

# A Novel Base-Promoted Cyclization: Synthesis of Substituted Benzo[b]furans

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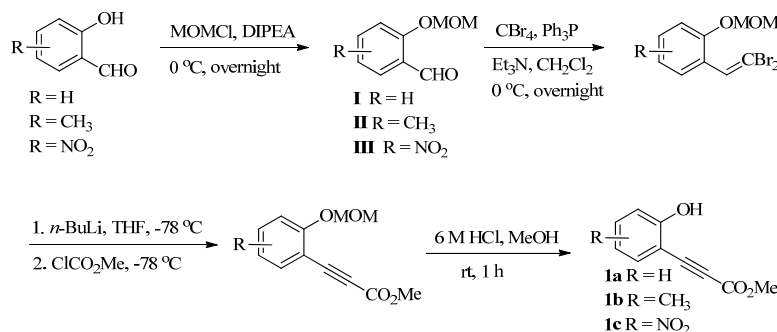
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## Experimental Section

### General methods and materials

All reagents and solvents were reagent grade or were purified by standard methods before use. Column chromatography was carried out on flash silica gel (Sorbent 230–400 mesh). TLC analysis was conducted on silica gel plates (Sorbent Silica G UV254). NMR spectra were recorded at <sup>1</sup>H (400 MHz) and <sup>13</sup>C (100 MHz) on a Bruker instrument. Chemical shifts ( $\delta$  values) and coupling constants ( $J$  values) are given in ppm and hertz, respectively, using solvents (<sup>1</sup>H NMR, <sup>13</sup>C NMR) as the internal standard.



Scheme 1

### General procedure for the synthesis of Arylpropiolates (1a-c)

**Preparation of 1b:** To a solution of CBr<sub>4</sub> (3.03 g, 6.11 mmol) and PPh<sub>3</sub> (4.0 g, 15.27 mmol) in dry CH<sub>2</sub>Cl<sub>2</sub> (20 mL) was added drop wise a solution of aldehyde II (1.1 g, 6.11 mmol) and Et<sub>3</sub>N (2.5 mL, 18.3 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (5 mL) the solution was stirred at 0 °C for overnight, and then *n*-hexane (20 mL) was added and stirred for another 30 min at this temperature. After removing insoluble materials by filtration through Celite, the filtrate was concentrated in vacuo. The residue was purified by silica gel

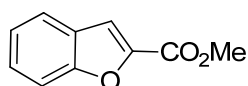
flash column chromatography (hexane- AcOEt 10:1) to give dibromoalkene (1.50 g, 75%) as pale yellow oil.

To a stirred solution of dibromoalkene (1.50 g, 0.93 mmol) was added drop wise *n*-BuLi (2.5 M solution in hexane, 4.5 mL) at -78 °C and the reaction mixture was stirred at this temperature for 30 min, and then at 0 °C for 2 h. To this solution methyl chloroformate (0.5 mL 1.1 mmol) was added at -78 °C, and the reaction mixture was further stirred at 0 °C for 2 h. The reaction mixture was quenched with sat. NH<sub>4</sub>Cl (10 mL), and extracted with Et<sub>2</sub>O (10 mL × 3). The combined organic layers was washed with H<sub>2</sub>O (20 mL) and brine (20 mL), dried over MgSO<sub>4</sub>, and concentrated in vacuo. The residue was purified by silica gel flash chromatography (hexane-EtOAc 25:1) to give propiolate (0.85 g, 71%) as yellow oil.

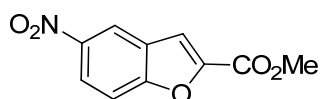
To a solution of arylpropionate (0.85 g, 3.2 mmol) in MeOH (4 mL) was added 6 M HCl (5 mL) and the reaction mixture was stirred at room temperature for 1 h. The resultant mixture was extracted with AcOEt (10 mL × 3). The combined organic layers was washed with H<sub>2</sub>O (10 mL), brine (10 mL), dried over MgSO<sub>4</sub>, and concentrated in vacuo. The residue was purified by silica gel flash column chromatography (hexane-AcOEt 4:1) to give **1b** (0.51 g, 71%) as pale yellow oil.<sup>1</sup>

#### General procedure and Spectral data for all final compounds (2a-d):

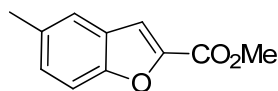
To the solution of arylpropionate **1a** (40 mg, 0.22 mmol) in dry DMF (3 mL) was added Cs<sub>2</sub>CO<sub>3</sub> (147 mg, 0.45 mmol). The reaction mixture was stirred at 60 °C under N<sub>2</sub> atmosphere for 1 h. The resulting mixture was diluted with AcOEt (20 mL). The organic layer was washed with water (15 mL) and brine (15 mL), dried over MgSO<sub>4</sub>, and concentrated in vacuo. The residue was purified by silica gel flash column chromatography (hexane-AcOEt 9:1) to give benzofuran **2a** (35 mg, 87%) as pale yellow syrup. The following spectral data were in good agreement with those reported previously.<sup>2</sup>



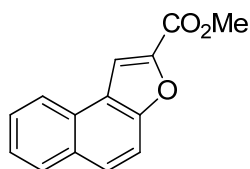
**Methyl benzofuran-2-carboxylate (2a):** <sup>1</sup>H NMR (CDCl<sub>3</sub>): δ = 3.98 (s, 3 H), 7.29 (t, *J* = 1.9 Hz, 1 H), 7.45 (t, *J* = 1.9 Hz, 1 H), 7.53 (s, 1 H), 7.60 (d, *J* = 21 Hz, 1 H), 7.69 (d, *J* = 1.9 Hz, 1 H); <sup>13</sup>C NMR (CDCl<sub>3</sub>): δ = 52.38, 112.37, 114.01, 122.85, 123.82, 126.93, 127.68, 145.40, 155.73, 160.00.



**Methyl 5-nitrobenzofuran-2-carboxylate (2b):** <sup>1</sup>H NMR (CDCl<sub>3</sub>): δ = 4.01 (s, 3 H), 7.65 (s, 1 H), 7.71 (d, *J* = 2.3 Hz, 1 H), 8.38 (d, *J* = 2.3 Hz, 1 H), 8.66 (s, 1 H); <sup>13</sup>C NMR (CDCl<sub>3</sub>): δ = 52.83, 113.00, 114.13, 119.55, 123.05, 127.22, 144.85, 148.39, 158.02, 159.03.



**Methyl 5-methylbenzofuran-2-carboxylate (2c):**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 2.35 (s, 3H), 3.88 (s, 3 H), 7.17 (d,  $J$  = 2.2 Hz, 1 H), 7.36-7.38 (m, 3 H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 21.27, 52.30, 111.84, 113.79, 122.33, 127.01, 129.22, 133.41, 145.43, 154.24, 160.04.



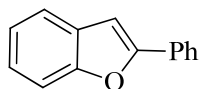
**Methyl naphtho[1,2-b]furan-2-carboxylate (2d):**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 3.93 (s, 3 H), 7.46 (t,  $J$  = 2.0 Hz, 1 H), 7.56 (t,  $J$  = 2.0 Hz, 1 H), 7.62 (d,  $J$  = 2.3 Hz, 1 H), 7.80 (d,  $J$  = 2.3 Hz, 1 H), 7.88 (d,  $J$  = 2.0 Hz, 1 H), 7.94 (s, 1 H), 8.08 (d,  $J$  = 2.0 Hz, 1 H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 52.35, 112.73, 113.00, 122.73, 123.32, 125.45, 127.31, 127.99, 129.01, 129.22, 130.51, 144.75, 154.04, 159.88; ESIMS  $m/z$ : 227 (M+1).

#### General procedure for Sonogashira reaction:

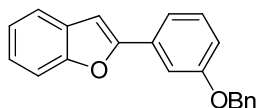
To a solution of 2-iodophenol (600 mg, 2.72 mmol) in a THF- $\text{Et}_3\text{N}$  mixture (30 mL, 4:1, v/v) were added  $\text{PdCl}_2(\text{PPh}_3)_2$  (380 mg, 0.054 mmol), CuI (22 mg, 0.11 mmol) and 1-ethynyl-4-methylbenzene (632 mg, 5.44 mmol). The mixture was stirred at 25 °C for 12 h. A saturated aqueous solution of saturated  $\text{NH}_4\text{Cl}$  was added and the mixture was extracted with  $\text{CH}_2\text{Cl}_2$ . The combined organic layer was dried ( $\text{Na}_2\text{SO}_4$ ) and the solvent was evaporated. The residue was purified by column chromatography to give **6e** as a yellow solid 562 mg (97%).

#### General procedure and Spectral data for final compounds (4a-m):

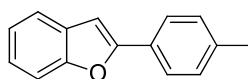
To the solution of 2-(*p*-tolylethynyl)phenol **3c** (104 mg, 0.5 mmol) in dry DMF (8 mL) was added  $\text{Cs}_2\text{CO}_3$  (326 mg, 1 mmol). The reaction mixture was stirred at 60 °C under  $\text{Ar}_2$  for 1 h. The resulting mixture was diluted with AcOEt (30 mL). The organic layer was washed with water (30 mL) and brine (30 mL), dried over  $\text{Na}_2\text{SO}_4$ , and concentrated in vacuo. The residue was purified by silica gel flash column chromatography (hexane-AcOEt 15:1) to give 2-(*p*-tolyl)benzofuran (**4c**) (94 mg, 90%) as yellow oil. The following spectral data were in good agreement with those reported previously.<sup>3</sup>



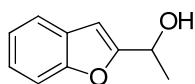
**2-Phenylbenzofuran (4a)**<sup>3</sup> <sup>1</sup>H NMR (CDCl<sub>3</sub>): δ = 7.04 (s, 1H), 7.22–7.38 (m, 3H), 7.44–7.48 (m, 2H), 7.49–7.61 (m, 2H), 7.95 (d, *J* = 7.6 Hz, 2H); <sup>13</sup>C NMR (CDCl<sub>3</sub>): δ = 154.81, 154.80, 130.50, 129.23, 128.78, 128.54, 124.94, 124.25, 122.92, 120.90, 111.17, 101.29.



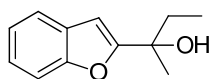
**2-(3-(Benzyloxy)phenyl)benzofuran (4b)**: <sup>1</sup>H NMR (CDCl<sub>3</sub>): δ = 5.18 (s, 2H), 7.01 (dd, *J* = 8.4 Hz, *J* = 2.0 Hz, 1H), 7.04 (s, 1H), 7.62–7.24 (m, 12H). <sup>13</sup>C NMR (CDCl<sub>3</sub>): δ = 70.17, 101.68, 111.21, 111.31, 115.19, 117.81, 120.96, 122.98, 124.37, 127.60, 128.09, 128.66, 129.18, 129.92, 131.84, 136.85, 154.88, 155.70, 159.19.



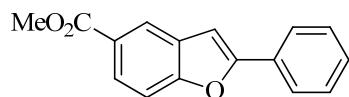
**2-(p-Tolyl)benzofuran (4c)**<sup>3</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>): δ = 2.44 (s, 3H), 7.00 (s, 1H), 7.30–7.26 (m, 4H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 7.2 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 2H). <sup>13</sup>C NMR (CDCl<sub>3</sub>): δ = 21.41, 100.59, 111.12, 120.77, 122.88, 124.02, 124.92, 127.79, 129.39, 129.52, 138.62, 154.81, 156.23.



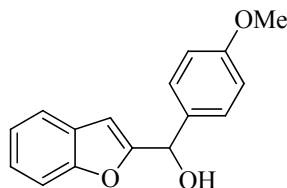
**1-(Benzofuran-2-yl)ethanol (4d)**<sup>4</sup>: <sup>1</sup>H NMR (CDCl<sub>3</sub>): δ = 1.65 (d, *J* = 6.8 Hz, 2H), 2.55 (s, 1H), 5.02 (q, *J* = 6.4, 1H), 6.61 (s, 1H), 7.31–7.22 (m, 2H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.56 (d, *J* = 7.6 Hz, 1H). <sup>13</sup>C NMR (CDCl<sub>3</sub>): δ = 21.43, 64.78, 101.80, 111.22, 121.09, 122.79, 124.17, 128.18, 154.79, 160.28.



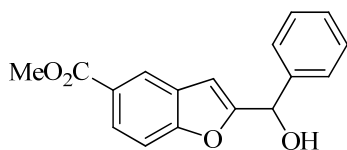
**2-(Benzofuran-2-yl)butan-2-ol (4e)**: <sup>1</sup>H NMR (CDCl<sub>3</sub>): δ = 0.916 (t, *J* = 7.6 Hz, 3H), 1.64 (s, 3H), 1.99 (q, *J* = 7.6 Hz, 2H), 2.12 (s, 1H), 6.61 (s, 1H), 7.27–7.22 (m, 2H), 7.47 (d, *J* = 7.6 Hz, 1H), 7.55 (d, *J* = 7.2 Hz, 1H). <sup>13</sup>C NMR (CDCl<sub>3</sub>): δ = 8.39, 26.27, 34.26, 72.38, 101.49, 111.15, 120.89, 122.69, 123.84, 128.34, 154.71, 162.31.



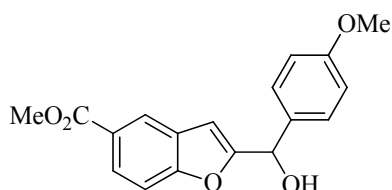
**Methyl 2-phenylbenzofuran-5-carboxylate (4f):**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 3.95 (s, 3H), 7.07 (s, 1H), 7.38 (t, 1H,  $J$  = 2.2 Hz), 7.46 (t, 2H,  $J$  = 1.9 Hz), 7.55 (d, 1H,  $J$  = 2.2 Hz), 7.88 (d, 2H,  $J$  = 19 Hz), 8.02 (d, 1H,  $J$  = 2.2 Hz), 8.32 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 52.11, 101.52, 111.00, 123.31, 125.08, 125.34, 126.06, 128.88, 129.04, 129.25, 129.89, 157.43, 16.30.



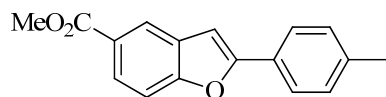
**Benzofuran-2-yl(4-methoxyphenyl)methanol (4g):**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 2.48 (s, 1H), 3.81 (s, 3H), 5.90 (s, 1H), 6.52 (s, 1H), 6.92 (d, 2H,  $J$  = 2.2 Hz), 7.17-7.26 (m, 2H), 7.39 (d, 2H,  $J$  = 2.2 Hz), 7.44 (d, 1H,  $J$  = 19 Hz), 7.51 (d, 1H,  $J$  = 1.9 Hz);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 55.33, 70.38, 103.83, 111.32, 114.03, 121.10, 122.81, 124.23, 128.08, 132.56, 155.10, 158.80, 159.70; ESIMS  $m/z$ : 277  $[\text{M}+\text{Na}]^+$ .



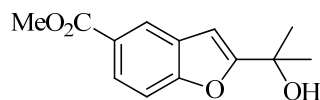
**Methyl 2-(hydroxy(phenyl)methyl)benzofuran-5-carboxylate (4h):**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 2.62 (s, 1H), 3.92 (s, 3H), 5.95 (s, 1H), 6.60 (s, 1H), 7.33-7.42 (m, 4H), 7.49 (d, 2H,  $J$  = 2.3 Hz), 7.96 (d, 2H,  $J$  = 2.3 Hz), 8.24 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 52.14, 70.60, 104.31, 111.19, 123.61, 125.19, 126.11, 126.80, 128.07, 128.57, 128.72, 140.00, 157.66, 160.10, 167.30; ESIMS  $m/z$ : 305  $[\text{M}+\text{Na}]^+$ .



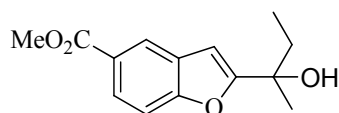
**Methyl 2-(hydroxy(4-methoxyphenyl)methyl)benzofuran-5-carboxylate (4i):**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 2.63 (s, 1H), 3.81 (s, 3H), 3.91 (s, 3H), 5.89 (s, 1H), 6.60 (s, 1H), 6.93 (d, 2H,  $J$  = 2.1 Hz), 7.41 (d, 2H,  $J$  = 2.1 Hz), 7.44 (d, 1H,  $J$  = 2.1 Hz), 7.98 (d, 1H,  $J$  = 2.1 Hz), 8.23 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 52.12, 55.33, 70.30, 104.10, 111.16, 114.11, 123.56, 125.19, 126.04, 128.20, 132.23, 157.66, 159.81, 160.37, 167.29; ESIMS  $m/z$ : 335  $[\text{M}+\text{Na}]^+$ .



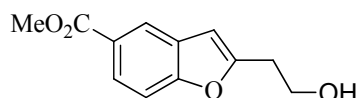
**Methyl 2-(p-tolyl)benzofuran-5-carboxylate (4j):**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 2.41 (s, 3H), 3.95 (s, 3H), 6.99 (s, 1H), 7.27 (d, 2H,  $J$  = 20 Hz), 7.53 (d, 1H,  $J$  = 21 Hz), 7.76 (d, 2H,  $J$  = 20 Hz), 8.02 (d, 2H,  $J$  = 21 Hz), 8.30 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 21.41, 52.08, 100.75, 110.89, 123.12, 125.01, 125.23, 125.81, 127.14, 129.57, 139.14, 157.64, 167.33.



**Methyl 2-(2-hydroxypropan-2-yl)benzofuran-5-carboxylate (4k):**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 1.67 (s, 6H), 2.72 (s, 1H), 3.92 (s, 3H), 6.60 (s, 1H), 7.44 (d, 1H,  $J$  = 21 Hz), 7.96 (d, 1H,  $J$  = 21 Hz), 8.21 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 28.68, 52.18, 69.20, 100.78, 110.98, 123.43, 124.96, 125.78, 128.35, 157.28, 164.72, 167.41.



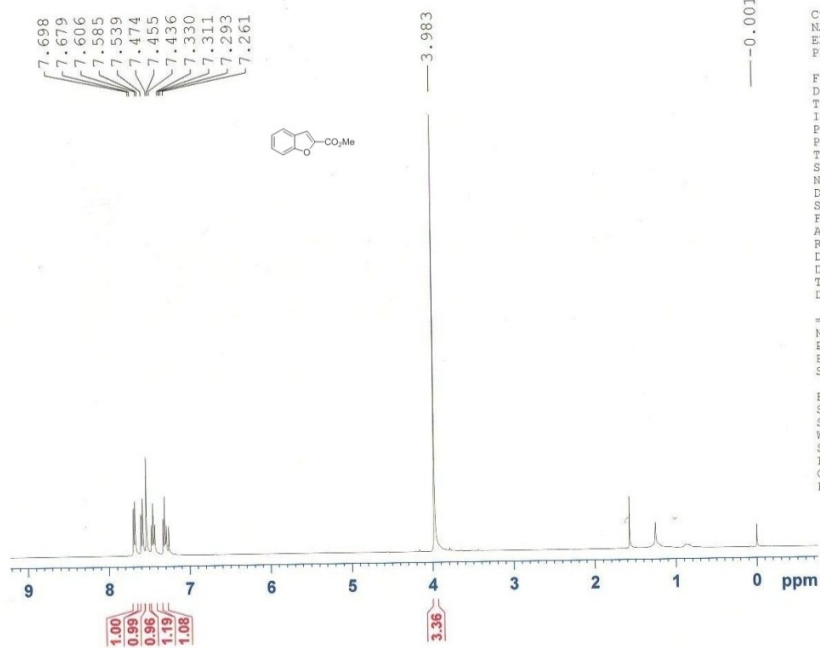
**Methyl 2-(2-hydroxybutan-2-yl)benzofuran-5-carboxylate (4l):**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 0.90 (t, 3H,  $J$  = 19 Hz), 1.63 (s, 3H), 1.98 (q, 2H,  $J$  = 19 Hz), 2.32 (s, 1H), 3.94 (s, 3H), 6.65 (s, 1H), 7.47 (d, 1H,  $J$  = 21 Hz), 7.99 (d, 1H,  $J$  = 21 Hz), 8.26 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 8.31, 26.24, 34.17, 52.10, 72.31, 101.95, 110.97, 123.35, 125.04, 125.70, 128.37, 157.32, 163.98, 167.36.



**Methyl 2-(2-hydroxyethyl)benzofuran-5-carboxylate (4m):**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 1.81 (s, 1H), 3.07 (t, 2H,  $J$  = 15 Hz), 3.94 (s, 3H), 4.03 (t, 2H,  $J$  = 15 Hz), 6.58 (s, 1H), 7.46 (d, 1H,  $J$  = 21 Hz), 7.98 (d, 1H,  $J$  = 21 Hz), 8.24 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  = 32.03, 52.08, 60.53, 100.08, 110.69, 122.86, 124.99, 125.44, 128.75, 157.63, 167.40.

## References:

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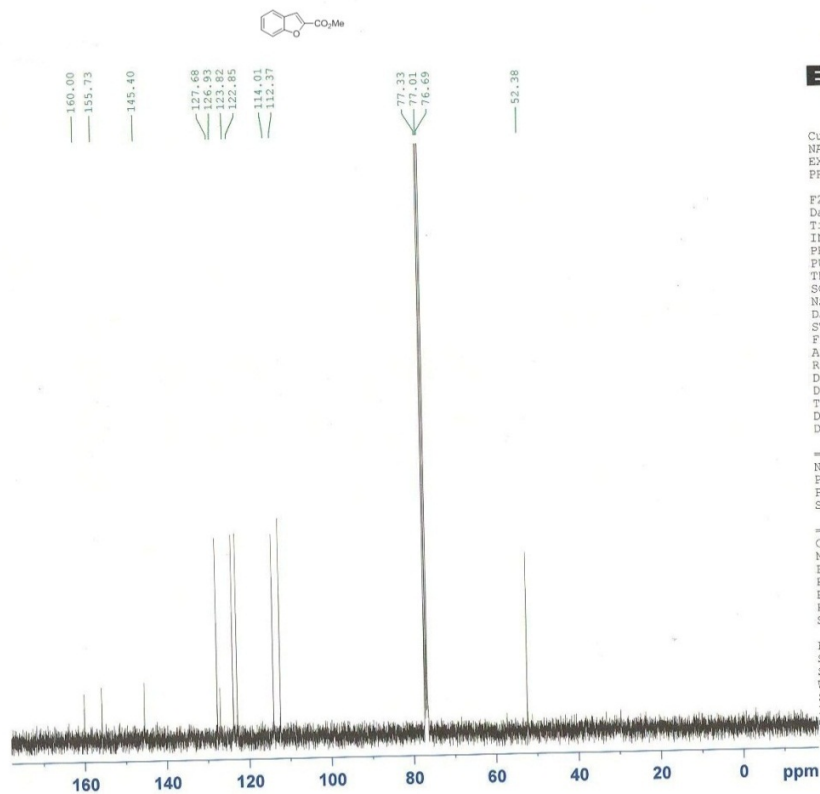


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PC 1.40



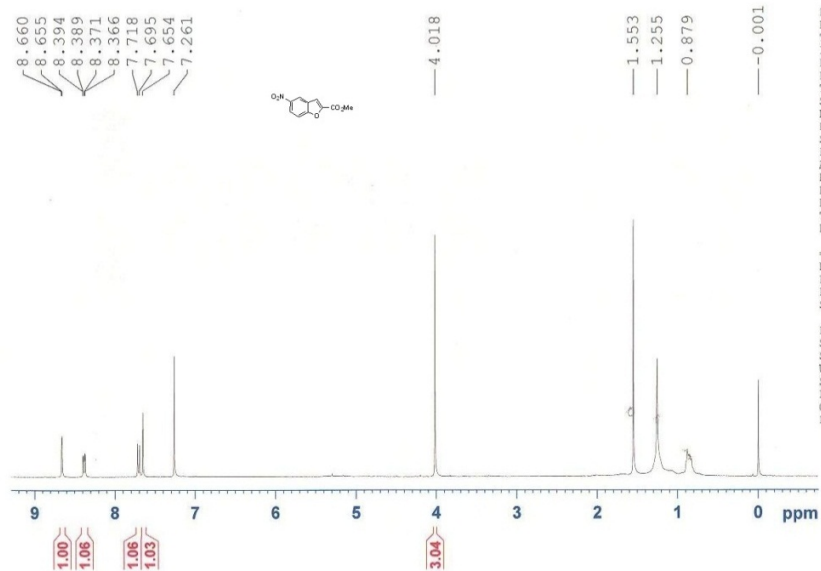


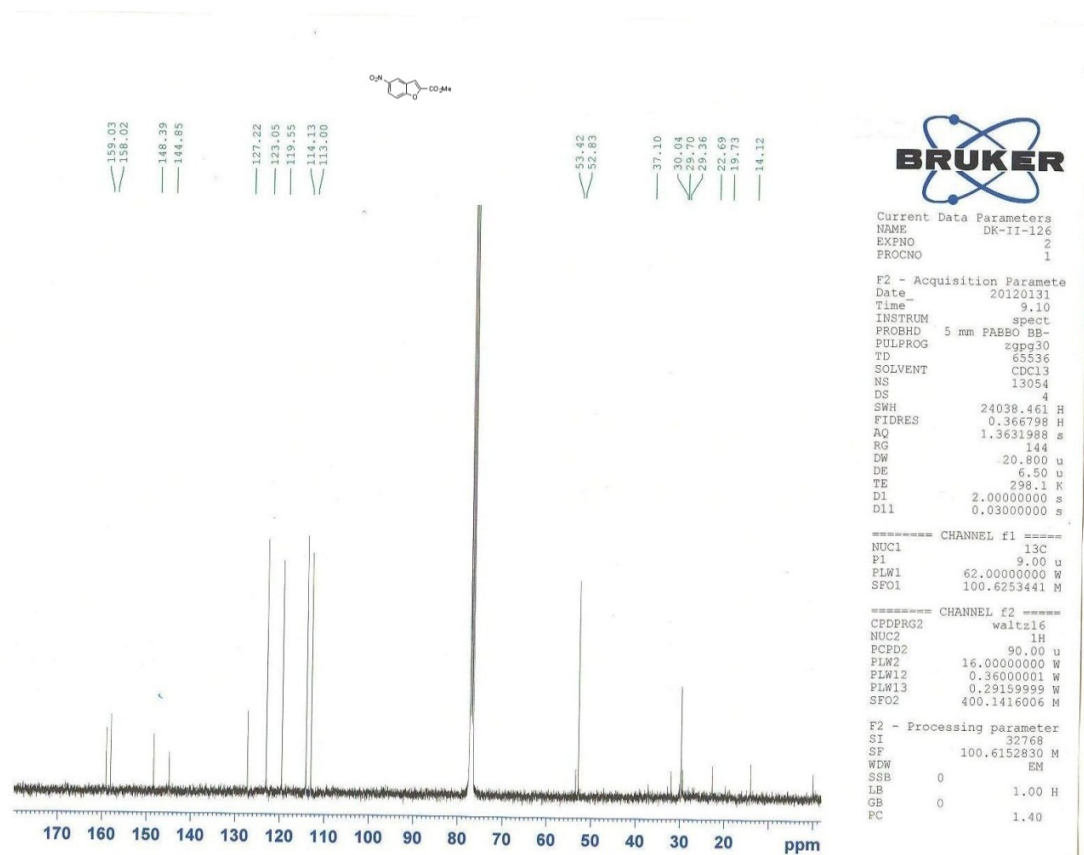
Current Data Parameters  
NAME DK-III-g5  
EXPNO 1  
PROCNO 1

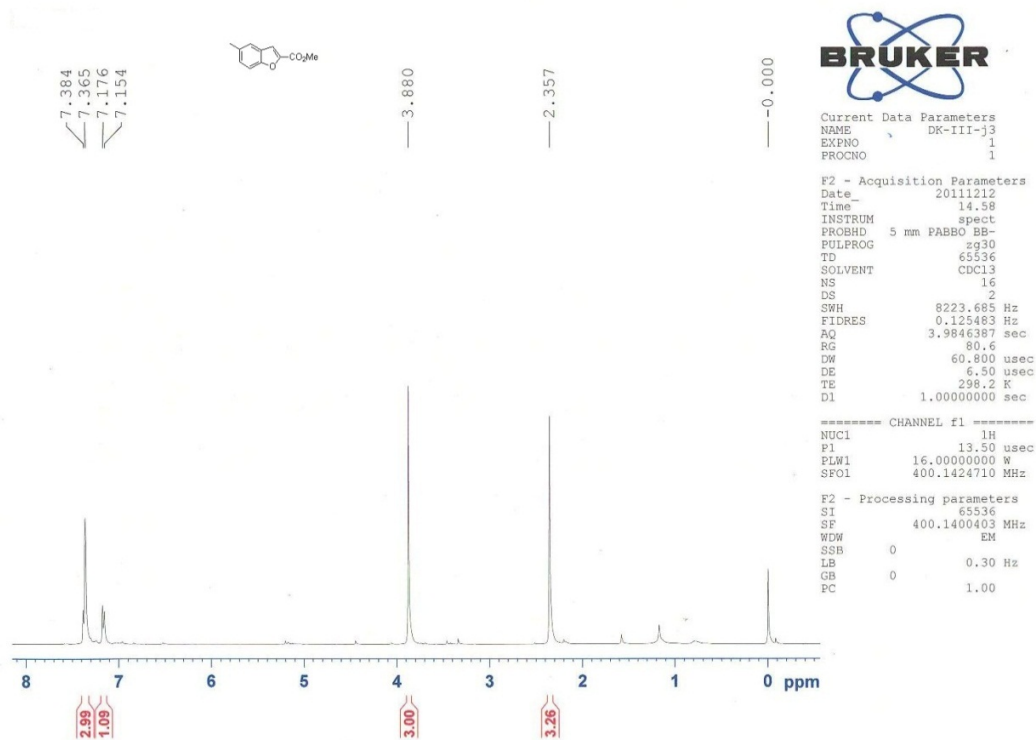
F2 - Acquisition Parameters  
Date\_ 20111229  
Time\_ 10.34  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 203  
DW 60.800 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec

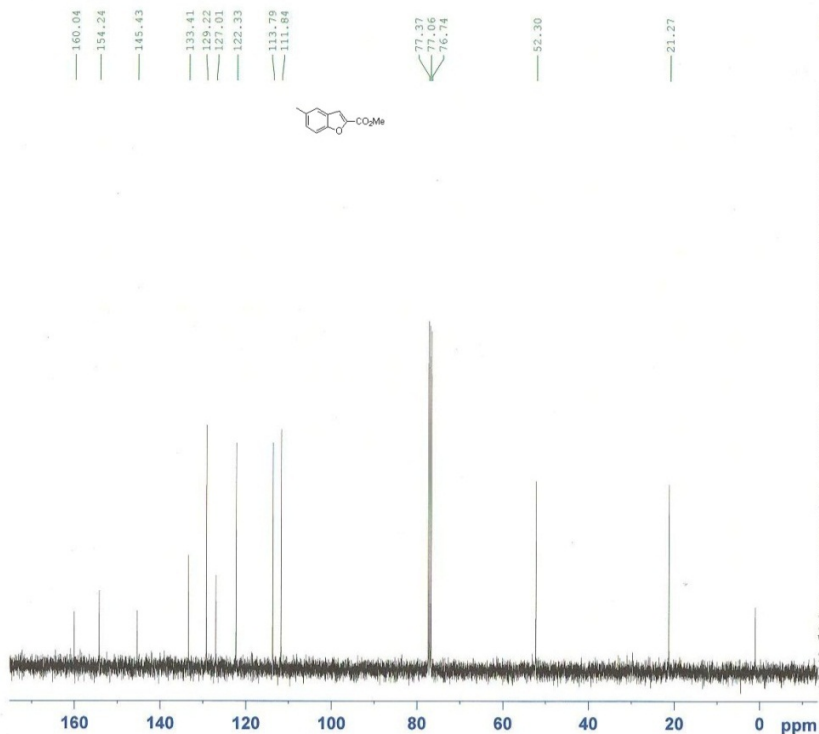
===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W  
SF01 400.1424710 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1400076 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00









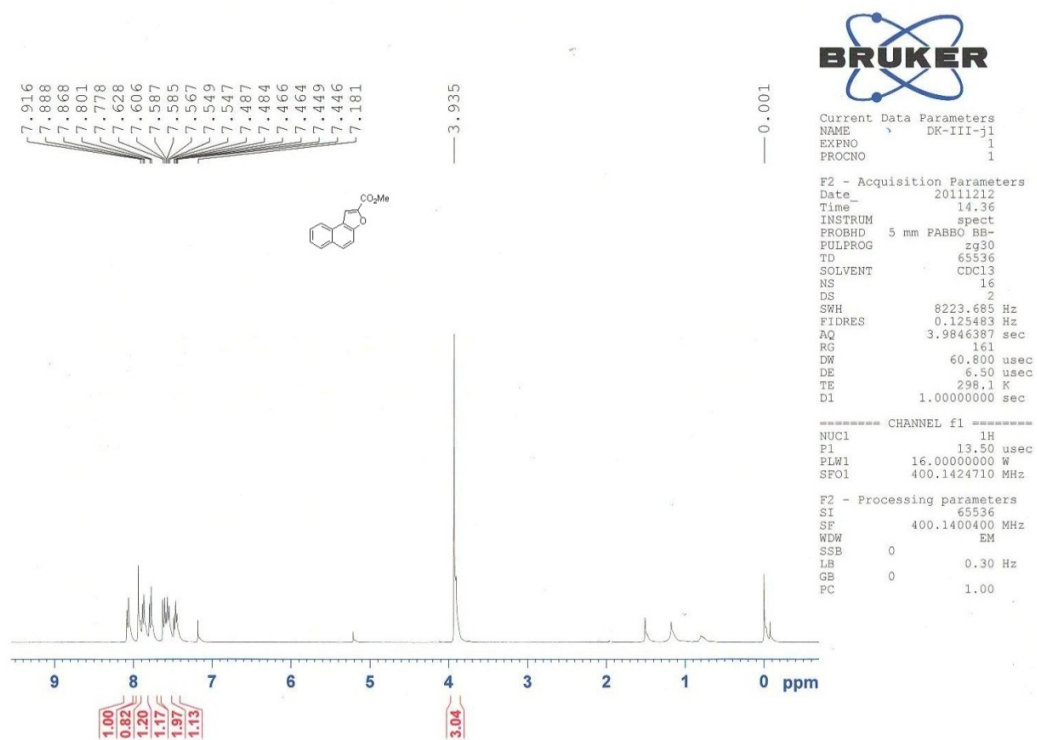
Current Data Parameters  
NAME DK-III-j4  
EXPNO 1  
PROCNO 1

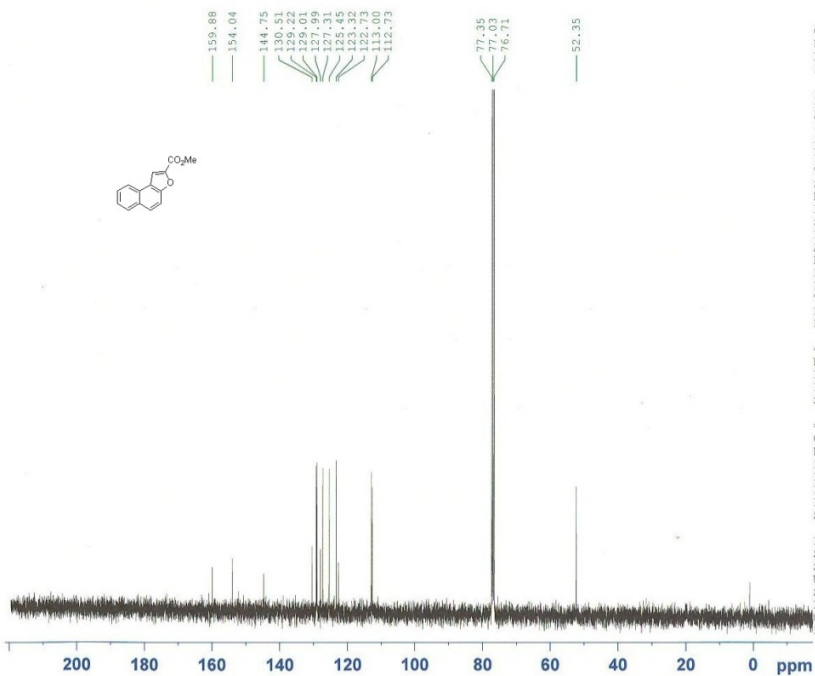
F2 - Acquisition Parameters  
Date\_ 20111212  
Time\_ 15.03  
INSTRUM spect  
PROBHD 5 mm FAPBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 38  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 161  
DW 20.800 usec  
DE 6.50 usec  
TE 298.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.00 usec  
PLW1 62.00000000 W  
SFO1 100.6253441 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 16.00000000 W  
PLW12 0.36000001 W  
PLW13 0.29159999 W  
SFO2 400.1416006 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6152830 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





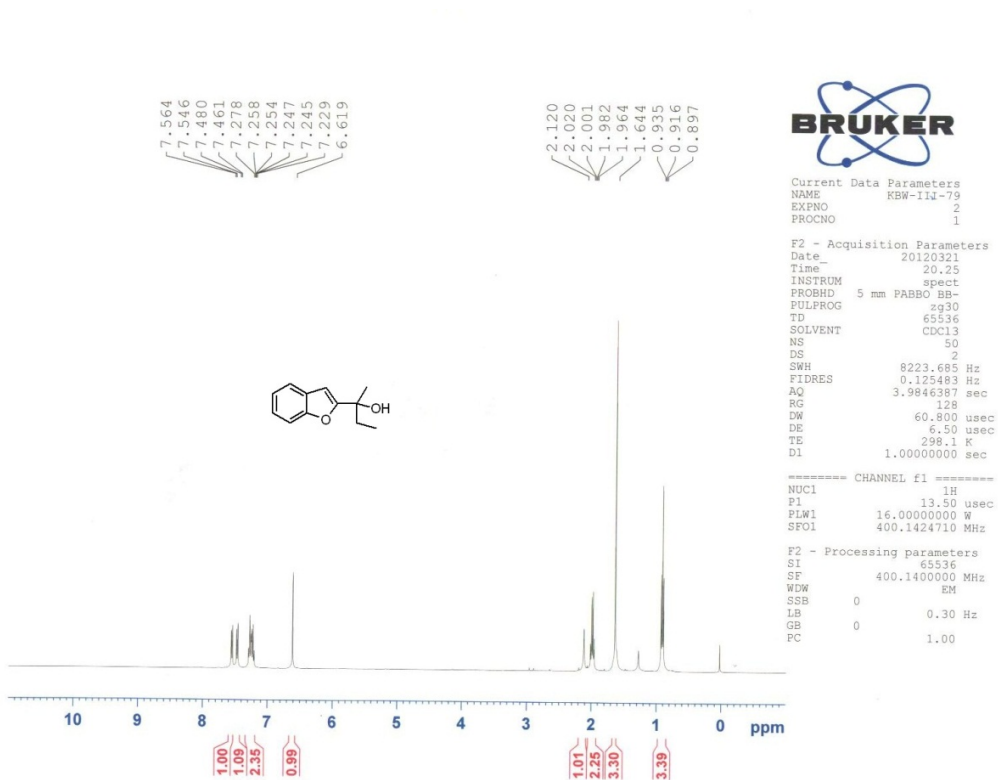
Current Data Parameters  
NAME DK-III-j2  
EXPNO 1  
PROCNO 1

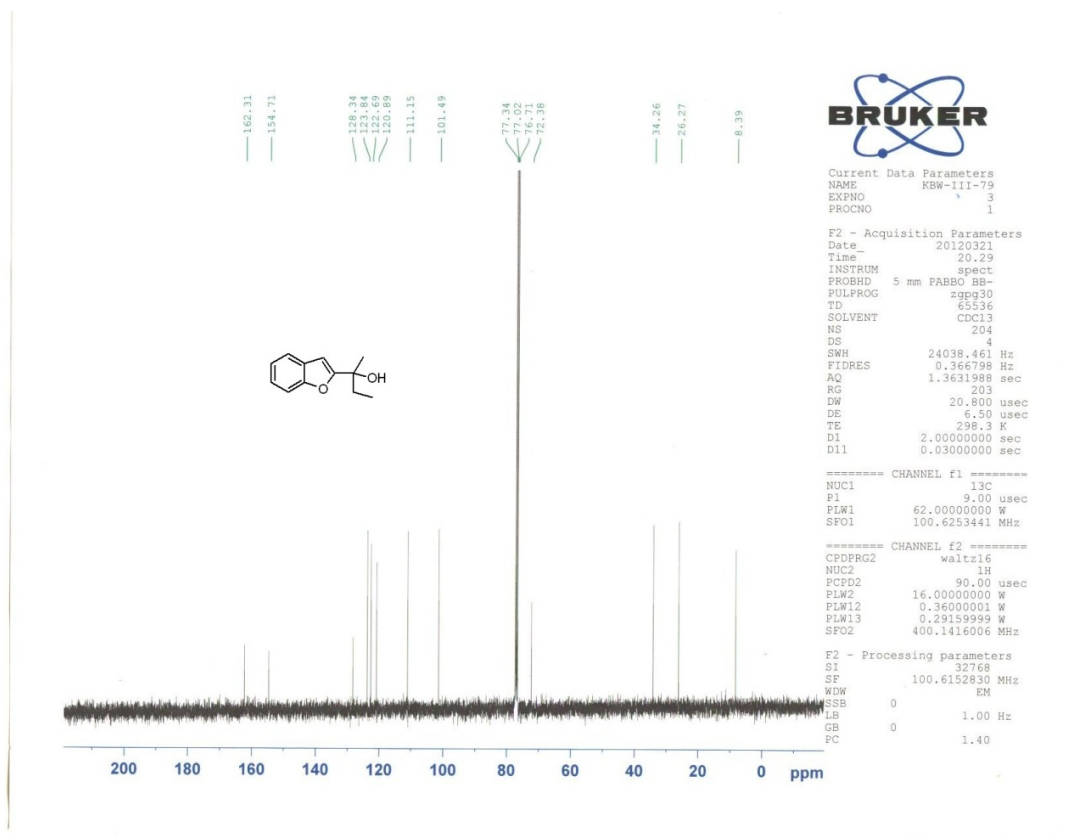
F2 - Acquisition Parameters  
Date\_ 20111212  
Time 14.42  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 184  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 161  
DW 20.800 usec  
DE 6.50 usec  
TE 298.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec

----- CHANNEL f1 -----  
NUC1 13C  
P1 9.00 usec  
PLW1 62.0000000 W  
SFO1 100.6253441 MHz

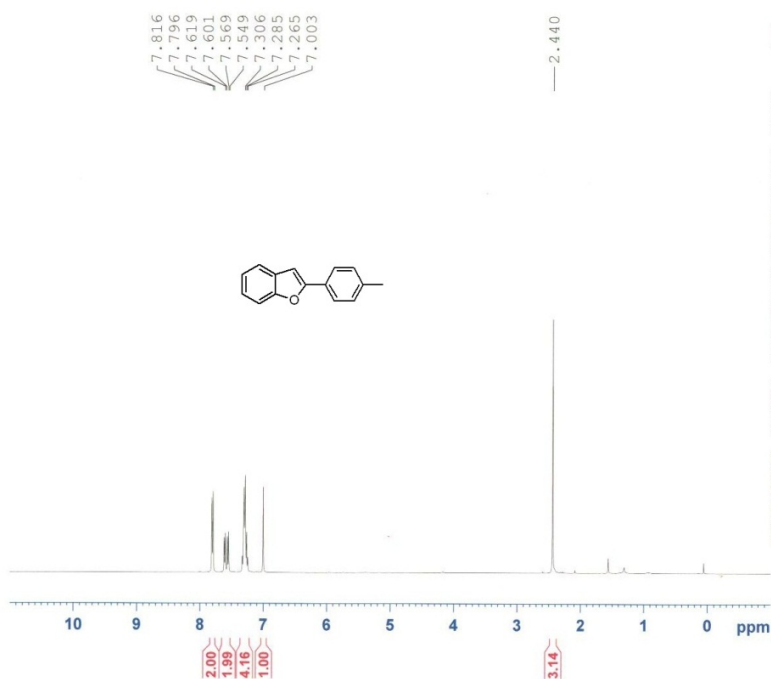
----- CHANNEL f2 -----  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 16.00000000 W  
PLW12 0.36000001 W  
PLW13 0.29159999 W  
SFO2 400.1416006 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6152830 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40







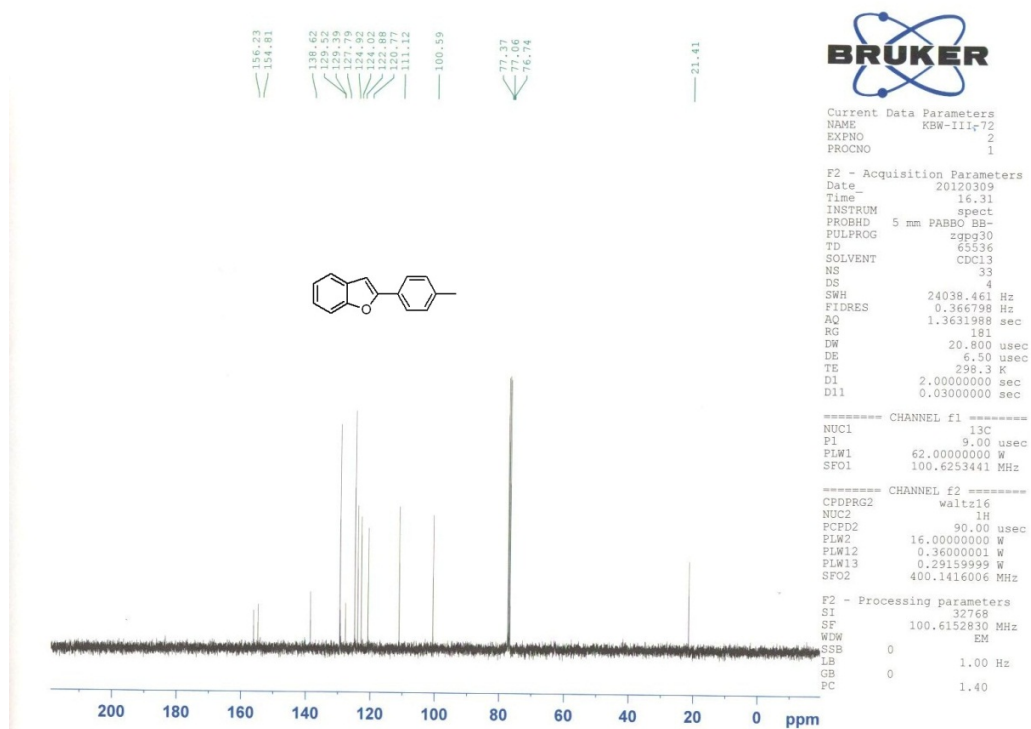


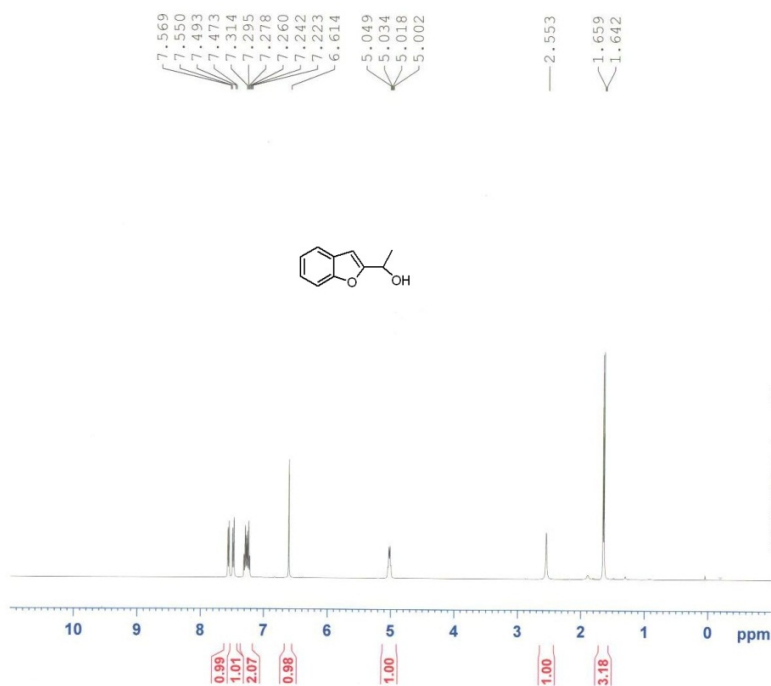
Current Data Parameters  
NAME KBW-III-72  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120309  
Time 16.26  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 6  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 90.5  
EW 60.800 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W  
SF01 400.1424710 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1400000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



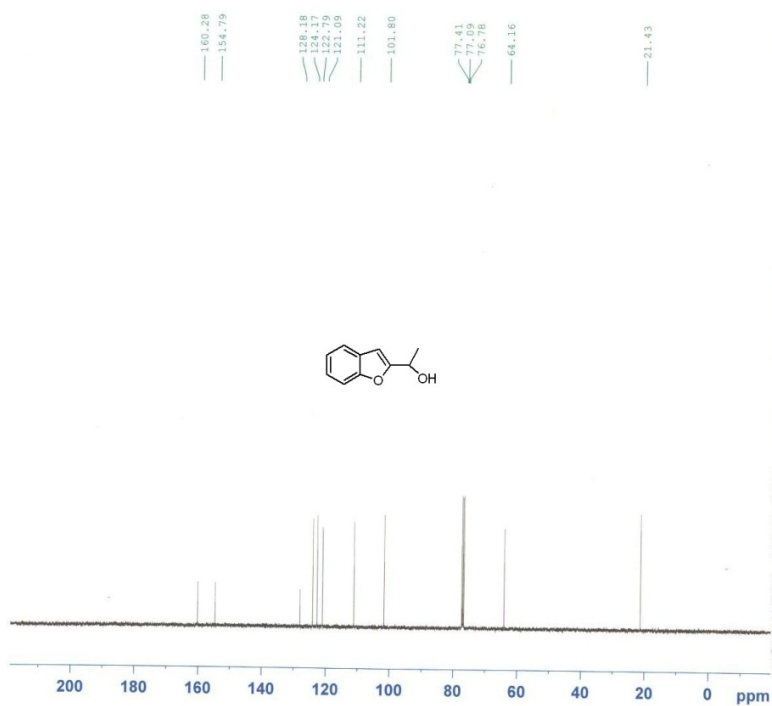


Current Data Parameters  
NAME KBW-III-75  
EXPNO 3  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120318  
Time 23.01  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 39  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
FQ 3.9846387 sec  
RG 32  
DW 60.800 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PLW1 16.0000000 W  
SF01 400.1424710 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1400000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



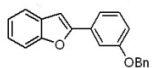
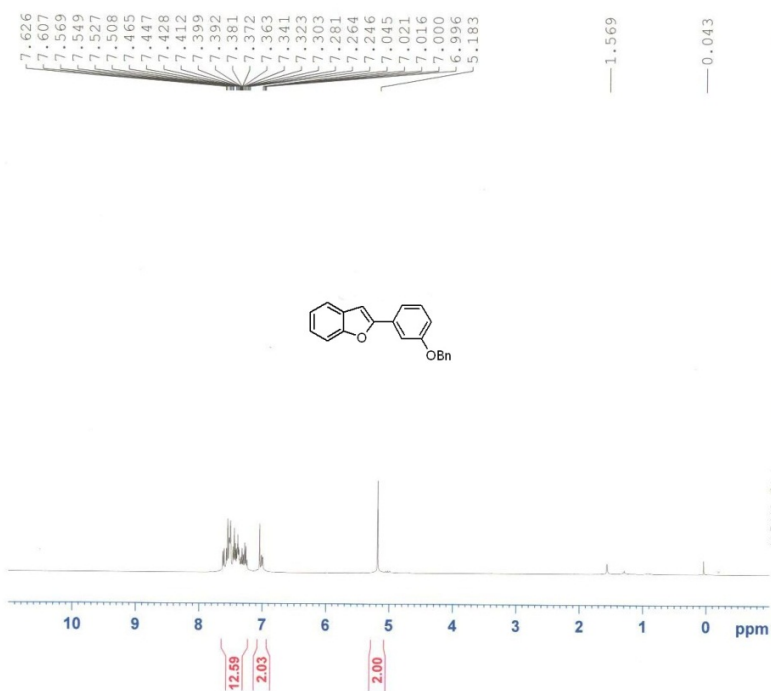
Current Data Parameters  
NAME KBW-111-75  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120318  
Time 23.05  
INSTRUM spect  
PROBHD 5 mm PABBO DP-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 41  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 203  
DW 20.800 usec  
DE 6.50 usec  
TE 298.4 K  
D1 2.0000000 sec  
D11 0.03000000 sec

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.00 usec  
PLW1 62.00000000 W  
SFO1 100.6253441 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 16.00000000 W  
PLW12 0.36000001 W  
PLW13 0.29159999 W  
SFO2 400.1416006 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6152630 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

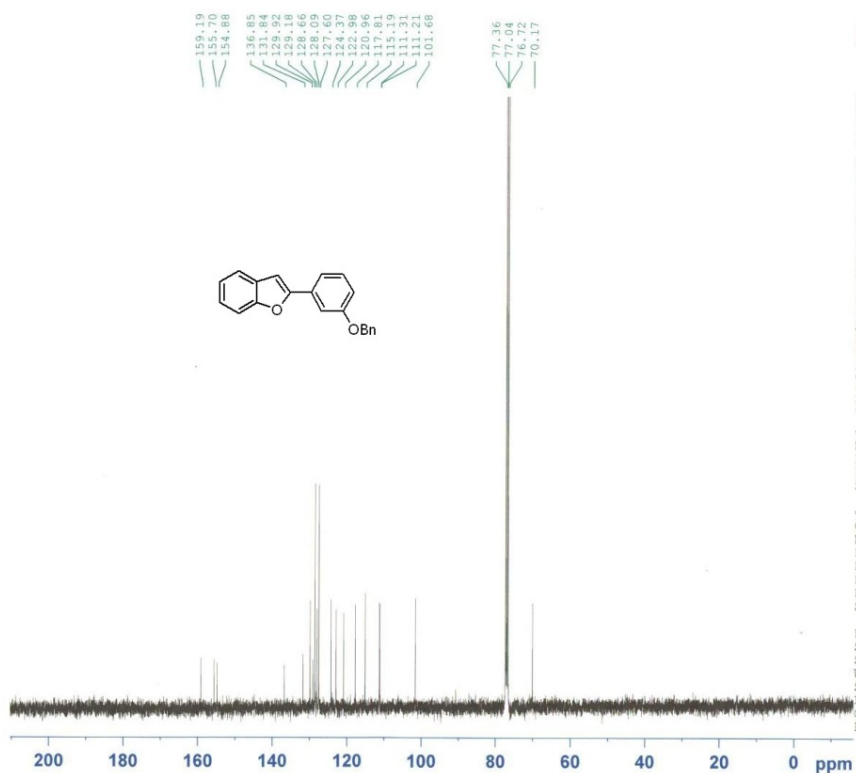


Current Data Parameters  
NAME KBW-IIJ-78  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120321  
Time 12.44  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 50  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 114  
DW 60.800 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec

----- CHANNEL f1 -----  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W  
SF01 400.1424710 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1400000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Current Data Parameters  
NAME KBW-III-78  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120321  
Time 12.52  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 127  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 203  
DW 20.800 usec  
DE 6.50 usec  
TE 298.1 K  
D1 2.0000000 sec  
D11 0.0300000 sec

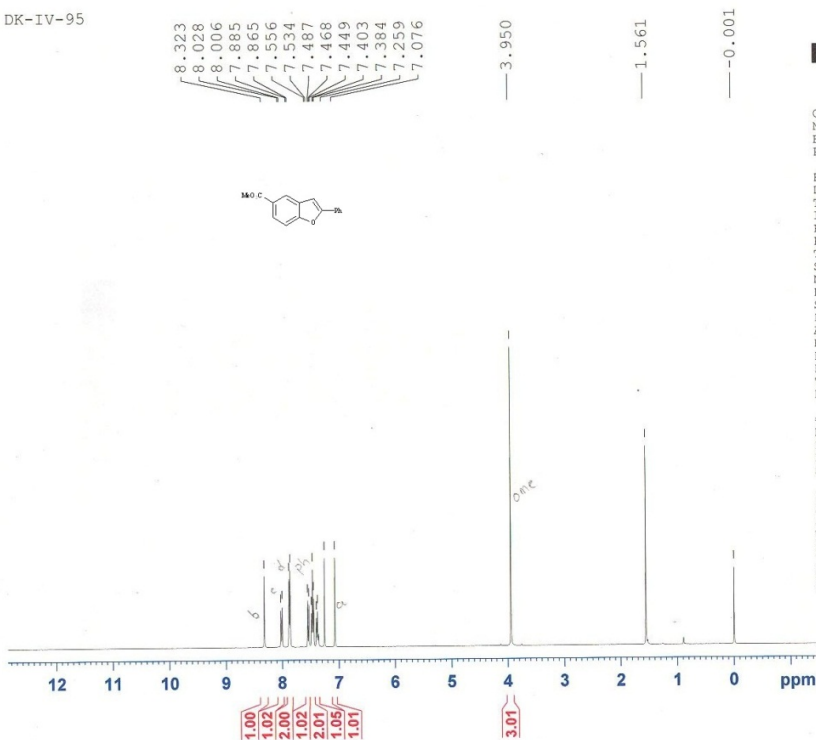
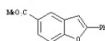
===== CHANNEL f1 =====  
NUC1 13C  
P1 9.00 usec  
PLW1 62.00000000 W  
SFO1 100.6253441 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 16.00000000 W  
PLW12 0.36000001 W  
PLW13 0.29159999 W  
SFO2 400.1416006 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6152830 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

DK-IV-95

8.323  
8.028  
8.006  
7.885  
7.865  
7.556  
7.534  
7.487  
7.468  
7.449  
7.403  
7.384  
7.259  
7.076



Current Data Parameters  
NAME DK-IV-95  
EXPNO 1  
PROCNO 1

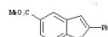
F2 - Acquisition Parameters  
Date\_ 20120116  
Time 12:02  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 6536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.885 Hz  
FIDRES 0.12583 Hz  
AQ 3.984687 sec  
RG 403  
DW 60.800 usec  
DE 6.50 usec  
TE 298.2 K  
D1 1.0000000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PLW1 16.0000000 W  
SFO1 400.1424710 MHz

F2 - Processing parameters  
SI 6536  
SF 400.140080 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

DK-IV-96a

167.30  
157.43  
157.40  
129.89  
129.25  
129.04  
128.08  
125.34  
125.08  
123.31  
111.00  
101.52



77.33  
77.02  
76.10  
53.42  
52.11  
31.59  
22.65  
14.11



Current Data Parameters  
NAME DK-IV-96a  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120519  
Time 22.48  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 867  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 128  
DW 20.800 usec  
DE 6.50 usec  
TE 298.9 K  
D1 2.0000000 sec  
D11 0.03000000 sec

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.00 usec  
PLW1 62.00000000 W  
SF01 100.6253441 MHz

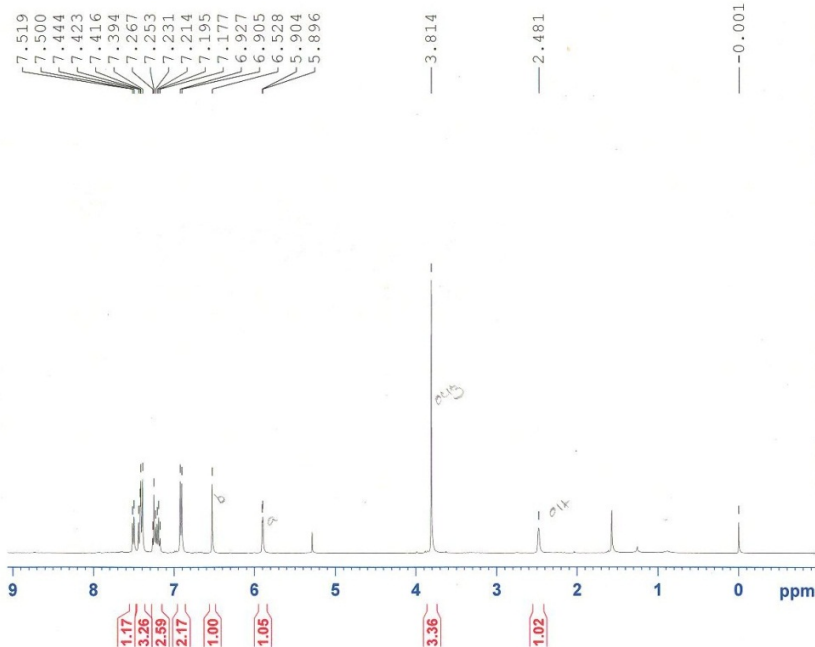
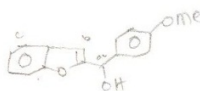
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 16.00000000 W  
PLW12 0.36000001 W  
PLW13 0.29159999 W  
SFO2 400.1416006 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6152830 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





DK-IV-98



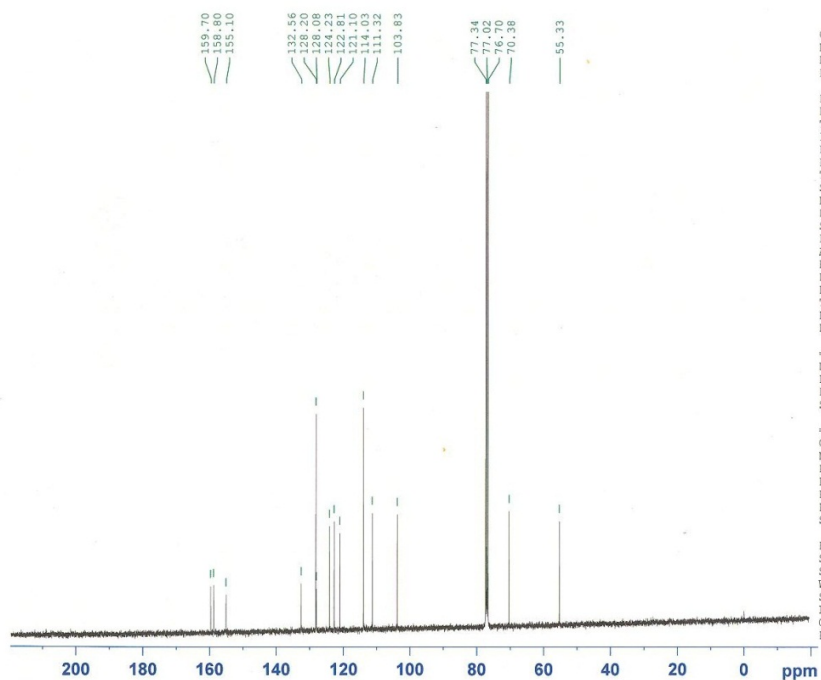
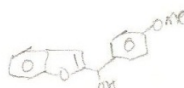
Current Data Parameters  
NAME DK-IV-98  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120519  
Time\_ 23.44  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.635 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 181  
DW 60.800 usec  
DE 6.50 usec  
TE 298.15 K  
D1 1.00000000 sec

----- CHANNEL f1 -----  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W  
SF01 400.1424710 MHz

F2 - Processing parameters  
SI 65586  
SF 400.1400108 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

DK-IV-98a



Current Data Parameters  
NAME DK-IV-98a  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120519  
Time\_ 23.52  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 128  
DW 20.800 usec  
DE 6.50 usec  
TE 298.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec

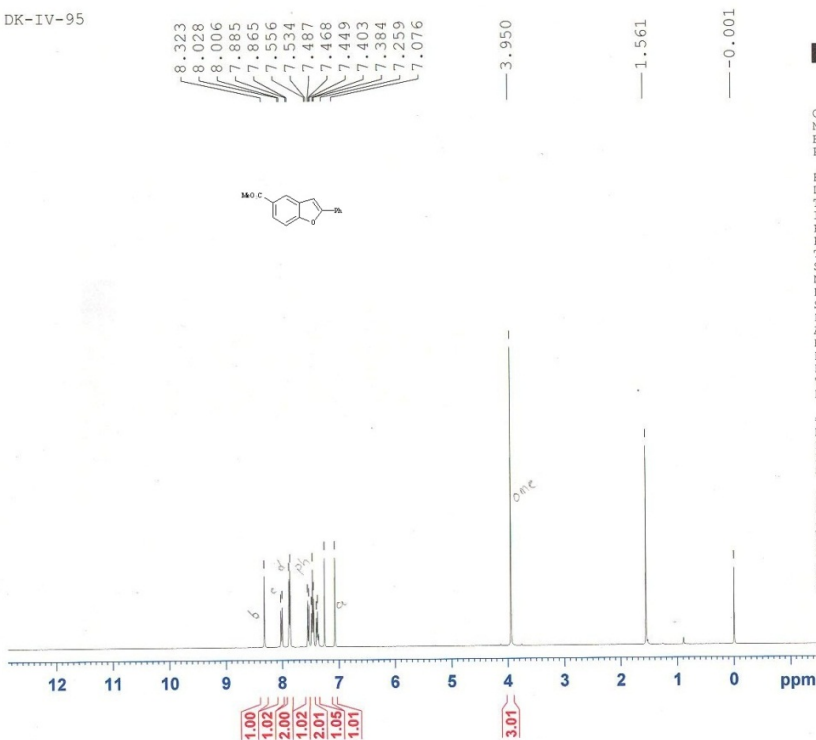
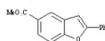
===== CHANNEL f1 =====  
NUC1 13C  
P1 9.00 usec  
PLW1 62.00000000 W  
SFO1 100.6253441 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 16.00000000 W  
PLW12 0.36000001 W  
PLW13 0.29159999 W  
SFO2 400.1416006 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6152830 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

DK-IV-95

8.323  
8.028  
8.006  
7.885  
7.865  
7.556  
7.534  
7.487  
7.468  
7.449  
7.403  
7.384  
7.259  
7.076



Current Data Parameters  
NAME DK-IV-95  
EXPNO 1  
PROCNO 1

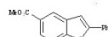
F2 - Acquisition Parameters  
Date\_ 20120116  
Time 12:02  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 6536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.885 Hz  
FIDRES 0.12583 Hz  
AQ 3.984687 sec  
RG 403  
DW 60.800 usec  
DE 6.50 usec  
TE 298.2 K  
D1 1.00000000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W  
SFO1 400.1424710 MHz

F2 - Processing parameters  
SI 6536  
SF 400.140080 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

DK-IV-96a

167.30  
157.43  
157.40  
129.89  
129.25  
129.04  
128.08  
125.34  
125.08  
123.31  
111.00  
101.52



77.33  
77.02  
76.10  
53.42  
52.11  
31.59  
22.65  
14.11



Current Data Parameters  
NAME DK-IV-96a  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120519  
Time 22.48  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 867  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 128  
DW 20.800 usec  
DE 6.50 usec  
TE 298.9 K  
D1 2.0000000 sec  
D11 0.03000000 sec

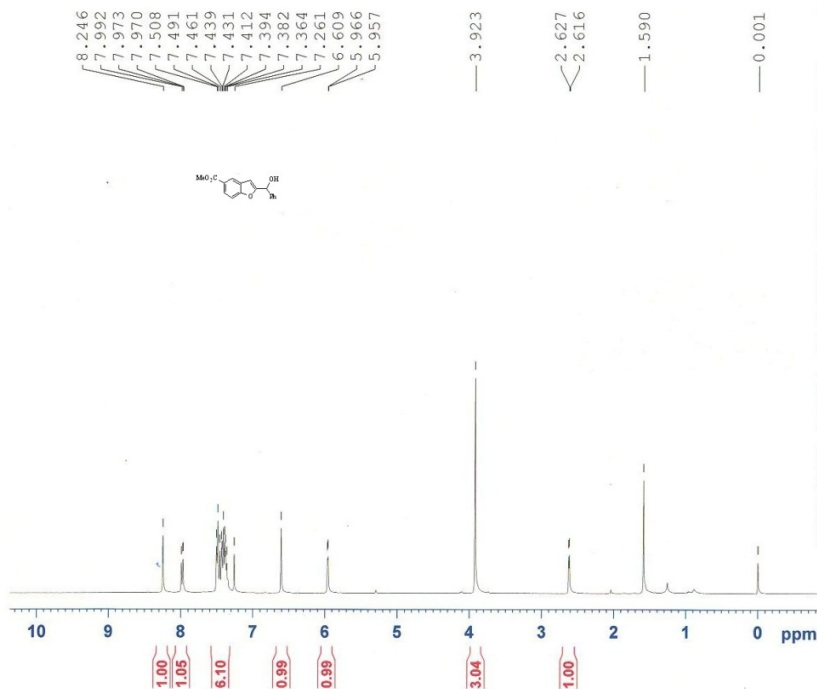
==== CHANNEL f1 =====  
NUC1 13C  
P1 9.00 usec  
PLW1 62.00000000 W  
SF01 100.6253441 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 16.00000000 W  
PLW12 0.36000001 W  
PLW13 0.29159999 W  
SFO2 400.1416006 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6152830 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

DK-IV-105



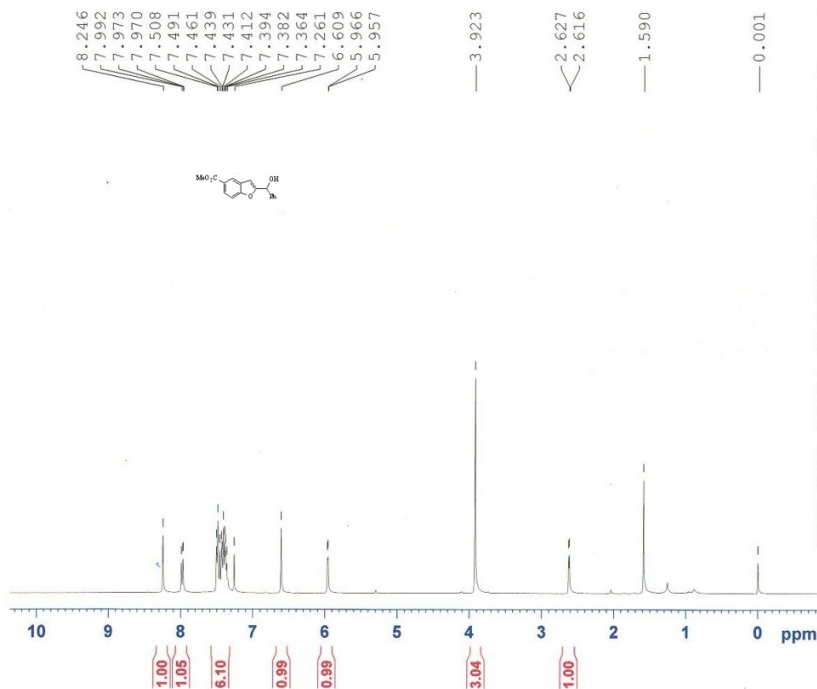
Current Data Parameters  
NAME DK-IV-105  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120523  
Time 13.20  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 181  
DW 60.800 usec  
DE 6.50 usec  
TE 298.3 K  
D1 1.00000000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W  
SF01 400.1424710 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1400075 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

DK-IV-105



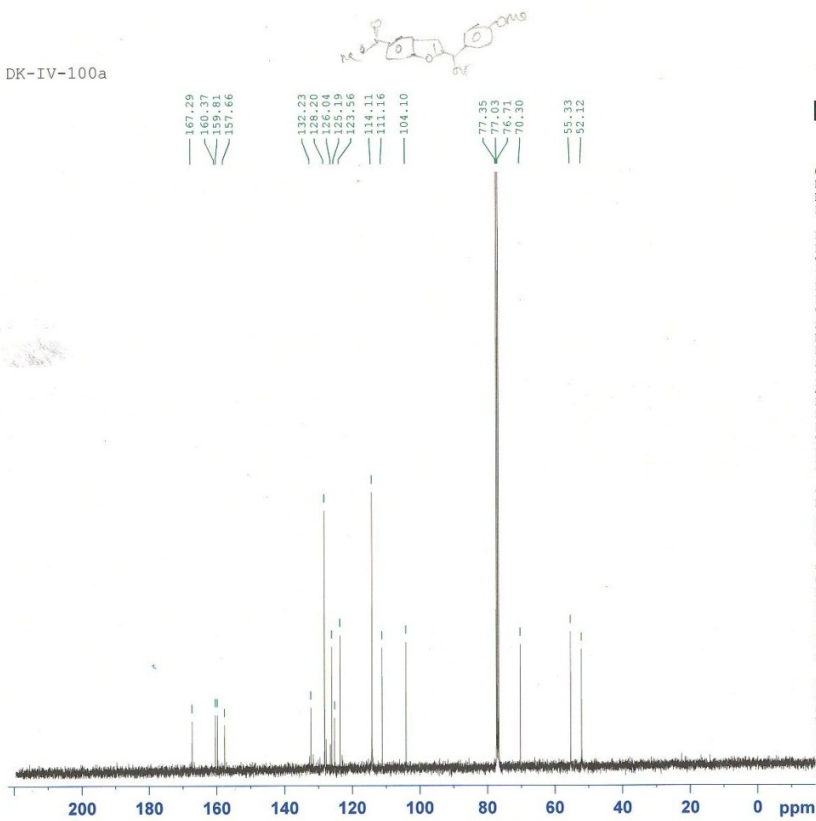
Current Data Parameters  
NAME DK-IV-105  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120523  
Time 13.20  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 181  
DW 60.800 usec  
DE 6.50 usec  
TE 298.3 K  
D1 1.00000000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W  
SF01 400.1424710 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1400075 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

DK-IV-100a



Current Data Parameters  
NAME DK-IV-100a  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120520  
Time 1.25  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 343  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 80.6  
DW 20.800 usec  
DE 6.50 usec  
TE 298.6 K  
D1 2.0000000 sec  
D11 0.03000000 sec

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.00 usec  
PLW1 62.00000000 W  
SFO1 100.6253441 MHz

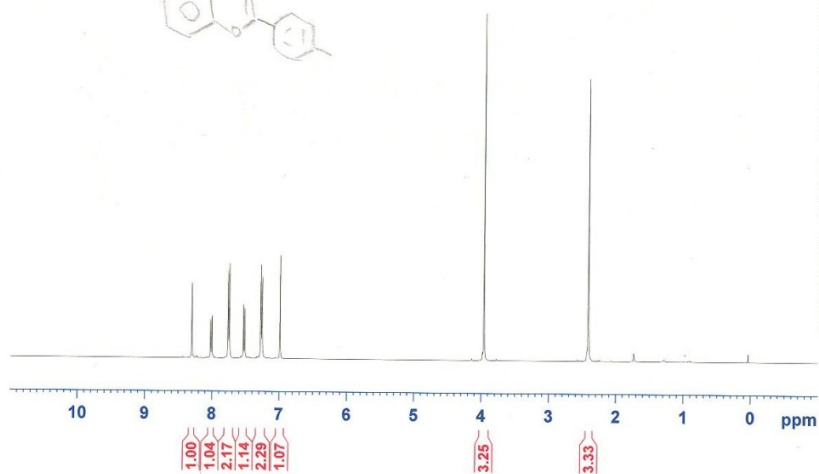
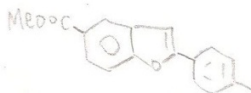
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 16.00000000 W  
PLW12 0.36000001 W  
PLW13 0.29159999 W  
SFO2 400.1416006 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6152830 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

KBW-III-99H

8.303  
8.026  
8.004  
7.767  
7.747  
7.538  
7.517  
7.279  
7.260  
6.991

2.416



Current Data Parameters  
NAME KBW-III-99  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date 20120521  
Time 10.53  
INSTRUM spect  
PROBHD 5 mm FAPBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 6  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 57  
DW 60.800 usec  
DE 6.50 usec  
TE 298.2 K  
D1 1.00000000 sec

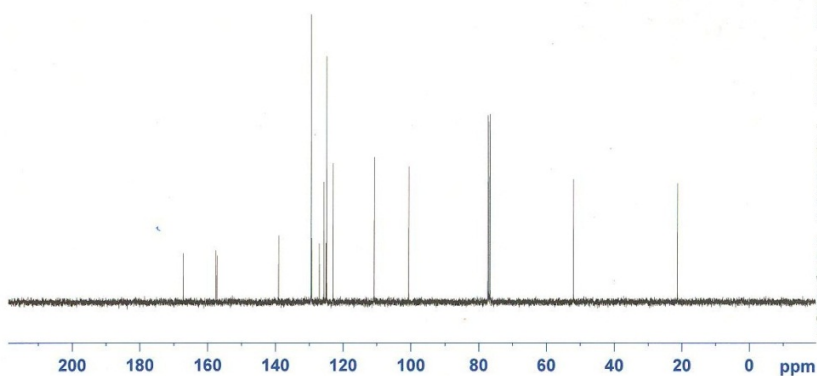
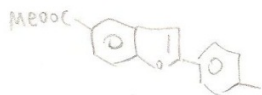
===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W  
SFO1 400.1424710 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1400000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



100  
KBW-III-99C

167.33  
157.64  
157.31  
139.14  
129.57  
129.38  
129.28  
125.81  
125.23  
125.01  
123.12  
110.89  
100.75  
77.40  
77.08  
76.76  
52.08  
21.41



Current Data Parameters  
NAME KBW-III-99  
EXPO 2  
PROCNO 1

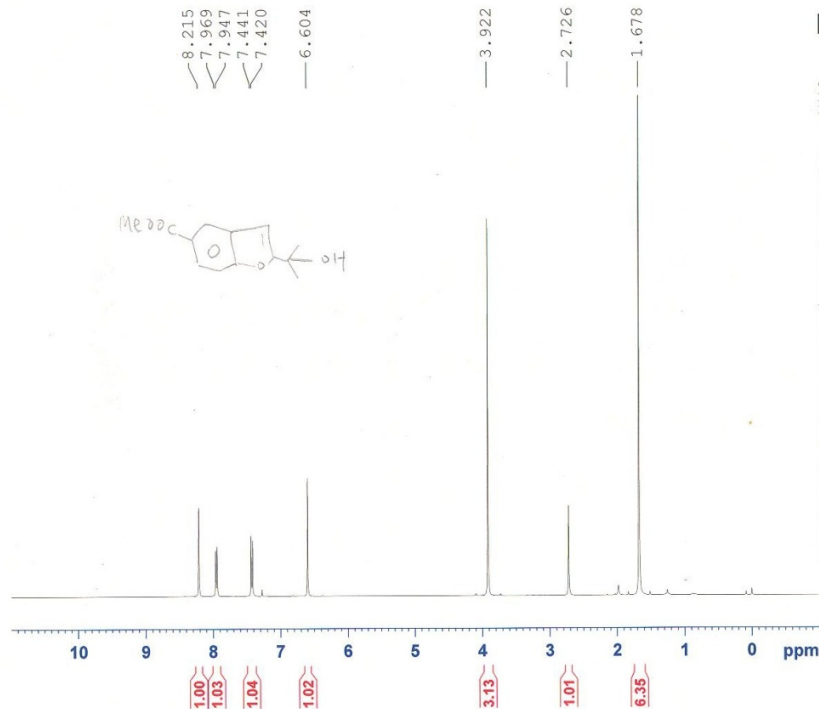
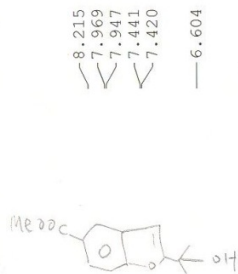
F2 - Acquisition Parameters  
Date\_ 20120521  
Time 10.57  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 25  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 181  
DW 20.800 usec  
DE 6.50 usec  
TE 298.7 K  
D1 2.00000000 sec  
D11 0.03000000 sec

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.00 usec  
PLW1 62.00000000 W  
SFO1 100.6253441 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 16.00000000 W  
PLW12 0.36000001 W  
PLW13 0.29159999 W  
SFO2 400.1416006 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6152830 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

KBW-III-102H



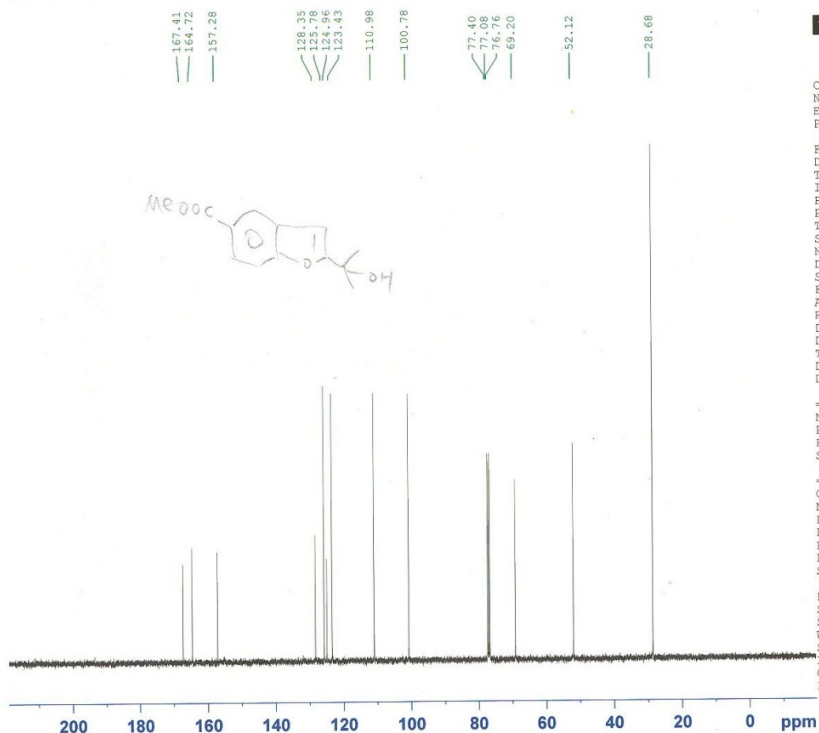
Current Data Parameters  
NAME KBW-III-102  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120522  
Time\_ 16:05  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 6536  
SOLVENT CDCl3  
NS 9  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846897 sec  
RG 32  
DW 60.800 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W  
SF01 400.1424710 MHz

F2 - Processing parameters  
SI 6536  
SF 400.1400000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

KBW-III-102C



Current Data Parameters  
NAME KBW-III-102  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120522  
Time 16.09  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 74  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 203  
DW 20.800 usec  
DE 6.50 usec  
TE 298.7 K  
D1 2.0000000 sec  
D11 0.0300000 sec

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.00 usec  
PLW1 62.0000000 W  
SFO1 100.6253441 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 16.0000000 W  
PLW12 0.3600000 W  
PLW13 0.2915999 W  
SFO2 400.1416006 MHz

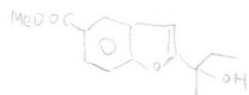
F2 - Processing parameters  
SI 32768  
SF 100.6152830 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

KBW-III-103H

8.260  
7.993  
7.972  
7.470  
7.448  
6.659

3.942

2.322  
1.988  
1.970  
1.638  
0.924  
0.905  
0.887



Current Data Parameters  
NAME KBW-III-103  
EXNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date 20120521  
Time 15.20  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 12  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 71.8  
DW 60.800 usec  
DE 6.50 usec  
TE 298.2 K  
D1 1.00000000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W  
SFO1 400.1424710 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1400000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



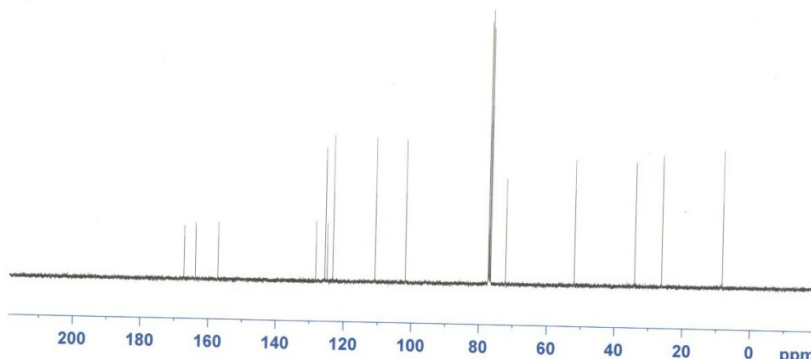
1.00  
1.04  
1.02  
1.03

3.15

1.02  
2.14  
3.25  
3.28

KBW-III-103C

167.36  
163.98  
157.32  
128.37  
125.70  
123.04  
123.55  
110.97  
101.95  
77.36  
76.72  
72.31  
52.10  
34.17  
26.24  
8.31



Current Data Parameters  
NAME KBW-III-103  
EXPCNO 2  
PROCNO 1

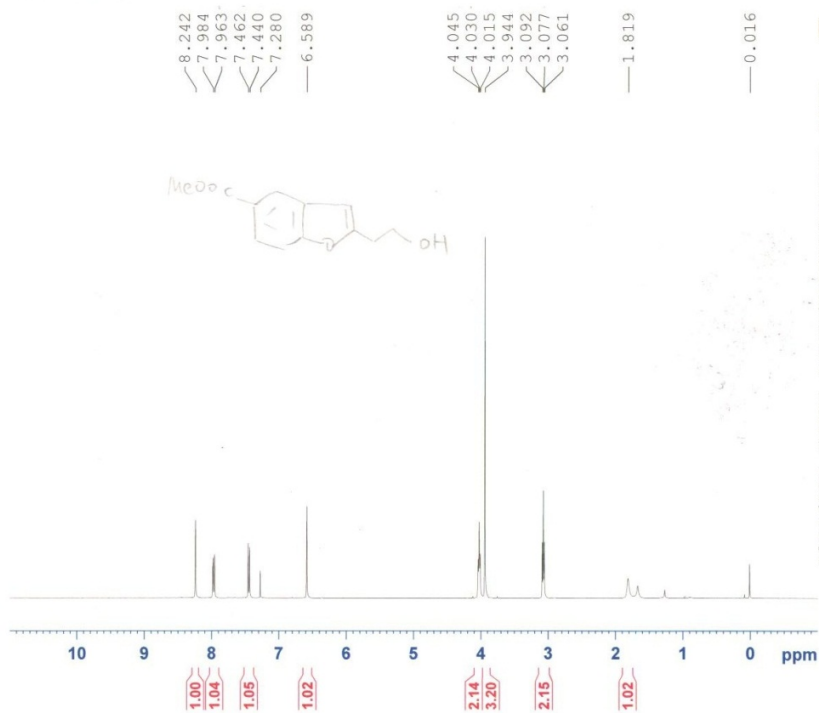
F2 - Acquisition Parameters  
Date 20120521  
Time 15.31  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 148  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 181  
DW 20.800 usec  
DE 6.50 usec  
TE 299.1 K  
D1 2.0000000 sec  
D11 0.0300000 sec

==== CHANNEL f1 =====  
NUC1 13C  
PI 9.00 usec  
PLW1 62.0000000 W  
SFO1 100.6253441 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 16.0000000 W  
PLW12 0.36000001 W  
PLW13 0.29159999 W  
SFO2 400.1416006 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6152830 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

KBW-III-101H



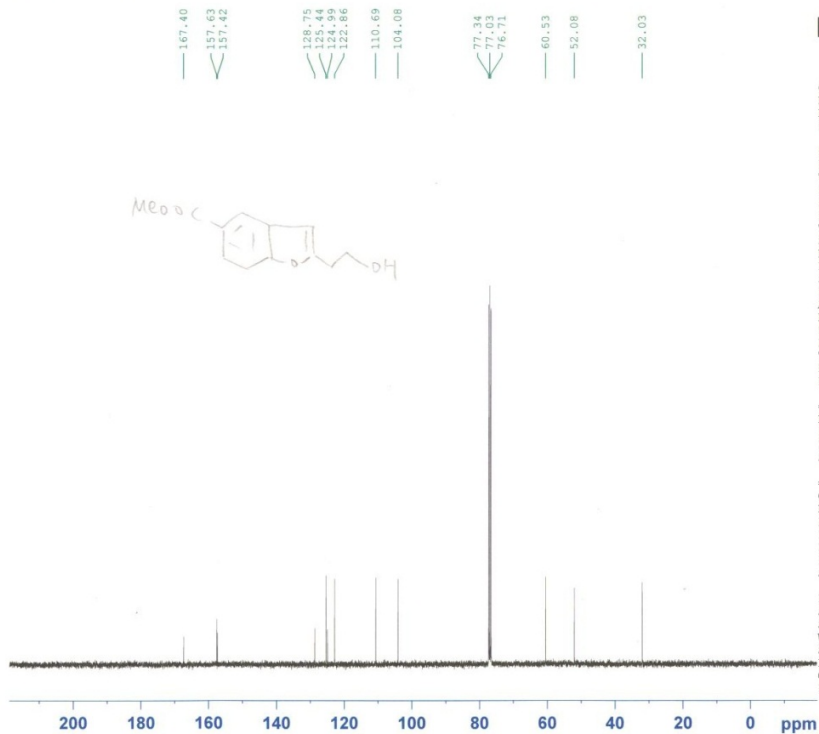
Current Data Parameters  
NAME KBW-III-101  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120518  
Time 18.07  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 14  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9846387 sec  
RG 144  
DW 60.800 usec  
DE 6.50 usec  
TE 298.4 K  
D1 1.00000000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PLW1 16.00000000 W  
SFO1 400.1424710 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1400000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

KBW-III-101C



Current Data Parameters  
NAME KBW-III-101  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120518  
Time 18.13  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 128  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 71.8  
DW 20.800 usec  
DE 6.50 usec  
TE 299.2 K  
D1 2.0000000 sec  
D11 0.0300000 sec

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.00 usec  
PLW1 62.00000000 W  
SFO1 100.6253441 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 16.00000000 W  
PLW12 0.36000001 W  
PLW13 0.29159999 W  
SFO2 400.1416006 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6152830 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40