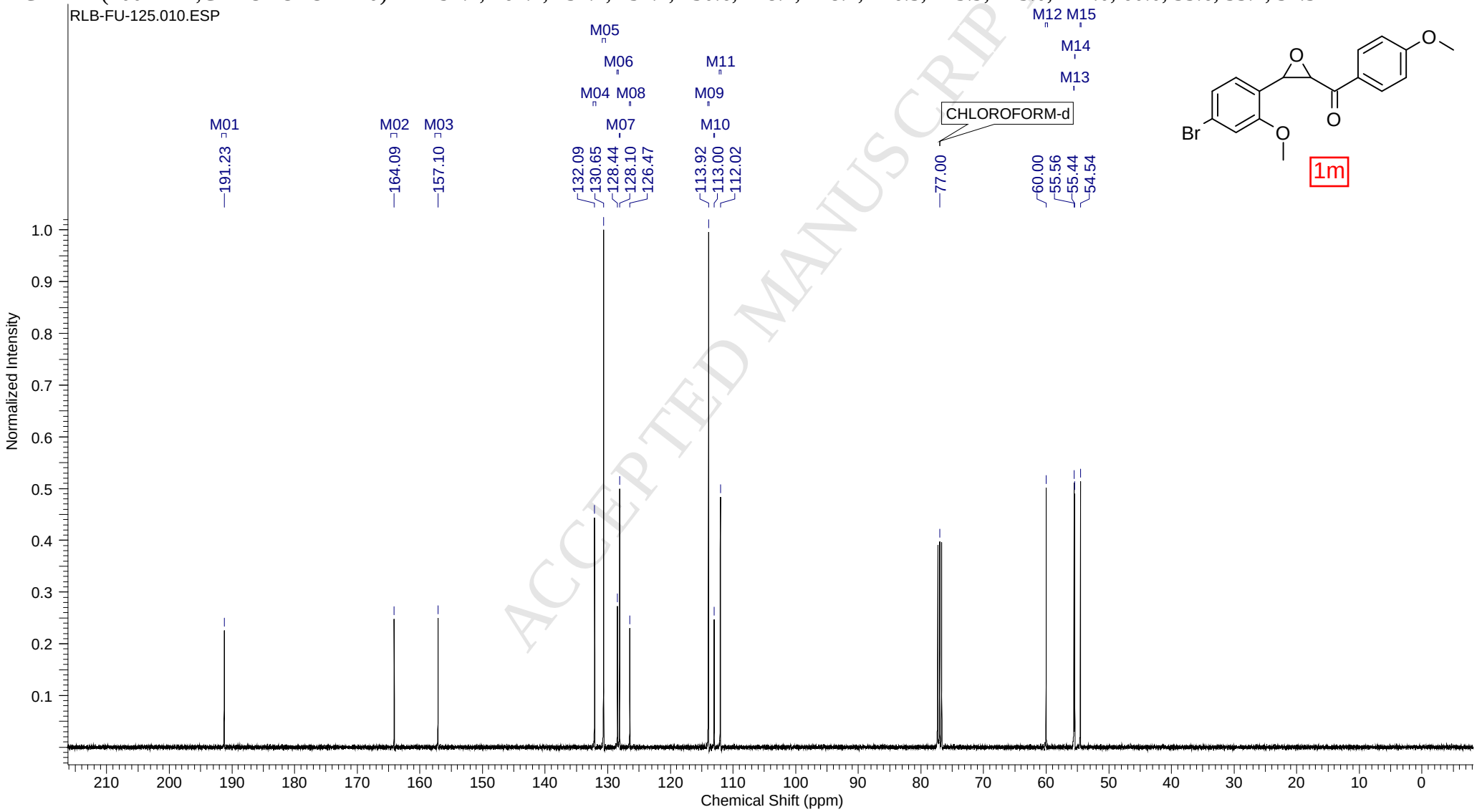
^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 8.04 (d, *J* = 8.8 Hz, 2 H), 7.45 - 7.37 (m, 2 H), 6.96 (d, *J* = 8.8 Hz, 2 H), 6.78 (d, *J* = 8.8 Hz, 1 H), 4.34 (d, *J* = 2.0 Hz, 1 H), 4.11 (d, *J* = 2.0 Hz, 1 H), 3.89 (s, 3 H), 3.81 (s, 3 H)



13/8/2013 PM 8:09:32

Acquisition Time (sec)	1.3631	***Comment***		***Date***	29 Jun 2013 10:18:40				
Date Stamp	29 Jun 2013 10:18:40			***File Name***	E:\ \ \ &MAss\RLB-FU-125\10\fid			***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	256	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10045.1719	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	25.257		

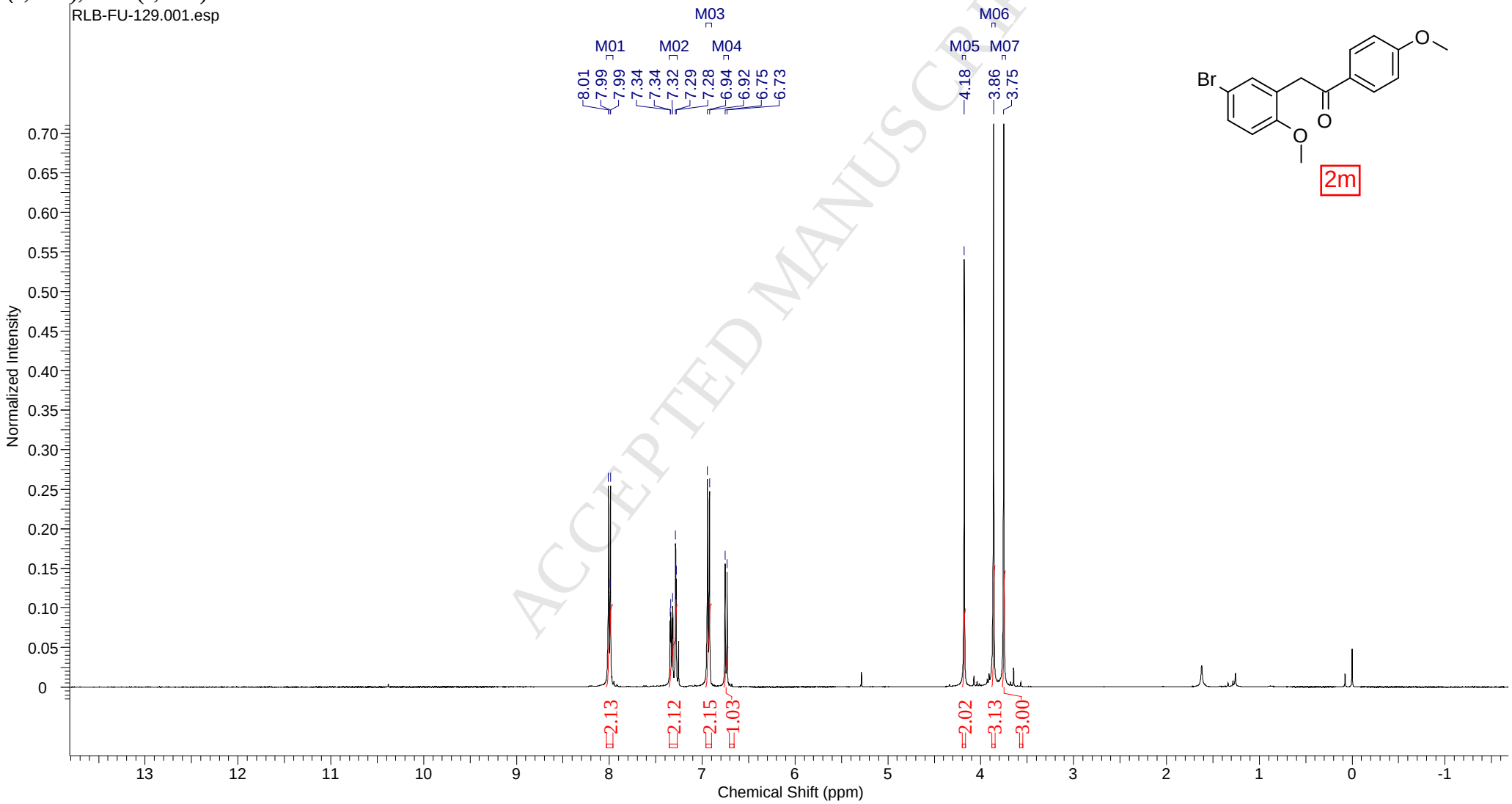
^{13}C NMR (100MHz ,CHLOROFORM-d) δ = 191.2, 164.1, 157.1, 132.1, 130.6, 128.4, 128.1, 126.5, 113.9, 113.0, 112.0, 60.0, 55.6, 55.4, 54.5



2/7/2013 PM 1:38:46

Acquisition Time (sec)	3.9846	***Comment***		***Date***	02 Jul 2013 12:16:00			***Date Stamp***	02 Jul 2013 12:16:00
File Name	E:\ \ \ &MAss\RLB-FU-129\1\fid			***Frequency (MHz)***	400.13	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	31.69	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2459.5967
Spectrum Type	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	27.387				

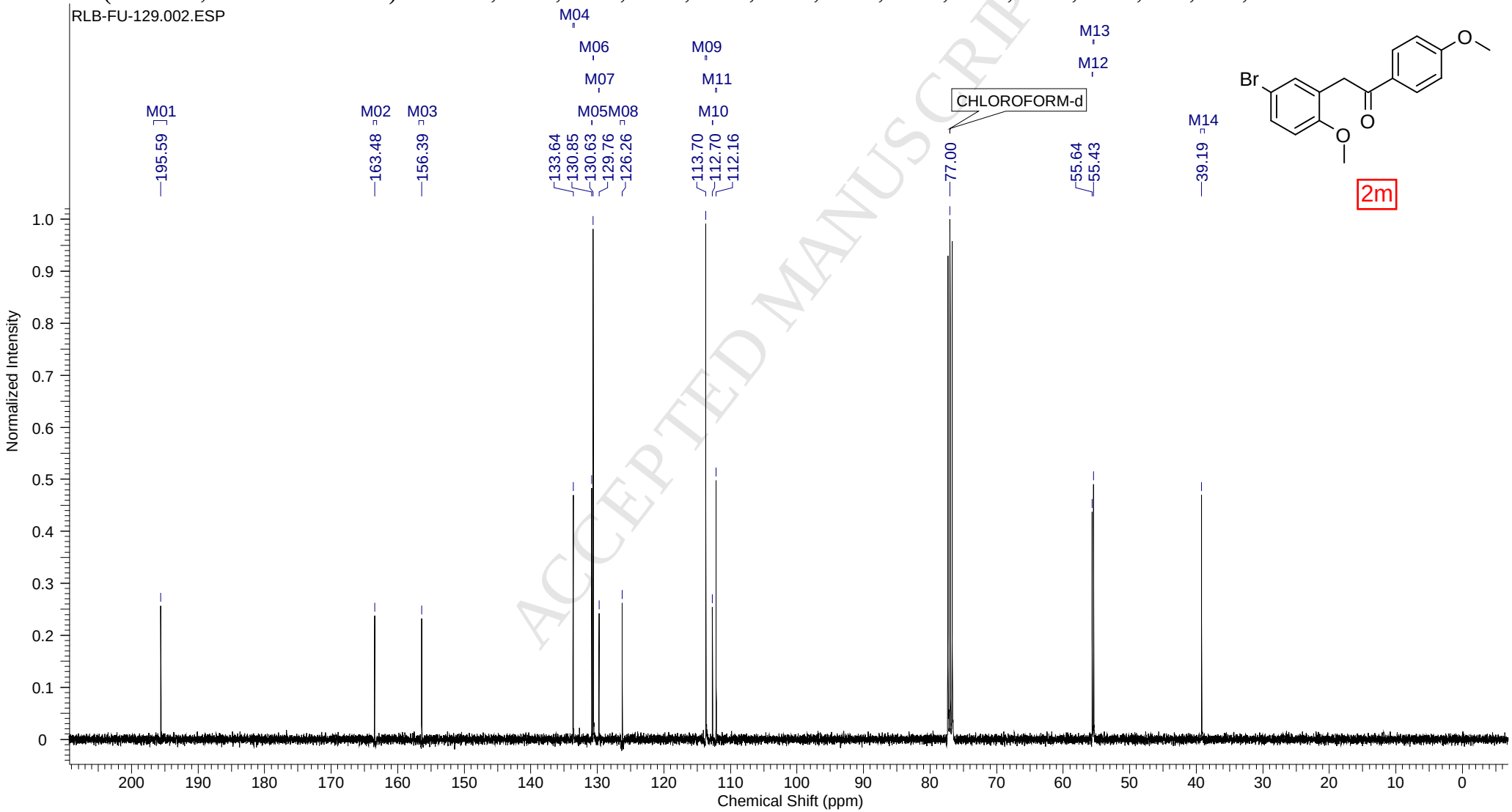
^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 8.03 - 7.96 (m, 2 H), 7.36 - 7.27 (m, 2 H), 6.93 (d, *J* = 8.5 Hz, 2 H), 6.74 (d, *J* = 8.5 Hz, 1 H), 4.18 (s, 2 H), 3.86 (s, 3 H), 3.75 (s, 3 H)



14/8/2013 PM 1:37:15

Acquisition Time (sec)	1.3631	***Comment***		***Date***	02 Jul 2013 12:33:04			***Date Stamp***	02 Jul 2013 12:33:04
File Name	E:\ \ \ &MAss\RLB-FU-129\2\fid			***Frequency (MHz)***	100.61	***Nucleus***	13C	***Number of Transients***	256
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10054.7080
Spectrum Type	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	27.699				

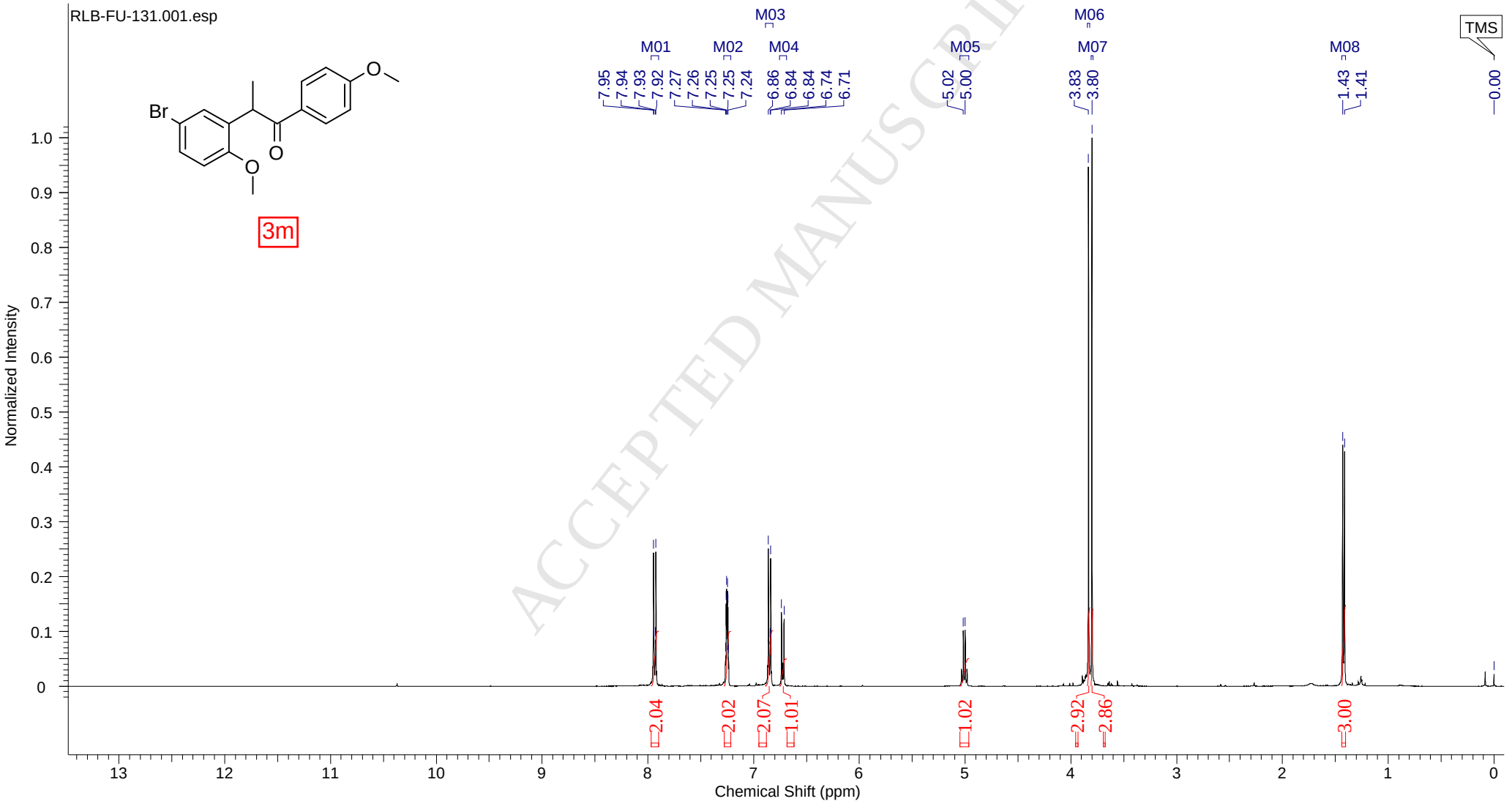
^{13}C NMR (100MHz ,CHLOROFORM-d) δ = 195.6, 163.5, 156.4, 133.6, 130.9, 130.6, 129.8, 126.3, 113.7, 112.7, 112.2, 55.6, 55.4, 39.2



4/7/2013 PM 2:08:02

Acquisition Time (sec)	3.9846	***Comment***				***Date***	03 Jul 2013 11:09:52		
Date Stamp	03 Jul 2013 11:09:52			***File Name***	E:\ \ \ &MAss\RLB-FU-131\1\fid			***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	31.69	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	2460.3542	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	27.727		

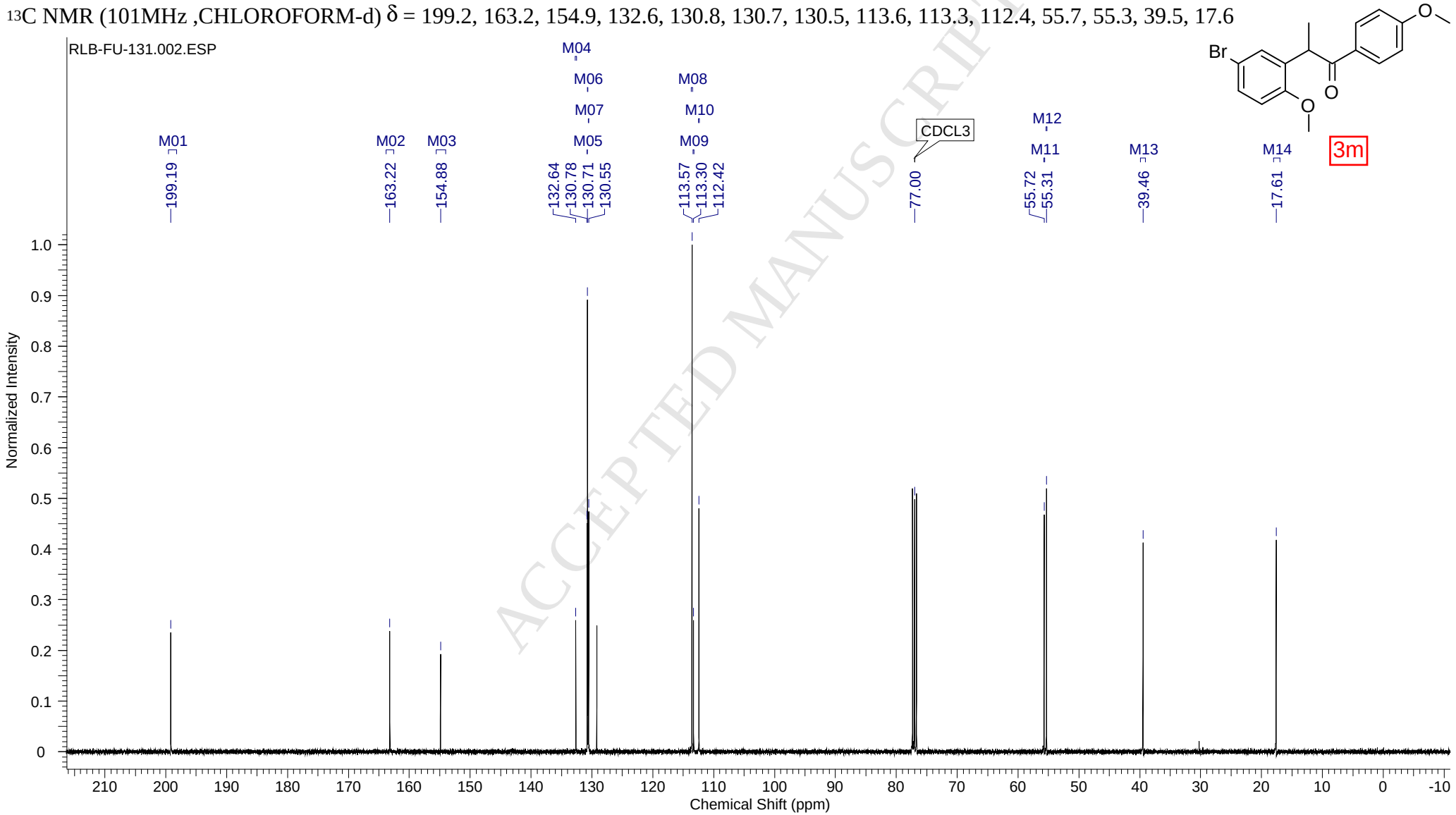
^{1}H NMR (400MHz ,CHLOROFORM-d) δ = 7.97 - 7.90 (m, 2 H), 7.28 - 7.22 (m, 2 H), 6.89 - 6.82 (m, 2 H), 6.72 (d, *J* = 9.3 Hz, 1 H), 5.01 (d, *J* = 6.8 Hz, 1 H), 3.83 (s, 3 H), 3.80 (s, 3 H), 1.42 (d, *J* = 6.8 Hz, 3 H)



13/8/2013 PM 8:04:38

Acquisition Time (sec)	1.3631	***Comment***		***Date***	03 Jul 2013 11:26:56			***Date Stamp***	03 Jul 2013 11:26:56
File Name	E:\ \ \ &MAss\RLB-FU-131\2\fid			***Frequency (MHz)***	100.61	***Nucleus***	13C	***Number of Transients***	256
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10051.7734
Spectrum Type	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	28.056				

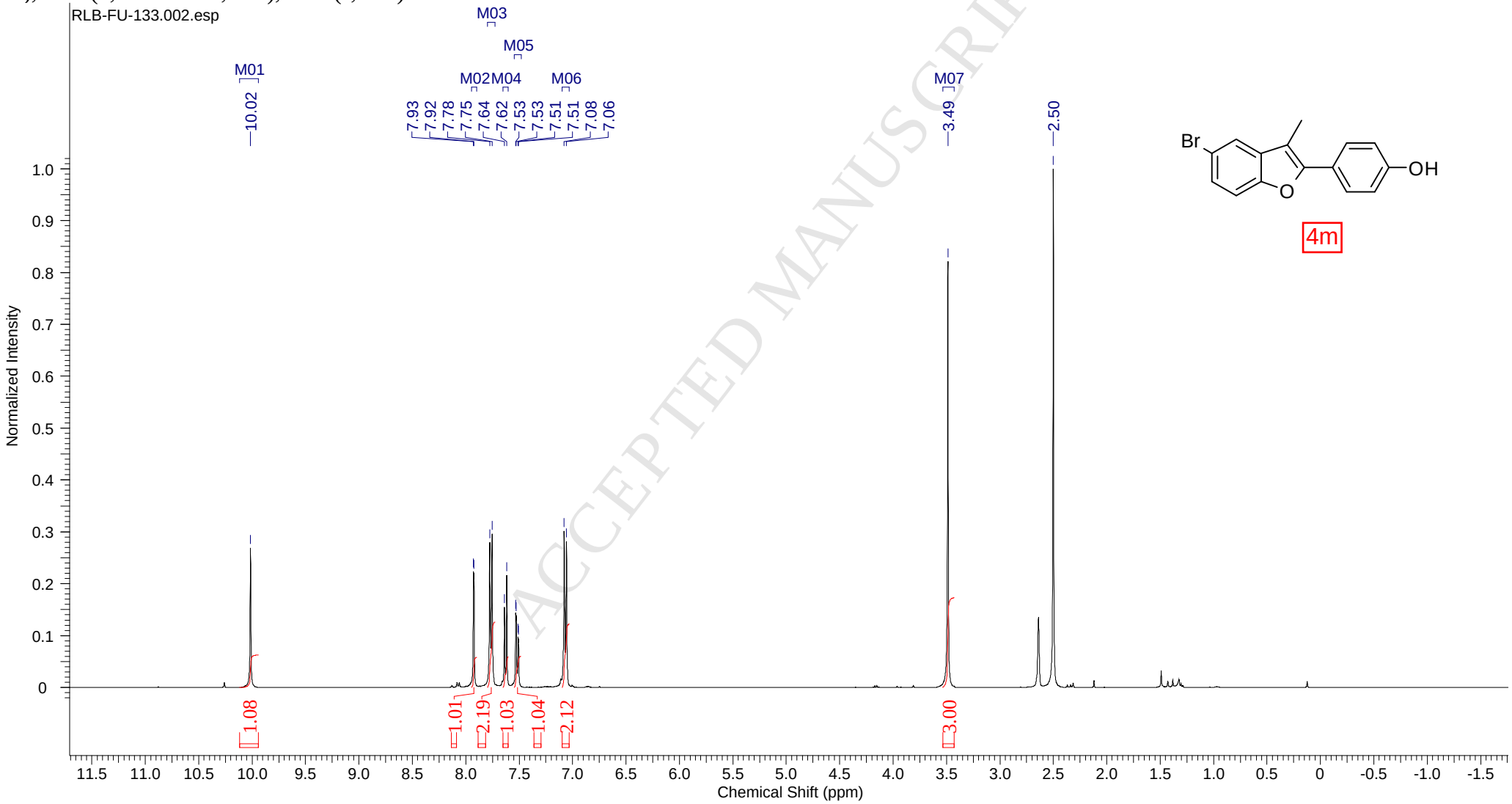
^{13}C NMR (101MHz ,CHLOROFORM-d) δ = 199.2, 163.2, 154.9, 132.6, 130.8, 130.7, 130.5, 113.6, 113.3, 112.4, 55.7, 55.3, 39.5, 17.6



14/8/2013 PM 2:16:24

Acquisition Time (sec)	3.9846	***Comment***				***Date***	04 Jul 2013 15:23:44		
Date Stamp	04 Jul 2013 15:23:44			***File Name***	E:\ \ \ &MAss\RLB-FU-133\2\fid			***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768	***Owner***	root
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	56.68	***SW(cyclical) (Hz)***	8223.68	***Solvent***	$DMSO\text{-}d_6$
Spectrum Offset (Hz)	623.2471	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	28.937		

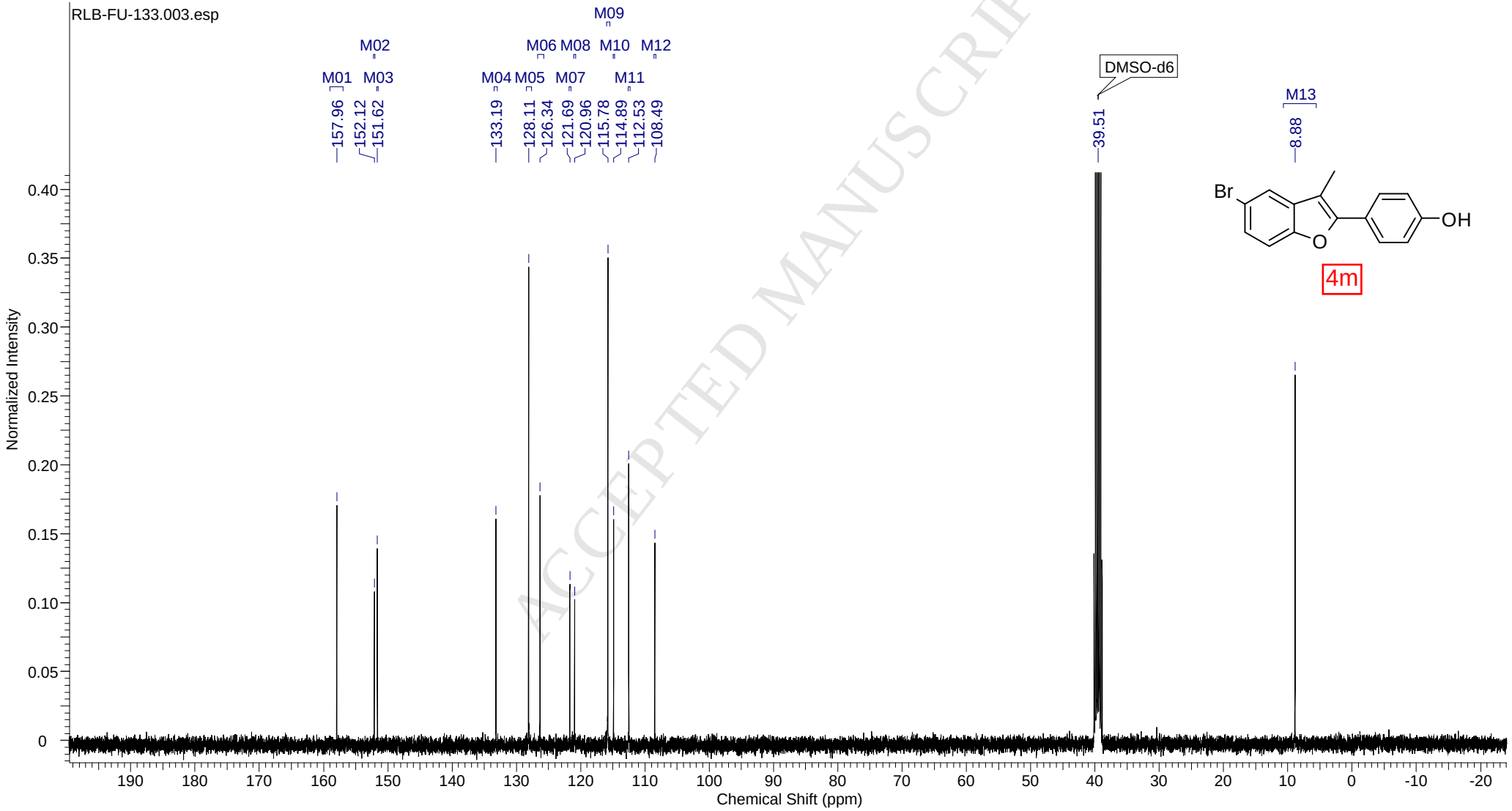
^{1}H NMR (400MHz ,DMSO-d_6) δ = 10.02 (s, 1 H), 7.93 (d, *J* = 1.5 Hz, 1 H), 7.76 (d, *J* = 8.5 Hz, 2 H), 7.63 (d, *J* = 8.5 Hz, 1 H), 7.52 (dd, *J* = 1.5, 8.5 Hz, 1 H), 7.07 (d, *J* = 8.5 Hz, 2 H), 3.49 (s, 3 H)



14/8/2013 PM 2:21:28

Acquisition Time (sec)	1.3631	***Comment***		***Date***	04 Jul 2013 15:38:40			***Date Stamp***	04 Jul 2013 15:38:40
File Name	E:\ \ \ &MAss\RLB-FU-133\3\fid			***Frequency (MHz)***	100.61	***Nucleus***	13C	***Number of Transients***	256
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	189.81	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	9531.0967
Spectrum Type	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	29.367				

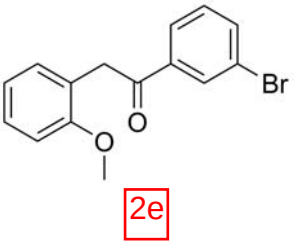
^{13}C NMR (100MHz ,CHLOROFORM-d) δ = 158.0, 152.1, 151.6, 133.2, 128.1, 126.3, 121.7, 121.0, 115.8, 114.9, 112.5, 108.5, 8.9



Elemental Composition Report

Single Mass Analysis

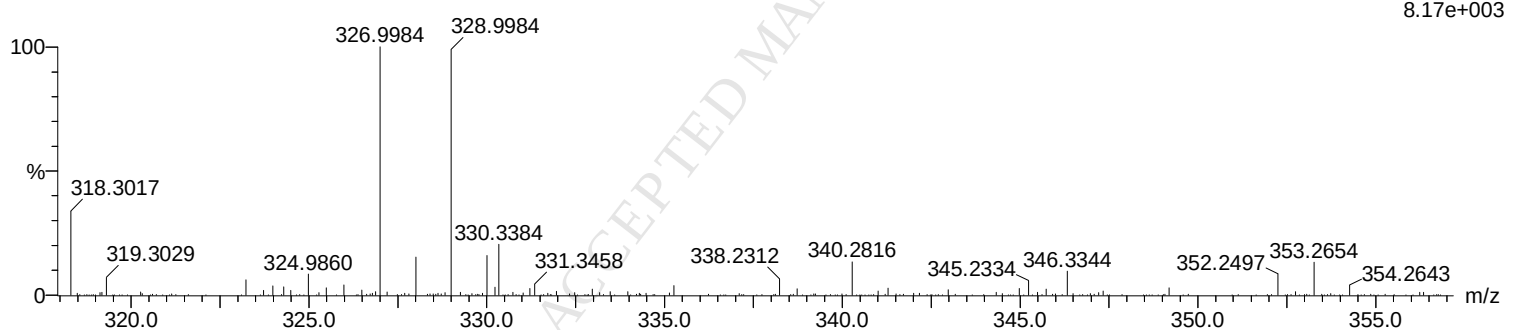
Tolerance = 500.0 mDa / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9



Monoisotopic Mass, Even Electron Ions
1 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 15-15 H: 8-15 O: 2-2 Na: 1-1 Br: 1-1

11:06:54
RLB-D-304 89 (3.928)

1: TOF MS ES+
8.17e+003

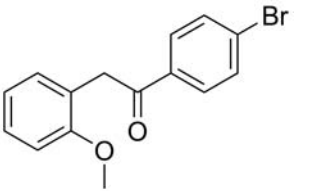


Minimum:				-1.5			
Maximum:		500.0	1000.0	500.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
326.9984	326.9997	-1.3	-4.0	8.5	392.3	0.0	C15 H13 O2 Na Br

Elemental Composition Report

Single Mass Analysis

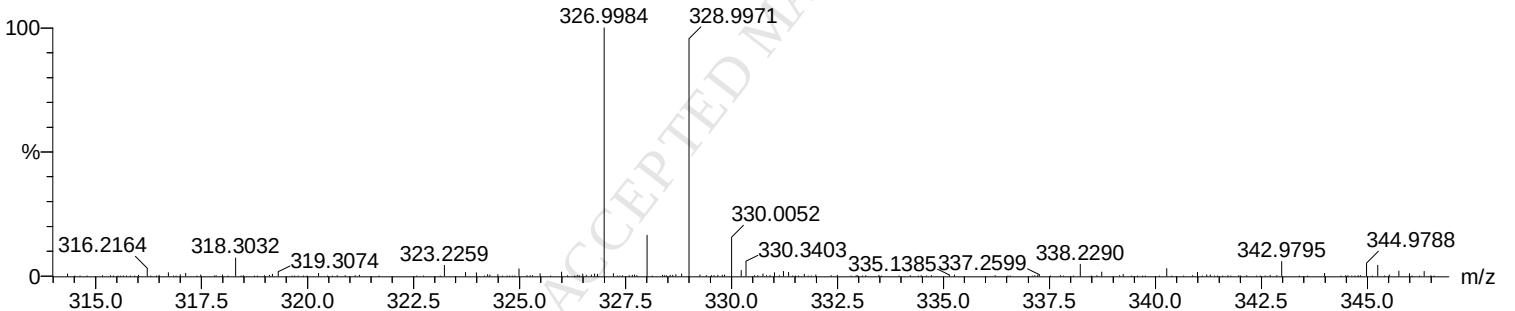
Tolerance = 500.0 mDa / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9



Monoisotopic Mass, Even Electron Ions
1 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 15-15 H: 8-15 O: 2-2 Na: 1-1 Br: 1-1

11:14:07
RLB-D-304-2 88 (3.874)

1: TOF MS ES+
1.74e+004

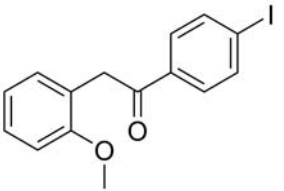


Minimum:				-1.5			
Maximum:		500.0	1000.0	500.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
326.9984	326.9997	-1.3	-4.0	8.5	398.5	0.0	C15 H13 O2 Na Br

Elemental Composition Report

Single Mass Analysis

Tolerance = 500.0 mDa / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

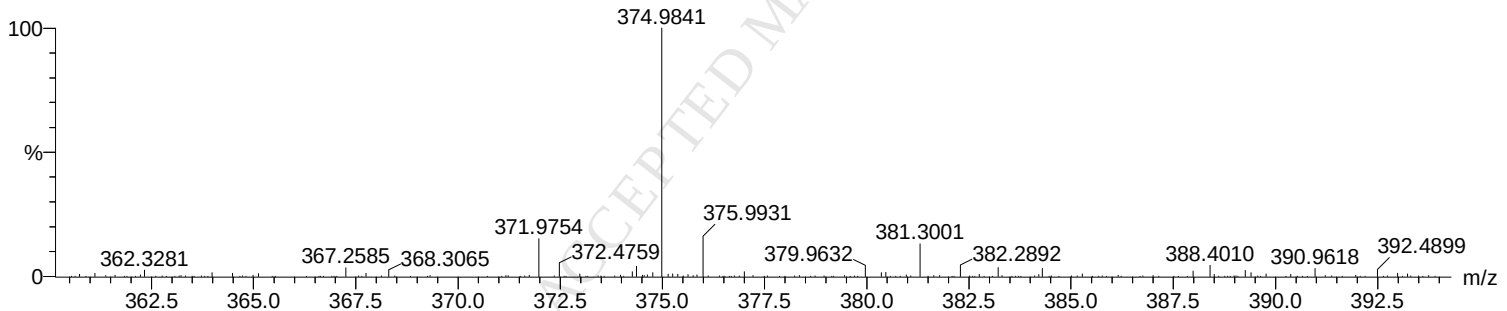


2g

Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 15-15 H: 8-15 O: 2-2 Na: 1-1 I: 0-1

11:20:12
RLB-D-352 39 (1.736)

1: TOF MS ES+
1.87e+004

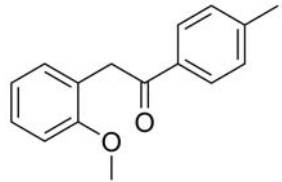


Minimum:				-1.5			
Maximum:		500.0	1000.0	500.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
374.9841	374.9858	-1.7	-4.5	8.5	362.4	0.0	C15 H13 O2 Na I

Elemental Composition Report

Single Mass Analysis

Tolerance = 500.0 mDa / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

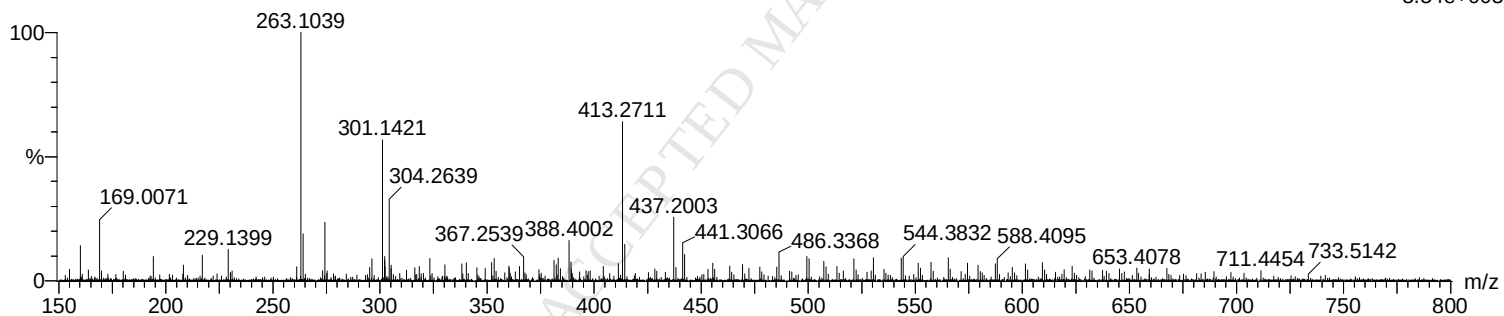


2h

Monoisotopic Mass, Even Electron Ions
1 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 15-16 H: 8-17 O: 2-2 Na: 1-1

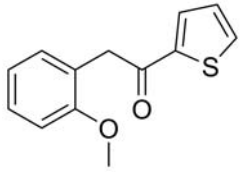
11:23:02
RLB-D-240 137 (6.032)

1: TOF MS ES+
5.54e+003



Minimum:				-1.5			
Maximum:		500.0	1000.0	500.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
263.1039	263.1048	-0.9	-3.4	8.5	345.1	0.0	C16 H16 O2 Na

Elemental Composition Report



2i

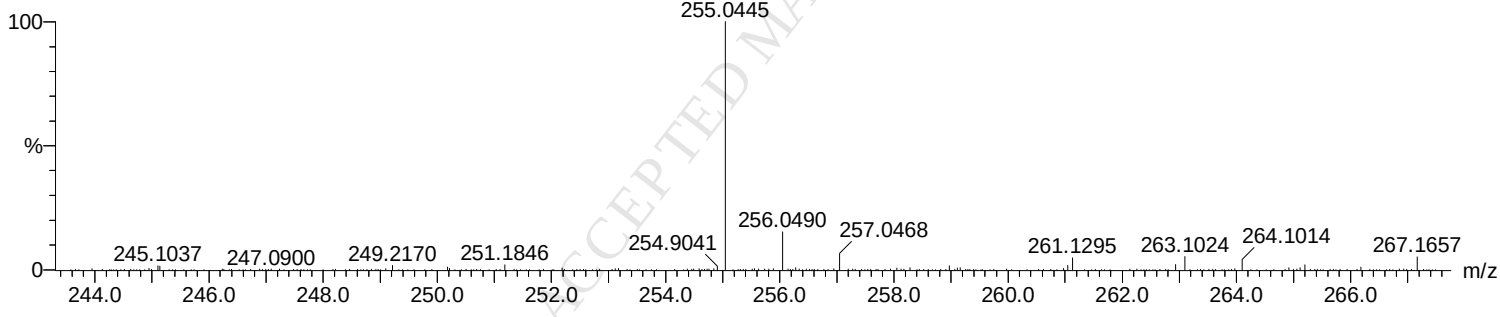
Single Mass Analysis

Tolerance = 500.0 mDa / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
1 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 13-16 H: 8-17 O: 2-2 Na: 1-1 S: 1-1

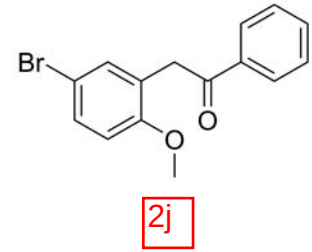
11:31:48
RLB-232 37 (1.648)

1: TOF MS ES+
4.64e+003



Minimum:				-1.5			
Maximum:		500.0	1000.0	500.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
255.0445	255.0456	-1.1	-4.3	7.5	382.5	0.0	C13 H12 O2 Na S

Elemental Composition Report



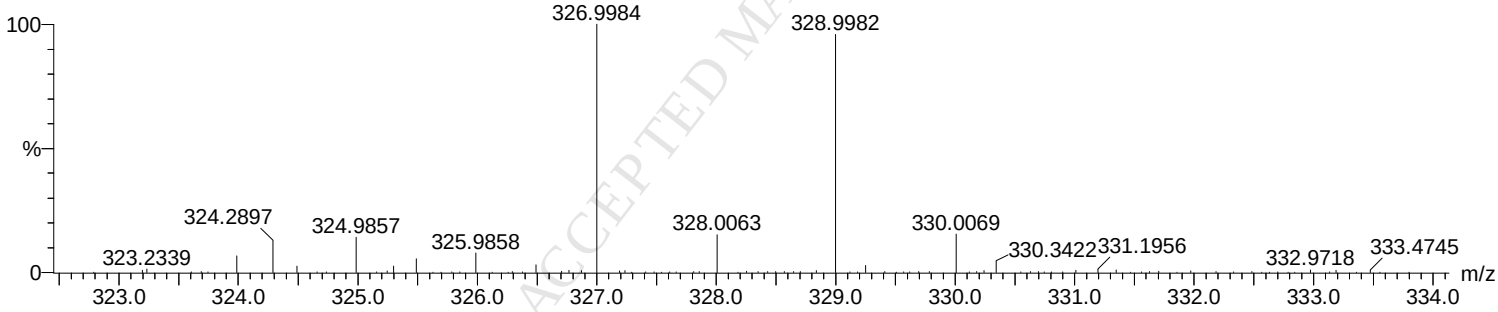
Single Mass Analysis

Tolerance = 500.0 mDa / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
1 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 13-16 H: 8-17 O: 2-2 Na: 1-1 Br: 1-1

12:49:28
RLB-304-4 30 (1.332)

1: TOF MS ES+
1.27e+004

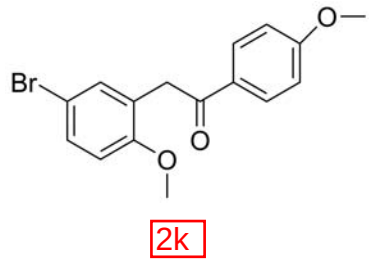


Minimum:				-1.5			
Maximum:		500.0	1000.0	500.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
326.9984	326.9997	-1.3	-4.0	8.5	408.4	0.0	C15 H13 O2 Na Br

Elemental Composition Report

Single Mass Analysis

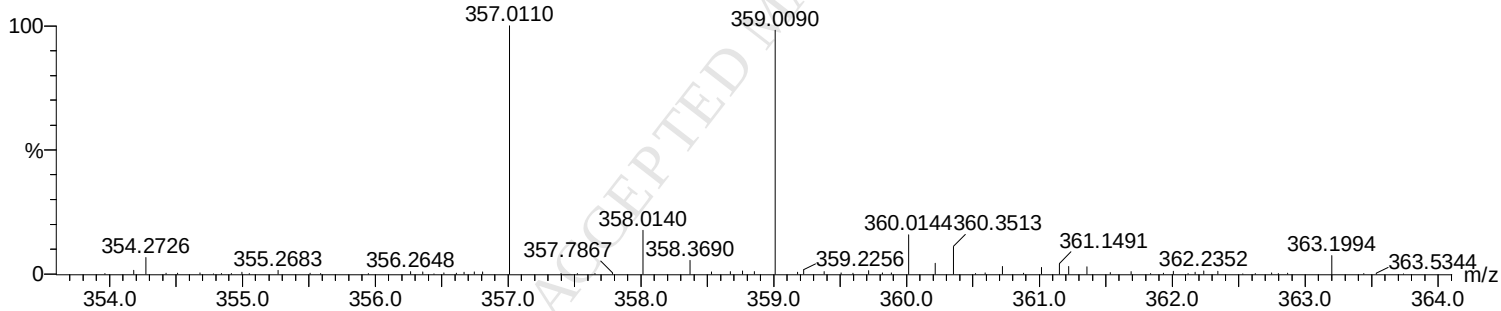
Tolerance = 500.0 mDa / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9



Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 13-16 H: 8-19 O: 3-3 Na: 1-1 Br: 1-1 I: 0-1

13:44:03
RLB-C-334 63 (2.788)

1: TOF MS ES+
3.58e+003

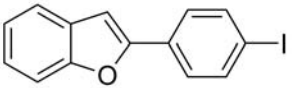


Minimum:				-1.5			
Maximum:		500.0	1000.0	500.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
357.0110	357.0102	0.8	2.2	8.5	278.3	0.0	C16 H15 O3 Na Br

Elemental Composition Report

Single Mass Analysis

Tolerance = 500.0 mDa / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

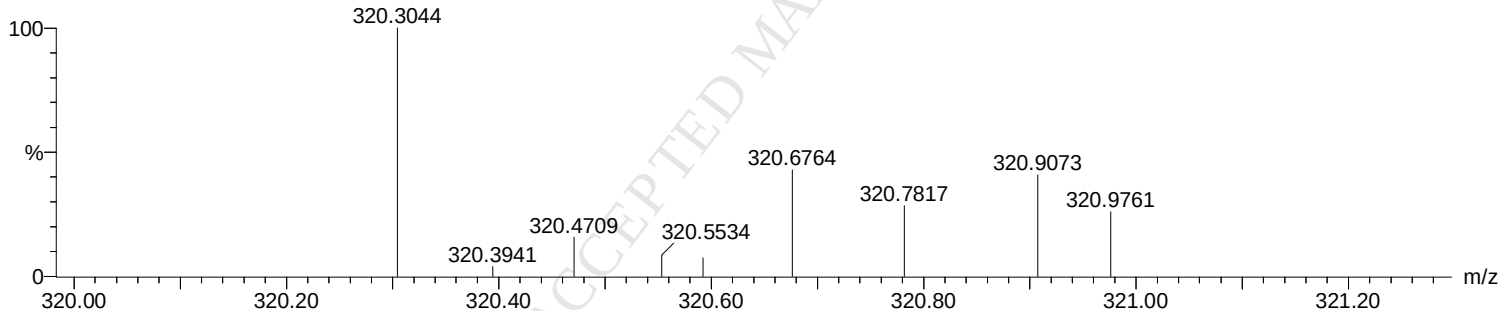


3g

Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 14-14 H: 9-10 O: 1-1 I: 0-1

10:36:39
RLB-320-0911 133 (5.856)

1: TOF MS ES+
1.39e+002

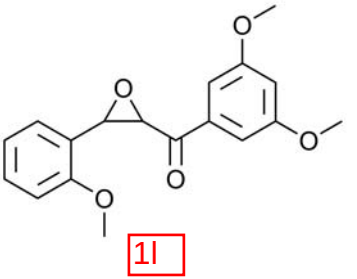


Minimum:				-1.5			
Maximum:		500.0	1000.0	500.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
320.9761	320.9776	-1.5	-4.7	9.5	23.0	0.0	C14 H10 O I

Elemental Composition Report

Single Mass Analysis

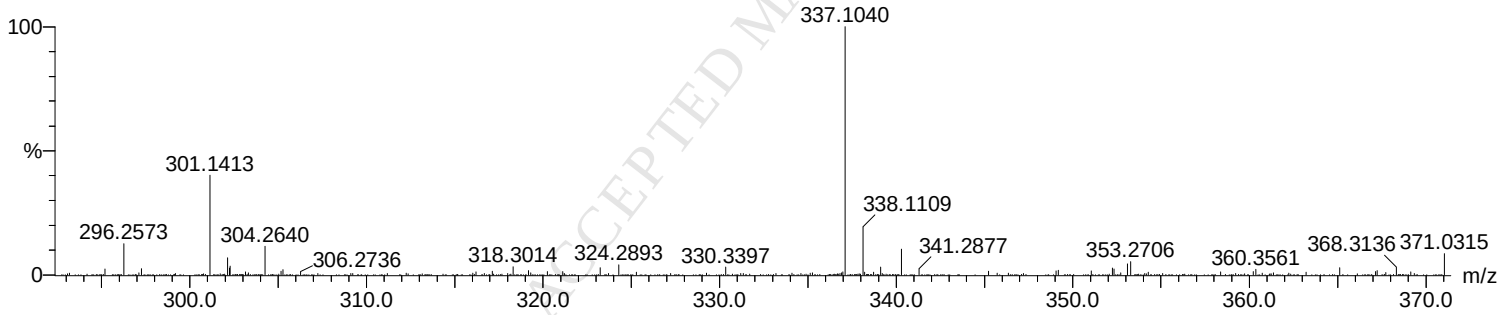
Tolerance = 500.0 mDa / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9



Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 13-18 H: 8-19 O: 4-5 Na: 1-1 I: 0-1

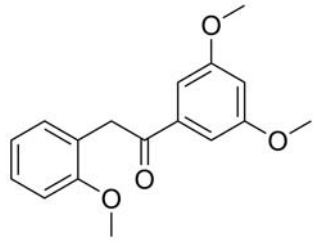
13:55:41
RLB-314 49 (2.174)

1: TOF MS ES+
1.34e+004



Minimum:				-1.5			
Maximum:		500.0	1000.0	500.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
337.1040	337.1052	-1.2	-3.6	9.5	338.3	0.0	C18 H18 O5 Na

Elemental Composition Report



2l

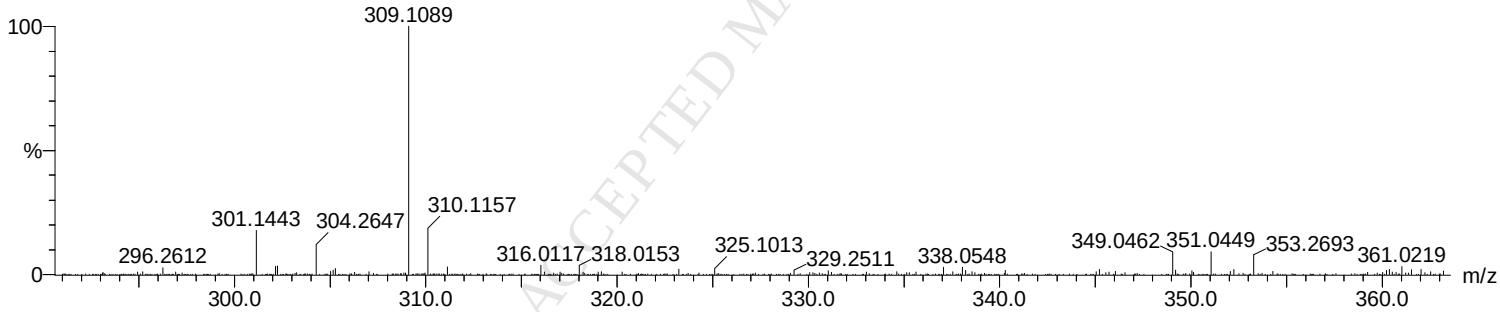
Single Mass Analysis

Tolerance = 500.0 mDa / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 13-17 H: 8-19 O: 4-4 Na: 1-1 I: 0-1

13:19:52
RLB-348 102 (4.488)

1: TOF MS ES+
1.23e+004

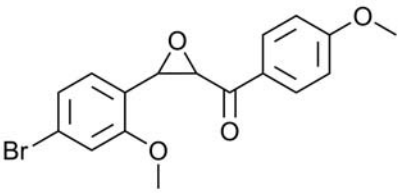


Minimum:				-1.5			
Maximum:		500.0	1000.0	500.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
309.1089	309.1103	-1.4	-4.5	8.5	344.3	0.0	C17 H18 O4 Na

Elemental Composition Report

Single Mass Analysis

Tolerance = 500.0 mDa / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

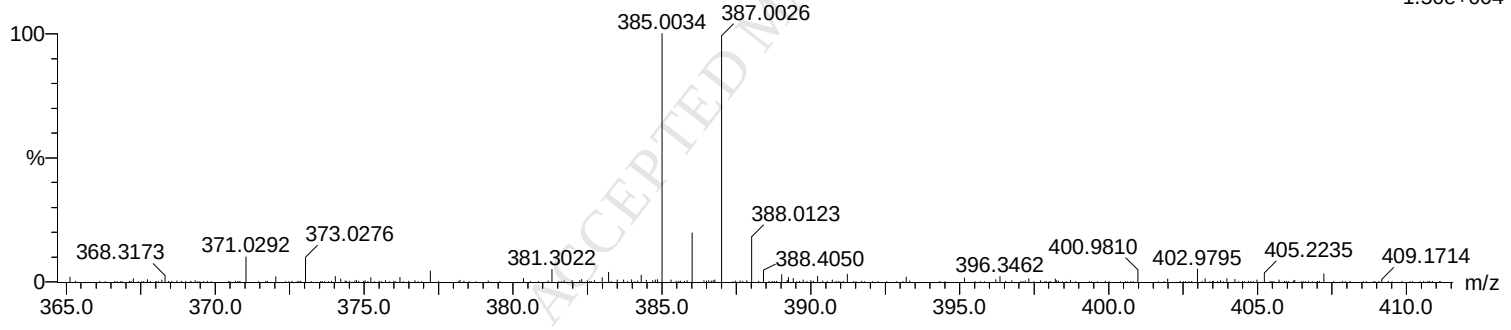


1m

Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 13-17 H: 8-19 O: 4-4 Na: 1-1 Br: 1-1 I: 0-1

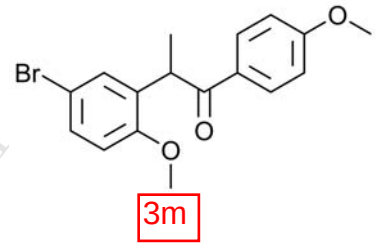
13:51:01
RLB-362 67 (2.963)

1: TOF MS ES+
1.50e+004



Minimum:				-1.5			
Maximum:		500.0	1000.0	500.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
385.0034	385.0051	-1.7	-4.4	9.5	359.3	0.0	C17 H15 O4 Na Br

Elemental Composition Report



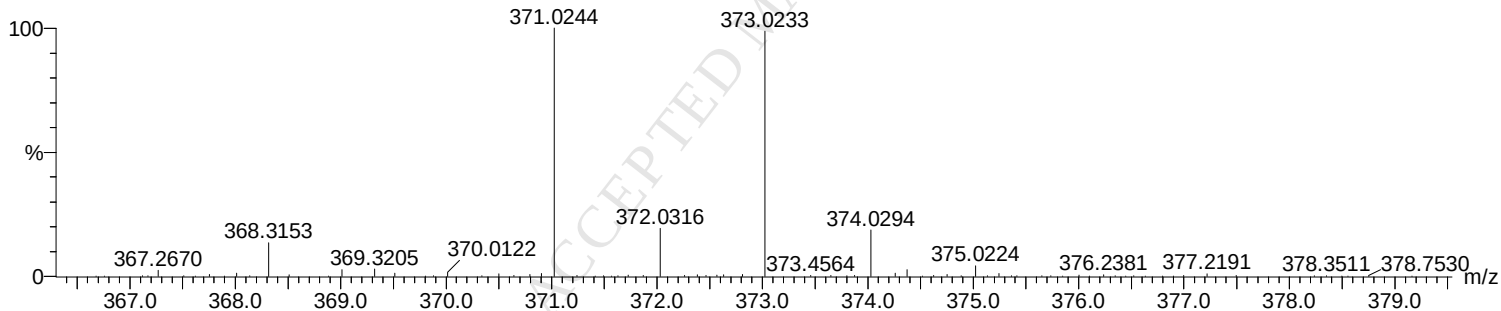
Single Mass Analysis

Tolerance = 500.0 mDa / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 13-17 H: 8-19 O: 3-3 Na: 1-1 Br: 1-1 I: 0-1

13:38:08
RLB-348 32 (1.419)

1: TOF MS ES+
1.27e+004



Minimum:				-1.5			
Maximum:		500.0	1000.0	500.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
371.0244	371.0259	-1.5	-4.0	8.5	312.4	0.0	C17 H17 O3 Na Br