

Supporting Information

For

Efficient Chiral Monophosphorus Ligands for Asymmetric Suzuki-Miyaura Coupling Reactions

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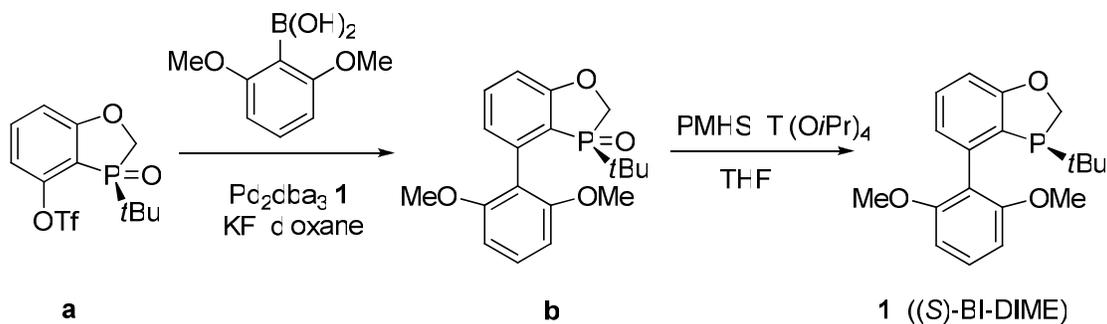
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1. General Methods. All reactions were carried out under a nitrogen atmosphere unless otherwise specified. THF (<0.02% water content), CH₂Cl₂, hexane, *n*-butanol, dioxane and toluene were purchased from J. T. Baker and used directly without further 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-dicyclohexylphosphino-2',6'-dimethoxybiphenyl, PMHS = polymethylhydrosiloxane,

¹H, ³¹P and ¹³C NMR data were recorded on a Bruker-Biospin DRX500 or DRX400 NMR Spectrometer with CDCl₃ or CD₂Cl₂ as the solvent. ¹H shifts were referenced to CDCl₃ at 7.26 ppm and CD₂Cl₂ at 5.32 ppm. ³¹P shifts were referenced to 85% H₃PO₄ in D₂O at 0.0 ppm as external standard and obtained with ¹H decoupling. ¹³C shifts were referenced to CDCl₃ at 77 ppm and CD₂Cl₂ at 54 ppm and obtained with ¹H decoupling. MS was measured on Agilent 1100 Series LC/MSD mass spectrometer. Chiral HPLC analyses were 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)

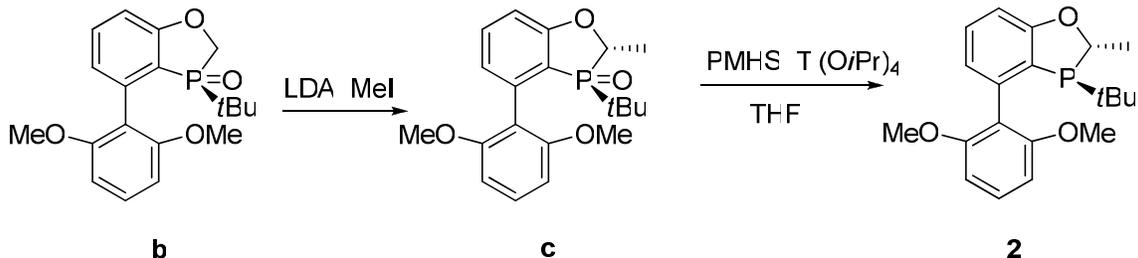


The synthesis of ligand **1** ((*S*)-BI-DIME) was carried out from chiral triflate **1** through a Suzuki coupling with 2,6-dimethoxyphenylboronic acid to form **b** followed by a stereospecific reduction of the phosphane oxide **b** mediated by PMHS/Ti(OiPr)₄. The synthetic procedures were similar to those for racemic BI-DIME published in our previous paper.²

Phosphane oxide **b**: white solid; >99% ee; [α]_D²⁰ = -66.4° (c = 0.64, CHCl₃); 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; [α]_D²⁰ = -175.3° (c = 0.3, CHCl₃); The enantiomeric excess was determined by converting to its phosphine oxide via stereospecific oxidation with H₂O₂ as the oxidant.

b. Synthesis of ligand 2

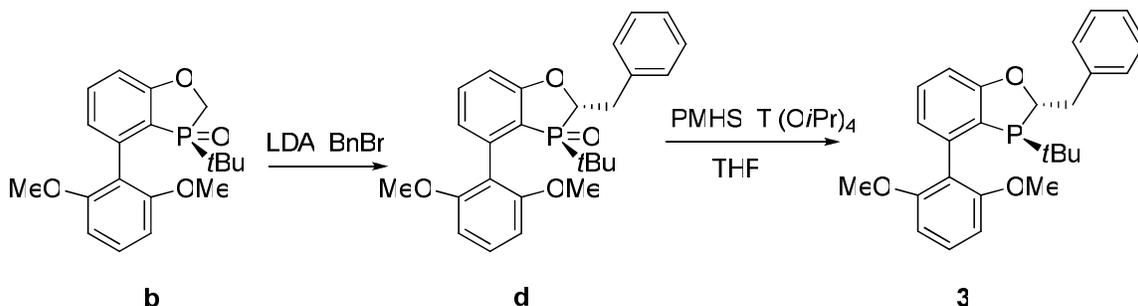


The synthesis of ligand **2** was carried out from chiral phosphane oxide **b** through methylation to form **c** followed by a stereospecific reduction of the phosphane oxide **c** under conditions of PMHS/Ti(OiPr)₄. The synthetic procedures were similar to those for its racemic form published in our previous paper.³ The relative configuration between P chirality and C chirality was determined by NOE experiments.

Phosphane oxide **c**: white solid; $[\alpha]_{\text{D}}^{20} = -12.8^{\circ}$ ($c = 0.53$, CHCl₃).

Phosphane **2**: white solid; $[\alpha]_{\text{D}}^{20} = -121.6^{\circ}$ ($c = 0.55$, CHCl₃).

c: Synthesis of ligand 3

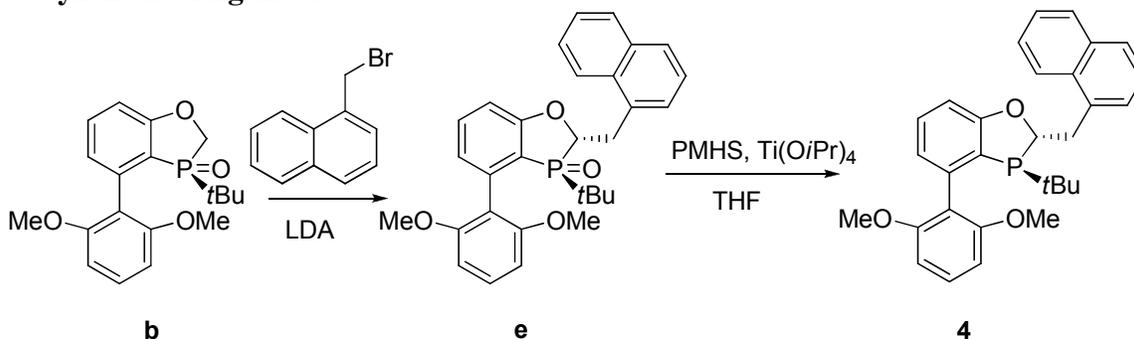


To a solution of (*R*)-3-*tert*-butyl-4-(2,6-dimethoxyphenyl)-2,3-dihydrobenzo[d][1,3]oxaphosphole oxide (**b**, 5.0 g, 14.4 mmol) in THF (50 mL) at -70 °C was charged LDA (9.6 mL, 1.8 M, 17.3 mmol, 1.2 equiv) over 5 min. The mixture was kept at -70 °C for 1 h. To the mixture was charged BnBr (2.96 g, 17.3 mmol, 1.2 equiv) over 5 min while controlling the reaction temperature below -60 °C. The resulting mixture was stirred at -70 °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**: $[\alpha]_{\text{D}}^{20} = +55.9^{\circ}$ ($c = 0.42$, CHCl₃); ¹H NMR (400 MHz, CDCl₃) 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); ³¹P NMR (162 MHz, CDCl₃) δ 59.9; ¹³C NMR (100 MHz, CDCl₃) 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 carefully 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 °C 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**: $[\alpha]_D^{20} = -16.2^\circ$ ($c = 0.49$, $CHCl_3$); 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 $[M + H]^+$.

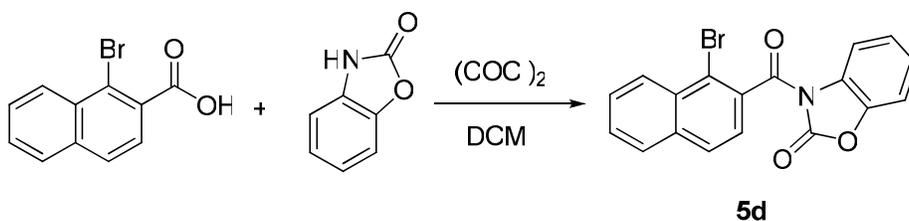
d: Synthesis of ligand 4



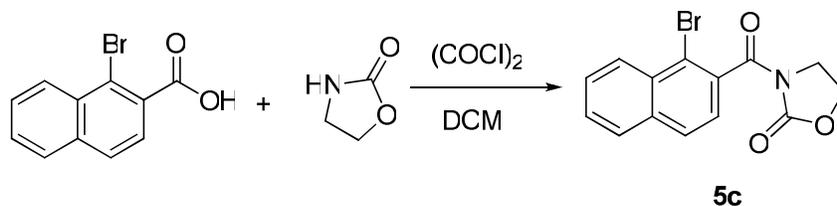
The synthesis of compound **e** from compound **b** was carried out following a procedure similar to the preparation of compound **d** for the synthesis of ligand **3**. **e**: 85% yield (white solid); $[\alpha]_D^{20} = +43.4^\circ$ ($c = 0.35$, $CHCl_3$); 1H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, $J = 7.8$ 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); $[\alpha]_D^{20} = -28.6^\circ$ ($c = 0.29$, CHCl_3); $^1\text{H NMR}$ (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); $^{31}\text{P NMR}$ (162 MHz, CDCl_3) δ 7.5; $^{13}\text{C NMR}$ (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 $[\text{M} + \text{H}]^+$.

3. Procedures for substrate preparation



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 oxalyl 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**: $^1\text{H NMR}$ (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); $^{13}\text{C NMR}$ (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 $[\text{M} + \text{Na}]^+$.



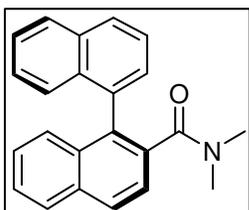
Preparation of **5c** was carried out according to a procedure similar to that for the synthesis of **5d**. **5c**: 85% yield; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.30 (d, $J = 8.5$ Hz, 1H),

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 $[\text{M} + \text{Na}]^+$.

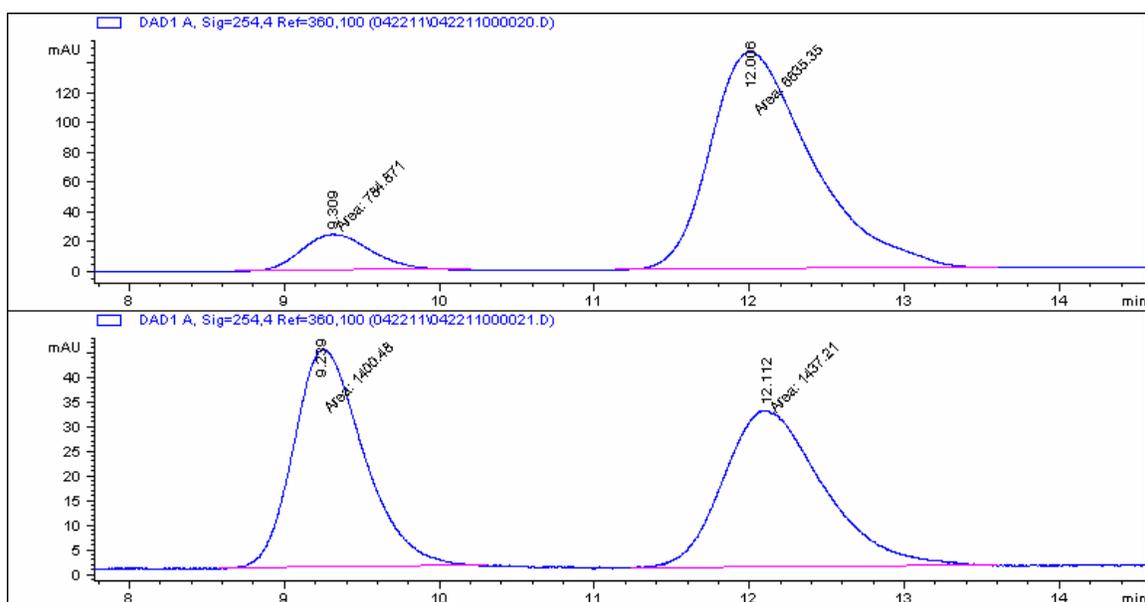
4. General procedure for asymmetric Suzuki-Miyaura couplings

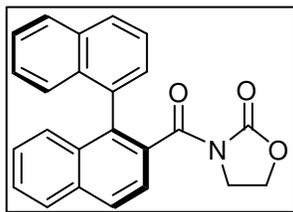
To a mixture of aryl bromide (1.0 mmol), arylboronic acid (2.0 mmol), potassium phosphate (3 mmol, 3 equiv), $\text{Pd}(\text{OAc})_2$ (0.01-0.05 mmol), and ligand **2** or **4** (0.012-0.06 mmol, Pd/ligand ratio = 1/1.2) was charged dry THF (2 mL). The mixture was stirred at room temperature or 40 °C 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



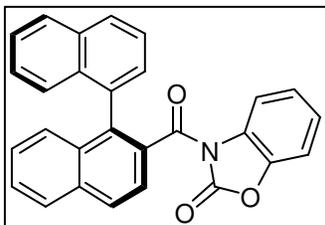
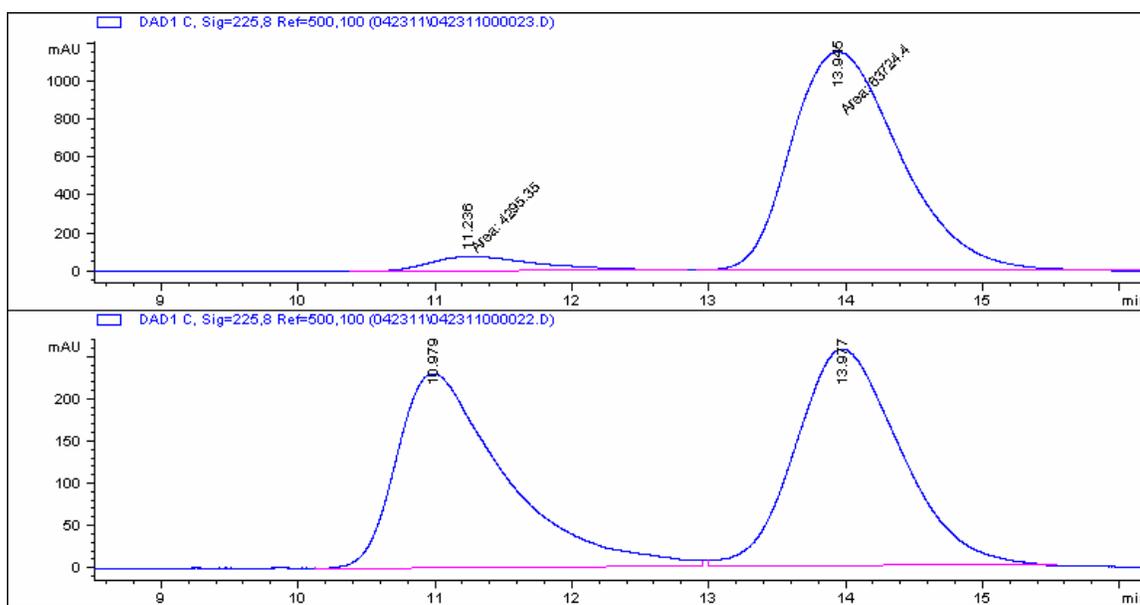
(*R*)-*N,N*-Dimethyl-1,1'-binaphthyl-2-carboxamide: white solid (95% yield); 79% ee; $[\alpha]_{\text{D}}^{20} = +66.0^\circ$ ($c = 0.80$, CHCl_3); ^1H NMR (500 MHz, CDCl_3) δ 8.02 (d, $J = 7.3$ Hz, 1H), 7.95 (br m, 3H), 7.40-7.75 (m, 5H), 7.29 (m, 4H), 2.20-3.10 (br m, 4H); ^{13}C NMR (125 MHz, CDCl_3) 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 $[\text{M} + \text{H}]^+$. 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, 9.30 min (*S*), 12.00 min (*R*).





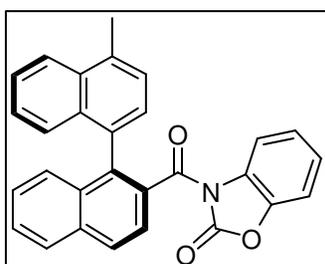
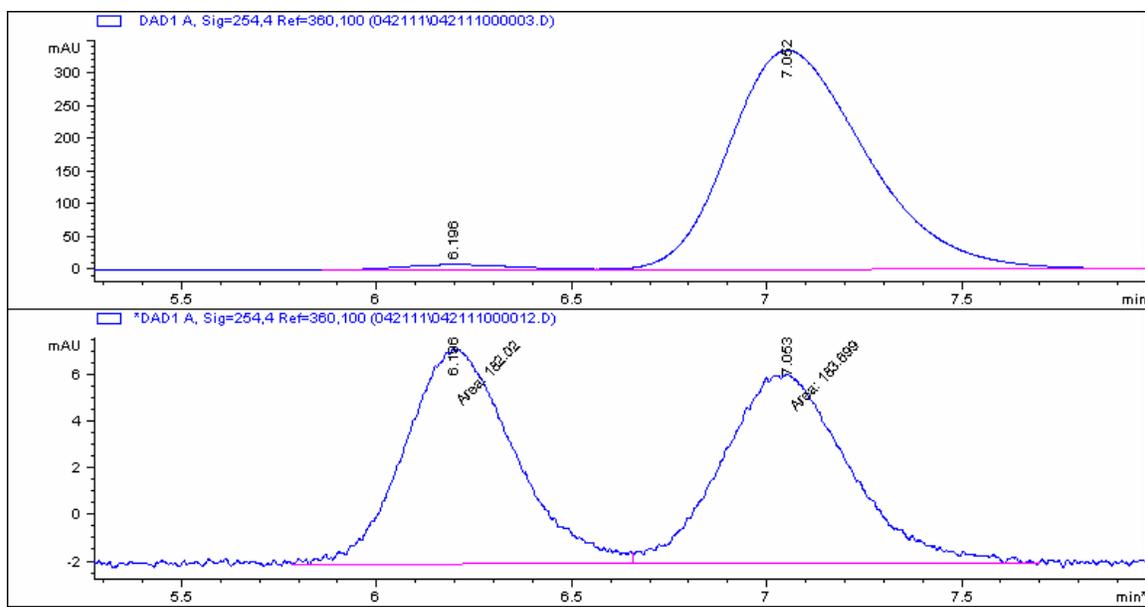
(R)-3-(1,1'-binaphthyl-2-carbonyl)oxazolidin-2-one:

yellowish solid (96% yield). 87% ee; $[\alpha]_D^{20} = -61.6^\circ$ (c = 0.55, CHCl₃); ¹H NMR (400 MHz, CD₂Cl₂) 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); ¹³C NMR (100 MHz, CD₂Cl₂) 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*).

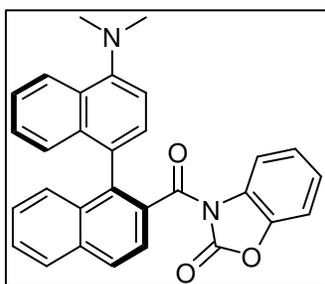
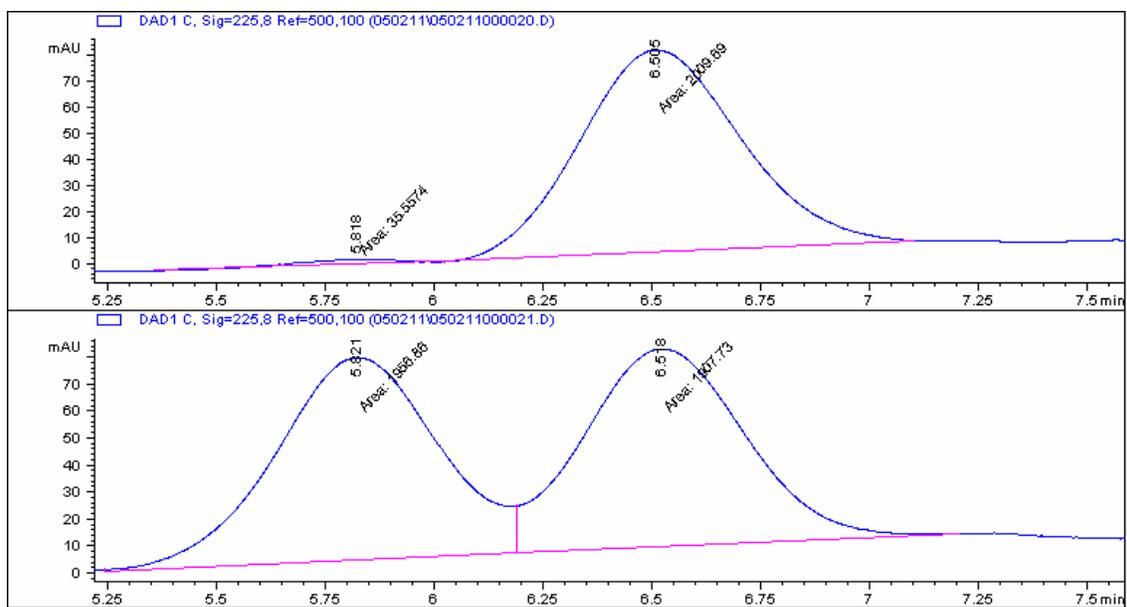


(R)-3-(1,1'-binaphthyl-2-carbonyl)benzo[d]oxazol-2(3H)-one:

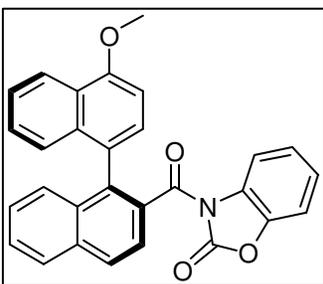
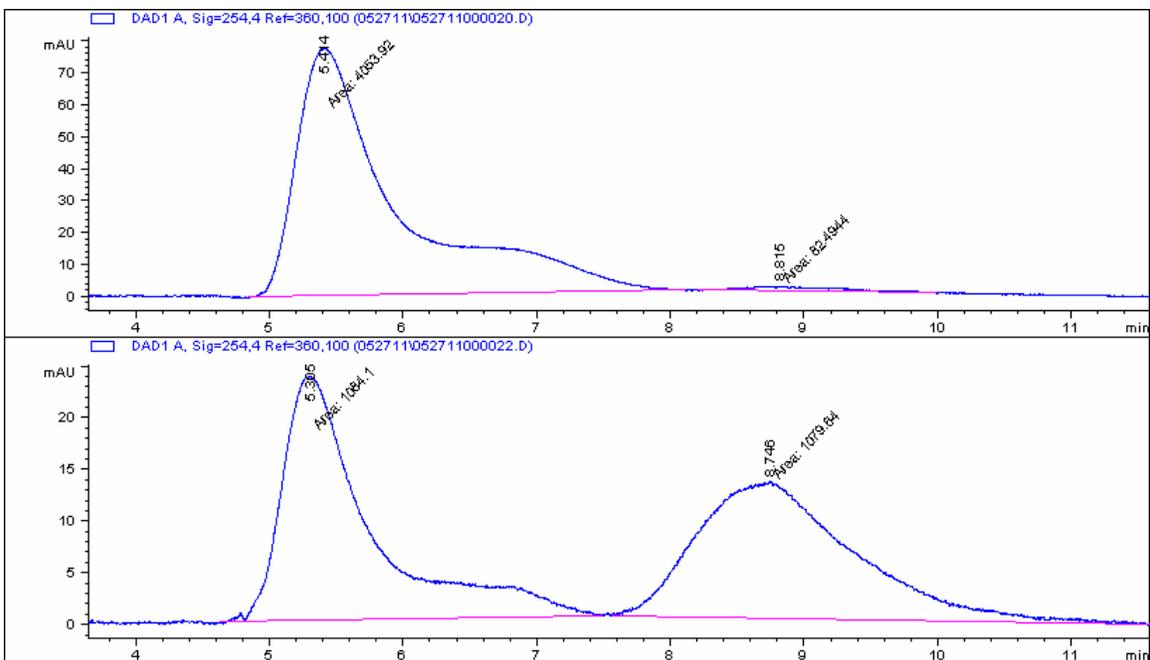
white solid (96% yield); 96% ee; $[\alpha]_D^{20} = -126.1^\circ$ (c = 1.33, CHCl₃); ¹H NMR (400 MHz, CD₂Cl₂) δ 8.11 (d, *J* = 6.7 Hz, 1H), 8.04 (d, *J* = 6.4 Hz, 1H), 7.79 (m, 2H), 7.72 (d, *J* = 6.7 Hz, 1H), 7.60 (m, 1H), 7.25-7.50 (m, 8H), 7.14 (t, *J* = 6.0 Hz, 1H), 7.04 (m, 2H); ¹³C NMR (100 MHz, CD₂Cl₂) 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*).



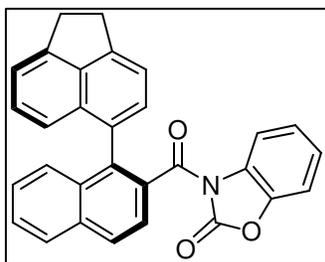
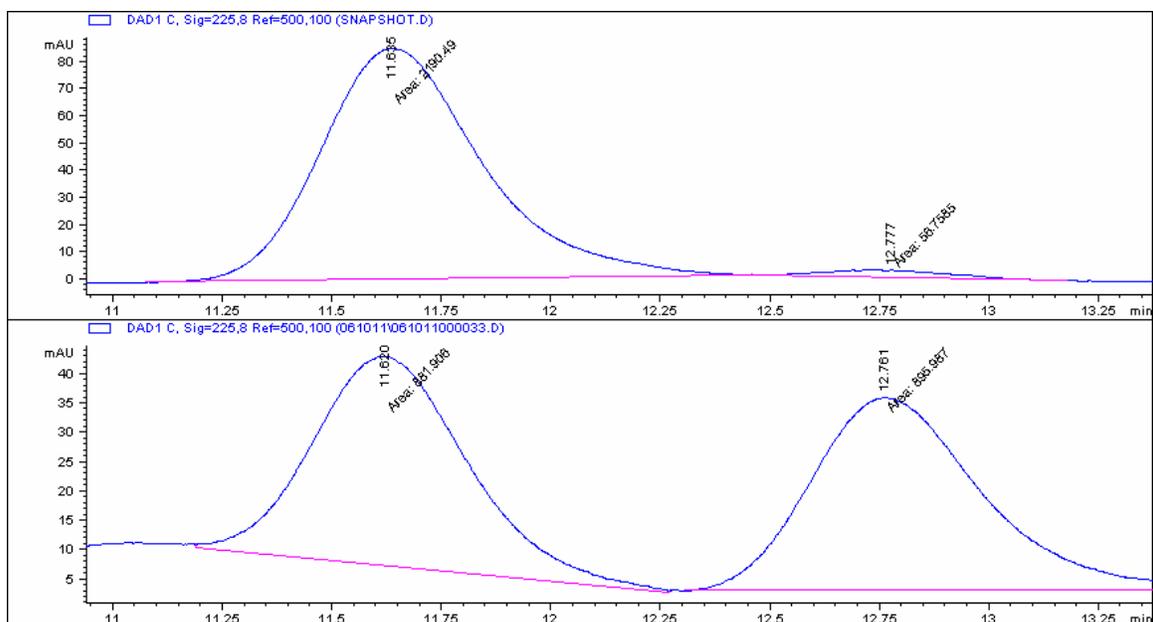
(R)-3-(4'-Methyl-1,1'-binaphthyl-2-carbonyl)benzo[d]oxazol-2(3H)-one: white solid (95% yield); 96% ee; $[\alpha]_D^{20} = -128.8^\circ$ ($c = 0.49$, CHCl_3); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.07 (d, $J = 8.5$ Hz, 1H), 7.98 (d, $J = 8.3$ Hz, 1H), 7.87 (d, $J = 8.4$ Hz, 1H), 7.70 (d, $J = 8.4$ Hz, 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); $^{13}\text{C NMR}$ (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 $[\text{M} + \text{Na}]^+$; 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*).



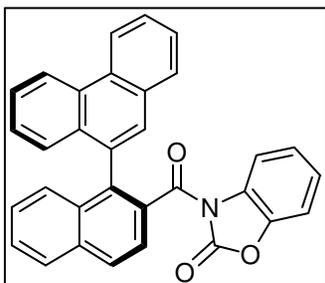
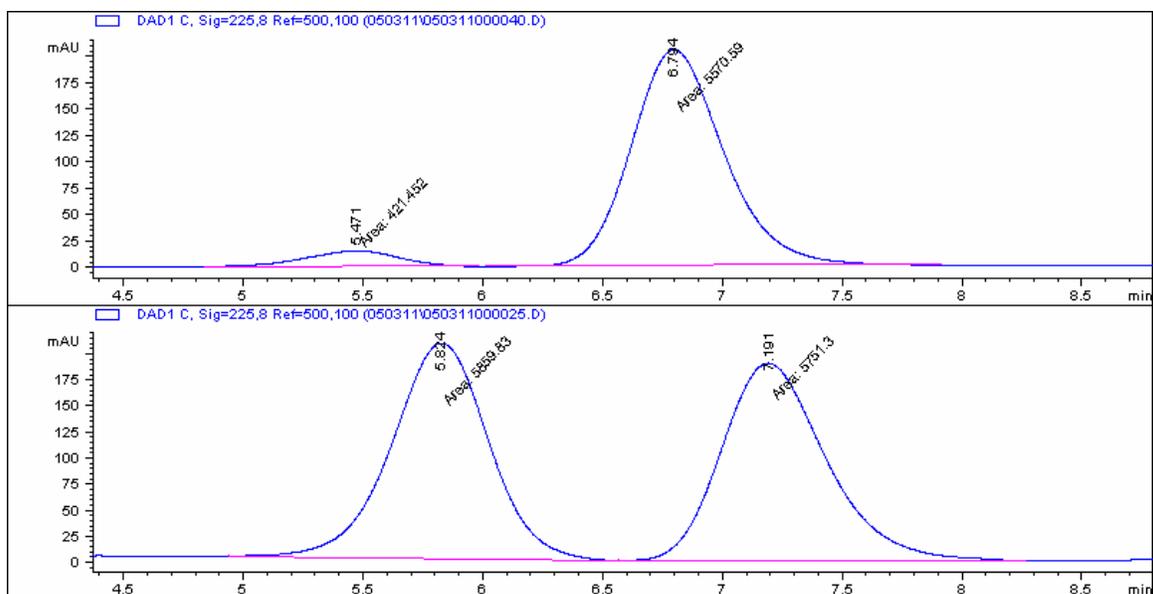
(R)-3-(4'-(dimethylamino)-1,1'-binaphthyl-2-carbonyl)benzo[d]oxazol-2(3H)-one: 95% yield; 96% ee; $[\alpha]_D^{20} = -175.2^\circ$ ($c = 0.65$, CHCl_3); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.09 (d, $J = 8.4$ Hz, 1H), 8.07 (d, $J = 8.3$ Hz, 1H), 7.99 (d, $J = 8.2$ Hz, 1H), 7.73 (d, $J = 8.4$ Hz, 1H), 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); $^{13}\text{C NMR}$ (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 $[\text{M} + \text{Na}]^+$; 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*).



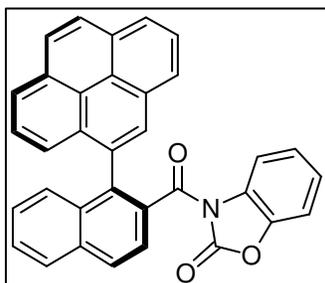
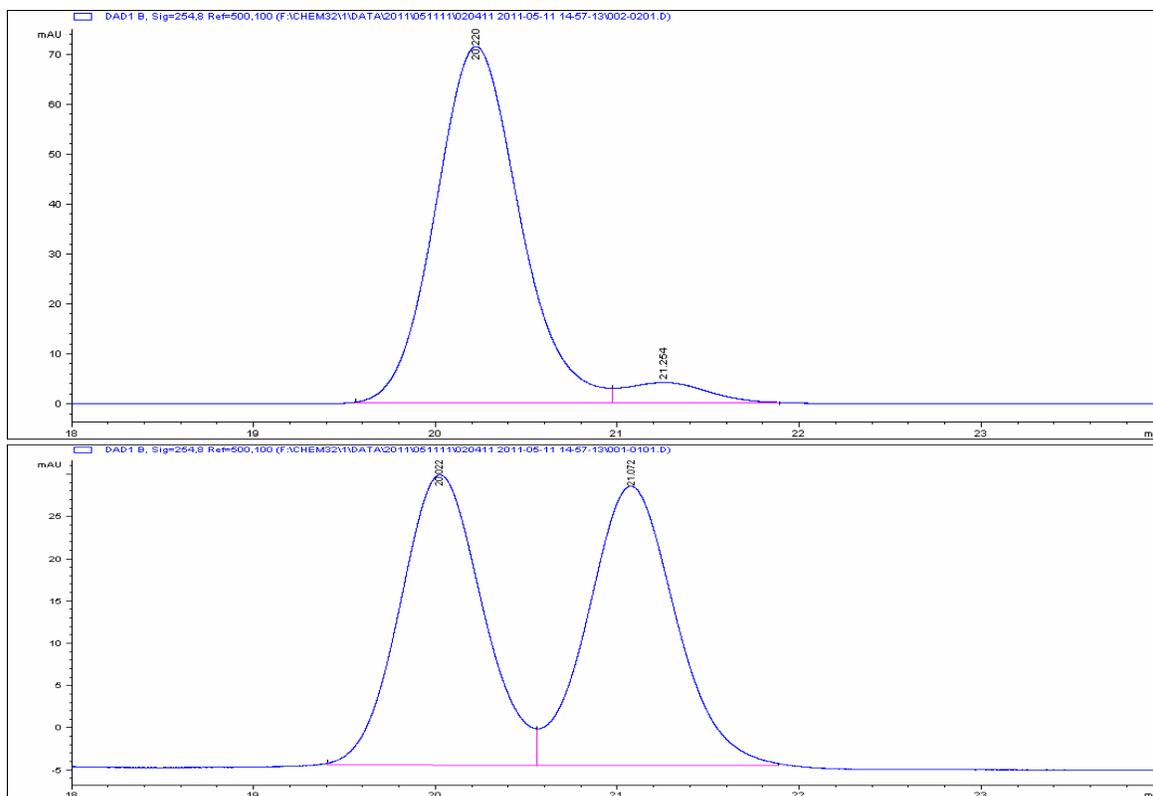
(R)-3-(4'-methoxy-1,1'-binaphthyl-2-carbonyl)benzo[d]oxazol-2(3H)-one: white solid (95% yield); 94% ee; $[\alpha]_D^{20} = -70.6^\circ$ ($c = 0.17$, CHCl_3); $^1\text{H NMR}$ (400 MHz, CD_2Cl_2) δ 8.19 (d, $J = 8.3$ Hz, 1H), 8.10 (d, $J = 8.5$ Hz, 1H), 8.03 (d, $J = 8.3$ Hz, 1H), 7.70 (d, $J = 8.5$ Hz, 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); $^{13}\text{C NMR}$ (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 $[\text{M} + \text{Na}]^+$; 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, 11.53 min (*R*), 12.78 min (*S*).



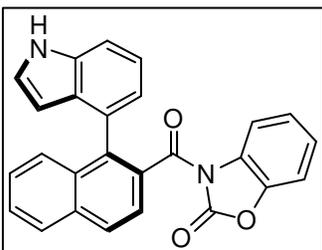
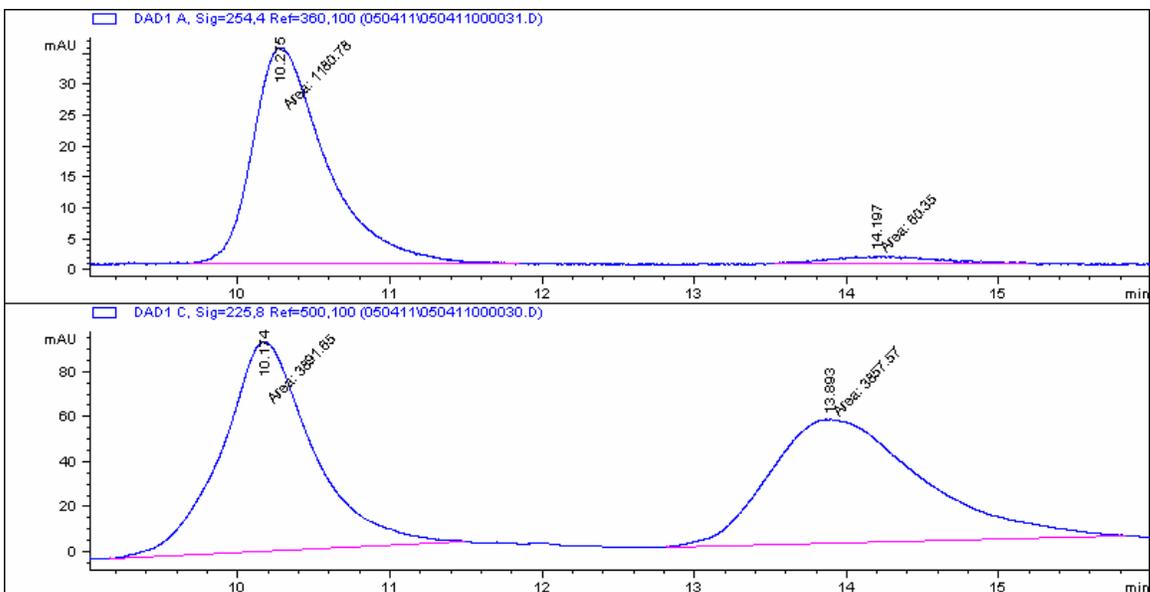
(R)-3-(1-(1,2-dihydroacenaphthylen-5-yl)-2-naphthoyl)benzo[d]oxazol-2(3H)-one: white solid (96% yield); 88% ee; $[\alpha]_D^{20} = -96.8^\circ$ ($c = 0.41$, CHCl_3); ^1H NMR (400 MHz, CD_2Cl_2) δ 8.10 (d, $J = 8.5$ Hz, 1H), 8.03 (d, $J = 8.2$ Hz, 1H), 7.73 (d, $J = 8.5$ Hz, 1H), 7.61 (m, 1H), 7.54 (d, $J = 8.6$ 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 $[\text{M} + \text{Na}]^+$; 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*).



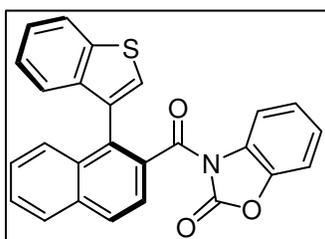
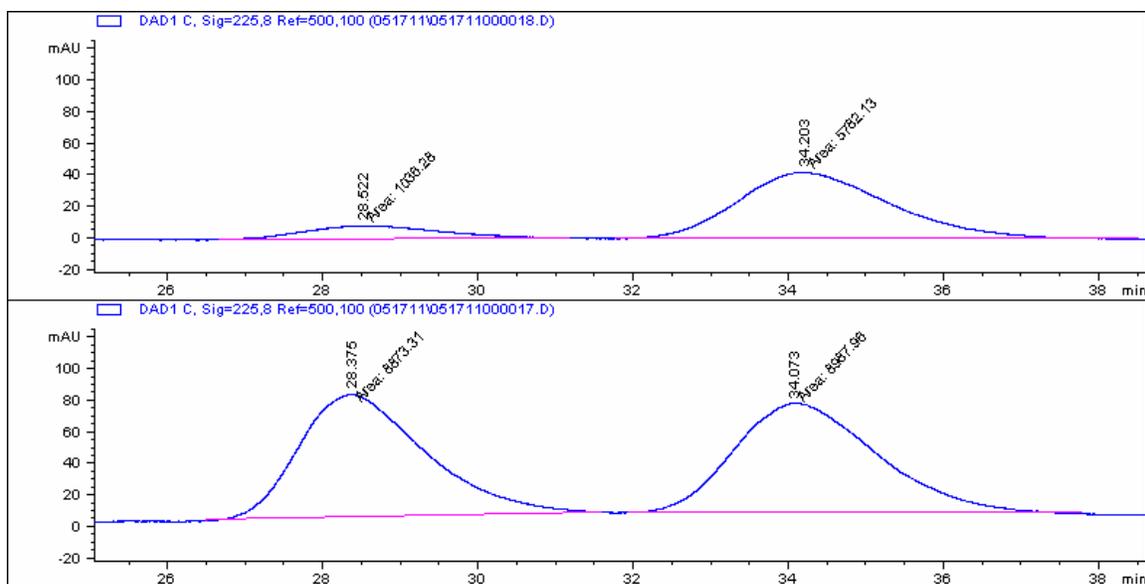
(R)-3-(1-(phenanthren-9-yl)-2-naphthoyl)benzo[d]oxazol-2(3H)-one: white solid (96% yield); 90% ee; $[\alpha]_D^{20} = -91.7^\circ$ ($c = 0.36$, CHCl_3); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.61 (d, $J = 8.3$ Hz, 1H), 8.57 (d, $J = 8.2$ Hz, 1H), 8.11 (d, $J = 8.5$ Hz, 1H), 8.01 (d, $J = 8.3$ Hz, 1H), 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); $^{13}\text{C NMR}$ (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 $[\text{M} + \text{Na}]^+$; Chiral HPLC conditions: Chiralpak AD-3, 4.6 mm X 250 mm, 25 °C, flow rate: 1.2 mL/min, heptane/isopropanol: 85/15, 254 nm, 20.0 min (*R*), 21.1 min (*S*).



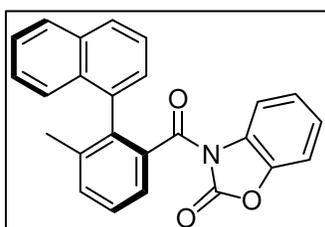
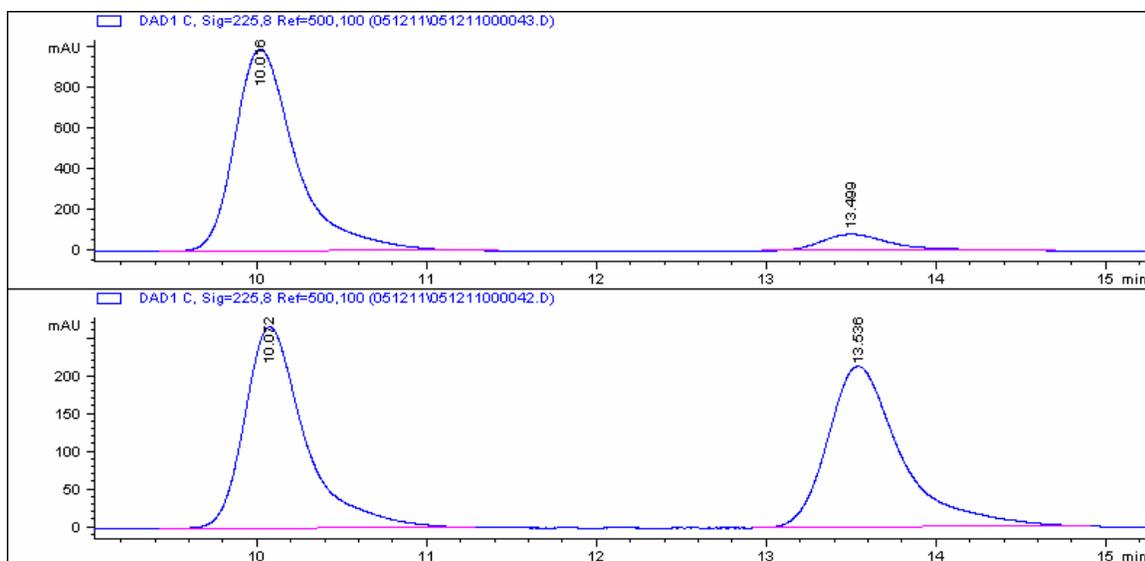
(R)-3-(1-(pyren-4-yl)-2-naphthoyl)benzo[d]oxazol-2(3H)-one: white solid (95% yield); 90% ee; $[\alpha]_D^{20} = -129.5^\circ$ (c = 0.44, CHCl_3); $^1\text{H NMR}$ (400 MHz, CD_2Cl_2) δ 8.13-8.25 (m, 4H), 8.00-8.12 (m, 5H), 7.94 (d, $J = 9.2$ Hz, 1H), 7.79 (d, $J = 8.5$ Hz, 1H), 7.63 (m, 2H), 7.36 (m, 2H), 7.29 (d, $J = 7.9$ Hz, 1H), 6.88 (m, 2H), 6.75 (t, $J = 7.8$ Hz, 1H); $^{13}\text{C NMR}$ (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 $[\text{M} + \text{Na}]^+$; Chiral HPLC conditions: Chiralcel AD-H, 4.6 mm X 250 mm, 30 °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; ^1H 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 $[\text{M} + \text{Na}]^+$; Chiral HPLC conditions: Chiralcel OD-H, 4.6 mm X 250 mm, 30 °C, flow rate: 2 mL/min, heptane/isopropanol: 93/7, 225 nm, 28.5 min (*S*), 34.2 min (*R*).

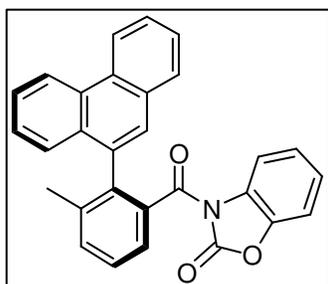
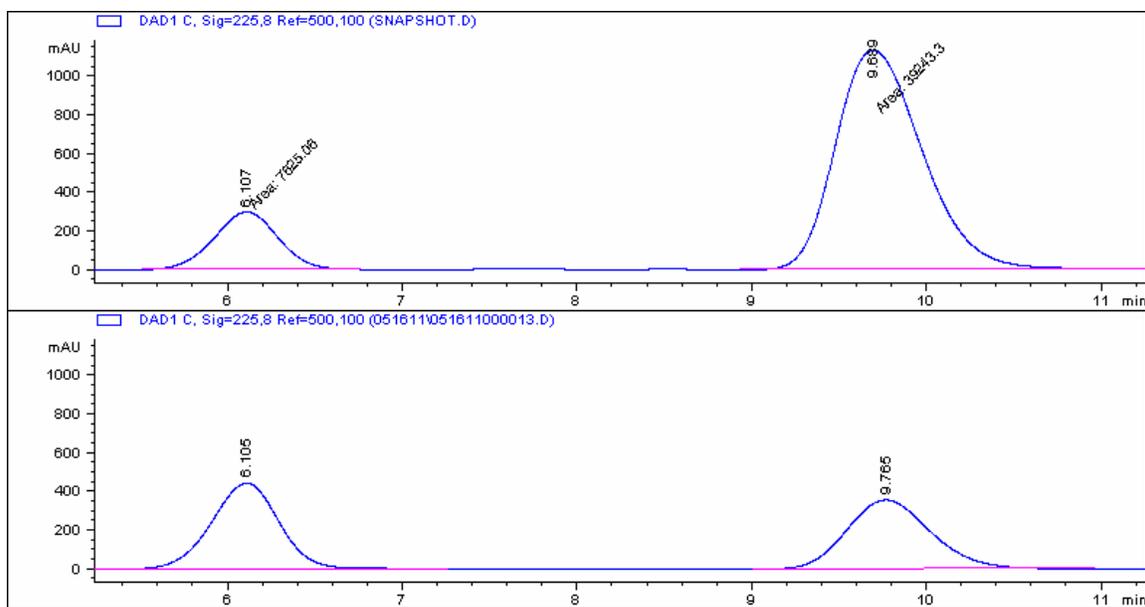


(S)-3-(1-(benzo[b]thiophen-3-yl)-2-naphthoyl)benzo[d]oxazol-2(3H)-one: 95% yield; 82% ee; $[\alpha]_D^{20} = -121.8^\circ$ ($c = 0.61$, CHCl_3); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.09 (d, $J = 8.5$ Hz, 1H), 8.99 (d, $J = 8.3$ Hz, 1H), 7.71 (m, 2H), 7.64 (d, $J = 8.6$ Hz, 1H), 7.60 (t, $J = 8.0$ Hz, 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); $^{13}\text{C NMR}$ (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 $[\text{M} + \text{Na}]^+$; 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*).



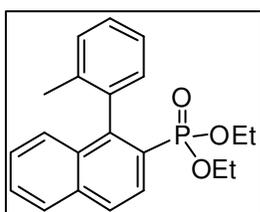
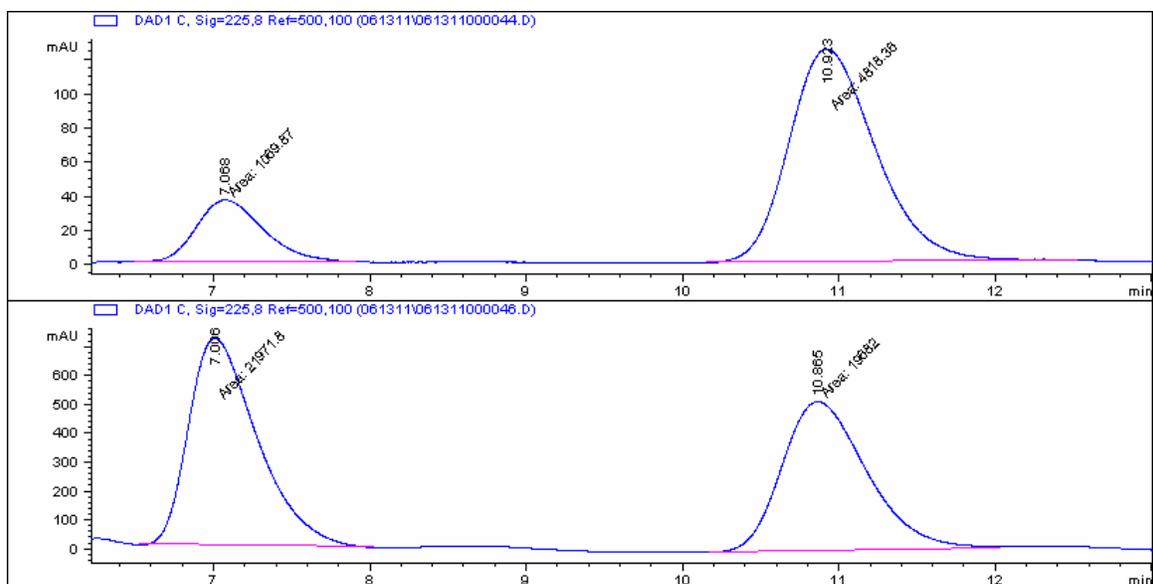
(R)-3-(3-methyl-2-(naphthalen-1-yl)benzoyl)benzo[d]oxazol-2(3H)-one: 85% yield; 70% ee; $[\alpha]_{\text{D}}^{20} = -121.8^{\circ}$ ($c = 0.66$, CHCl_3); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.70 (m, 1H), 7.66 (dd, $J = 7.4, 1.6$ Hz, 1H), 7.56 (m, 1H), 7.51 (m, 3H), 7.42 (m, 2H), 7.27-7.45 (m, 3H), 7.06 (m, 1H), 6.97 (m, 2H), 2.06 (s, 3H); $^{13}\text{C NMR}$ (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 $[\text{M} + \text{Na}]^+$; 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*).

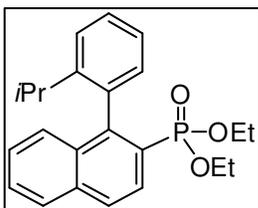
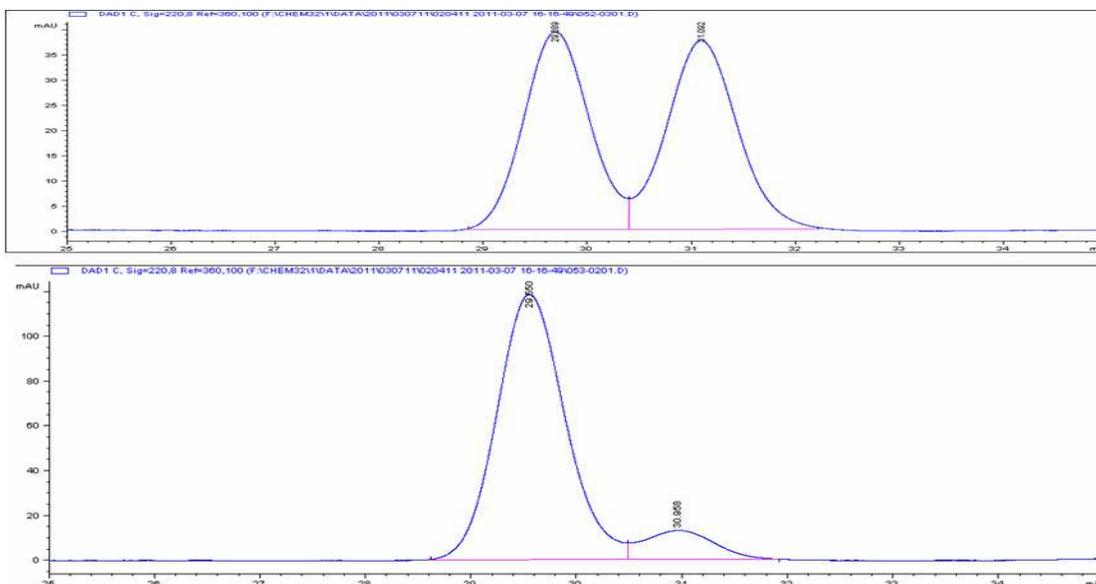


(R)-3-(3-Methyl-2-(phenanthren-9-yl)benzoyl)benzo[d]oxazol-2(3H)-one: white solid (90% yield); 64% ee; $[\alpha]_D^{20} = -17.8^\circ$ (c = 0.45, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 8.57 (d, *J* = 8.2 Hz, 1H), 8.51 (d, *J* = 7.4 Hz, 1H), 7.80 (m, 1H), 7.50-7.65 (m, 9H), 7.22 (d, *J* = 7.8 Hz, 1H), 6.93 (t, *J* = 7.9 Hz, 1H), 6.81(m, 2H), 2.10 (s, 3H); ¹H NMR (100 MHz, CDCl₃) 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,

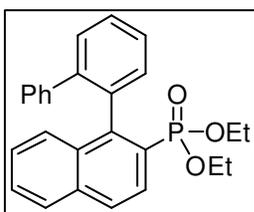
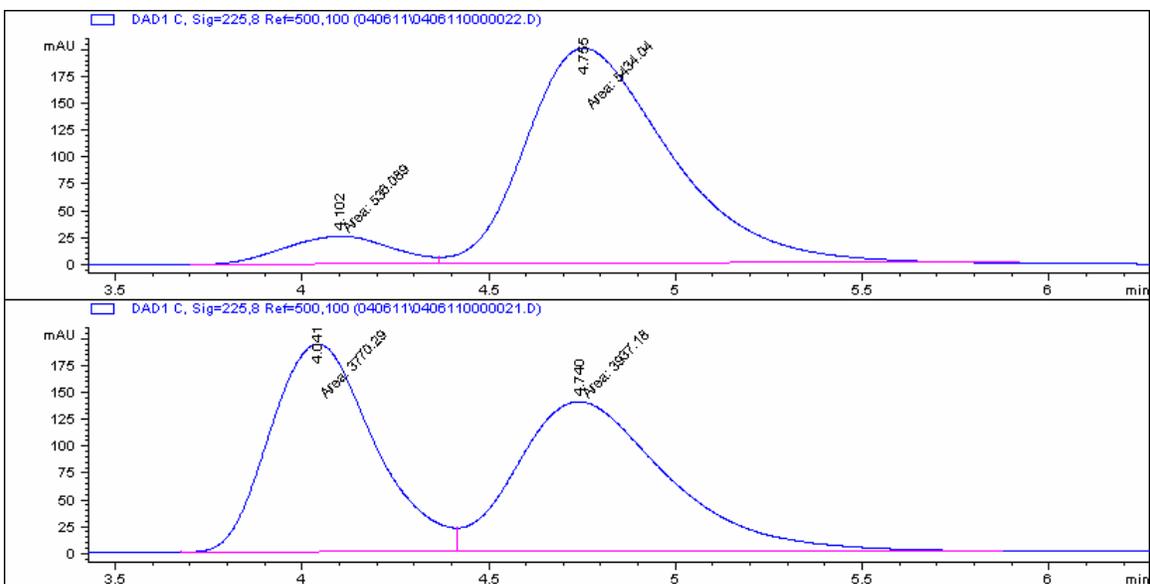
128.7, 127.9, 127.8, 127.2, 126.9, 126.8, 126.72, 126.7, 125.1, 124.6, 124.1, 122.7, 122.3, 113.9, 109.3, 20.1; ESI-MS: *m/z* 452 [M + Na]⁺; Chiral HPLC conditions: Chiralcel OD-H, 4.6 mm X 250 mm, 30 °C, flow rate: 2 mL/min, heptane/isopropanol: 94/6, 225 nm, 7.07 min (*S*), 10.92 min (*R*).



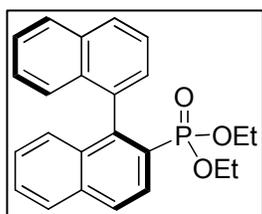
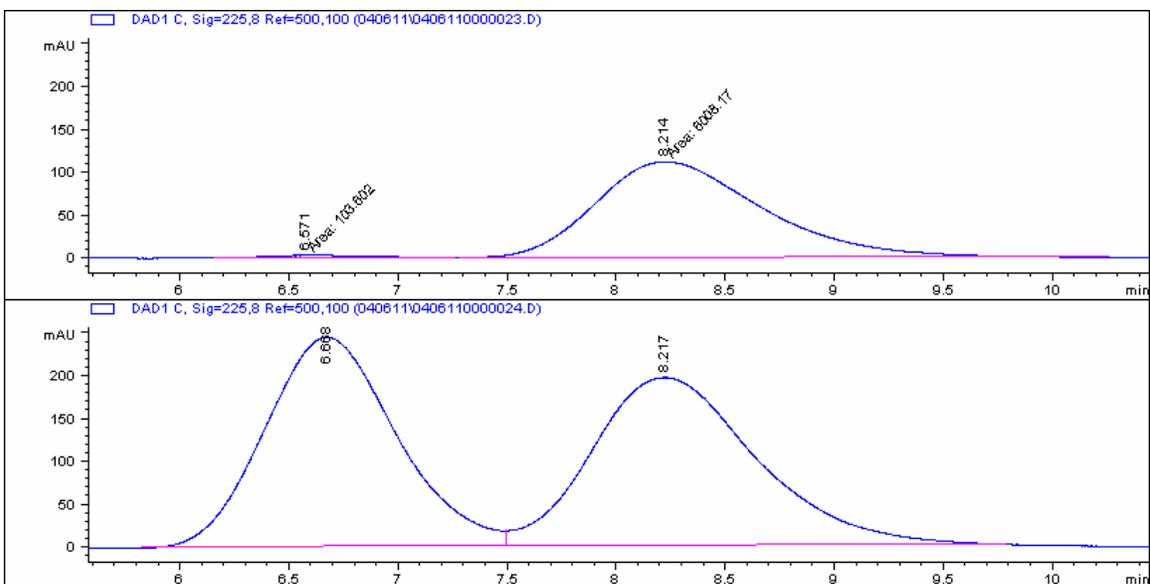
Diethyl 1-*o*-tolynaphthalen-2-ylphosphonate: white solid (95% yield); 80% ee; $[\alpha]_{\text{D}}^{20} = -5.5^{\circ}$ ($c = 0.53$, CHCl_3); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.09 (dd, $J = 11.8, 8.8$ Hz, 1H), 7.92 (m, 2H), 7.55 (t, $J = 7.3$ Hz, 1H), 7.25-7.43 (m, 5H), 7.21 (d, $J = 7.3$ Hz, 1H), 3.82-4.00 (m, 3H), 3.70-3.82 (m, 1H), 1.92 (s, 3H), 1.85 (m, 6H); $^{13}\text{C NMR}$ (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 $[\text{M} + \text{H}]^+$; 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; $[\alpha]_{\text{D}}^{20} = -19.8^\circ$ ($c = 0.4$, CHCl_3); $^1\text{H NMR}$ (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); $^{13}\text{C NMR}$ (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 $[\text{M} + \text{H}]^+$; 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.

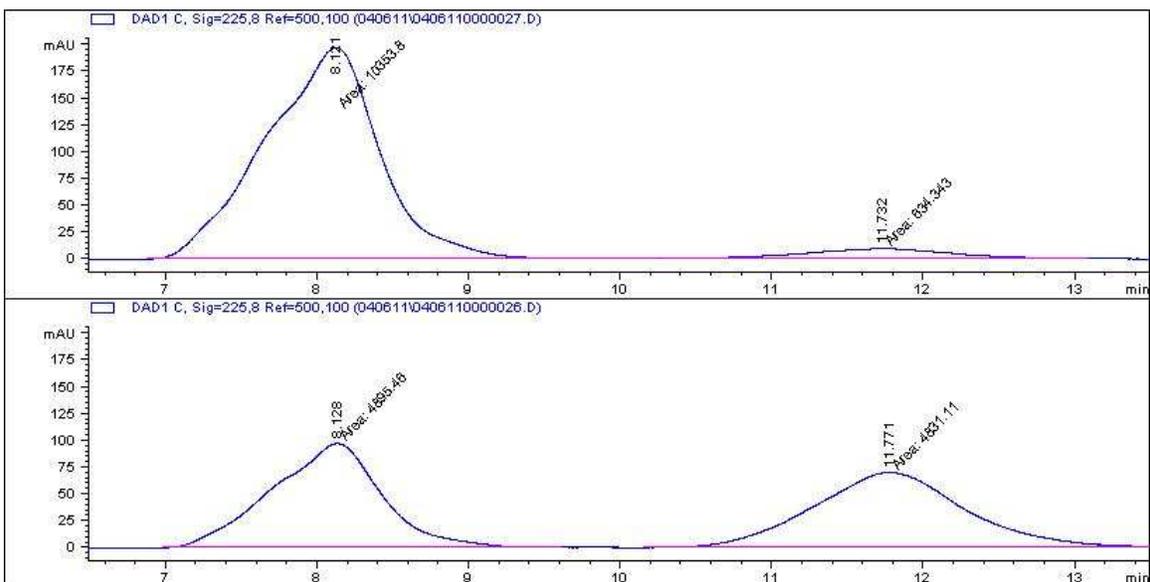


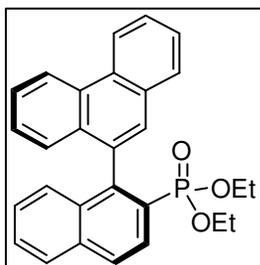
Diethyl 1-(biphenyl-2-yl)naphthalen-2-ylphosphonate: 74% yield; 96% ee; $[\alpha]_D^{20} = -4.7^\circ$ ($c = 0.6$, CHCl_3); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.98 (dd, $J = 12.0, 8.8$ Hz, 1H), 7.81 (dd, $J = 8.4, 3.6$ Hz, 1H), 7.73 (d, $J = 8.3$ Hz, 1H), 7.54 (m, 2H), 7.37-7.49 (m, 3H), 7.33 (d, $J = 8.6$ 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); $^{13}\text{C NMR}$ (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 $[\text{M} + \text{H}]^+$; 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; $[\alpha]_{\text{D}}^{20} = +46.4^{\circ}$ ($c = 0.29$, 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,

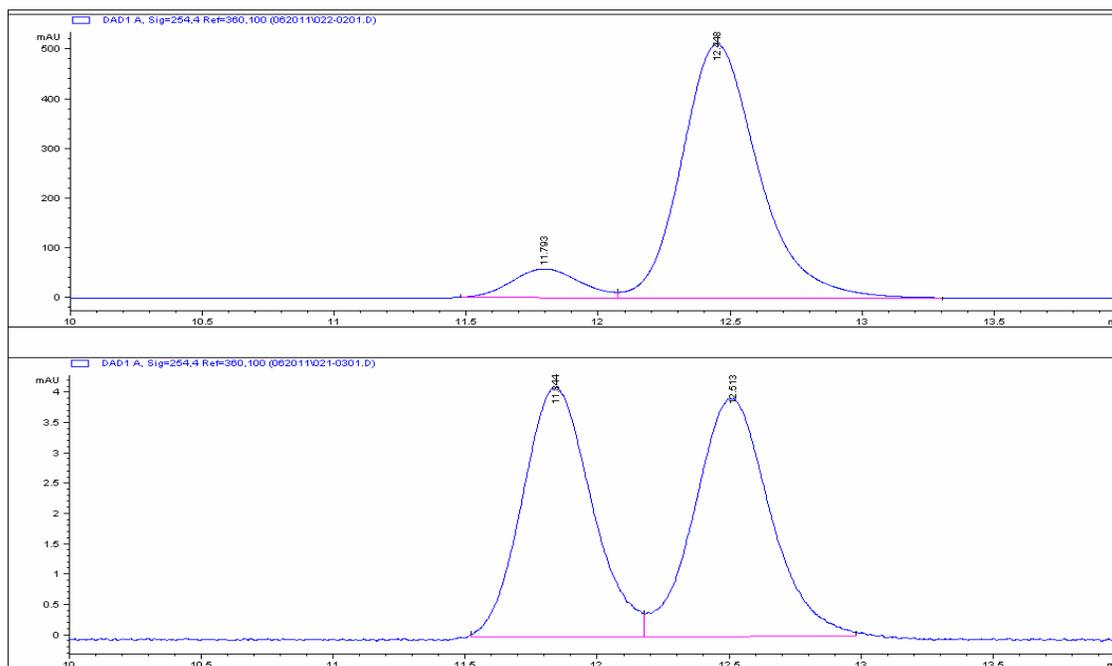
1H), 3.58 (m 2H), 0.97 (t, $J = 7.0$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 135.9, 134.9, 133.4, 133.2, 128.73, 128.71, 128.6, 128.3, 128.0, 127.9, 127.8, 127.7, 127.6, 126.72, 126.7, 125.9, 125.6, 124.9, 61.8 (d, $J = 6.0$ Hz), 61.6 (d, $J = 6.0$ Hz), 15.9 (d, $J = 6.7$ Hz), 15.4 (d, $J = 7.2$ Hz); ESI-MS: m/z 391 $[\text{M} + \text{H}]^+$; Chiral HPLC conditions: Chiralcel AD-H, 4.6 mm X 250 mm, 30 $^{\circ}\text{C}$, flow rate: 2 mL/min, heptane/isopropanol: 96/4, 225 nm, 8.13 min (*R*), 11.7 min (*S*).



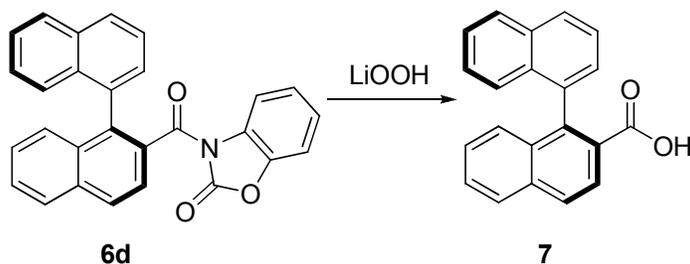


(R)-diethyl 1-(phenanthren-9-yl)naphthalen-2-ylphosphonate:
 90% yield; 82% ee; $[\alpha]_D^{20} = +30.4^\circ$ (c = 0.25, CHCl₃); ¹H NMR (500 MHz, CDCl₃) δ 8.79 (d, *J* = 8.3 Hz, 2H), 8.26 (dd, *J* = 12.2, 8.6 Hz, 1H), 8.06 (dd, *J* = 8.6, 3.7 Hz, 1H), 8.96 (d, *J* = 8.3 Hz, 1H), 7.89 (d, *J* = 7.8 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); ¹³C NMR (125 MHz, CDCl₃)

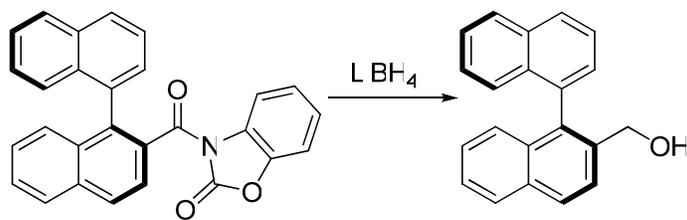
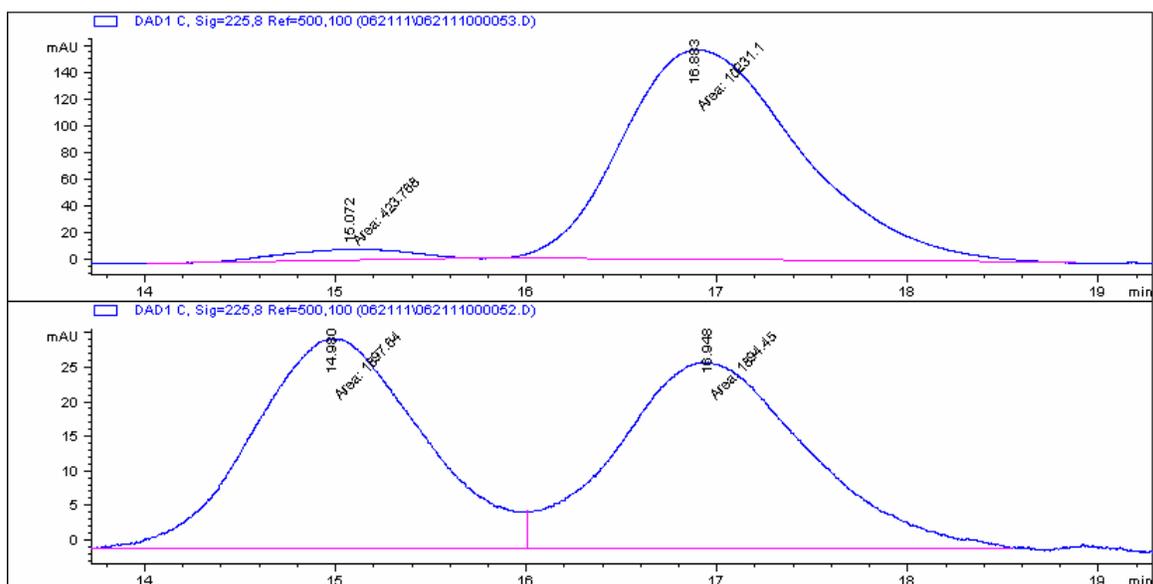
δ 143.3 (d, *J* = 9.3 Hz), 135.0 (d, *J* = 2.6 Hz), 134.5 (d, *J* = 5.3 Hz), 133.3 (d, *J* = 15.7 Hz), 132.6, 131.3, 130.3, 129.9, 129.63, 129.62, 128.9, 128.8, 128.79, 128.0 (d, *J* = 1.0 Hz), 127.9 (d, *J* = 1.0 Hz), 127.87, 127.8, 127.7, 127.1, 127.6, 126.9, 126.7 (d, *J* = 1.4 Hz), 126.5, 126.3, 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: Chiralcel 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



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% H₂O₂ 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; $[\alpha]_D^{20} = +23.6^\circ$ (c = 0.70, CHCl₃); ¹H NMR (400 MHz, CDCl₃) 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); ¹³C NMR (100 MHz, CDCl₃) 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*).

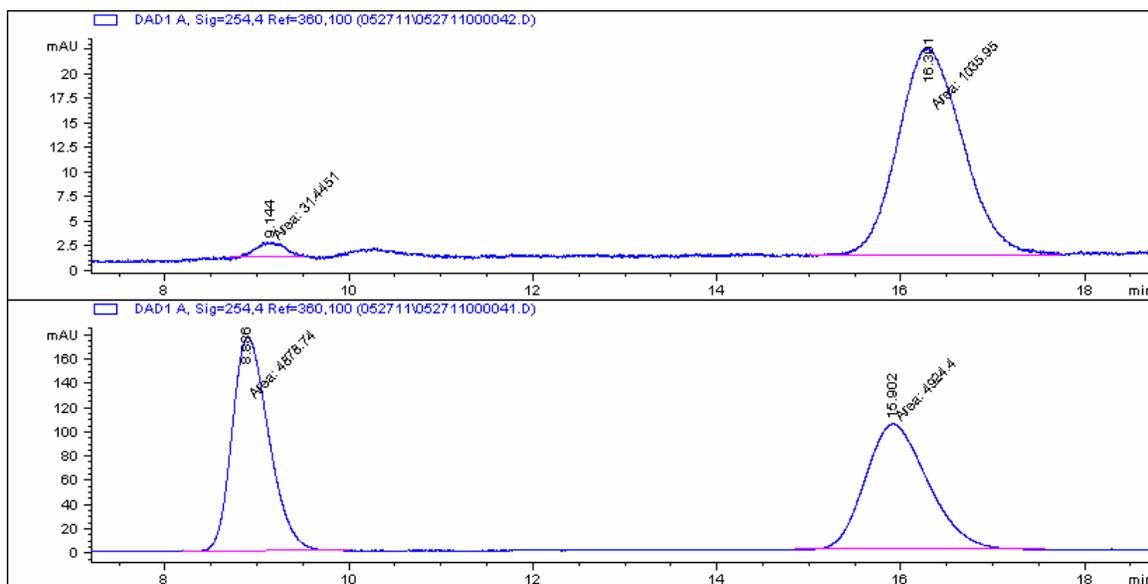


6d

8

To a solution of **6d** (100 mg, 0.24 mmol, 94% ee) in THF (5 mL) at 0 °C was charged LiBH₄ (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; $[\alpha]_D^{20} = +46.3^\circ$ (c = 1.0, CHCl₃); ¹H NMR (400

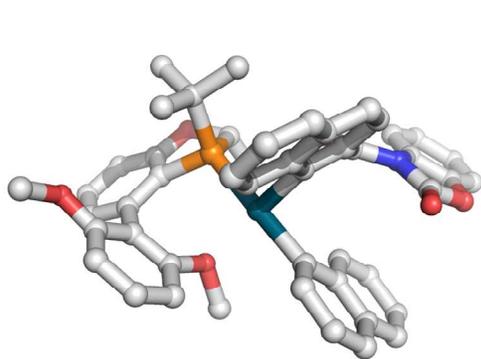
MHz, CDCl₃) δ 7.85-8.05 (m, 4H), 7.78 (d, J = 8.3 Hz, 1H), 7.59 (t, J = 7.7 Hz, 1H), 7.33-7.50 (m, 3H), 7.12-7.30 (m, 4H), 4.4 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 136.7, 135.8, 135.7, 133.6, 133.1, 132.9, 132.8, 128.3, 128.1, 127.9, 127.8, 126.6, 126.4, 126.2, 126.1, 125.8, 125.7, 125.5, 63.4; ESI-MS: m/z 285[M +H]⁺; Chiral HPLC conditions: Chiralcel OD-H, 4.6 mm X 250 mm, 30 °C, flow rate: 2 mL/min, heptane/isopropanol: 96/4, 254 nm, 9.14 min (*S*), 16.30 min (*R*).



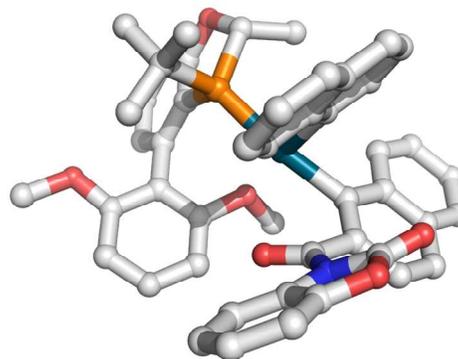
7. Computational studies

Both Buchwald⁶ and Baudoin⁷ 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° 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 Waals 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-workers⁹, 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 bulk¹⁰ 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.

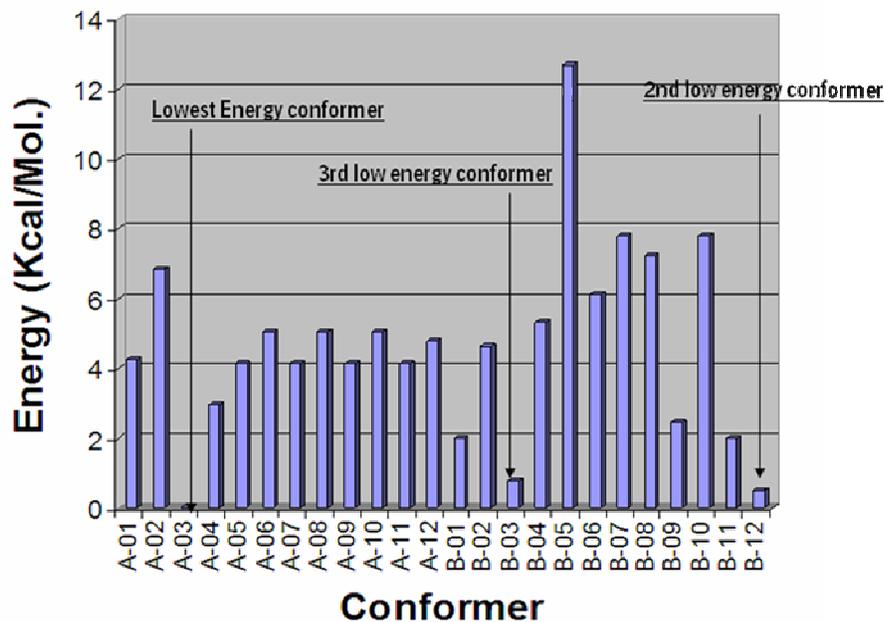


Figure S2: The relative energy of all the sample conformations in the energy-minimized state

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.

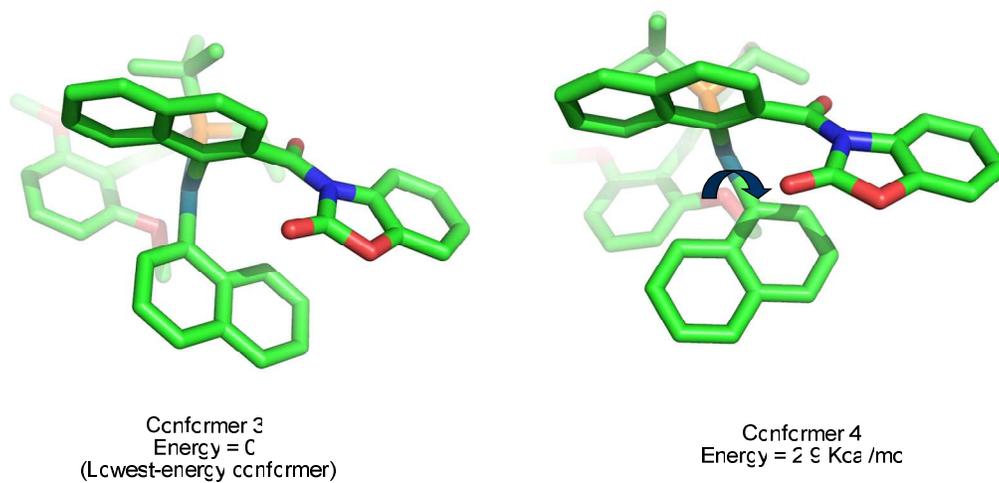


Figure S3: Comparison of the lowest-energy conformation and the local energy minimum in which the naphthyl group approximately flaps by 180° with respect to the first conformation

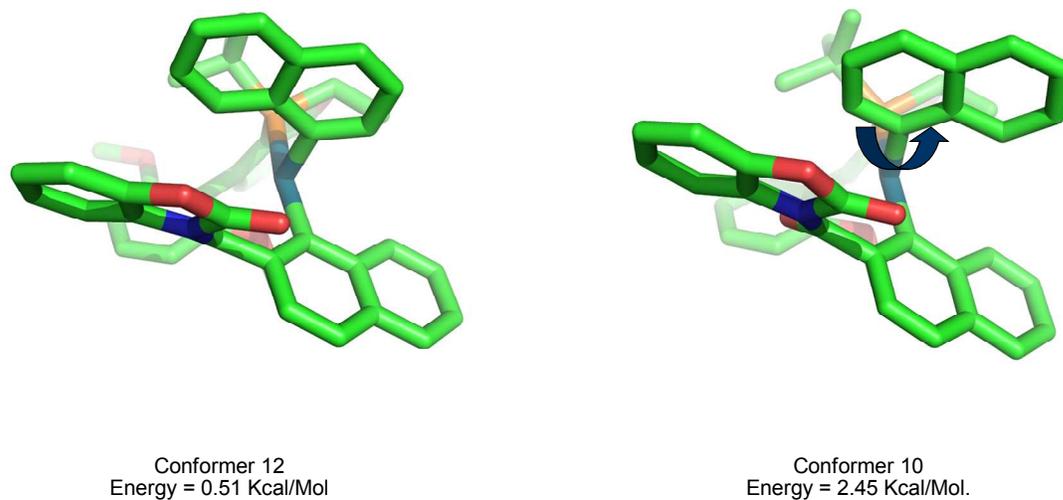
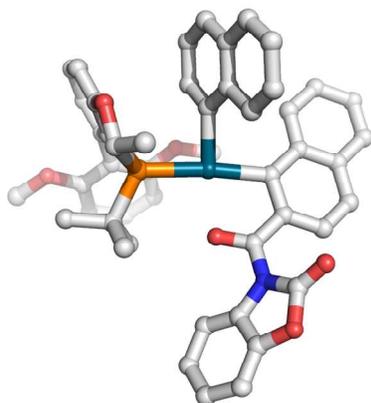


Figure S4: Comparison of the 2nd lowest-energy conformation and the local energy minimum in which the naphthyl group approximately flaps by 180° with respect to the first conformation



Ccncfmer B-C5 Energy = 0.78 Kcal/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:

- (1) (a) Tang, W.; Qu, B.; Capacci, A. G.; Rodriguez, S.; Wei, X.; Haddad, N.; Narayanan, B.; Ma, S.; Grinberg, N.; Yee, N. K.; Krishnamurthy, D.; Senanayake, C. H. *Org. Lett.* **2010**, *12*, 176. (b) Tang, W.; Capacci, A. G.; White, A.; Ma, S.; Rodriguez, S.; Qu, B.; Savoie, J.; Patel, N. D.; Wei, X.; Haddad, N.; Grinberg, N.; Yee, N. K.; Krishnamurthy, D.; Senanayake, C. H. *Org. Lett.* **2010**, *12*, 1104.
- (2) Tang, W.; Capacci, A. G.; Wei, X.; Li, W.; White, A.; Patel, N. D.; Savoie, J.; Gao, J. J.; Rodriguez, S.; Qu, B.; Haddad, N.; Lu, B. Z.; Krishnamurthy, D.; Yee, N. K.; Senanayake, C. H. *Angew. Chem., Int. Ed.* **2010**, *49*, 5879.
- (3) Rodriguez, S.; Qu, B.; Haddad, N.; Reeves, D.; Tang, W.; Krishnamurthy, D.; Senanayake, C. H. *Adv. Asy. Cat.* **2011**, *353*, 533.
- (4) (a) Yin, J. J.; Buchwald, S. L. *J. Am. Chem. Soc.* **2000**, *122*, 12051. (b) Kurz, L.; Lee, G.; Morgans, D., Jr.; Waldyke, M. J.; Ward, T. *Tetrahedron Lett.* **1990**, *31*, 6321.
- (5) (a) Meyers, A. I.; Lutomski, K. A. *J. Am. Chem. Soc.* **1982**, *104*, 879. (b) Aoyagi, N.; Ohwada, T.; Izumi, T. *Tetrahedron Lett.* **2003**, *44*, 8269.
- (6) Shen, X.; Jones, G. O.; Watson, D. A.; Bhayana, B.; Buchwald, S. L. *J. Am. Chem. Soc.* **2010**, *132*, 11278.
- (7) Joncour, A.; Décor, A.; Liu, J.M.; Dau, M.; Baudoin, O. *Chem. Eur. J.* **2007**, *13*, 5450.
- (8) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D.

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.
(9) (a) Zhou, Y.; Truhlar, D.G. *J. Phys. Chem. A* **2006**, *110*, 10478. (b) Zhou, Y.; Truhlar, D.G. *J. Chem. Theory Comput.* **2007**, *3*, 289.
(10) <http://www.chimifm.unito.it/teprica/crystal/crystal.html>



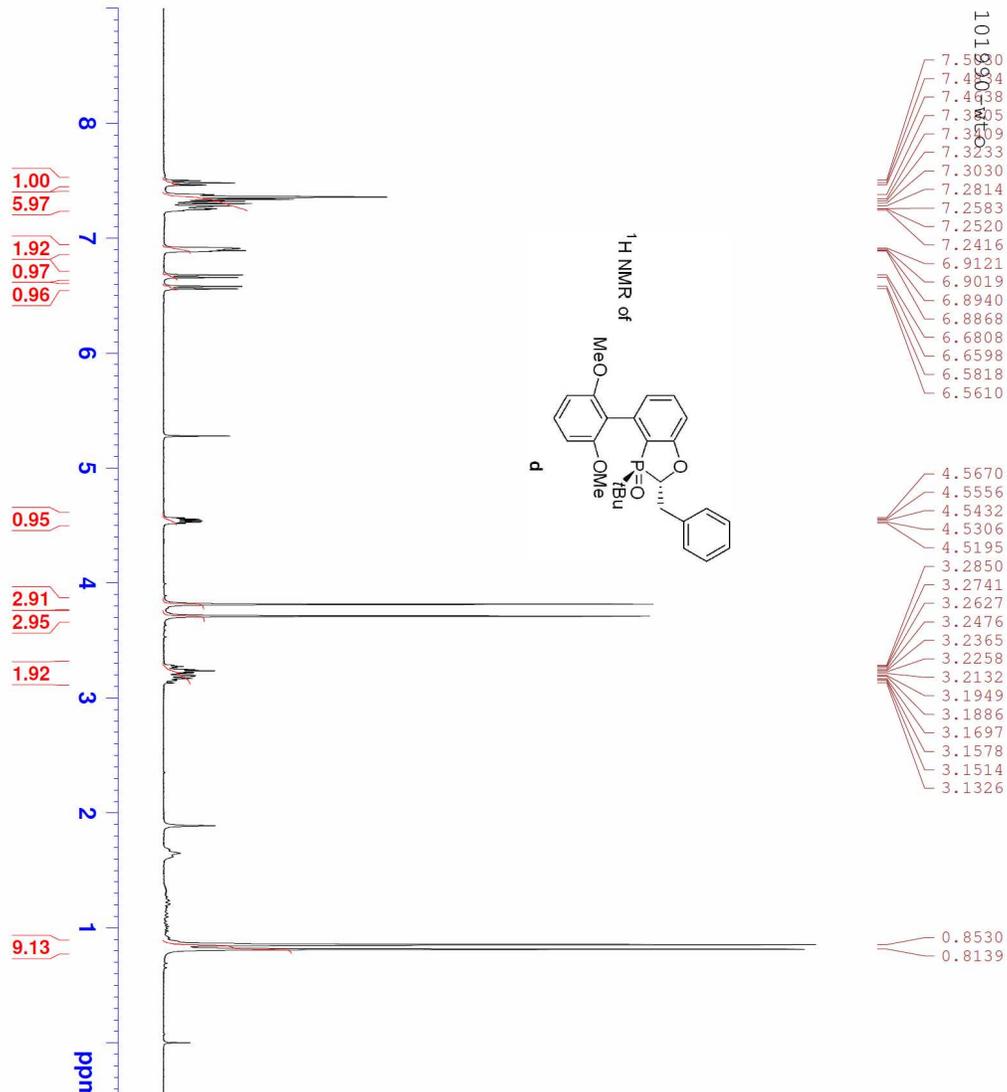
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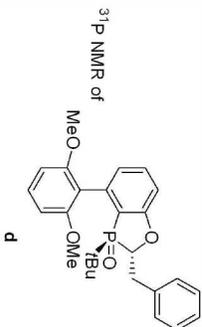
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101990-wtco

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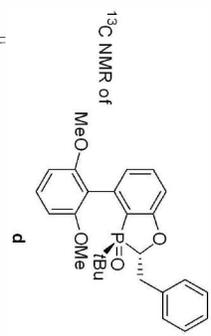
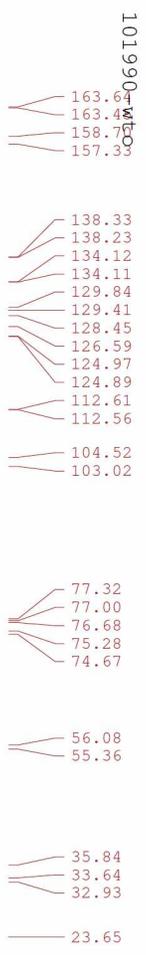
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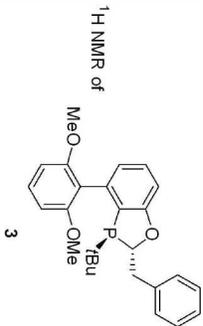
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101990-wt



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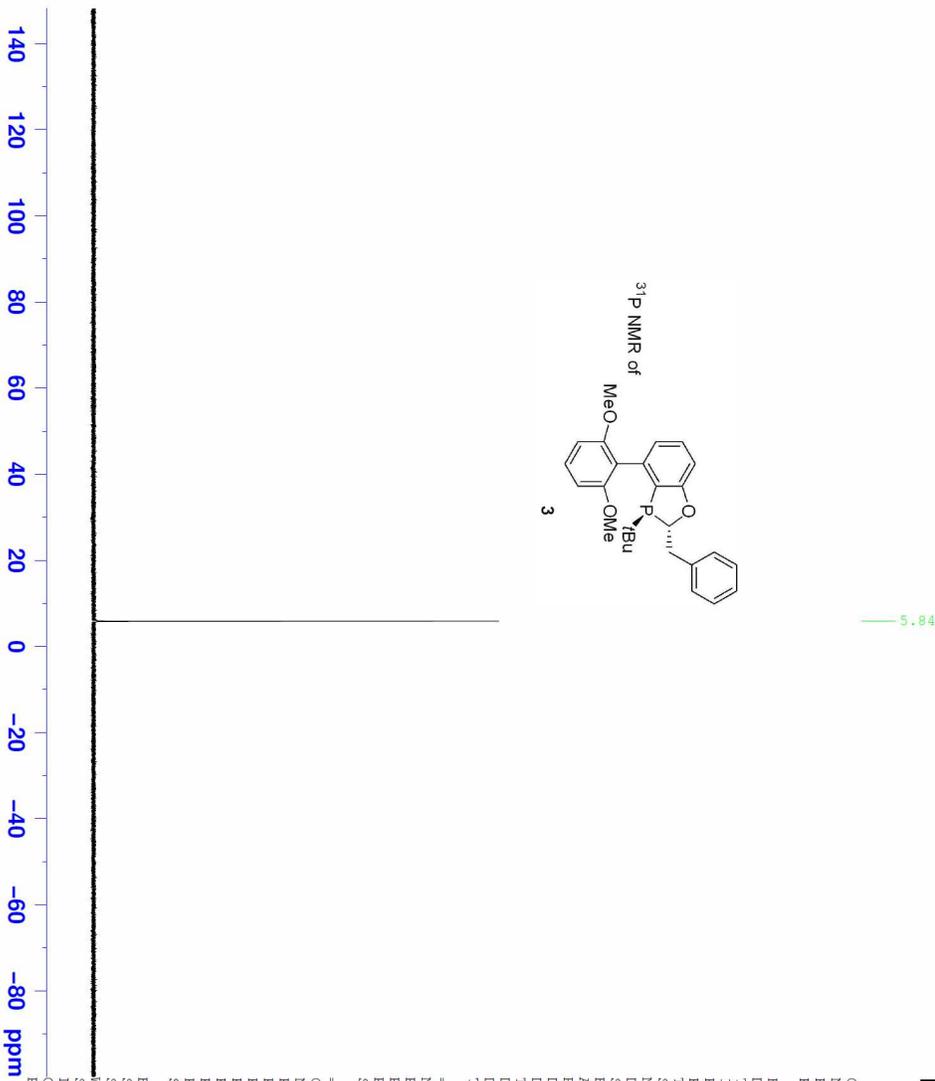
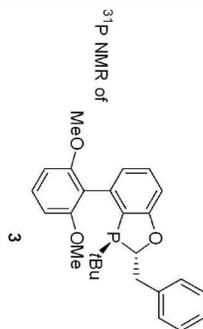
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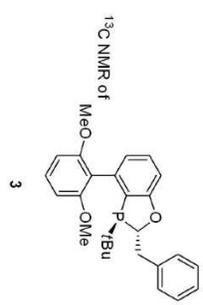
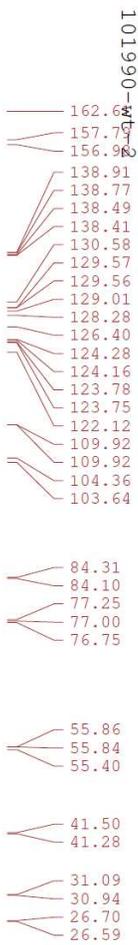
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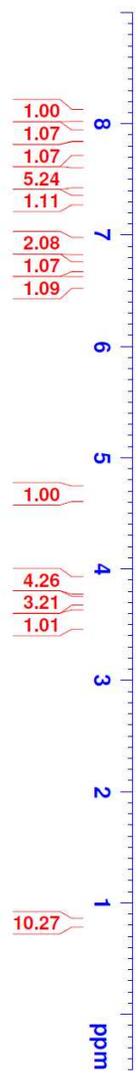
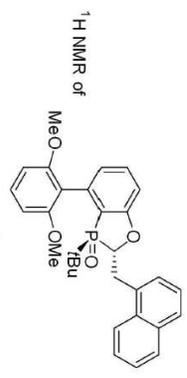
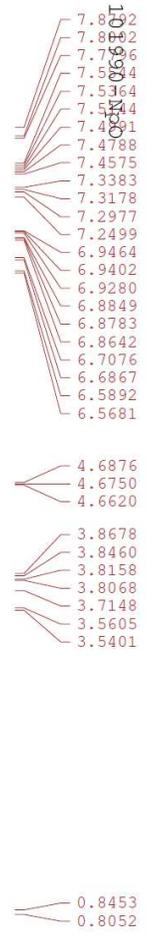
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 ID0 1

CHANNEL F1
 NUCL1 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



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
D11 2.00000000 sec
D1 0.03000000 sec
TD0 1

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

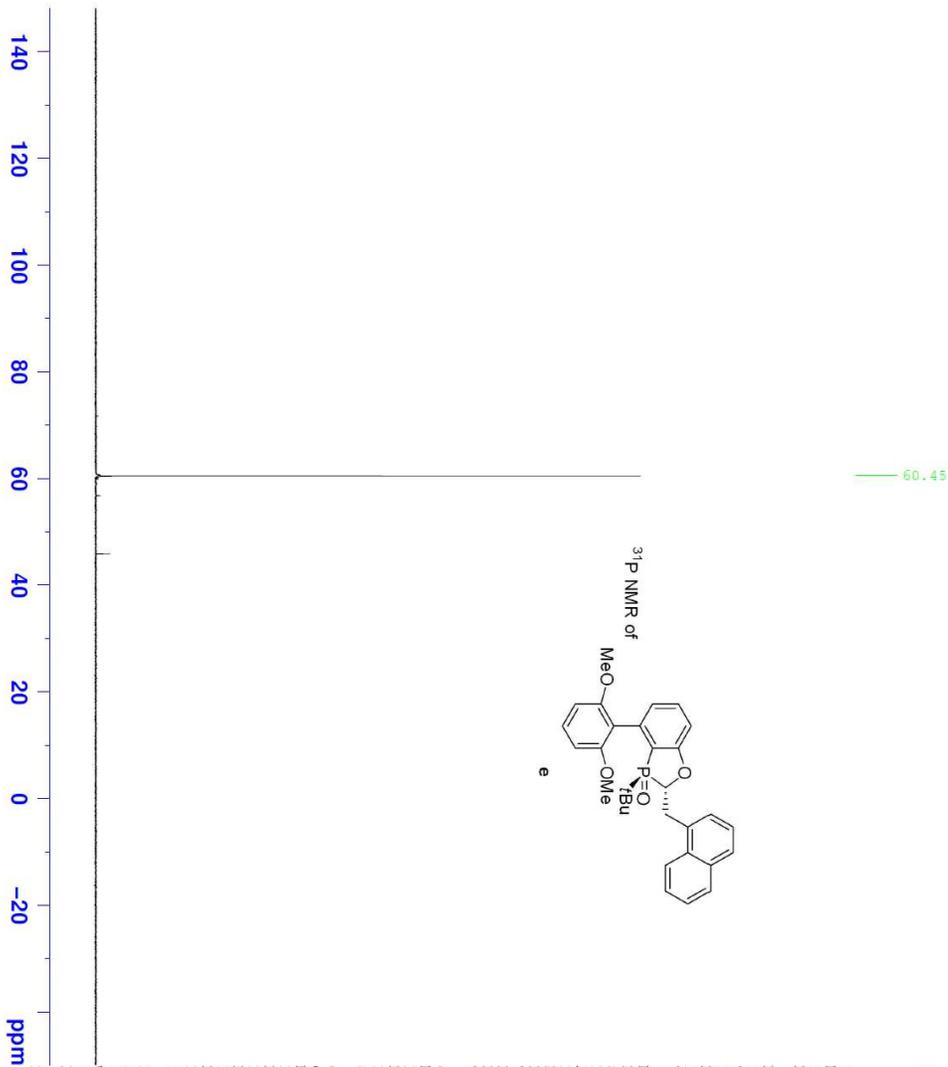
NUC1 31P
P1 13.75 usec
PL1 4.00 dB
PL1W 9.7600023 W
SFO1 161.9674942 MHz

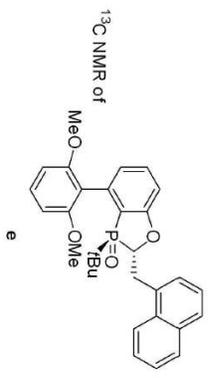
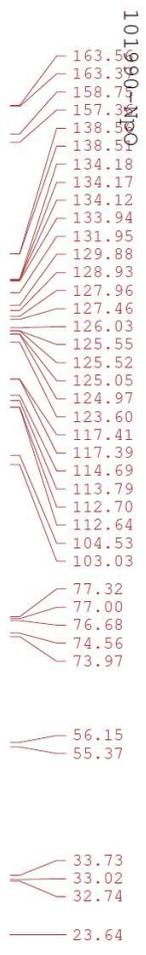
===== CHANNEL f2 =====

CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2D2 0.00 dB
PL12 15.14 dB
PL13 15.14 dB
PL12W 10.49968529 W
PL12M 0.32149649 W
PL13M 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





Current Data Parameters
 NAME 101990-npo
 EXPNO 3
 PROCNO 1



F2 - Acquisition Parameters
 Date_ 20110324
 Time 1.52
 INSTRUM spect
 PROBD 5 mm PABBO BB-
 PULPROG zgpg
 TD 32768
 SOLVENT CDCl3
 NS 5000
 DS 4
 SWH 24038.461 Hz
 FIDRRS 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 =====
 NUCL1 13C
 P1 9.75 usec
 PL1 -1.00 dB
 PL1W 43.00697708 W
 SF01 100.6243395 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUCC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.14 dB
 PL13 15.14 dB
 PL14 15.14 dB
 PL1Z 10.43968529 W
 PL1ZM 0.32149649 W
 PL13M 0.32149649 W
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 100.6127742 MHz
 SF 100.6127742 MHz
 MDW 0
 EX 0
 SSB 0
 LB 1.00 Hz
 GB 0
 EC 1.40

7.7327
7.7315
7.7299
7.6983
7.4244
7.4230
7.3832
7.3627
7.3425
7.3224
7.2933
7.2741
7.2552
7.2242
7.2042
7.1834
6.8208
6.7997
6.7796
6.5978
6.5773
6.5127
6.4917
5.0697
5.0506
5.0322

3.7596
3.6200
3.4875
3.4607
3.4547
3.4271
3.4008
3.2795
3.2627
3.2442
3.2263

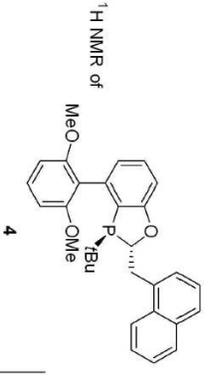
0.5644
0.5343



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 zgpg30
TD 32768
SOLVENT CDCl3
NS 16
DS 4
SWH 5896.227 Hz
FIDRES 0.17939 Hz
AQ 2.7787764 sec
RG 456
DW 84.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TDO 1

CHANNEL f1
NUC1 1H
PI 14.00 usec
PL1 0.00 dB
PL1W 10.49968529 W
SFO1 400.1327209 MHz
F2 - Processing parameters
SI 63536
SF 400.1300562 MHz
WDW EM
SSB 0
LB 0.05 Hz
GB 0
PC 1.00



101990-NP



Current Data Parameters
NAME 101990-np
EXNO 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
FIDRRS 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

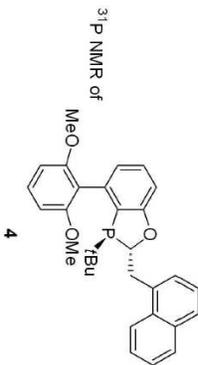
NUC1 ³¹P
P1 13.75 usec
E11 4.00 dB
P11W 9.7600023 W
SFO1 161.9674942 MHz

CHANNEL f2

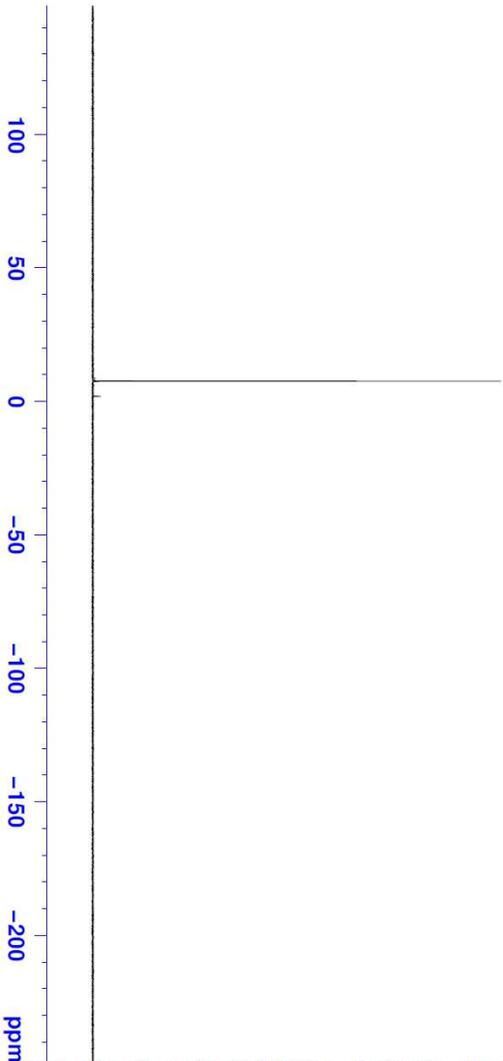
CPDPRG2 waltz16
NUC2 ¹H
NOB2 30.01 usec
PTD2 0.00 dB
P12 15.14 dB
P13 15.14 dB
P12W 10.43968529 W
P112W 0.32149649 W
P113W 0.32149649 W
SFO2 400.1316005 MHz

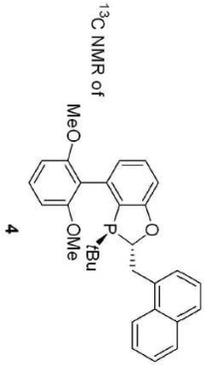
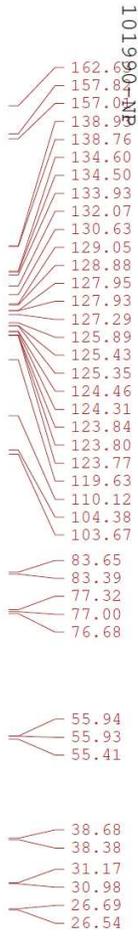
F2 - Processing parameters

SI 32768
SF 161.975588 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.54





Current Data Parameters
 NAME 101990-pp
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110325
 Time 13.41
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg4
 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
 PLI -1.00 dB
 PLIw 43.00697708 W
 SF01 100.6243395 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUCC2 IH
 PCPD2 80.00 usec
 PL2 0.00 dB
 PLI2 12.14 dB
 PLI3 12.14 dB
 PLI2w 10.499868328 W
 PLI2M 0.32148649 W
 PLI3w 0.32148649 W
 SF02 400.1316005 MHz

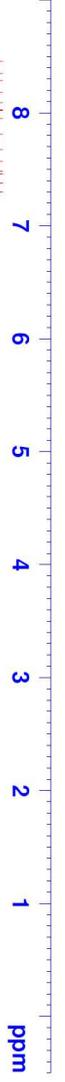
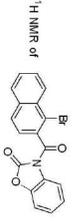
F2 - Processing parameters
 SI 6553
 SF 100.6127725 MHz
 DS 4
 SSB 0
 GB 1.00 Hz
 PC 1.40



8.062
8.053
8.045
7.997
7.944
7.886
7.792
7.770
7.773
7.699
7.583
7.514
7.418
7.408
7.398
7.354
7.343



Current Data Parameters
NAME 101990-drom-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
RG 406
DM 84.800 usec
DE 6.50 usec
TE 298.0 K
DI 2.00000000 sec
TD0 1

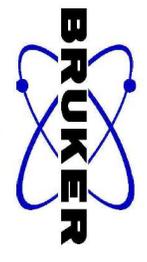
==== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
PL1W 10.49968529 W
SFO1 400.1327209 MHz

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

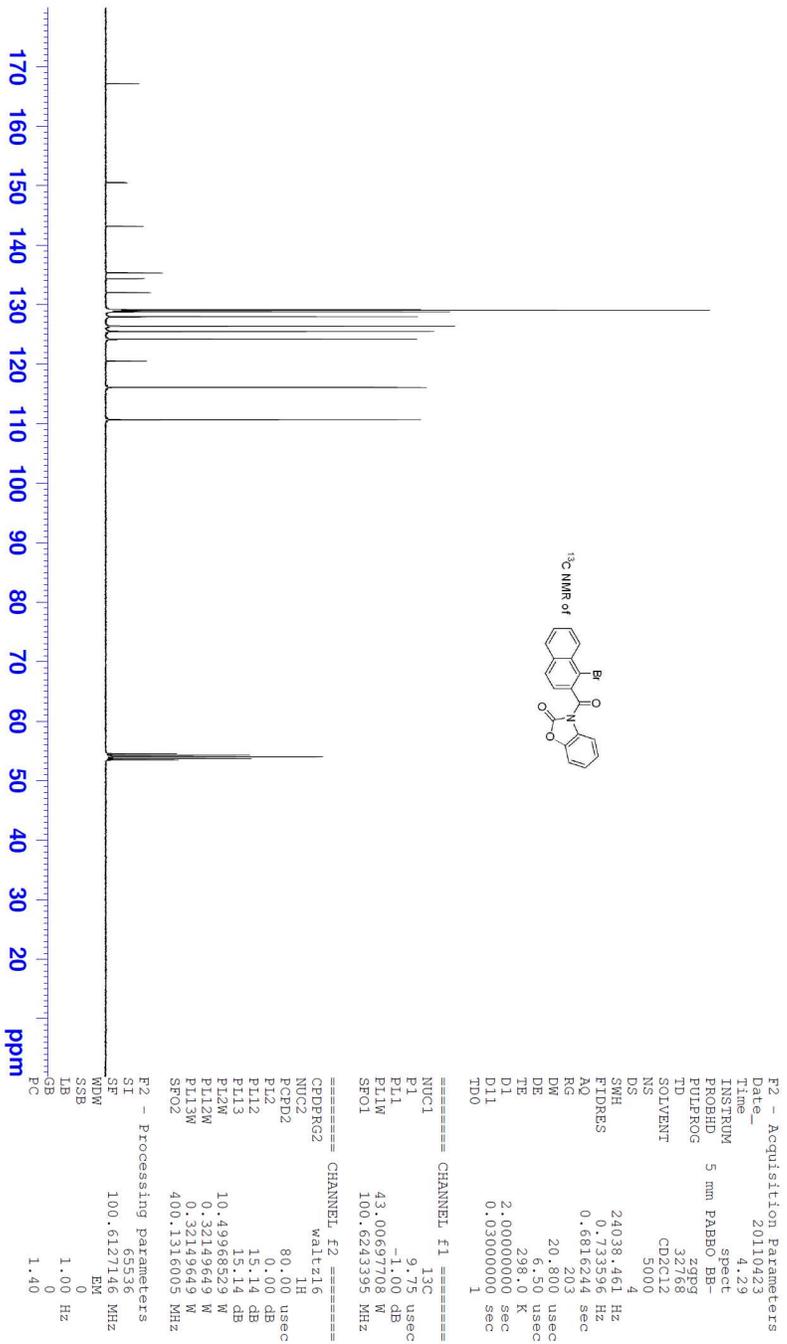
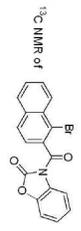
tang-bromo-imide

167.11
150.54
143.22
135.33
134.33
132.04
129.19
129.07
128.89
128.80
127.99
127.96
126.41
125.52
124.19
120.52
116.11
110.68

54.54
54.27
54.00
53.73
53.46



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





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

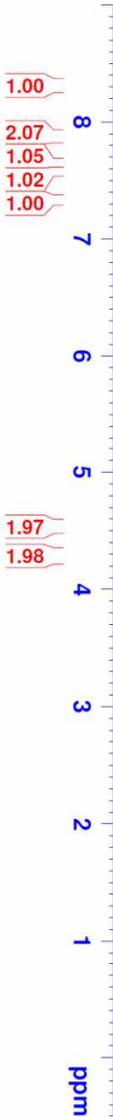
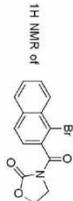
SWH 7500.000 Hz
 FIDRES 0.228882 Hz
 AQ 2.1845834 sec
 RG 456
 DW 66.667 usec
 DE 6.50 usec
 TE 299.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUCL1 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

7.81805
 7.8177
 7.81634
 7.81533
 7.6588
 7.6570
 7.6450
 7.6427
 7.6284
 7.6262
 7.6009
 7.5989
 7.5848
 7.5709
 7.3482
 7.3315
 7.2603

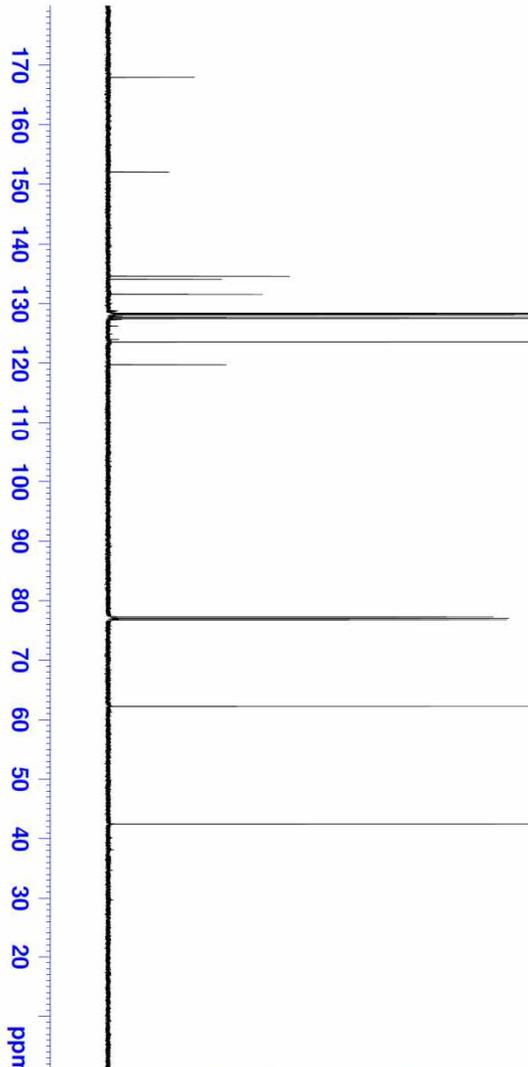
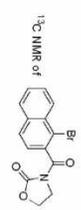
4.5409
 4.5253
 4.5089
 4.2965
 4.2800
 4.2644



amide2
 167.92
 152.08
 134.60
 134.09
 131.57
 128.40
 128.25
 128.15
 127.76
 127.51
 123.58
 119.77
 77.26
 77.01
 76.75
 62.24
 42.47

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
 TDO 1



==== CHANNEL f1 =====
 NUCL ¹³C
 P1 9.88 usec
 PL1 -0.50 dB
 PL1M 124.00885010 W
 SFO1 125.7698617 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUCL2 ¹H
 PCPD2 80.00 usec
 PL2 2.10 dB
 PL12 19.30 dB
 PL13 19.30 dB
 PL2M 18.43091324 W
 PL12M 0.32119326 W
 PL13M 0.32119326 W
 SFO2 500.1325007 MHz

F2 - Processing parameters
 SI 31072
 SF 125.7577920 MHz
 MDW 0
 SSB 0
 GB 0
 PC 1.40



8.0308
8.0163
7.9533
7.5939
7.5565
7.5340
7.5188
7.5050
7.4873
7.4737
7.4596
7.3067
7.2866

2.6869
2.4327



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 B-
PULPROG zg10
TD 32768
SOLVENT CDCl3
NS 32

DS 0
SMH 7500.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 512
DM 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
IB 0
GB 0
PC 1.00





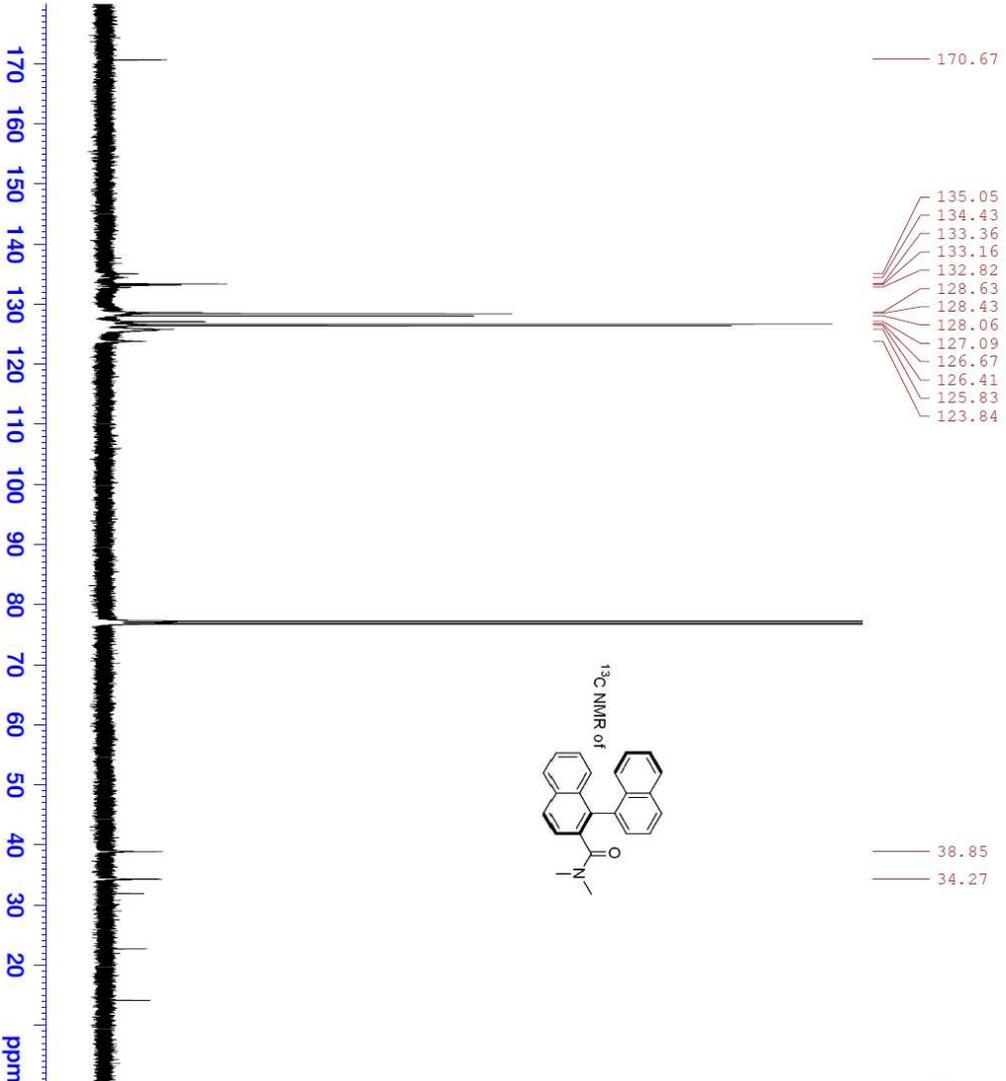
Current Data Parameters
 NAME 102190-87e-3
 EXPNO 2
 PROCNO 1

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 4.194341 sec
 RG 2050
 DW 16.000 usec
 DE 6.50 usec
 TE 299.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 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 18.443091774 W
 PL3W 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



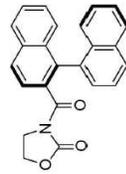
101990-dephlmide
 8.0199
 8.0196
 8.0193
 8.0189
 8.0186
 7.9920
 7.6610
 7.6609
 7.6608
 7.6604
 7.5579
 7.5158
 7.4975
 7.3731
 7.3618

4.0150
 3.9951
 3.9747
 3.6401
 3.6188
 3.4612



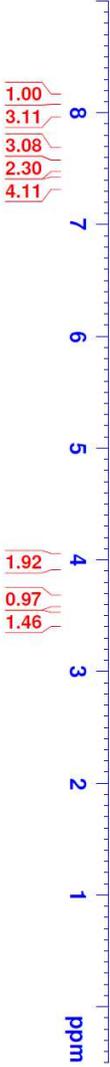
Current Data Parameters
 NAME 101990-dephlmide
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110425
 Time 12.30



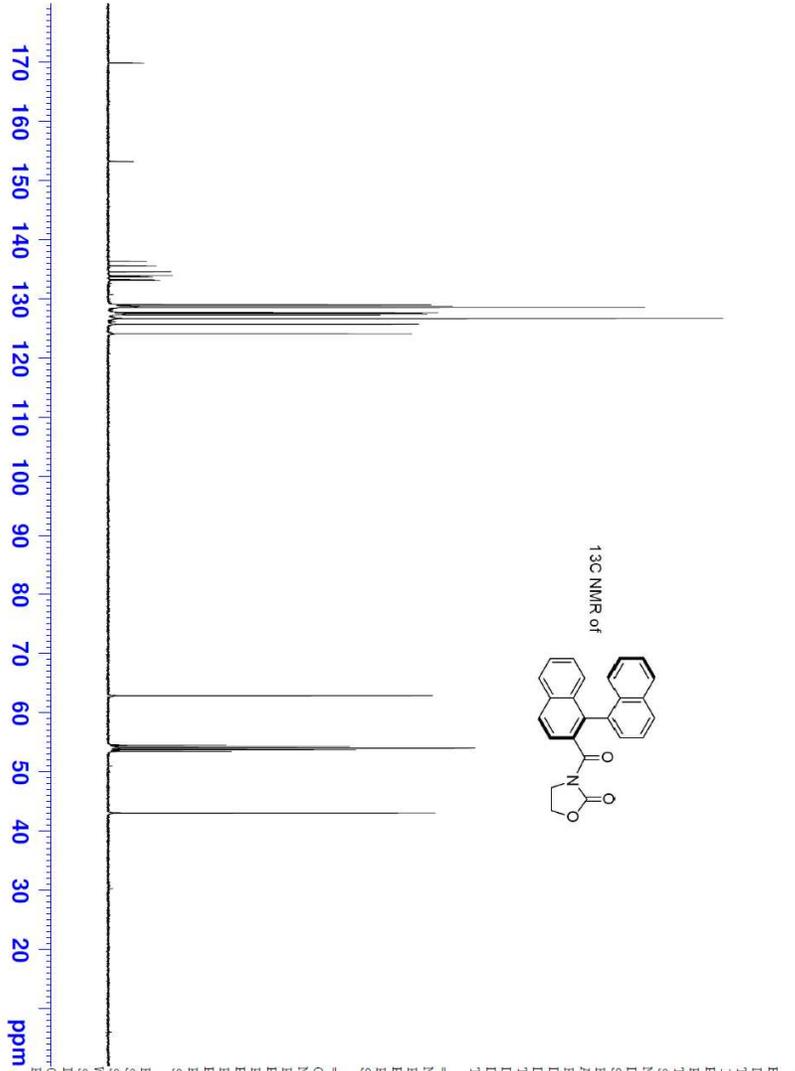
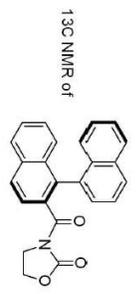
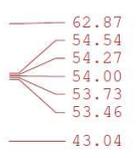
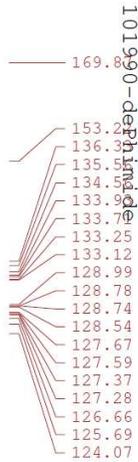
INSTRUM 5 mm PABBO BR-
 PROBHD zg10
 PULPROG 32768
 TD CD2C12
 SOLVENT 16
 NS 4
 DS 5896.227 Hz
 SWH 0.17939 Hz
 FIDRES 2.7787764 sec
 AQ 456
 RG 84.800 usec
 DW 6.50 usec
 DE 298.0 K
 TE 2.00000000 sec
 D1 1
 TD0 1

===== 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
 MDW EM
 SSB 0
 LB 0.05 Hz
 GB 0
 PC 1.00



1.00
 3.11
 3.08
 2.30
 4.11

1.92
 0.97
 1.46



Current Data Parameters
 NAME 101990-dephlimide
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110425
 Time 22.52
 INSTRUM spect
 PROBH0 5 mm PABHO BB-
 PULPROG zgpg4
 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 =====
 NUCL1 13C
 P1 9.75 usec
 PL1 -1.00 dB
 PL1W 43.00697708 W
 SF01 100.6243395 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUCL2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 12.14 dB
 PL13 12.14 dB
 PL14 12.14 dB
 PL12W 10.49968523 W
 PL12W 0.32149649 W
 PL13W 0.32149649 W
 SF02 400.1516005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127139 MHz
 NPM 32
 SSB 0
 GB 0
 PC 1.40



102253-002 CDCl3
 7.7716
 7.7711
 7.7703
 7.7692
 7.6049
 7.5033
 7.4888
 7.4794
 7.4777
 7.4636
 7.4632
 7.4621
 7.4026
 7.3685
 7.3536
 7.3308
 7.3172
 7.1405
 7.1255
 7.0596
 7.0434
 7.0275
 5.3204



Current Data Parameters
 NAME 102253-002
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

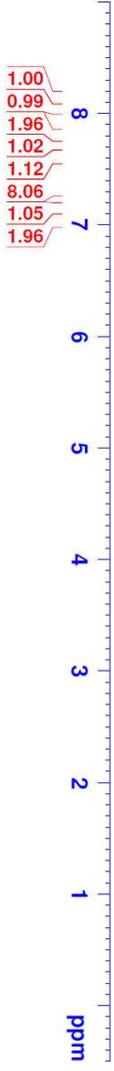
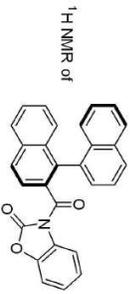
Date_ 20110425
 Time 16.57
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg10
 TD 32768
 SOLVENT CDCl2
 NS 16
 DS 0
 SWH 7500.000 Hz
 FIDRES 0.228882 Hz
 AQ 2.1845834 sec
 RG 512
 DW 66.667 usec
 DE 6.50 usec
 TE 299.0 K
 DL 1.00000000 sec
 TDO 1

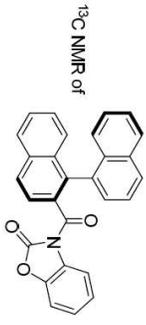
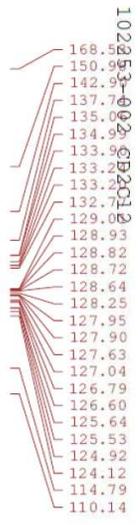
CHANNEL F1

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





54.54
53.46



Current Data Parameters
 NAME 102253--002
 EXNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110426
 Time 22:52
 INSTRUM spect
 PROBHD 5 mm PABBO-2HPC
 PULPROG zgpg30
 TD 32768
 CQDC12
 SOLVENT 5000
 NS 4
 DS 24038.461 Hz
 SWH 0.733596 Hz
 FIDRES 0.6816244 sec
 AQ 20.203
 RG 20,800 usec
 DW 6.250 usec
 DE 24.50 K
 DI 2.0000000 K
 D11 0.0300000 sec
 TDO 1

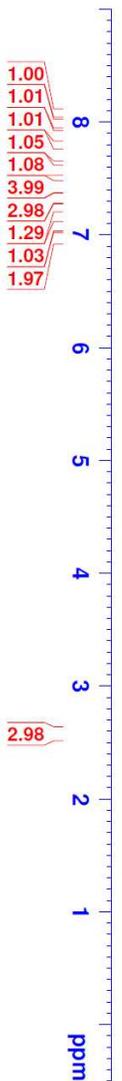
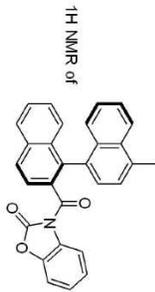
===== CHANNEL F1 =====
 NUCL1 13C
 P1 9.75 usec
 PL1 -1.00 dB
 PL1W 43.00697708 W
 SFO1 100.6243395 MHz

===== CHANNEL F2 =====
 CPDPRG2 waltz16
 NUC2 13C
 NO2 80.40 usec
 PL2 0.00 dB
 PL12 15.14 dB
 PL13 15.14 dB
 PL1W 10.4968529 W
 PL12W 0.32149649 W
 PL13W 0.32149649 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SE 100.6127117 MHz
 WMW EM
 SSB 0
 GB 1.40
 PC 1.40

4-Methyl-2-(3-methylphenyl)-1H-benzimidazole
 7.5544
 7.5531
 7.4605
 7.4477
 7.4271
 7.4288
 7.3300
 7.3318
 7.3330
 7.3347
 7.3349
 7.3366
 7.3322
 7.2502
 7.2590
 7.2500
 7.2449
 7.0829
 7.0808
 7.0671
 7.0513
 7.0496
 6.9881
 6.9770
 6.9739
 6.9608

2.5624



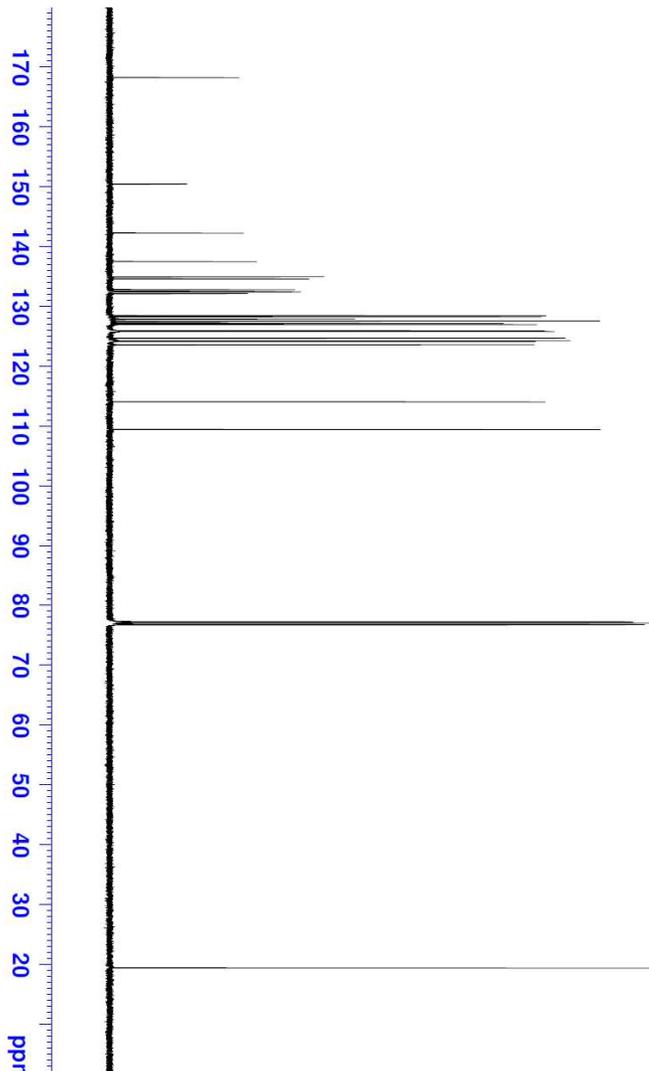
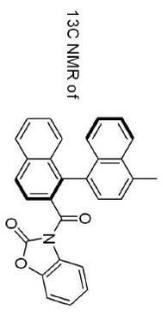
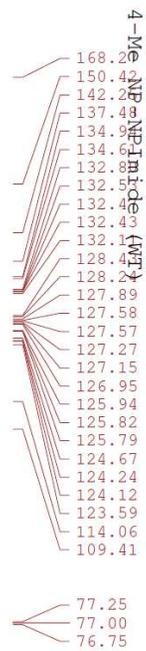
Current Data Parameters
 NAME 102190-4meimp-1p
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110824
 Time 19.05
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg10
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SMH 7500.000 Hz
 FIDRES 0.228882 Hz
 AQ 2.1845834 sec
 RG 405
 DW 66.667 usec
 DE 66.50 usec
 TE 299.0 K
 D1 1.00000000 sec
 ID0 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
 GB 0.30 Hz
 PC 1.00





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

F2 - Acquisition Parameters
 Date_ 20110524
 Time 23.29
 INSTRUM spect
 PROBHID 5 mm PABBO BB-
 PULPROG zgpg9
 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 =====
 NUCL1 13C
 P1 9.88 usec
 PL1 -0.50 dB
 PL1W 124.00885010 W
 SFO1 125.7698617 MHz

==== CHANNEL F2 =====
 CEPRG2 waltz16
 NUCL2 1H
 FOCPD2 80.00 usec
 P12 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
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40

DATA LIST

8.0001
7.9987
7.7931
7.7232
7.5588
7.5589
7.5585
7.487
7.3831
7.3789
7.3748
7.3653
7.3111
7.2959
7.2605
7.0439
7.0283
6.9672
6.9517
6.9330
6.9164

2.7095

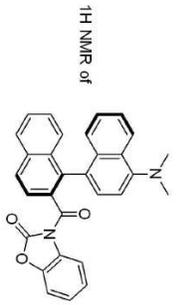


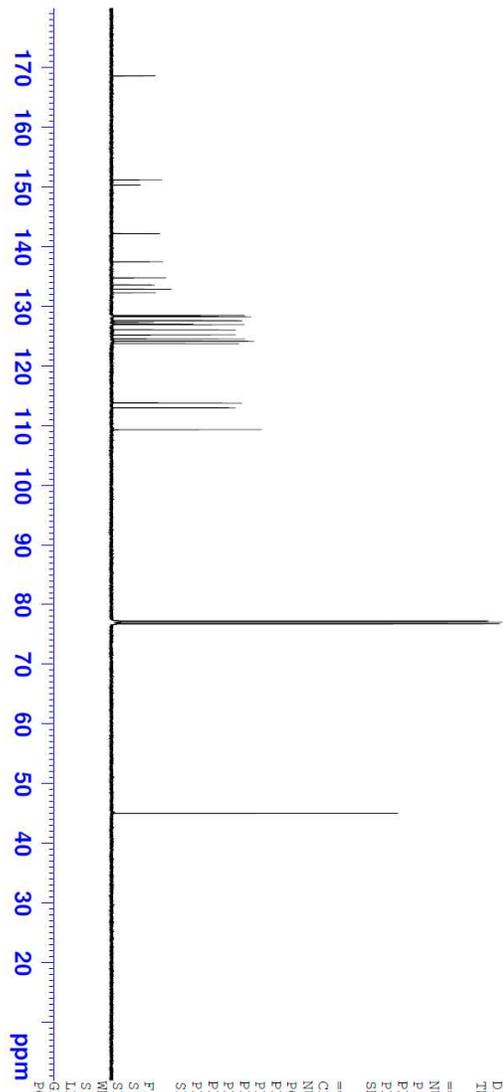
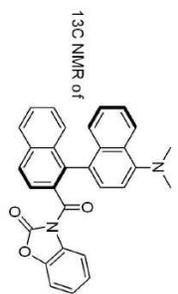
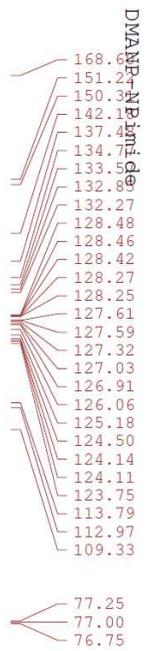
Current Data Parameters
 NAME 102190-e70-1
 EXPNO 1
 PROCNO 1

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
 DI 1.00000000 sec
 TDO 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
 KDPW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





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 282144
 SOLVENT CDCl3
 NS 4000
 DS 0
 SMH 31250.000 Hz
 FIDRES 0.119209 Hz
 AQ 4.1943541 sec
 RG 2050
 DM 16.000 usec
 DE 6.50 usec
 TE 299.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL F1 =====
 NUCL 13C
 P1 9.88 usec
 PL1 -0.50 dB
 PL1W 124.00885010 W
 SFO1 125.7698617 MHz

==== CHANNEL F2 =====
 CPDPRG2 waltz16
 NUCL2 1H
 PCPBP2 80.00 usec
 PL2 2.10 dB
 PL12 19.30 dB
 PL13 19.30 dB
 PL1Z 18.43091774 W
 PL2W 0.35119396 W
 PL1W 0.35119396 W
 SFO2 500.1325007 MHz

F2 - Processing Parameters
 SI 151072
 SF 125.7577909 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40



101990-meomp
 7.6037
 7.6006
 7.5986
 7.5511
 7.4417
 7.4429
 7.4405
 7.3381
 7.3846
 7.3786
 7.3678
 7.3495
 7.3297
 7.3118
 7.2901
 7.1636
 7.1450
 7.1248
 7.0730
 7.0586
 7.0397
 6.8093
 6.7897
 5.3316



Current Data Parameters
 NAME 101990-meomp
 EXPNO 1
 PROCNO 1

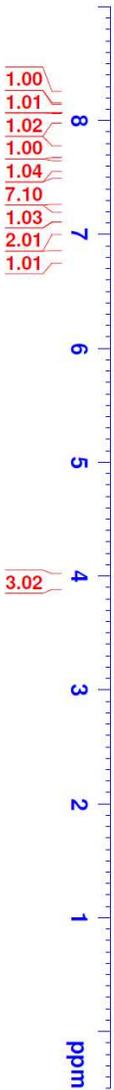
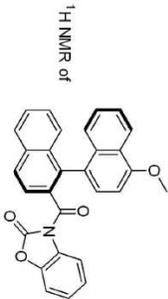
F2 - Acquisition Parameters

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
 TDO 1

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

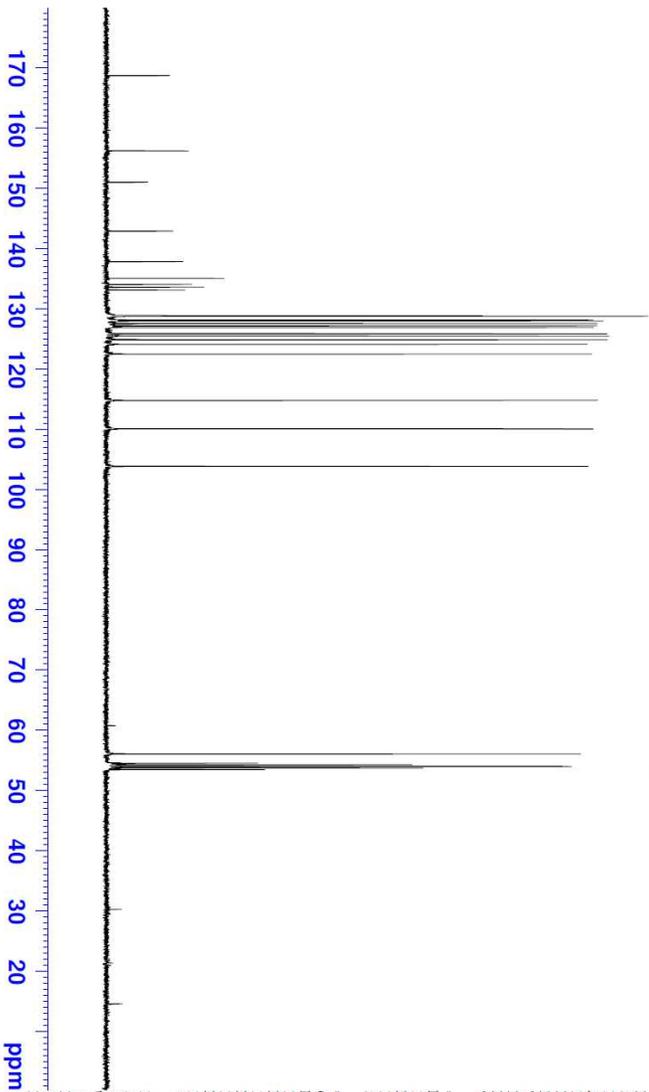
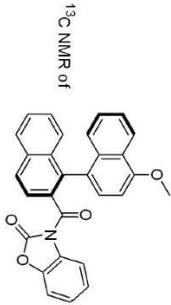
F2 - Processing parameters

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



101990-Meomp
 168.7
 156.22
 151.06
 142.06
 137.88
 135.06
 134.05
 133.62
 133.12
 128.87
 128.80
 128.76
 128.14
 127.98
 127.53
 127.19
 126.92
 125.87
 125.49
 124.88
 124.09
 122.49
 114.78
 110.08
 103.83

56.08
 54.54
 54.27
 54.00
 53.73
 53.46



Current Data Parameters
 NAME 101990-meomp
 EXPNO 2
 PROCNO 1

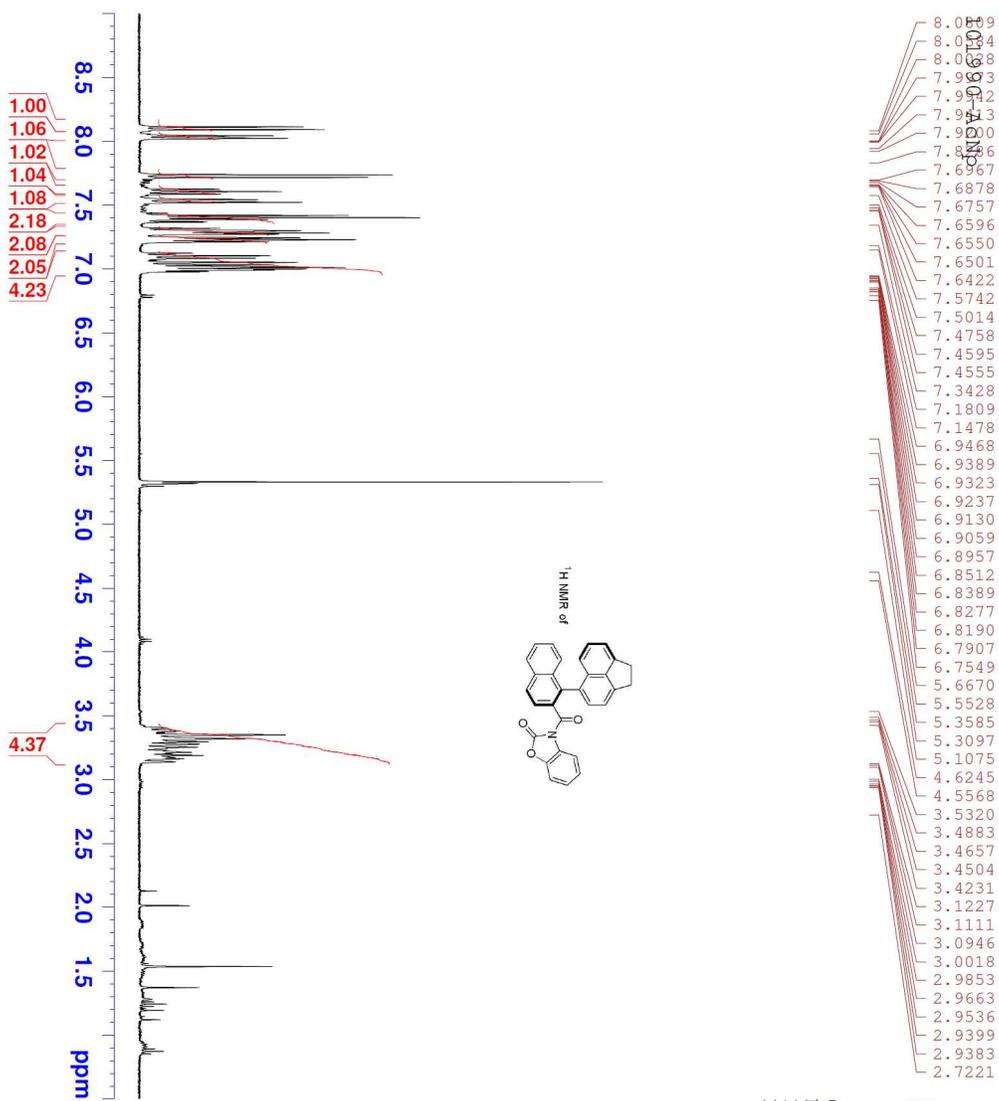


F2 - Acquisition Parameters
 Date_ 20110610
 Time 22.38
 INSTRUM spect
 PROBD 5 mm PABBO BB-
 PULPROG zgpg
 TD 32768
 CD2C12
 SOLVENT 3000
 NS 4
 DS 24038.461 Hz
 SWH 0.733596 Hz
 FIDRES 0.6816244 sec
 AQ 322
 RG 20.800 usec
 DW 6.50 usec
 DE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUCL1 13C
 P1 9.75 usec
 PL1 -1.00 dB
 PL1W 43.00697708 W
 SFO1 100.6243395 MHz

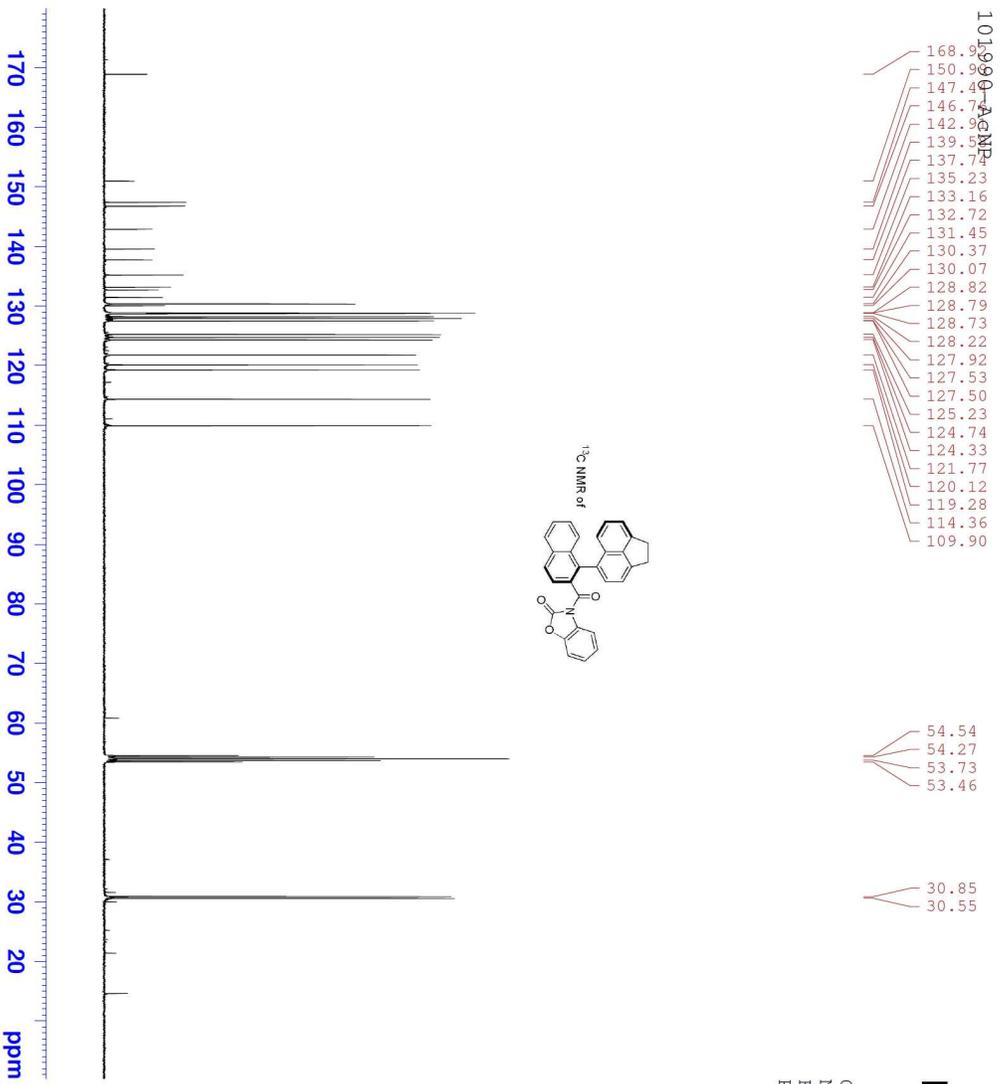
===== CHANNEL f2 =====
 CPPPRG2 waltz16
 NUCL2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PLI2 15.14 dB
 PLI3 15.14 dB
 PLI2W 10.49968829 W
 PLI2W 0.32149649 W
 PLI3W 0.32149649 W
 SFO2 400.1316005 MHz

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



Current Data Parameters
 NAME 101990-acmp
 EXPNO 1
 PROCNO 1





Current Data Parameters
 NAME 101990-acnfp
 EXPNO 4
 PROCNO 1



101990-pyrene
 8.0190
 8.0182
 8.0175
 8.0169
 8.0165
 7.9925
 7.9919
 7.7773
 7.7761
 7.6887
 7.6206
 7.6240
 7.6159
 7.6044
 7.3676
 7.3534
 7.2966
 7.2768
 6.9138
 6.8950
 6.8828
 6.8644
 6.7666
 6.7471
 5.3323
 5.3202



Current Data Parameters
 NAME 101990-pyrene
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

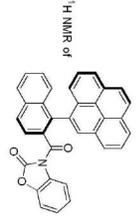
Date_ 20110506
 Time 14.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT CD2Cl2
 NS 16
 DS 4
 SWH 5896.227 Hz
 FIDRES 0.179939 Hz
 AQ 2.7787764 sec
 RG 575
 DW 84.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 TDO 1

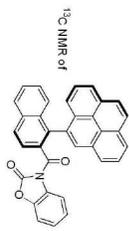
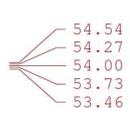
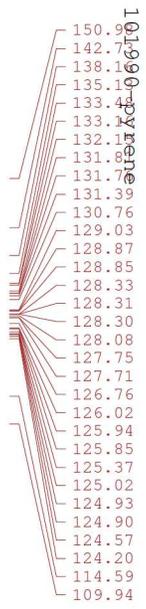
===== CHANNEL f1 =====

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
 MDW EM
 SSB 0
 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

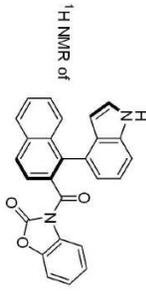
DS 4
 SMH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6816244 sec
 RG 228
 DW 20.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 1

===== 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
 P12 0.00 dB
 PL12 15.14 dB
 PL13 15.14 dB
 PL1W 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

7.55165
7.54949
7.44227
7.44042
7.39552
7.39228
7.3903
7.2587
7.1690
7.1531
7.1220
7.1100
7.1074
7.0993
7.0916
7.0762
7.0620
7.0467
7.0441
7.0163
7.0145
7.0008
6.9989
6.9396
6.9239
6.1486
6.1443
6.1399

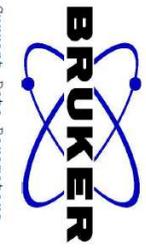
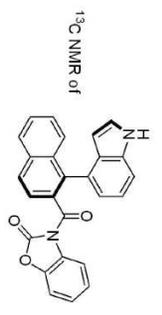
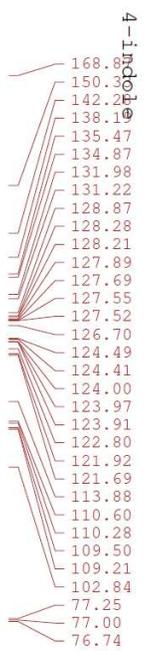


Current Data Parameters
NAME 102190-e57-4
EXPNO 1
PROCNO 1



F2 - Acquisition Parameters
Date_ 20110609
Time 0.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
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
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.70 usec
PL 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



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 zgpg3
 TD 262144
 SOLVENT CDCl3
 NS 3000
 DS 0
 SWH 31250.000 Hz
 FIDRRS 0.119209 Hz
 AQ 4.1943541 sec
 RG 2056
 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
 SF01 125.7698617 MHz

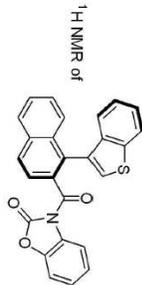
==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NDC2 IH
 PCPD2 80.00 usec
 PL2 2.10 dB
 PL12 19.30 dB
 PL13 19.30 dB
 PL1Z 18.43091774 W
 PL1ZW 0.35118396 W
 PL13W 0.35118396 W
 SF02 500.1325007 MHz

F2 - Processing Parameters
 SI 131072
 SF 125.7577916 MHz
 WDM EX
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME 102208-thio
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110916
 Time 17.01



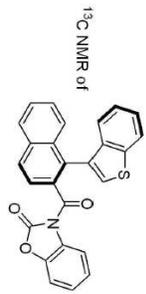
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 7.4374
 7.4227
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 7.3694
 7.3551
 7.3522
 7.2977
 7.2949
 7.2825
 7.2789
 7.2639
 7.2608
 7.1183
 7.1161
 7.1026
 7.1004
 7.0704
 7.0561
 7.0549
 6.9960
 6.9801



===== CHANNEL f1 =====
 NUCL1 1H
 P1 11.70 usec
 PL1 2.10 dB
 P1LW 18.43091774 W
 SFO1 500.1325007 MHz

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

- 168.36
 - 150.38
 - 142.27
 - 139.51
 - 138.97
 - 134.67
 - 132.42
 - 132.38
 - 132.30
 - 129.05
 - 128.39
 - 127.74
 - 127.28
 - 127.16
 - 127.05
 - 126.55
 - 124.93
 - 124.70
 - 124.47
 - 124.39
 - 123.75
 - 123.57
 - 122.36
 - 114.21
 - 109.54
-
- 77.25
 - 77.00
 - 76.75



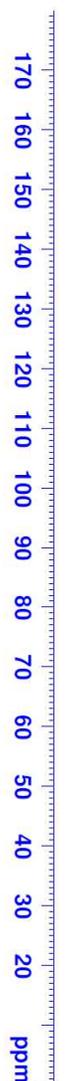
Current Data Parameters
 NAME 102208-thio
 EXPNO 2
 PROCNO 1

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
 TDO 1

===== CHANNEL f1 =====
 NUCC1 13C
 P1 9.88 usec
 PL1 -0.50 dB
 PL1W 124.00885010 W
 SFO1 125.7698617 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUCC2 1H
 PCPD2 80.00 usec
 P12 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
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40

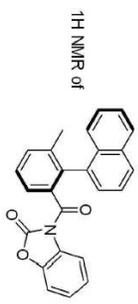




7.7744
7.7753
7.7755
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7.6618
7.6612
7.6659
7.5338
7.5726
7.5636
7.5608
7.5584
7.5508
7.5496
7.5399
7.5369
7.5180
7.5141
7.5045
7.4973
7.4412
7.4386
7.4312
7.4243
7.4217
7.4168
7.4137
7.4071
7.3838
7.3789
7.3663
7.3607
7.3416
7.3237
7.3201
7.3023
7.3004
7.2601
7.0861
7.0828
7.0665
7.0645
7.0620
7.0468
7.0435
6.9849
6.9818
6.9708
6.9676
6.9639
6.9510
6.9500
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6.9457
6.9423
2.0644

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

F2 - Acquisition Parameters
Date_ 20110517

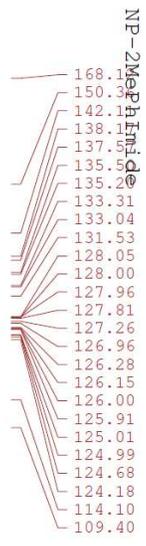


Time 17.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg10
TD 32768
SOLVENT CDCl3
NS 16
DS 4
SWH 5896.227 Hz
FIDRES 0.17939 Hz
AQ 2.7787764 sec
RG 456
DW 84.800 usec
DE 66.50 usec
TE 298.0 K
D1 2.00000000 sec
ID0 1

==== 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 0.05 Hz
LB 0
GB 0
PC 1.00



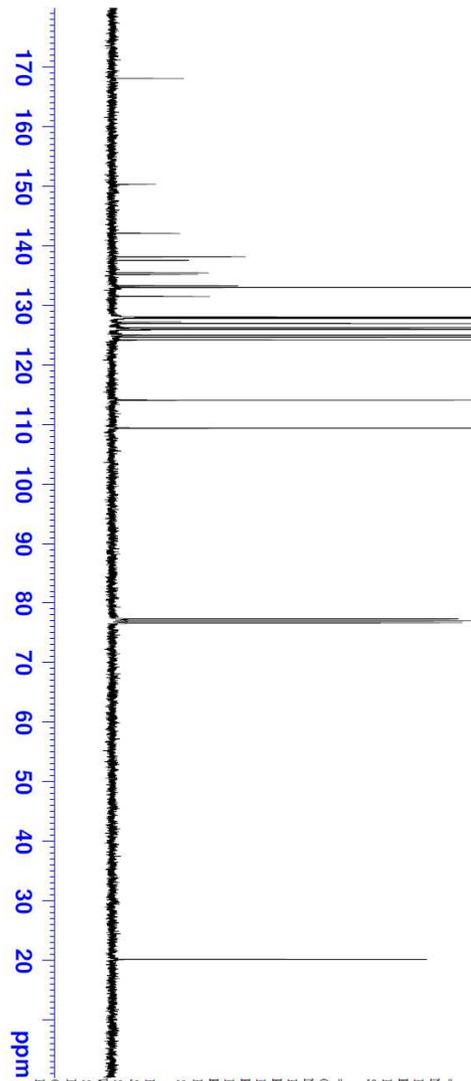
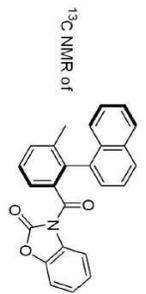


20.13



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
 TDO 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
 PL14 15.86 dB
 PL15 15.86 dB
 PL16 15.86 dB
 PL17 15.86 dB
 PL18 15.86 dB
 PL19 15.86 dB
 PL20 15.86 dB
 PL21 15.86 dB
 PL22 15.86 dB
 PL23 15.86 dB
 PL24 15.86 dB
 PL25 15.86 dB
 PL26 15.86 dB
 PL27 15.86 dB
 PL28 15.86 dB
 PL29 15.86 dB
 PL30 15.86 dB
 PL31 15.86 dB
 PL32 15.86 dB
 PL33 15.86 dB
 PL34 15.86 dB
 PL35 15.86 dB
 PL36 15.86 dB
 PL37 15.86 dB
 PL38 15.86 dB
 PL39 15.86 dB
 PL40 15.86 dB
 PL41 15.86 dB
 PL42 15.86 dB
 PL43 15.86 dB
 PL44 15.86 dB
 PL45 15.86 dB
 PL46 15.86 dB
 PL47 15.86 dB
 PL48 15.86 dB
 PL49 15.86 dB
 PL50 15.86 dB
 PL51 15.86 dB
 PL52 15.86 dB
 PL53 15.86 dB
 PL54 15.86 dB
 PL55 15.86 dB
 PL56 15.86 dB
 PL57 15.86 dB
 PL58 15.86 dB
 PL59 15.86 dB
 PL60 15.86 dB
 PL61 15.86 dB
 PL62 15.86 dB
 PL63 15.86 dB
 PL64 15.86 dB
 PL65 15.86 dB
 PL66 15.86 dB
 PL67 15.86 dB
 PL68 15.86 dB
 PL69 15.86 dB
 PL70 15.86 dB
 PL71 15.86 dB
 PL72 15.86 dB
 PL73 15.86 dB
 PL74 15.86 dB
 PL75 15.86 dB
 PL76 15.86 dB
 PL77 15.86 dB
 PL78 15.86 dB
 PL79 15.86 dB
 PL80 15.86 dB
 PL81 15.86 dB
 PL82 15.86 dB
 PL83 15.86 dB
 PL84 15.86 dB
 PL85 15.86 dB
 PL86 15.86 dB
 PL87 15.86 dB
 PL88 15.86 dB
 PL89 15.86 dB
 PL90 15.86 dB
 PL91 15.86 dB
 PL92 15.86 dB
 PL93 15.86 dB
 PL94 15.86 dB
 PL95 15.86 dB
 PL96 15.86 dB
 PL97 15.86 dB
 PL98 15.86 dB
 PL99 15.86 dB
 PL100 15.86 dB
 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

Peak Name
 7.6077
 7.6041
 7.6039
 7.6039
 7.5987
 7.5887
 7.5758
 7.5727
 7.5631
 7.5564
 7.5445
 7.5362
 7.5247
 7.2599
 7.2325
 7.2130
 6.9342
 6.9144
 6.8349
 6.8139
 6.8123
 6.7925

2.1028
 1.5563



Current Data Parameters
 NAME 102190-e79-1
 EXPNO 1
 F2OCNO 1

F2 - Acquisition Parameters
 Date_ 20110614

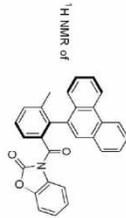
Time 23.04
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg10
 TD 32768
 SOLVENT CDCl3
 NS 64
 DS 4
 SMH 5896.227 Hz
 FIDRES 0.179939 Hz
 AO 2.7787764 sec
 RG 812
 DM 84.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 Sec
 TD0 1

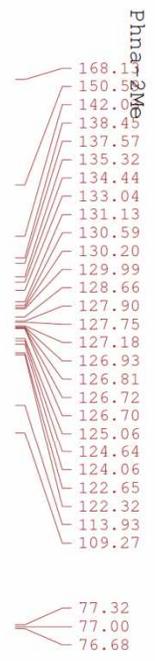
===== CHANNEL f1 =====

NUC1 1H
 P1 14.00 usec
 PL1 0.00 dB
 PLI1 W
 SFO1 400.1327209 MHz

F2 - Processing parameters

SI 65536
 SF 400.1300127 MHz
 MDW EM
 SSB 0
 LB 0.05 Hz
 GB 0
 PC 1.00





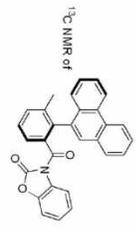
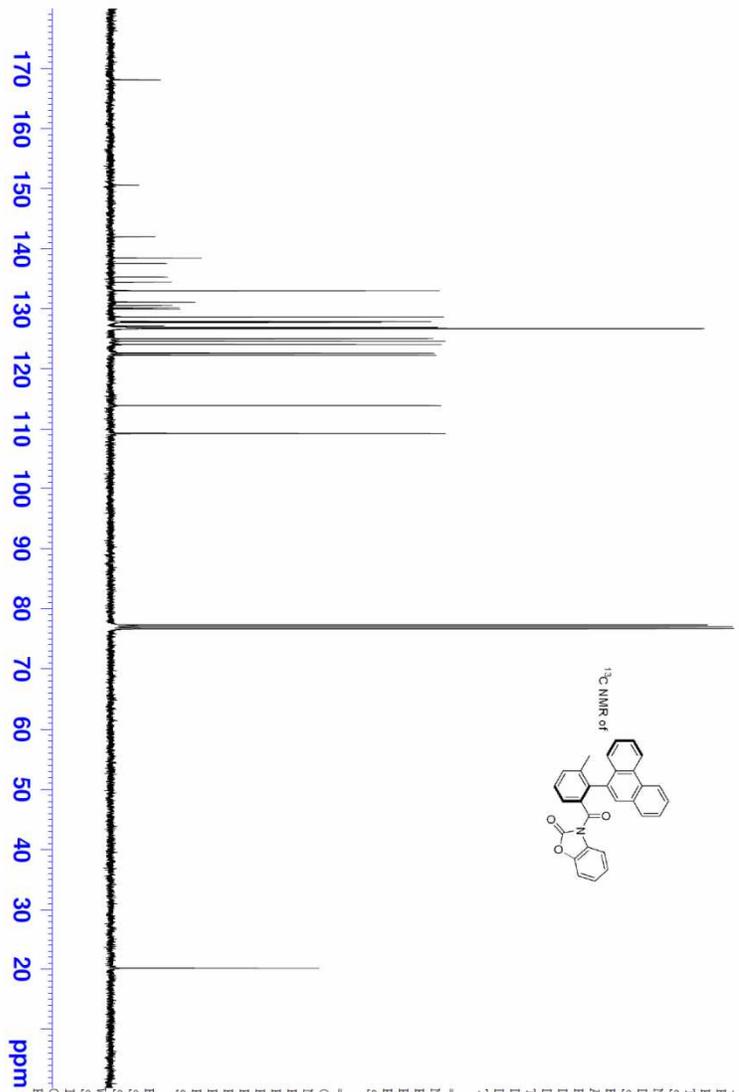
Current Data Parameters
 NAME 102190-e79-1
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110614
 Time 22.57
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg2
 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
 NUCL1 13C
 P1 9.75 usec
 PL1 -1.00 dB
 PL1W 43.00697708 W
 SFO1 100.6243395 MHz

CHANNEL F2
 walTz16
 NUCL2 1H
 PCHD2 80.00 usec
 PL2 0.00 dB
 PL12 15.14 GB
 PL13 15.14 GB
 PL14 15.14 GB
 PL15 15.14 GB
 PL16 15.14 GB
 PL17 15.14 GB
 PL18 15.14 GB
 PL19 15.14 GB
 PL20 15.14 GB
 PL21 15.14 GB
 PL22 15.14 GB
 PL23 15.14 GB
 PL24 15.14 GB
 PL25 15.14 GB
 PL26 15.14 GB
 PL27 15.14 GB
 PL28 15.14 GB
 PL29 15.14 GB
 PL30 15.14 GB
 PL31 15.14 GB
 PL32 15.14 GB
 PL33 15.14 GB
 PL34 15.14 GB
 PL35 15.14 GB
 PL36 15.14 GB
 PL37 15.14 GB
 PL38 15.14 GB
 PL39 15.14 GB
 PL40 15.14 GB
 PL41 15.14 GB
 PL42 15.14 GB
 PL43 15.14 GB
 PL44 15.14 GB
 PL45 15.14 GB
 PL46 15.14 GB
 PL47 15.14 GB
 PL48 15.14 GB
 PL49 15.14 GB
 PL50 15.14 GB
 PL51 15.14 GB
 PL52 15.14 GB
 PL53 15.14 GB
 PL54 15.14 GB
 PL55 15.14 GB
 PL56 15.14 GB
 PL57 15.14 GB
 PL58 15.14 GB
 PL59 15.14 GB
 PL60 15.14 GB
 PL61 15.14 GB
 PL62 15.14 GB
 PL63 15.14 GB
 PL64 15.14 GB
 PL65 15.14 GB
 PL66 15.14 GB
 PL67 15.14 GB
 PL68 15.14 GB
 PL69 15.14 GB
 PL70 15.14 GB
 PL71 15.14 GB
 PL72 15.14 GB
 PL73 15.14 GB
 PL74 15.14 GB
 PL75 15.14 GB
 PL76 15.14 GB
 PL77 15.14 GB
 PL78 15.14 GB
 PL79 15.14 GB
 PL80 15.14 GB
 PL81 15.14 GB
 PL82 15.14 GB
 PL83 15.14 GB
 PL84 15.14 GB
 PL85 15.14 GB
 PL86 15.14 GB
 PL87 15.14 GB
 PL88 15.14 GB
 PL89 15.14 GB
 PL90 15.14 GB
 PL91 15.14 GB
 PL92 15.14 GB
 PL93 15.14 GB
 PL94 15.14 GB
 PL95 15.14 GB
 PL96 15.14 GB
 PL97 15.14 GB
 PL98 15.14 GB
 PL99 15.14 GB
 PL100 15.14 GB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 1
 SF 100.612717 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



8.0037
8.0045
7.9923
7.9988
7.9914
7.8909
7.5599
7.5586
7.5598
7.3999
7.3972
7.3902
7.3840
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



Current Data Parameters
NAME 102130-2mephos
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

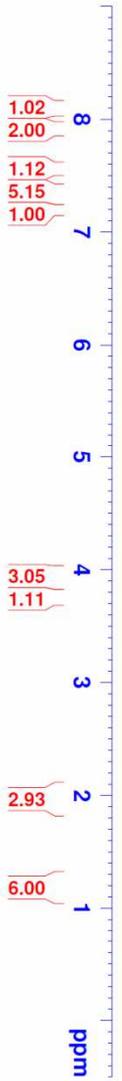
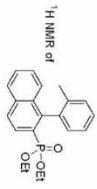
Date_ 20110614
Time 13.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg10
TD 32768
SOLVENT CDCl3
NS 64
DS 4
SWH 5896.227 Hz
FIDRES 0.179939 Hz
AQ 2.7787764 sec
RG 645
DM 84.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1

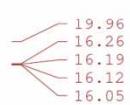
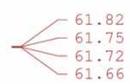
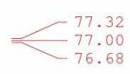
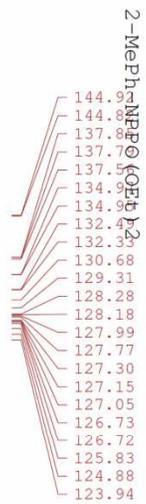
==== CHANNEL f1 =====

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
IB 0
GB 0
PC 1.00





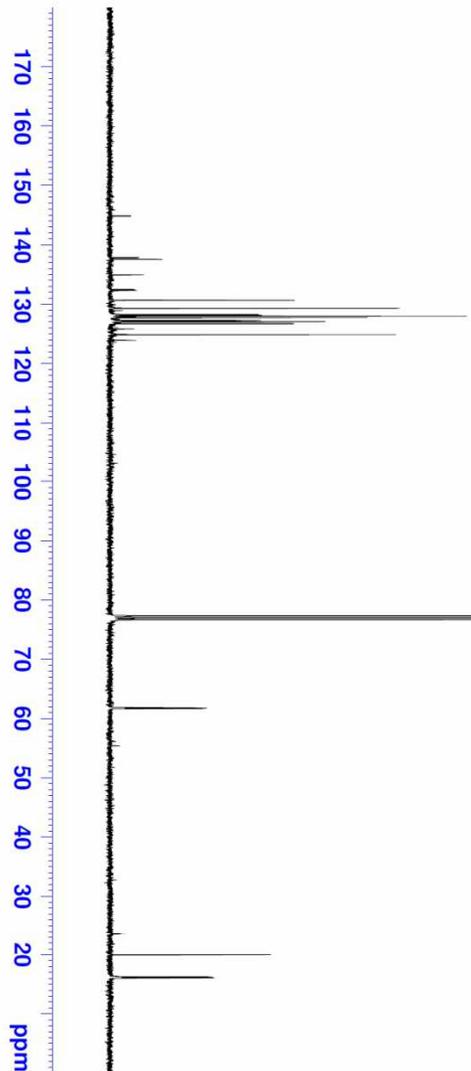
Current Data Parameters
 NAME 102190-2mephos
 EXPNO 3
 PROCNO 1

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 =====
 NUCL1 13C
 P1 9.75 usec
 PL1 -1.00 dB
 ELW 43.00697708 W
 SFO1 100.624395 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NOC2 1H
 FQ2 80.00 usec
 FID2 15.00 dB
 PL2 15.14 dB
 PL12 15.14 dB
 PL13 15.14 dB
 PL14 15.14 dB
 PL15 15.14 dB
 PL16 15.14 dB
 PL17 15.14 dB
 PL18 15.14 dB
 PL19 15.14 dB
 PL20 15.14 dB
 PL21 15.14 dB
 PL22 15.14 dB
 PL23 15.14 dB
 PL24 15.14 dB
 PL25 15.14 dB
 PL26 15.14 dB
 PL27 15.14 dB
 PL28 15.14 dB
 PL29 15.14 dB
 PL30 15.14 dB
 PL31 15.14 dB
 PL32 15.14 dB
 PL33 15.14 dB
 PL34 15.14 dB
 PL35 15.14 dB
 PL36 15.14 dB
 PL37 15.14 dB
 PL38 15.14 dB
 PL39 15.14 dB
 PL40 15.14 dB
 PL41 15.14 dB
 PL42 15.14 dB
 PL43 15.14 dB
 PL44 15.14 dB
 PL45 15.14 dB
 PL46 15.14 dB
 PL47 15.14 dB
 PL48 15.14 dB
 PL49 15.14 dB
 PL50 15.14 dB
 PL51 15.14 dB
 PL52 15.14 dB
 PL53 15.14 dB
 PL54 15.14 dB
 PL55 15.14 dB
 PL56 15.14 dB
 PL57 15.14 dB
 PL58 15.14 dB
 PL59 15.14 dB
 PL60 15.14 dB
 PL61 15.14 dB
 PL62 15.14 dB
 PL63 15.14 dB
 PL64 15.14 dB
 PL65 15.14 dB
 PL66 15.14 dB
 PL67 15.14 dB
 PL68 15.14 dB
 PL69 15.14 dB
 PL70 15.14 dB
 PL71 15.14 dB
 PL72 15.14 dB
 PL73 15.14 dB
 PL74 15.14 dB
 PL75 15.14 dB
 PL76 15.14 dB
 PL77 15.14 dB
 PL78 15.14 dB
 PL79 15.14 dB
 PL80 15.14 dB
 PL81 15.14 dB
 PL82 15.14 dB
 PL83 15.14 dB
 PL84 15.14 dB
 PL85 15.14 dB
 PL86 15.14 dB
 PL87 15.14 dB
 PL88 15.14 dB
 PL89 15.14 dB
 PL90 15.14 dB
 PL91 15.14 dB
 PL92 15.14 dB
 PL93 15.14 dB
 PL94 15.14 dB
 PL95 15.14 dB
 PL96 15.14 dB
 PL97 15.14 dB
 PL98 15.14 dB
 PL99 15.14 dB
 PL100 15.14 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127722 MHz
 KW 0
 SSB 0
 LB 0
 GB 0
 PC 1.40





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

F2 - Acquisition Parameters

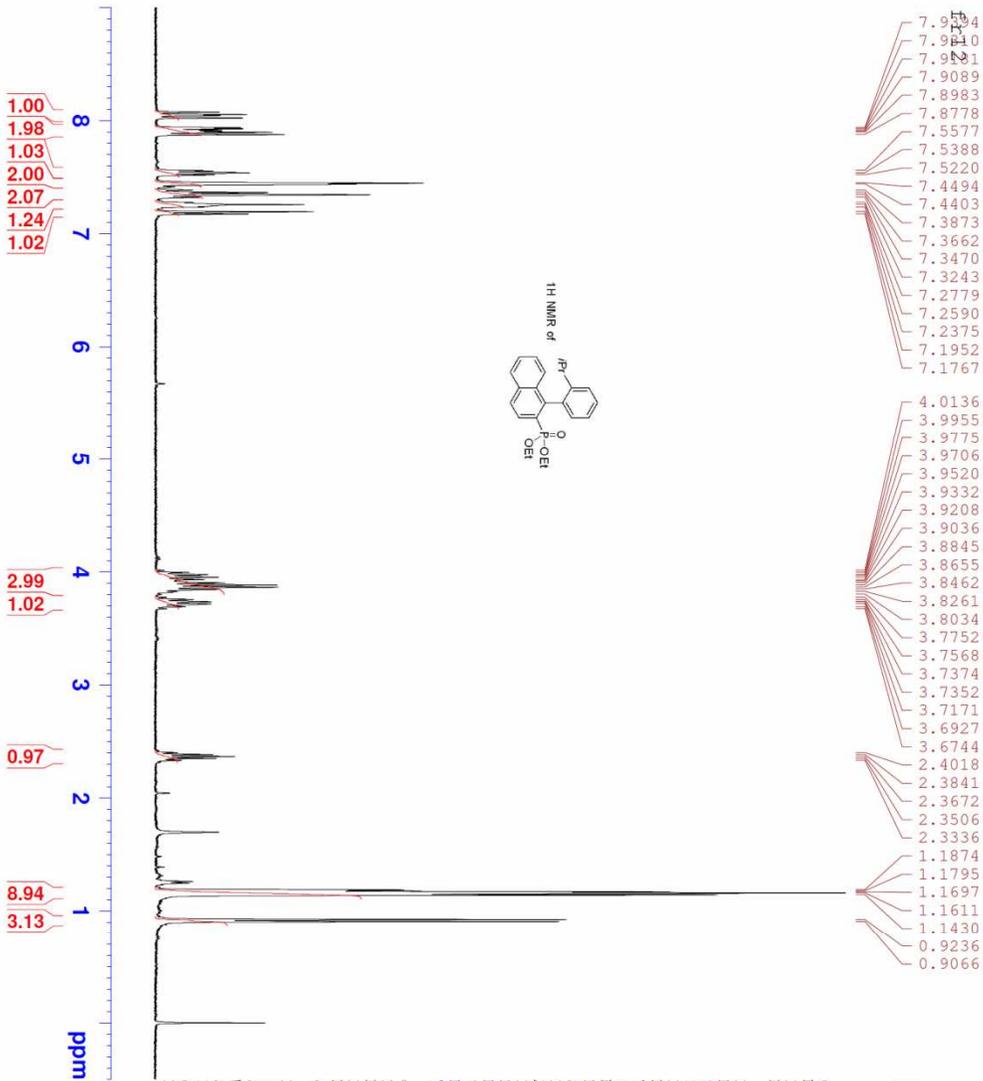
Date_ 20110405
 Time 16:14
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 4
 SWH 5896.227 Hz
 FIDRES 0.179939 Hz
 AQ 2.7787764 sec
 RG 456
 DW 84.800 usec
 DE 6.50 usec
 TE 298.0 K
 DI 2.00000000 sec
 TDO 1

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

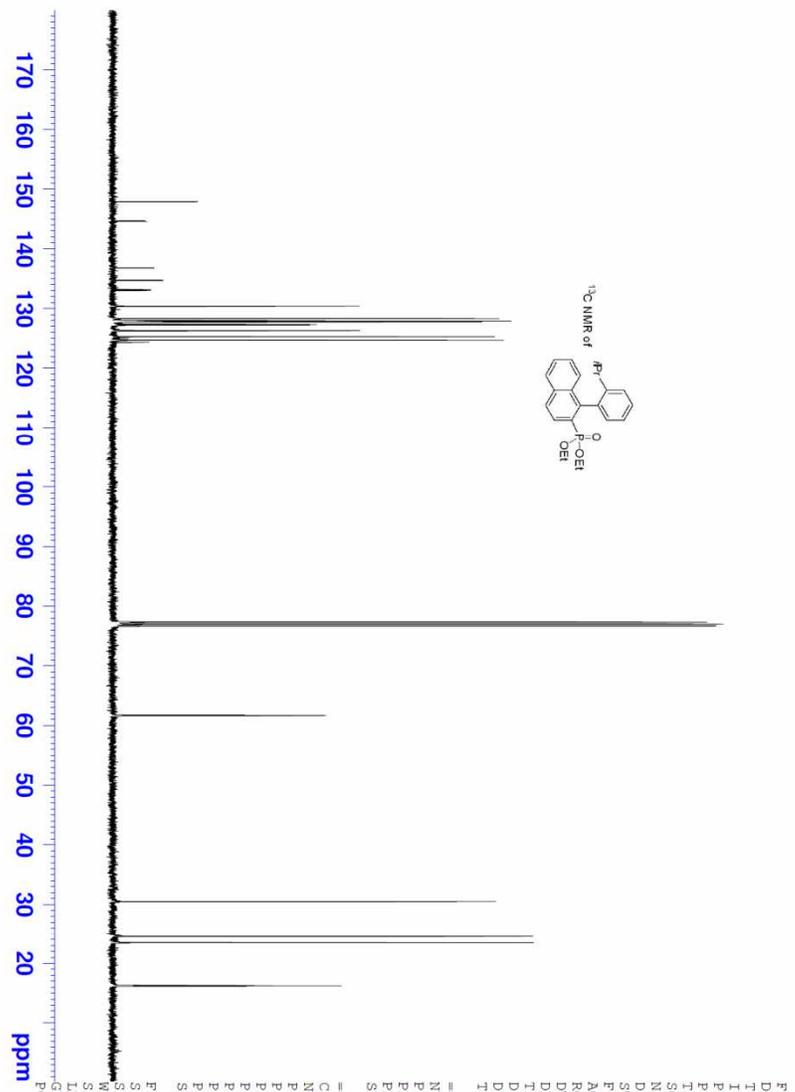
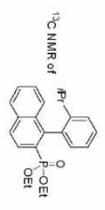
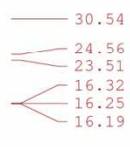
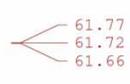
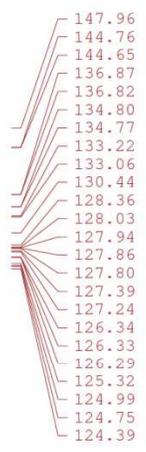
NUC1 1H
 P1 14.00 usec
 PL1 0.00 dB
 PL1W 10.49968529 W
 SFO1 400.1327209 MHz

F2 - Processing parameters

SI 65536
 SF 400.1300123 MHz
 WDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.00



F112



Current Data Parameters
 NAME 102190-e-3f12
 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
 DE 20.800 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 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
 PL1W 10.49968529 W
 PL2W 0.32149649 W
 PL13W 0.32149649 W
 SFO2 400.1316005 MHz

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



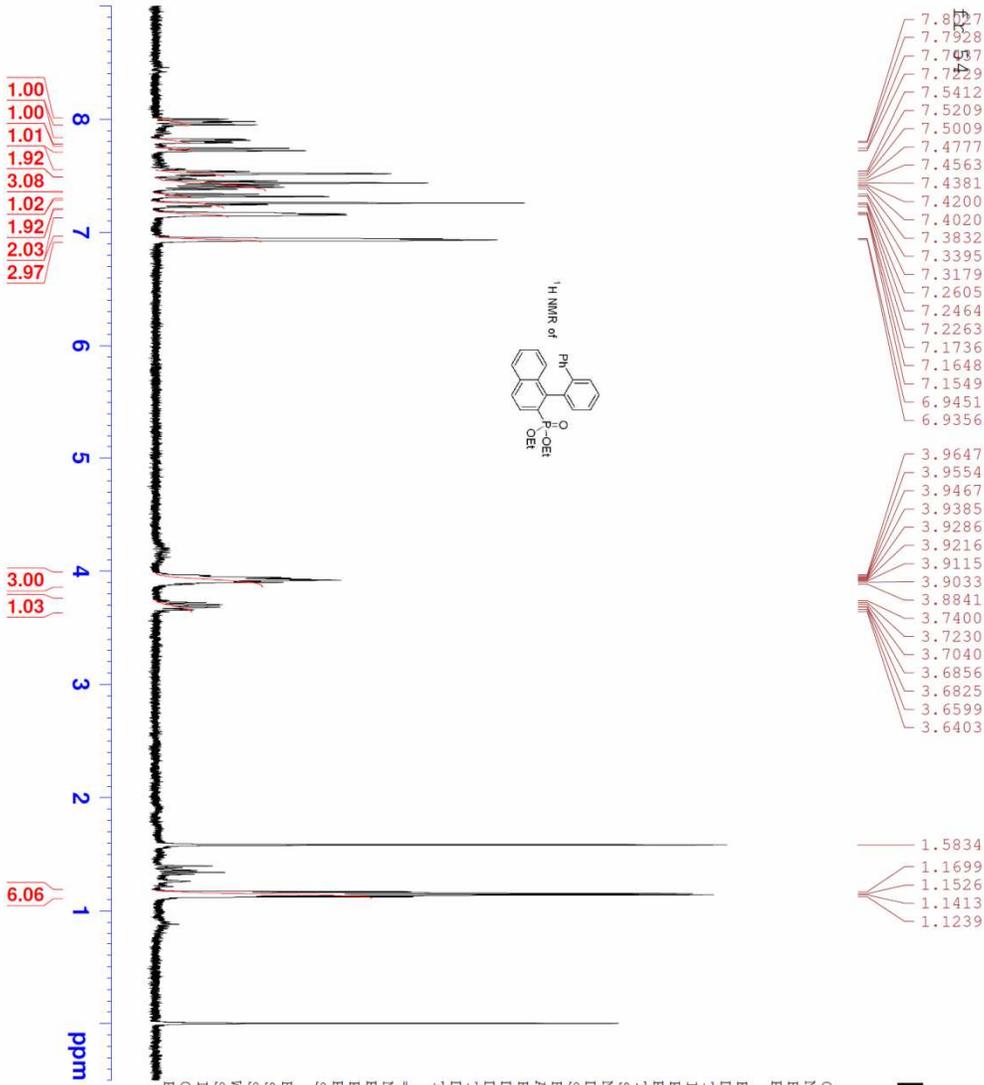
Current Data Parameters
 NAME 102190-e-1-F154
 EXPNO 1
 PROCNO 1

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 0.178939 Hz
 AQ 2.7787764 sec
 RG 724
 DM 84.800 usec
 DE 6.30 usec
 TE 298.0 K
 D1 2.00000000 sec
 TD0 1

==== CHANNEL F1 =====
 NUCL 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



- 7.8027
- 7.7928
- 7.7837
- 7.7829
- 7.5412
- 7.5209
- 7.5009
- 7.4777
- 7.4563
- 7.4381
- 7.4200
- 7.4020
- 7.3832
- 7.3395
- 7.3179
- 7.2605
- 7.2464
- 7.2263
- 7.1736
- 7.1648
- 7.1549
- 6.9451
- 6.9356
- 3.9647
- 3.9554
- 3.9467
- 3.9385
- 3.9286
- 3.9216
- 3.9115
- 3.9033
- 3.8841
- 3.7400
- 3.7230
- 3.7040
- 3.6856
- 3.6825
- 3.6599
- 3.6403
- 1.5834
- 1.1699
- 1.1526
- 1.1413
- 1.1239

- 1.00
- 1.00
- 1.01
- 3.08
- 1.02
- 1.92
- 2.03
- 2.97

- 3.00
- 1.03

- 6.06

Fr 54

142.01
141.25
136.89
134.57
131.68
129.66
129.10
128.33
127.88
127.78
127.73
127.69
127.51
127.40
127.33
127.26
126.50
126.33
126.29

61.87
61.84
61.82
61.78

16.30
16.24
16.19
16.13



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

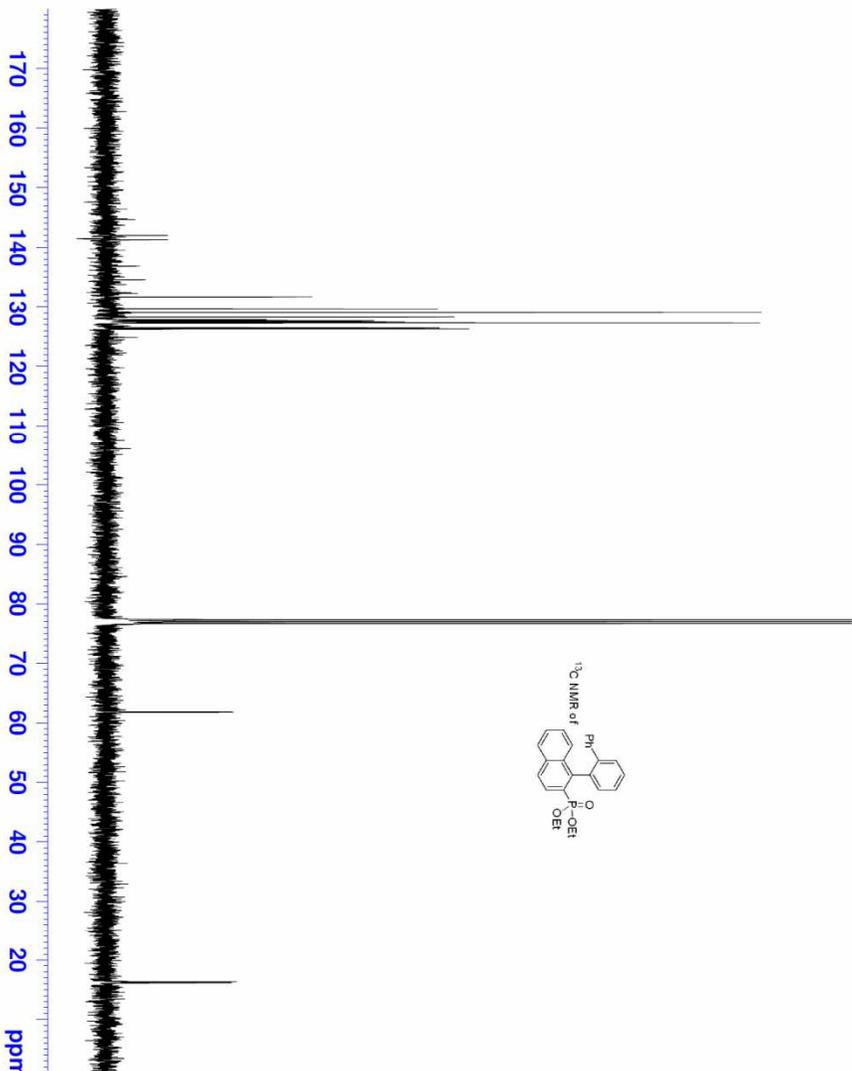
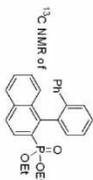
F2 - Acquisition Parameters

Date_ 20110406
Time 0.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 32768
SOLVENT 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
TDO 1

===== CHANNEL F1 =====
NUC1 13C
P1 9.75 usec
PL1 -1.00 dB
PL1W 43.006597708 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
PL14 15.14 dB
PL15 15.14 dB
PL16 10.49968529 W
PL17 0.32149649 W
PL18 0.32149649 W
PL19 400.1316005 MHz
SFO2

F2 - Processing parameters
SI 65336
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
FC 1.40





Current Data Parameters
 NAME 102190-e-2-1
 EXPTNO 4
 PROCNO 1

F2 - Acquisition Parameters

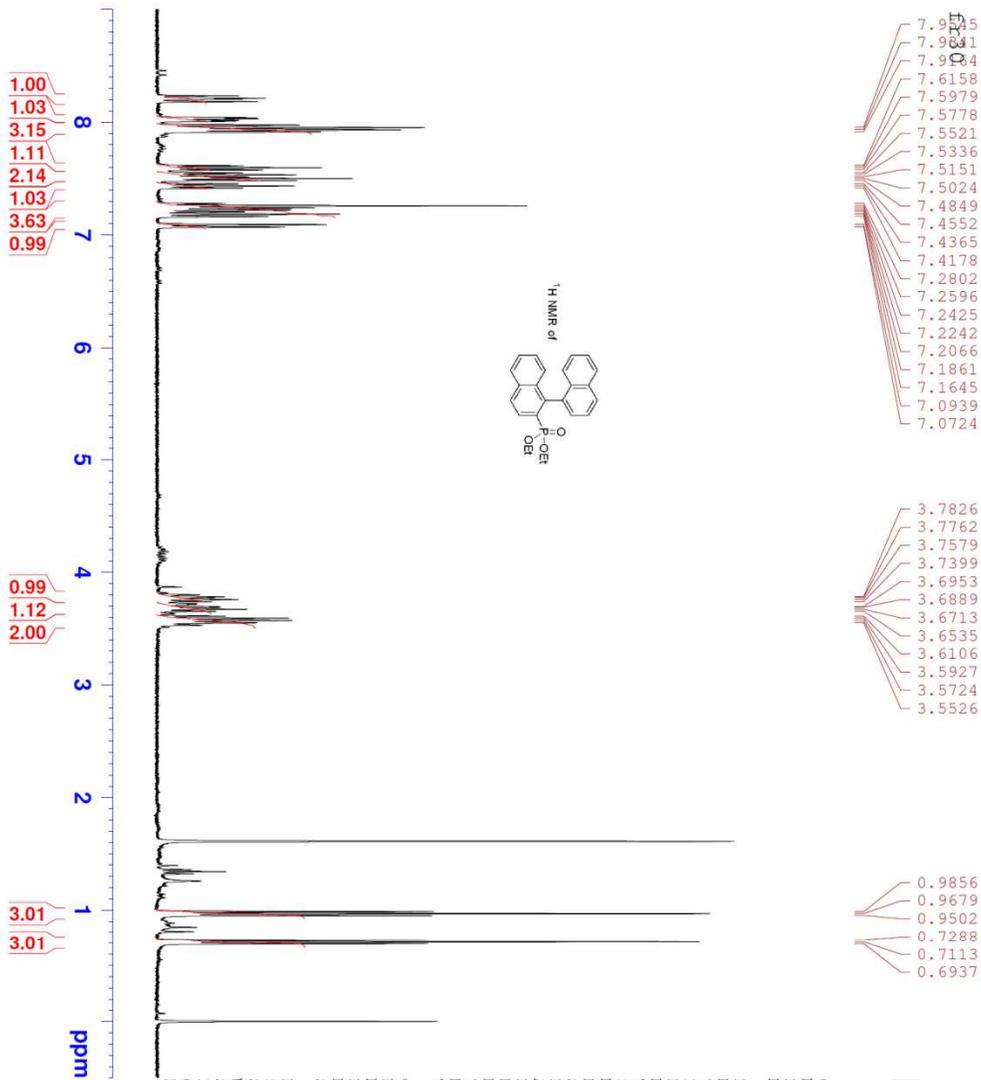
Date_ 20110405
 Time 18.44
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg10
 TD 32768
 SOLVENT CDCl3
 NS 64
 DS 4
 SWH 5896.227 Hz
 FIDRES 0.179939 Hz
 AQ 2.7787764 sec
 RG 645
 DW 84.800 usec
 DE 298.0 usec
 TE 298.0 K
 D1 2.00000000 sec
 TD0 1

===== 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
 GB 0
 PC 1.00



Clean Oil

- 135.81
- 134.92
- 133.36
- 133.19
- 133.13
- 128.74
- 128.71
- 128.64
- 128.26
- 128.02
- 127.92
- 127.84
- 127.76
- 127.62
- 126.72
- 126.70
- 125.88
- 125.61
- 124.95

- 77.35
- 77.03
- 76.71
- 61.80
- 61.74

- 15.99
- 15.92
- 15.50
- 15.43



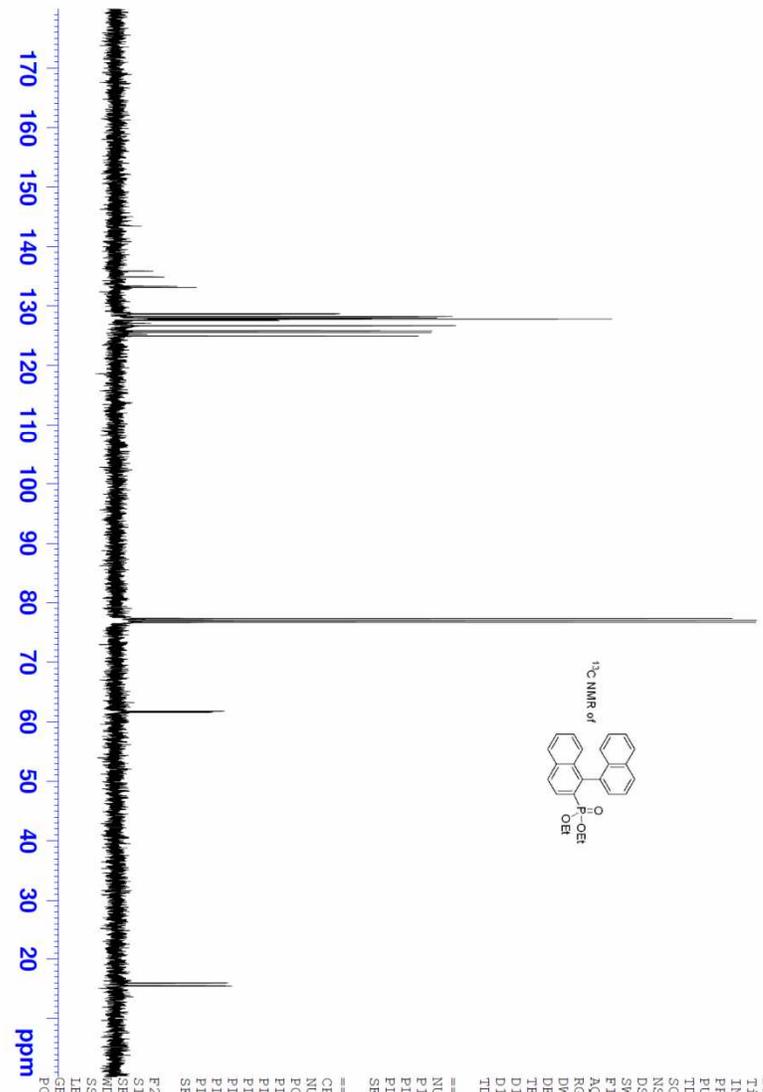
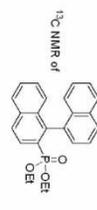
Current Data Parameters
 NAME 102190-e-2-1
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110405
 Time 12.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg
 TD 32768
 SOLVENT CDCl3
 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
 TDO 1

===== CHANNEL f1 =====
 NUCL 13C
 P1 9.75 usec
 EL1 -1.00 dB
 ELI 43.006597708 W
 SFO1 100.6243395 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUCL2 1H
 FCFD2 80.00 usec
 P12 0.00 dB
 P112 13.14 dB
 P113 13.14 dB
 P12M 10.49968529 W
 P112M 0.32149649 W
 P113M 0.32149649 W
 SFO2 400.1516005 MHz

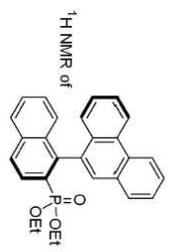
F2 - Processing parameters
 SI 65936
 SF 100.6127690 MHz
 RDW 0
 SSB 0
 IB 1.00 Hz
 PC 1.40



8.2659
8.2660
8.2689
8.2717
8.2735
8.2735
8.0391
8.0420
8.0420
7.9655
7.9490
7.9017
7.8861
7.7715
7.7295
7.7154
7.7129
7.6610
7.6599
7.6458
7.6311
7.6149
7.6008
7.5986
7.5519
7.5379
7.3494
7.3347
7.3212
7.3070
7.2601
7.2463
7.1548
7.1394
3.7755
3.7697
3.7555
3.7413
3.6482
3.6450
3.6394
3.6336
3.6310
3.6278
3.6254
3.6115
3.5642
3.5500
3.5359
3.5302
0.9614
0.9472
0.9331
0.6251
0.6110
0.5969
0.0022



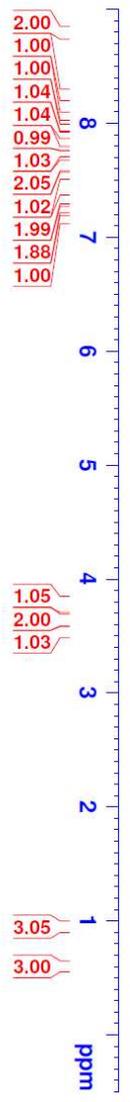
Current Data Parameters
 NAME 102190-Phna-phos
 EXPNO 1
 PROCNO 1

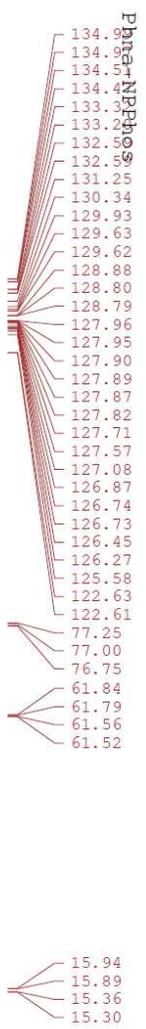


F2 - Acquisition Parameters
 Date_ 20110623
 Time 14.48
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 64
 DS 0
 SWH 7500.000 Hz
 FIDRES 0.228882 Hz
 AQ 2.1845834 sec
 RG 512
 DW 66.667 usec
 DE 6.50 usec
 TE 299.0 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUCL1 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
 GB 0
 PC 1.00





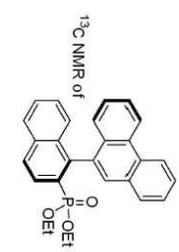
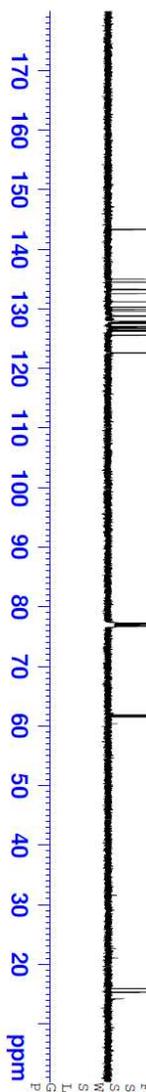
Current Data Parameters
 NAME 102190-phna-phos
 EXPNO 2
 PROCNO 1

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
 TDO 1

CHANNEL F1
 NUCC1 13C
 P1 9.88 usec
 PL1 -0.50 dB
 PL1W 124.00885010 W
 SFO1 125.7698617 MHz

CHANNEL F2
 CPDPRG2 waltz16
 NUCC2 1H
 PCPD2 80.00 usec
 P12 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
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40



8.119088
 8.119066
 8.119044
 8.002066
 7.889044
 7.889022
 7.889000
 7.888978
 7.888956
 7.888934
 7.471555
 7.463566
 7.3967
 7.3938
 7.3723
 7.3592
 7.2825
 7.1778
 7.0985
 7.0831



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

F2 - Acquisition Parameters

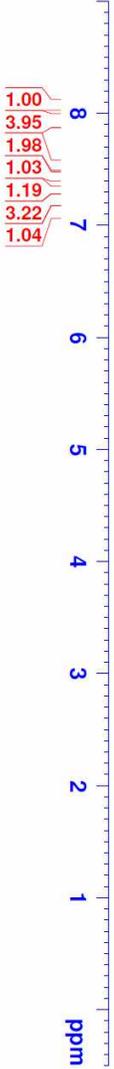
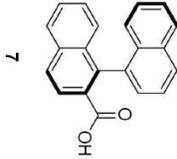
Date_ 20110621
 Time 12.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg10
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 4
 SWH 5896.227 Hz
 FIDRES 0.179939 Hz
 AQ 2.778764 sec
 RG 812
 DM 84.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 ID0 1

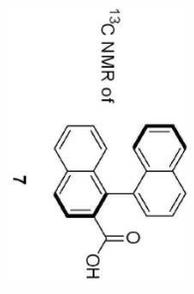
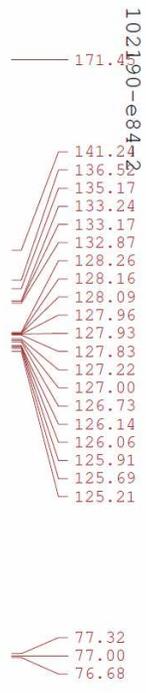
CHANNEL f1

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 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 =====
 NUCL1 13C
 P1 9.75 usec
 PL1 -1.00 dB
 PL1W 43.00697708 W
 SFO1 100.6243395 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUCL2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.14 dB
 PL13 15.14 dB
 PL1W 10.49968529 W
 PL12W 0.32149649 W
 PL13W 0.32149649 W
 SFO2 400.1316005 MHz

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

10.1990
 7.9855
 7.9822
 7.9800
 7.9824
 7.9823
 7.8894
 7.7899
 7.7891
 7.6809
 7.5895
 7.5703
 7.4788
 7.4595
 7.4401
 7.4194
 7.4006
 7.3841
 7.2714
 7.2534
 7.2355
 7.2165
 7.1982
 7.1763
 7.1554

4.4044



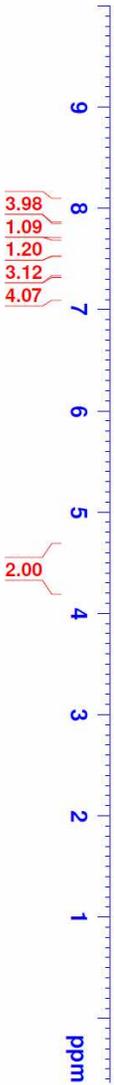
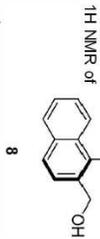
Current Data Parameters
 NAME 101990-alcohol
 EXNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110528

Time 1.54
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 4
 SWH 5896.227 Hz
 FIDRES 0.179939 Hz
 AQ 2.787764 sec
 RG 436
 DW 84.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 TDO 1

CHANNEL F1

NUC1 1H
 P1 14.00 usec
 PL 0.00 dB
 PL1W 10.49968529 W
 SFO1 400.1327209 MHz
 F2 - Processing parameters
 SI 65336
 SF 400.1300263 MHz
 WDW EM
 SSB 0
 LB 0.05 Hz
 GB 0
 PC 1.00



101990-1-alcohol1
 136.7
 135.7
 135.6
 133.3
 133.1
 132.9
 132.8
 128.3
 128.1
 127.92
 127.86
 126.63
 126.42
 126.15
 126.06
 125.81
 125.76
 125.46

77.31
 76.99
 76.68

63.43



Current Data Parameters
 NAME 101990-1alcohol1
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110528
 Time 5.46

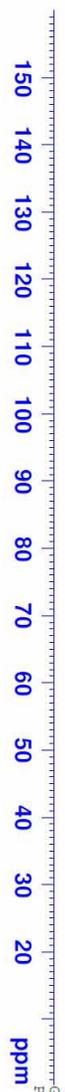
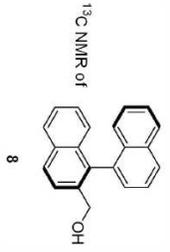
INSTRUM spect
 PROBD 5 mm PABBO BB-
 PULPROG zgpg
 TD 32768
 SOLVENT CDCl3
 NS 5000

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
 NUCL 13C
 P1 9.75 usec
 PL1 -1.00 dB
 PL1W 43.00697708 W
 SFO1 100.6243395 MHz

CHANNEL F2
 CPDPRG2 waltz16
 NUCL2 1H
 PCPDZ 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 100.612769 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



7.6229
7.6181
7.6072
7.6045
7.6018
7.5908
7.5883
7.5248
7.5232
7.5109
7.5092
7.4948
7.4930
7.3916
7.3749
7.3523
7.3501
7.3389
7.3363
7.3332
7.3197
7.3168
7.3143
7.3026
7.3006
7.2607
7.2275
7.2105



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

F2 - Acquisition Parameters

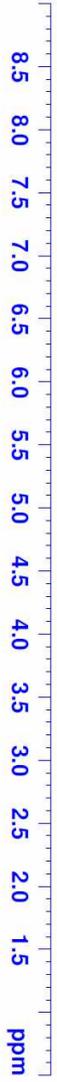
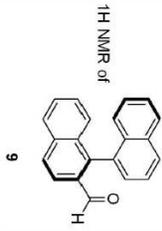
Date_ 20110609
Time_ 23.39
INSTRUM spect
PROBHD 5 mm PABBO BBI
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 64
DS 0
SWH 7500.000 Hz
FIDRES 0.228882 Hz
AQ 2.184534 sec
RG 322
DW 66.667 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
TDO 1

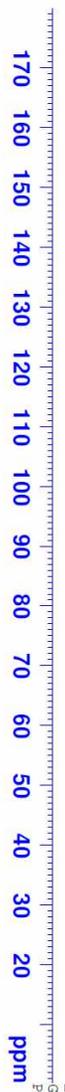
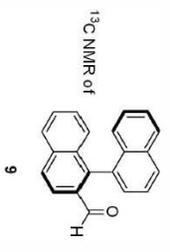
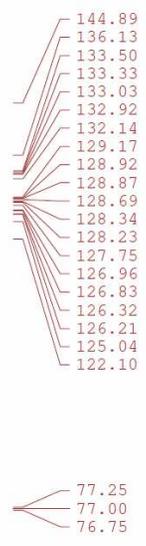
CHANNEL f1

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
 TDO 1

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

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 P2 2.10 dB
 PL2 19.30 dB
 PL3 19.30 dB
 PL2W 18.43091774 W
 PL2W 0.35119396 W
 PL3W 0.35119396 W
 SFO2 500.1325007 MHz

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

