Supporting Information

For

Efficient Chiral Monophosphorus Ligands for Asymmetric Suzuki-Miyaura Coupling Reactions

Wenjun Tang,*,[†] Nitinchandra D. Patel,[‡] Guangqing Xu,[†] Xiaobing Xu,[†] Jolaine Savoie,[‡] Shengli Ma,[‡] Ming-Hong Hao,[‡] Santosh Keshipeddy,[‡] Andrew G. Capacci,[‡] Xudong Wei,[‡] Yongda Zhang,[‡] Joe J. Gao,[‡] Wenjie Li,[‡] Sonia Rodriguez,[‡] Bruce Z. Lu,[‡] Nathan K. Yee,[‡] and Chris H. Senanayake[‡]

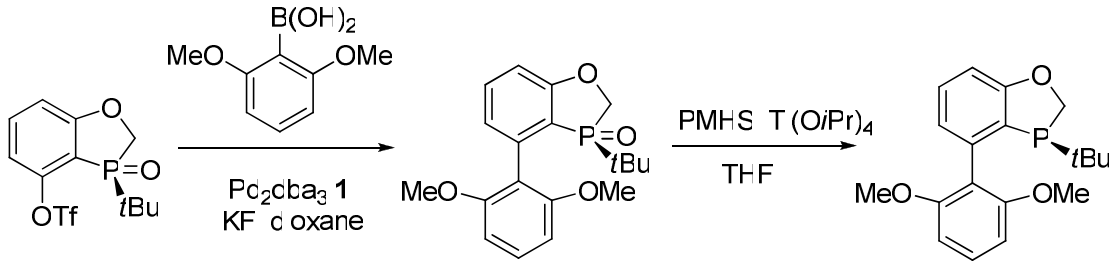
State Key Laboratory of Bio-Organic and Natural Products Chemistry, Shanghai Institute of Organic Chemistry,345 Ling Ling Road, Shanghai 200032,China, and Chemical Development, Boehringer Ingelheim Pharmaceuticals Inc., Ridgefield, CT06877, USA

1. General Methods. All reactions were carried out under a nitrogen atomosphere unless otherwise specified. THF (<0.02% water content), CH_2Cl_2, hexane, *n*-butanol, dioxane and toluene were purchased from J. T. Baker and used directly without further purifications. Commercialized reagents were used without further purifications. Chiral triflate **2** were prepared according to our reported procedure.[1] Tf = trifluoromethylsulfonate, dba = dibenzylideneacetone, Cy = cyclohexyl, S-Phos = 2-dicylohexylphosphino-2',6'-dimethoxybiphenyl, PMHS = polymethylhydrosiloxane,

^1H, ^{31}P and ^{13}C NMR data were recorded on a Bruker-Biospin DRX500 or DRX400 NMR Spectrometer with $CDCl_3$ or CD_2Cl_2 as the solvent. ^1H shifts were referenced to $CDCl_3$ at 7.26 ppm and CD_2Cl_2 at 5.32 ppm. ^{31}P shifts were referenced to 85% H_3PO_4 in D_2O at 0.0 ppm as external standard and obtained with ^1H decoupling. ^{13}C shifts were referenced to $CDCl_3$ at 77 ppm and CD_2Cl_2 at 54 ppm and obtained with 1H decoupling. MS was measured on Agilent 1100 Series LC/MSD mass spectrometer. Chiral HPLC analyses wee performed on a Hewlett-Packard 1100 system using a Chiralcel OD-H or Chiralpak AD-H column. Racemic compounds were prepared by reaction using S-Phos or racemic BI-DIME[2] as the ligand at 65 °C. The optical rotations were recorded on a Rudolph Research Automatic Polarimeter.

2. Synthetic procedures for ligand 1a-d

a. Synthesis of ligand 1 ((*S*)-BI-DIME)

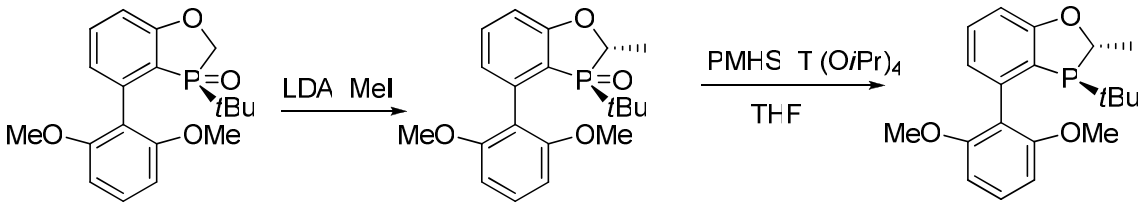


The synthesis of ligand **1** ((*S*)-BI-DIME) was carried out from chiral triflate[1] **a** through a Suzuki coupling with 2,6-dimethoxyphenylboronic acid to form **b** followed by a stereospecific reduction of the phosphane oxide **b** mediated by PMHS/$Ti(OiPr)_4$. The synthetic procedures were similar to those for racemic BI-DIME published in our previous paper.[2]

Phosphane oxide **b**: white solid; >99% ee; $[\alpha]_D^{20}$ = -66.4° (c = 0.64, $CHCl_3$); Chiral HPLC conditions: Chiralcel AD-H, heptane/*n*-propanol = 90:10, 1 mL/min, 25 °C, 4.93 min (*S*-enantiomer), 10.22 min (*R*-enantiomer, **b**).

1 ((*S*)-BI-DIME): white solid; >99% ee; $[\alpha]_D^{20}$ = -175.3° (c = 0.3, $CHCl_3$); The enantiomeric excess was determined by converting to its phosphine oxide via stereospecific oxidation with H_2O_2 as the oxidant.

b. Synthesis of ligand 2

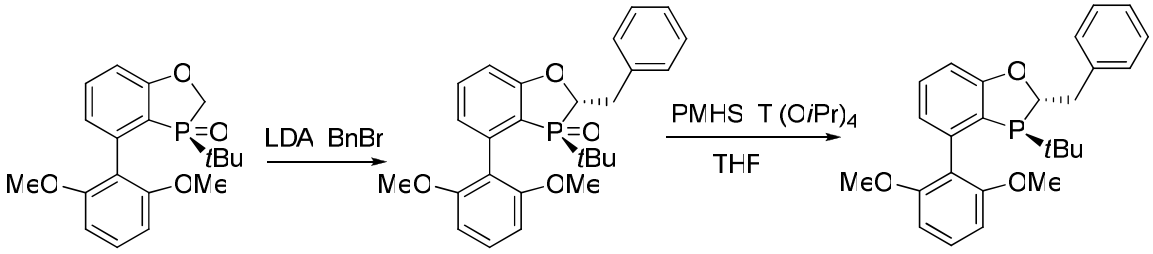


b **c** **2**

The synthesis of ligand **2** was carried out from chiral phosphane oxide **b** through methylation to form **c** followed by a stereospecific reduction of the phosphane oxide **c** under conditions of PMHS/Ti(O*i*Pr)$_4$. The synthetic procedures were similar to those for its racemic form published in our previous paper.[3] The relative configuration between P chirality and C chirality was determined by NOE experiments.

Phosphane oxide **c**: white solid; $[\alpha]_D^{20}$ = -12.8^o (c = 0.53, $CHCl_3$).
Phosphane **2**: white solid; $[\alpha]_D^{20}$ = -121.6^o (c = 0.55, $CHCl_3$).

c: Synthesis of ligand 3



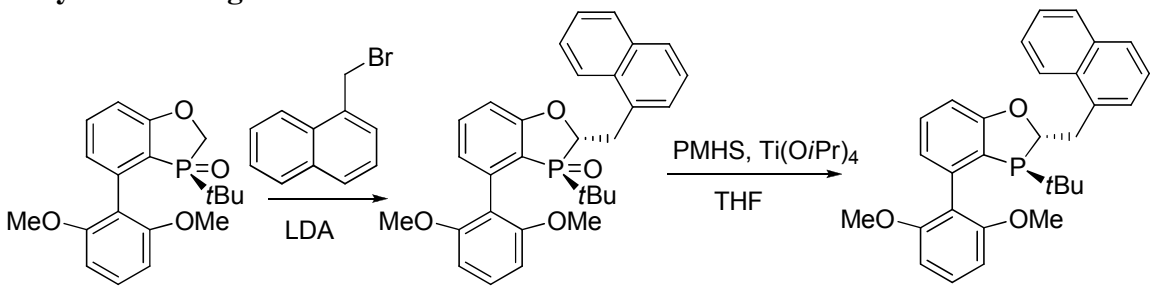
b **d** **3**

To a solution of (*R*)-3-*tert*-butyl-4-(2,6-dimethoxyphenyl)-2,3-dihydrobenzo[*d*][1,3]oxaphosphole oxide (**b**, 5.0 g, 14.4 mmol) in THF (50 mL) at -70 ^{o}C was charged LDA (9.6 mL, 1.8 M, 17.3 mmol, 1.2 equiv) over 5 min. The mixture was kept at -70 ^{o}C for 1 h. To the mixture was charged BnBr (2.96 g, 17.3 mmol, 1.2 equiv) over 5 min while controlling the reaction temperature below -60 ^{o}C. The resulting mixture was stirred at -70 ^{o}C for additional 1 h and then allowed to warm to rt over 2 h. Water (50 mL) and dichloromethane (50 mL) was charged. The dichloromethane layer was separated, washed with brine (50 mL), dried over sodium sulfate, and concentrated. The residue was purified by silica gel column chromatography (eluent: hexane to EtOAc) to provide the desired product **d** as white solid (5.0 g, 11.5 mmol, 80% yield). **d**: $[\alpha]_D^{20}$ = +55.9^o (c = 0.42, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (t, *J* = 7.8 Hz, 1H), 7.20-7.40 (m, 6H), 6.90 (m, 2H), 6.67 (d, *J* = 8.4 Hz, 1H), 6.57 (d, *J* = 8.3 Hz, 1H), 4.54 (m, 1H), 2.91 (s, 3H), 2.95 (s, 3H), 3.10-3.30 (m, 2H), 0.83 (d, *J* = 15.6 Hz, 9H); ^{31}P NMR (162 MHz, $CDCl_3$) δ 59.9; ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.5 (d, *J* = 18.6 Hz), 158.7, 157.3, 138.4 (d, *J* = 4.7 Hz), 138.3 (d, *J* = 9.4 Hz), 134.1 (d, *J* = 1.6 Hz), 129.8, 129.4,

128.5, 126.6, 124.9 (d, J = 8.3 Hz), 117.5, 114.5 (d, J = 89.9 Hz), 112.6 (d, J = 5.5 Hz), 104.5, 103.1, 75.0 (d, J = 60.4 Hz), 55.1, 56.4, 35.8, 33.3 (d, J = 70.8 Hz), 23.7; ESI-MS: m/z 437 $[M+H]^+$.

To a solution of (2*S*,3*R*)-2-benzyl-3-*tert*-butyl-4-(2,6-dimethoxyphenyl)-2,3-dihydrobenzo[d][1,3]oxaphosphole oxide (**d**, 3.0 g, 6.87 mmol, 1.0 equiv) in THF (30 mL) at rt was added PMHS (3 g) and $Ti(OiPr)_4$ (1.95 g, 6.87 mmol, 1.0 equiv). The mixture was stirred at reflux for 24 h and then distilled under reduced pressure to remove most THF. To the residue was charging carfully 30% NaOH solution (30 mL). Gas was generated during the addition. To the mixture at rt was charged Me-THF (30 mL). The resulting mixture was stirred at 60 ^oC for 0.5 h. The organic layer was separated and the most of the aqueous slurry was discarded. To the organic layer was charged water (30 mL). The aqueous layer was discarded. The organic layer was further washed with water (30 mL X2) and 5% NaCl solution (30 mL), and then concentrated at rt. The residue was purified by passing through a neutral alumina plug to provide **3** as white solid (2.5 g, 5.95 mmol, 87% yield). **3**: $[\alpha]_D^{20}$ = -16.2^o (c = 0.49, $CHCl_3$); ^1H NMR (500 MHz, $CDCl_3$) δ 7.10-7.30 (m, 7H), 6.79 (m, 2H), 6.56 (d, J = 8.4 Hz, 1H), 6.49 (d, J = 8.4 Hz, 1H), 4.87 (t, J = 7.7 Hz, 1H), 3.71 (s, 3H), 3.61 (s, 3H), 3.00 (m, 1H), 2.77 (m, 1H), 0.58 (d, J = 12.0 Hz, 9H); ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.84; ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.6, 157.8, 157.0, 138.8 (d, J = 17.2 Hz), 138.5 (d, J = 10.0 Hz), 130.6, 129.6, 129.5, 129.0, 128.3, 126.4, 124.2 (d, J = 14.9 Hz), 123.8 (d, J = 4.1 Hz), 119.6, 109.9, 104.4, 103.6, 84.2 (d, J = 26.4 Hz), 55.8 (d, J = 1.8 Hz), 53.4, 41.4 (d, J = 28.1 Hz), 31.0 (d, J = 18.4 Hz), 26.6 (d, d, J = 14.3 Hz); ESI-MS: m/z 421 $[M+H]^+$.

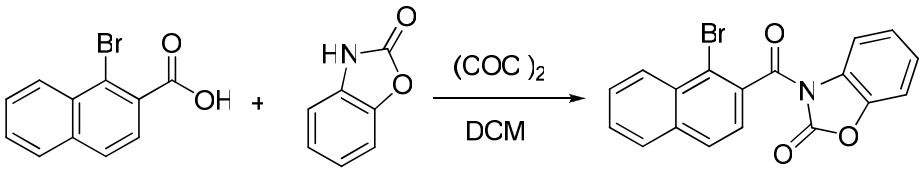
d: Synthesis of ligand 4



The synthesis of compound **e** from compound **b** was carried out following a procedure similar to the preparation of compound **d** for the synthesis of ligand **3**. **e**: 85% yield (white solid); $[\alpha]_D^{20}$ = +43.4^o (c = 0.35, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, J = 7.8 Hz, 1H), 7.89 (d, J = 7.7 Hz, 1H), 7.79 (d, J = 8.2 Hz, 1H), 7.40-7.60 (m, 5H), 7.32 (t, J = 8.2 Hz, 1H), 6.90 (m, 2H), 6.69 (d, J = 8.4 Hz, 1H), 6.58 (d, J = 8.4 Hz, 1H), 4.68 (m, 1H), 3.87 (s, 3H), 3.82 (m, 1H), 3.71 (s, 3H), 3.55 (m, 1H), 0.82 (d, J = 16.0 Hz, 9H); ^{31}P NMR (162 MHz, $CDCl_3$) δ 60.5; ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.5 (d, J = 18.8 Hz), 158.7, 157.4, 138.5 (d, J = 5.1 Hz), 134.2 (d, J = 1.5 Hz), 133.9, 131.9, 129.9, 128.9, 128.0, 127.5, 126.0, 125.6, 125.5, 125.0 (d, J = 8.3 Hz), 123.6, 117.4, 114.2 (d, J = 89.5 Hz), 112.7 (d, J = 5.5 Hz), 104.5, 103.0, 74.3 (d, J = 59.7 Hz), 56.1, 55.4, 35.4, 33.4 (d, J = 70.6 Hz), 23.6; ESI-MS: m/z 487 $[M+H]^+$.

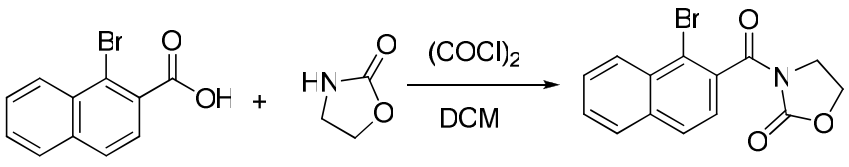
The synthesis of ligand **4** from compound **e** was carried out following a procedure similar to the preparation of ligand **3** from compound **d**. **4**: 83% yield (white solid); $[\alpha]_D^{20}$ = -28.6° (c = 0.29, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.1 Hz, 1H), 7.77 (d, *J* = 7.7 Hz, 1H), 7.67 (d, *J* = 7.4 Hz, 1H), 7.12-7.50 (m, 6H), 6.80 (m, 2H), 6.59 (d, *J* = 8.2 Hz, 1H), 6.50 (d, *J* = 8.4 Hz, 1H), 5.05 (t, *J* = 7.6 Hz, 1H), 3.76 (s, 3H), 3.62 (s, 3H), 3.45 (m, 1H), 3.25 (m, 1H), 0.55 (d, *J* = 12.0 Hz, 9H); ^{31}P NMR (162 MHz, $CDCl_3$) δ 7.5; ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.6, 157.8, 157.0, 138.8 (d, *J* = 17.0 Hz), 134.6 (d, *J* = 10.7 Hz), 133.9, 132.1, 130.6, 129.1, 128.9, 127.9 (d, *J* = 1.8 Hz), 127.3, 125.9, 125.4, 125.3, 123.8 (d, *J* = 4.1 Hz), 123.8, 119.6, 110.1, 104.4, 103.7, 83.5 (d, *J* = 26.2 Hz), 55.9 (d, *J* = 1.5 Hz), 55.4, 38.5 (d, *J* = 29.3 Hz), 31.0 (d, *J* = 18.4 Hz), 26.6 (d, *J* = 14.3 Hz); ESI-MS: m/z 471 $[M+H]^+$.

3. Procedures for substrate preparation



5d

To a suspension of 1-bromo-2-naphthoic acid (1.0g, 4.0 mmol) in DCM (10 mL) was charged DMF (14.5 mg, 0.2 mmol, 0.05 equiv) followed by slow addition of oxaly chloride (0.56 g, 4.38 mmol, 1.1 equiv). Gas was generated during the addition and the resulting mixture was stirred at rt for 1 h. In a separated flask was charged benzo[*d*]oxazol-2(3*H*)-one (0.54 g, 3.98 mmol, 1.0 equiv), triethylamine (1.21 g, 11.9 mmol, 3.0 equiv) and DCM (10 mL). To the mixture at rt was charged the aforementioned solution. The resulting mixture was stirred at rt overnight. Water (20 mL) was charged to quench the reaction. The DCM layer was separated, washed with water (25 mL X 2) and brine (25 mL), dried over sodium sulfate, concentrated and solvent-switched to EtOAc (10 mL). The slurry was heated to 55 °C for 10 min and then cooled to rt. Filtration of the slurry provided the desired product **5d** as yellow solid (1.2 g, 3.3 mmol, 82% yield). **5d**: ^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.39 (d, *J* = 8.3 Hz, 1H), 8.23 (m, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 8.00 (d, *J* = 7.9 Hz, 1H), 7.74 (m, 2H), 7.52 (d, *J* = 8.4 Hz, 1H), 7.41 (m, 2H), 7.35 (m, 1H); ^{13}C NMR (100 MHz, CD_2Cl_2) δ 167.2, 150.5, 143.2, 135.4, 134.4, 132.0, 129.2, 129.1, 128.9, 128.8, 128.0, 127.9, 126.4, 125.5, 124.2, 120.5, 116.1, 110.7; ESI-MS: m/z 390 $[M+Na]^+$.



5c

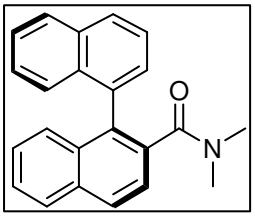
Preparation of **5c** was carried out according to a procedure similar to that for the synthesis of **5d**. **5c**: 85% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.5 Hz, 1H),

7.89 (d, J = 8.4 Hz, 1H), 7.86 (d, J = 8.1 Hz, 1H), 7.65 (m, 1H), 7.58 (m, 1H), 7.34 (d, J = 8.4 Hz, 1H), 4.53 (t, J = 7.8 Hz, 2H), 4.28 (t, J = 8.3 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.0, 152.1, 134.6, 134.1, 131.6, 128.4, 128.3, 128.2, 127.8, 127.5, 123.6, 119.8, 62.2, 42.5; ESI-MS: m/z 342 $[M+Na]^+$.

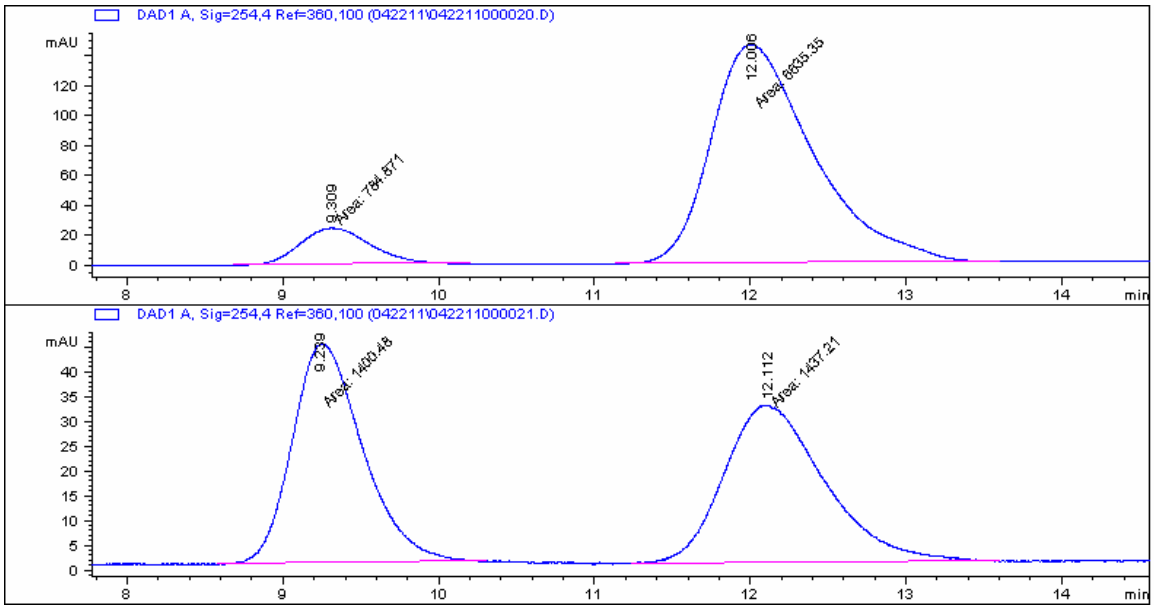
4. General procedure for asymmetric Suzuki-Miyaura couplings

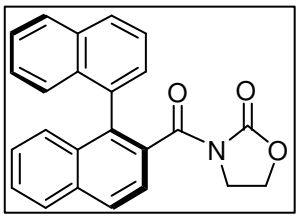
To a mixture of aryl bromide (1.0 mmol), arylboronic acid (2.0 mmol), potassium phosphate (3 mmol, 3 equiv), $Pd(OAc)_2$ (0.01-0.05 mmol), and ligand **2** or **4** (0.012-0.06 mmol, Pd/ligand ratio = 1/1.2) was charged dry THF (2 mL). The mixture was stirred at room temperature or 40 ^{o}C under nitrogen for 4-36 h and then quenched by addition of 10% citric acid solution (4 mL). EtOAc (4 mL) was added and the EtOAc layer was separated, washed sequentially with water (4 mL) and brine (4 mL), dried over sodium sulfate, concentrated, and purified by silica gel column chromatography to provide biaryl products. Their ee's were determined by chiral HPLC on a chiralcel OD-H or chiralpak AD-H column.

5. Analytical data of asymmetric Suzuki-Miyaura coupling products

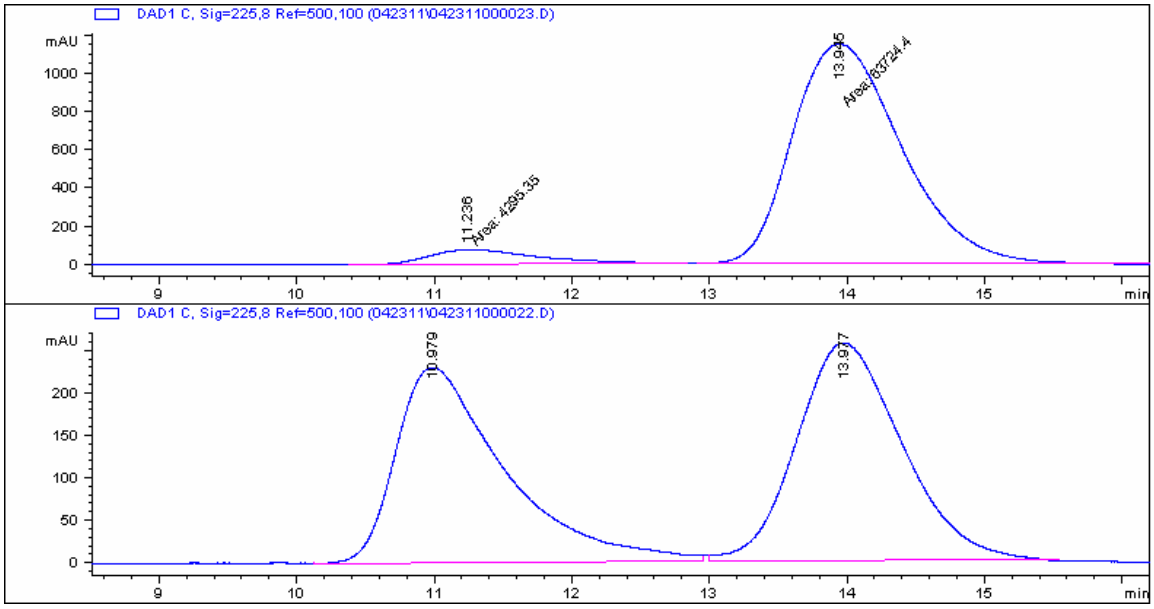


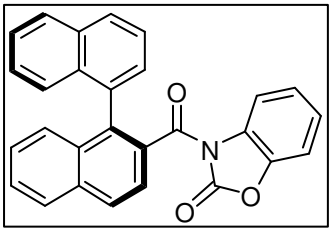
(*R*)-***N,N*-Dimethyl-1,1'-binaphthyl-2-carboxamide**: white solid (95% yield); 79% ee; $[\alpha]_D^{20}$ = +66.0^o (c = 0.80, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ8.02 (d, J = 7.3 Hz, 1H), 7.95 (br m, 3H), 7.40-7.75 (m, 5H), 7.29 (m, 4H), 2.20-3.10 (br m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.7, 135.1, 134.4, 133.4, 133.2, 132.8, 128.6, 128.4, 128.1, 127.1, 126.7, 126.4, 125.8, 123.8, 38.8, 34.3. ESI-MS: m/z 326 $[M+H]^+$. Chiral HPLC conditions: Chiralcel OD-H, 4.6 mm X 250 mm, 30 ^{o}C, flow rate: 2 mL/min, heptane/isopropanol: 96/4, 254 nm, 9.30 min (*S*), 12.00 min (*R*).



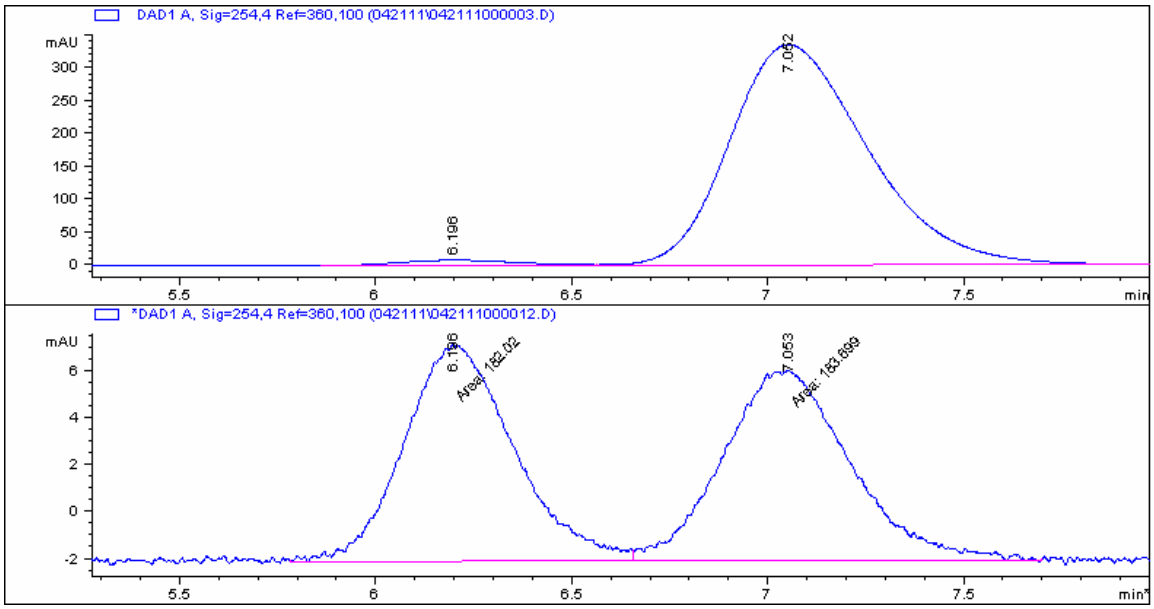


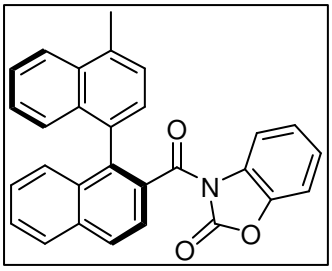
(*R*)-3-(1,1'-binaphthyl-2-carbonyl)oxazolidin-2-one: yellowish solid (96% yield). 87% ee; $[\alpha]_D^{20}$ = -61.6° (c = 0.55, $CHCl_3$); ^1H NMR (400 MHz, CD_2Cl_2) δ 8.10 (d, J = 8.4 Hz, 1H), 7.95-8.07 (m, 3H), 7.55-7.70 (m, 3H), 7.52 (m, 2H), 7.38 (m, 4H), 3.99 (m, 2H), 3.63 (m, 1H), 3.46 (m, 1H); ^{13}C NMR (100 MHz, CD_2Cl_2) δ 169.9, 153.2, 136.3, 135.6, 134.6, 133.9, 133.7, 133.2, 133.1, 129.0, 128.8, 128.7, 128.5, 127.7, 127.6, 127.4, 127.3, 126.7, 125.7, 124.1, 62.9, 43.0; ESI-MS: m/z 390 $[M+Na]^+$. Chiral HPLC conditions: Chiralcel OD-H, 4.6 mm X 250 mm, 30 °C, flow rate: 2 mL/min, heptane/isopropanol: 85/15, 225 nm, 11.00 min (*S*), 13.98 min (*R*).



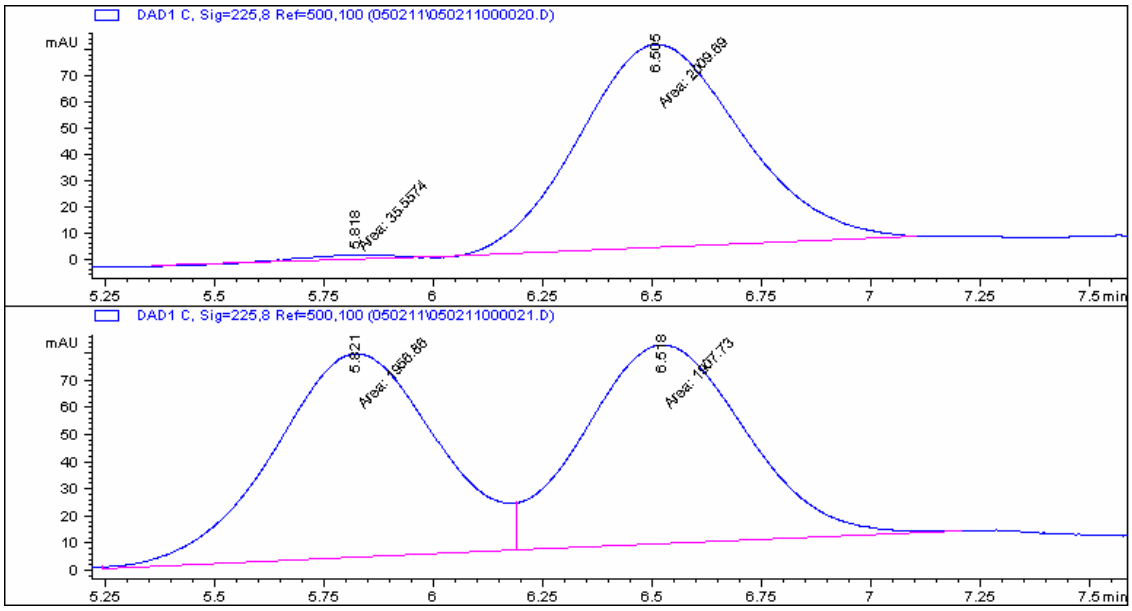


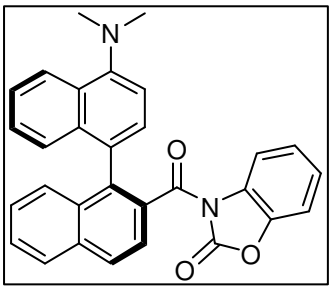
(*R*)-3-(1,1'-binaphthyl-2-carbonyl)benzo[d]oxazol-2(3*H*)-one: white solid (96% yield); 96% ee; $[\alpha]_D^{20}$ = -126.1° (c = 1.33, $CHCl_3$); ^1H NMR (400 MHz, CD_2Cl_2) δ 8.11 (d, J = 6.7 Hz, 1H), 8.04 (d, J = 6.4 Hz, 1H), 7.79 (m, 2H), 7.72 (d, J = 6.7 Hz, 1H), 7.60 (m, 1H), 7.25-7.50 (m, 8H), 7.14 (t, J = 6.0 Hz, 1H), 7.04 (m, 2H); ^{13}C NMR (100 MHz, CD_2Cl_2) δ 168.5, 151.0, 142.9, 137.7, 135.1, 135.0, 133.9, 133.3, 133.2, 132.8, 129.0, 128.9, 128.8, 128.7, 128.6, 128.2, 128.0, 127.9, 127.6, 127.0, 126.8, 126.6, 125.6, 125.5, 124.9, 124.1, 114.8, 110.1. ESI-MS: m/z 438 $[M+Na]^+$; Chiral HPLC conditions: Chiralcel OD-H, 4.6 mm X 250 mm, 30 °C, flow rate: 2 mL/min, heptane/isopropanol: 96/4, 254 nm, 6.19 min (*S*), 7.05 min (*R*).



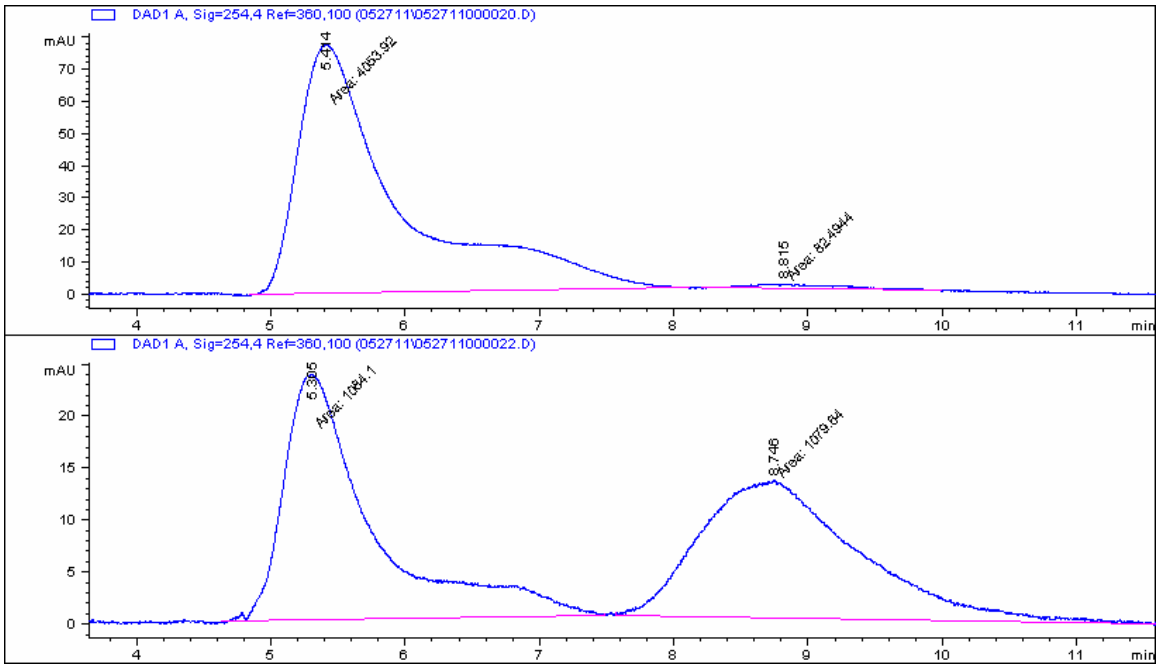


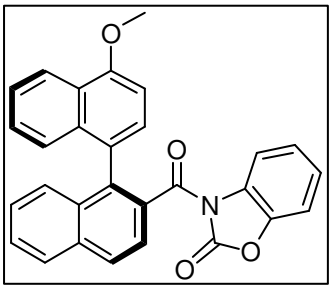
(*R*)-3-(4'-Methyl-1,1'-binaphthyl-2-carbonyl)benzo[d]oxazol-2(3H)-one: white solid (95% yield); 96% ee; $[\alpha]_D^{20}$ = -128.8° (c = 0.49, $CHCl_3$); ^1H NMR (500 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.5 Hz, 1H), 7.98 (d, *J* = 8.3 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.56 (m, 1H), 7.37-7.48 (m, 4H), 7.32 (m, 3H), 7.25 (d, *J* = 7.0 Hz, 1H), 7.06 (m, 1H), 6.97 (m, 2H), 2.56 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.3, 150.4, 142.3, 137.5, 134.9, 134.6, 132.8, 132.5, 132.4, 132.3, 132.1, 128.4, 128.2, 127.9, 127.6, 127.5, 127.3, 127.1, 126.9, 125.9, 125.8, 125.7, 124.7, 124.2, 124.1, 123.6, 114.1, 109.4, 19.4; ESI-MS: m/z 452 $[M+Na]^+$; Chiral HPLC conditions: Chiralcel OD-H, 4.6 mm X 250 mm, 30 °C, flow rate: 2 mL/min, heptane/isopropanol: 96/4, 254 nm, 5.82 min (*S*), 6.52 min (*R*).



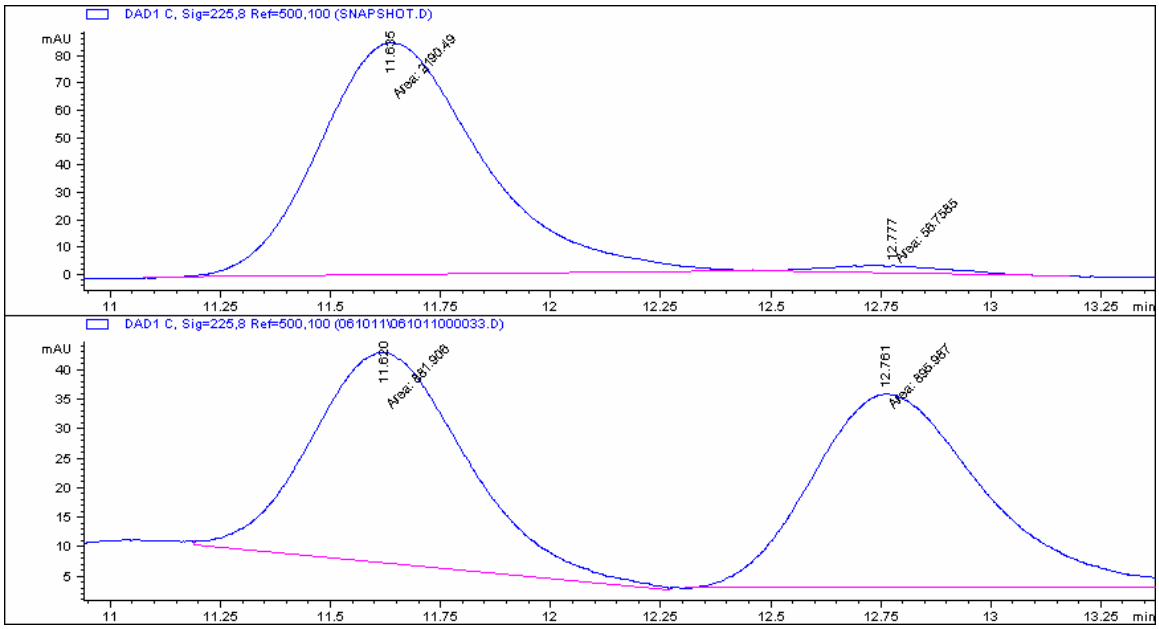


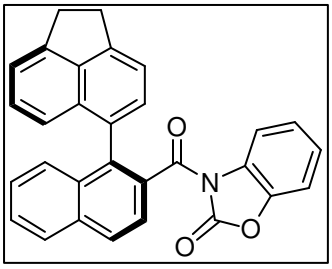
(*R*)-3-(4'-(dimethylamino)-1,1'-binaphthyl-2-carbonyl)benzo[d]oxazol-2(3H)-one: 95% yield; 96% ee; $[\alpha]_D^{20}$ = -175.2° (c = 0.65, $CHCl_3$); ^1H NMR (500 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.4 Hz, 1H), 8.07 (d, *J* = 8.3 Hz, 1H), 7.99 (d, *J* = 8.2 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.56 (m, 2H), 7.38 (m, 4H), 7.30 (m, 1H), 7.23 (m, 1H), 7.04 (m, 1H), 7.94 (m, 3H), 2.71 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.6, 151.2, 150.3, 142.2, 137.5, 134.8, 133.6, 132.9, 132.3, 128.5, 128.45, 128.4, 128.3, 128.2, 127.6, 127.5, 127.3, 127.1, 127.0, 126.9, 126.0, 125.2, 124.5, 124.2, 124.1, 123.8, 113.8, 113.0, 109.3, 45.0; ESI-MS: m/z 481 $[M+Na]^+$; Chiral HPLC conditions: Chiralcel AD-H, 4.6 mm X 250 mm, 30 °C, flow rate: 2 mL/min, heptane/isopropanol: 97/3, 254 nm, 5.30 min (*R*), 8.75 min (*S*).



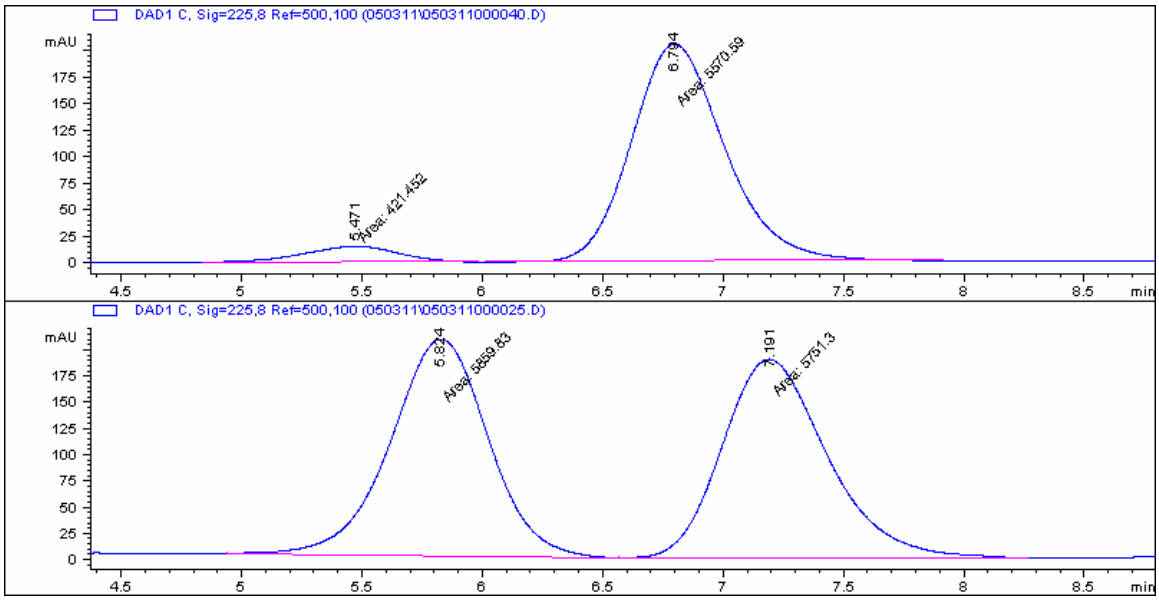


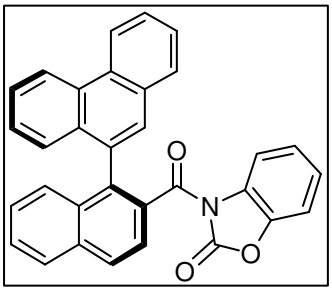
(*R*)-3-(4'-methoxy-1,1'-binaphthyl-2-carbonyl)benzo[d]oxazol-2(3H)-one: white solid (95% yield); 94% ee; $[\alpha]_D^{20} = -70.6^o$ (c = 0.17, $CHCl_3$); ^1H NMR (400 MHz, CD_2Cl_2) δ 8.19 (d, *J* = 8.3 Hz, 1H), 8.10 (d, *J* = 8.5 Hz, 1H), 8.03 (d, *J* = 8.3 Hz, 1H), 7.70 (d, *J* = 8.5 Hz, 1H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.28-7.50 (m, 7H), 7.15 (t, *J* = 7.4 Hz, 1H), 7.06 (m, 2H), 6.80 (d, *J* = 7.8 Hz, 1H), 3.94 (s, 3H); ^{13}C NMR (100 MHz, CD_2Cl_2) δ 168.7, 156.2, 151.0, 142.9, 137.8, 135.1, 134.1, 133.6, 133.1, 128.9, 128.8, 128.7, 128.1, 128.0, 127.5, 127.2, 126.9, 125.9, 125.5, 124.9, 124.1, 122.5, 114.8, 110.1, 103.8, 56.1; ESI-MS: m/z 468 $[M+Na]^+$; Chiral HPLC conditions: Chiralcel AD-H, 4.6 mm X 250 mm, 30 ^oC, flow rate: 2 mL/min, heptane/isopropanol: 96/4, 225 nm, 11.53 min (*R*), 12.78 min (*S*).



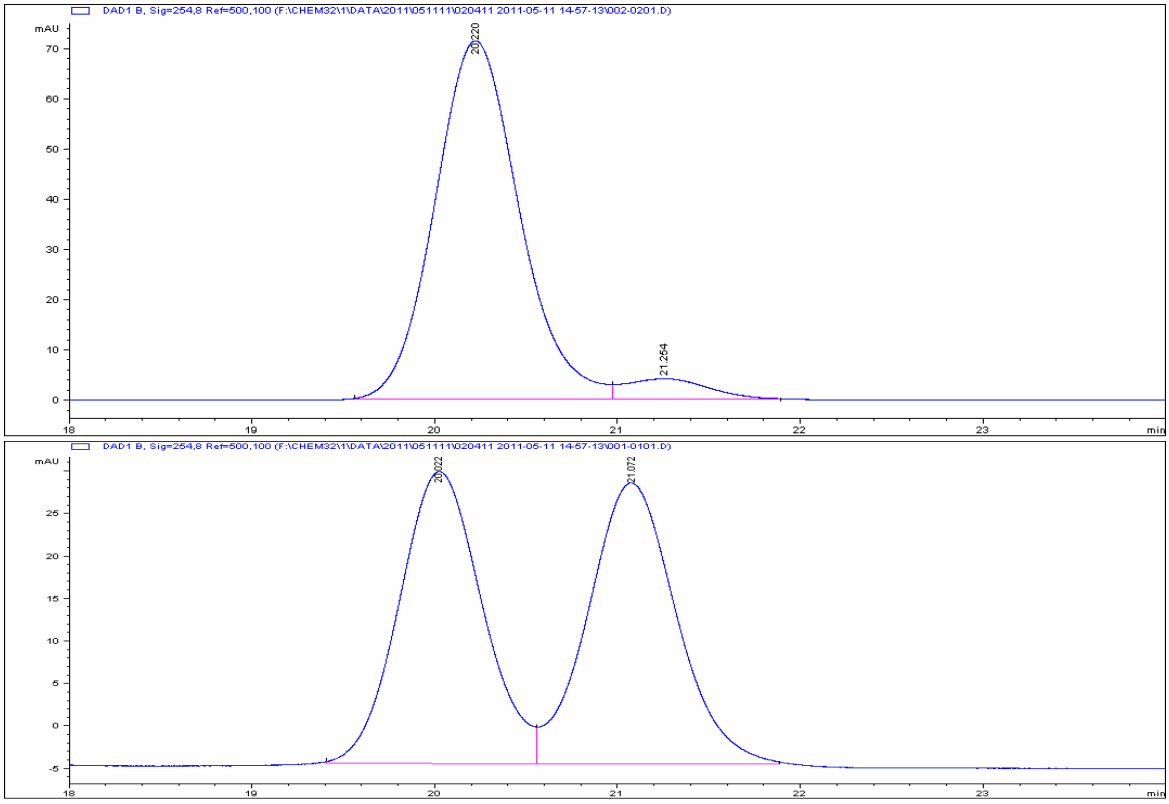


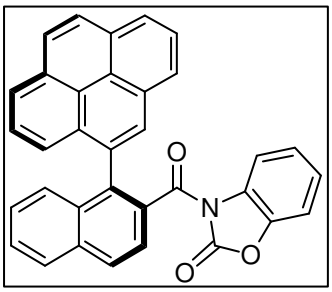
(*R*)-3-(1-(1,2-dihydroacenaphthylen-5-yl)-2-naphthoyl)benzo[d]oxazol-2(3H)-one: white solid (96% yield); 88% ee; $[\alpha]_D^{20}$ = -96.8° (c = 0.41, $CHCl_3$); ^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.10 (d, *J* = 8.5 Hz, 1H), 8.03 (d, *J* = 8.2 Hz, 1H), 7.73 (d, *J* = 8.5 Hz, 1H), 7.61 (m, 1H), 7.54 (d, *J* = 8.6 Hz, 1H), 7.40 (m, 2H), 2.31 (m, 2H), 7.23 (m, 2H), 6.95-7.13 (m, 4H), 3.13-3.42 (m, 4H); ^{13}C NMR (100 MHz, CD_2Cl_2) δ 168.9, 151.0, 147.4, 146.8, 142.9, 139.6, 137.7, 135.2, 133.2, 132.7, 131.4, 130.4, 130.1, 128.82, 128.8, 128.7, 128.2, 127.9, 127.5, 125.2, 124.7, 124.3, 121.8, 120.1, 119.3, 114.4, 109.9, 30.8, 30.6; ESI-MS: m/z 464 $[M+Na]^+$; Chiral HPLC conditions: Chiralcel OD-H, 4.6 mm X 250 mm, 30 °C, flow rate: 2 mL/min, heptane/isopropanol: 96/4, 225 nm, 5.47 min (*S*), 6.80 min (*R*).



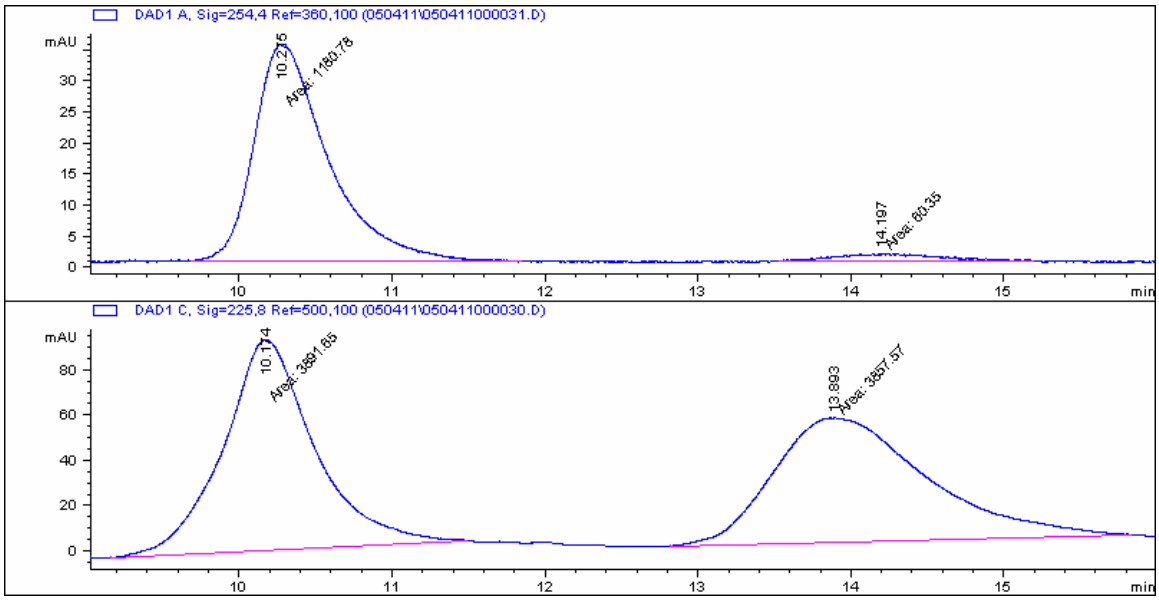


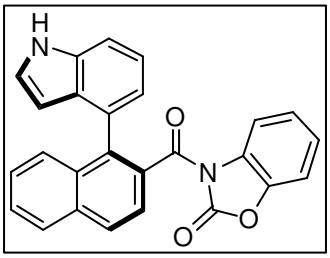
(*R*)-3-(1-(phenanthren-9-yl)-2-naphthoyl)benzo[d]oxazol-2(3H)-one: white solid (96% yield); 90% ee; $[\alpha]_D^{20} = -91.7^o$ (c = 0.36, $CHCl_3$); ^1H NMR (500 MHz, $CDCl_3$) δ 8.61 (d, J = 8.3 Hz, 1H), 8.57 (d, J = 8.2 Hz, 1H), 8.11 (d, J = 8.5 Hz, 1H), 8.01 (d, J = 8.3 Hz, 1H), 7.83 (d, J = 7.3 Hz, 1H), 7.78 (s, 1H), 7.74 (d, J = 8.6 Hz, 1H), 7.53-7.65 (m, 4H), 7.40-7.53 (m, 3H), 7.34 (t, J = 7.3 Hz, 1H), 7.29 (d, J = 8.0 Hz, 1H), 6.96 (m, 1H), 6.85 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.1, 150.6, 142.1, 137.1, 134.6, 133.2, 132.8, 132.2, 131.5, 131.0, 130.2, 130.1, 129.1, 128.8, 128.6, 128.3, 127.7, 127.6, 127.5, 127.2, 127.1, 126.9, 126.8, 126.78, 126.77, 124.7, 124.2, 123.6, 122.6, 122.4, 114.0, 109.4; ESI-MS: m/z 488 $[M + Na]^+$; Chiral HPLC conditions: Chiralpak AD-3, 4.6 mm X 250 mm, 25 ^oC, flow rate: 1.2 mL/min, heptane/isopropanol: 85/15, 254 nm, 20.0 min (*R*), 21.1 min (*S*).



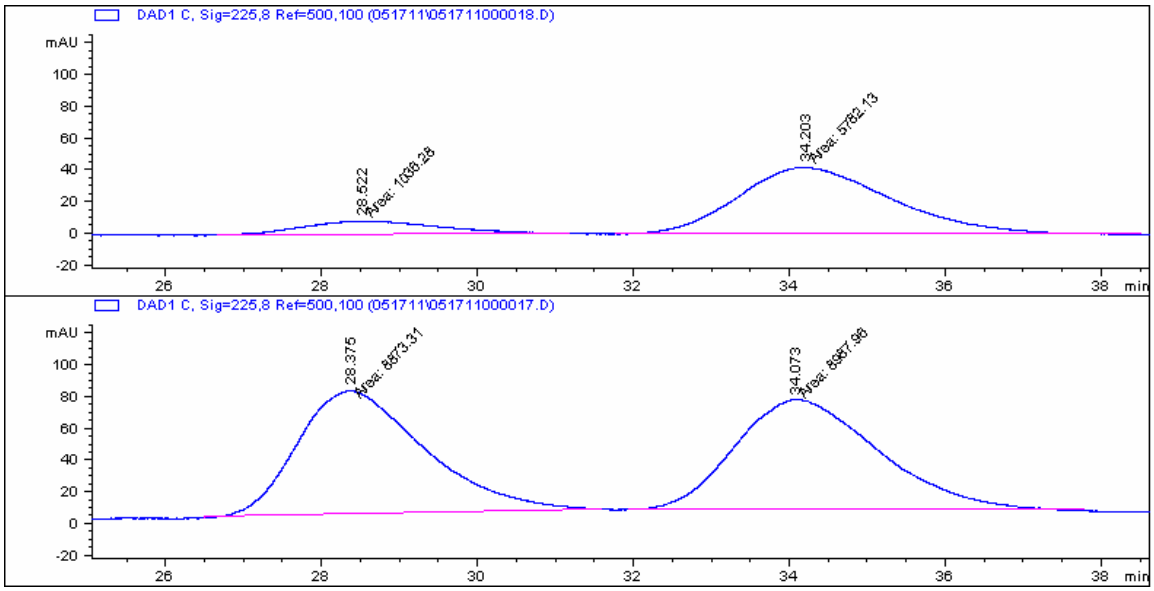


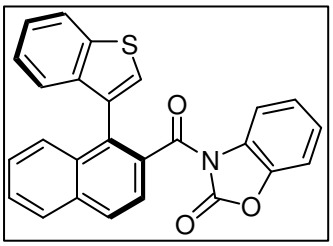
(*R*)-3-(1-(pyren-4-yl)-2-naphthoyl)benzo[d]oxazol-2(3H)-one: white solid (95% yield); 90% ee; $[\alpha]_D^{20}$ = -129.5^o (c = 0.44, $CHCl_3$); ^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.13-8.25 (m, 4H), 8.00-8.12 (m, 5H), 7.94 (d, J = 9.2 Hz, 1H), 7.79 (d, J = 8.5 Hz, 1H), 7.63 (m, 2H), 7.36 (m, 2H), 7.29 (d, J = 7.9 Hz, 1H), 6.88 (m, 2H), 6.75 (t, J = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, CD_2Cl_2) δ 168.5, 151.0, 142.7, 138.2, 135.1, 133.5, 133.2, 132.1, 131.8, 131.7, 131.4, 130.8, 129.0, 128.9, 128.8, 128.32, 128.31, 128.29, 128.1, 127.8, 127.7, 126.8, 126.0, 125.9, 125.9, 125.4, 125.0, 124.93, 124.9, 124.6, 124.2, 114.6, 109.9; ESI-MS: m/z 512 $[M+Na]^+$; Chiral HPLC conditions: Chiralcel AD-H, 4.6 mm X 250 mm, 30 ^{o}C, flow rate: 2 mL/min, heptane/isopropanol: 96/4, 254 nm, 10.17 min (*R*), 13.89 min (*S*).



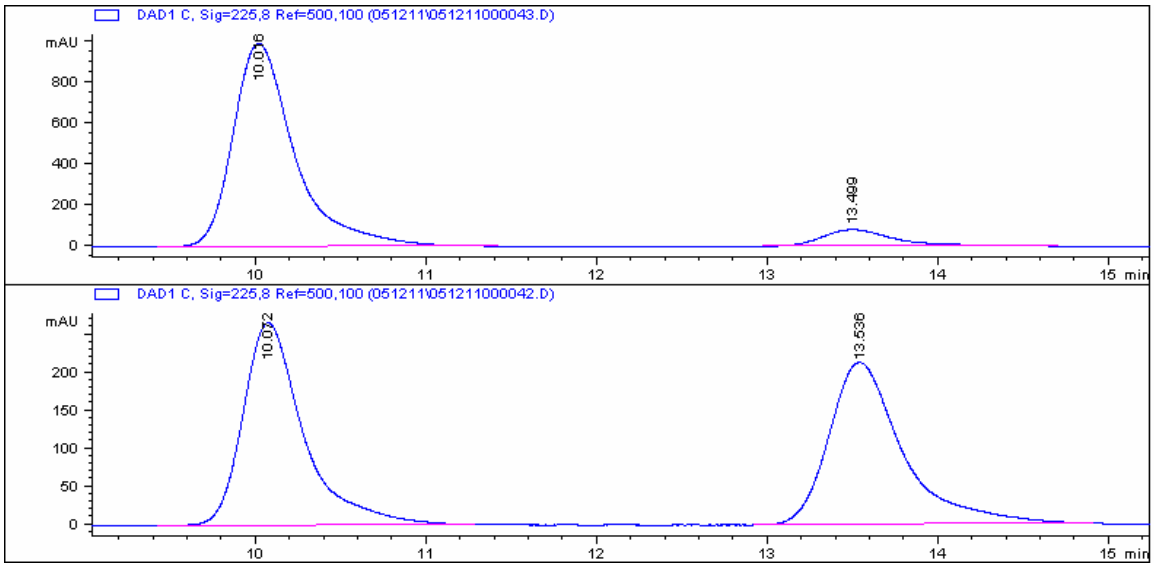


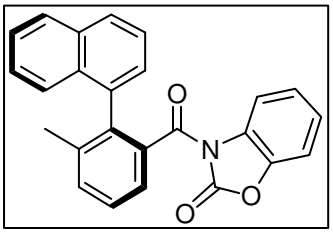
(*R*)-3-(1-(1H-indol-4-yl)-2-naphthoyl)benzo[d]oxazol-2(3H)-one: 95%; 68% ee; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (d, J = 8.4 Hz, 1H), 8.04 (br, 1H), 7.98 (d, J = 8.3 Hz, 1H), 7.72 (d, J = 8.4 Hz, 2H), 7.57 (t, J = 7.2 Hz, 1H), 7.40 (m, 2H), 6.95-7.20 (m, 6H), 6.93 (d, J = 7.9 Hz, 1H), 6.14 (t, J = 2.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.9, 150.3, 142.3, 138.2, 135.5, 134.9, 132.0, 131.2, 128.9, 128.3, 128.2, 127.9, 127.7, 127.5, 126.7, 124.5, 124.4, 124.0, 123.9, 122.8, 121.9, 121.7, 113.9, 110.6, 109.2, 102.8; ESI-MS: m/z 427 $[M+Na]^+$; Chiral HPLC conditions: Chiralcel OD-H, 4.6 mm X 250 mm, 30 ^{o}C, flow rate: 2 mL/min, heptane/isopropanol: 93/7, 225 nm, 28.5 min (*S*), 34.2 min (*R*).



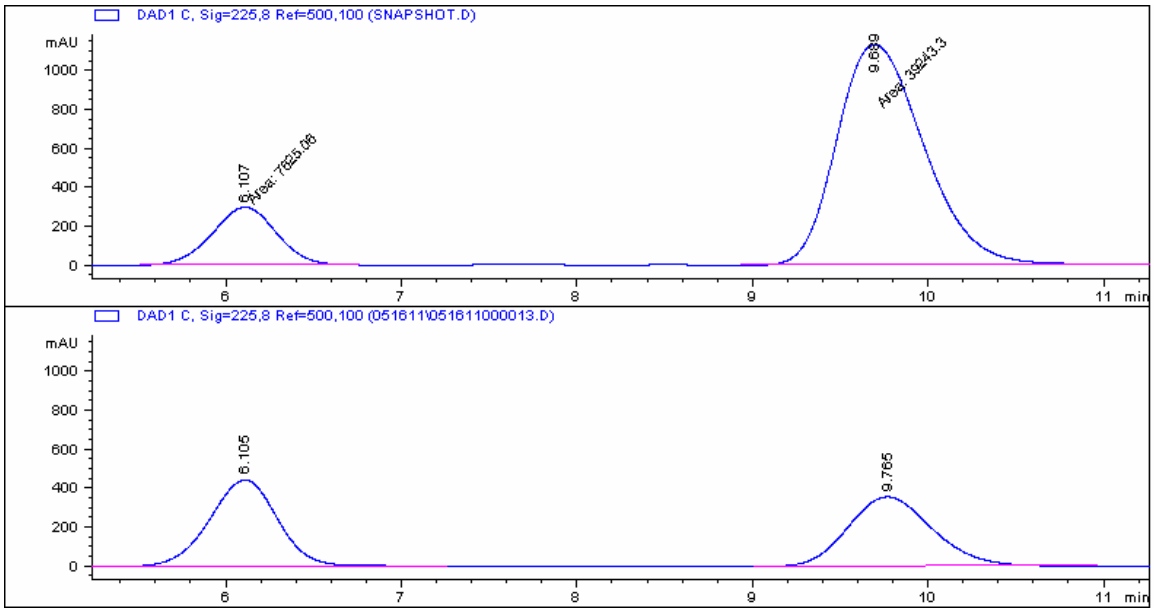


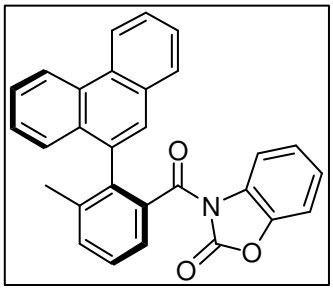
(*S*)-3-(1-(benzo[b]thiophen-3-yl)-2-naphthoyl)benzo[d]oxazol-2(3H)-one: 95% yield; 82% ee; $[\alpha]_D^{20}$ = -121.8° (c = 0.61, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.5 Hz, 1H), 8.99 (d, *J* = 8.3 Hz, 1H), 7.71 (m, 2H), 7.64 (d, *J* = 8.6 Hz, 1H), 7.60 (t, *J* = 8.0 Hz, 1H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.49 (s, 1H), 7.42 (m, 1H), 7.35 (m, 1H), 7.23-7.32 (m, 2H), 7.11 (m, 1H), 7.05 (m, 1H), 6.99 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.4, 150.4, 142.3, 139.5, 139.0, 134.7, 132.42, 132.38, 132.3, 129.1, 128.4, 127.7, 127.3, 127.2, 127.0, 126.5, 124.9, 124.7, 124.5, 124.4, 123.7, 123.6, 122.4, 114.2, 109.5; ESI-MS: m/z 431 $[M+Na]^+$; Chiral HPLC conditions: Chiralcel AD-H, 4.6 mm X 250 mm, 30 °C, flow rate: 2 mL/min, heptane/isopropanol: 96/4, 225 nm, 10.02 min (*S*), 13.50 min (*R*).



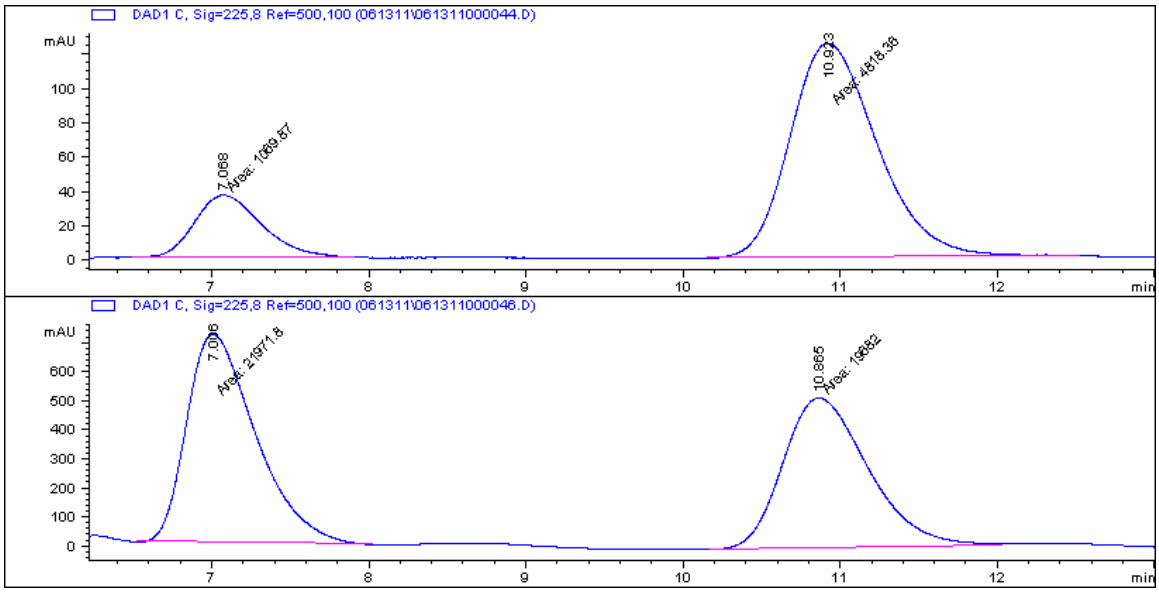


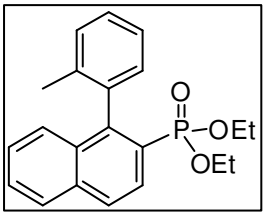
(*R*)-3-(3-methyl-2-(naphthalen-1-yl)benzoyl)benzo[d]oxazol-2(3H)-one: 85% yield; 70% ee; $[\alpha]_D^{20}$ = -121.8° (c = 0.66, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (m, 1H), 7.66 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.56 (m, 1H), 7.51 (m, 3H), 7.42 (m, 2H), 7.27-7.45 (m, 3H), 7.06 (m, 1H), 6.97 (m, 2H), 2.06 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.1, 150.4, 142.1, 138.2, 137.6, 135.5, 135.2, 133.3, 133.0, 131.5, 128.1, 128.0, 127.8, 127.3, 127.0, 126.3, 126.0, 125.9, 125.0, 124.99, 124.7, 124.2, 114.1, 109.4, 20.1; ESI-MS: m/z 402 $[M+Na]^+$; Chiral HPLC conditions: Chiralcel OD-H, 4.6 mm X 250 mm, 30 °C, flow rate: 2 mL/min, heptane/isopropanol: 96/4, 225 nm, 6.11 min (*S*), 9.69 min (*R*).



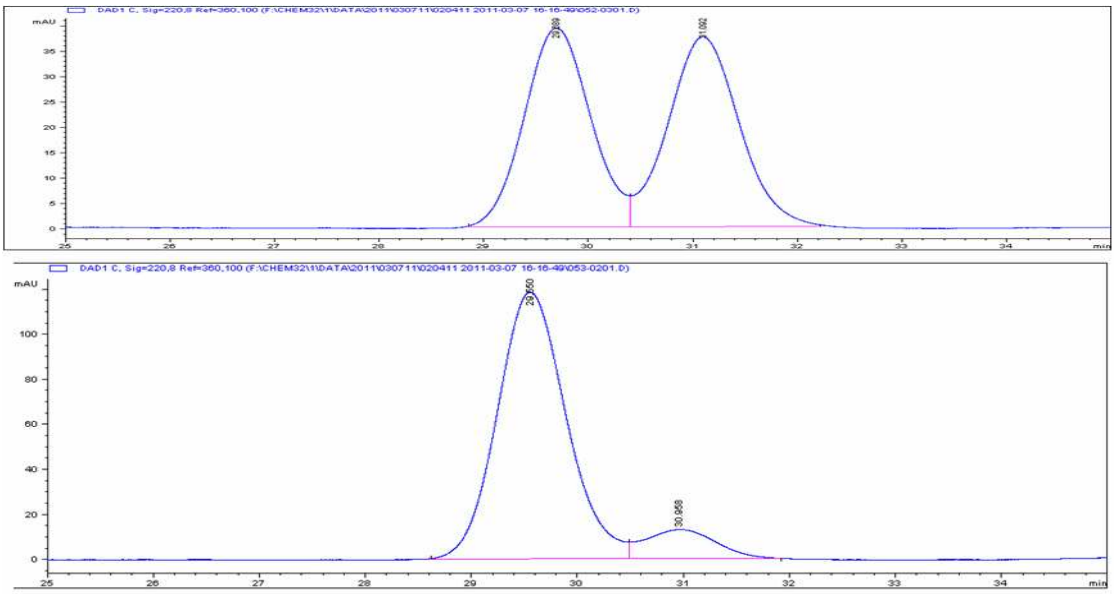


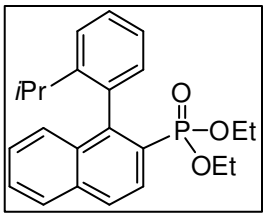
(*R*)-3-(3-Methyl-2-(phenanthren-9-yl)benzoyl)benzo[d]oxazol-2(3H)-one: white solid (90% yield); 64% ee; $[\alpha]_D^{20}$ = -17.8° (c = 0.45, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, *J* = 8.2 Hz, 1H), 8.51 (d, *J* = 7.4 Hz, 1H), 7.80 (m, 1H), 7.50-7.65 (m, 9H), 7.22 (d, *J* = 7.8 Hz, 1H), 6.93 (t, *J* = 7.9 Hz, 1H), 6.81(m, 2H), 2.10 (s, 3H); ^{1}H NMR (100 MHz, $CDCl_3$) δ 168.1, 150.6, 142.0, 138.4, 137.6, 135.3, 134.4, 133.0, 131.1, 130.6, 130.2, 130.0, 128.7, 127.9, 127.8, 127.2, 126.9, 126.8, 126.72, 126.7, 125.1, 124.6, 124.1, 122.7, 122.3, 113.9, 109.3, 20.1; ESI-MS: m/z 452 $[M+Na]^+$; Chiral HPLC conditions: Chiralcel OD-H, 4.6 mm X 250 mm, 30 °C, flow rate: 2 mL/min, heptane/isopropanol: 94/6, 225 nm, 7.07 min (*S*), 10.92 min (*R*).



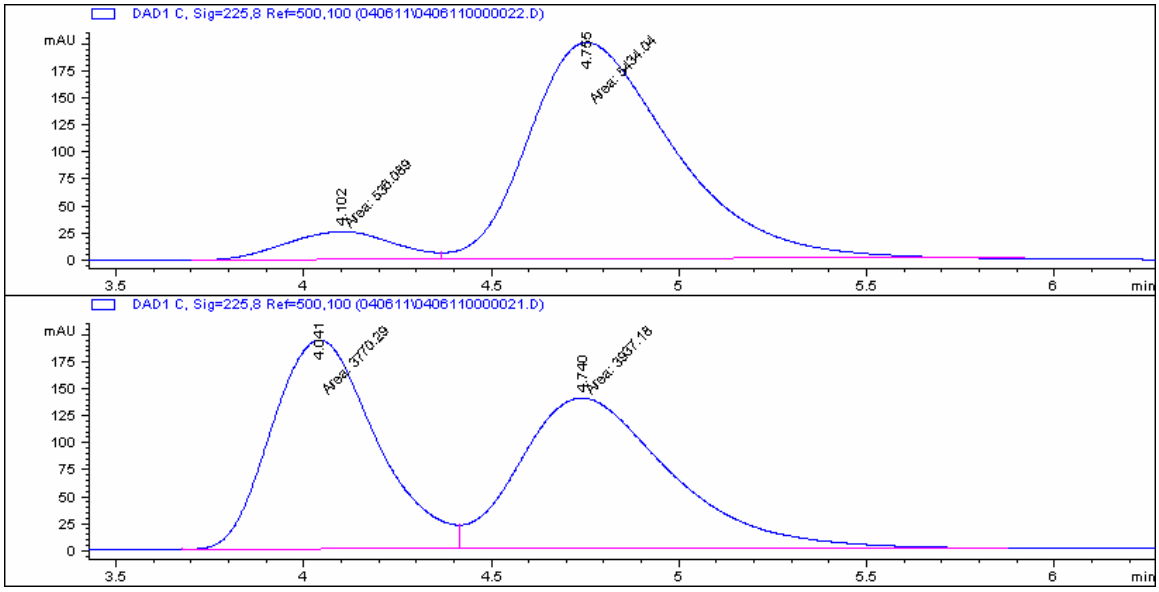


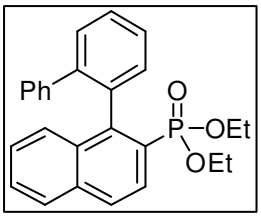
Diethyl 1-*o*-tolylnaphthalen-2-ylphosphonate: white solid (95% yield); 80% ee; $[\alpha]_D^{20}$ = -5.5° (c = 0.53, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (dd, J = 11.8, 8.8 Hz, 1H), 7.92 (m, 2H), 7.55 (t, J = 7.3 Hz, 1H), 7.25-7.43 (m, 5H), 7.21 (d, J = 7.3 Hz, 1H), 3.82-4.00 (m, 3H), 3.70-3.82 (m, 1H), 1.92 (s, 3H), 1.85 (m, 6H); ^{1}H NMR (100 MHz, $CDCl_3$) δ 144.9 (d, J = 10.0 Hz), 137.8 (d, J = 5.2 Hz), 137.6, 134.9 (d, J = 2.6 Hz), 132.4 (d, J = 16.1 Hz), 130.7, 129.3, 128.3, 128.2, 128.0, 127.8, 127.3, 127.2, 127.0, 126.7 (d, J = 1.2 Hz), 124.9, 124.8 (d, J = 129.0 Hz), 61.7 (m), 20.0, 16.2 (m); ESI-MS: m/z 355 $[M+H]^+$; Chiral HPLC conditions: Chiralpak AD-3, 4.6 mm X 250 mm, 30 °C, flow rate: 1.0 mL/min, heptane/ethanol: 90/10, 220 nm, 29.6 min, 31.0 min;



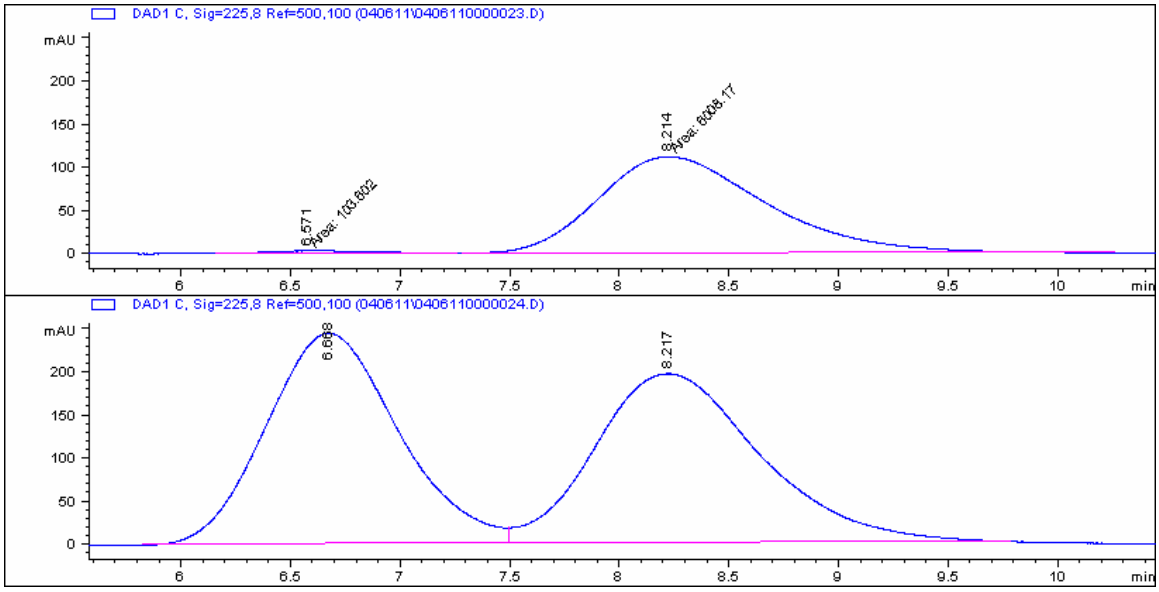


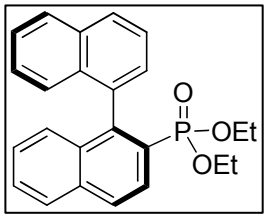
Diethyl 1-(2-isopropylphenyl)naphthalen-2-ylphosphonate: 75% yield; 80% ee; $[\alpha]_D^{20}$ = -19.8° (c = 0.4, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, J = 8.5 Hz, 1H), 8.03 (d, J = 8.7 Hz, 1H), 7.92 (dd, J = 8.5, 3.4 Hz, 1H), 7.88 (d, J = 8.2 Hz, 1H), 7.54 (t, J = 7.6 Hz, 1H), 7.44 (m, 2H), 7.36 (m, 2H), 7.26 (m, 1H), 7.18 (d, J = 7.4 Hz, 1H), 3.98 (m, 1H), 3.88 (m, 2H), 3.84 (m, 1H), 2.37 (m 1H), 1.17 (m, 9H), 0.91 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.0, 144.7 (d, J = 10.2 Hz), 136.8 (d, J = 5.1 Hz), 134.8 (d, J = 2.6 Hz), 133.1 (d, J = 16.4 Hz), 130.4, 128.4, 128.0, 127.9, 127.86, 127.8, 127.3, 127.2, 126.3 (d, J = 1.1 Hz), 125.3, 124.8, 61.7 (t, J = 6.0 Hz), 30.5, 24.6, 23.5, 16.3 (t, J = 6.4 Hz); ESI-MS: m/z 383 $[M+H]^+$; Chiral HPLC conditions: Chiralcel OD-H, 4.6 mm X 250 mm, 30 °C, flow rate: 2 mL/min, heptane/isopropanol: 96/4, 225 nm, 4.04 min , 4.74 min.



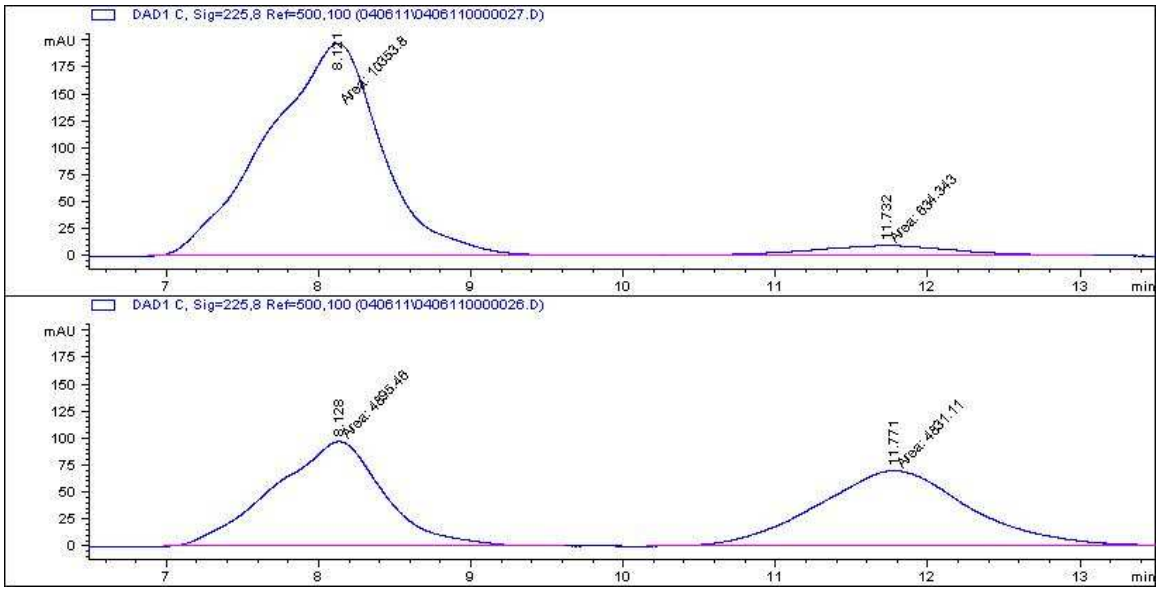


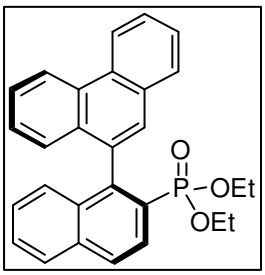
Diethyl 1-(biphenyl-2-yl)naphthalen-2-ylphosphonate: 74% yield; 96% ee; $[\alpha]_D^{20}$ = -4.7° (c = 0.6, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.98 (dd, *J* = 12.0, 8.8 Hz, 1H), 7.81 (dd, *J* = 8.4, 3.6 Hz, 1H), 7.73 (d, *J* = 8.3 Hz, 1H), 7.54 (m, 2H), 7.37-7.49 (m, 3H), 7.33 (d, *J* = 8.6 Hz, 1H), 7.25 (t, *J* = 8.0 Hz, 1H), 7.16 (m, 2H), 6.94 (m, 3H), 3.92 (m, 3H), 3.68 (m, 1H), 1.15 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.0, 141.2, 136.9, 134.6, 131.7, 129.7, 129.1, 128.3, 127.9, 127.8, 127.7, 127.68, 127.5, 127.4, 127.3, 127.26, 126.5, 126.3, 126.29, 61.9 (d, *J* = 5.8 Hz), 61.8 (d, *J* = 6.6 Hz), 16.3 (d, *J* = 6.2 Hz), 16.2 (d, *J* = 6.5 Hz); ESI-MS: m/z 417 $[M+H]^+$; Chiral HPLC conditions: Chiralcel OD-H, 4.6 mm X 250 mm, 30 °C, flow rate: 2 mL/min, heptane/isopropanol: 96/4, 225 nm, 6.57 min , 8.21 min.



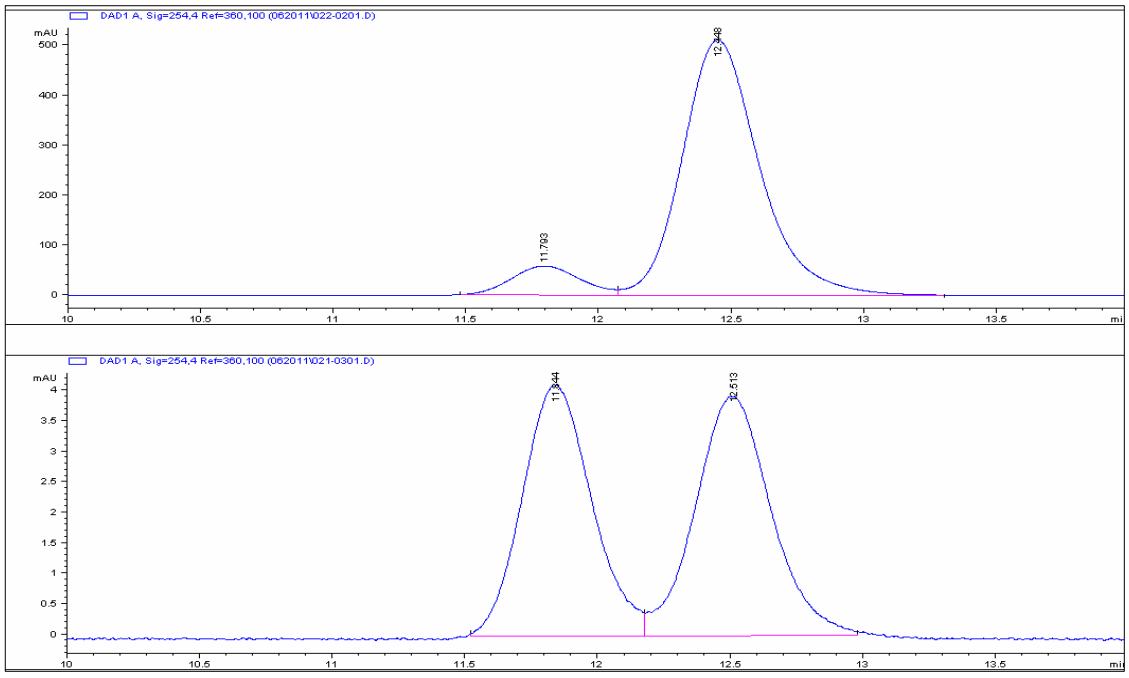


(*R*)-Diethyl 1,1'-binaphthyl-2-ylphosphonate:[5] 88% yield; 90% ee; $[\alpha]_D^{20}$ = +46.4° (c = 0.29, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 8.21 (dd, *J* = 12.0, 8.7 Hz, 1H), 8.02 (dd, *J* = 8.6, 3.7 Hz, 1H), 7.94 (m, 3H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.49 (d, *J* = 7.0 Hz, 1H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.15-7.30 (m, 3H), 7.08 (d, *J* = 8.4 Hz, 1H), 3.80 (m, 1H), 3.69 (m, 1H), 3.58 (m 2H), 0.97 (t, *J* = 7.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.9, 134.9, 133.4, 133.2, 128.73, 128.71, 128.6, 128.3, 128.0, 127.9, 127.8, 127.7, 127.6, 126.72, 126.7, 125.9, 125.6, 124.9, 61.8 (d, *J* = 6.0 Hz), 61.6 (d, *J* = 6.0 Hz), 15.9 (d, *J* = 6.7 Hz), 15.4 (d, *J* = 7.2 Hz); ESI-MS: m/z 391 $[M+H]^+$; Chiral HPLC conditions: Chiralcel AD-H, 4.6 mm X 250 mm, 30 °C, flow rate: 2 mL/min, heptane/isopropanol: 96/4, 225 nm, 8.13 min (*R*), 11.7 min (*S*).

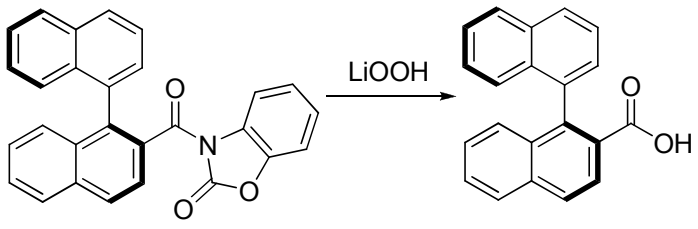




(*R*)-diethyl 1-(phenanthren-9-yl)naphthalen-2-ylphosphonate: 90% yield; 82% ee; $[\alpha]_D^{20}$ = +30.4° (c = 0.25, $CHCl_3$); ^1H NMR (500 MHz, $CDCl_3$) δ 8.79 (d, *J* = 8.3 Hz, 2H), 8.26 (dd, *J* = 12.2, 8.6 Hz, 1H), 8.06 (dd, *J* = 8.6, 3.7 Hz, 1H), 8.96 (d, *J* = 8.3 Hz, 1H), 7.89 (d, *J* = 7.8 Hz, 1H), 7.77 (s, 1H), 7.74 (m, 1H), 7.65 (m, 2H), 7.54 (t, *J* = 7.0 Hz, 1H), 7.34 (m, 2H), 7.23 (m, 1H), 7.15 (d, *J* = 7.7 Hz, 1H), 3.77 (m, 1H), 3.64 (m, 2H), 3.54 (m, 1H), 0.95 (t, *J* = 7.1 Hz, 3H), 0.61 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.3 (d, *J* = 9.3 Hz), 135.0 (d, *J* = 2.6 Hz), 134.5 (d, *J* = 5.3 Hz), 133.3 (d, *J* = 15.7 Hz), 132.6, 131.3, 130.3, 129.9, 129.63, 129.62, 128.9, 128.8, 128.79, 128.0 (d, *J* = 1.0 Hz), 127.9 (d, *J* = 1.0 Hz), 127.87, 127.8, 127.7, 127.1, 127.6, 126.9, 126.7 (d, *J* = 1.4 Hz), 126.5, 126.3, 125.6, 122.63, 122.61, 61.8 (d, *J* = 6.1 Hz), 61.5 (d, *J* = 6.1 Hz), 15.9 (d, *J* = 7.1 Hz), 15.3 (d, *J* = 7.2 Hz); ESI-MS: m/z 441 $[M+H]^+$; Chiral HPLC conditions: Chiracel OD-H, 4.6 X150 mm, flow rate: 2 mL/min, Water/Acetonitrile: 50/50; 225 nm, 11.70 min (*S*), 12.50 min (*R*).

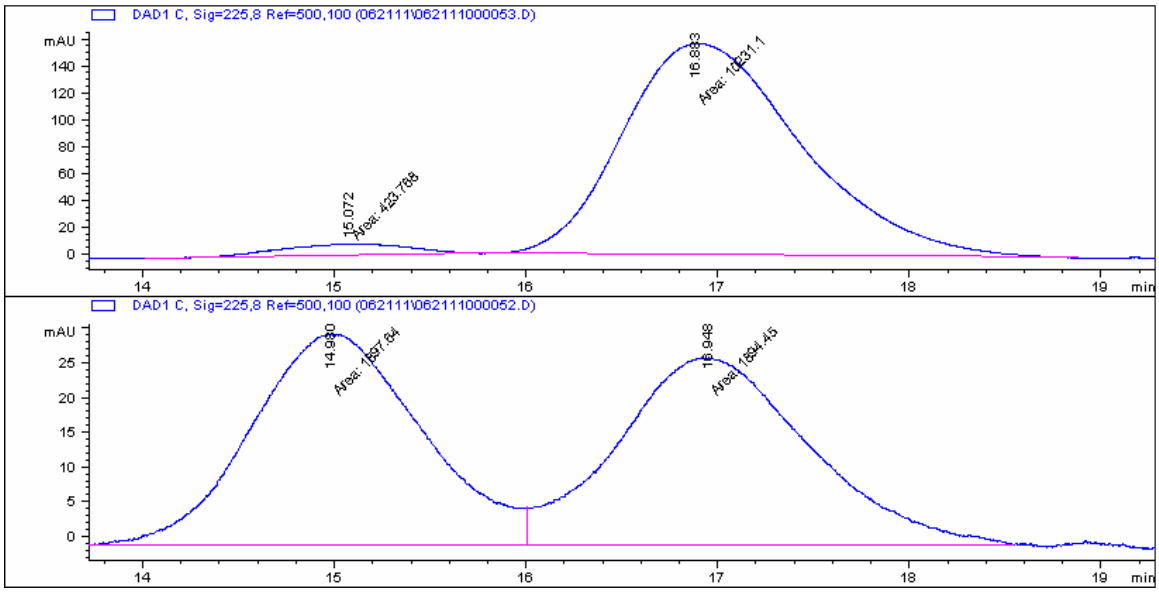


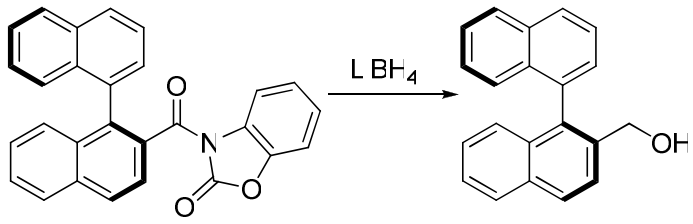
6. Derivatization of chiral biaryl coupling product 6d



6d **7**

To a solution of **6d** (100 mg, 0.24 mmol, 92% ee) in THF/water (4 mL, 3/1 v/v) at 0 °C was charged 30% H_2O_2 solution (109 mg, 0.96 mmol, 3 equiv) followed by lithium hydroxide (11.5 mg, 0.48 mmol, 2 equiv). The resulting mixture was stirred at 0-25 °C for ~ 0.5 h. The starting material was totally consumed. To the mixture was charged 10 % sodium bisulfite solution (4 mL) and dichloromethane (4 mL). The DCM layer was separated, washed with brine, concentrated, and purified by column chromatography to provide **7** as white solid (71 mg, 0.238 mmol, 99% yield). **7**: 92% ee; $[\alpha]_D^{20}$ = +23.6° (c = 0.70 , $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 8.7 Hz, 1H), 7.95 (m, 4H), 7.54 (m, 2H), 7.44 (t, J = 7.3 Hz, 1H), 7.31 (d, J = 6.8 Hz, 1H), 7.20-7.28 (m, 3H), 7.13 (d, J = 8.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5, 141.2, 136.5, 135.2, 133.2, 133.1, 132.9, 128.3, 128.2, 128.1, 128.0, 127.9, 127.8, 127.2, 127.0, 126.7, 126.1, 126.0, 125.7, 125.2; ESI-MS: m/z 299[M +H]$^+$; Chiral HPLC conditions: Chiralcel OD-H, 4.6 mm X 250 mm, 30 °C, flow rate: 2 mL/min, heptane/isopropanol: 94/6, 225 nm, 15.07 min (*S*) , 16.88 min (*R*).

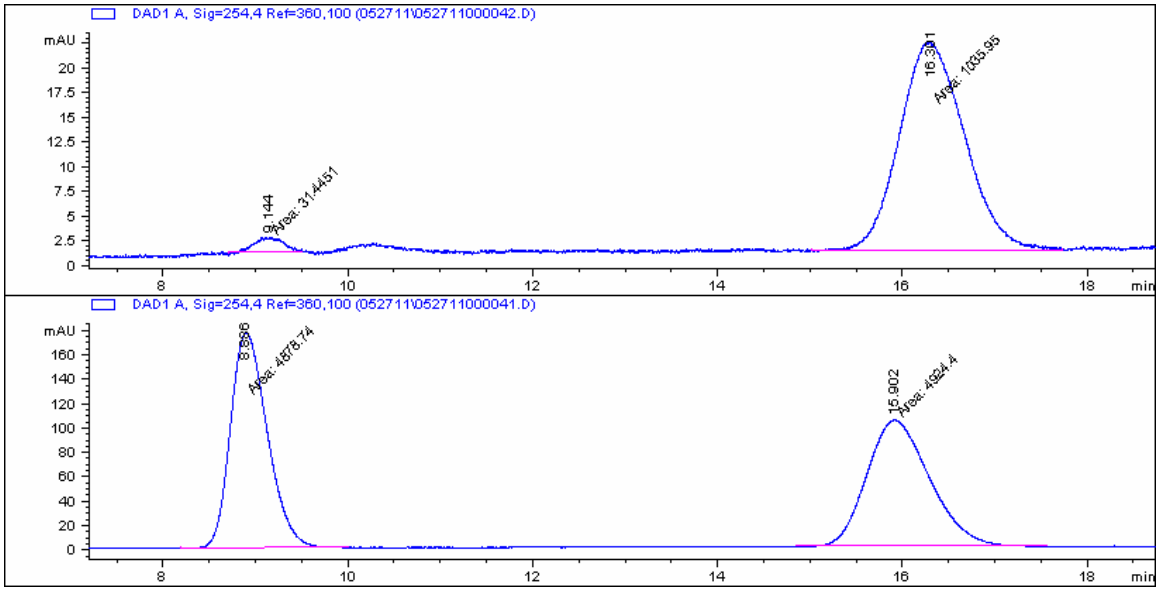




6d **8**

To a solution of **6d** (100 mg, 0.24 mmol, 94% ee) in THF (5 mL) at 0 °C was charged $LiBH_4$ (8 mg, 0.36 mmol, 1.5 equiv) in one portion. The mixture was then stirred at 0-25 °C for 1 h and then quenched by addition of water (5 mL) and EtOAc (5 mL). The organic layer was separated, washed with brine, dried over sodium sulfate, concentrated, and purified by silica gel column chromatography to provide alcohol **8** as white solid (63 mg, 0.22 mmol, 94% ee). **8**: 94% ee; $[\alpha]_D^{20}$ = +46.3° (c = 1.0, $CHCl_3$);[5] ^{1}H NMR (400

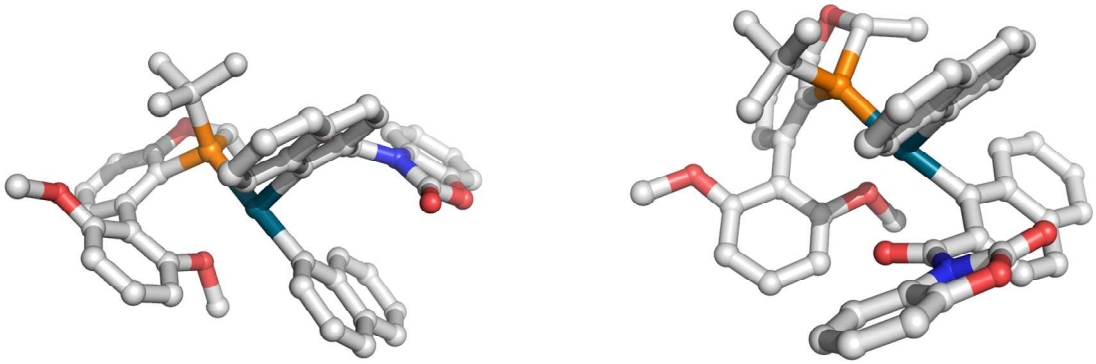
MHz, $CDCl_3$) δ 7.85-8.05 (m, 4H), 7.78 (d, J =8.3 Hz, 1H), 7.59 (t, J = 7.7 Hz, 1H), 7.33-7.50 (m, 3H), 7.12-7.30 (m, 4H), 4.4 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.7, 135.8, 135.7, 133.6, 133.1, 132.9, 132.8, 128.3, 128.1, 127.9, 127.8, 126.6, 126.4, 126.2, 126.1, 125.8, 125.7, 125.5, 63.4; ESI-MS: m/z 285[M +H]$^+$; Chiral HPLC conditions: Chiralcel OD-H, 4.6 mm X 250 mm, 30 ^{o}C, flow rate: 2 mL/min, heptane/isopropanol: 96/4, 254 nm, 9.14 min (*S*) , 16.30 min (*R*).



7. Computational studies

Both Buchwald[6] and Baudoin[7] have made a reasonable hypothesis that the enantioselectivities in the Suzuki-Miyaura coupling reactions are determined in the transition state of reductive elimination. The occurrence of a particular conformation of reaction intermediate is determined by its energy. The chirality of the product follows the shortest path from the conformation of the transition state. To determine the most probable conformation of the intermediates, we first sampled all possible conformations of the palladium complex at the reductive elimination step in the reaction of **5d** and 1-naphthylboronic acid with the Pd-**2** catalyst. This was accomplished by fixing the conformation of the ligand and systematically rotating the bonds between the Pd center and the two reactants in 30^o intervals. Two differently probable coordination configurations were considered as shown in Figure 1S. After eliminating conformations that have obvious steric clashes, 28 unique conformations were obtained. The geometry of each of these conformations was then optimized by energy minimized. All calculations were carried out with Gaussian 03 package.[8] The DFT/B3LYP method was used in the optimization. Because our system consists of bulky aromatic system, non-bonded van der Walls interactions are expected to make a significant contribution to the relative energy of different conformations. We therefore employed the MIDI basis set developed by

Truhlar and co-workers[9], supplied by the Gaussian 03 package (MidiX) for the first-row atoms (H, C, N and O). This functional was reported to produce good results for non-bonded interactions comparable with higher-order theories. For phosphorus, the 6-31G(d) basis set was employed; and for palladium, the all-electron basis set from optimization of fcc Pd bulk[10] was employed.



Conformer class A (A-01 to A-12)
Naphthyl group is 180° with respect to phosphorus ligand

Conformer class B (B-01 to B-12)
Naphthyl group is 90° with respect to phosphorus ligand

Figure S1: Two different conformation classes that were sampled

Although there were 28 unique starting conformations, four pairs of conformations were found to be almost duplicates after full energy minimization for each conformation. The coordinates of the 24 unique energy-minimized conformations are provided in the enclosed minimized-conformation.cif file. Figure S2 shows the relative energy of the 24 conformations. Three lowest-energy conformations were found with relative energy of 0, 0.51 and 0.78 kcal/mol, respectively. All other conformations have energy > 2 kcal/mol or higher than the lowest-energy state.

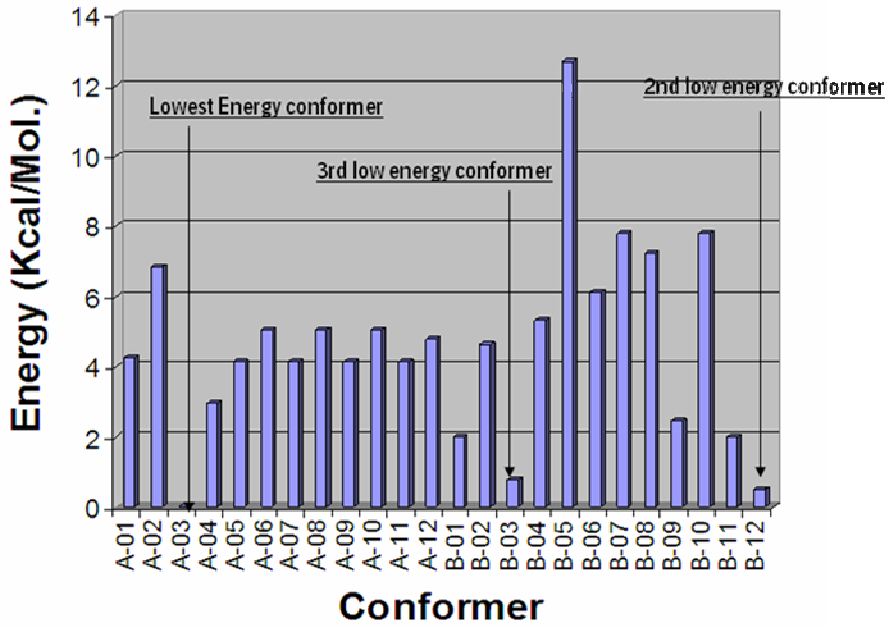


Figure S2: The relative energy of all the sample conformations in the energy-minimized state

There are two main interesting observations from calculation results. First, all three lowest-energy conformations turn out to lead to the same chirality in the coupling product that is in agreement with the inferred axial chirality of **6d**. This result suggests that the energetics of non-bonded π-interaction of the aromatic systems indeed dictate the conformation of the intermediate and the chirality of the product. Secondly, the origin of the π-stacking interaction in determining the energetics of this system is most clearly seen in the lowest and 2nd lowest-energy conformations. Figure S3 and S4 compare the conformations of these two conformations. In each case, there is a π-stacking interaction between the naphthal group and the benzooxazolidinone; and more revealing, in each case, there is a related energy-minimum conformation in which the naphthal group rotates by 180 that reverses the chirality of the system and that has higher energy by ~ 2 kcal/mol.

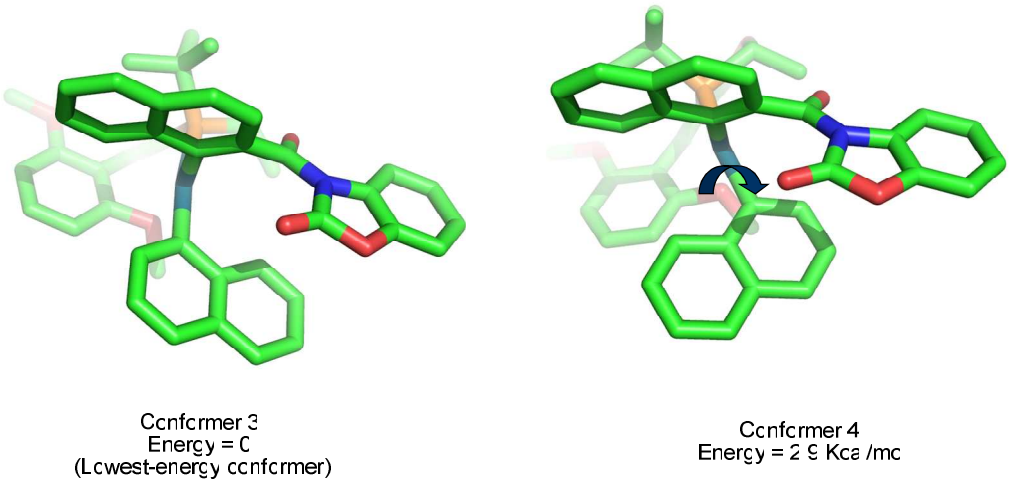


Figure S3: Comparison of the lowest-energy conformation and the local energy minimum in which the napthtyl group approximately flaps by 180° with respect to the first conformation

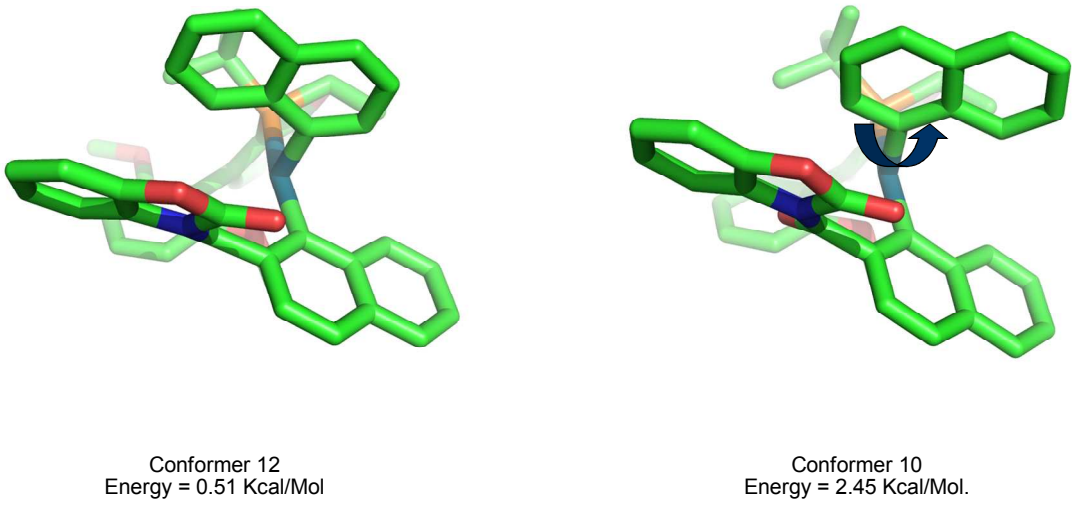
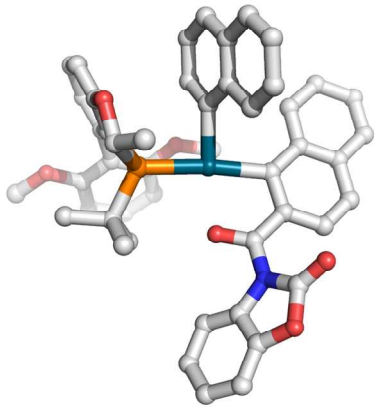


Figure S4: Comparison of the 2nd lowest-energy conformation and the local energy minimum in which the napthtyl group approximately flaps by 180° with respect to the first conformation



Ccnfcrmer B-C5 Energy = C 78 Kca /Mc

Figure S5: The conformation of the 3rd lowest-energy conformation. Interestingly, the chirality of the coupling product from this intermediate conformation is the same as the 1st and 2nd lowest energy conformations.

8. References:

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K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian 03 ; Gaussian, Inc. ; Wallingford CT, 2004.
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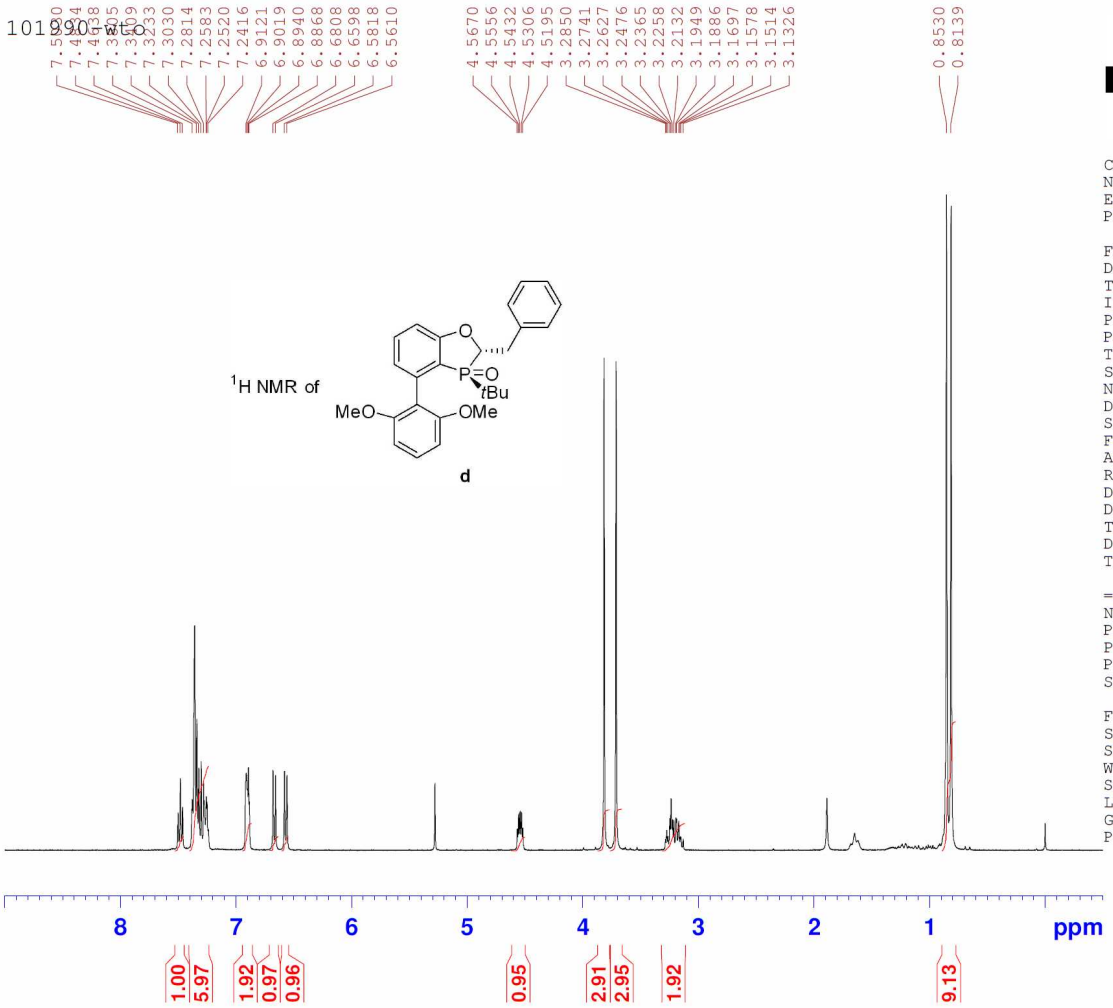

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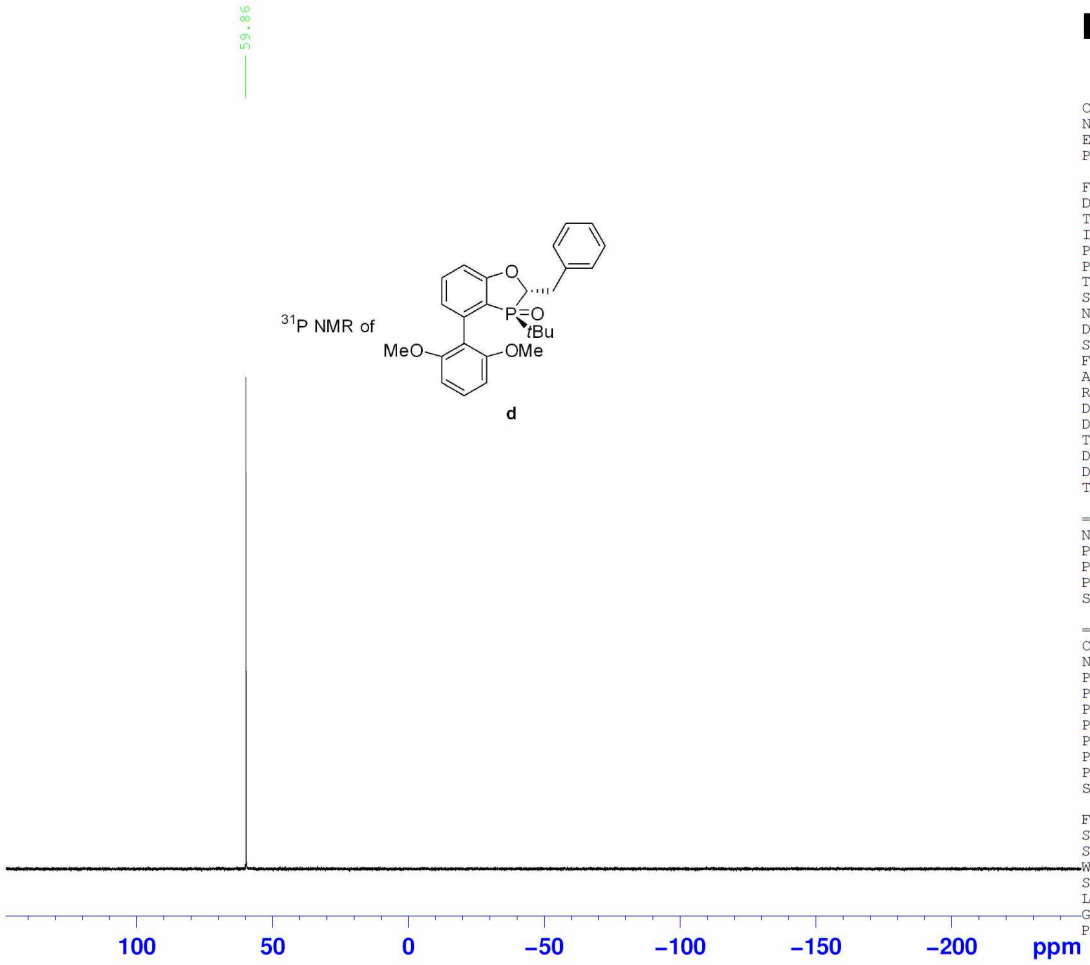


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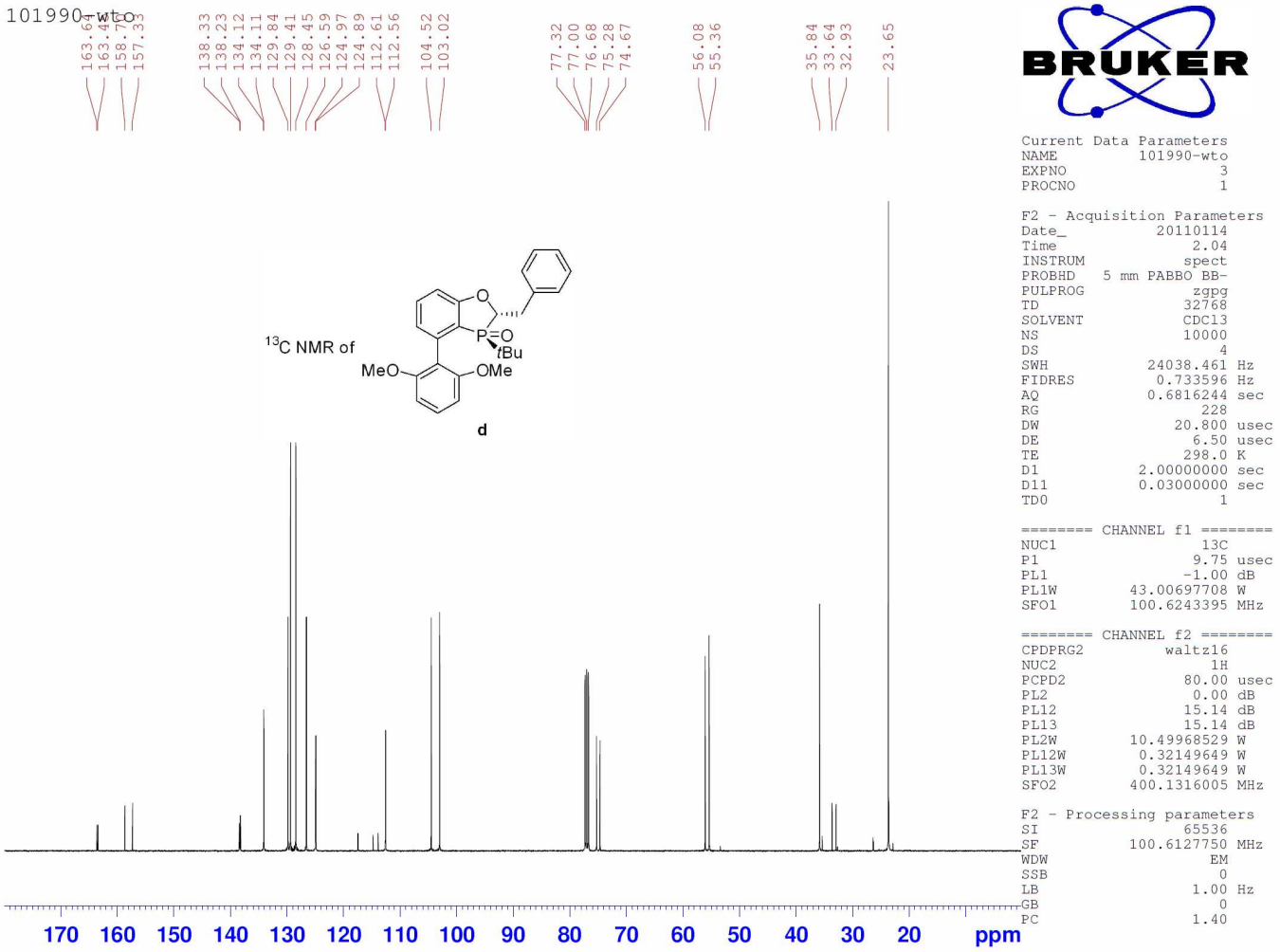

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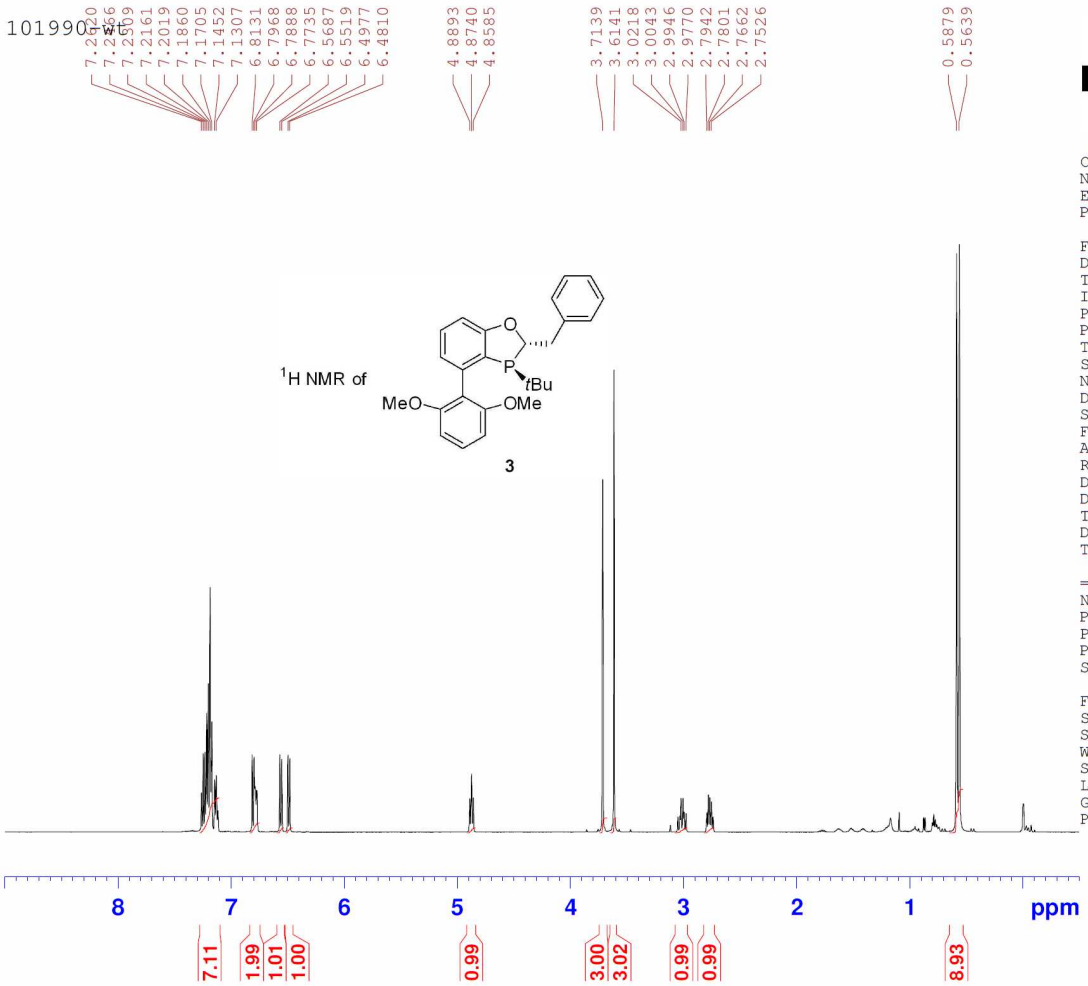
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.75 usec
PL1 -1.00 dB
PL1W 43.00697708 W
SFO1 100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.14 dB
PL13 15.14 dB
PL2W 10.49968529 W
PL12W 0.32149649 W
PL13W 0.32149649 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127750 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40




```
Current Data Parameters
NAME           101990-wt
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110119
Time               14.10
INSTRUM            spect
PROBHD   5 mm PABBI 1H-
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   32
DS                    0
SWH             7500.000 Hz
FIDRES          0.228882 Hz
AQ             2.1845834 sec
RG                  228
DW                66.667 usec
DE                 6.50 usec
TE                299.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                 8.00 usec
PL1                3.00 dB
PL1W        14.98121262 W
SFO1        500.1325007 MHz

F2 - Processing parameters
SI                16384
SF          500.1300709 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

101990-wt

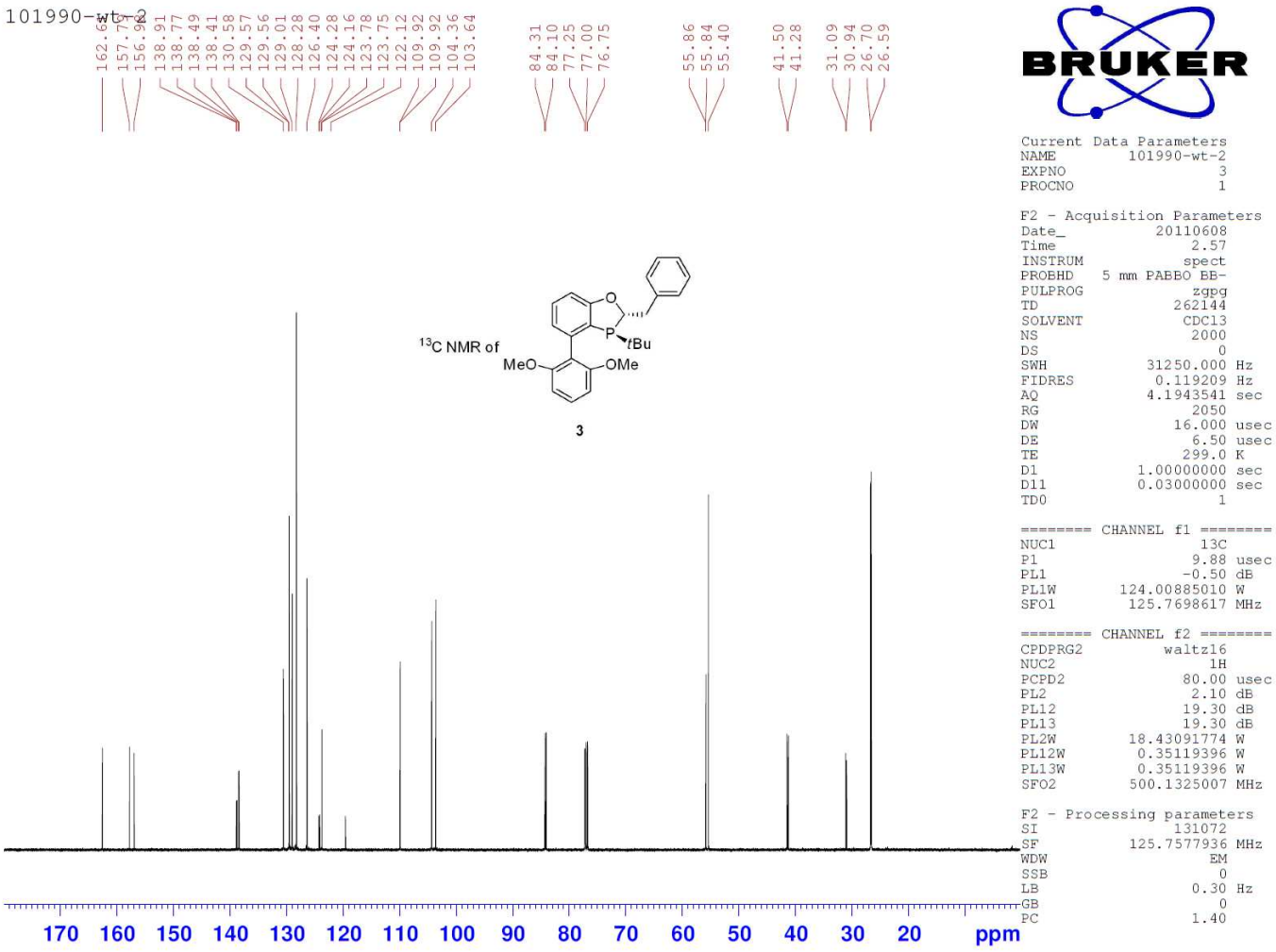

```
Current Data Parameters
NAME          101990-wt
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20110119
Time              14.07
INSTRUM           spect
PROBHD   5 mm PABBI 1H-
PULPROG           zgpg
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    0
SWH           81521.742 Hz
FIDRES         1.243923 Hz
AQ            0.4020041 sec
RG                 2050
DW                6.133 usec
DE                 6.50 usec
TE                299.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                31P
P1                25.00 usec
PL1                2.50 dB
PL1W        65.68299866 W
SFO1       202.4644333 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             80.00 usec
PL2                3.00 dB
PL12              23.00 dB
PL13              23.00 dB
PL2W        14.98121262 W
PL12W        0.14981212 W
PL13W        0.14981212 W
SFO2       500.1325007 MHz

F2 - Processing parameters
SI                131072
SF           202.4563066 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.40
```



BRUKER

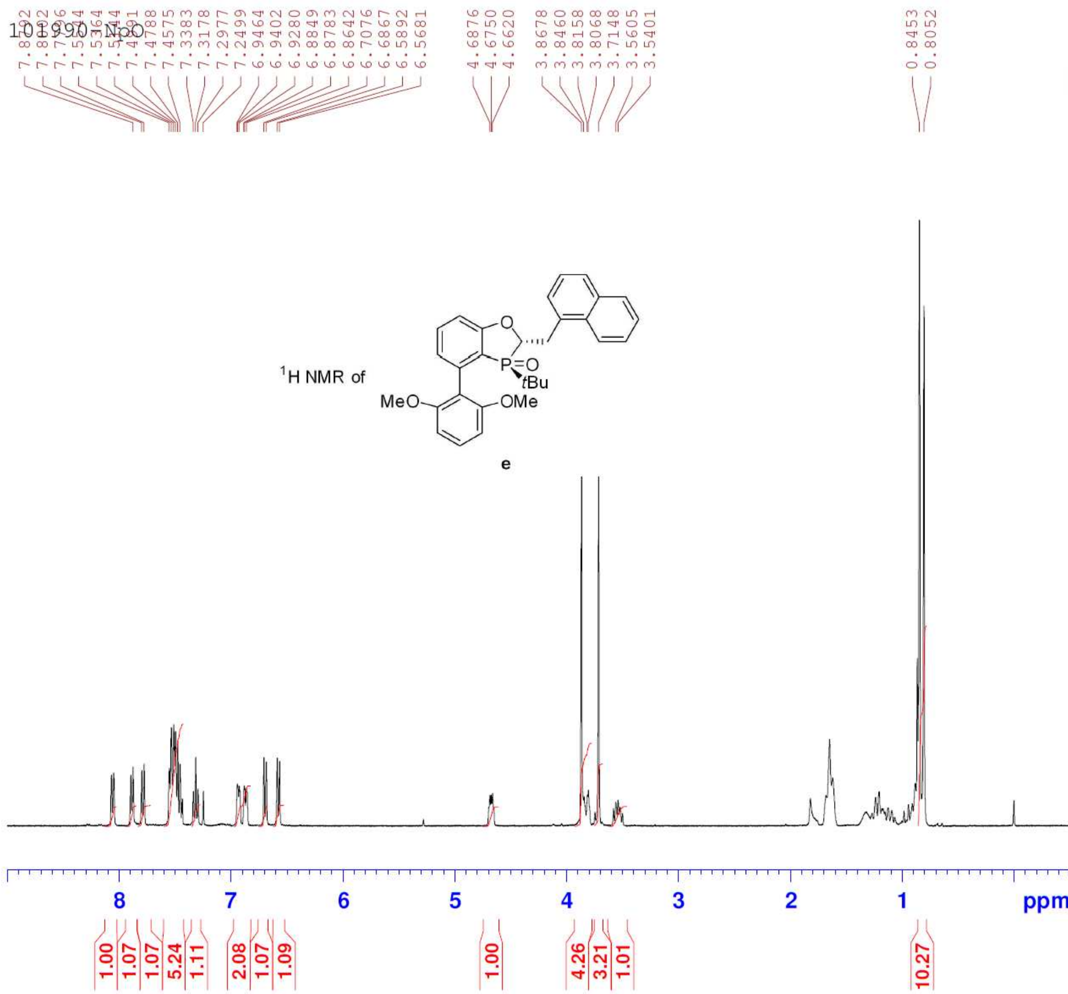
Current Data Parameters
NAME 101990-wt-2
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110608
Time 2.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 262144
SOLVENT CDCl3
NS 2000
DS 0
SWH 31250.000 Hz
FIDRES 0.119209 Hz
AQ 4.1943541 sec
RG 2050
DW 16.000 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.88 usec
PL1 -0.50 dB
PL1W 124.00885010 W
SFO1 125.7698617 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.10 dB
PL12 19.30 dB
PL13 19.30 dB
PL2W 18.43091774 W
PL12W 0.35119396 W
PL13W 0.35119396 W
SFO2 500.1325007 MHz

F2 - Processing parameters
SI 131072
SF 125.7577936 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



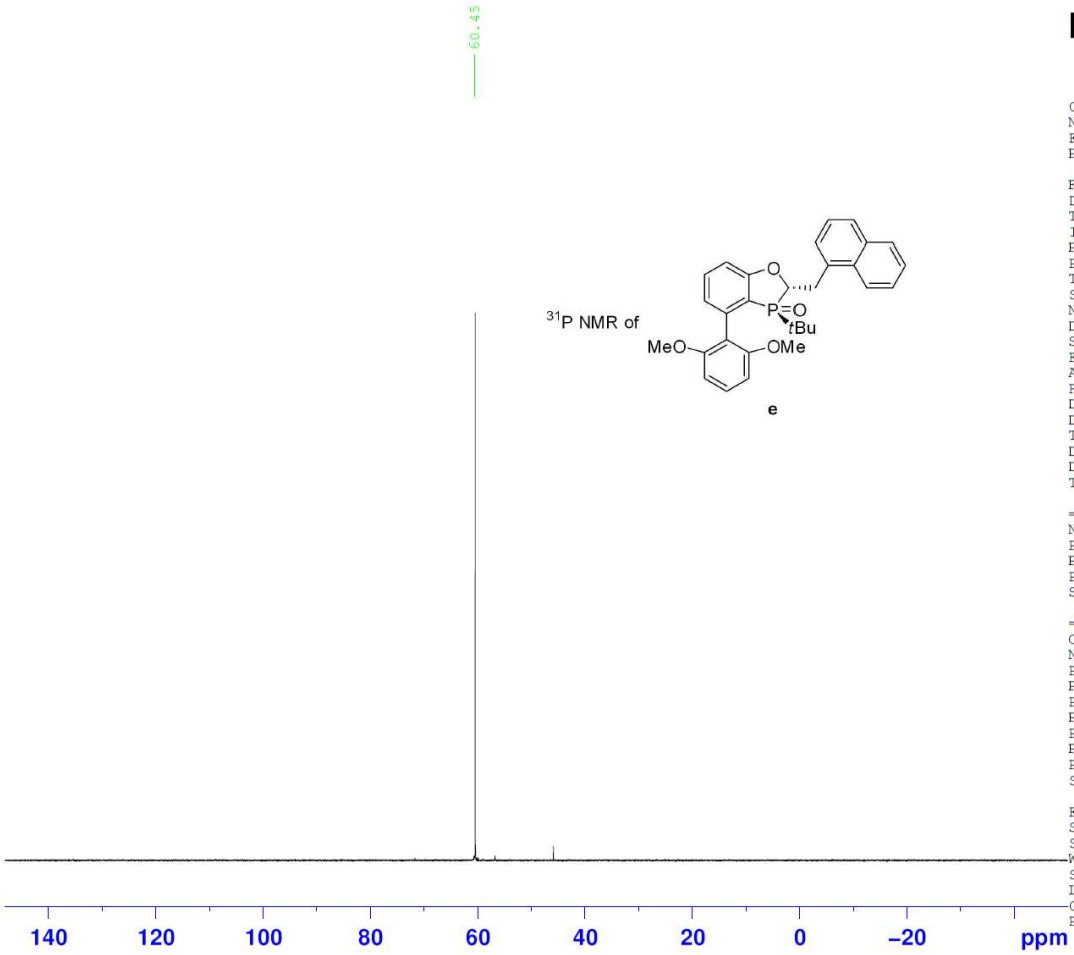

```
Current Data Parameters
NAME             101990-npo
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20110323
Time                  16.08
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG                zg10
TD                    32768
SOLVENT               CDCl3
NS                       16
DS                        4
SWH              5896.227 Hz
FIDRES           0.179939 Hz
AQ              2.7787764 sec
RG                      322
DW                   84.800 usec
DE                     6.50 usec
TE                    298.0 K
D1               2.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    14.00 usec
PL1                    0.00 dB
PL1W            10.49968529 W
SFO1            400.1327209 MHz

F2 - Processing parameters
SI                    65536
SF              400.1300163 MHz
WDW                      EM
SSB                       0
LB                     0.05 Hz
GB                        0
PC                     1.00
```

101990-NpO



^{31}P NMR of

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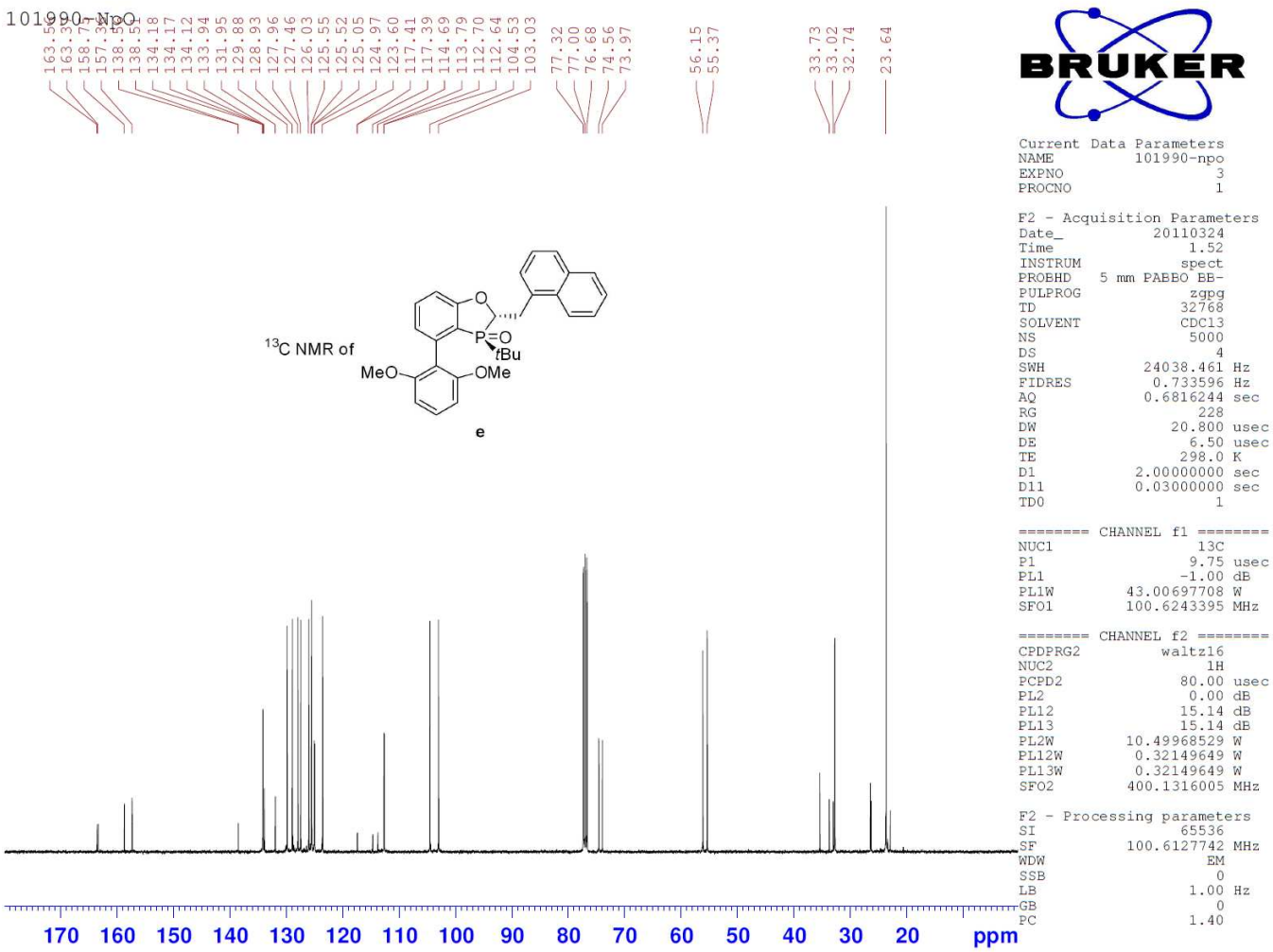
```
Current Data Parameters
NAME          101990-npo
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110323
Time               16.10
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    4
SWH           64102.563 Hz
FIDRES        0.978127 Hz
AQ            0.5112308 sec
RG                 2050
DW                7.800 usec
DE                6.50 usec
TE                298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                31P
P1                13.75 usec
PL1                4.00 dB
PL1W         9.76000023 W
SFO1        161.9674942 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               15.14 dB
PL13               15.14 dB
PL2W        10.49968529 W
PL12W        0.32149649 W
PL13W        0.32149649 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          161.9755588 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```



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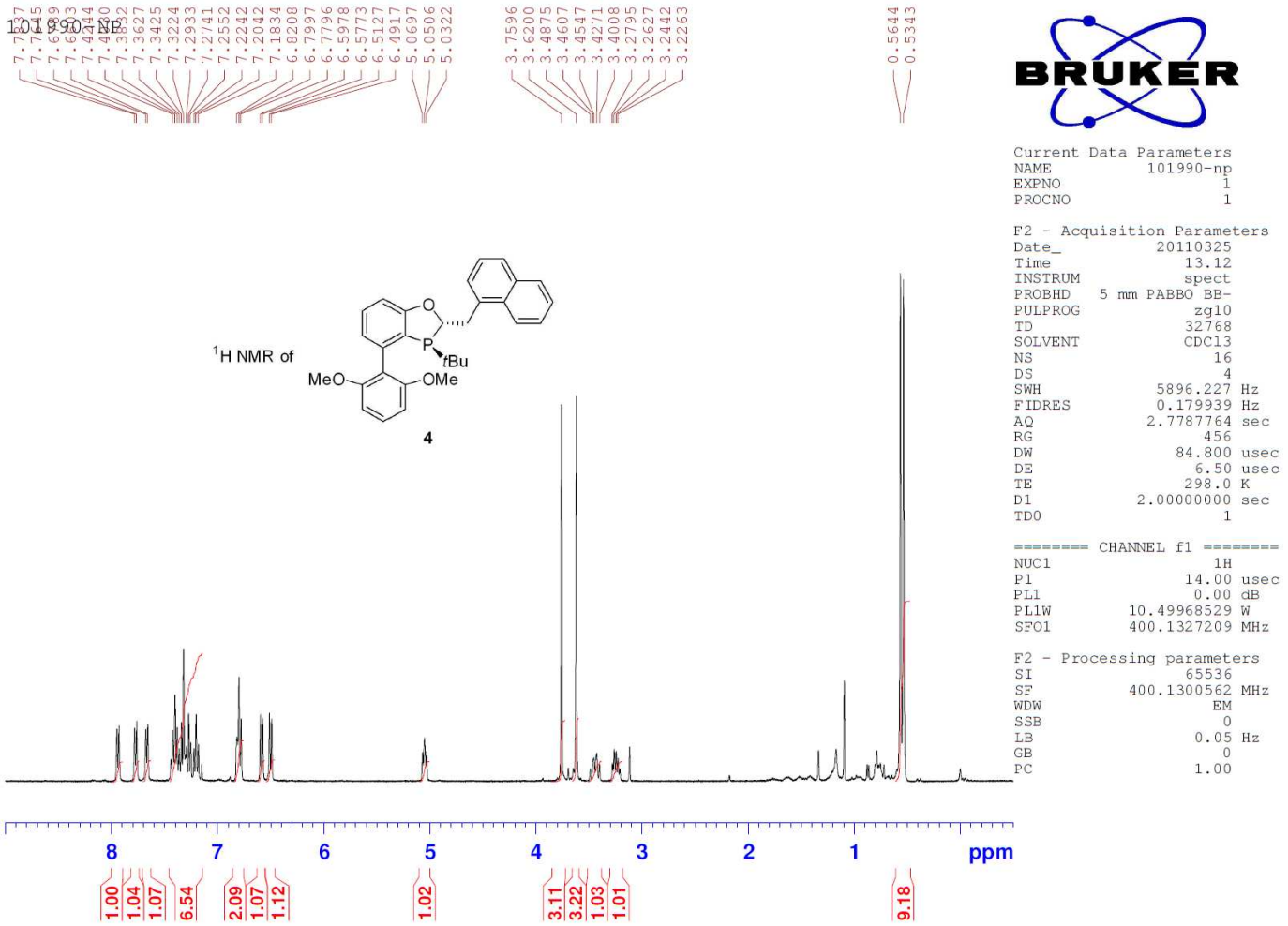
Current Data Parameters
NAME 101990-npo
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110324
Time 1.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 5000
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 228
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.75 usec
PL1 -1.00 dB
PL1W 43.00697708 W
SFO1 100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.14 dB
PL13 15.14 dB
PL2W 10.49968529 W
PL12W 0.32149649 W
PL13W 0.32149649 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127742 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



BRUKER

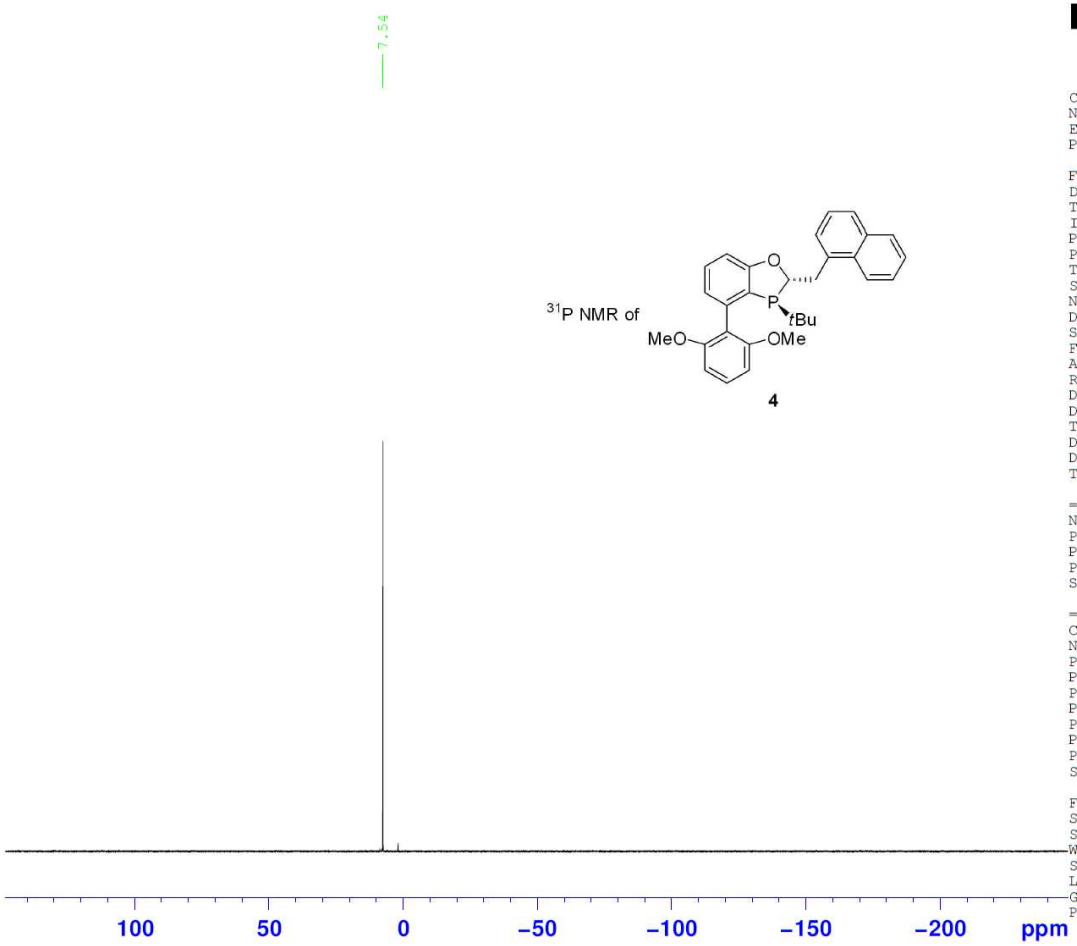
Current Data Parameters
NAME 101990-np
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110325
Time 13.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg10
TD 32768
SOLVENT CDCl3
NS 16
DS 4
SWH 5896.227 Hz
FIDRES 0.179939 Hz
AQ 2.7787764 sec
RG 456
DW 84.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
PL1W 10.49968529 W
SFO1 400.1327209 MHz

F2 - Processing parameters
SI 65536
SF 400.1300562 MHz
WDW EM
SSB 0
LB 0.05 Hz
GB 0
PC 1.00

101990-NP



^{31}P NMR of

4

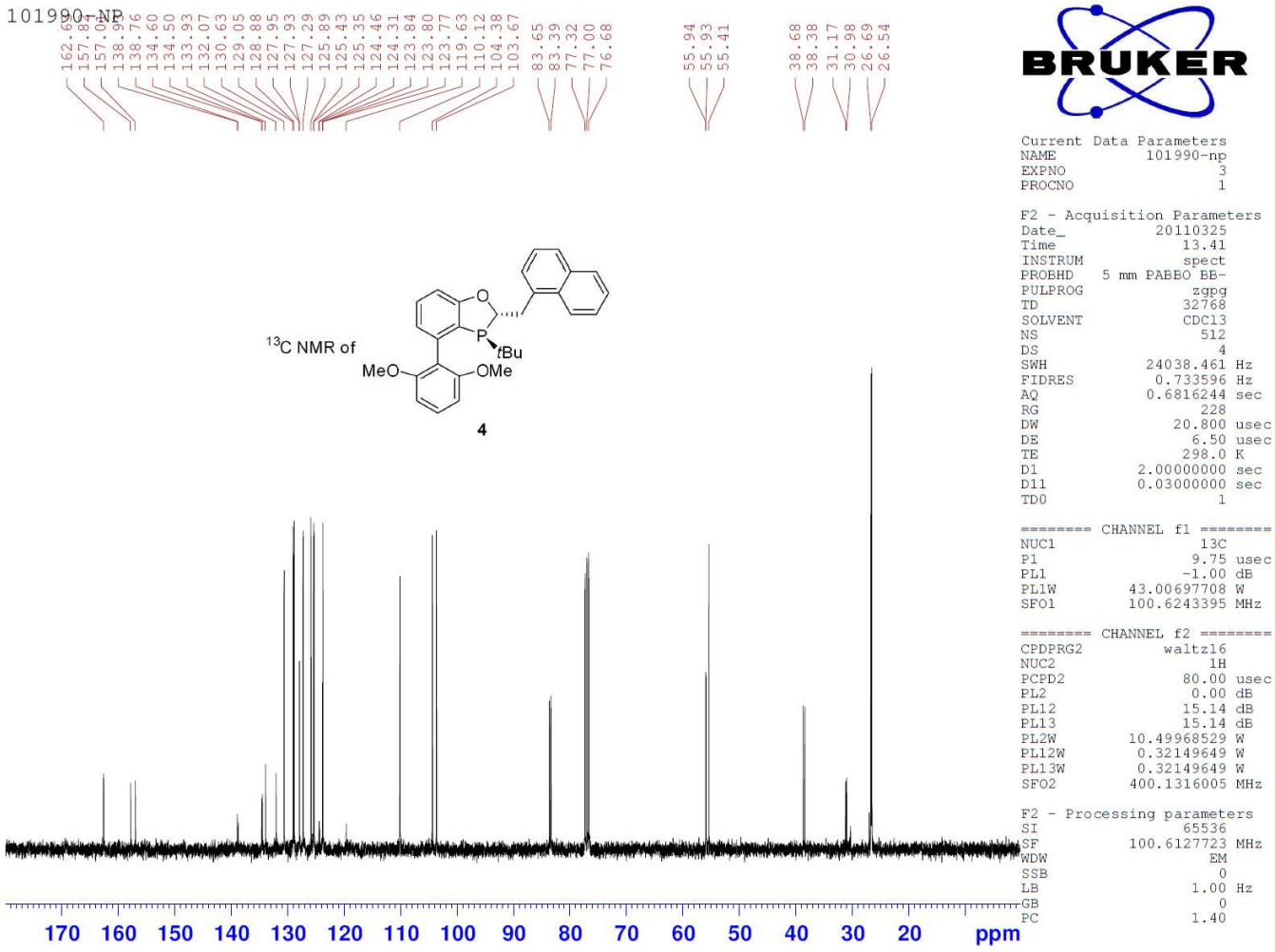
```
Current Data Parameters
NAME           101990-np
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110325
Time               13.15
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    4
SWH           64102.563 Hz
FIDRES        0.978127 Hz
AQ            0.5112308 sec
RG                 2050
DW                7.800 usec
DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                31P
P1                13.75 usec
PL1                4.00 dB
PL1W         9.76000023 W
SFO1        161.9674942 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               15.14 dB
PL13               15.14 dB
PL2W        10.49968529 W
PL12W        0.32149649 W
PL13W        0.32149649 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          161.9755588 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



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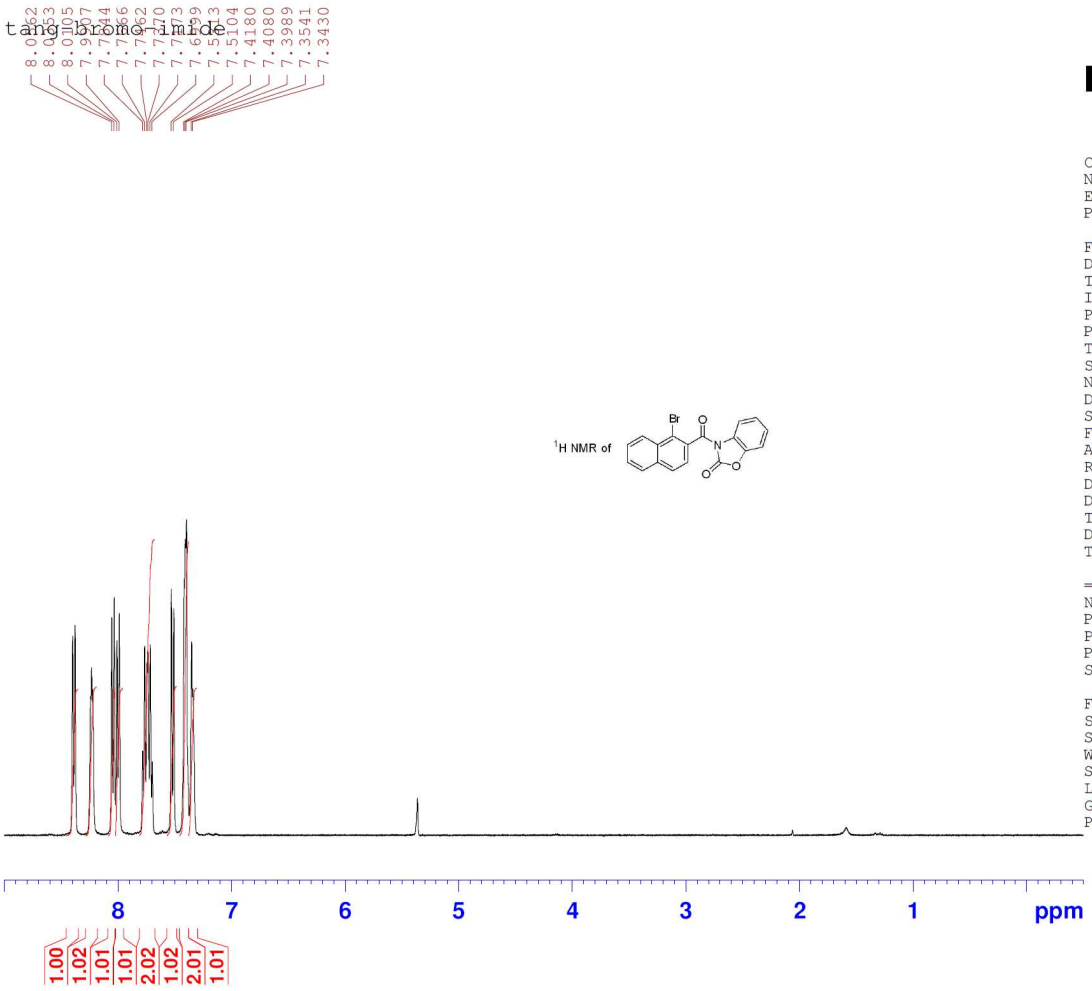
Current Data Parameters
NAME 101990-np
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110325
Time 13.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 228
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.75 usec
PL1 -1.00 dB
PL1W 43.00697708 W
SFO1 100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.14 dB
PL13 15.14 dB
PL2W 10.49968529 W
PL12W 0.32149649 W
PL13W 0.32149649 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127723 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



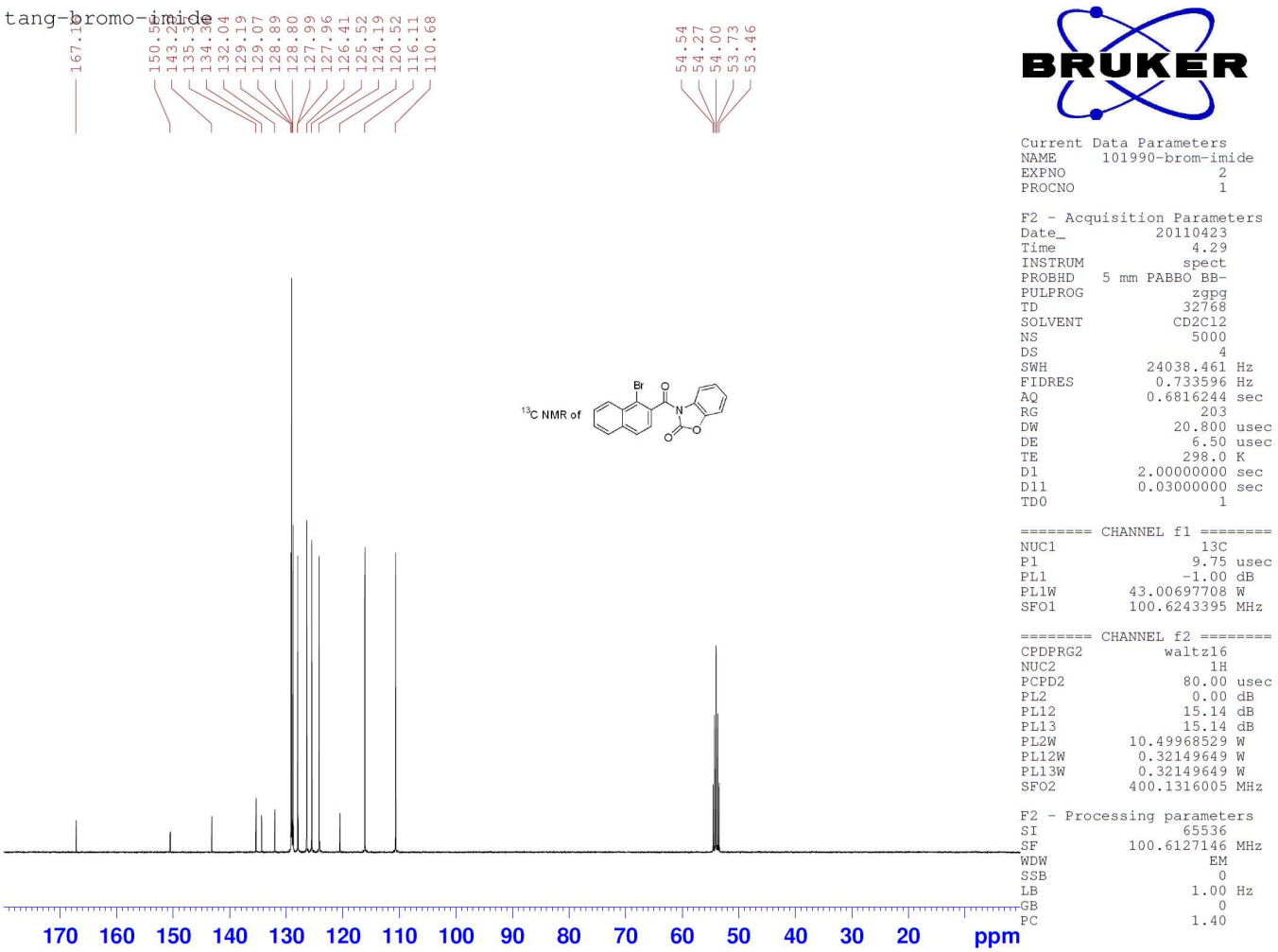
BRUKER

```
Current Data Parameters
NAME      101990-brom-imide
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20110423
Time                   0.38
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG                zg10
TD                    32768
SOLVENT            CD2Cl2
NS                        16
DS                         4
SWH               5896.227 Hz
FIDRES            0.179939 Hz
AQ                2.7787764 sec
RG                      406
DW                 84.800 usec
DE                  6.50 usec
TE                  298.0 K
D1             2.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                 14.00 usec
PL1                 0.00 dB
PL1W          10.49968529 W
SFO1          400.1327209 MHz

F2 - Processing parameters
SI                    65536
SF            400.1300000 MHz
WDW                      EM
SSB                       0
LB                   0.05 Hz
GB                        0
PC                     1.00
```



BRUKER

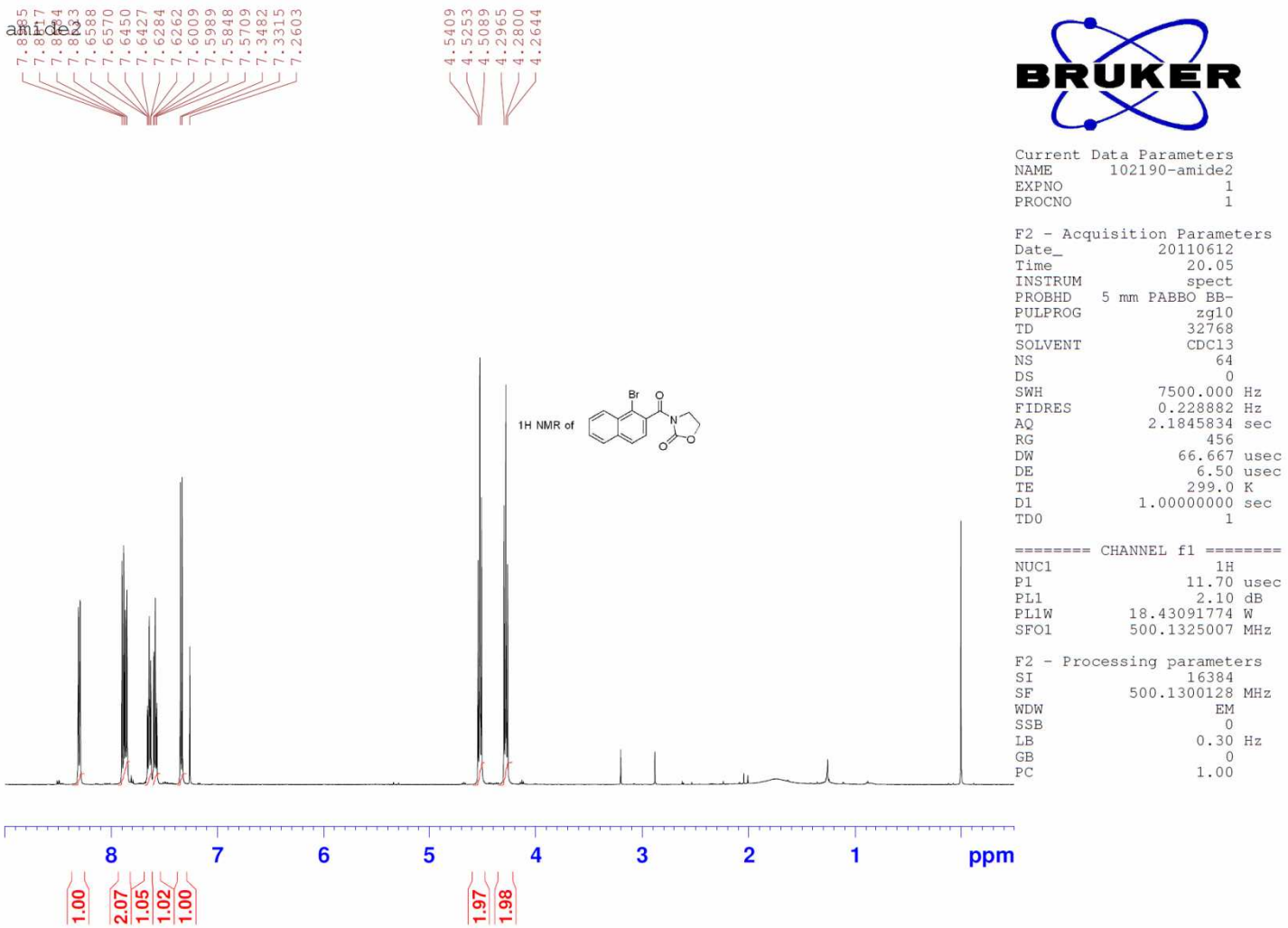
Current Data Parameters
NAME 101990-brom-imide
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110423
Time 4.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 32768
SOLVENT CD2C12
NS 5000
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.75 usec
PL1 -1.00 dB
PL1W 43.00697708 W
SFO1 100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.14 dB
PL13 15.14 dB
PL2W 10.49968529 W
PL12W 0.32149649 W
PL13W 0.32149649 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127146 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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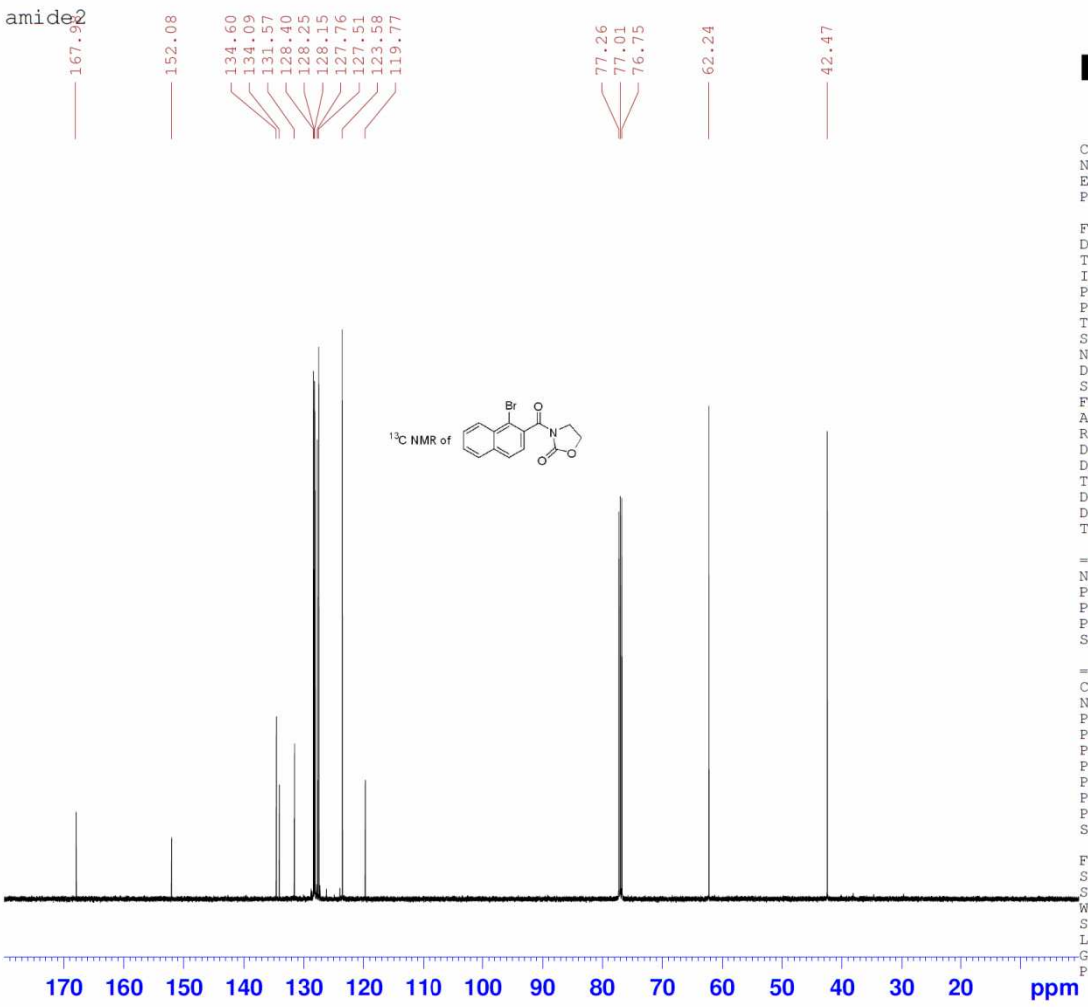
```
Current Data Parameters
NAME       102190-amide2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110612
Time               20.05
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg10
TD                 32768
SOLVENT            CDCl3
NS                    64
DS                     0
SWH             7500.000 Hz
FIDRES          0.228882 Hz
AQ              2.1845834 sec
RG                   456
DW                66.667 usec
DE                 6.50 usec
TE                299.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.70 usec
PL1                 2.10 dB
PL1W         18.43091774 W
SFO1         500.1325007 MHz

F2 - Processing parameters
SI                 16384
SF           500.1300128 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



BRUKER

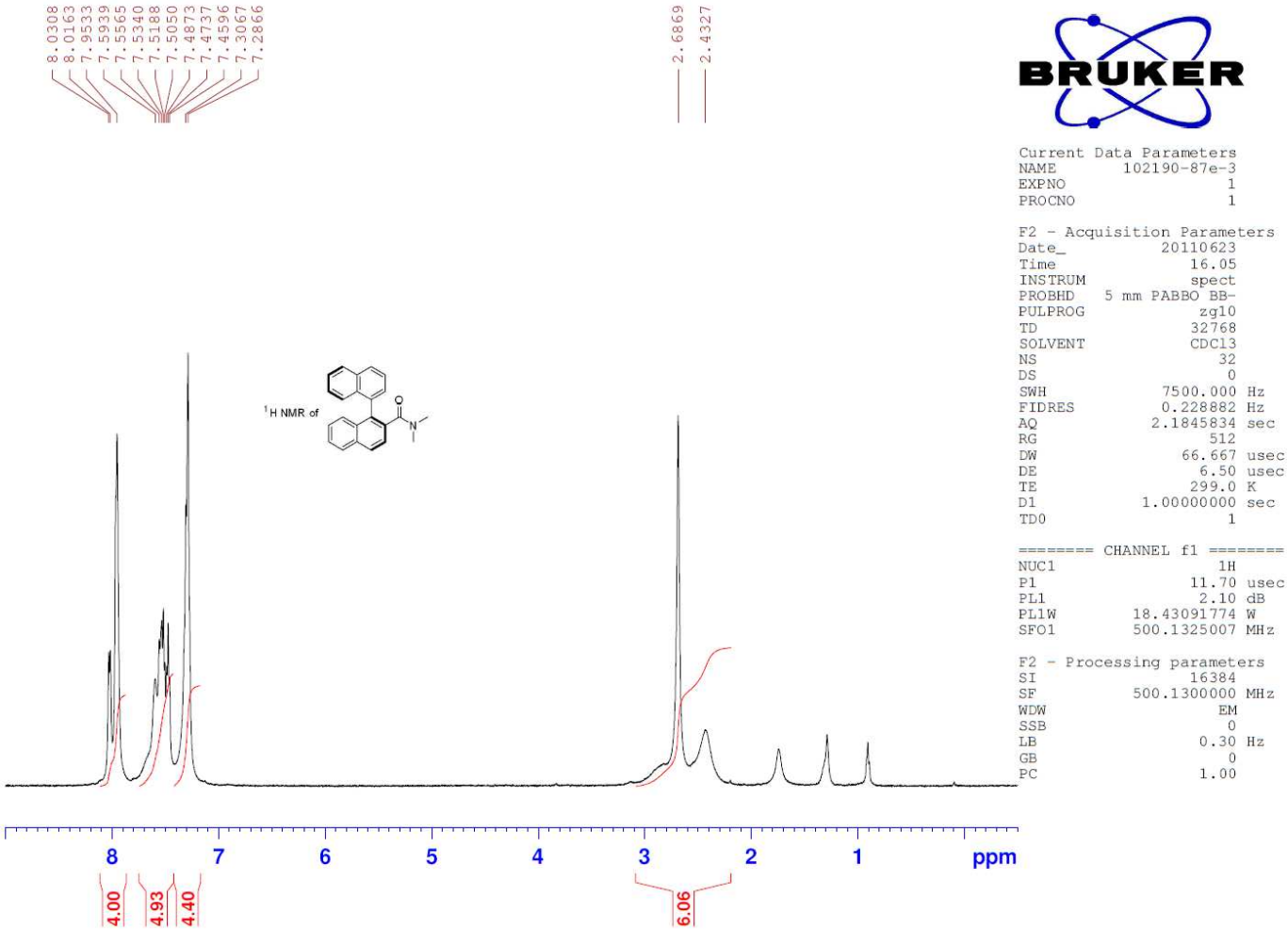
```
Current Data Parameters
NAME      102190-amide2
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20110613
Time               0.29
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg
TD                262144
SOLVENT            CDCl3
NS                  3000
DS                     0
SWH            31250.000 Hz
FIDRES             0.119209 Hz
AQ                 4.1943541 sec
RG                    2050
DW                   16.000 usec
DE                    6.50 usec
TE                   299.0 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.88 usec
PL1                 -0.50 dB
PL1W        124.00885010 W
SFO1         125.7698617 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2                80.00 usec
PL2                   2.10 dB
PL12                 19.30 dB
PL13                 19.30 dB
PL2W         18.43091774 W
PL12W         0.35119396 W
PL13W         0.35119396 W
SFO2        500.1325007 MHz

F2 - Processing parameters
SI                  131072
SF           125.7577920 MHz
WDW                    EM
SSB                    0
LB                   0.30 Hz
GB                     0
PC                   1.40
```



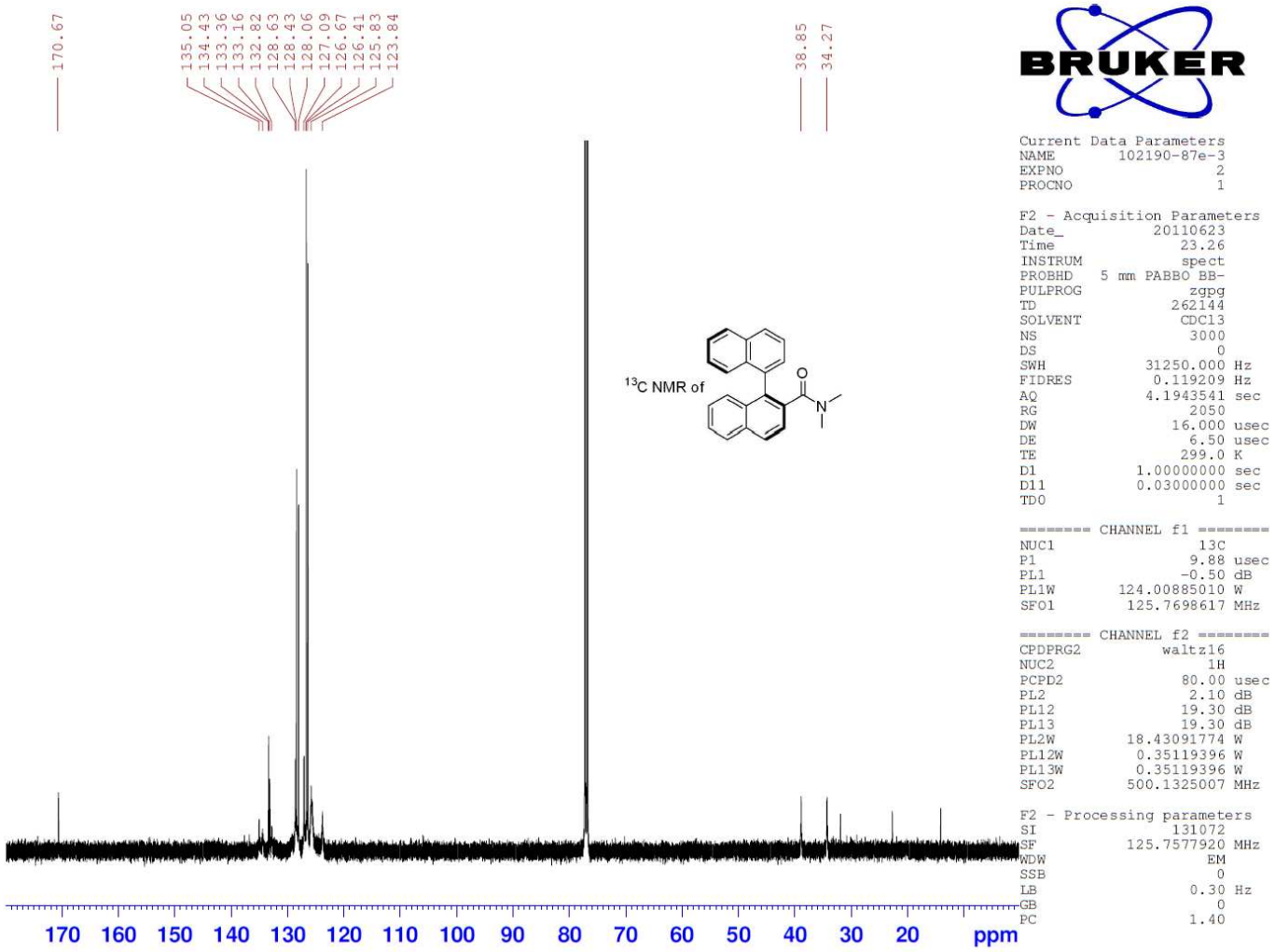
BRUKER

```
Current Data Parameters
NAME        102190-87e-3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110623
Time               16.05
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg10
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             7500.000 Hz
FIDRES             0.228882 Hz
AQ              2.1845834 sec
RG                   512
DW                66.667 usec
DE                 6.50 usec
TE                299.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.70 usec
PL1                 2.10 dB
PL1W         18.43091774 W
SFO1         500.1325007 MHz

F2 - Processing parameters
SI                 16384
SF           500.1300000 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```



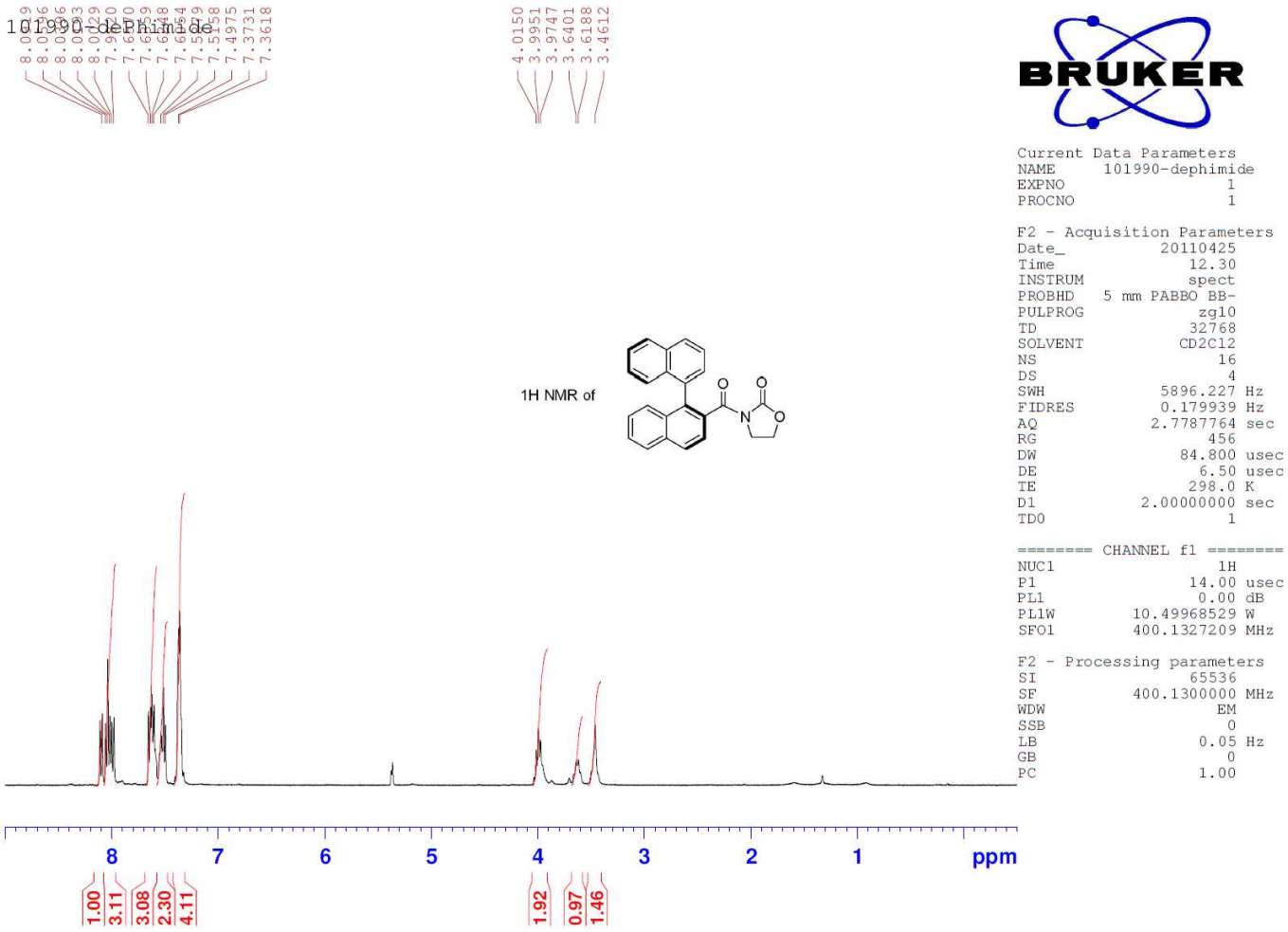

```
Current Data Parameters
NAME       102190-87e-3
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20110623
Time              23.26
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg
TD               262144
SOLVENT          CDCl3
NS                3000
DS                   0
SWH          31250.000 Hz
FIDRES        0.119209 Hz
AQ            4.1943541 sec
RG                2050
DW              16.000 usec
DE               6.50 usec
TE              299.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                9.88 usec
PL1              -0.50 dB
PL1W       124.00885010 W
SFO1        125.7698617 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               2.10 dB
PL12             19.30 dB
PL13             19.30 dB
PL2W       18.43091774 W
PL12W       0.35119396 W
PL13W       0.35119396 W
SFO2       500.1325007 MHz

F2 - Processing parameters
SI              131072
SF        125.7577920 MHz
WDW               EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.40
```

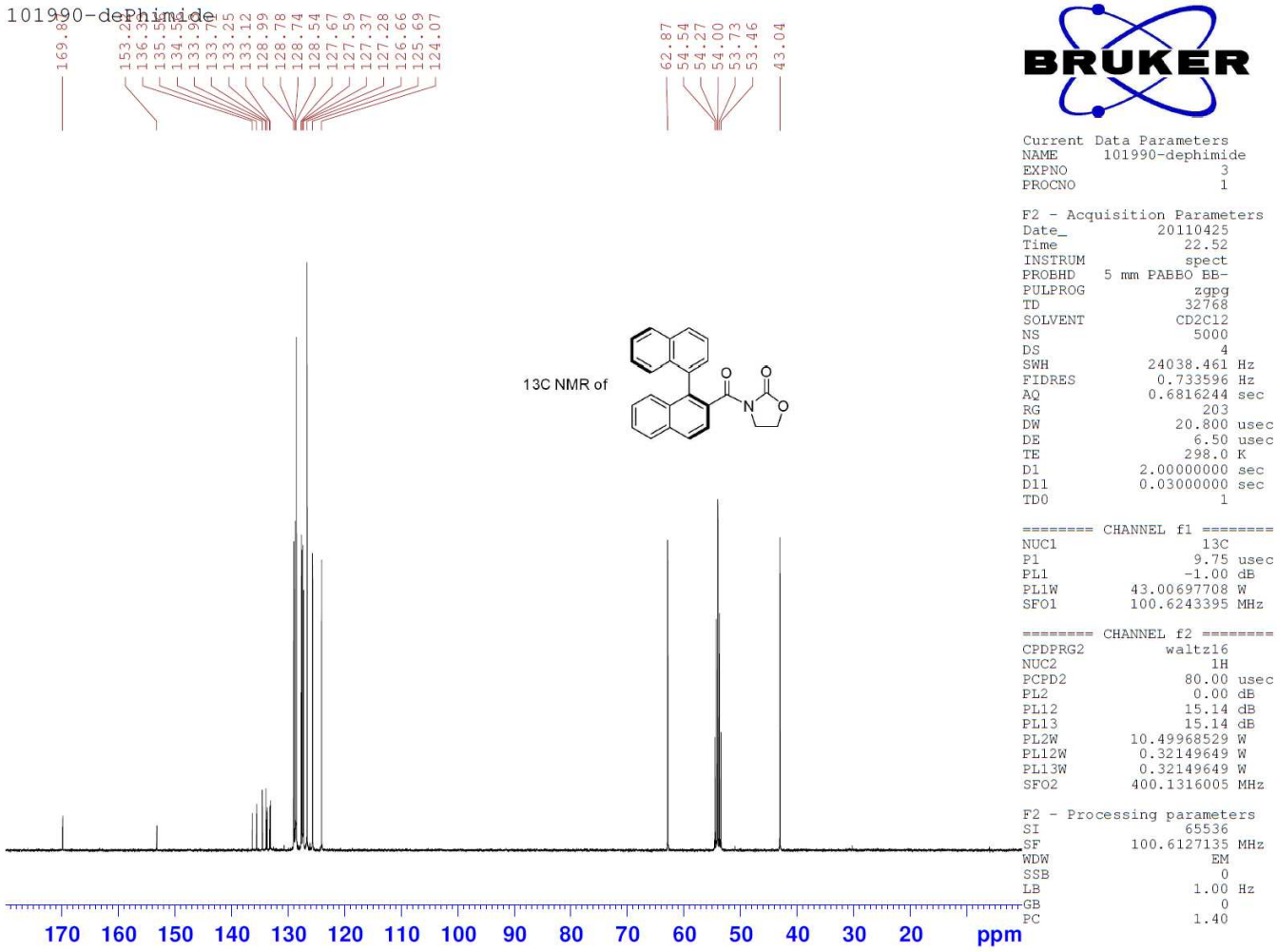


Current Data Parameters
NAME 101990-dephimide
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110425
Time 12.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg10
TD 32768
SOLVENT CD2C12
NS 16
DS 4
SWH 5896.227 Hz
FIDRES 0.179939 Hz
AQ 2.7787764 sec
RG 456
DW 84.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
PL1W 10.49968529 W
SFO1 400.1327209 MHz

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.05 Hz
GB 0
PC 1.00



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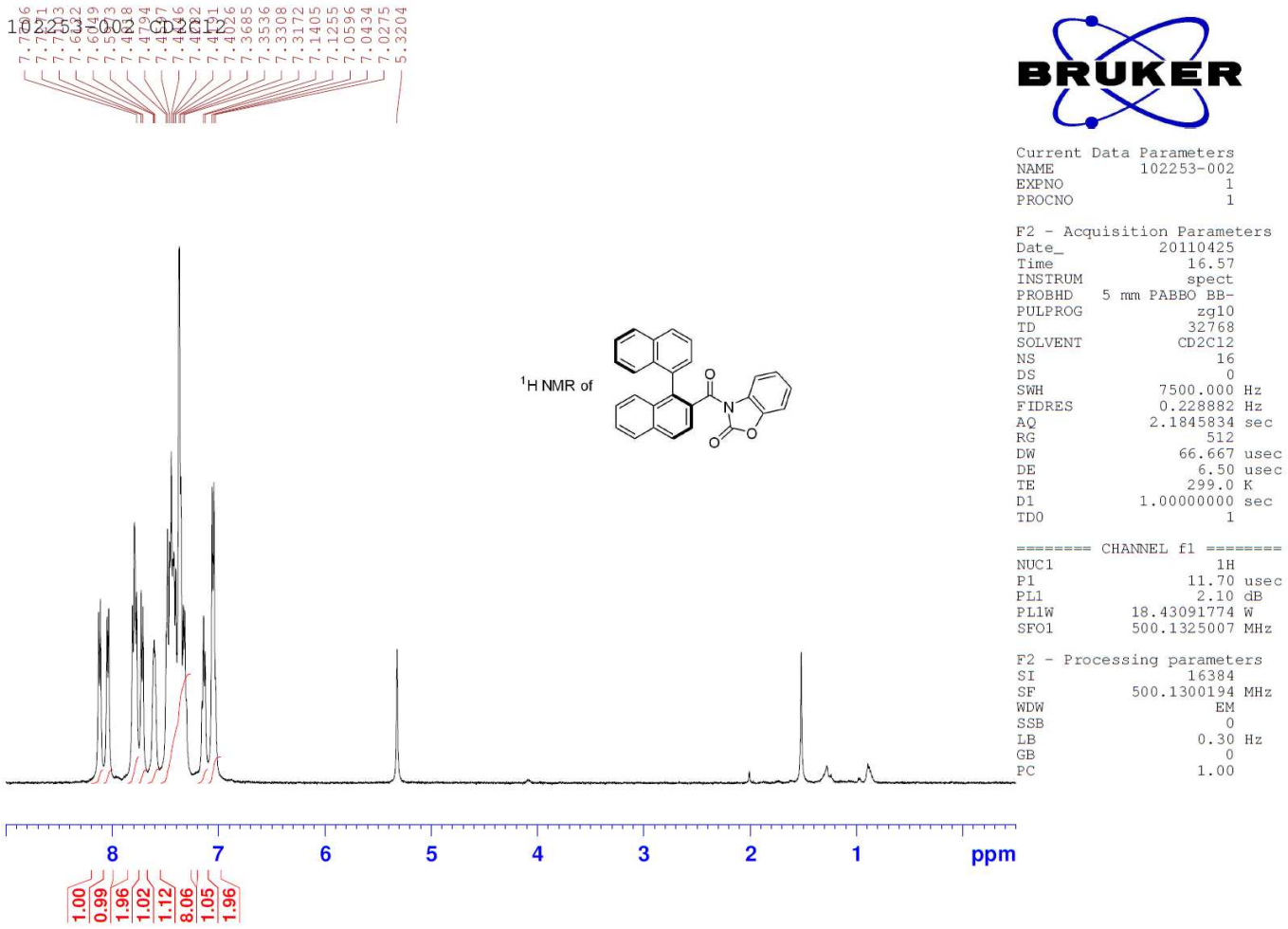
Current Data Parameters
NAME 101990-dephimide
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110425
Time 22.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 32768
SOLVENT CD2Cl2
NS 5000
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.75 usec
PL1 -1.00 dB
PL1W 43.00697708 W
SFO1 100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.14 dB
PL13 15.14 dB
PL2W 10.49968529 W
PL12W 0.32149649 W
PL13W 0.32149649 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127135 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



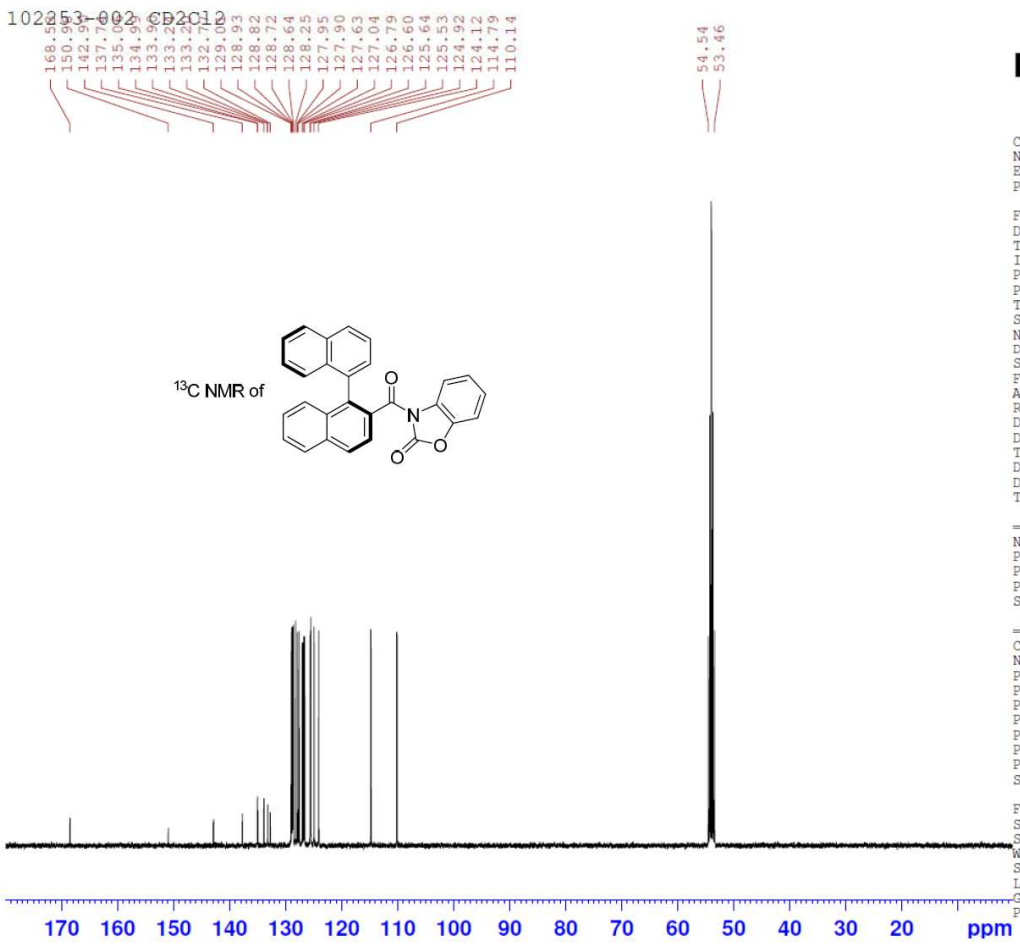
BRUKER

Current Data Parameters
NAME 102253-002
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110425
Time 16.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg10
TD 32768
SOLVENT CD2Cl2
NS 16
DS 0
SWH 7500.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 512
DW 66.667 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 2.10 dB
PL1W 18.43091774 W
SFO1 500.1325007 MHz

F2 - Processing parameters
SI 16384
SF 500.1300194 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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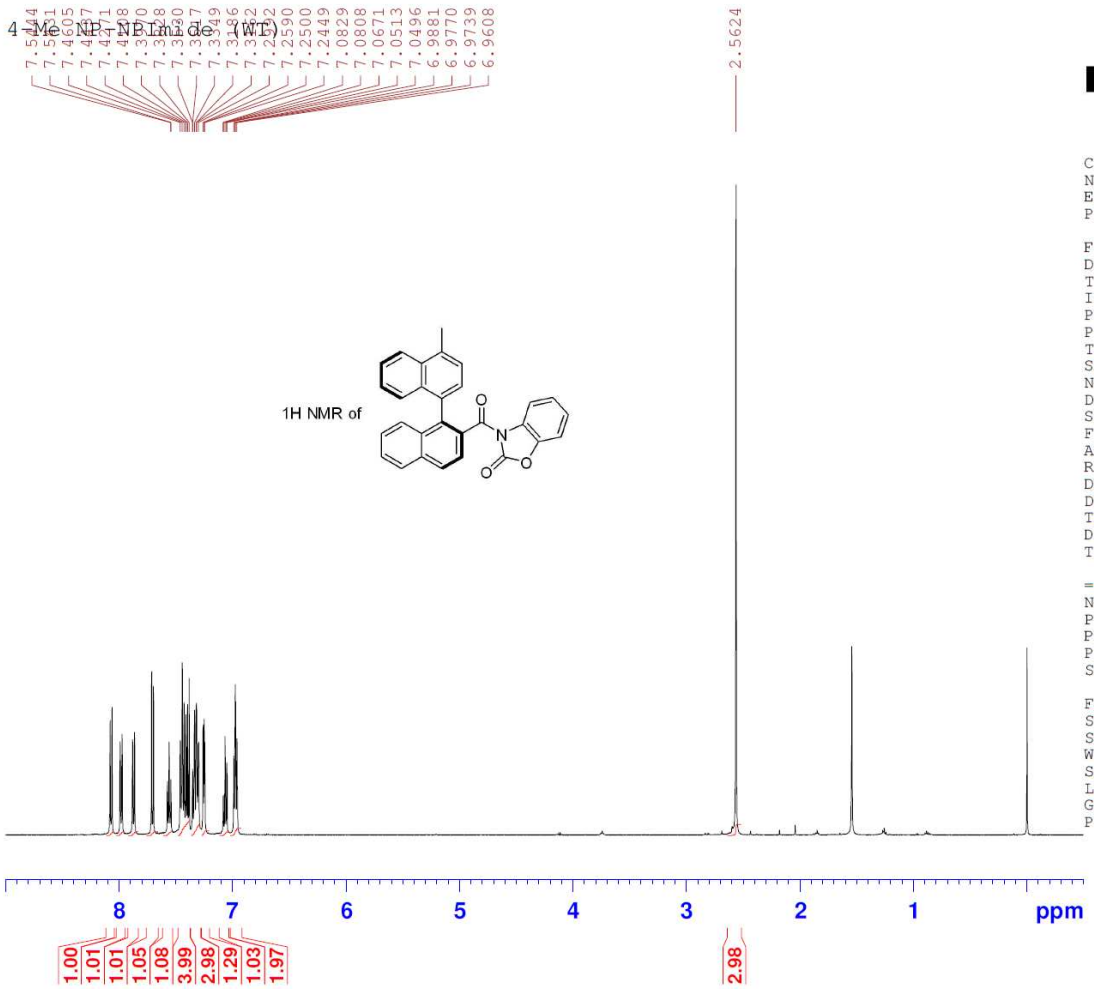
```
Current Data Parameters
NAME          102253-002
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110426
Time              22.53
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg
TD                32768
SOLVENT           CD2C12
NS                 5000
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6816244 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.75 usec
PL1                -1.00 dB
PL1W        43.00697708 W
SFO1        100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               15.14 dB
PL13               15.14 dB
PL2W        10.49968529 W
PL12W        0.32149649 W
PL13W        0.32149649 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                65536
SF          100.6127117 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



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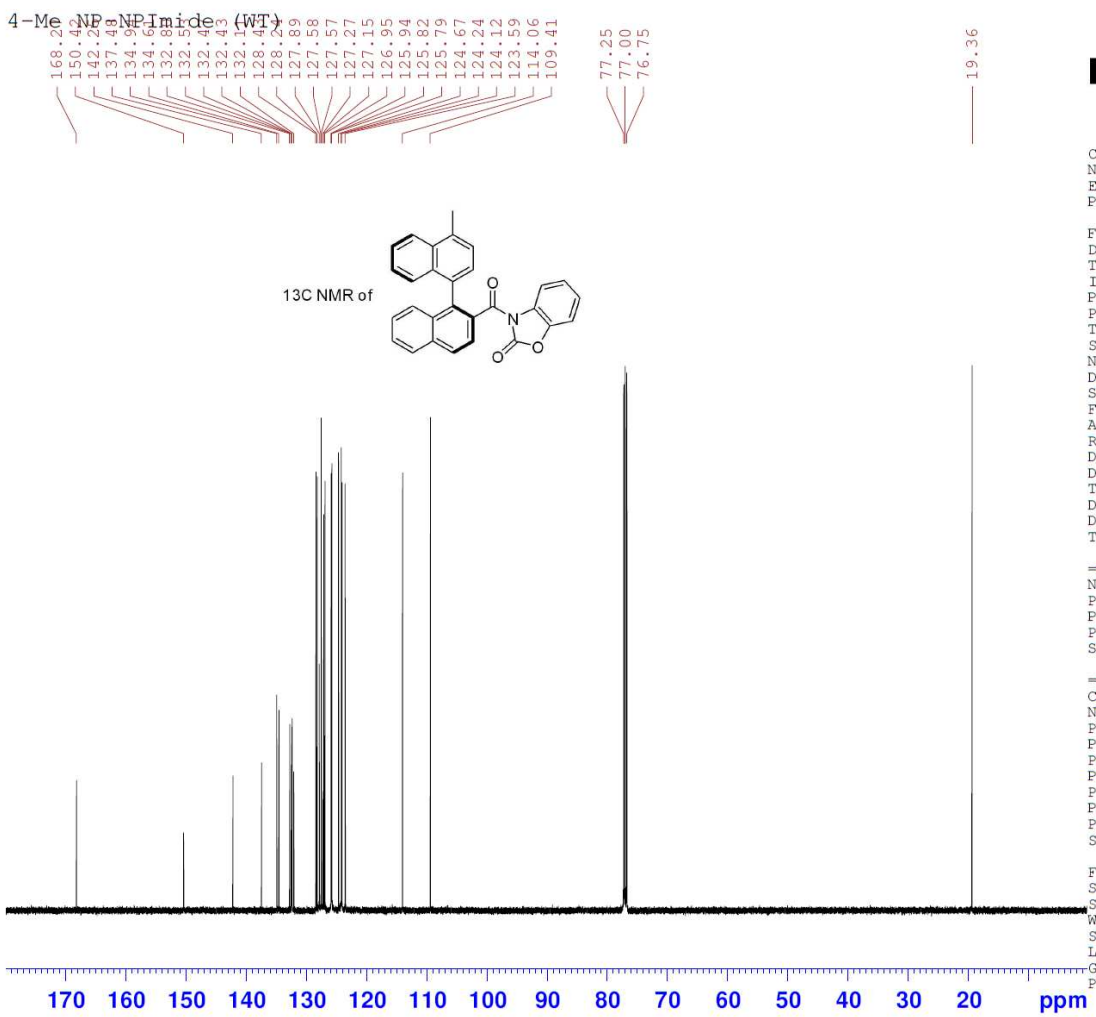
Current Data Parameters
NAME 102190-4menp-np
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110524
Time 19.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg10
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7500.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 406
DW 66.667 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 2.10 dB
PL1W 18.43091774 W
SFO1 500.1325007 MHz

F2 - Processing parameters
SI 16384
SF 500.1300178 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



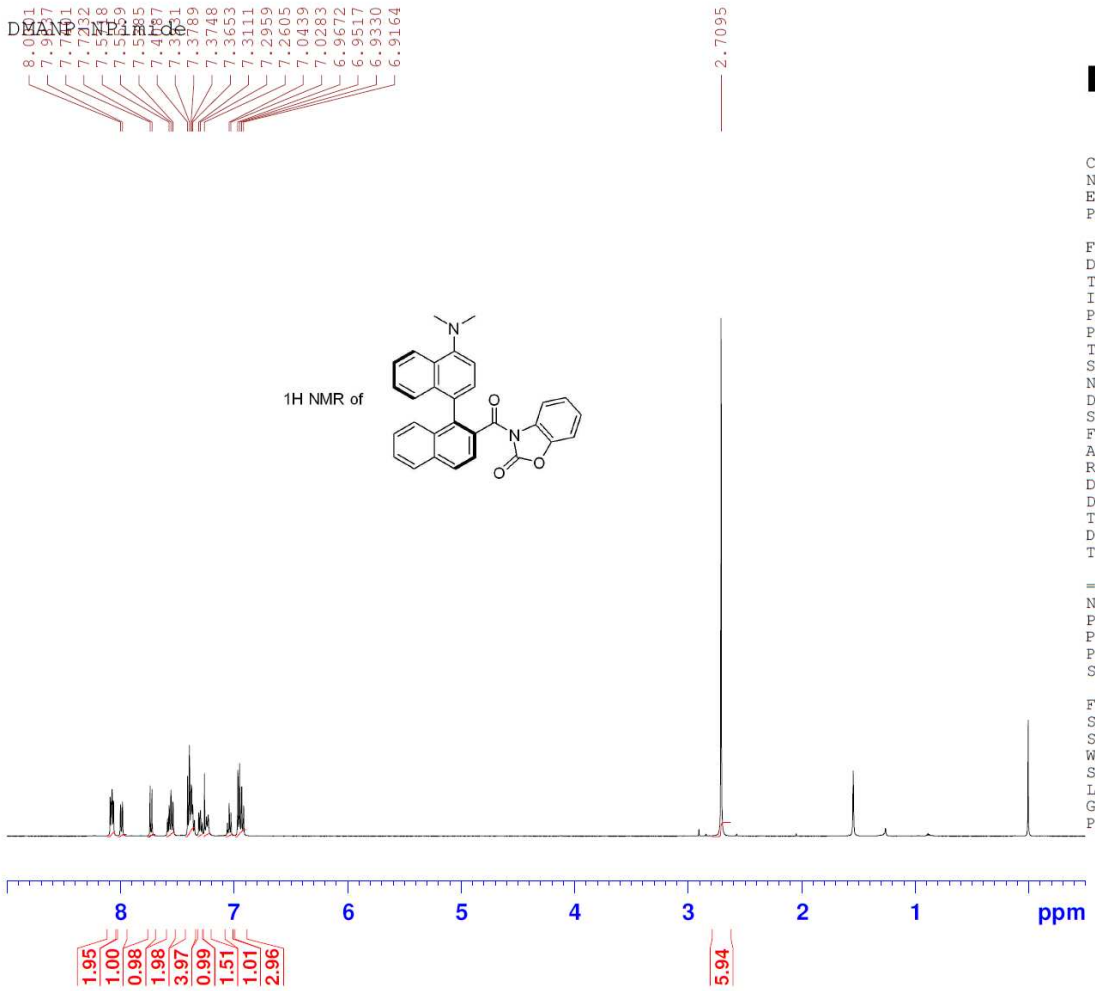
Current Data Parameters
NAME 102190-4menp-np
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110524
Time 23.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 262144
SOLVENT CDCl3
NS 3000
DS 0
SWH 31250.000 Hz
FIDRES 0.119209 Hz
AQ 4.1943541 sec
RG 2050
DW 16.000 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.88 usec
PL1 -0.50 dB
PL1W 124.00885010 W
SFO1 125.7698617 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.10 dB
PL12 19.30 dB
PL13 19.30 dB
PL2W 18.43091774 W
PL12W 0.35119396 W
PL13W 0.35119396 W
SFO2 500.1325007 MHz

F2 - Processing parameters
SI 131072
SF 125.7577929 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



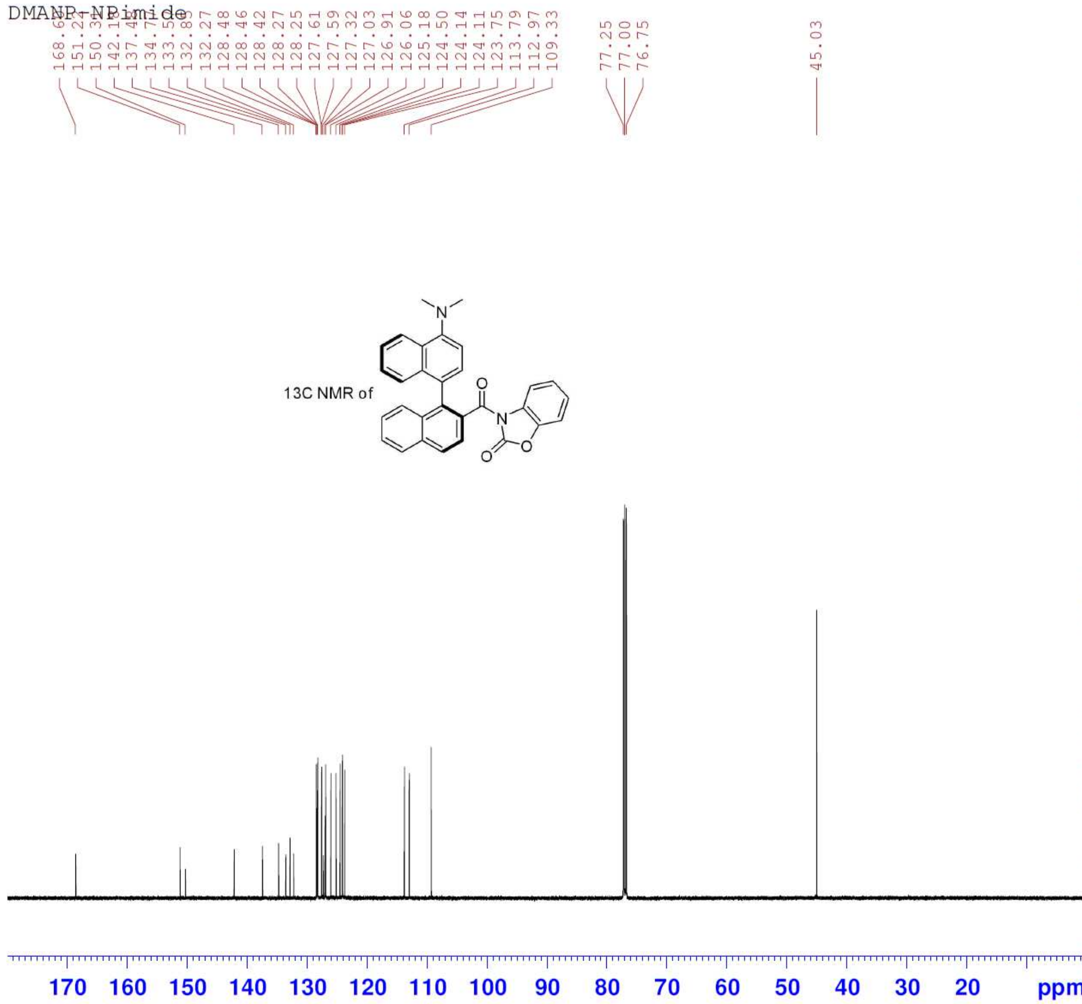
Current Data Parameters
NAME 102190-e70-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110531
Time 21.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg10
TD 32768
SOLVENT CDCl3
NS 64
DS 0
SWH 7500.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 575
DW 66.667 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 2.10 dB
PL1W 18.43091774 W
SFO1 500.1325007 MHz

F2 - Processing parameters
SI 16384
SF 500.1300127 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13C NMR of



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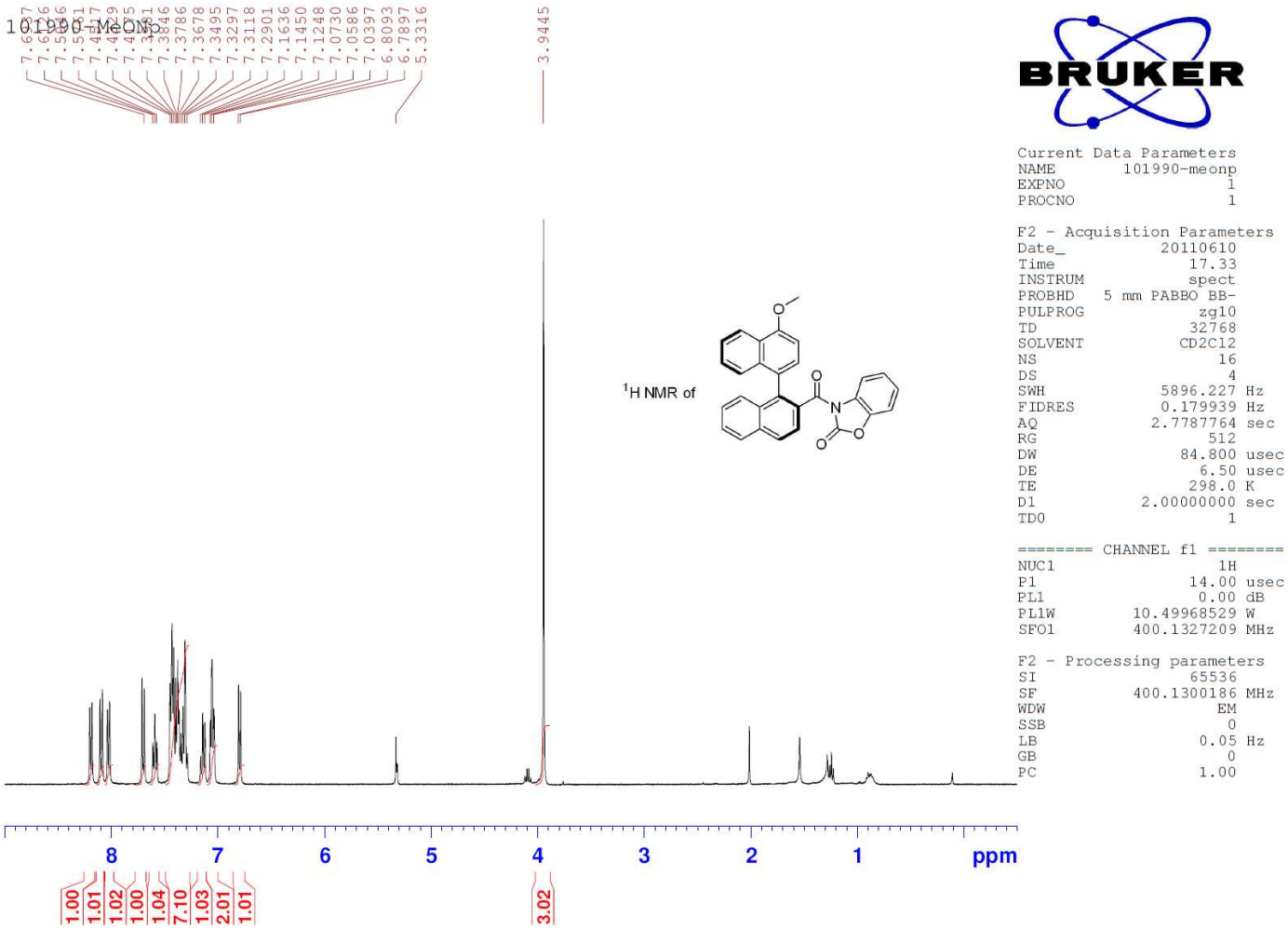
```
Current Data Parameters
NAME        102190-e70-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110601
Time                3.03
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                262144
SOLVENT            CDCl3
NS                  4000
DS                     0
SWH            31250.000 Hz
FIDRES          0.119209 Hz
AQ             4.1943541 sec
RG                  2050
DW                16.000 usec
DE                  6.50 usec
TE                 299.0 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.88 usec
PL1                -0.50 dB
PL1W        124.00885010 W
SFO1         125.7698617 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 2.10 dB
PL12               19.30 dB
PL13               19.30 dB
PL2W         18.43091774 W
PL12W         0.35119396 W
PL13W         0.35119396 W
SFO2         500.1325007 MHz

F2 - Processing parameters
SI                131072
SF           125.7577909 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.40
```



Current Data Parameters

NAME	101990-meonp
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

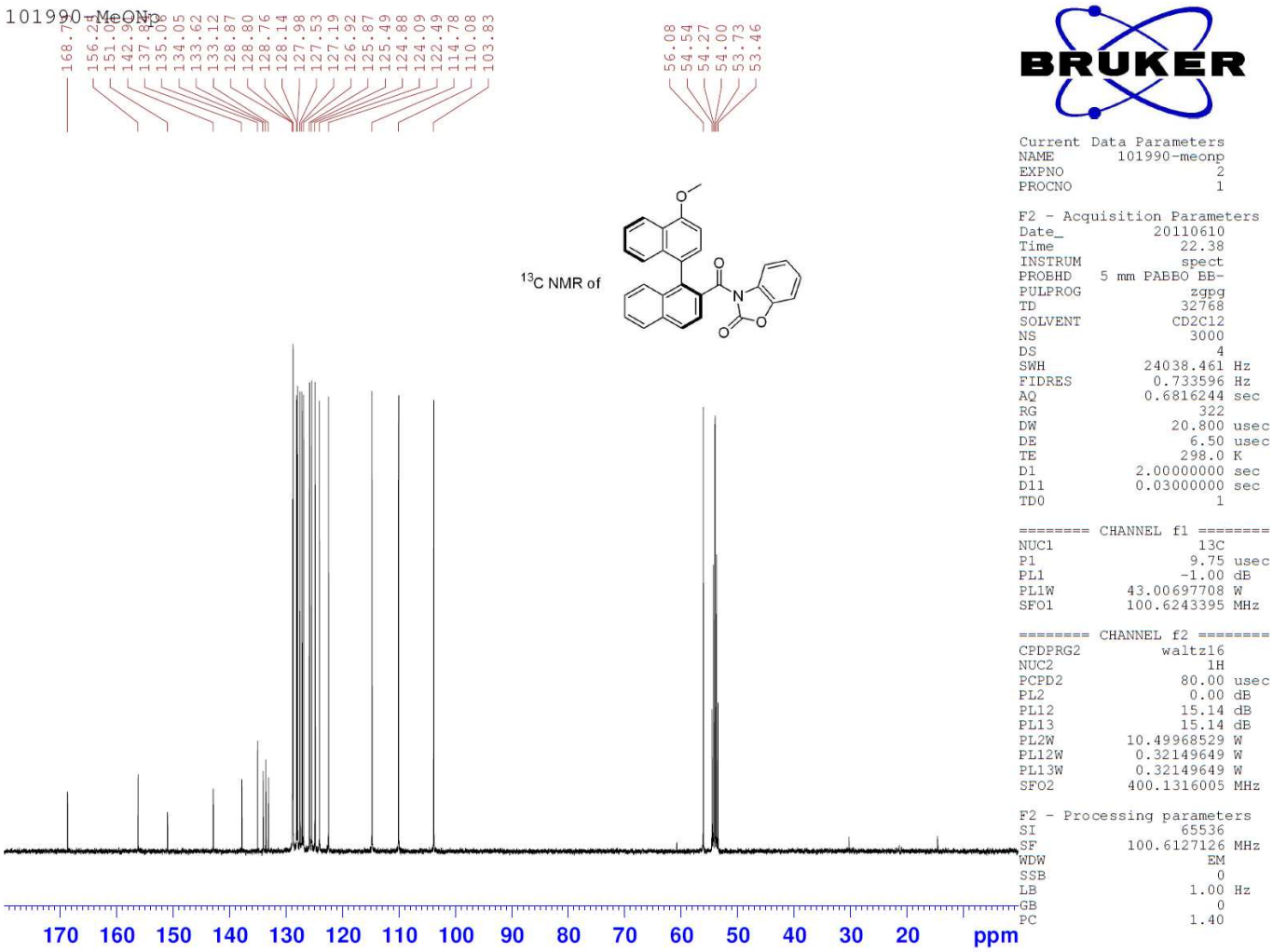
Date_	20110610
Time	17.33
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg10
TD	32768
SOLVENT	CD2Cl2
NS	16
DS	4
SWH	5896.227 Hz
FIDRES	0.179939 Hz
AQ	2.7787764 sec
RG	512
DW	84.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	14.00 usec
PL1	0.00 dB
PL1W	10.49968529 W
SFO1	400.1327209 MHz

F2 - Processing parameters

SI	65536
SF	400.1300186 MHz
WDW	EM
SSB	0
LB	0.05 Hz
GB	0
PC	1.00



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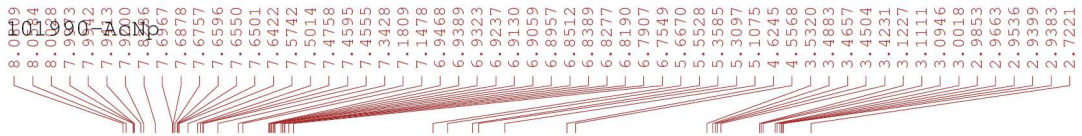
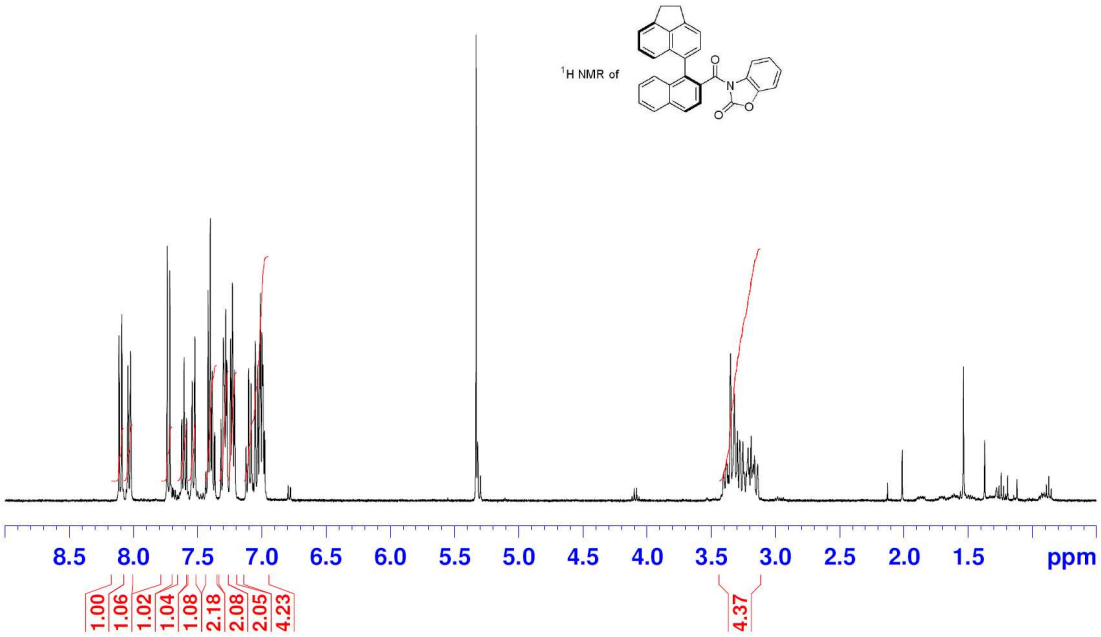
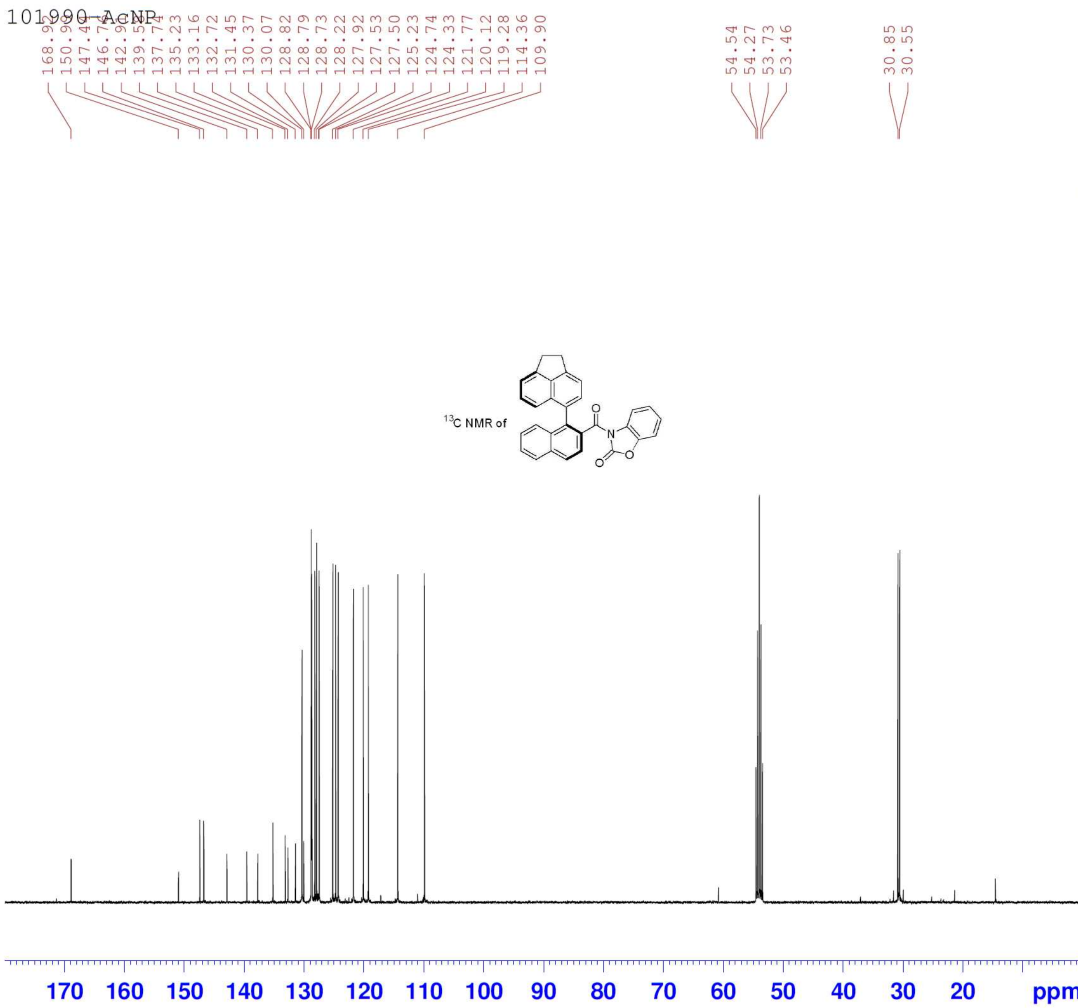
```
Current Data Parameters
NAME         101990-meonp
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20110610
Time               22.38
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg
TD                 32768
SOLVENT           CD2Cl2
NS                   3000
DS                      4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6816244 sec
RG                    322
DW                 20.800 usec
DE                  6.50 usec
TE                 298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.75 usec
PL1                 -1.00 dB
PL1W         43.00697708 W
SFO1        100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               15.14 dB
PL13               15.14 dB
PL2W         10.49968529 W
PL12W         0.32149649 W
PL13W         0.32149649 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                  65536
SF         100.6127126 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

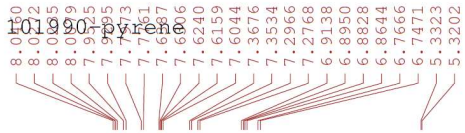


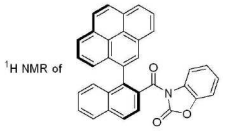
BRUKER

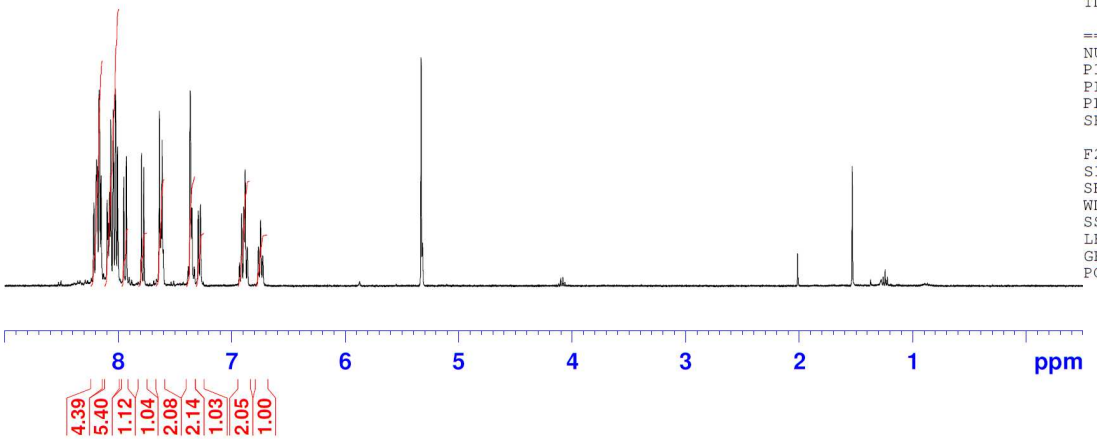
Current Data Parameters
NAME 101990-acnp
EXPNO 1
PROCNO 1



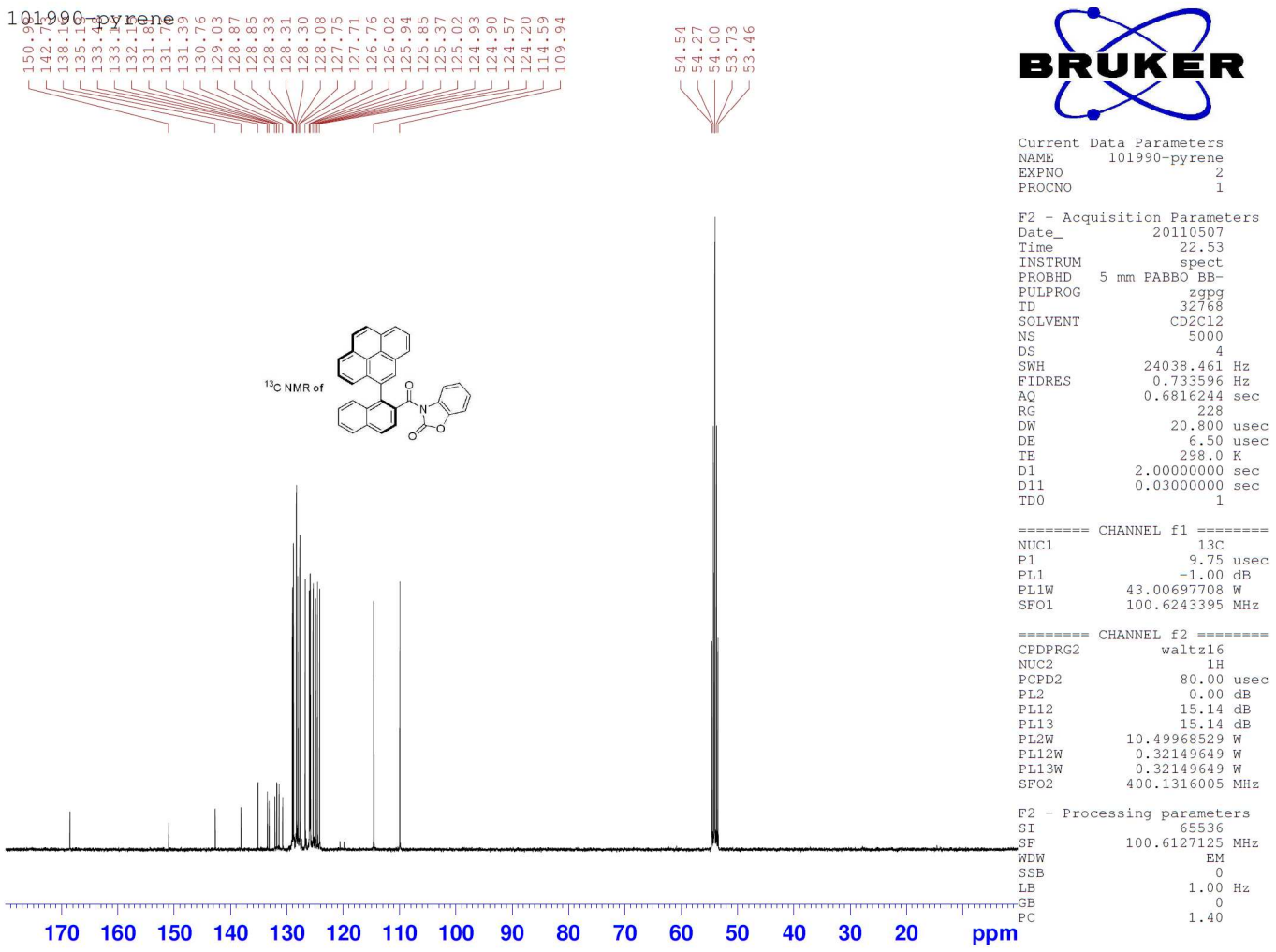

101990-AcNP
168.9
150.9
147.4
146.7
142.9
139.5
137.7
135.23
133.16
132.72
131.45
130.37
130.07
128.82
128.79
128.73
128.22
127.92
127.53
127.50
125.23
124.74
124.33
121.77
120.12
119.28
114.36
109.90
54.54
54.27
53.73
53.46
30.85
30.55
BRUKER
Current Data Parameters
NAME 101990-acnp
EXPNO 4
PROCNO 1
^{13}C NMR of
O
N
O
O
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm








```
Current Data Parameters
NAME      101990-pyrene
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20110506
Time              14.49
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg10
TD                32768
SOLVENT          CD2Cl2
NS                   16
DS                    4
SWH            5896.227 Hz
FIDRES         0.179939 Hz
AQ            2.7787764 sec
RG                  575
DW                84.800 usec
DE                 6.50 usec
TE                298.0 K
D1           2.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1                14.00 usec
PL1                0.00 dB
PL1W       10.49968529 W
SFO1       400.1327209 MHz

F2 - Processing parameters
SI                65536
SF         400.1300175 MHz
WDW                EM
SSB                 0
LB                0.05 Hz
GB                  0
PC                1.00
```



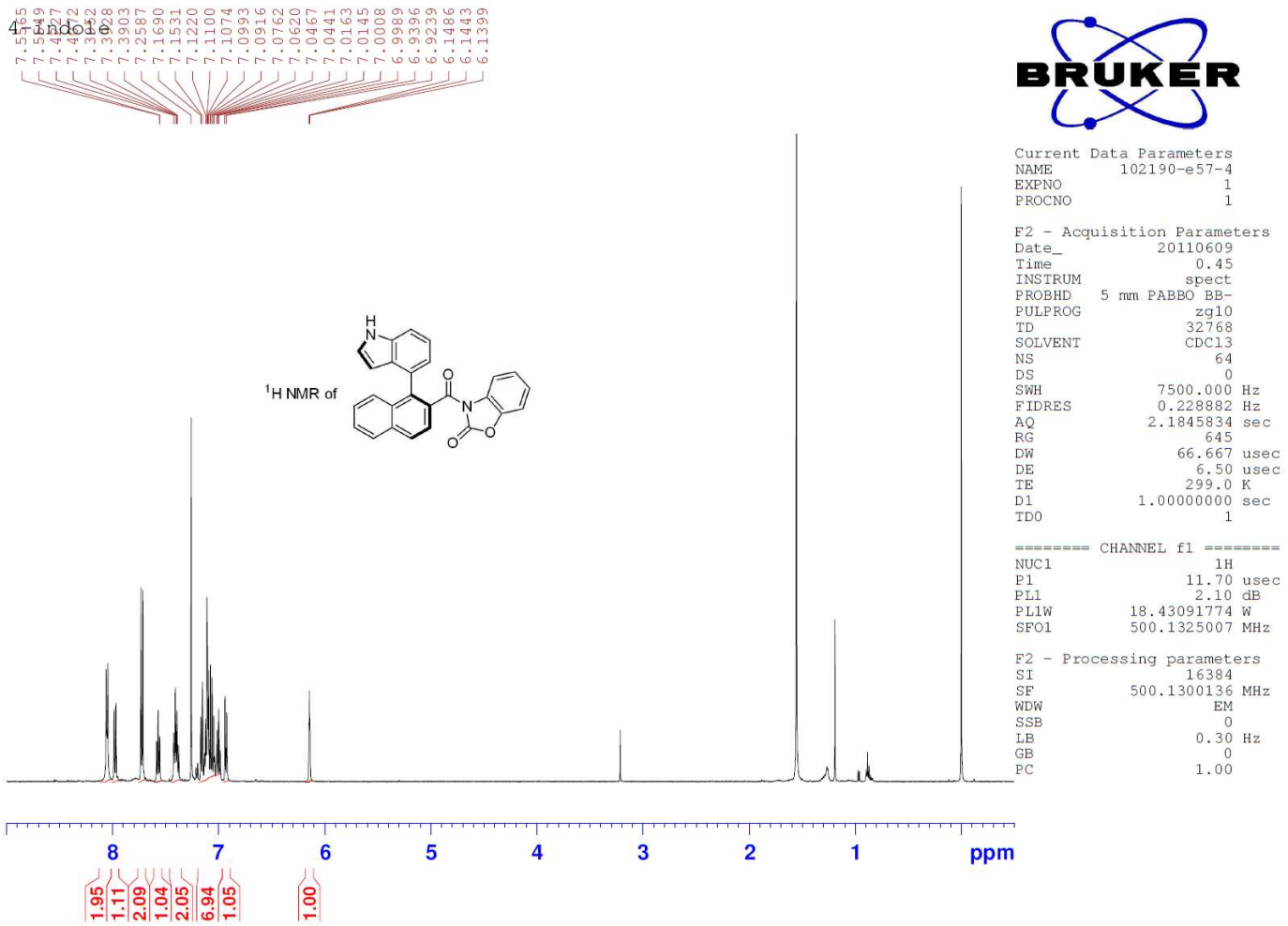
Current Data Parameters
NAME 101990-pyrene
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110507
Time 22.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 32768
SOLVENT CD2Cl2
NS 5000
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 228
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.75 usec
PL1 -1.00 dB
PL1W 43.00697708 W
SFO1 100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.14 dB
PL13 15.14 dB
PL2W 10.49968529 W
PL12W 0.32149649 W
PL13W 0.32149649 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127125 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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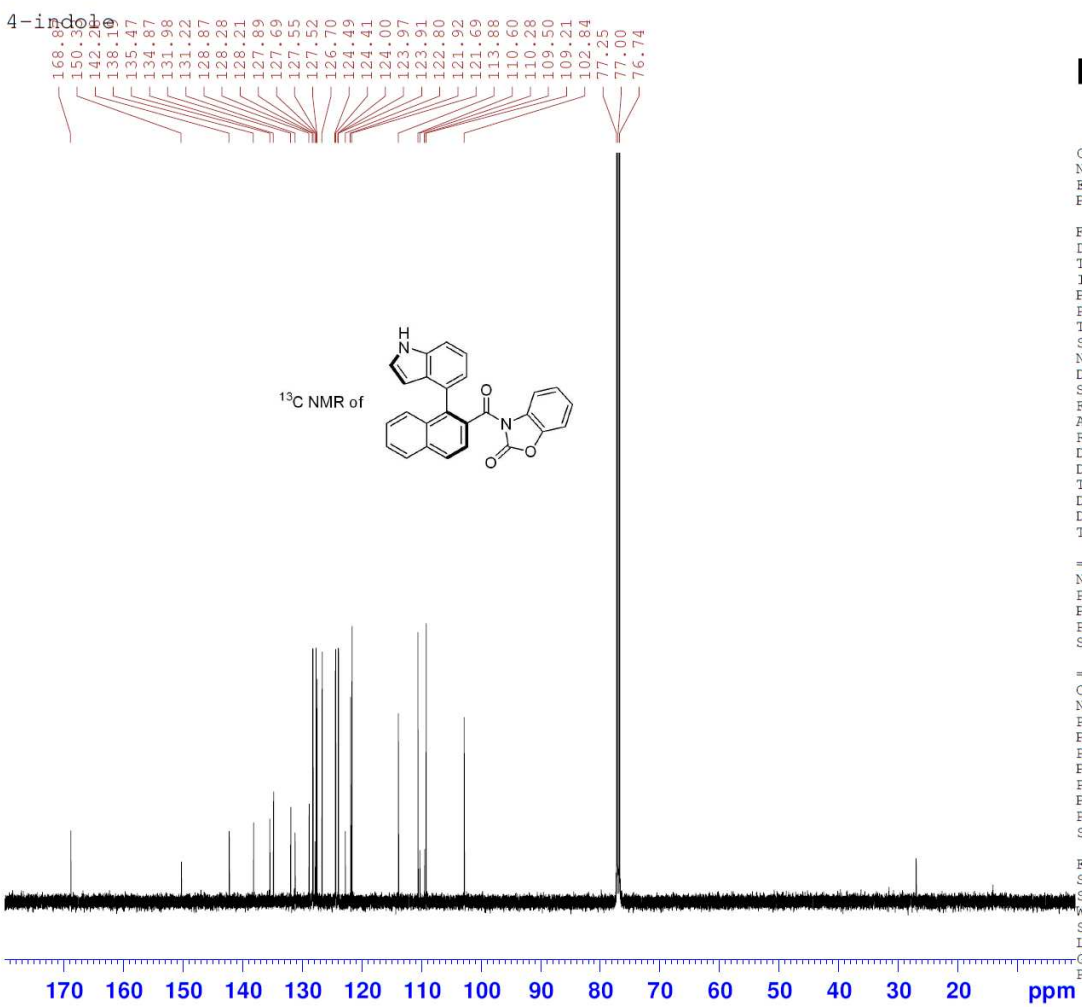
```
Current Data Parameters
NAME        102190-e57-4
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110609
Time                0.45
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg10
TD                 32768
SOLVENT            CDCl3
NS                    64
DS                     0
SWH             7500.000 Hz
FIDRES          0.228882 Hz
AQ             2.1845834 sec
RG                   645
DW                66.667 usec
DE                 6.50 usec
TE                299.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.70 usec
PL1                2.10 dB
PL1W         18.43091774 W
SFO1         500.1325007 MHz

F2 - Processing parameters
SI                 16384
SF          500.1300136 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

4-indole



BRUKER

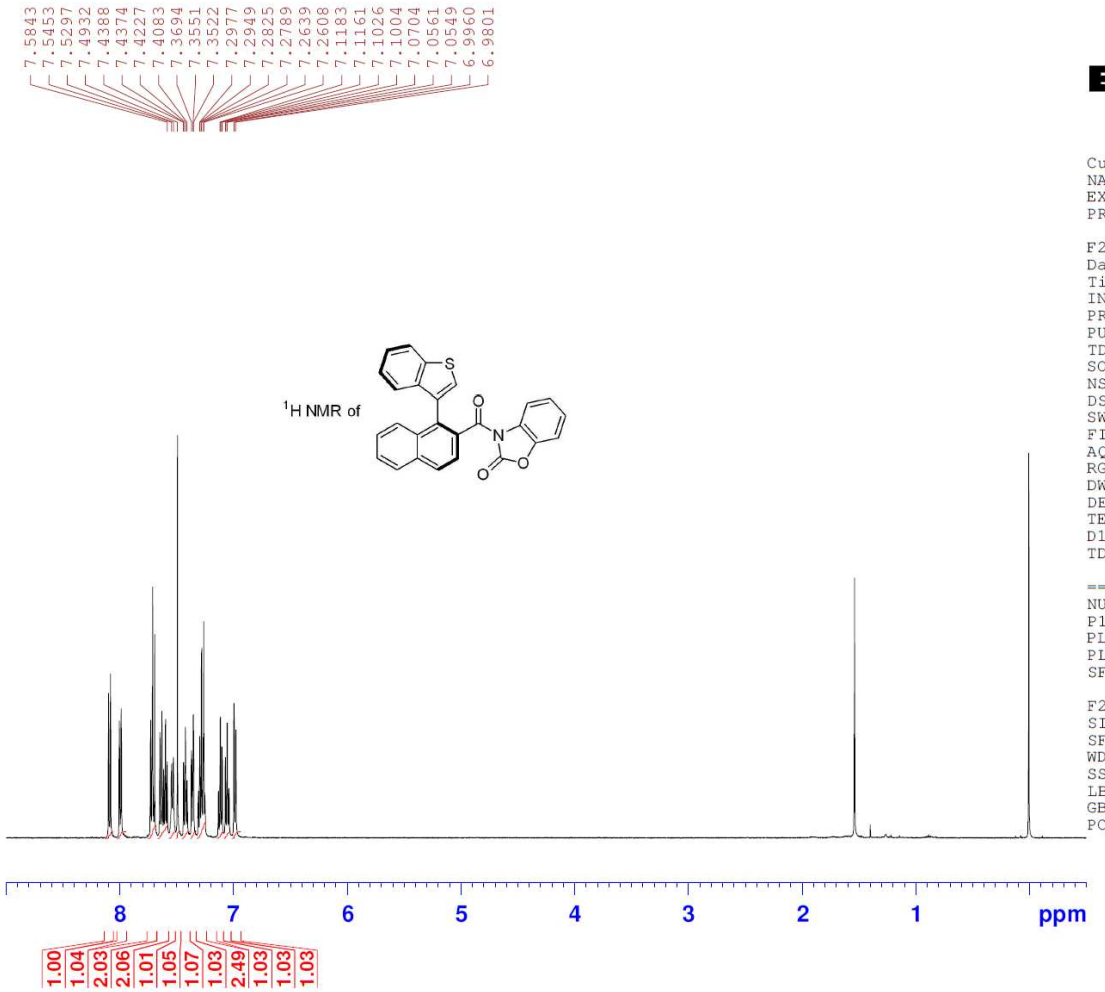
```
Current Data Parameters
NAME        102190-e57-4
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110609
Time                5.10
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                262144
SOLVENT             CDCl3
NS                   3000
DS                      0
SWH             31250.000 Hz
FIDRES          0.119209 Hz
AQ              4.1943541 sec
RG                   2050
DW                 16.000 usec
DE                  6.50 usec
TE                 299.0 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.88 usec
PL1                 -0.50 dB
PL1W        124.00885010 W
SFO1         125.7698617 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 2.10 dB
PL12               19.30 dB
PL13               19.30 dB
PL2W         18.43091774 W
PL12W         0.35119396 W
PL13W         0.35119396 W
SFO2        500.1325007 MHz

F2 - Processing parameters
SI                131072
SF          125.7577916 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.40
```



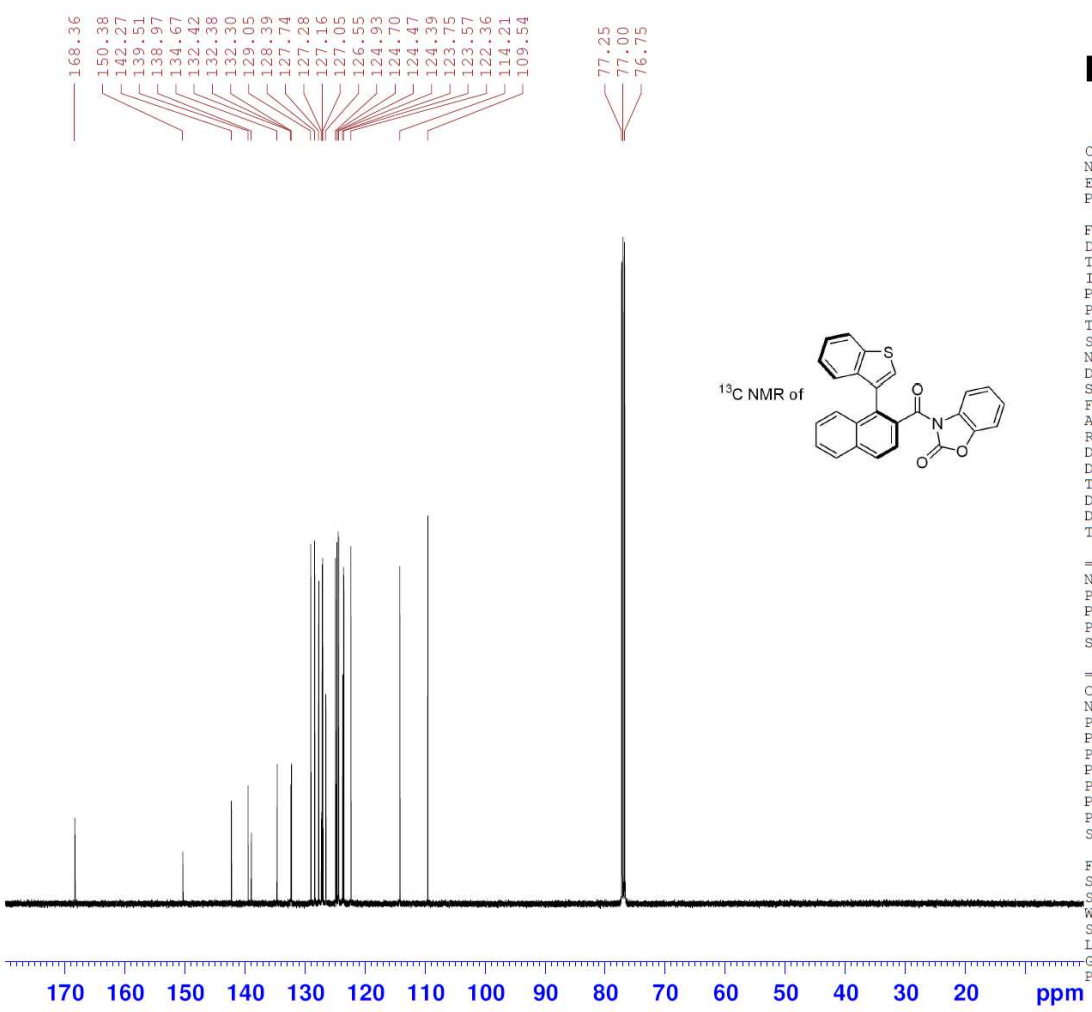
BRUKER

```
Current Data Parameters
NAME         102208-thio
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110516
Time               17.01
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg10
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             7500.000 Hz
FIDRES          0.228882 Hz
AQ             2.1845834 sec
RG                   512
DW                66.667 usec
DE                 6.50 usec
TE                299.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.70 usec
PL1                2.10 dB
PL1W         18.43091774 W
SFO1         500.1325007 MHz

F2 - Processing parameters
SI                 16384
SF          500.1300125 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



^{13}C NMR of

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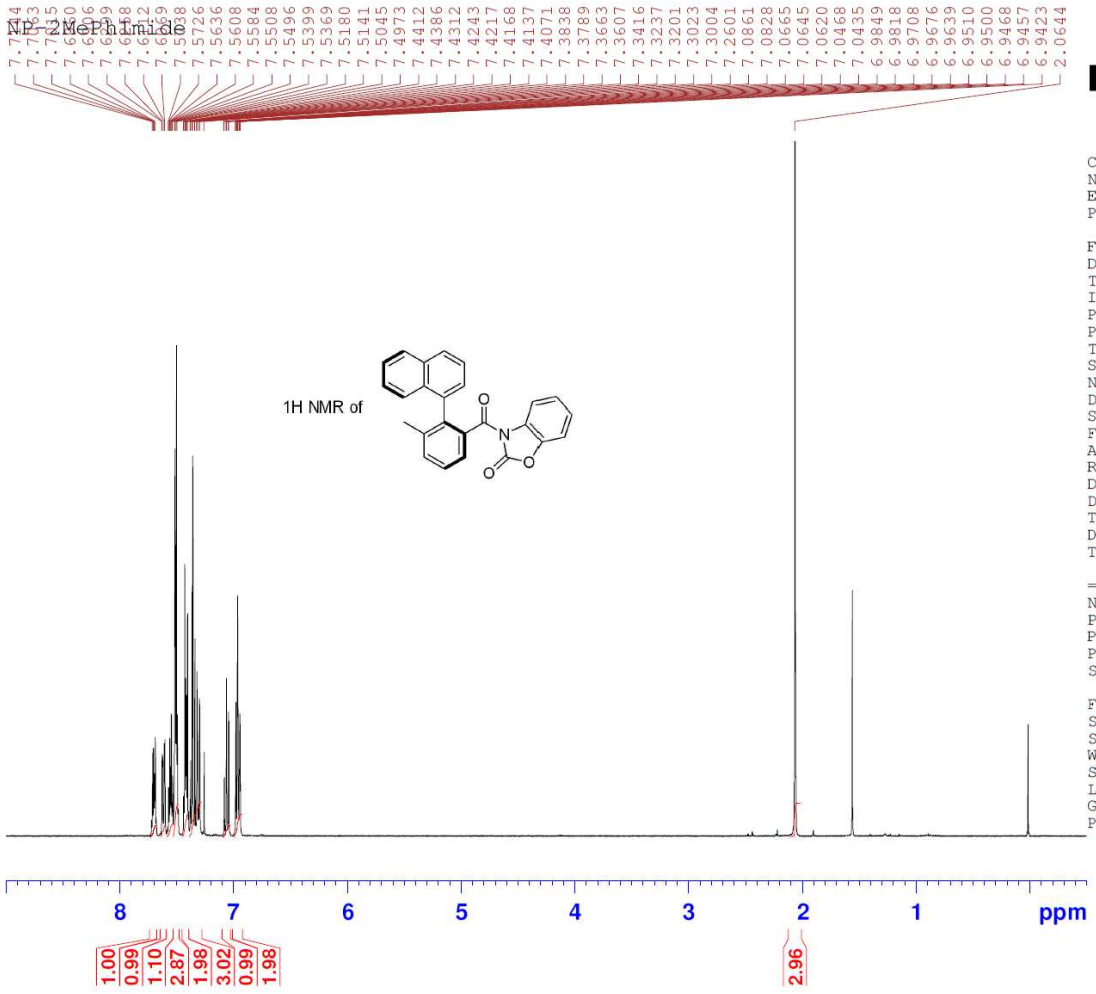
Current Data Parameters
NAME 102208-thio
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110517
Time 0.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 262144
SOLVENT CDCl3
NS 3500
DS 0
SWH 31250.000 Hz
FIDRES 0.119209 Hz
AQ 4.1943541 sec
RG 2050
DW 16.000 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.88 usec
PL1 -0.50 dB
PL1W 124.00885010 W
SFO1 125.7698617 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.10 dB
PL12 19.30 dB
PL13 19.30 dB
PL2W 18.43091774 W
PL12W 0.35119396 W
PL13W 0.35119396 W
SFO2 500.1325007 MHz

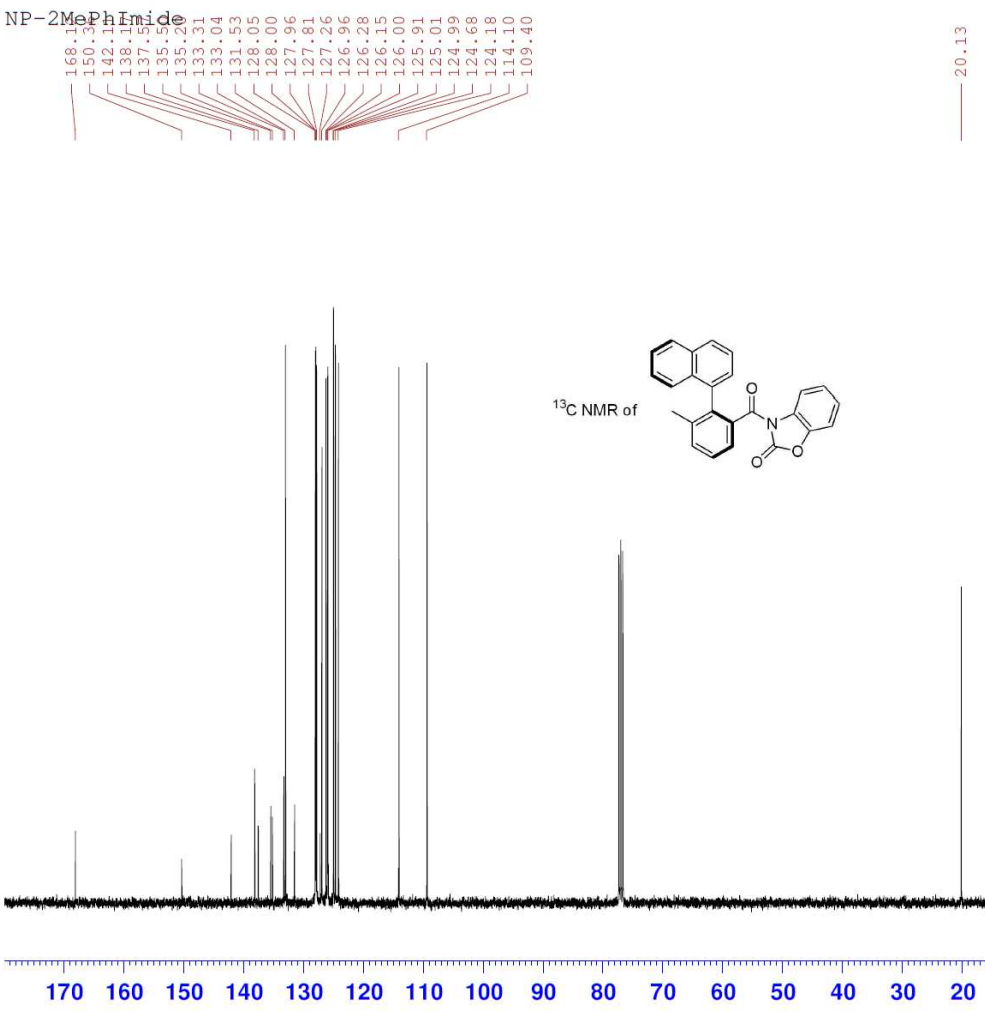
F2 - Processing parameters
SI 131072
SF 125.7577919 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



BRUKER

```
Current Data Parameters
NAME        102190-052-2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110517
Time               17.06
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg10
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     4
SWH             5896.227 Hz
FIDRES          0.179939 Hz
AQ             2.7787764 sec
RG                   456
DW                84.800 usec
DE                 6.50 usec
TE                298.0 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                13.80 usec
PL1                0.00 dB
PL1W         10.49968529 W
SFO1         400.1327209 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300098 MHz
WDW                   EM
SSB                    0
LB                  0.05 Hz
GB                     0
PC                  1.00
```

NP-2MePhImide



BRUKER

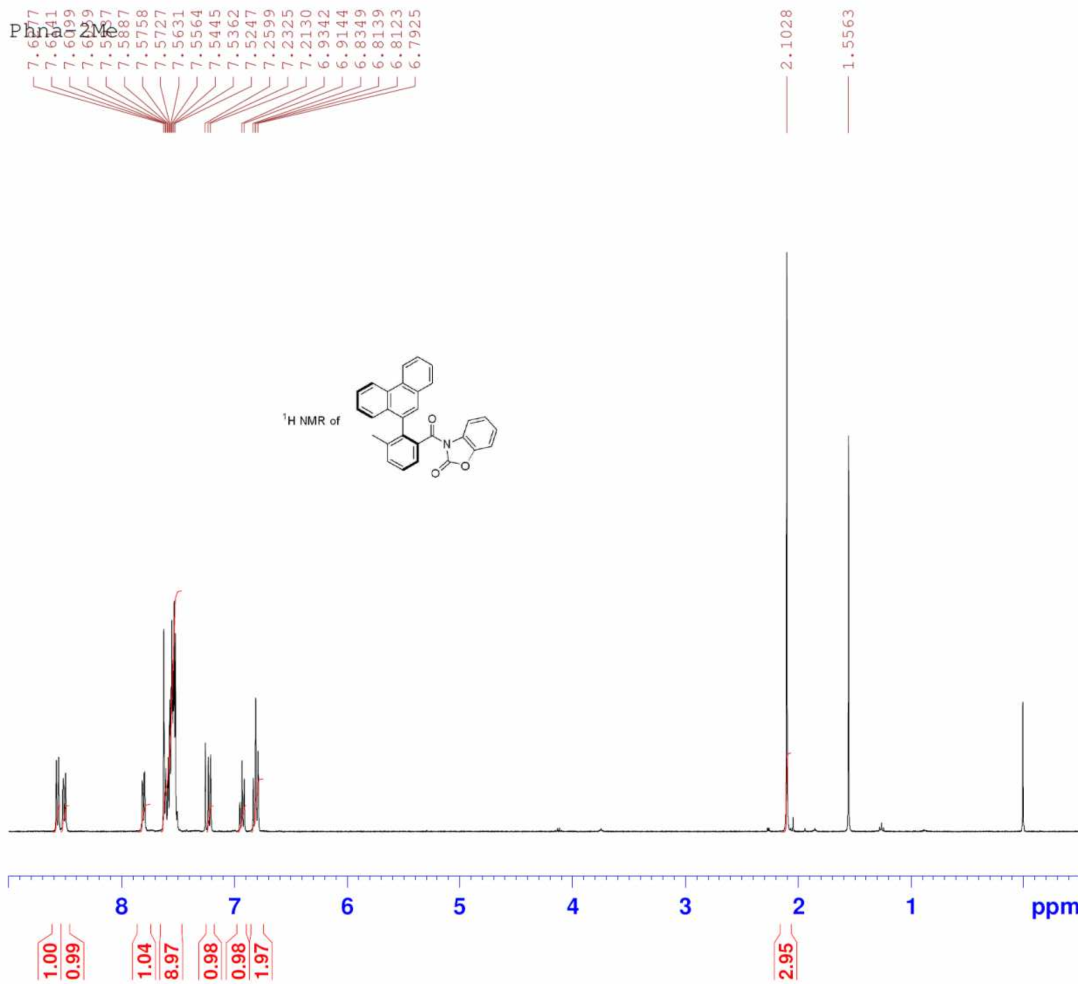
Current Data Parameters
NAME 102190-052-2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110517
Time 17.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.65 usec
PL1 -1.00 dB
PL1W 43.00697708 W
SFO1 100.6243395 MHz

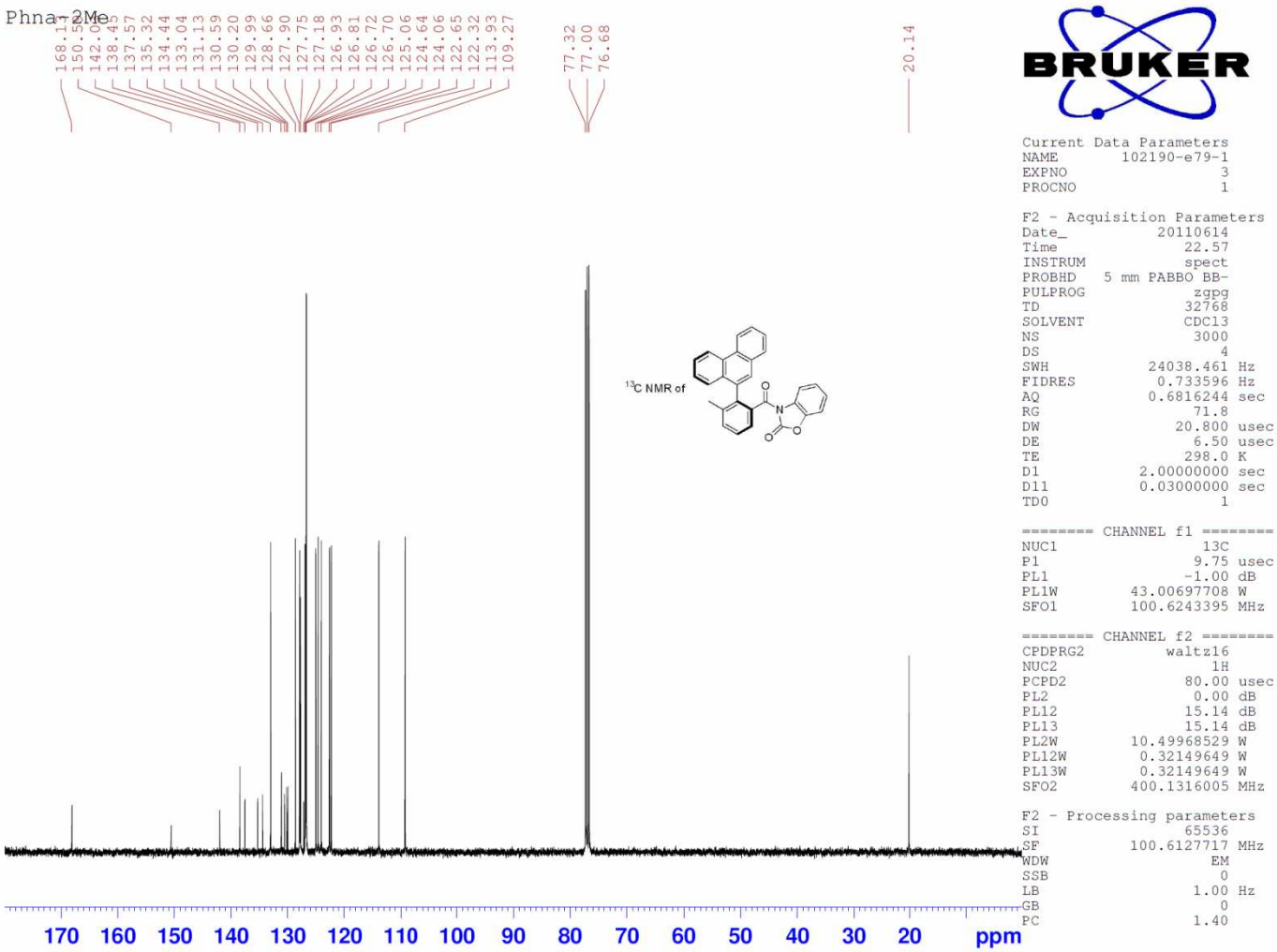
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 15.86 dB
PL13 15.86 dB
PL2W 10.49968529 W
PL12W 0.27238068 W
PL13W 0.27238068 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127745 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



BRUKER

```
Current Data Parameters
NAME        102190-e79-1
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110614
Time               23.04
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg10
TD                 32768
SOLVENT            CDCl3
NS                    64
DS                     4
SWH             5896.227 Hz
FIDRES          0.179939 Hz
AQ             2.7787764 sec
RG                   812
DW                84.800 usec
DE                  6.50 usec
TE                 298.0 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.00 usec
PL1                 0.00 dB
PL1W         10.49968529 W
SFO1         400.1327209 MHz

F2 - Processing parameters
SI                 65536
SF           400.1300127 MHz
WDW                   EM
SSB                    0
LB                  0.05 Hz
GB                     0
PC                  1.00
```



BRUKER

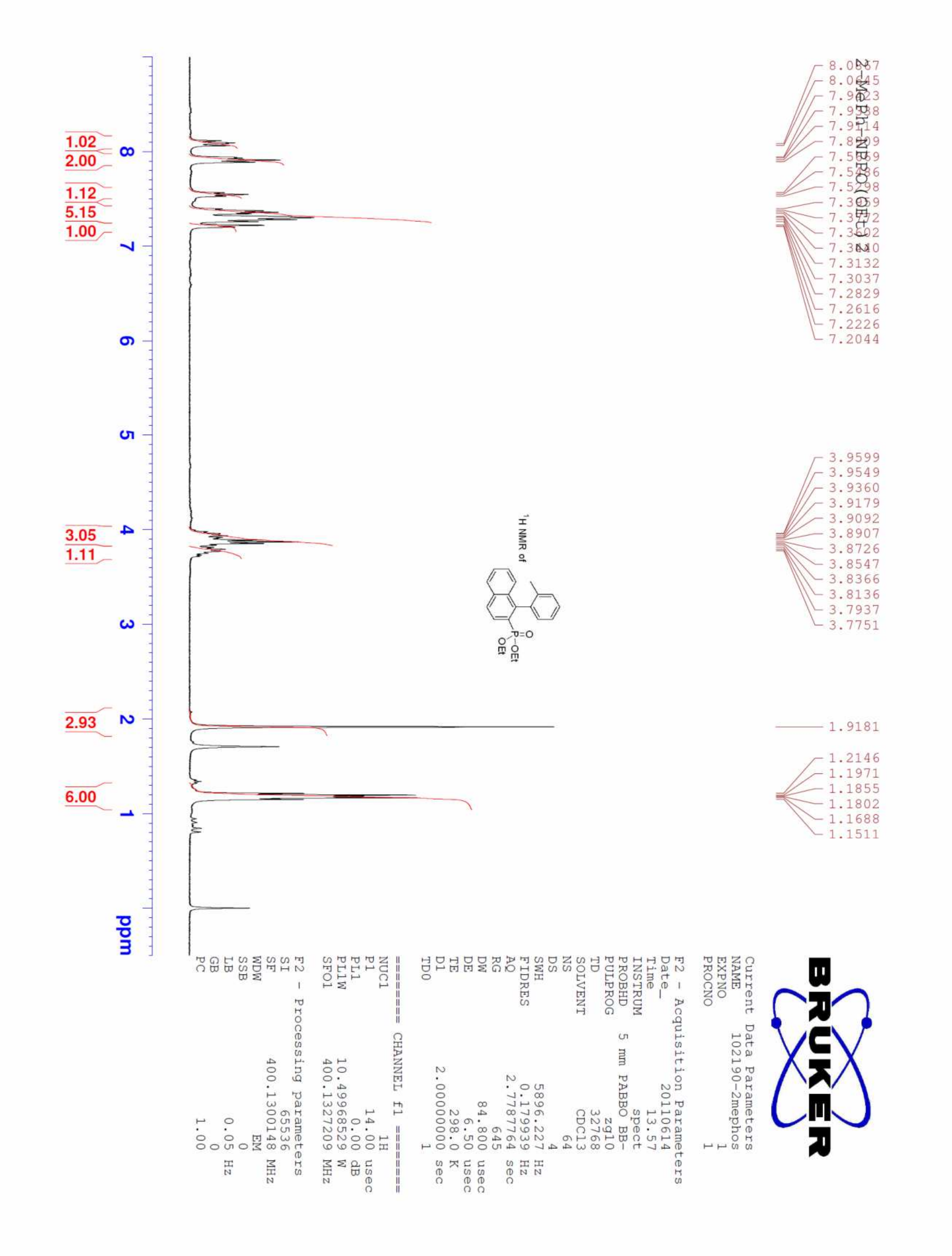
Current Data Parameters
NAME 102190-e79-1
EXPNO 3
PROCNO 1

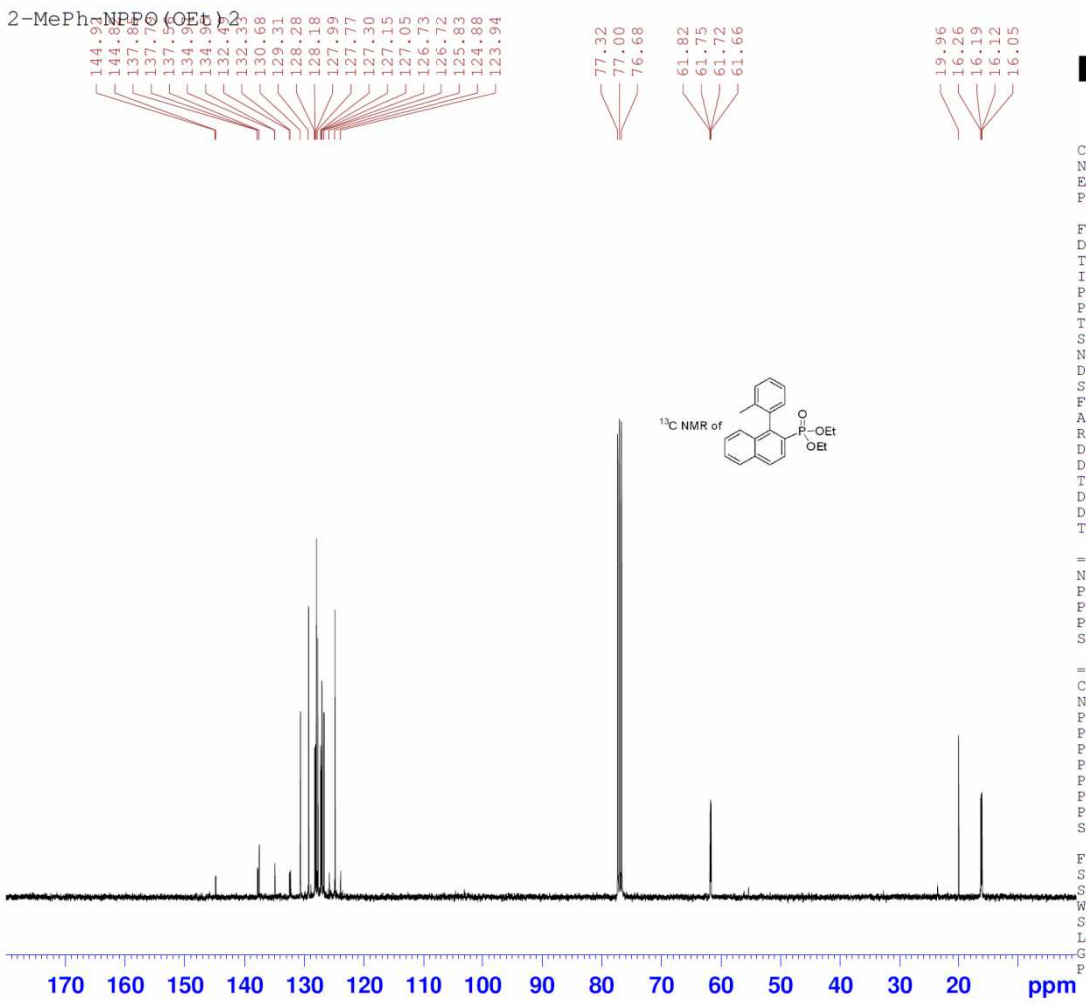
F2 - Acquisition Parameters
Date_ 20110614
Time 22.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 3000
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 71.8
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.75 usec
PL1 -1.00 dB
PL1W 43.00697708 W
SFO1 100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.14 dB
PL13 15.14 dB
PL2W 10.49968529 W
PL12W 0.32149649 W
PL13W 0.32149649 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127717 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


2-MePh-NEPO(OEt)2
8.0267
8.0145
7.9623
7.9388
7.9114
7.8899
7.5569
7.5436
7.5298
7.3369
7.3272
7.3202
7.3230
7.3132
7.3037
7.2829
7.2616
7.2226
7.2044
3.9599
3.9549
3.9360
3.9179
3.9092
3.8907
3.8726
3.8547
3.8366
3.8136
3.7937
3.7751
1.9181
1.2146
1.1971
1.1855
1.1802
1.1688
1.1511
¹H NMR of
P
O
OEt
OEt
1.02
2.00
1.12
5.15
1.00
3.05
1.11
2.93
6.00
8
7
6
5
4
3
2
1
ppm
BRUKER
Current Data Parameters
NAME 102190-2mephos
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110614
Time 13.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg10
TD 32768
SOLVENT CDCl3
NS 64
DS 4
SWH 5896.227 Hz
FIDRES 0.179939 Hz
AQ 2.7787764 sec
RG 645
DW 84.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
PL1W 10.49968529 W
SFO1 400.1327209 MHz
F2 - Processing parameters
SI 65536
SF 400.1300148 MHz
WDW EM
SSB 0
LB 0.05 Hz
GB 0
PC 1.00



BRUKER

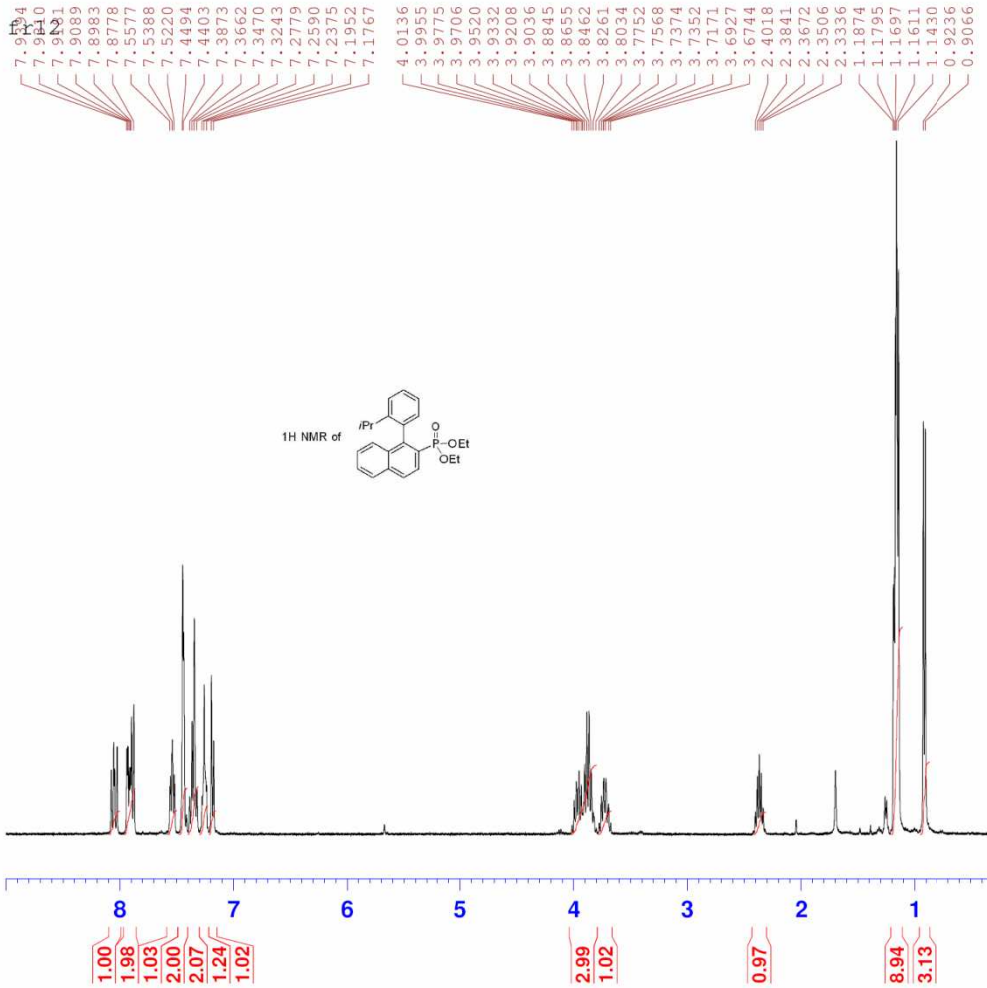
Current Data Parameters
NAME 102190-2mephos
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110615
Time 1.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 3000
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 71.8
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

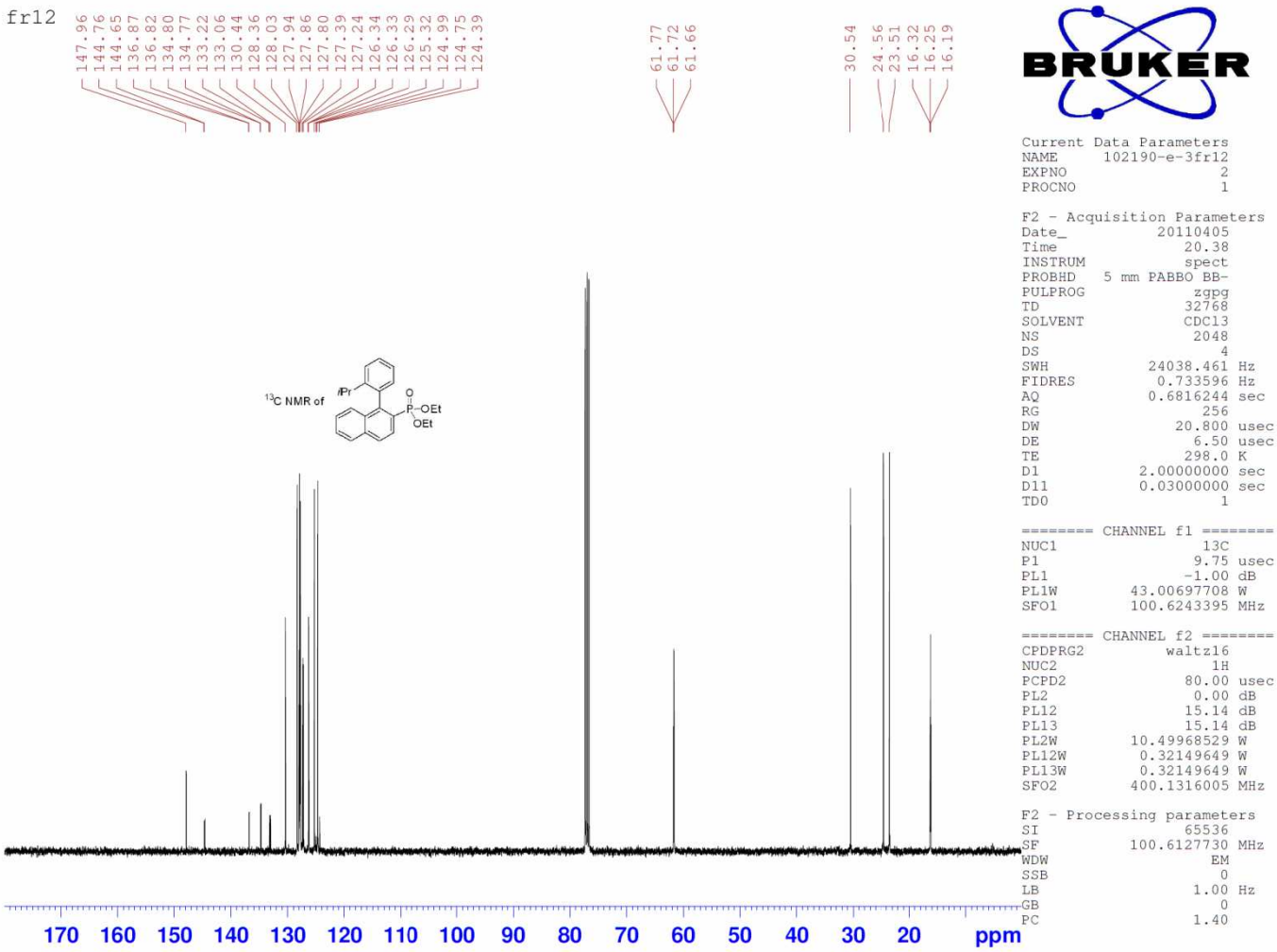
======== CHANNEL f1 ========
NUC1 13C
P1 9.75 usec
PL1 -1.00 dB
PL1W 43.00697708 W
SFO1 100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.14 dB
PL13 15.14 dB
PL2W 10.49968529 W
PL12W 0.32149649 W
PL13W 0.32149649 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127722 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40




```
Current Data Parameters
NAME      102190-e-3fr12
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110405
Time               16.14
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg10
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     4
SWH             5896.227 Hz
FIDRES          0.179939 Hz
AQ             2.7787764 sec
RG                   456
DW                84.800 usec
DE                 6.50 usec
TE                298.0 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.00 usec
PL1                0.00 dB
PL1W         10.49968529 W
SFO1         400.1327209 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300123 MHz
WDW                   EM
SSB                    0
LB                 0.05 Hz
GB                     0
PC                  1.00
```



BRUKER

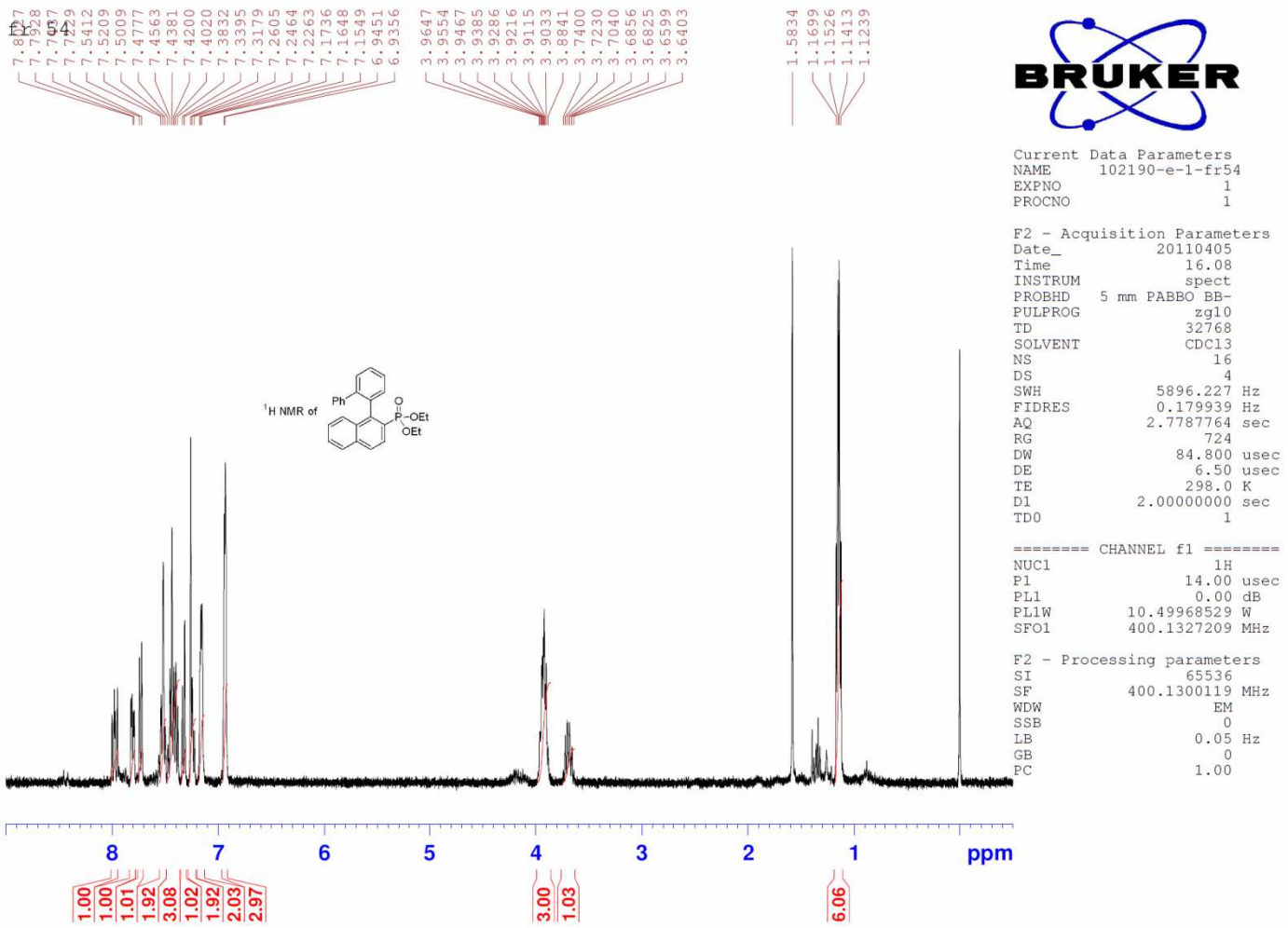
Current Data Parameters
NAME 102190-e-3fr12
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110405
Time 20.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 256
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.75 usec
PL1 -1.00 dB
PL1W 43.00697708 W
SFO1 100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.14 dB
PL13 15.14 dB
PL2W 10.49968529 W
PL12W 0.32149649 W
PL13W 0.32149649 W
SFO2 400.1316005 MHz

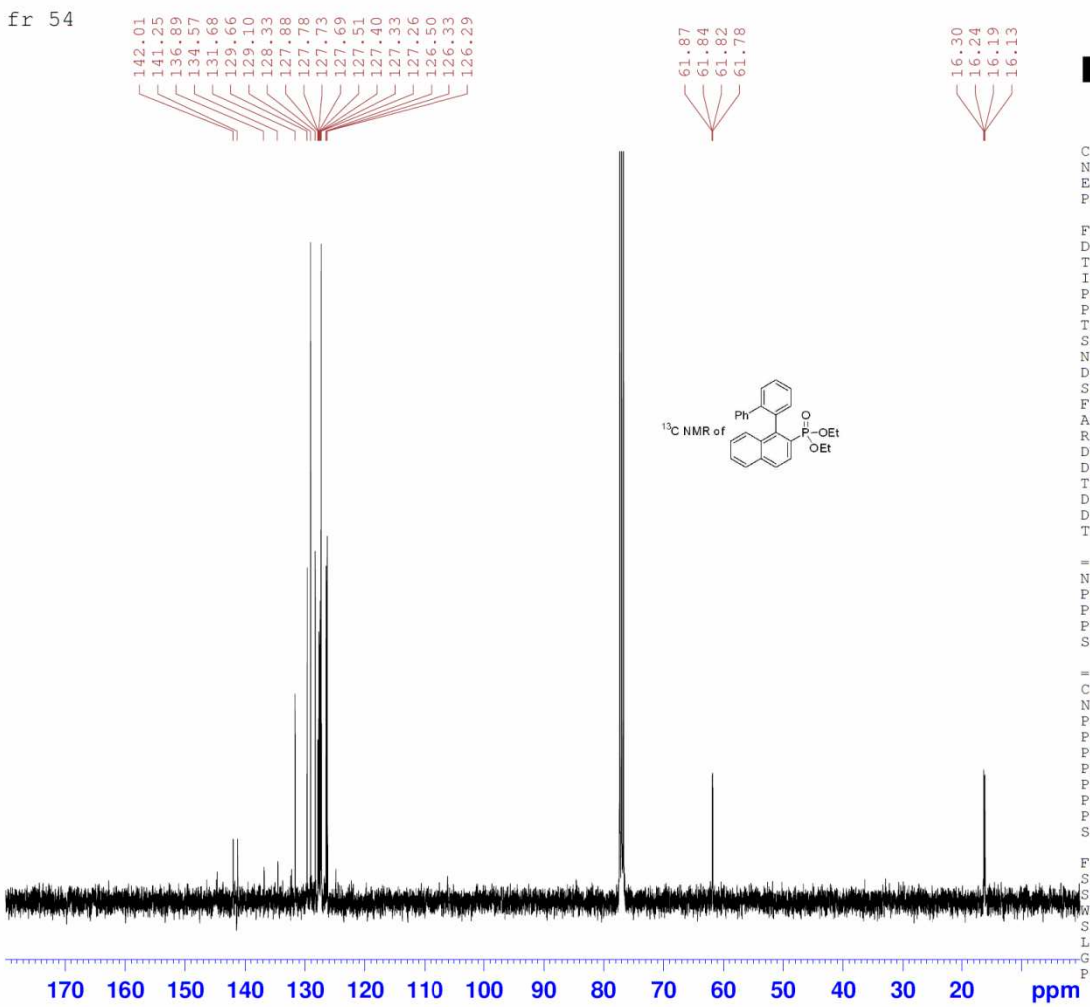
F2 - Processing parameters
SI 65536
SF 100.6127730 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



BRUKER

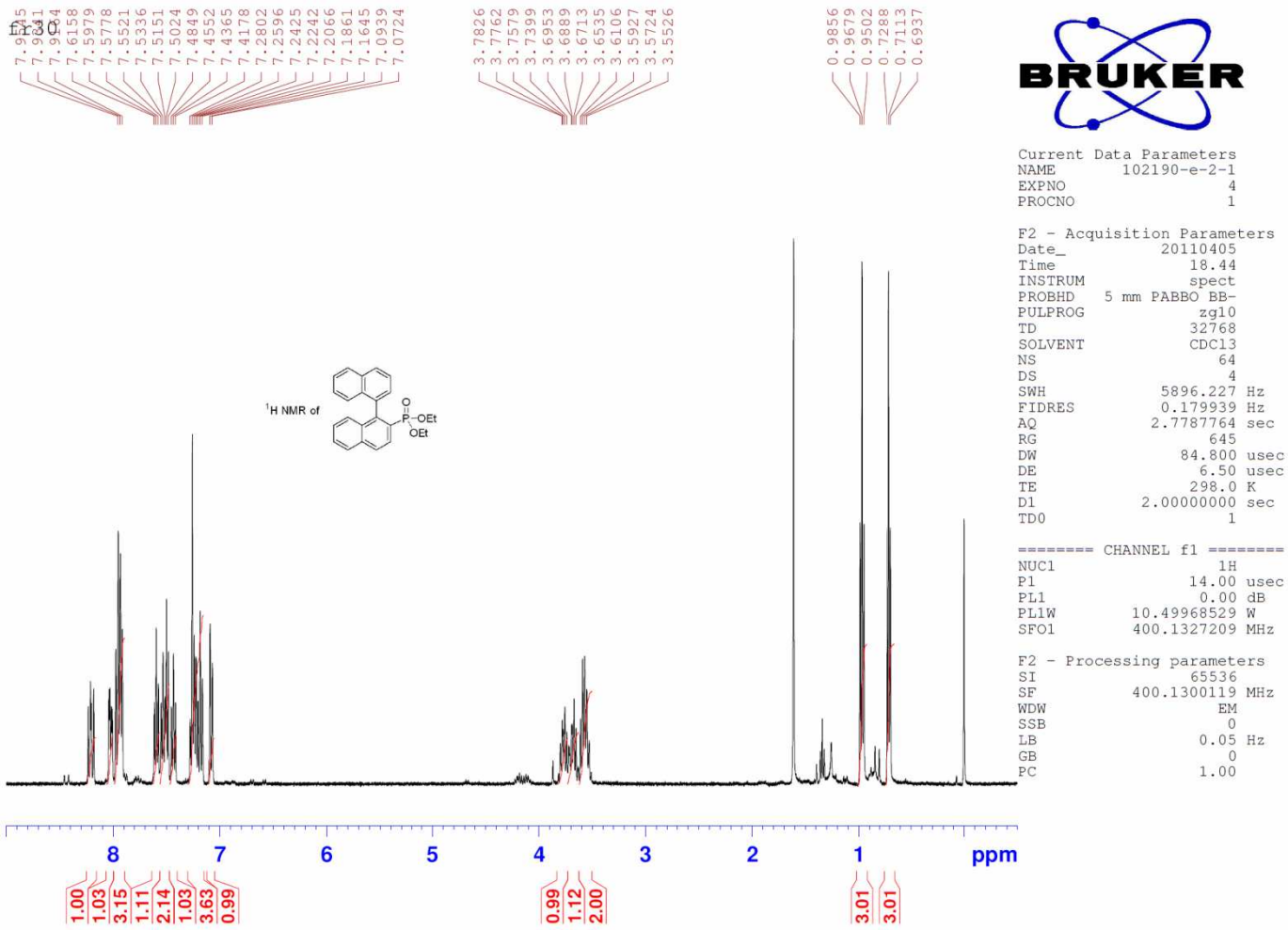
```
Current Data Parameters
NAME      102190-e-1-fr54
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110405
Time               16.08
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg10
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     4
SWH             5896.227 Hz
FIDRES          0.179939 Hz
AQ              2.7787764 sec
RG                   724
DW                84.800 usec
DE                 6.50 usec
TE                298.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.00 usec
PL1                0.00 dB
PL1W         10.49968529 W
SFO1         400.1327209 MHz

F2 - Processing parameters
SI                 65536
SF           400.1300119 MHz
WDW                   EM
SSB                    0
LB                  0.05 Hz
GB                     0
PC                  1.00
```

fr 54



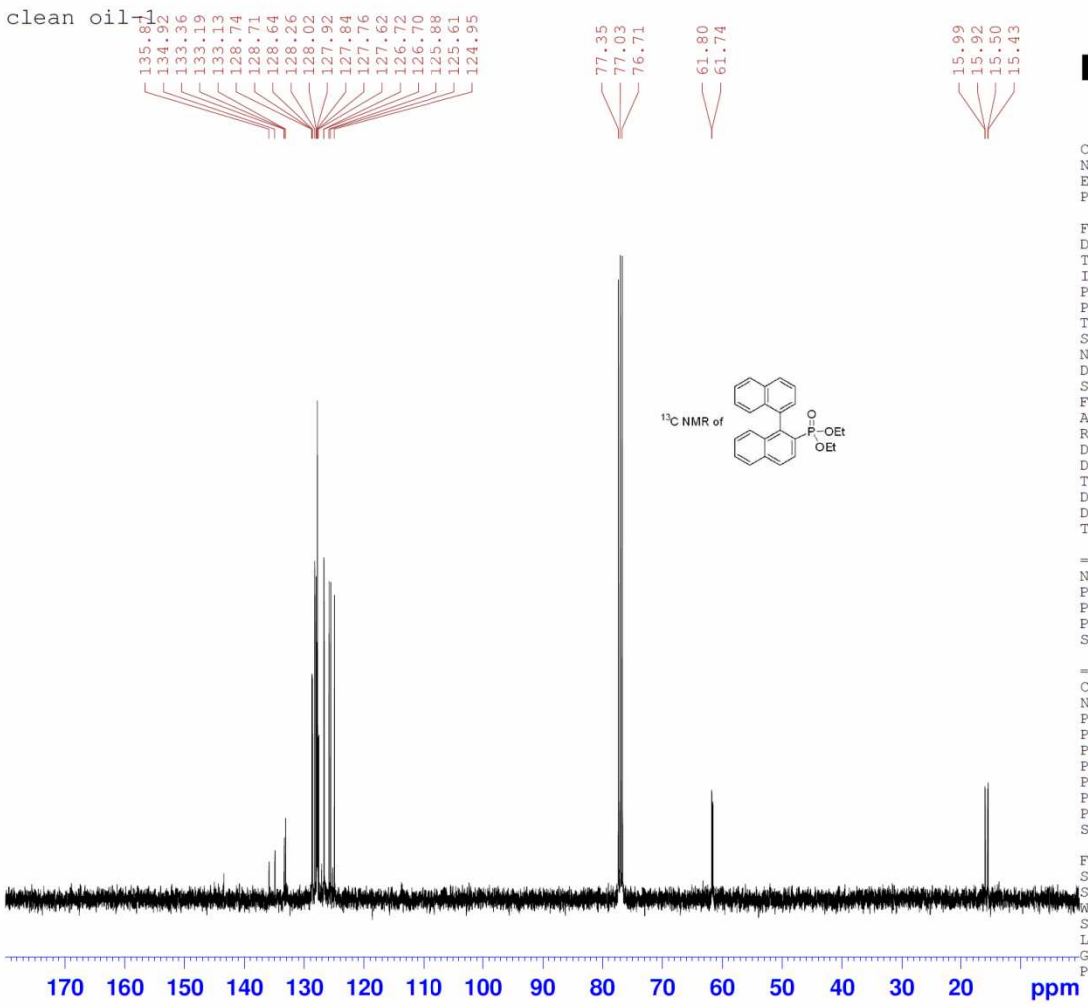
BRUKER

```
Current Data Parameters
NAME      102190-e-1-fr54
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110406
Time                0.46
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                 32768
SOLVENT            CDC13
NS                  2048
DS                     4
SWH            24038.461 Hz
FIDRES             0.733596 Hz
AQ                 0.6816244 sec
RG                   256
DW                  20.800 usec
DE                   6.50 usec
TE                  298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.75 usec
PL1                 -1.00 dB
PL1W          43.00697708 W
SFO1          100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2               80.00 usec
PL2                  0.00 dB
PL12                15.14 dB
PL13                15.14 dB
PL2W          10.49968529 W
PL12W          0.32149649 W
PL13W          0.32149649 W
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                  65536
SF            100.6127690 MHz
WDW                    EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

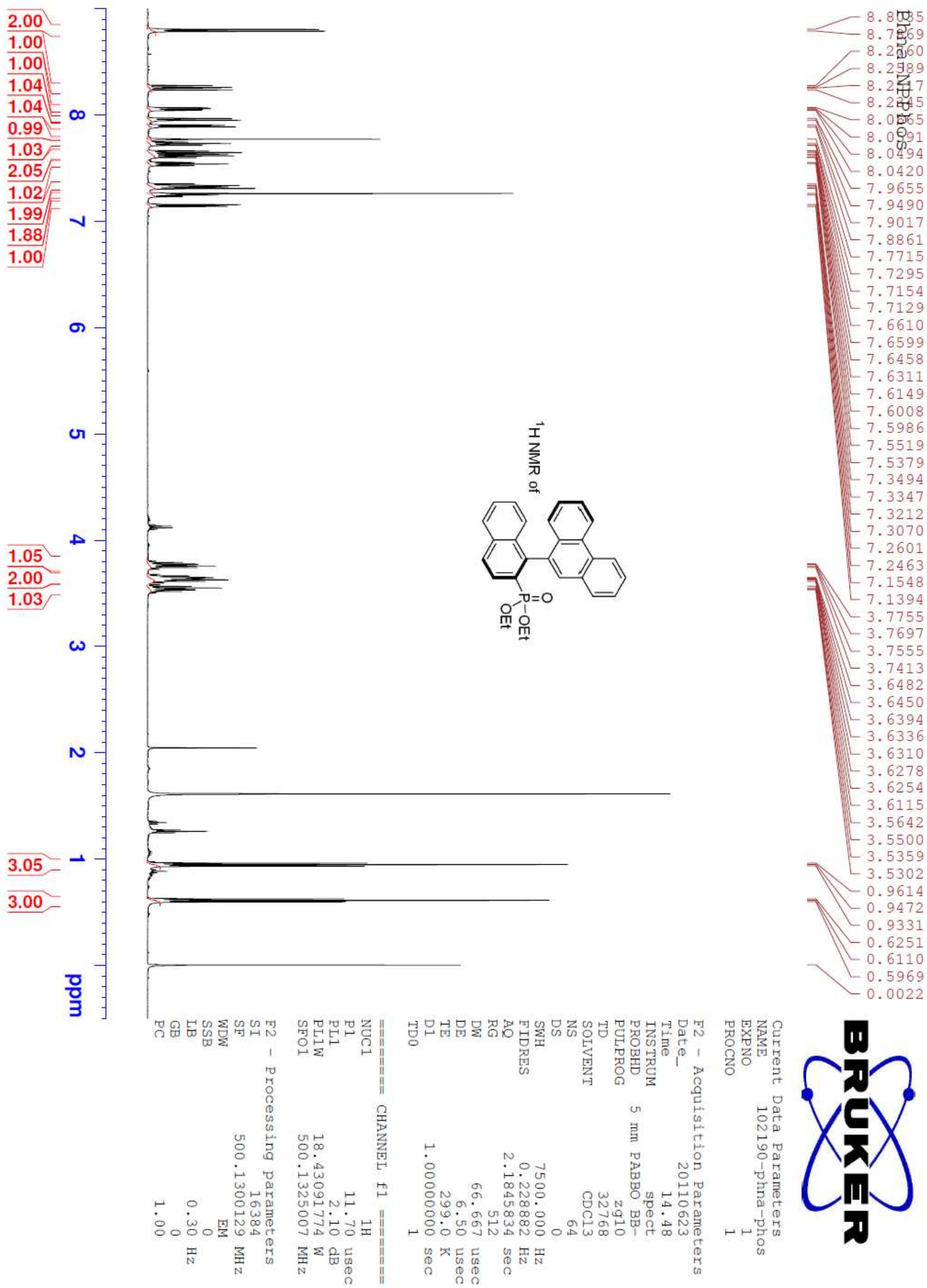



```
Current Data Parameters
NAME       102190-e-2-1
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20110405
Time              18.44
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   64
DS                    4
SWH            5896.227 Hz
FIDRES        0.179939 Hz
AQ            2.7787764 sec
RG                  645
DW               84.800 usec
DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.00 usec
PL1                0.00 dB
PL1W        10.49968529 W
SFO1        400.1327209 MHz

F2 - Processing parameters
SI                65536
SF          400.1300119 MHz
WDW                  EM
SSB                   0
LB                 0.05 Hz
GB                    0
PC                 1.00
```

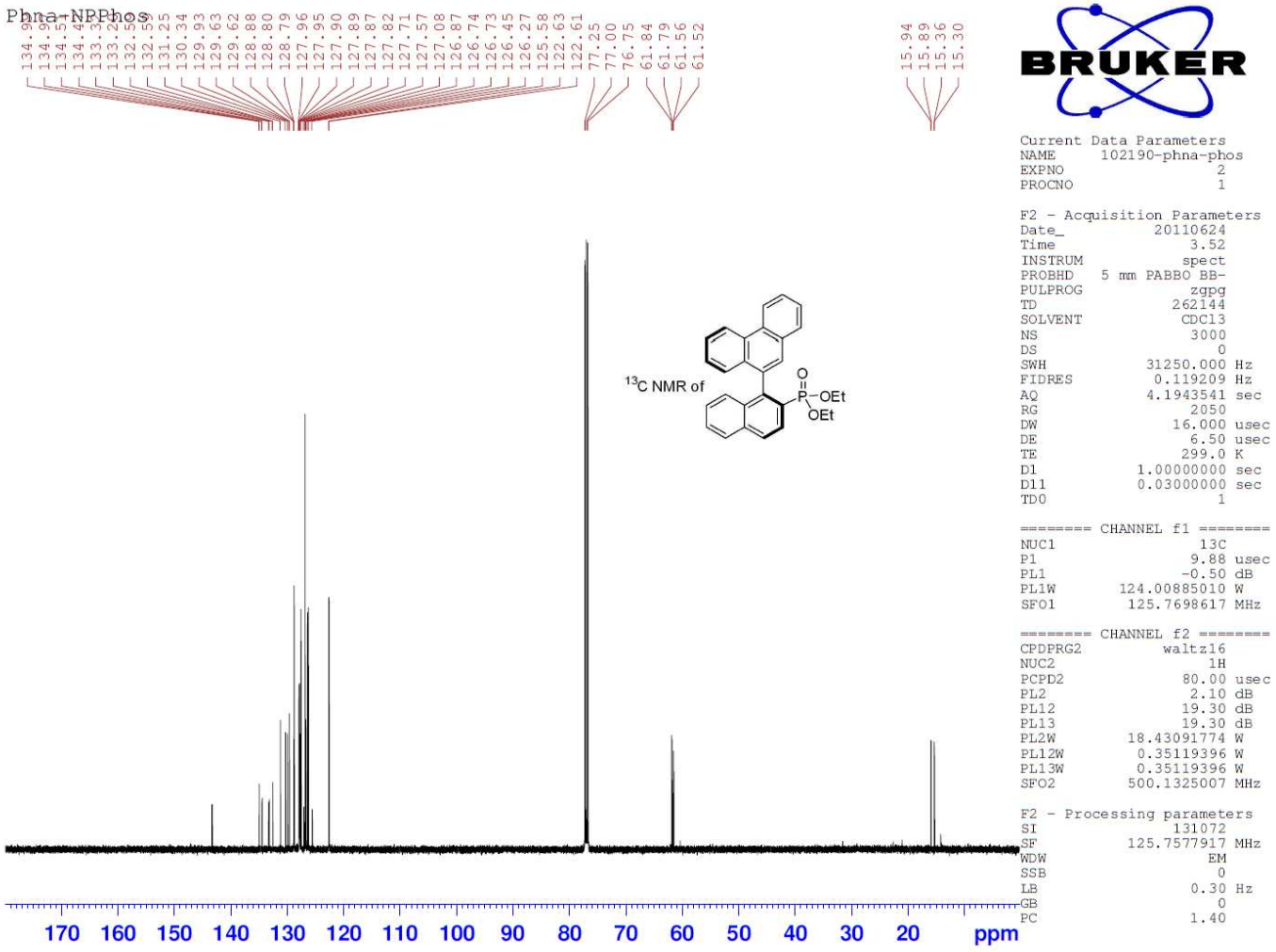
clean oil-1




```
Current Data Parameters
NAME       102190-e-2-1
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20110405
Time              12.47
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg
TD                32768
SOLVENT           CDC13
NS                  512
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6816244 sec
RG                  287
DW                20.800 usec
DE                 6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.75 usec
PL1                -1.00 dB
PL1W        43.00697708 W
SFO1        100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               15.14 dB
PL13               15.14 dB
PL2W        10.49968529 W
PL12W        0.32149649 W
PL13W        0.32149649 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 65536
SF          100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



1H NMR of
O
P–OEt
OEt
PhnaNIPhos
Current Data Parameters
NAME 102190-phna-phos
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110623
Time 14.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg10
TD 32768
SOLVENT CDCl3
NS 64
DS 0
SWH 7500.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 512
DW 66.667 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 2.10 dB
PL1W 18.43091774 W
SFO1 500.1325007 MHz
F2 - Processing parameters
SI 16384
SF 500.1300129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ppm



BRUKER

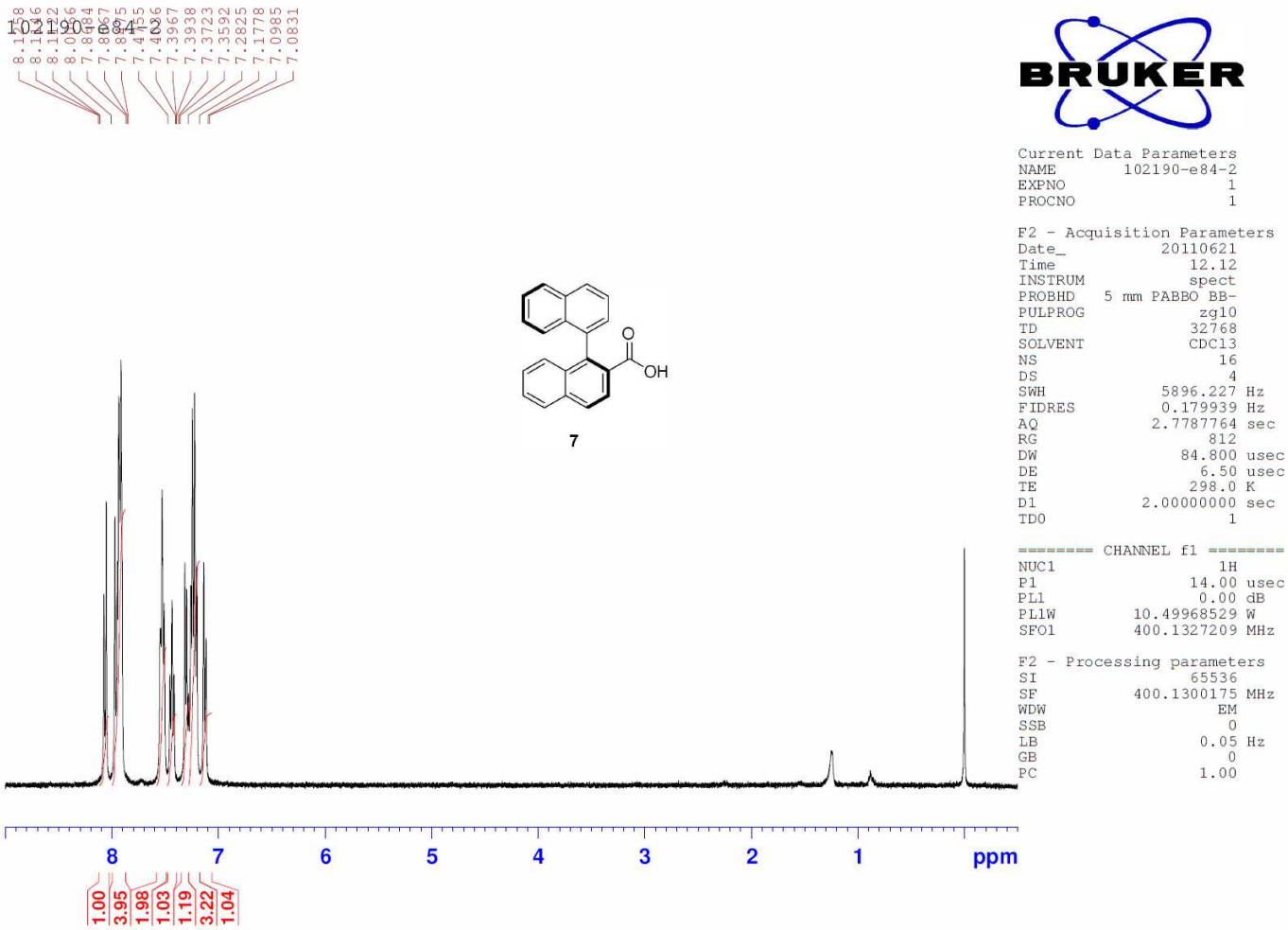
Current Data Parameters
NAME 102190-phna-phos
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110624
Time 3.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 262144
SOLVENT CDCl3
NS 3000
DS 0
SWH 31250.000 Hz
FIDRES 0.119209 Hz
AQ 4.1943541 sec
RG 2050
DW 16.000 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.88 usec
PL1 -0.50 dB
PL1W 124.00885010 W
SFO1 125.7698617 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.10 dB
PL12 19.30 dB
PL13 19.30 dB
PL2W 18.43091774 W
PL12W 0.35119396 W
PL13W 0.35119396 W
SFO2 500.1325007 MHz

F2 - Processing parameters
SI 131072
SF 125.7577917 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

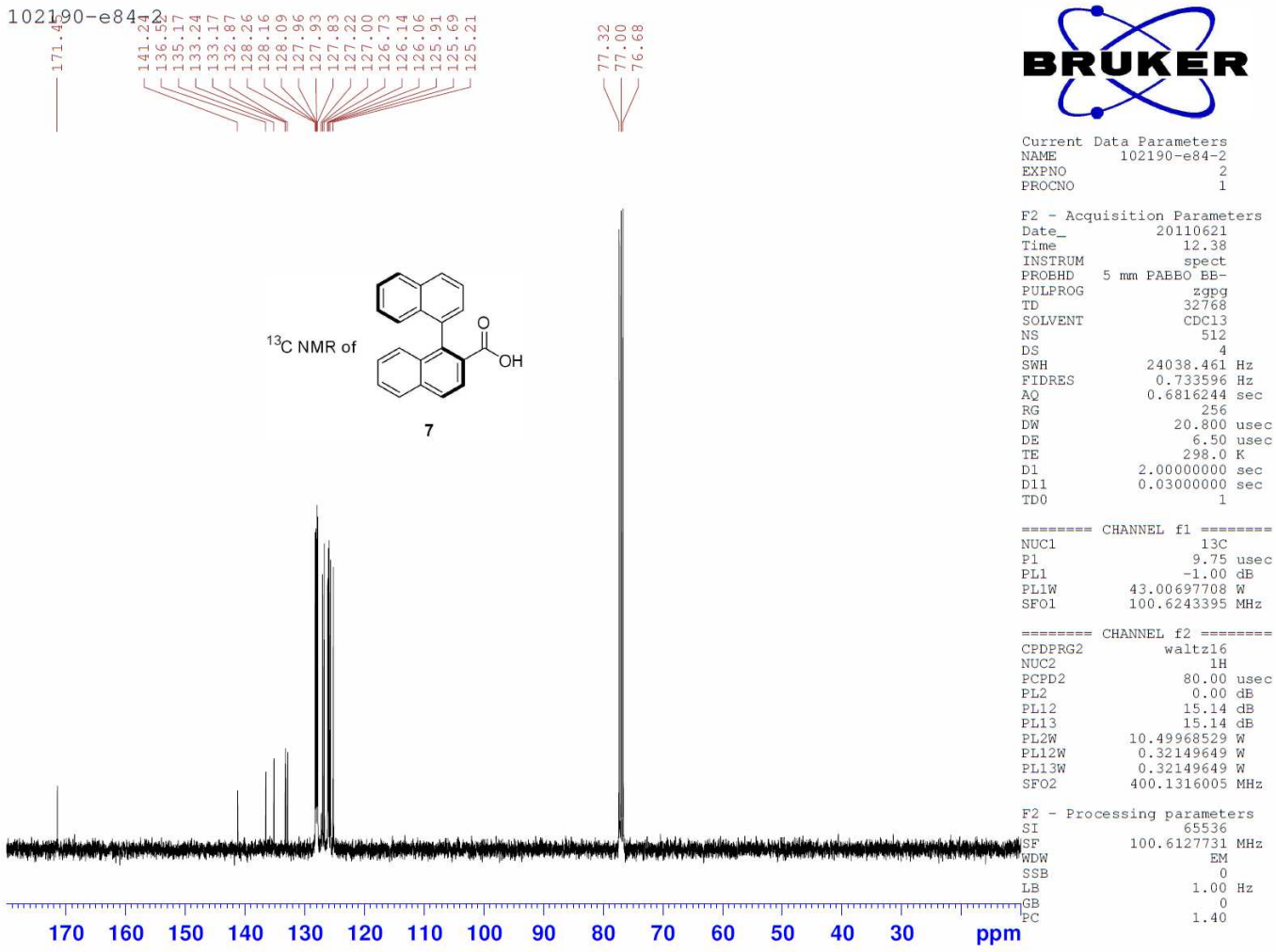


Current Data Parameters
NAME 102190-e84-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110621
Time 12.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg10
TD 32768
SOLVENT CDCl3
NS 16
DS 4
SWH 5896.227 Hz
FIDRES 0.179939 Hz
AQ 2.7787764 sec
RG 812
DW 84.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
PL1W 10.49968529 W
SFO1 400.1327209 MHz

F2 - Processing parameters
SI 65536
SF 400.1300175 MHz
WDW EM
SSB 0
LB 0.05 Hz
GB 0
PC 1.00



BRUKER

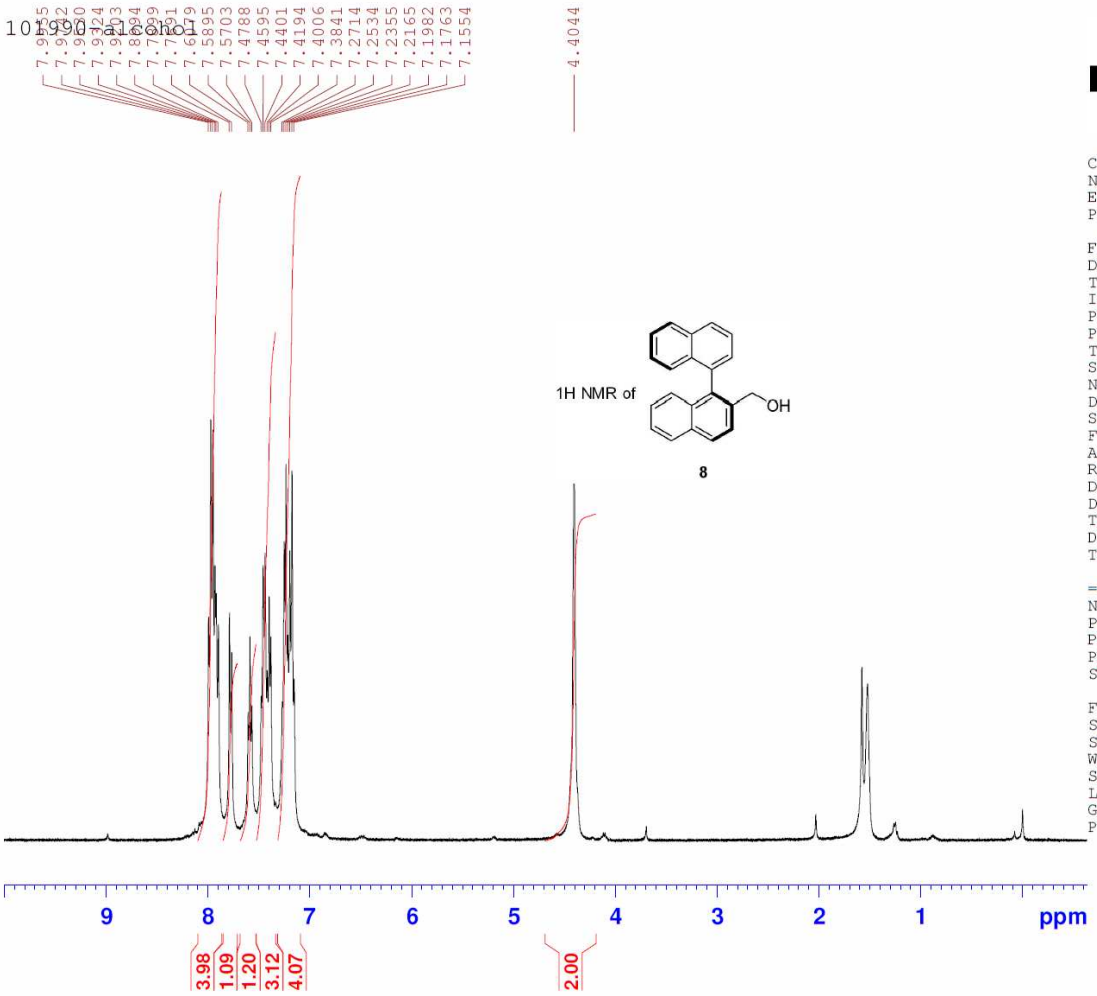
Current Data Parameters
NAME 102190-e84-2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110621
Time 12.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 256
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.75 usec
PL1 -1.00 dB
PL1W 43.00697708 W
SFO1 100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.14 dB
PL13 15.14 dB
PL2W 10.49968529 W
PL12W 0.32149649 W
PL13W 0.32149649 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127731 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

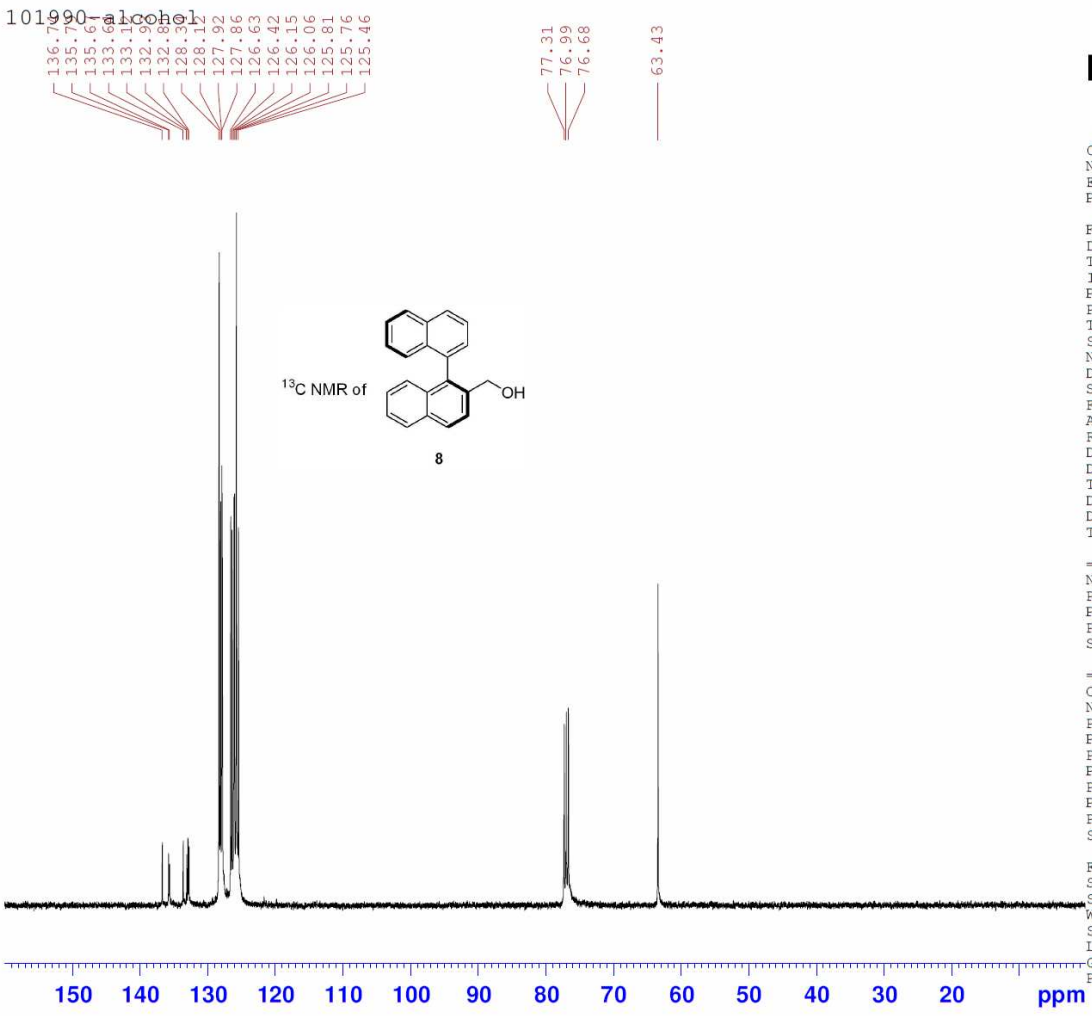


Current Data Parameters
NAME 101990-alcohol
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110528
Time 1.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg10
TD 32768
SOLVENT CDCl3
NS 32
DS 4
SWH 5896.227 Hz
FIDRES 0.179939 Hz
AQ 2.7787764 sec
RG 456
DW 84.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
PL1W 10.49968529 W
SFO1 400.1327209 MHz

F2 - Processing parameters
SI 65536
SF 400.1300263 MHz
WDW EM
SSB 0
LB 0.05 Hz
GB 0
PC 1.00



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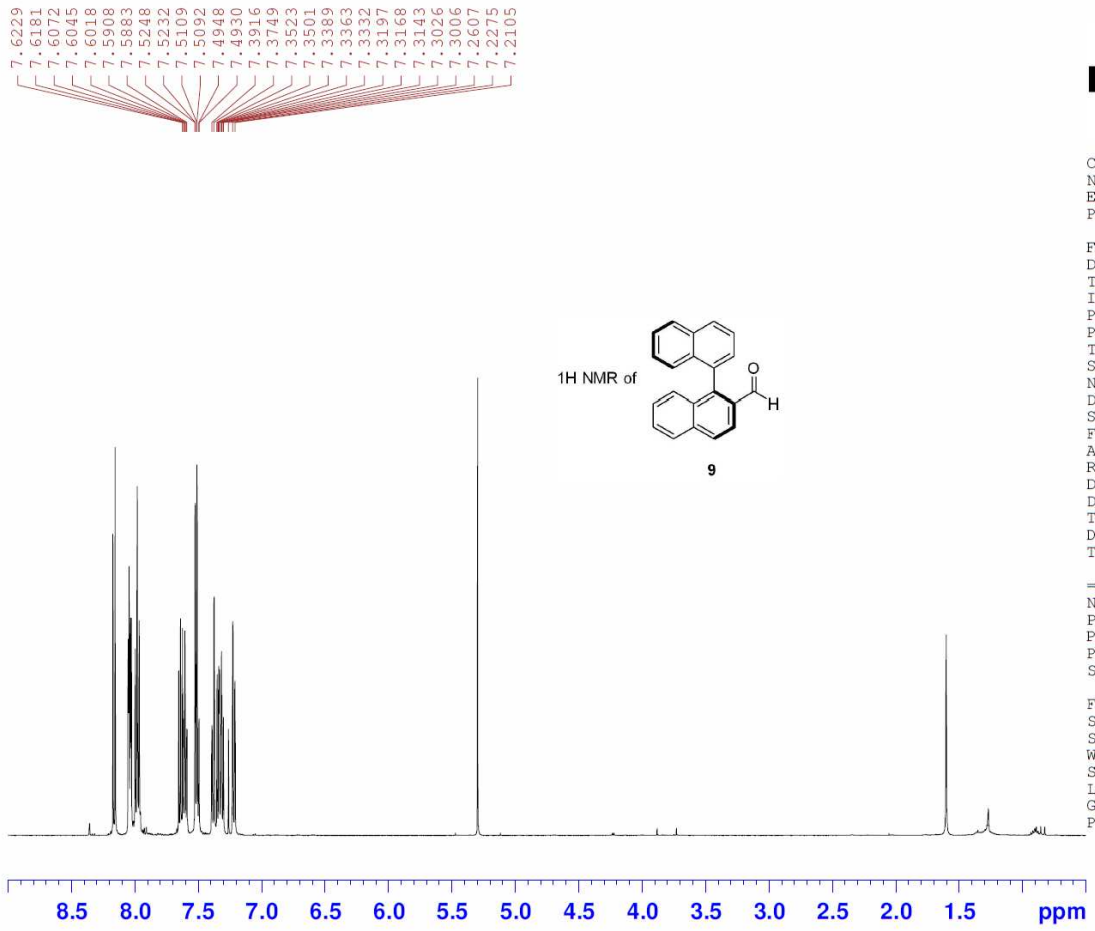
```
Current Data Parameters
NAME      101990-alcohol
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110528
Time                5.46
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                 32768
SOLVENT            CDCl3
NS                  5000
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6816244 sec
RG                  71.8
DW                20.800 usec
DE                 6.50 usec
TE                300.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.75 usec
PL1                -1.00 dB
PL1W        43.00697708 W
SFO1       100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               15.14 dB
PL13               15.14 dB
PL2W        10.49968529 W
PL12W        0.32149649 W
PL13W        0.32149649 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                 65536
SF         100.6127769 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



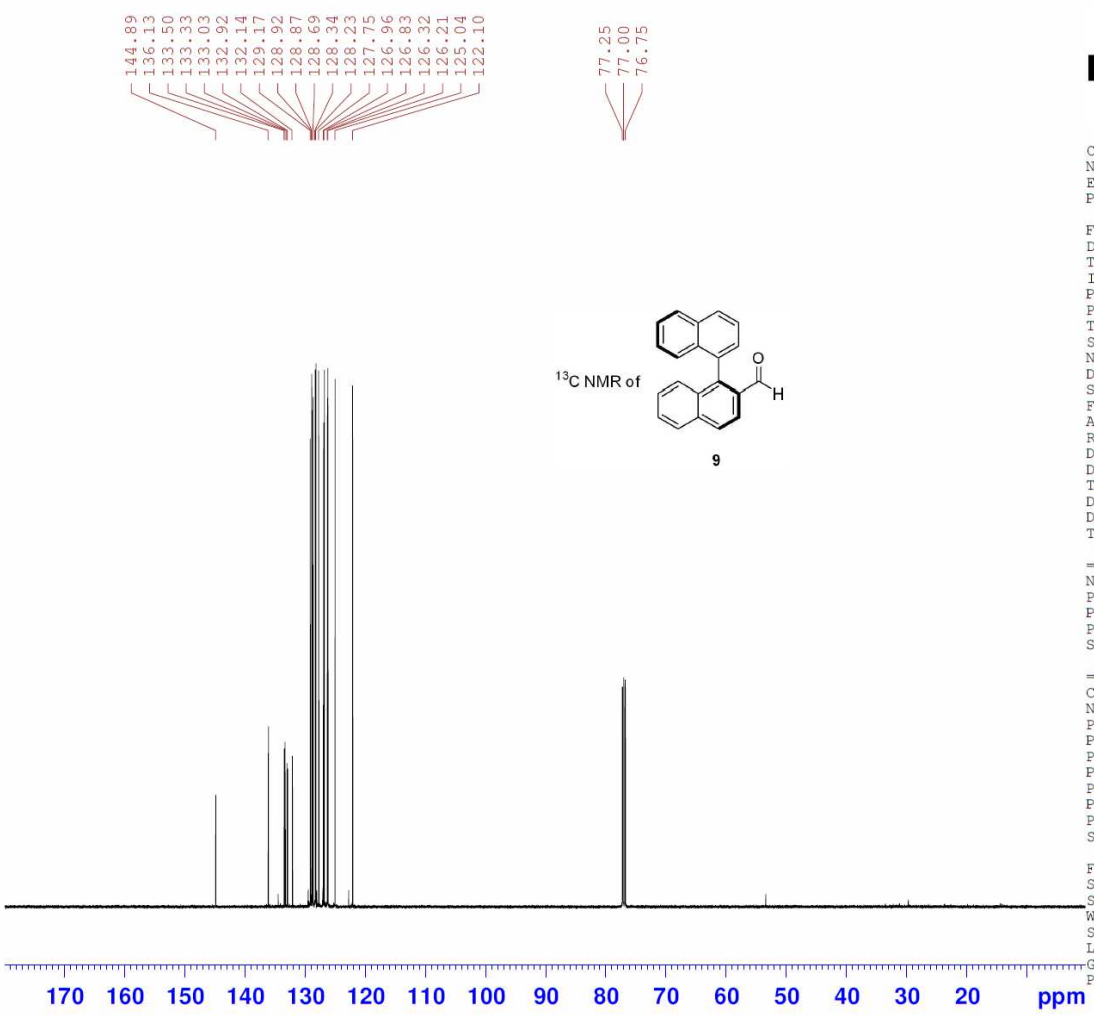
BRUKER

```
Current Data Parameters
NAME      102190-e68-cho
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110609
Time               23.39
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg10
TD                 32768
SOLVENT            CDCl3
NS                    64
DS                     0
SWH             7500.000 Hz
FIDRES          0.228882 Hz
AQ             2.1845834 sec
RG                   322
DW                66.667 usec
DE                 6.50 usec
TE                299.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.70 usec
PL1                 2.10 dB
PL1W        18.43091774 W
SFO1        500.1325007 MHz

F2 - Processing parameters
SI                 16384
SF          500.1300126 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



Current Data Parameters
NAME 102190-e68-cho
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110610
Time 4.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 262144
SOLVENT CDCl3
NS 3000
DS 0
SWH 31250.000 Hz
FIDRES 0.119209 Hz
AQ 4.1943541 sec
RG 2050
DW 16.000 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.88 usec
PL1 -0.50 dB
PL1W 124.00885010 W
SFO1 125.7698617 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.10 dB
PL12 19.30 dB
PL13 19.30 dB
PL2W 18.43091774 W
PL12W 0.35119396 W
PL13W 0.35119396 W
SFO2 500.1325007 MHz

F2 - Processing parameters
SI 131072
SF 125.7577938 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40