Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Highly Chemoselective Hydrogenation of Cyclic Imides to ω-hydroxylactams or ω-hydroxyamides Catalysed by Iridium Catalysts

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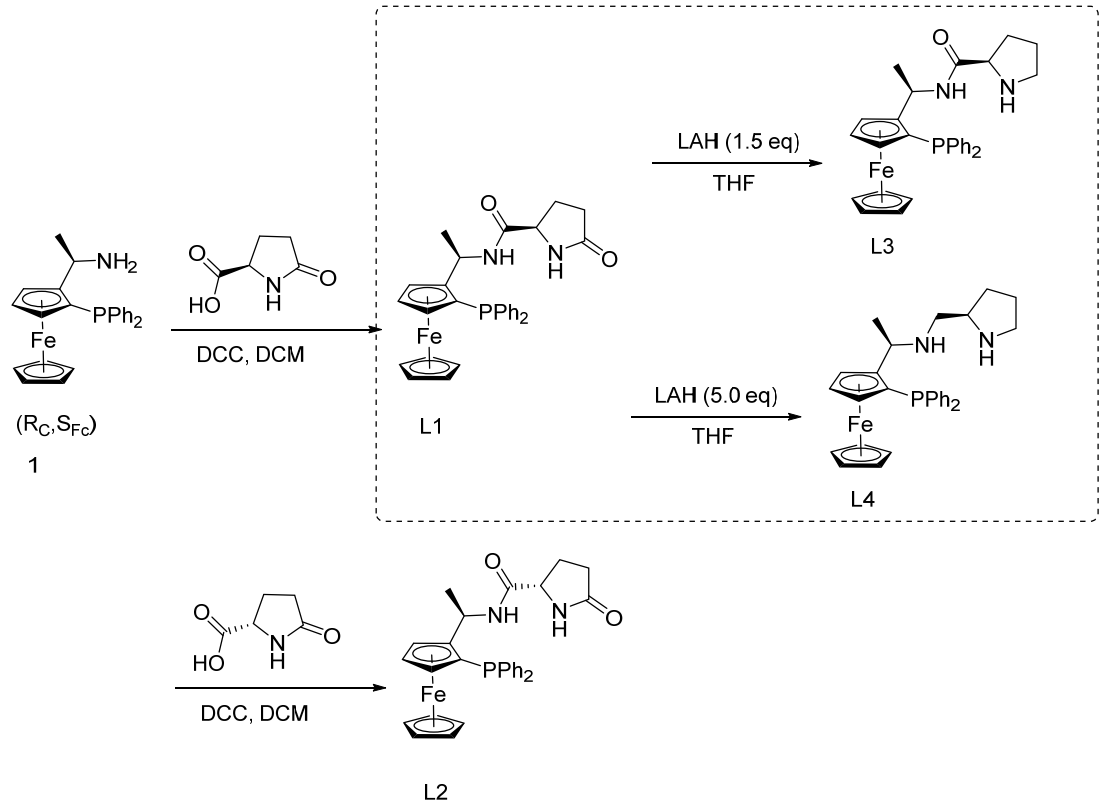
Supporting Information

Content

1. General Information

Unless otherwise mentioned, all experiments were carried out under an atmosphere of argon in a glovebox or using standard Schlenk techniques. Solvents were dried with standard procedures and degassed with Ar_2. Flash column chromatography was performed using Tsingdao silica gel (60, particle size 300-400 mesh). NMR spectra were recorded on a Bruker DPX 400 spectrometer at 400 MHz for ^{1}H NMR, 101 MHz for ^{13}C NMR and 162 MHz for ^{31}P NMR or a Bruker DPX 600 spectrometer at 600 MHz for ^{1}H NMR, 150 MHz for ^{13}C NMR in $CDCl_3$, DMSO-*d6* and CD_3OD with tetramethylsilane (TMS) as internal standard. Chemical shifts are reported in ppm and coupling constants are given in Hz.

2. General procedure for synthesis of L1-4 Ligands



The chiral ferrocenyl aminophosphine compound 1 (R_C, S_{FC}) was prepared according to the procedure of literatures. The synthesis of L1-L4 were based on the literatures.[1]

To a solution of chiral ferrocenyl aminophosphine compound 1 (3.0 mmol) and 5-oxopyrrolidine-2-carboxylic acid (3.0 mmol) in anhydrous DCM (50.0 mL) was added DCC (3.3 mmol) at rt. The reaction mixture obtained was stirred at rt for 5 h (monitored by TLC). After completion of the reaction, filter with diatomite, remove the solvent under the vacuum, the mixture was diluted with water and extracted with ethyl acetate. The organic layer was dried with anhydrous Na_2SO_4 and concentrated in vacuo to afford the crude product. After chromatography on silica-gel column (CH_2Cl_2/MeOH = 100/1 to 20/1), the corresponding were obtained.

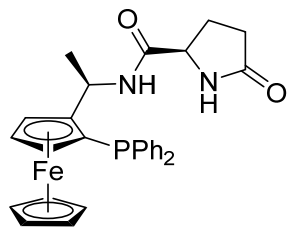
The following ligands can be obtained by adding different equivalent of lithium aluminum hydride to reduce one amide or two amides.

To a solution of L1 (1.0 mmol) in anhydrous THF (50.0 mL) at 0 ^oC was added LAH (1.5 mmol) under a nitrogen atmosphere. After 30min, move to 60 ^oC stirred for

3h (monitored by TLC). After completion of the reaction, quenched with saturated ammonium chloride and extracted with ethyl acetate. The organic layer was dried with anhydrous Na_2SO_4 and concentrated in vacuo to afford the crude product. After chromatography on silica-gel column (CH_2Cl_2/MeOH = 50/1 to 20/1), the corresponding were obtained.

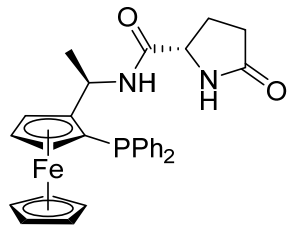
To a solution of L1(1.0 mmol) in anhydrous THF (50.0 mL) at 0 ^oC was added LAH (5.0 mmol) under a nitrogen atmosphere. After 30min, move to 80 ^oC stirred for 2h (monitored by TLC). After completion of the reaction, quenched with saturated ammonium chloride and extracted with ethyl acetate. The organic layer was dried with anhydrous Na_2SO_4 and concentrated in vacuo to afford the crude product. After chromatography on silica-gel column (CH_2Cl_2/MeOH = 30/1 to 10/1), the corresponding ere obtained with moderate yields.

L1



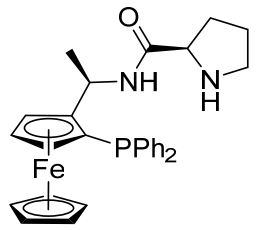
Yellow foam, 92% yield, ^1H NMR (400 MHz, $CDCl_3$) δ 7.50-7.46 (m, 2H), 7.36-7.35 (m, 6H), 7.32-7.29 (m, 2H), 5.68 (d, *J* = 4.0 Hz, 1H), 5.39-5.35 (m, 1H), 4.50 (s, 1H), 4.35-4.33 (m, 1H), 4.05 (s, 5H), 3.96 (s, 1H), 3.84 (s, 1H), 3.39-3.36 (m, 1H), 2.33-2.25 (m, 1H), 2.16-2.09 (m, 2H), 1.93-1.85 (m, 1H), 1.471 (d, *J* = 4.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 178.48, 169.35, 140.72 (d, *J* = 12.0 Hz), 140.13 (d, *J* = 9.1 Hz), 134.81 (d, *J* = 21.0 Hz), 133.13 (d, *J* = 19.0 Hz), 129.20, 128.80, 128.52 (d, *J* = 6.0 Hz), 128.18 (d, *J* = 8.0 Hz), 93.26 (d, *J* = 25.3 Hz), 75.92 (d, *J* = 9.1 Hz), 72.27 (d, *J* = 5.1 Hz), 69.94, 69.75 (d, *J* = 4.0 Hz), 69.28, 56.56, 44.16 (d, *J* = 9.1 Hz), 28.78, 25.94, 19.80; ^{31}P NMR (101 MHz, $CDCl_3$) δ -27.30; HRMS (ESI) calcd. for $C_{29}H_{30}FeN_2O_2P$ $[M+H]^+$: 525.1316, Found: 525.1391.

L2



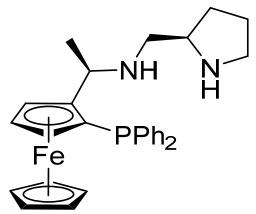
Yellow foam, 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.49 (m, 2H), 7.38-7.36 (m, 3H), 7.25-7.24 (m, 3H), 7.16-7.13 (m, 2H), 6.47-6.45 (m, 1H), 5.79 (s, 1H), 5.19-5.15 (m, 1H), 4.50 (s, 1H), 4.34-4.33 (m, 1H), 3.97 (s, 5H), 3.85-3.84 (m, 1H), 3.60-3.57 (m, 1H), 2.21-2.22 (m, 1H), 2.10-1.97 (m, 2H), 1.64-1.57 (m, 1H), 1.46 (d, *J* = 4.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 178.57, 168.82, 140.26 (d, *J* = 9.0 Hz), 136.65 (d, *J* = 7.0 Hz), 135.21 (d, *J* = 21.0 Hz), 132.22 (d, *J* = 18.0 Hz), 129.42, 128.31 (t, *J* = 6.0 Hz), 128.16 (d, *J* = 2.0 Hz), 94.49 (d, *J* = 25.0 Hz), 74.43 (d, *J* = 10.0 Hz), 72.12 (d, *J* = 4.0 Hz), 70.25 (d, *J* = 4.0 Hz), 69.66, 56.66, 45.16 (d, *J* = 6.6 Hz), 29.31, 25.35, 21.22; ^{31}P NMR (101 MHz, $CDCl_3$) δ -25.20; HRMS (ESI) calcd. for $C_{29}H_{30}FeN_2O_2P$ $[M+H]^+$: 525.1316, Found: 525.1391.

L3



Yellow foam, 70% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.49 (m, 2H), 7.42-7.39 (m, 1H), 7.35-7.34 (m, 3H), 7.24-7.22 (m, 4H), 5.25-5.21 (m, 1H), 4.48 (s, 1H), 4.30-4.29 (m, 1H), 4.20-4.19 (m, 1H), 4.02 (s, 5H), 3.82-3.81 (m, 1H), 2.92-2.89 (m, 1H), 2.71-2.67 (m, 1H), 1.93-1.86 (m, 1H), 1.71-1.67 (m, 2H), 1.55-1.51 (m, 1H), 1.43-1.41 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.63, 140.34 (d, *J* = 4.0 Hz), 137.20 (d, *J* = 4.0 Hz), 134.99 (d, *J* = 8.0 Hz), 132.97 (d, *J* = 8.0 Hz), 129.00, 128.08, 127.99, 127.92, 68.48, 60.32, 46.83, 43.38 (d, *J* = 8.0 Hz), 30.39, 25.83, 20.82; ^{31}P NMR (101 MHz, $CDCl_3$) δ -25.99; HRMS (ESI) calcd. for $C_{29}H_{32}FeN_2OP$ $[M+H]^+$: 511.1523, Found: 511.1598.

L4

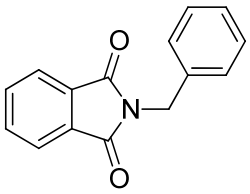


Yellow foam, 67 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56-7.52 (m, 2H), 7.38-7.36 (m, 3H), 7.25-7.24 (m, 5H), 5.25-5.21 (m, 1H), 4.49-4.47 (m, 1H), 4.29-4.28 (m, 1H), 4.14-4.09 (m, 1H), 4.06-4.03 (m, 1H), 3.98 (s, 5H), 3.82-3.81 (m, 1H), 2.65-2.61 (m, 1H), 2.58-2.51 (m, 1H), 2.42-2.37 (m, 1H), 2.33-2.29 (m, 1H), 1.49-1.45 (m, 3H), 1.27-1.24 (m, 2H), 1.15-1.12 (m, 1H), 1.05-1.11 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.43 (d, *J* = 10.1 Hz), 137.22 (d, *J* = 8.1 Hz), 135.08 (d, *J* = 21.2 Hz), 132.58 (d, *J* = 19.2 Hz), 129.14, 128.33, 128.27, 128.15, 128.06, 97.80 (d, *J* = 24.2 Hz), 74.92 (d, *J* = 7.1 Hz), 71.31 (d, *J* = 4.0 Hz), 69.64, 69.23 (d, *J* = 4.0 Hz), 69.10, 58.36, 51.40 (d, *J* = 9.1 Hz), 51.13, 45.92, 28.62, 24.98, 19.32; ^{31}P NMR (101 MHz, $CDCl_3$) δ -25.24; HRMS (ESI) calcd. for $C_{29}H_{34}FeN_2P$ $[M+H]^+$: 497.1731, Found: 497.1806.

3. General procedures for the synthesis of the cyclic imides

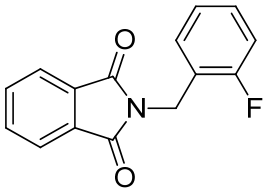
Method A: To a solution of the anhydride (10 mmol, 1.0 eq) in acetic acid (20 mL), was added slowly the substituted benzylamine or aniline (10 mmol, 1.0 eq), and then the reaction mixture was refluxed for 6 h. After removing acetic acid, the residue was added into water (50 mL). The product was precipitated in cold water and the solid recovered by filtration. Then crude product was recrystallized in an appropriate solvent to give the product.

2-benzylisoindoline-1,3-dione(1aa)[2]



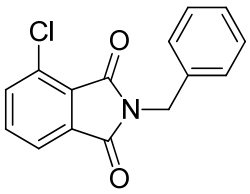
white solid, mp: 115-117 °C; 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84-7.82 (m, 2H), 7.70-7.68 (m, 2H), 7.44-7.42 (m, 2H), 7.33-7.25 (m, 3H), 4.48 (s,1H). ^{13}C NMR (101 MHz, CDCl3) δ 167.98, 136.32, 133.92, 132.08, 128.62, 128.55, 127.77, 123.28, 77.32, 77.00, 76.68, 41.56.

2-(2-fluorobenzyl)isoindoline-1,3-dione(1ae)[3]



white solid, mp: 184-186 °C; 87% yield. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 7.91-7.85 (m, 4H), 7.35-7.31 (m, 2H), 7.22-7.13 (m, 2H), 4.82 (s, 2H), ^{13}C NMR (101 MHz, DMSO-*d6*) δ 167.54, 161.10, 158.66, 134.63, 131.55, 129.71, 129.67, 129.58, 124.59, 124.56, 123.36, 123.28, 123.22, 115.49, 115.28, 35.01, 34.96.

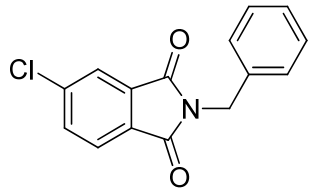
2-benzyl-4-chloroisoindoline-1,3-dione(1ba)



white solid, mp: 138-141 °C; 65% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76-7.74 (m, 1H), 7.62-7.61 (m, 2H), 7.46-7.43 (m, 2H), 7.33-7.26 (m, 3H), 4.84 (s,

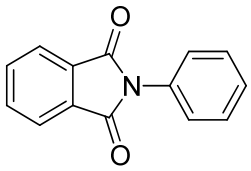
2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.66, 165.79, 136.13, 135.84, 135.05, 134.30, 131.55, 128.95, 128.84, 128.10, 127.90, 121.97, 41.95. HRMS (ESI) calcd. for $C_{15}H_{10}ClNO_2$ $[M+H]^+$: 272.0040, Found: 272.0110.

2-benzyl-5-chloroisoindoline-1,3-dione(1ca)



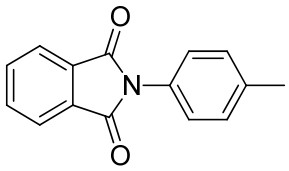
white solid, mp: 143-145 °C; 69% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.96 (m, 1H), 7.92-7.88 (m, 2H), 7.46-7.43 (m, 2H), 7.33-7.26 (m, 5H), 4.76 (s, 2H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 166.91, 166.55, 139.39, 136.45, 134.34, 133.64, 130.18, 128.61, 127.50, 127.43, 125.01, 123.42, 41.10. HRMS (ESI) calcd. for $C_{15}H_{12}ClNO_2$ $[M+H]^+$: 272.0040, Found: 272.0110.

2-phenylisoindoline-1,3-dione(1aj)[2]



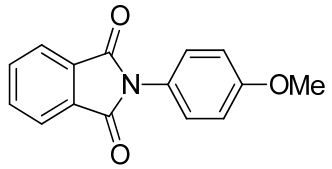
white solid, mp: 203-205 °C; 83% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-7.95 (m, 2H), 7.80-7.78 (m, 2H), 7.53-7.49 (m, 2H), 7.46-7.41 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.27, 134.38, 131.76, 129.10, 128.09, 126.56, 123.73.

2-(p-tolyl)isoindoline-1,3-dione(1ak)[2]



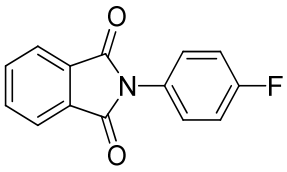
white solid, mp: 201-203 °C; 84% yield. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 7.97-7.95 (m, 2H), 7.91-7.89 (m, 2H), 3.37 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 167.17, 137.67, 134.71, 131.61, 129.38, 129.30, 127.30, 123.42, 20.80.

2-(4-methoxyphenyl)isoindoline-1,3-dione(1al)[2]



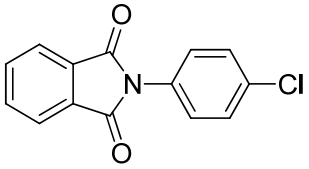
white solid, mp: 158-160 °C; 87% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94-7.92 (m, 2H), 7.78-7.76 (m, 2H), 7.35-7.32 (m, 2H), 7.03-7.01 (m, 2H), 3.84 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.68, 159.35, 134.41, 131.91, 128.05, 124.36, 123.76, 114.57, 55.61.

2-(4-fluorophenyl)isoindoline-1,3-dione(1am)[4]



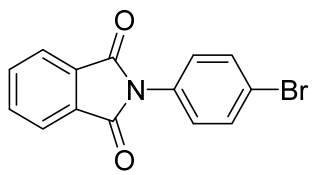
white solid, mp: 178-180 °C; 72% yield. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 7.99-7.97 (m, 2H), 7.93-7.91 (m, 2H), 7.53-7.49 (m, 2H), 7.40-7.36 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.06, 134.77, 131.61, 129.76, 129.67, 123.49, 115.95, 115.72.

2-(4-chlorophenyl)isoindoline-1,3-dione(1an)[2]



white solid, mp: 195-197 °C; 71% yield. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 7.99-7.97 (m, 2H), 7.93-7.90 (m, 2H), 7.62-7.60 (m, 2H), 7.51-7.49 (m, 2H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 166.85, 134.81, 132.57, 131.59, 130.86, 129.17, 128.95, 123.54.

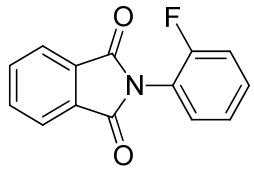
2-(4-bromophenyl)isoindoline-1,3-dione(1ao)[5]



white solid, mp: 201-203 °C; 70% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-7.95 (m, 2H), 7.81-7.79 (m, 2H), 7.65-7.61 (m, 2H), 7.37-7.33 (m, 2H). ^{13}C

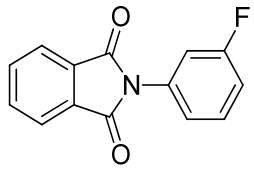
NMR (101 MHz, $CDCl_3$) δ 167.06, 134.73, 132.42, 131.74, 130.86, 128.08, 124.01, 121.96.

2-(2-fluorophenyl)isoindoline-1,3-dione(1ap)[4]



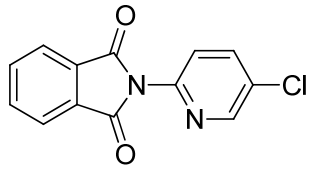
white solid, mp: 181-183 °C; 84% yield. ^1H NMR (400 MHz, $CDCl_3$) δ 7.98-7.97 (m, 2H), 7.81-7.80 (m, 2H), 7.47-7.44 (m, 1H), 7.38-7.36 (m, 1H), 7.31-7.26 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.66, 158.86, 157.19, 134.61, 132.10, 130.91, 130.85, 130.01, 124.80, 124.77, 124.08, 119.55, 119.47, 116.98, 116.85.

2-(3-fluorophenyl)isoindoline-1,3-dione(1aq)[4]



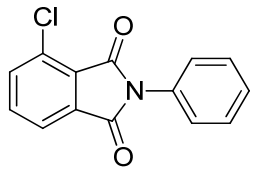
white solid, mp: 172-174 °C; 89% yield. ^1H NMR (400 MHz, $CDCl_3$) δ 7.98-7.96 (m, 2H), 7.82-7.80 (m, 2H), 7.49-7.45 (m, 1H), 7.31-7.28 (m, 1H), 7.26-7.23 (m, 1H), 7.14-7.09 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.99, 163.99, 161.54, 134.75, 133.12, 131.67, 130.38, 130.29, 124.04, 122.16, 122.12, 115.25, 115.04, 114.19, 113.94.

2-(5-chloropyridin-2-yl)isoindoline-1,3-dione(1ar)[6]



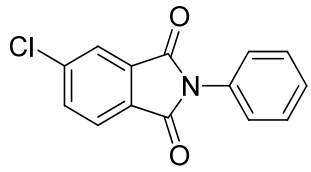
white solid, mp: 145-147 °C; 91% yield; ^1H NMR (400 MHz, $CDCl_3$) δ 8.63-8.62 (m, 1H), 7.99-7.96 (m, 2H), 7.87-7.85 (m, 1H), 7.83-7.80 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.48, 148.64, 144.42, 138.12, 134.90, 131.76, 131.73, 124.21, 122.71.

4-chloro-2-phenylisoindoline-1,3-dione(1bj)[7]



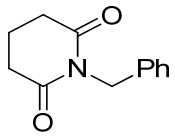
white solid, mp: 185-187 °C; 56% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88-7.86 (m, 1H), 7.71-7.70 (m, 2H), 7.53-7.49 (m, 2H), 7.44-7.41 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.96, 164.97, 136.26, 135.40, 133.96, 132.02, 131.43, 129.26, 128.43, 127.49, 126.69, 122.37.

5-chloro-2-phenylisoindoline-1,3-dione(1cj)[7]



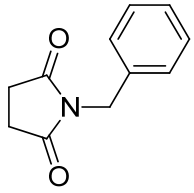
white solid, mp: 190-192 °C; 60% yield. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.06-8.05 (m, 1H), 7.99-7.94 (m, 2H), 7.56-7.52 (m, 2H), 7.47-7.43 (m, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 166.23, 165.87, 139.47, 134.49, 133.68, 131.76, 130.22, 128.94, 128.26, 127.38, 125.22, 123.54.

1-benzylpiperidine-2,6-dione(1da)[8]



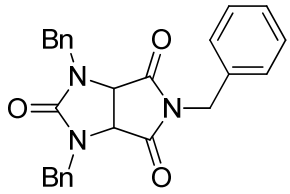
white solid, mp: 46-48 °C; 78% yield. ^{1}H NMR (600 MHz, CD_3OD) δ 7.25-7.23 (m, 4H), 7.19-7.17 (m, 1H), 4.89 (d, *J* = 6.0 Hz, 2H), 2.64-2.61 (m, 4H), 1.86-1.84 (m, 2H). ^{13}C NMR (150 MHz, CD_3OD) δ 174.69, 138.86, 129.29, 129.03, 128.15, 43.41, 33.45, 17.94.

1-benzylpyrrolidine-2,5-dione(1ea)[8]



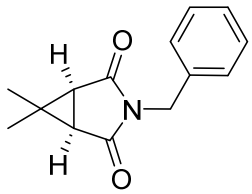
white solid, mp: 100-102 °C; 69% yield. ^{1}H NMR (400 MHz, CD_3OD) δ 7.73-7.24 (m, 5H), 4.62 (s, 2H), 2.70 (s, 4H). ^{13}C NMR (101 MHz, CD_3OD) δ 179.62, 137.57, 129.55, 129.30, 128.71, 29.12.

1,3,5-tribenzyltetrahydropyrrolo[3,4-d]imidazole-2,4,6(5H)-trione(1fa)[9]



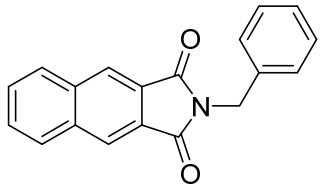
white solid, mp: 111-113 °C; 84% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.36-7.32 (m, 7H), 7.30-7.28 (m, 7H), 5.06 (d, *J* = 12 Hz, 2H), 4.65 (s, 2H), 4.26-4.23 (m, 2H), 3.98 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 172.76, 157.54, 135.72, 134.78, 129.00, 128.97, 128.91, 128.50, 128.13, 53.29, 46.45, 42.75.

(1R,5S)-3-benzyl-6,6-dimethyl-3-azabicyclo[3.1.0]hexane-2,4-dione(1ga)[10]



white solid, mp: 89-91 °C; 85% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.39-7.38 (m, 2H), 7.30-7.25 (m, 3H), 4.53 (s, 2H), 2.31 (s, 2H), 1.20 (s, 3H), 1.01 (s, 3H), 2.06 (t, *J* = 6.0 Hz, 2H), 1.60-1.57 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.72, 135.96, 129.31, 128.66, 128.06, 41.91, 35.78, 33.63, 26.42, 15.50.

2-benzyl-1H-benzo[f]isoindole-1,3(2H)-dione(1ha)[11]

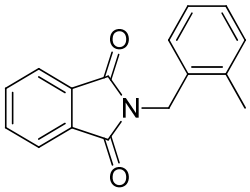


white solid, mp: 161-163 °C; 81% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.30-8.28 (m, 2H), 8.01-7.99 (m, 2H), 7.65-7.64 (m, 2H), 7.49-7.47 (m, 2H), 7.35-7.31 (m, 2H), 7.28-7.25 (m, 2H), 4.53 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.73, 136.41, 135.42, 130.27, 129.17, 128.73, 128.71, 127.86, 127.83, 127.82, 124.77, 124.76, 41.86.

Method B: Phthalimide (14 mmol, 2.06 g, 1.0 eq.), potassium carbonate (15.4 mmol, 2.14 g, 1.1 eq), potassium iodide (20 mg) and the corresponding alkyl or benzyl halide (14 mmol, 1.0 eq.) were heated at 40 ℃ in N,N-dimethylformamide (20 mL) for 16 hours. After solvents evaporation under vacuum, water was added to the

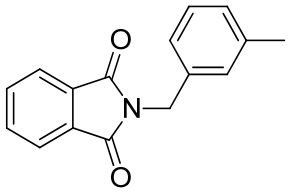
reaction mixture followed by extraction with DCM. The combined organic phases were dried over Na_2SO_4, filtered and concentrated in vacuo. The desired phthalimide was purified by silica gel column chromatography with a mixture of petroleum ether and ethyl acetate as eluent.

2-(2-methylbenzyl)isoindoline-1,3-dione(1ab)[12]



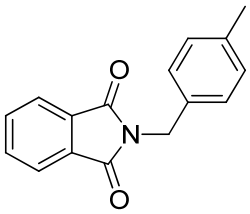
white solid, mp: 115-117 °C; 93% yield. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 7.91-7.84 (m, 4H), 7.23-7.19 (m, 1H), 7.11-7.06 (m, 3H), 4.72 (s, 2H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 167.73, 137.80, 136.62, 134.58, 131.57, 128.50, 128.07, 127.89, 124.47, 123.25, 40.82, 20.96.

2-(3-methylbenzyl)isoindoline-1,3-dione(1ac)[12]



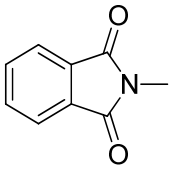
white solid, mp: 118-120 °C; 90% yield. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 7.92-7.85 (m, 4H), 7.19-7.06 (m, 4H), 4.75 (s, 2H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 167.86, 135.33, 134.61, 134.39, 131.58, 130.16, 127.24, 126.60, 126.03, 123.26, 18.84.

2-(4-methylbenzyl)isoindoline-1,3-dione(1ad)[12]



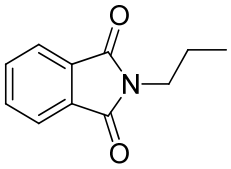
white solid, mp: 120-122 °C; 89% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.84-7.82 (m, 2H), 7.70-7.69 (m, 2H), 7.34-7.32 (m, 2H), 7.13-7.11 (m, 2H), 4.81 (s, 2H), 2.30 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.21, 137.71, 134.07, 133.56, 132.32, 129.47, 128.78, 123.44, 41.50, 21.26.

2-methylisoindoline-1,3-dione(1af)[5]



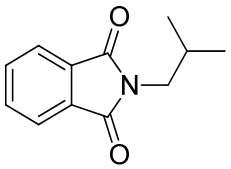
white solid, mp: 125-127 °C; 76% yield. ^{1}H NMR (400 MHz, DMSO-*d6*) δ7.94-7.91 (m, 1H), 7.81-7.75 (m, 4H), 2.98 (s,3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.08, 134.28, 131.85, 122.92, 23.74.

2-propylisoindoline-1,3-dione(1ag)[13]



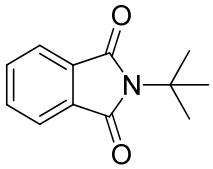
white solid, mp: 59-61 °C; 81% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84-7.82 (m, 2H), 7.71-7.69 (m, 1H), 7.33-7.29 (m, 2H), 3.66-3.63 (m, 2H), 1.73-1.65 (m, 1H), 0.94 (t, *J* = 8.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.64, 133.97, 132.29, 123.28, 39.74, 22.04, 11.46.

2-isobutylisoindoline-1,3-dione(1ah)[14]



white solid, mp: 94-96 °C; 80% yield. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 7.89-7.81 (m, 1H), 3.39 (s, 2H), 2.04-1.94 (m, 1H), 0.87 (d, *J* = 4.0 Hz, 6H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 168.17, 134.45, 131.49, 123.07, 44.77, 27.44.

2-(tert-butyl)isoindoline-1,3-dione(1ai)[15]



white solid, mp: 55-57 °C; 83% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77-7.74 (m, 2H), 7.69-7.65 (m, 2H), 1.69 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.83, 133.80, 132.30, 122.71, 57.98, 29.23.

4. General procedure for hydrogenation

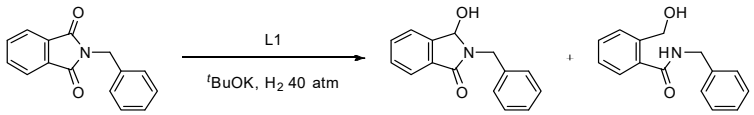
4.1 The optimization of the reaction conditions:

A study of the reaction with $[Ir(COD)Cl]_2$/ligand L_1 was performed in various solvents and bases. The results are summarized in Table 1 and Table 2.

A study of the reaction with $[Ir(COD)Cl]_2$/ligand L_4 was performed in various solvents and bases. The results are summarized in Table 3 and Table 4.

General procedure for S/C = 200 : To a 4.0 mL vial was added the catalyst precursor $[Ir(COD)Cl]_2$ (6.71 mg, 1.0×10^{-2} mmol, 1.0 eq), ligand L1 or L4 (2.1×10^{-2} mmol, 2.1 eq) and anhydrous ^{i}PrOH (2.0 mL) under argon atmosphere. The mixture was stirred for 2.0 h at 25 ℃ giving orange red solution in the argon-filled glovebox. The resulting solution (100 μL) and ^{t}BuOK (2.2 mg) were transferred by syringe into a 5.0 mL vial charged with substrate (0.2 mmol) in 1.0 mL anhydrous ^{i}PrOH. The vials were transferred to an autoclave, which was then charged with 40 atm of H_2 and stirred at 50 ℃ for 24 h. The hydrogen gas was released slowly in a well-ventilated hood and the solution was concentrated and passed through a short column of silica gel to remove the metal complex.

Table 1. The effect of solvents on the hydrogenation of the cyclic imide (**1aa**) by L1

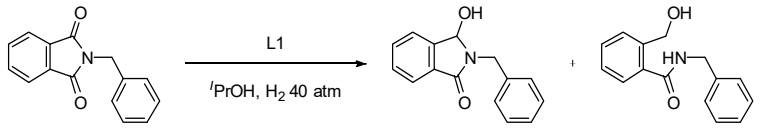


2aa 3aa

Entry	Solvent	Time (h)	Yield % (2aa)	Yield % (3aa)
1	Toluene	24	76	0
2	MTBE	24	46	0
3	DCM	24	0	0
4	THF	24	82	10
5	MeOH	24	0	0
6	EtOH	24	0	0

7	1,4-dioxane	24	0	0
8	^{i}PrOH	24	**97**	0

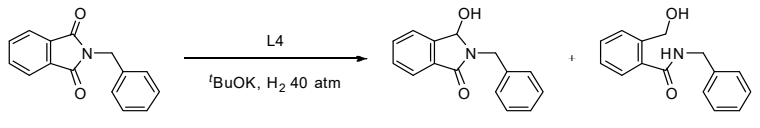
Table 2. The effect of base on the hydrogenation of the cyclic imide (**1aa**) by L1



2aa 3aa

Entry	Base	Time (h)	Yield % (2aa)	Yield % (3aa)
1	NaOH	24	0	0
2	KOH	24	0	0
3	Cs_2CO_3	24	0	0
4	K_2CO_3	24	0	0
5	MeOK	24	0	0
6	MeONa	24	87	0
7	^{t}BuONa	24	91	0
8	^{t}BuOK	24	**97**	0
9	^{t}BuOLi	24	92	0

Table 3. The effect of solvents on the hydrogenation of the cyclic imide (**1aa**) by L4

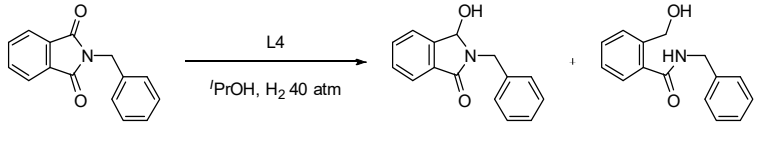


2aa 3aa

Entry	Solvent	Time (h)	Yield % (2aa)	Yield % (3aa)
1	Toluene	24	0	93
2	MTBE	24	52	41

3	DCM	24	33	31
4	THF	24	38	53
5	MeOH	24	45	51
6	EtOH	24	40	57
7	1,4-dioxane	24	43	44
8	*i*PrOH	24	0	**94**

Table 4. The effect of base on the hydrogenation of the cyclic imide (**1aa**) by L4



2aa 3aa

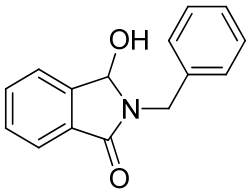
Entry	Base	Time (h)	Yield % (2aa)	Yield % (3aa)
1	NaOH	24	0	92
2	KOH	24	0	93
3	Cs_2CO_3	24	0	94
4	K_2CO_3	24	0	92
5	MeOK	24	0	93
6	MeONa	24	0	94
7	^{t}BuONa	24	0	92
8	^{t}BuOK	24	0	**98**
9	^{t}BuOLi	24	0	95

4.2 General procedure for type I hydrogenation (S/C = 1000, non-ring opening):

To a 4.0 mL vial was added the catalyst precursor $[Ir(COD)Cl]_2$ (6.71 mg,

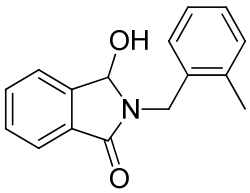
1.0×10^{-2} mmol, 1 eq), ligand L_1 (2.1×10^{-2} mmol, 2.1 eq) and anhydrous ^{i}PrOH (2.0 mL) under argon atmosphere. The mixture was stirred for 12.0 h at 25 ℃ giving orange red solution in the argon-filled glovebox. The resulting solution (20 μL) and ^{t}BuOK (2.2 mg) transferred by syringe into a 5.0 mL vial charged with substrate (0.2 mmol) in 1.0 mL anhydrous ^{i}PrOH. The vials were transferred to an autoclave, which was then charged with 40 atm of H_2 and stirred at 50 ℃ for 24 h. The hydrogen gas was released slowly in a well-ventilated hood and the solution was concentrated and passed through a short column of silica gel to remove the metal complex.

2-benzyl-3-hydroxyisoindolin-1-one(2aa)[16]



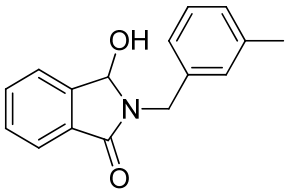
white solid, mp: 140-142 °C; 97% yield. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 7.71-7.69 (m, 1H), 7.66-7.55 (m, 3H), 7.35-7.25 (m, 5H), 5.67 (d, *J* = 8.0 Hz, 1H), 4.91 (d, *J* = 16 Hz, 1H), 4.37 (d, *J* = 12 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.15, 144.89, 137.74, 132.09, 131.42, 129.42, 128.49, 127.68, 127.11, 123.76, 122.47, 80.28, 42.11.

3-hydroxy-2-(2-methylbenzyl)isoindolin-1-one(2ab)



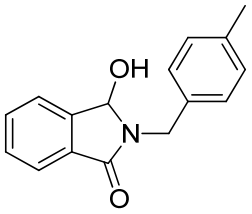
white solid, mp: 143-145 °C; 92% yield. ^{1}H NMR (400 MHz, CD_3OD) δ 7.78-7.76 (m, 1H), 7.65-7.56 (m, 3H), 7.21-7.08 (m, 4H), 5.66 (s, 1H), 5.06 (d, *J* = 16 Hz, 1H), 4.38 (d, *J* = 12Hz, 1H), 2.31 (d, *J* = 4 Hz, 3H). ^{13}C NMR (101 MHz, CD_3OD) δ 169.26, 146.13, 139.59, 138.39, 133.66, 132.61, 130.78, 129.73, 129.66, 129.25, 126.17, 124.68, 123.94, 82.07, 43.61, 21.42. HRMS (ESI) calcd. for $C_{16}H_{16}NO_2$ $[M+H]^+$: 254.1103, Found: 254.1175.

3-hydroxy-2-(3-methylbenzyl)isoindolin-1-one(2ac)



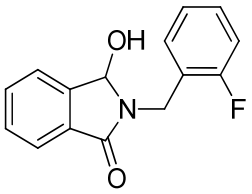
white solid, mp: 137-139 °C; 93% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62-7.60 (m, 1H), 7.56-7.54 (m, 2H), 7.46-7.43 (m, 1H), 7.16-7.13 (m, 4H), 5.50 (s, 1H), 4.68 (d, *J* = 16 Hz, 1H), 4.21 (d, *J* = 16 Hz, 1H), 2.31 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.47, 144.25, 136.63, 134.46, 132.48, 131.16, 130.64, 129.75, 128.85, 127.84, 126.30, 123.62, 123.44, 81.14, 40.32, 19.34. HRMS (ESI) calcd. for $C_{16}H_{16}NO_2$ $[M+H]^+$: 254.1103, Found: 254.1174.

3-hydroxy-2-(4-methylbenzyl)isoindolin-1-one(2ad)[17]



white solid, mp: 148-150 °C; 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64-7.63 (m, 1H), 7.55-7.54 (m, 2H), 7.46-7.43 (m, 1H), 7.20-7.18 (m, 2H), 7.10-7.08 (m, 2H), 5.57 (s, 1H), 4.80 (d, *J* = 16 Hz, 1H), 4.19 (d, *J* = 12 Hz, 1H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.43, 144.09, 137.49, 133.87, 132.43, 131.47, 129.86, 129.52, 128.60, 123.53, 123.49, 81.07, 42.49, 21.22.

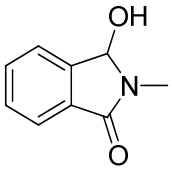
2-(2-fluorobenzyl)-3-hydroxyisoindolin-1-one(2ae)



white solid, mp: 131-133 °C; 91% yield. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 7.63-7.55 (m, 1H), 7.47-7.43 (m, 1H), 7.53-7.29 (m, 4H), 7.26-7.21 (m, 2H), 7.06-6.99 (m, 2H), 5.64 (s, 1H), 4.62 (d, *J* = 16 Hz, 1H), 4.42 (d, *J* = 16 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.70, 162.16, 159.71, 144.15, 132.57, 131.10, 130.76, 130.73, 129.84, 129.61, 129.53, 124.49, 124.45, 123.86, 123.71, 123.64, 123.47,

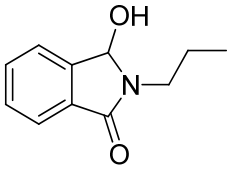
115.68, 115.46, 81.46, 81.45, 36.38, 36.34. HRMS (ESI) calcd. for $C_{15}H_{13}FNO_2$ $[M+H]^+$: 258.0852, Found: 258.0924.

3-hydroxy-2-methylisoindolin-1-one(2af)[16]



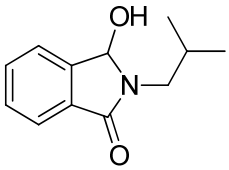
white solid, mp: 115-117 °C; 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60-7.58 (m, 1H), 7.56-7.52 (m, 2H), 7.42-7.38 (m, 1H), 5.29 (s, 1H), 2.91 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.70, 143.92, 132.27, 131.55, 129.83, 123.35, 123.19, 83.71, 26.23.

3-hydroxy-2-propylisoindolin-1-one(2ag)[18]



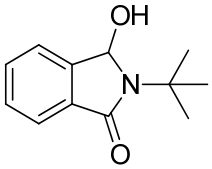
white solid, mp: 91-93 °C; 93% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54-7.47 (m, 2H), 7.43-7.41 (m, 1H), 7.36-7.32 (m, 1H), 5.67 (d, *J* = 8.0 Hz, 1H), 3.32-3.27 (m, 1H), 3.17-3.12 (m, 1H), 1.59-1.49 (m, 2H), 0.83 (t, *J* = 8.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.26, 144.11, 132.08, 131.44, 129.53, 123.31, 13.04, 81.61, 40.67, 21.48, 11.43.

3-hydroxy-2-isobutylisoindolin-1-one(2ah)[19]



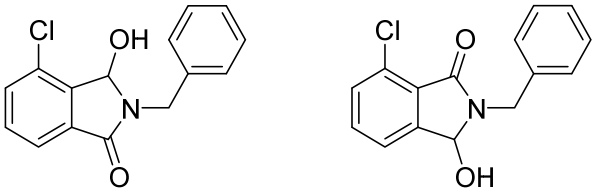
white solid, mp: 90-92 °C; 93% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62-7.54 (m, 3H), 7.46-7.42 (m, 1H), 5.74 (s, 1H), 3.30-3.24 (m, 1H), 3.15-3.10 (m, 1H), 2.07-2.00 (m, 1H), 0.95 (d, *J* = 4.0 Hz, 3H), 0.84 (d, *J* = 8.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.83, 144.01, 132.26, 131.67, 129.90, 123.46, 123.40, 82.24, 46.59, 27.59, 20.53, 20.12.

2-(tert-butyl)-3-hydroxyisoindolin-1-one(2ai)[20]



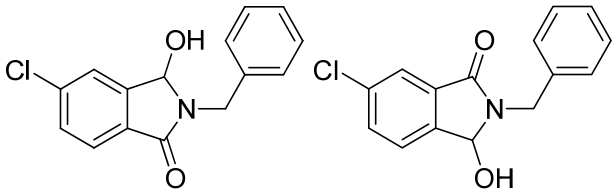
white solid, mp: 100-102 °C; 91% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77-7.68 (m, 1H), 7.53-7.44 (m, 3H), 5.99 (d, *J* = 8.0 Hz, 1H), 1.61 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.06, 143.62, 132.82, 132.14, 129.66, 123.16, 122.83, 82.41, 54.89, 28.72.

2-benzyl-4-chloro-3-hydroxyisoindolin-1-one(2ba, 2ba*)



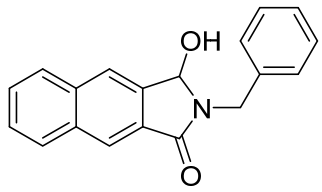
white solid, mp: 135-137 °C; 94% yield. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 7.69-7.53 (m, 3H), 7.36-7.26 (m, 5H), 7.53-7.29 (m, 4H), 7.28-7.23 (m, 1H), 6.92 (d, *J* = 8.0 Hz, 0.3 H), 6.82 (d, *J* = 8.0 Hz, 0.7 H), 5.72 (d, *J* = 8.0 Hz, 0.3 H), 5.66 (d, *J* = 8.0 Hz, 0.7 H), 4.93-4.85 (m, 1H), 4.38-4.34 (m, 1H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 165.01, 163.85, 147.71, 141.33, 137.51, 137.37, 133.62, 132.66, 131.71, 130.78, 129.44, 129.08, 128.60, 128.56, 127.78, 127.27, 127.22, 127.10, 122.88, 121.56, 79.64, 79.31, 40.15. HRMS (ESI) calcd. for $C_{15}H_{13}ClNO_2$ $[M+H]^+$: 274.0557, Found: 274.0628.

2-benzyl-5-chloro-3-hydroxyisoindolin-1-one(2ca, 2ca*)



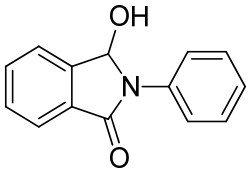
white solid, mp: 140-142 °C; 94% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54-7.39 (m, 3H), 7.31-7.27 (m, 5H), 5.56 (d, *J* = 8.0 Hz, 1 H), 4.94-4.89 (m, 1H), 4.29-4.25 (m, 1H), 4.00-3.91 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.51, 166.22, 145.65, 142.20, 139.00, 136.51, 136.45, 136.29, 133.05, 132.64, 130.37, 129.73, 128.98, 128.61, 128.57, 127.99, 127.97, 124.88, 124.60, 124.20, 123.60, 80.81, 80.65, 42.96. HRMS (ESI) calcd. for $C_{15}H_{13}ClNO_2$ $[M+H]^+$: 274.0557, Found: 274.0629.

2-benzyl-3-hydroxy-2,3-dihydro-1H-benzo[f]isoindol-1-one(2ha)



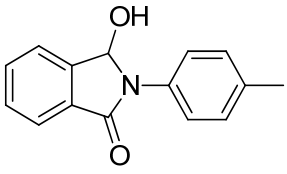
white solid, mp: 186-188 °C; 91% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.31 (s, 1H), 8.07-8.00 (m, 2H), 8.01 (d, *J* = 6.0 Hz, 1H), 7.63-7.59 (m, 2), 7.40-7.33 (m, 4H), 7.29-7.28 (m, 1), 5.82 (s, 1H), 5.15 (d, *J* = 12.0 Hz, 1H), 4.49 (d, *J* = 12.0 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.69, 139.60, 136.93, 135.63, 133.76, 129.18, 128.92, 128.39, 128.29, 127.85, 127.79, 127.25, 126.76, 123.10, 122.76, 80.76, 42.52, 30.42, 29.37. HRMS (ESI) calcd. for $C_{19}H_{15}NO_2$ $[M+H]^+$: 290.1103, Found: 290.1174.

3-hydroxy-2-phenylisoindolin-1-one(2aj)[16]



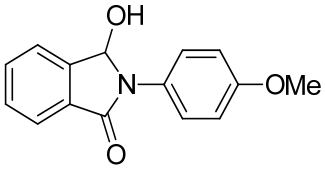
white solid, mp: 168-170 °C; 98% yield. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 7.78-7.67 (m, 5H), 7.63-7.60 (m, 1H), 7.46-7.42 (m, 2H), 7.23-7.19 (m, 1H), 6.54 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.43, 144.40, 137.46, 132.75, 131.28, 129.67, 128.66, 124.64, 123.66, 122.83, 122.30, 81.87.

3-hydroxy-2-(p-tolyl)isoindolin-1-one(2ak)[16]



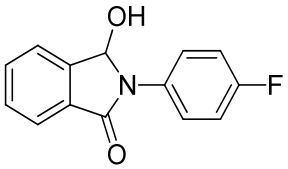
white solid, mp: 166-168 °C; 98% yield. ^{1}H NMR (400 MHz, CD_3OD) δ 7.80-7.78 (m, 2H), 7.69-7.67 (m, 2H), 7.60-7.53 (m, 3H), 7.27-7.24 (m, 2H), 6.36 (s, 1H), 2.36 (s, 3H). ^{13}C NMR (101 MHz, CD_3OD) δ 168.44, 145.66, 136.97, 135.54, 133.99, 132.70, 130.92, 130.48, 125.08, 124.63, 124.15, 84.37, 21.04.

3-hydroxy-2-(4-methoxyphenyl)isoindolin-1-one(2al)[21]



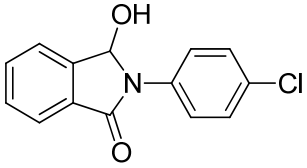
white solid, mp: 161-163 °C; 95% yield. ^{1}H NMR (600 MHz, CD_3OD) δ 7.81-7.79 (m, 1H), 7.71-7.67 (m, 2H), 7.61-7.58 (m, 1H), 7.54-7.52 (m, 2H), 7.02-7.00 (m, 2H), 6.31 (s, 1H), 3.83 (s, 3H). ^{13}C NMR (150 MHz, CD_3OD) δ 168.61, 159.61, 145.77, 133.94, 132.72, 130.92, 130.79, 127.32, 124.65, 124.14, 115.26, 84.82, 55.93.

2-(4-fluorophenyl)-3-hydroxyisoindolin-1-one(2am)[21]



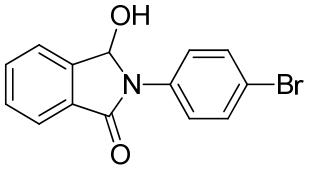
white solid, mp: 181-183 °C; 92% yield. ^{1}H NMR (600 MHz, CD_3OD) δ 7.82-7.81 (m, 1H), 7.72-7.69 (m, 4H), 7.62-7.59 (m, 1H), 7.21-7.18 (m, 2H), 6.40(s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.50, 162.87, 161.25, 145.70, 134.46, 134.44, 134.16, 132.51, 131.00, 127.16, 127.10, 124.69, 124.26, 116.64, 116.49, 84.56.

2-(4-chlorophenyl)-3-hydroxyisoindolin-1-one(2an)[22]



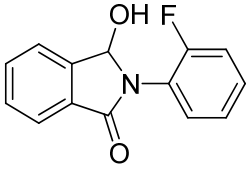
white solid, mp: 186-188 °C; 94% yield. ^{1}H NMR (600 MHz, DMSO-*d*$_6$) δ 7.84-7.82 (m, 2H), 7.78-7.77 (m, 1H), 7.74-7.72 (m, 1H), 7.69-7.68 (m, 1H), 7.62-7.60 (m, 1H), 7.51-7.50 (m, 2H), 6.53(d, J = 12 Hz, 1H). ^{13}C NMR (150 MHz, DMSO-*d*$_6$) δ 165.56, 144.29, 136.48, 133.01, 131.05, 129.82, 128.65, 128.57, 123.72, 123.54, 122.98, 81.95.

2-(4-bromophenyl)-3-hydroxyisoindolin-1-one(2ao)[23]



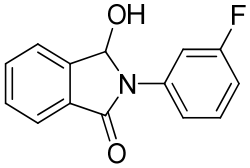
white solid, mp: 190-192 °C; 94% yield. ^{1}H NMR (600 MHz, CD_3OD) δ 7.83-7.81 (m, 1H), 7.72-7.70 (m, 4H), 7.62-7.58 (m, 3H), 6.46 (s, 1H). ^{13}C NMR (150 MHz, CD_3OD) δ 168.34, 145.56, 137.78, 134.31, 132.95, 132.44, 131.07, 125.88, 124.69, 124.32, 119.50, 84.05.

2-(2-fluorophenyl)-3-hydroxyisoindolin-1-one(2ap)[24]



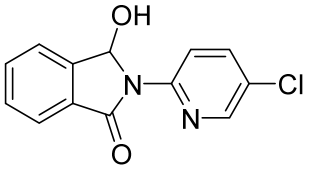
white solid, mp: 177-179 °C; 90% yield. ^{1}H NMR (400 MHz, CD_3OD) δ 7.82-7.80 (m, 1H), 7.72-7.65 (m, 3H), 7.62-7.58 (m, 2H), 7.44-7.42 (m, 1H), 6.99-6.94 (m, 1H), 6.45 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.36, 165.46, 163.04, 145.45, 140.34, 140.24, 135.44, 134.36, 132.37, 131.25, 131.16, 131.06, 130.09, 126.20, 124.66, 124.34, 123.65, 119.15, 119.12, 112.89, 112.68, 110.86, 110.60, 84.02, 71.42.

2-(3-fluorophenyl)-3-hydroxyisoindolin-1-one(2aq)[16]



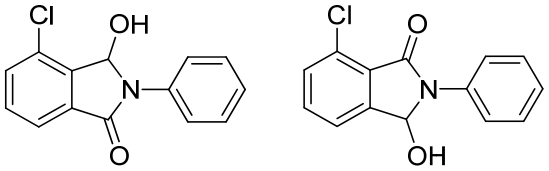
white solid, mp: 180-182 °C; 91% yield. ^{1}H NMR (400 MHz, CD_3OD) δ 7.84-7.82 (m, 1H), 7.73-7.70 (m, 2H), 7.69-7.67 (m, 1H), 7.63-7.60 (m, 2H), 7.46-7.44 (m, 1H), 7.00-6.97 (m, 1H), 6.49 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.39, 165.10, 163.49, 145.54, 140.38, 140.31, 134.38, 132.43, 131.26, 131.20, 131.08, 124.70, 124.36, 119.21, 119.19, 112.88, 112.74, 110.87, 110.70, 84.07.

2-(5-chloropyridin-2-yl)-3-hydroxyisoindolin-1-one(2ar)[25]



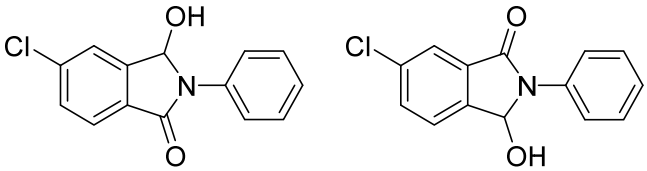
white solid, mp: 181-183 °C; 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, *J* = 8.0 Hz, 1H), 8.34 (d, *J* = 4.0 Hz, 1H), 7.91-7.89 (m, 1H), 7.79-7.76 (m, 1H), 7.72-7.67 (m, 2H), 7.60-7.56 (m, 1H), 6.73 (d, *J* = 4.0 Hz, 1H), 5.52 (d, *J* = 4.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.48, 150.39, 146.06, 142.20, 138.77, 133.68, 131.73, 130.33, 126.99, 124.30, 123.81, 115.12, 82.30.

4-chloro-3-hydroxy-2-phenylisoindolin-1-one(2bj-2bj*)[26]



white solid, mp: 124-126 °C; 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70-7.66 (m, 2H), 7.60-7.50 (m, 2H), 7.40-7.32 (m, 3H), 7.24-7.19 (m, 1H), 6.43 (d, *J* = 8.0 Hz, 0.5H), 6.26 (d, *J* = 8.0 Hz, 0.5H), 3.80 (d, *J* = 8.0 Hz, 0.5H), 3.70 (d, *J* = 8.0 Hz, 0.5H). ^{13}C NMR (101 MHz, CD_3OD) δ 165.54, 164.34, 145.53, 139.79, 136.88, 136.69, 133.76, 133.74, 133.44, 131.97, 131.80, 131.73, 130.22, 129.22, 129.12, 127.29, 125.88, 125.66, 122.39, 122.28, 122.14, 122.09.

5-chloro-3-hydroxy-2-phenylisoindolin-1-one(2cj-2cj*)[26]

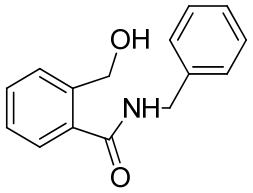


white solid, mp: 127-129 °C; 96% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66-7.62 (m, 2H), 7.60-7.51 (m, 2H), 7.39-7.34 (m, 3H), 7.24-7.20 (m, 1H), 6.33-6.29 (m, 1H), 3.93-3.74 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.81, 165.42, 144.50, 141.10, 139.47, 136.84, 136.70, 133.21, 130.81, 129.74, 129.24, 125.80, 125.74, 125.14, 124.77, 124.06, 123.97, 121.82, 121.75, 82.83, 82.59. HRMS (ESI) calcd. for $C_{14}H_{11}ClNO_2$ $[M+H]^+$: 260.0400, Found: 260.0471.

4.3 General procedure for type II hydrogenation (S/C = 1000, ring opening)

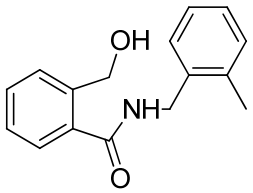
To a 4.0 mL vial was added the catalyst precursor $[Ir(COD)Cl]_2$ (6.71 mg, 1.0×10^{-2} mmol, 1 eq), ligand L4 (2.1×10^{-2} mmol, 2.1 eq) and anhydrous ^{i}PrOH (2.0 mL) under argon atmosphere. The mixture was stirred for 12.0 h at 25 ℃ giving orange red solution in the argon-filled glovebox. The resulting solution (20 μL) and ^{t}BuOK (2.2 mg) transferred by syringe into a 5.0 mL vial charged with substrate (0.2 mmol) in 1.0 mL anhydrous ^{i}PrOH. The vials were transferred to an autoclave, which was then charged with 40 atm of H_2 and stirred at 50 ℃ for 24 h. The hydrogen gas was released slowly in a well-ventilated hood and the solution was concentrated and passed through a short column of silica gel to remove the metal complex.

N-benzyl-2-(hydroxymethyl)benzamide(3aa)[27]



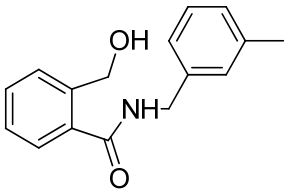
white solid, mp: 130-132 °C; 96% yield. ^{1}H NMR (400 MHz, CD_3OD) δ 7.54-7.51 (m, 2H), 7.49-7.45 (m, 1H), 7.40-7.32 (m, 5H), 7.28-7.24 (m, 1H), 4.69 (s, 2H), 4.56 (s, 2H). ^{13}C NMR (101 MHz, CD_3OD) δ 172.07, 140.72, 140.00, 136.42, 131.61, 129.86, 129.60, 128.82, 128.62, 128.60, 128.27, 63.48, 44.51.

2-(hydroxymethyl)-N-(2-methylbenzyl)benzamide(3ab)



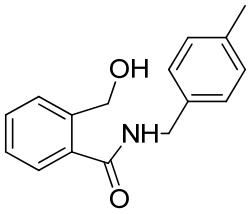
white solid, mp: 121-123 °C; 97% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55-7.53 (m, 1H), 7.43-7.41 (m, 3H), 7.38-7.31 (m, 1H), 7.27-7.23 (m, 3H), 7.16-7.10 (m, 3H), 4.60-4.58 (m, 4H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.97, 140.36, 138.71, 137.83, 135.58, 131.43, 130.96, 128.89, 128.71, 128.60, 128.26, 127.68, 124.94, 64.80, 44.35, 21.51. HRMS (ESI) calcd. for $C_{16}H_{18}NO_2$ $[M+H]^+$: 256.1259, Found: 256.1331.

2-(hydroxymethyl)-N-(3-methylbenzyl)benzamide(3ac)



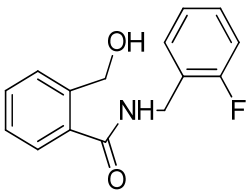
white solid, mp: 125-127 °C; 94% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51-7.49 (m, 1H), 7.41-7.37 (m, 1H), 7.31-7.25 (m, 3H), 7.21-7.17 (m, 3H), 4.58 (d, *J* = 4 Hz, 2H), 4.53 (s, 2H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.79, 140.08, 136.48, 135.54, 135.48, 131.30, 130.82, 130.71, 128.53, 128.19, 128.00, 127.80, 126.39, 64.65, 42.39, 19.12. HRMS (ESI) calcd. for $C_{16}H_{18}NO_2$ $[M+H]^+$: 256.1259, Found: 256.1331.

2-(hydroxymethyl)-N-(4-methylbenzyl)benzamide(3ad)



white solid, mp: 135-137 °C; 94% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.51 (m, 1H), 7.45-7.41 (m, 1H), 7.37-7.30 (m, 2H), 7.26-7.23 (m, 2H), 7.17-7.15 (m, 2H), 4.59-4.57 (m, 4H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.95, 140.34, 137.59, 135.62, 134.90, 131.40, 130.94, 129.64, 128.24, 127.94, 127.67, 64.82, 44.13, 21.24. HRMS (ESI) calcd. for $C_{16}H_{18}NO_2$ $[M+H]^+$: 256.1259, Found: 256.1330.

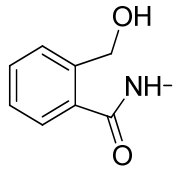
N-(2-fluorobenzyl)-2-(hydroxymethyl)benzamide(3ae)



white solid, mp: 127-129 °C; 90% yield. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 7.54-7.52 (m, 1H), 7.42-7.40 (m, 2H), 7.34-7.27 (m, 2H), 7.14-7.04 (m, 3H), 4.66 (d, *J* = 4 Hz, 2H), 4.55 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.98, 162.40, 159.95, 140.15, 135.42, 131.42, 130.89, 130.40, 130.36, 129.69, 129.61, 128.27, 127.84,

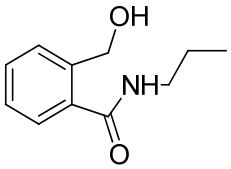
125.04, 124.89, 124.55, 124.51, 115.72, 115.50, 64.71, 38.39, 38.35. HRMS (ESI) calcd. for $C_{16}H_{18}NO_2$ $[M+H]^+$: 260.1009, Found: 260.1081.

2-(hydroxymethyl)-N-methylbenzamide(3af)[27]



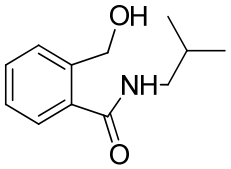
white solid, mp: 120-122 °C; 93% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54-7.51 (m, 1H), 7.46-7.34 (m, 3H), 4.61 (s, 2H), 3.03 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.85, 140.46, 135.78, 131.41, 131.02, 128.29, 127.59, 64.96, 27.12.

2-(hydroxymethyl)-N-propylbenzamide(3ag)



white solid, mp: 81-83 °C; 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.51 (m, 1H), 7.47-7.43 (m, 1H), 7.417.34 (m, 2H), 4.61 (d, *J* = 4.0 Hz, 2H), 4.41 (t, *J* = 8.0 Hz, 1H), 3.46-3.41 (m, 2H), 1.69-1.63 (m, 2H), 1.03-0.94 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.69, 140.40, 136.09, 131.33, 130.98, 128.28, 127.51, 64.94, 42.08, 22.99, 11.57. HRMS (ESI) calcd. for $C_{11}H_{15}NO_2$ $[M+H]^+$: 194.1103, Found: 194.1170.

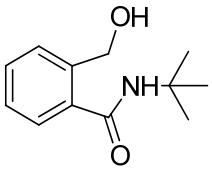
2-(hydroxymethyl)-N-isobutylbenzamide(3ah)



white solid, mp: 75-77 °C; 95% yield; 93% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.50 (m, 1H), 7.41-7.37 (m, 1H), 7.33-7.29 (m, 2H), 4.51 (s, 2H), 3.24-3.21 (m, 2H), 1.90-1.81 (m, 1H), 2.07-2.00 (m, 1H), 0.95 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.17, 139.74, 134.136.12, 131.07, 130.74, 128.19, 127.86, 64.62,

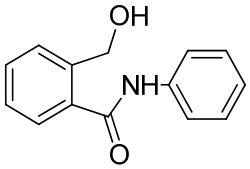
47.60, 28.61, 20.24. HRMS (ESI) calcd. for $C_{12}H_{17}NO_2$ $[M+H]^+$: 208.1259, Found: 208.1320.

N-(tert-butyl)-2-(hydroxymethyl)benzamide(3ai)[28]



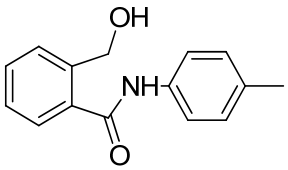
white solid, mp: 80-82 °C; 96% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48-7.46 (m, 1H), 7.38-7.36 (m, 1H), 7.32-7.28 (m, 2H), 4.51 (s, 2H), 1.45 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.80, 139.41, 137.26, 130.72, 130.60, 128.07, 127.65, 64.46, 52.10, 28.75.

2-(hydroxymethyl)-N-phenylbenzamide(3aj)[29]



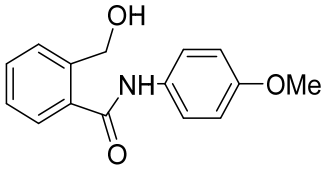
white solid, mp: 132-134 °C; 95% yield; 94% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.73 (m, 1H), 7.66-7.64(m, 2H), 7.51-7.49 (m, 1H), 7.46-7.37 (m, 4H), 7.20-7.16 (m, 1H), 4.70 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.91, 139.63, 137.96, 136.28, 131.74, 131.22, 129.31, 128.71, 128.33, 125.03, 120.42, 64.84.

2-(hydroxymethyl)-N-(p-tolyl)benzamide(3ak)[29]



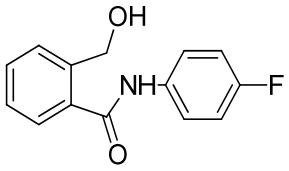
white solid, mp: 145-147 °C; 95% yield; 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72-7.70 (m, 1H), 7.53-7.51 (m, 2H), 7.48-7.47 (m, 1H), 7.43-7.40 (m, 2H), 7.19-7.17(m, 2H), 4.67 (s, 2H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.90, 139.68, 136.29, 135.34, 134.76, 131.63, 131.17, 129.77, 128.62, 128.25, 120.53, 64.80, 21.08.

2-(hydroxymethyl)-N-(4-methoxyphenyl)benzamide(3al)[29]



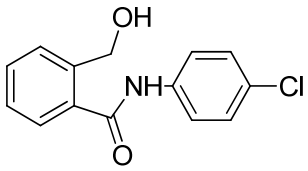
white solid, mp: 149-151 °C; 95% yield; 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73-7.70 (m, 1H), 7.56-7.53 (m, 2H), 7.49-7.47 (m, 1H), 7.44-7.41 (m, 2H), 6.92 (d, *J* = 8.0 Hz, 2H), 4.68 (d, *J* = 8.0 Hz, 2H), 3.82 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.83, 157.00, 139.79, 136.26, 131.62, 131.18, 130.99, 128.62, 128.20, 122.31, 114.45, 64.86, 55.68.

N-(4-fluorophenyl)-2-(hydroxymethyl)benzamide(3am)



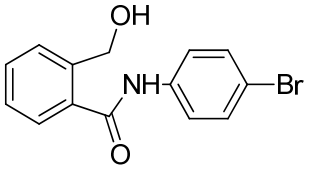
white solid, mp: 145-147 °C; 95% yield; 96% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75-7.72 (m, 1H), 7.63-7.60 (m, 2H), 7.50-7.47 (m, 1H), 7.45-7.39 (m, 2H), 7.09-7.05 (m, 2H), 4.69 (d, *J* = 4.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.77, 161.01, 158.59, 139.29, 136.09, 134.05, 134.02, 131.77, 131.19, 128.77, 128.58, 122.28, 122.20, 116.06, 115.83, 64.81. HRMS (ESI) calcd. for $C_{14}H_{13}FNO_2$ $[M+H]^+$: 246.0852, Found: 246.0924.

N-(4-chlorophenyl)-2-(hydroxymethyl)benzamide(3an)



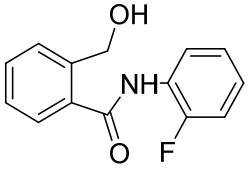
white solid, mp: 159-161 °C; 95% yield; 97% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76-7.74 (m, 1H), 7.63-7.61 (m, 2H), 7.51-7.42 (m, 3H), 7.35-7.33 (m, 2H), 4.71 (d, *J* = 4.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.69, 139.13, 136.66, 136.07, 131.85, 131.21, 129.92, 129.30, 128.85, 128.71, 121.59, 64.83. HRMS (ESI) calcd. for $C_{14}H_{13}ClNO_2$ $[M+H]^+$: 262.0557, Found: 262.0628.

N-(4-bromophenyl)-2-(hydroxymethyl)benzamide(3ao)[29]



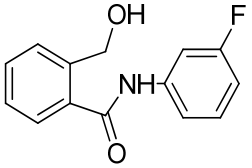
white solid, mp: 160-162 °C; 95% yield; 94% yield. ^{1}H NMR (600 MHz, CD_3OD) δ 7.65-7.63 (m, 3H), 7.56-7.55 (m, 1H), 7.52-7.48 (m, 3H), 7.43-7.41 (m, 1H), 4.76 (s, 2H). ^{13}C NMR (151 MHz, CD_3OD) δ 170.28, 140.68, 139.22, 136.73, 132.85, 131.89, 130.07, 129.13, 128.74, 123.29, 117.90, 63.47.

N-(2-fluorophenyl)-2-(hydroxymethyl)benzamide (3ap)



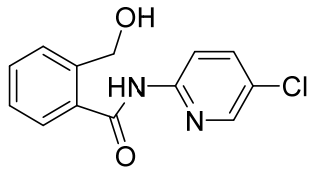
white solid, mp: 125-127 °C; 95% yield; 90% yield. ^{1}H NMR (600 MHz, CD_3OD) δ 7.97-7.96 (m, 1H), 7.72-7.70 (m, 1H), 7.57-7.51 (m, 2H), 7.45-7.44 (m, 1H), 7.24-7.18 (m, 3H), 4.79 (s, 2H). ^{13}C NMR (151 MHz, CD_3OD) δ 170.41, 157.65, 155.21, 140.56, 136.32 135.46, 132.09, 130.85, 130.23, 130.11, 129.55, 128.85, 127.66, 127.59, 126.99, 126.35, 125.40, 125.36, 116.68, 116.49, 63.52. HRMS (ESI) calcd. for $C_{14}H_{13}FNO_2$ $[M+H]^+$: 246.0852, Found: 246.0923.

N-(3-fluorophenyl)-2-(hydroxymethyl)benzamide(3aq)



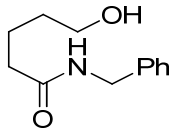
white solid, mp: 136-138 °C; 95% yield; 91% yield. ^{1}H NMR (400 MHz, CD_3OD) δ 7.68-7.63 (m, 2H), 7.57-7.52 (m, 2H), 7.44-7.33 (m, 3H), 6.90-6.85 (m, 1H), 4.77 (s, 2H). ^{13}C NMR (101 MHz, CD_3OD) δ 170.38, 165.53, 163.11, 141.75, 141.64, 140.67, 136.72, 131.91, 131.27, 131.17, 130.07, 129.15, 128.75, 116.96, 116.93, 111.93, 111.71, 108.65, 108.38, 66.67, 63.64. HRMS (ESI) calcd. for $C_{14}H_{13}FNO_2$ $[M+H]^+$: 246.0852, Found: 246.0925.

N-(5-chloropyridin-2-yl)-2-(hydroxymethyl)benzamide(3ar)



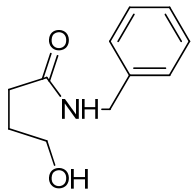
white solid, mp: 152-154 °C; 95% yield; 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 4.0 Hz, 2H), 7.94-7.91 (m, 1H), 7.71-7.67 (m, 1H), 7.52-7.50 (m, 1H), 7.52-7.48 (m, 1H), 7.39-7.36 (m, 2H), 6.46 (d, *J* = 8.0 Hz, 2H), 5.33 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.25, 156.83, 146.65, 146.23, 137.82, 134.16, 129.19, 125.93, 125.86, 122.22, 121.06, 109.70, 69.80. HRMS (ESI) calcd. for $C_{13}H_{12}ClN_2O_2$ $[M+H]^+$: 246.0852, Found: 246.0925.

N-benzyl-5-hydroxypentanamide(3da)[30]



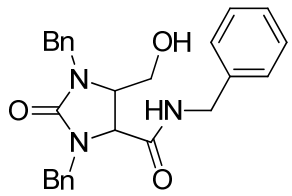
white solid, mp: 58-60 °C; 96% yield. ^{1}H NMR (600 MHz, CD_3OD) δ 7.32-7.22 (m, 5H), 4.36 (s, 2H), 3.56 (t, *J* = 6.0 Hz, 2H), 2.26 (t, *J* = 6.0 Hz, 2H), 1.71-1.68 (m, 2H), 1.57-1.54 (m, 2H). ^{13}C NMR (150 MHz, CD_3OD) δ 175.93, 140.08, 129.52, 128.56, 128.18, 62.49, 44.07, 36.76, 33.08, 23.44.

N-benzyl-4-hydroxybutanamide(3ea)[31]



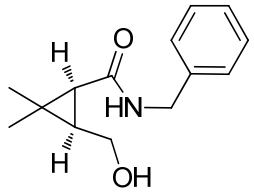
white solid, mp: 65-67 °C; 97% yield. ^{1}H NMR (600 MHz, CD_3OD) δ 7.28-6.18 (m, 5H), 4.32 (s, 2H), 3.53 (t, *J* = 6.0 Hz, 2H), 2.28 (t, *J* = 6.0 Hz, 2H), 1.82-1.79 (m, 2H). ^{13}C NMR (150 MHz, CD_3OD) δ 175.74, 140.06, 129.51, 128.54, 128.17, 62.26, 44.09, 33.60, 29.80.

N,1,3-tribenzyl-5-(hydroxymethyl)-2-oxoimidazolidine-4-carboxamide (3fa)[32]



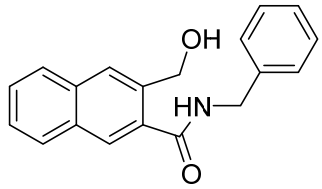
white solid, mp: 143-145 °C; 91% yield. ^{1}H NMR (600 MHz, CD_3OD) δ 7.36-7.30 (m, 7H), 7.22-7.15(m, 7H), 4.90 (d, *J* = 12.0 Hz, 1H), 4.81 (d, *J* = 12.0 Hz, 1H), 4.53 (d, *J* = 12.0 Hz, 1H), 4.46-4.35 (m, 2H), 4.15 (d, *J* = 12.0 Hz, 1H), 4.05 (d, *J* = 12.0 Hz, 1H), 3.82 (d, *J* = 6.0 Hz, 1H). ^{13}C NMR (150 MHz, CD_3OD) δ 172.14, 160.70, 137.96, 137.86, 137.05, 129.86, 129.84, 129.80, 129.75, 129.70, 129.35, 129.31, 129.03, 129.01, 128.82, 128.77, 84.99, 62.04, 55.99, 48.27, 46.69, 43.93.

(1S,3R)-N-benzyl-3-(hydroxymethyl)-2,2-dimethylcyclopropanecarboxamide(3ga)[33]



white solid, mp: 67-69 °C; 92% yield. ^{1}H NMR (600 MHz, CD_3OD) δ 7.32-7.26 (m, 4H), 7.24-7.22 (m, 1H), 4.37-4.31 (m, 2H), 4.00-3.96 (m, 1H), 3.88-3.84 (m, 1H), 1.53 (d, *J* = 6.0 Hz, 1H), 1.30-1.24 (m, 1H), 1.24 (s, 3H), 1.19 (s, 3H). ^{13}C NMR (150 MHz, CD_3OD) δ 173.39, 140.32, 129.48, 128.50, 128.10, 59.03, 44.08, 34.07, 31.86, 29.12, 24.68, 14.92.

N-benzyl-3-(hydroxymethyl)-2-naphthamide(3ha)

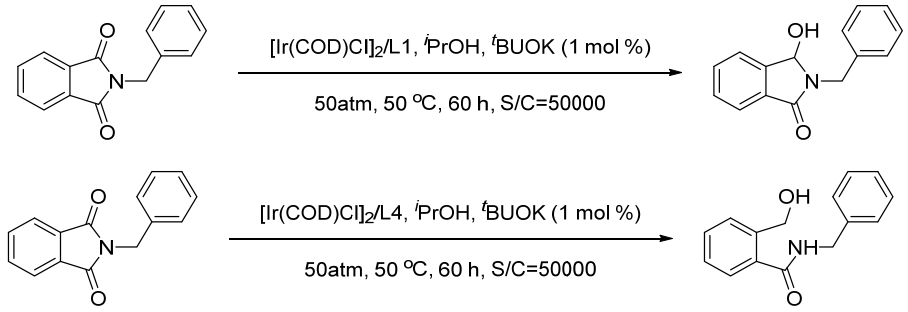


white solid, mp: 172-174 °C; 92% yield. ^{1}H NMR (600 MHz, CD_3OD) δ 8.07 (s, 1H), 7.96 (s, 1H), 7.92-7.88 (m, 2H), 7.56-7.52 (m, 2H), 7.43-7.42 (m, 2H), 7.37-7.34 (m, 2H), 7.28-7.26 (m, 1H), 4.85 (s, 2H), 4.61 (s, 2H). ^{13}C NMR (150 MHz, CD_3OD) δ 170.77, 138.66, 136.30, 134.10, 133.07, 132.03, 128.24, 127.92, 127.73, 127.37, 127.28, 127.27, 126.90, 126.36, 62.52, 43.21. HRMS (ESI) calcd. for $C_{19}H_{17}NO_2$ $[M+H]^+$: 292.1259, Found: 292.1330.

4.4 High TON experiment

General procedure for S/C = 50000: To a 4.0 mL vial was added the catalyst precursor $[Ir(COD)Cl]_2$ (6.71 mg, 1.0×10^{-2} mmol, 1 eq), ligand L1 or L4 (2.4×10^{-2} mmol, 2.4 eq) and anhydrous ^{i}PrOH (2.0 mL) under argon atmosphere. The mixture

was stirred for 12.0 h at 25 ℃ giving orange red solution in the argon-filled glovebox. The resulting solution (20 μL) and ^{t}BuOK (110 mg) transferred by syringe into a 10 mL vial charged with substrate (10 mmol) in 5.0 mL anhydrous ^{i}PrOH. The vials were transferred to an autoclave, which was then charged with 50 atm of H_2 and stirred at 50 ℃ for 60 h. The hydrogen gas was released slowly in a well-ventilated hood and the solution was concentrated and passed through a short column of silica gel to remove the metal complex.



5. Reference

[1] H. Nie, G. Zhou, Q. Wang, W. Chen and S. Zhang, *Tetrahedron: Asymmetry,* **2013**, *24*, 1567-1571.

[2] J.-C. Hsieh and C.-H. Cheng, *Chem. Commun.,* **2005**, 4554-4556.

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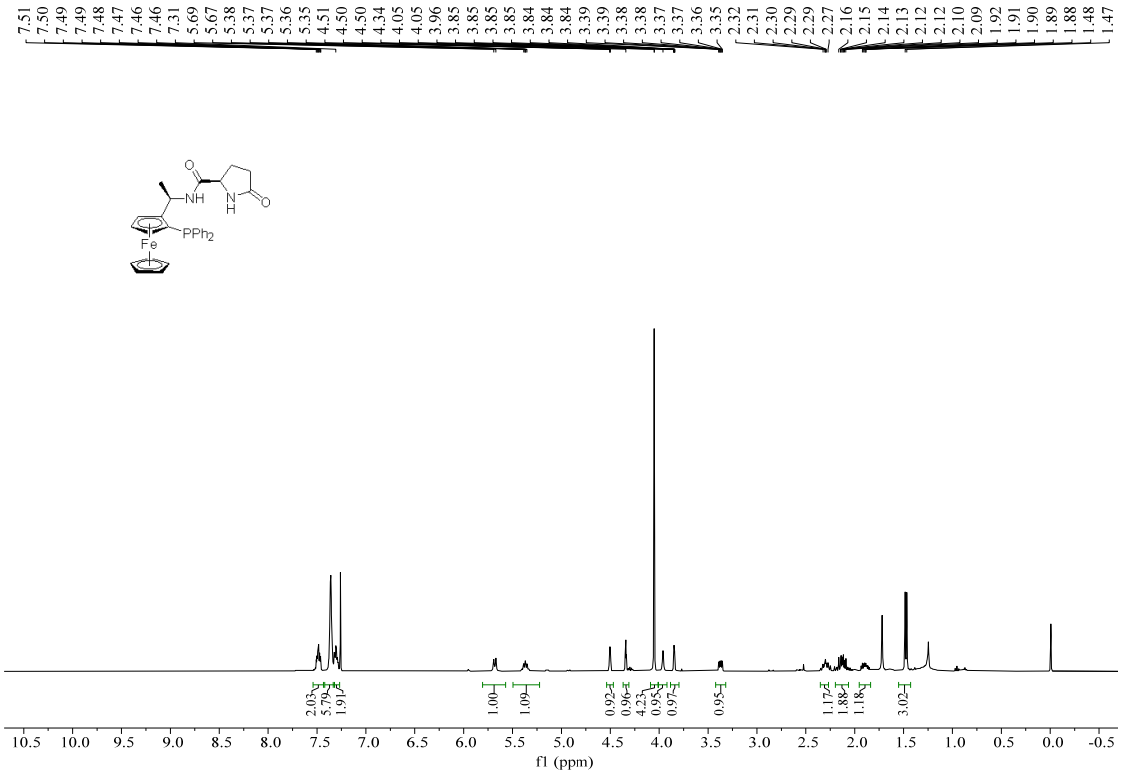
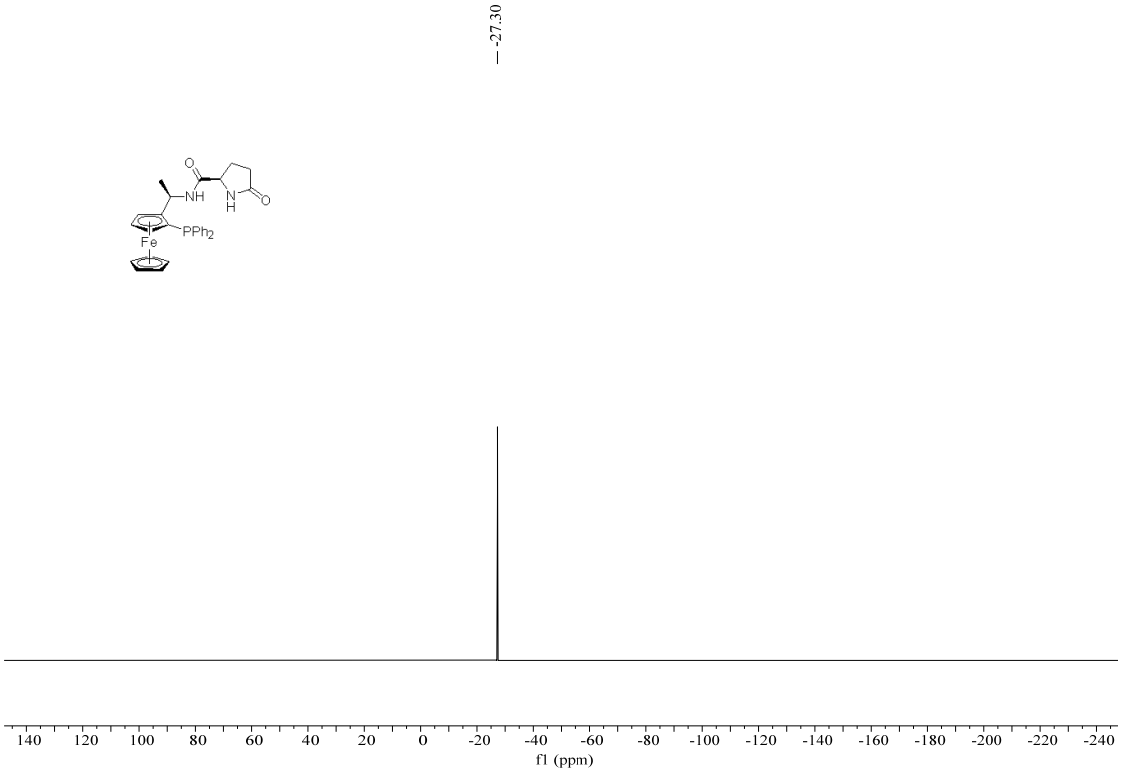
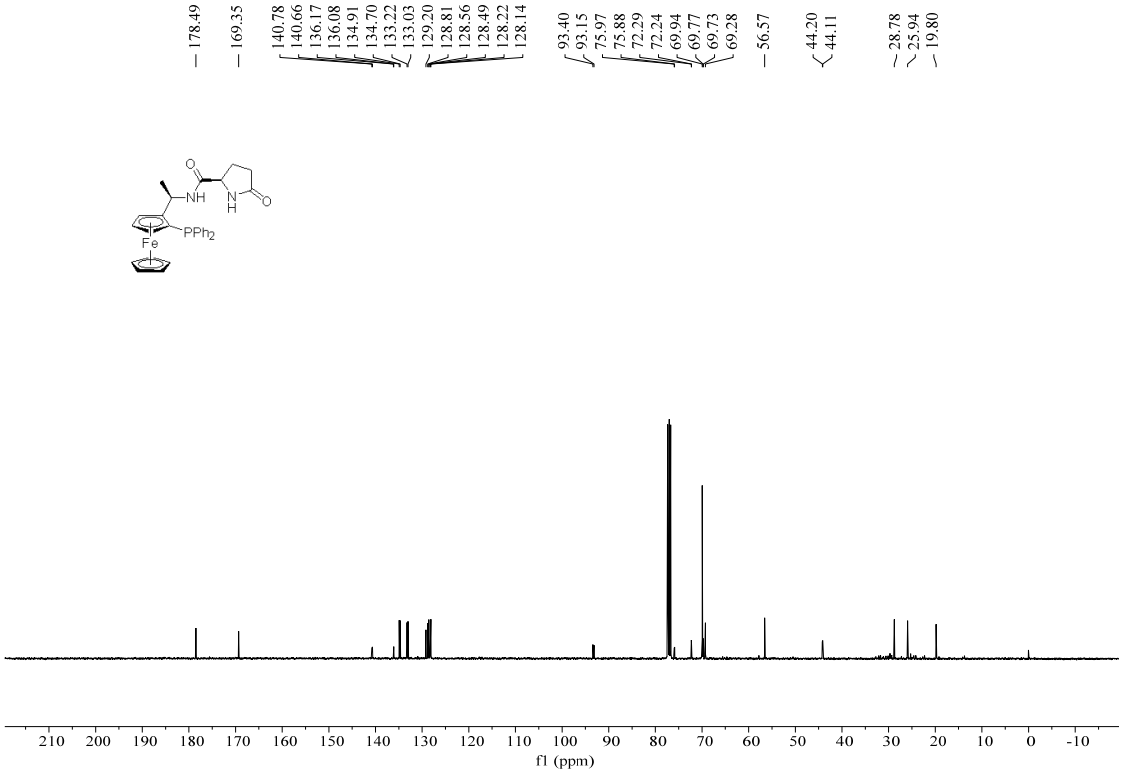
6. Spectroscopic data

L1



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128.56
128.49
128.22
128.14
93.40
93.15
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75.88
72.29
72.24
69.94
69.77
69.73
69.28
56.57
44.20
44.11
28.78
25.94
19.80
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N
H
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O
PPh2
Fe
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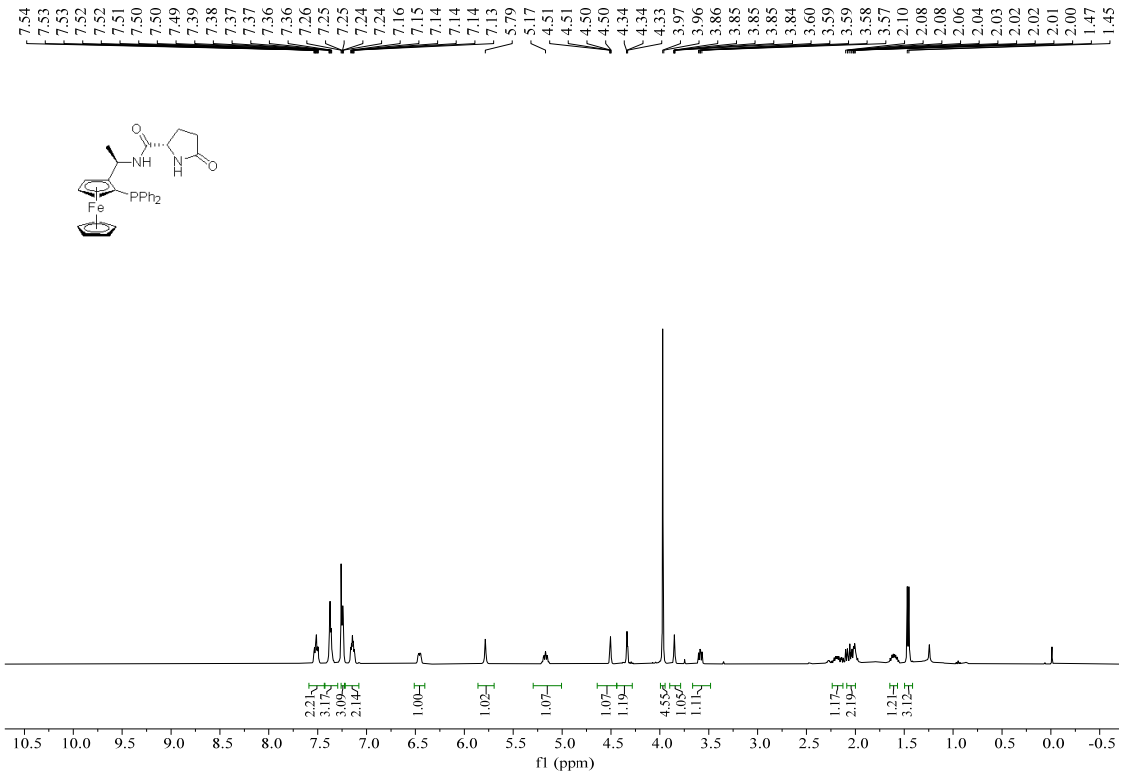
f1 (ppm)

L2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4.33
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3.86
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3.85
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3.59
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3.58
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2.08
2.08
2.06
2.04
2.03
2.02
2.02
2.01
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N
H
O
O
PPh2
Fe
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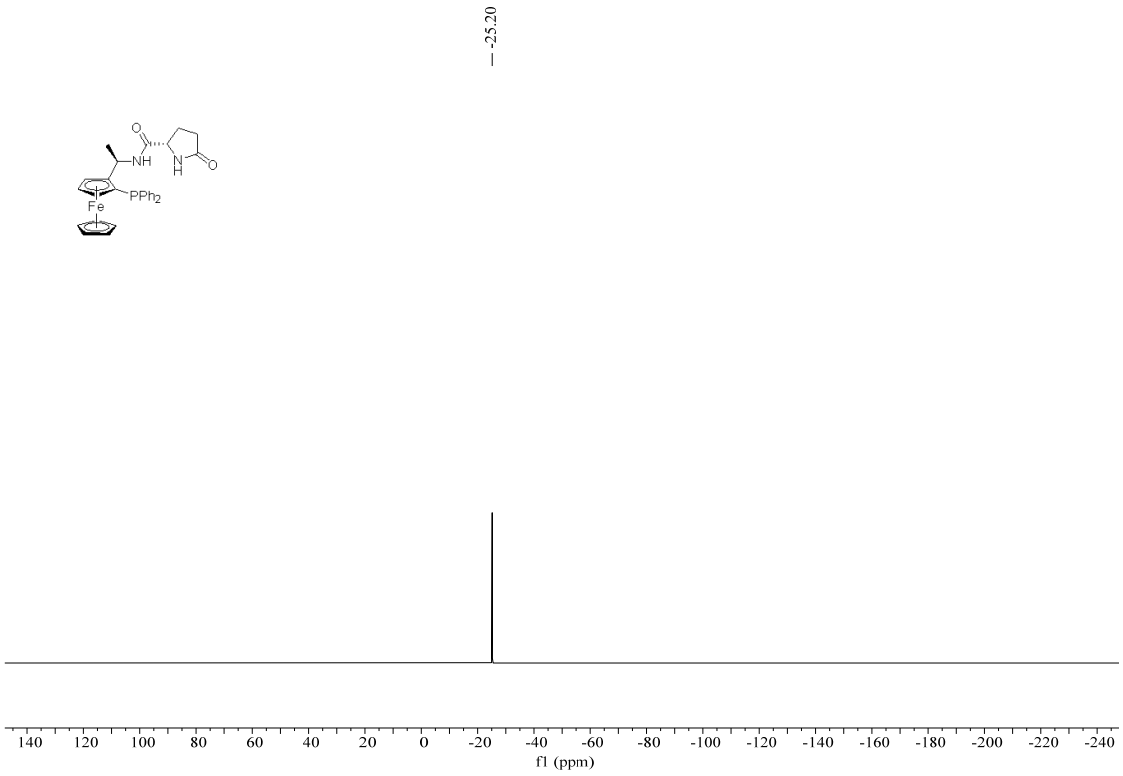
3.17
3.09
2.14
1.00
1.02
1.07
1.07
1.19
4.55
1.05
1.11
1.17
2.19
1.21
3.12
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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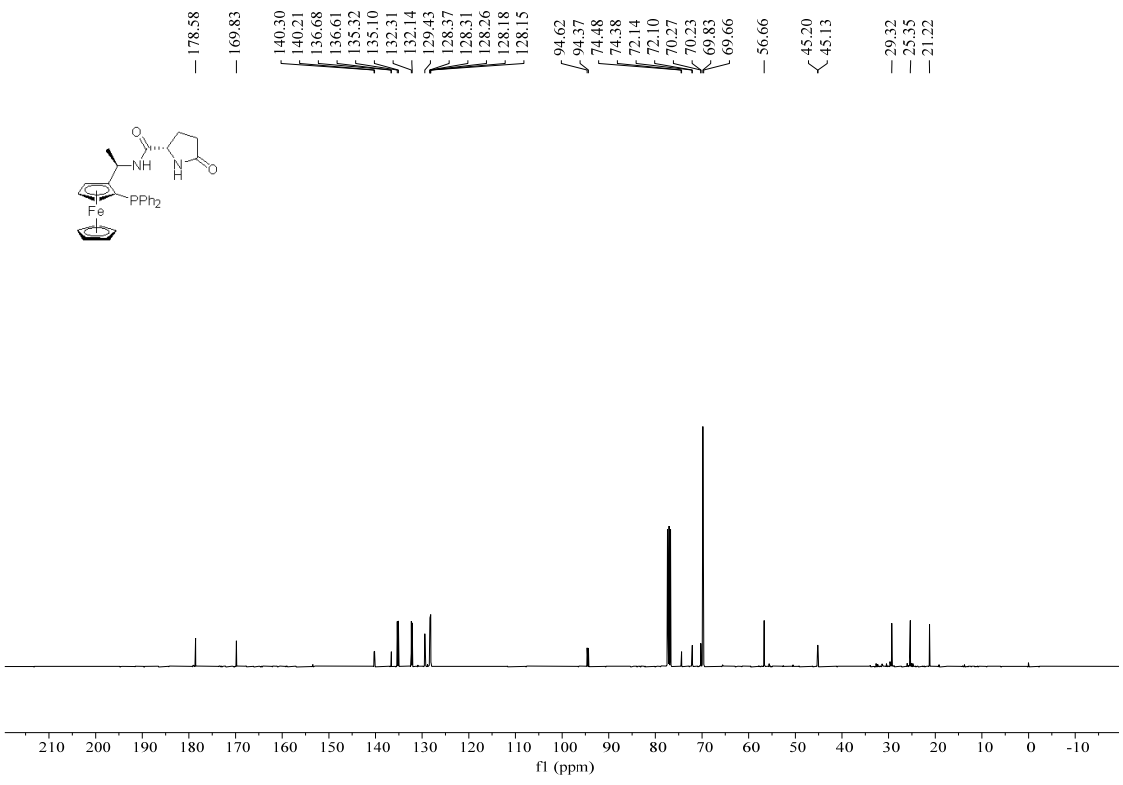
f1 (ppm)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45.13
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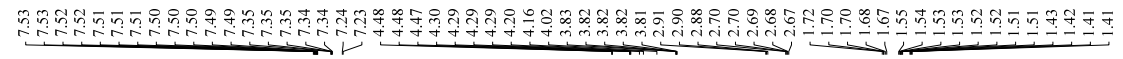
PPh2
Fe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

L3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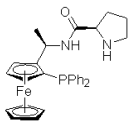
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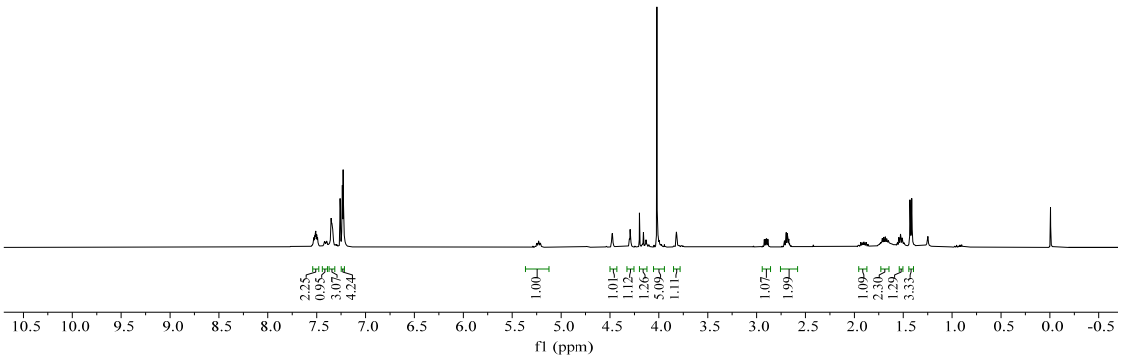
H
PPh2
Fe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3.33
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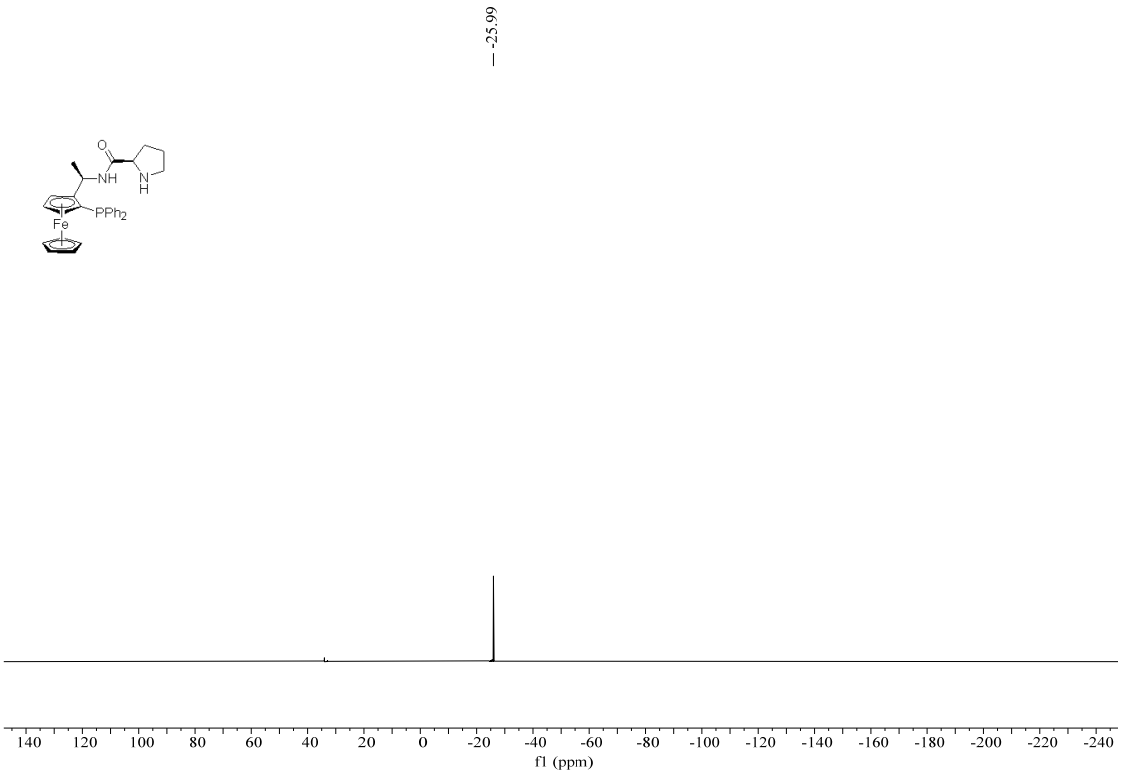
f1 (ppm)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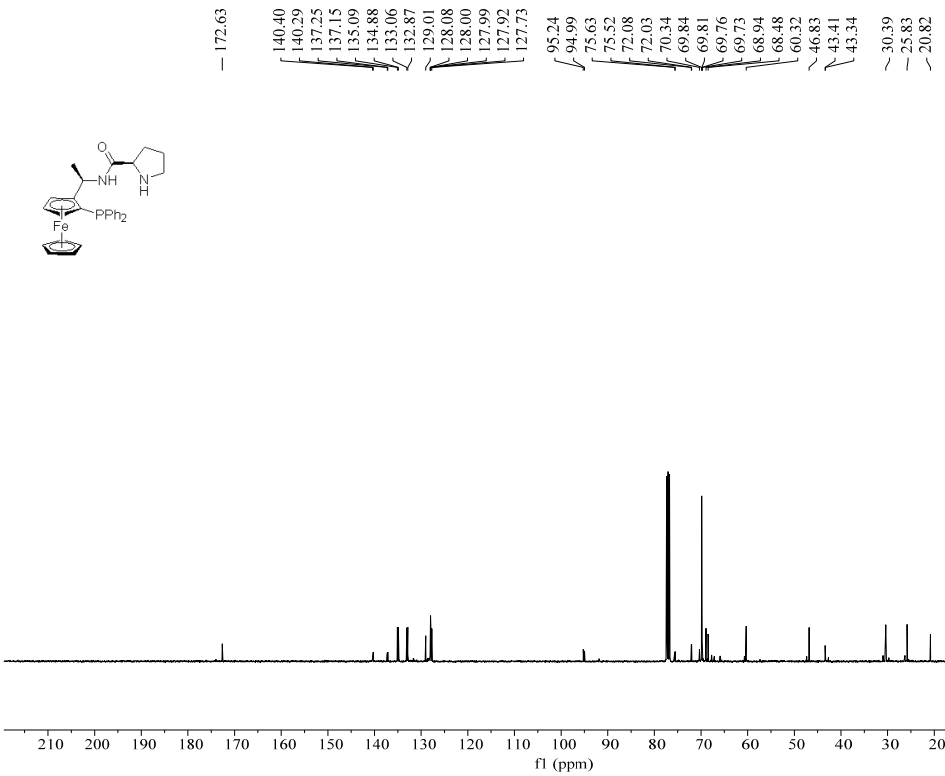
O
NH
N
H
PPh2
Fe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H
PPh2
Fe
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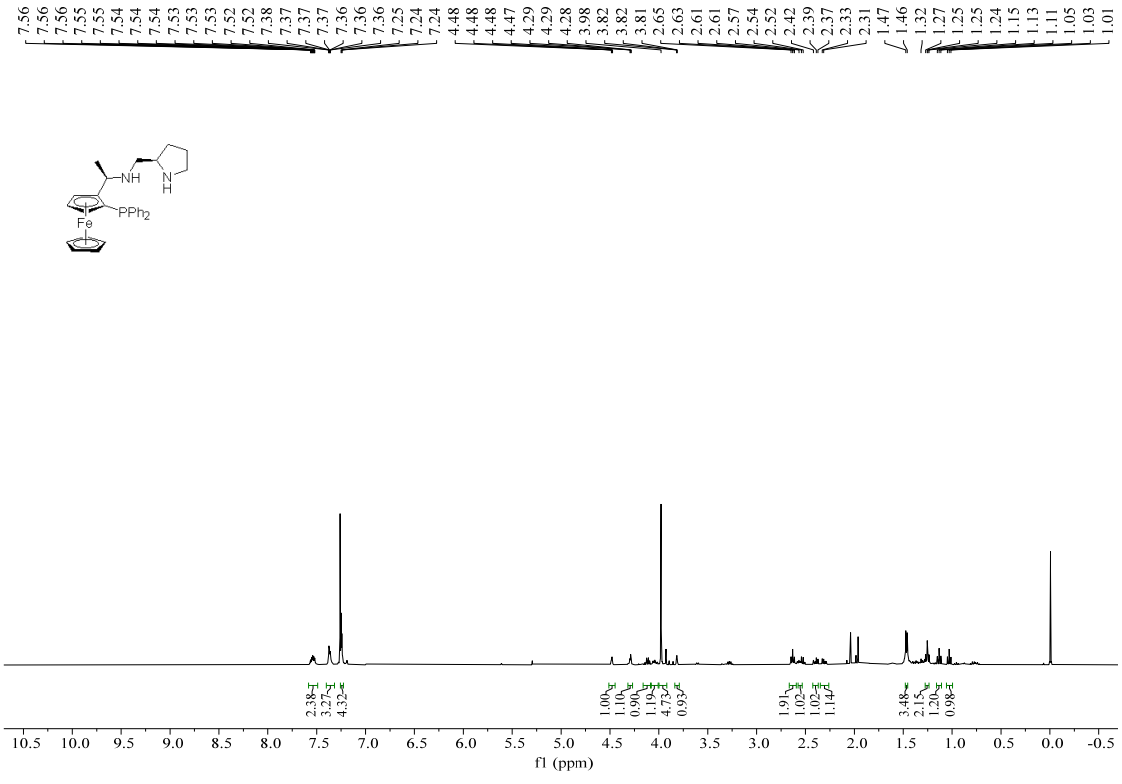
f1 (ppm)

L4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1.02
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2.15
1.20
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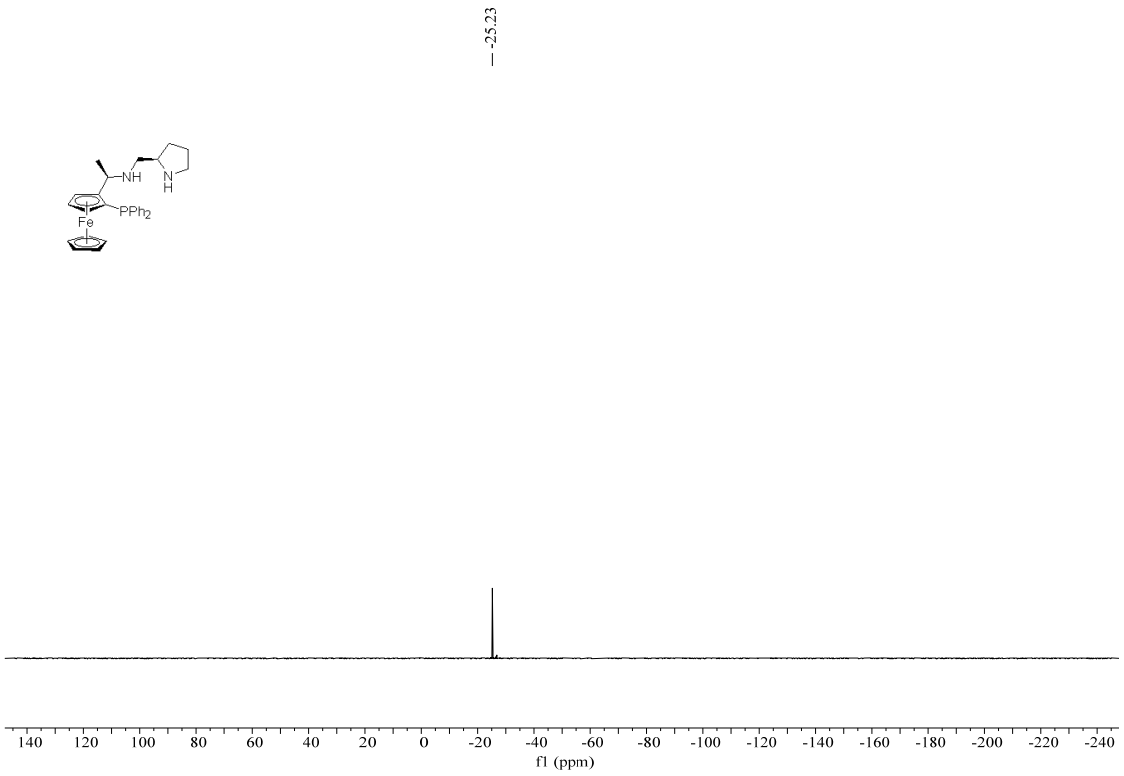
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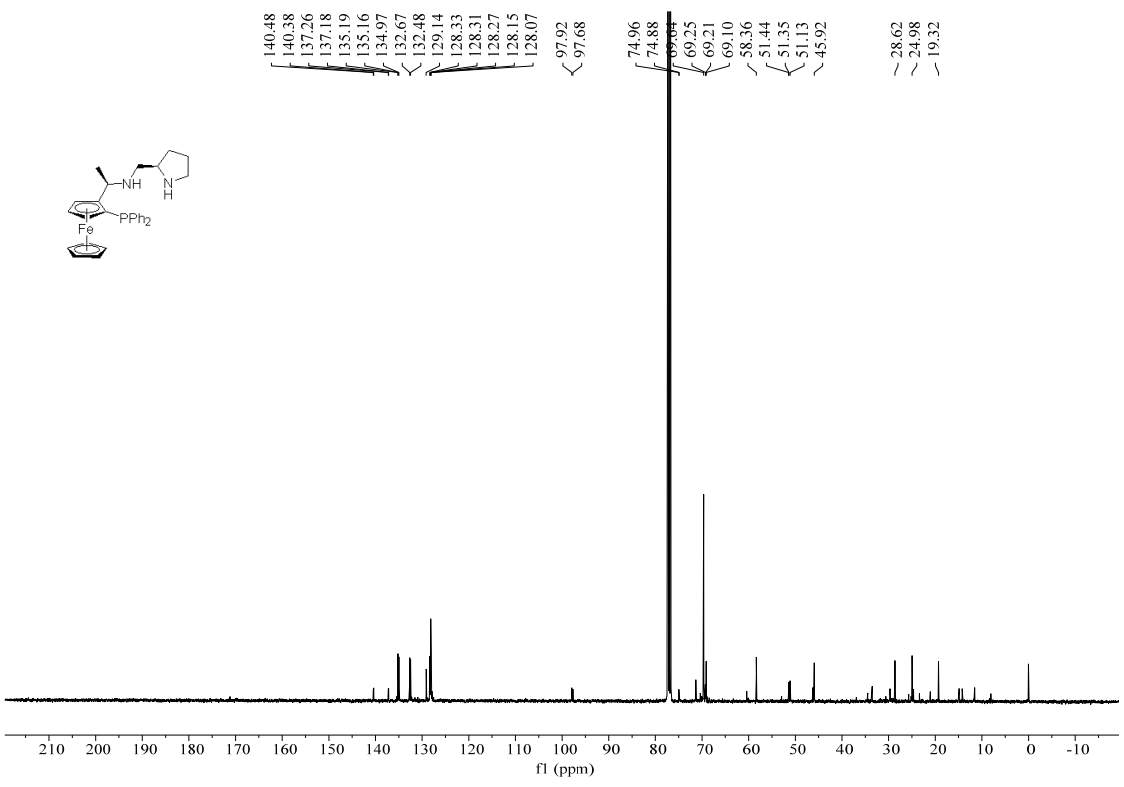
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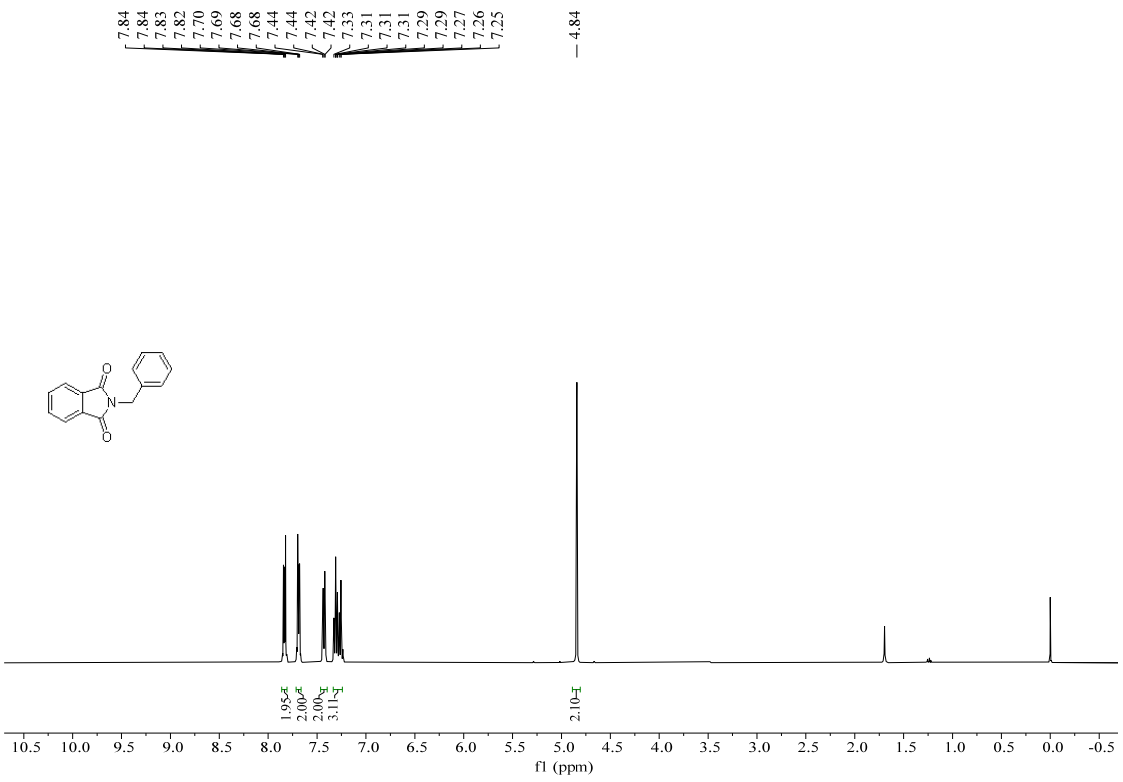
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7.29
7.27
7.26
7.25
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2.00
3.11
2.10
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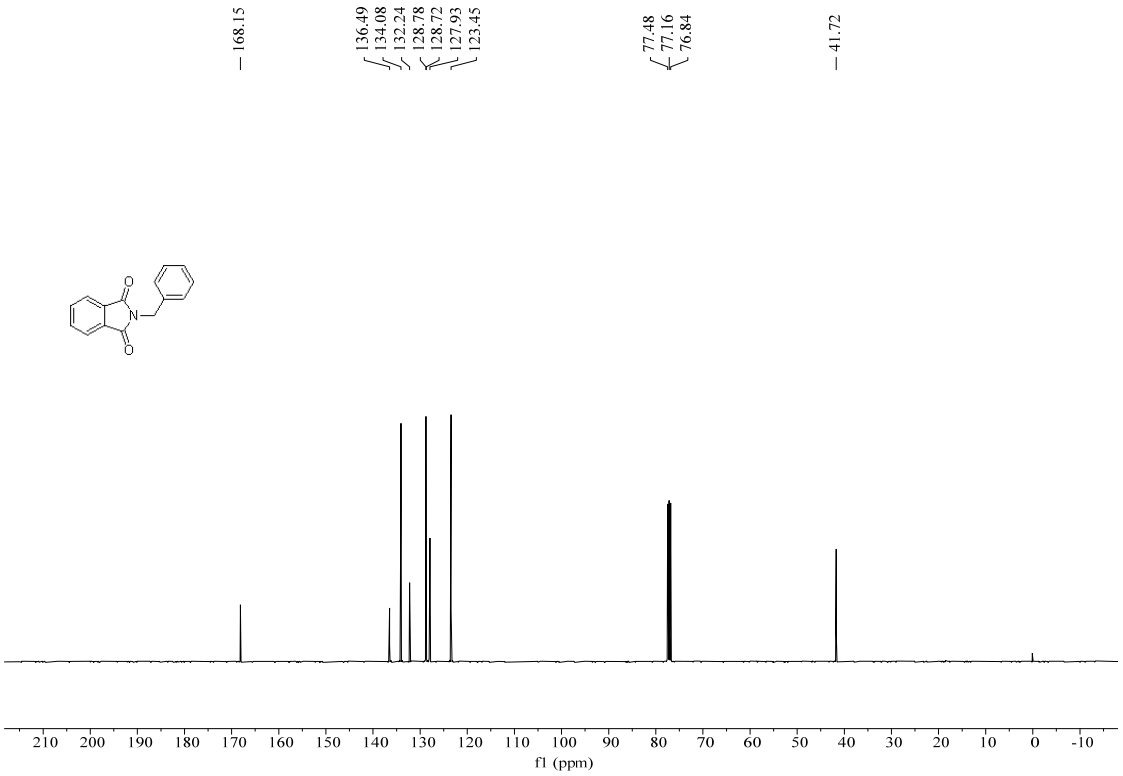
f1 (ppm)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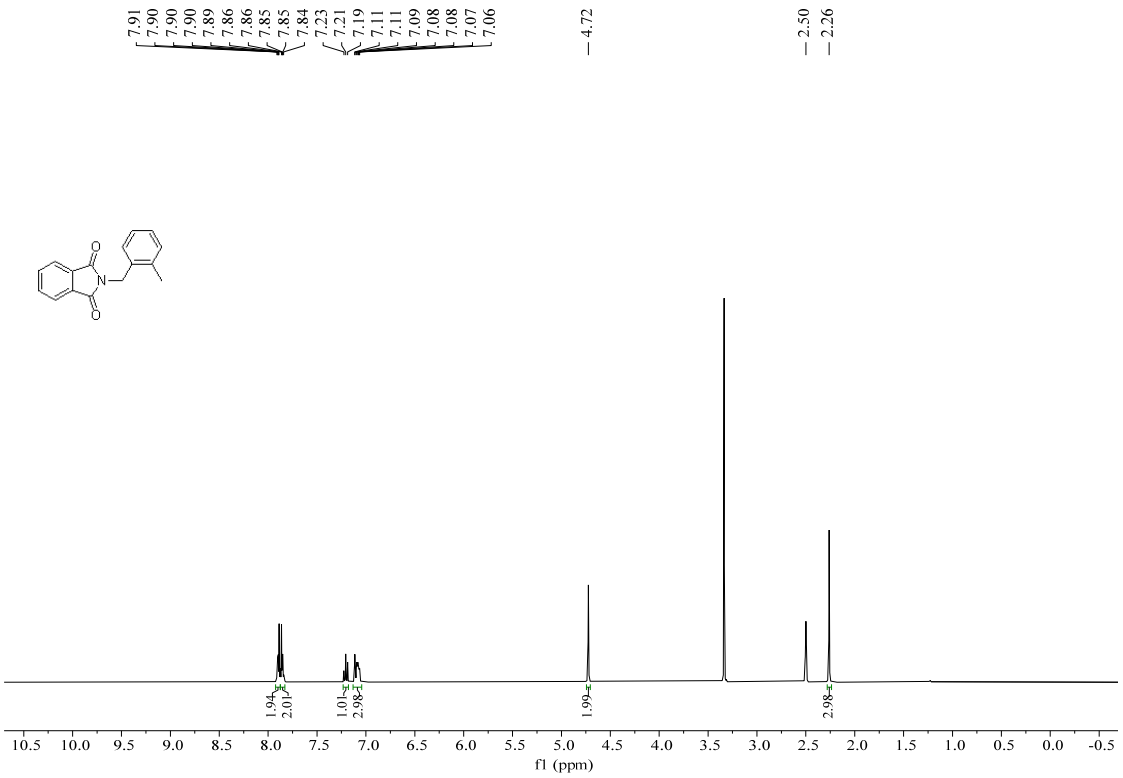
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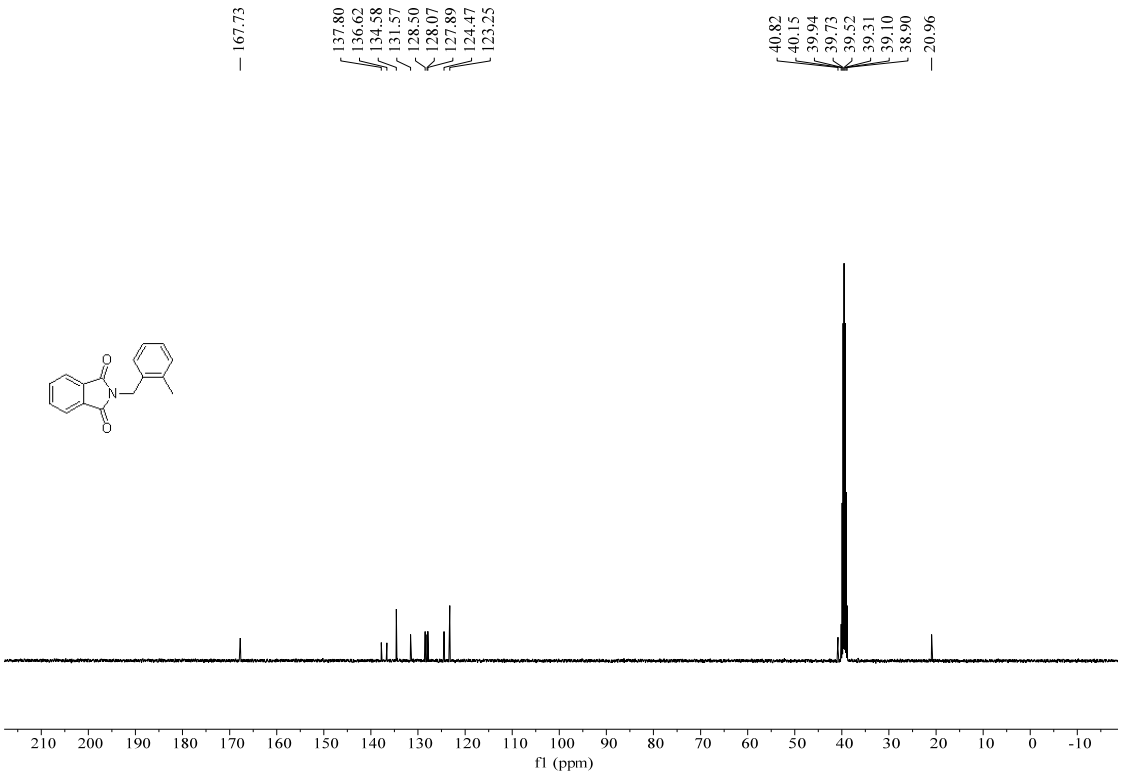
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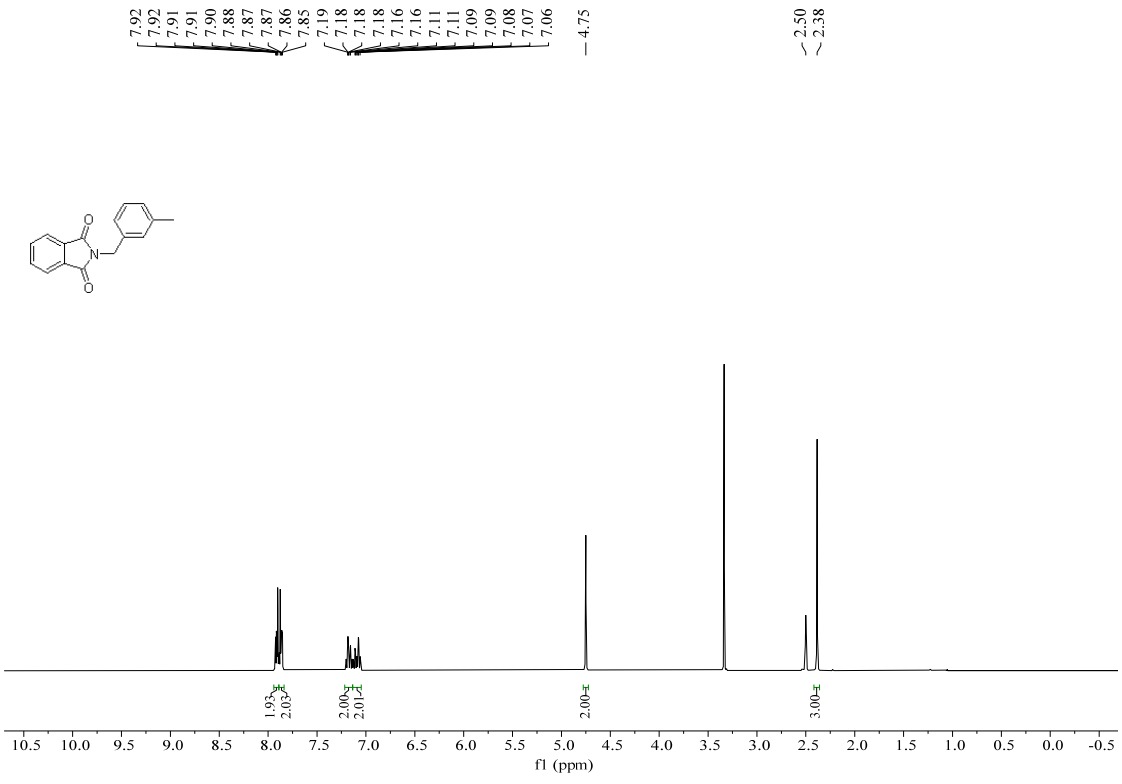
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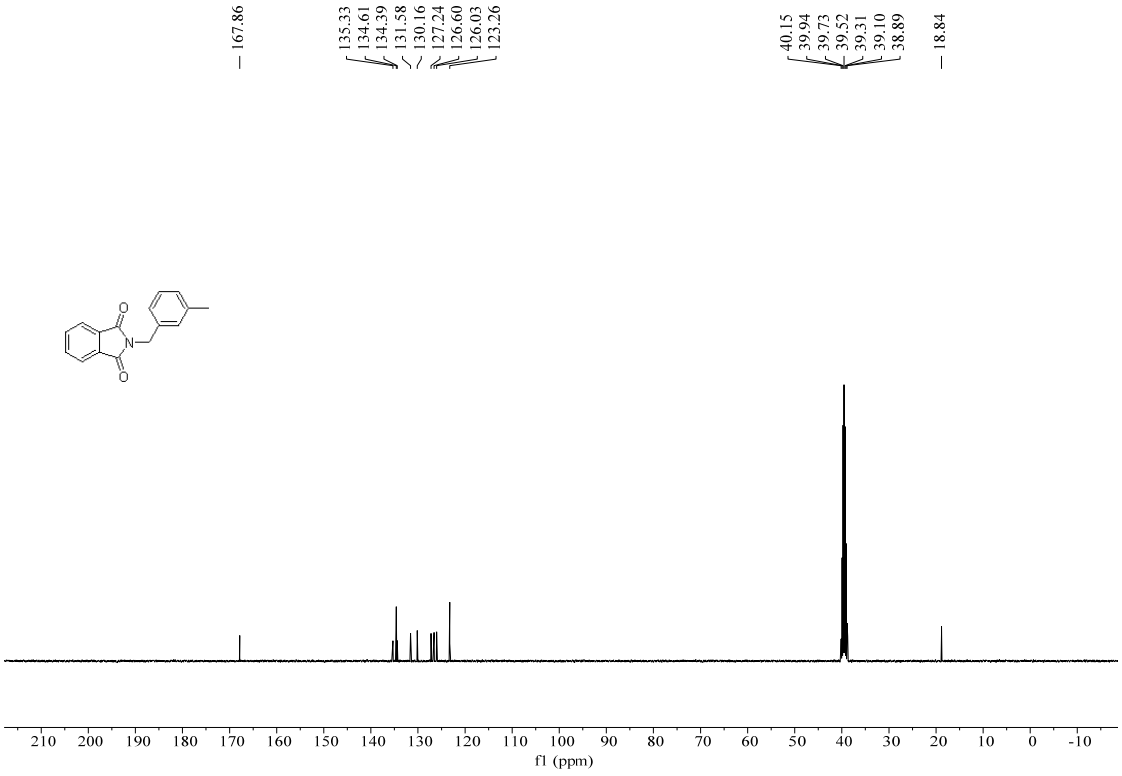
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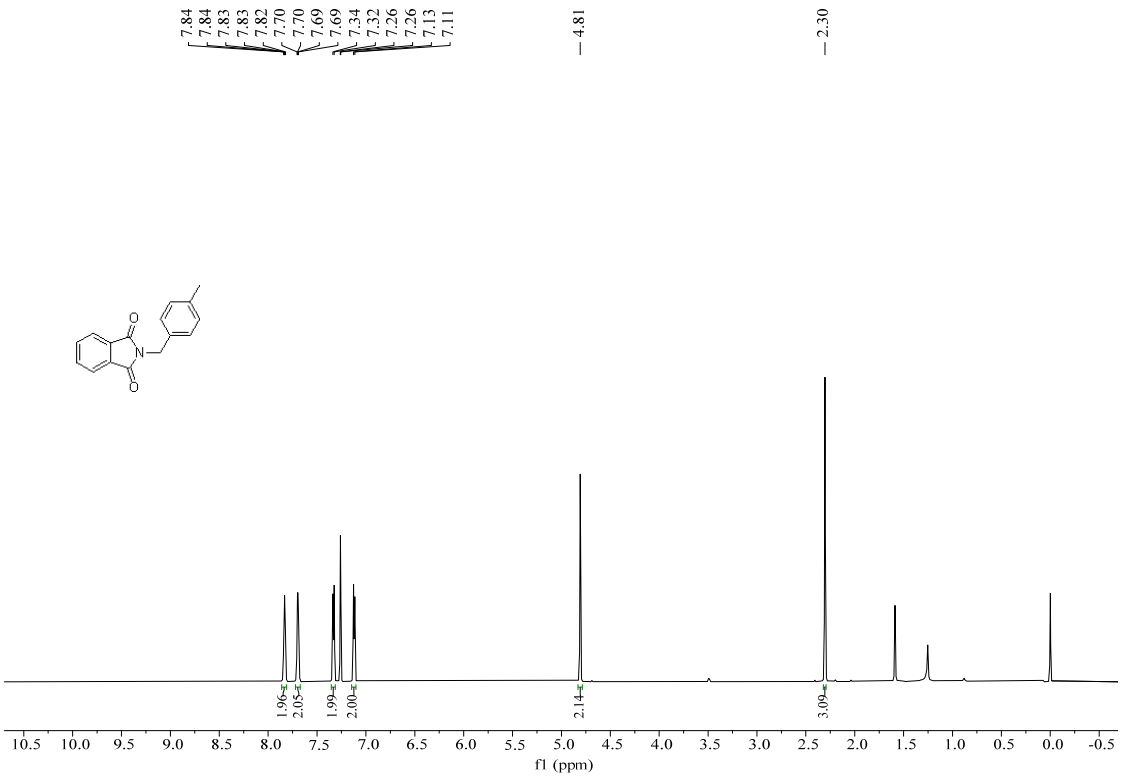
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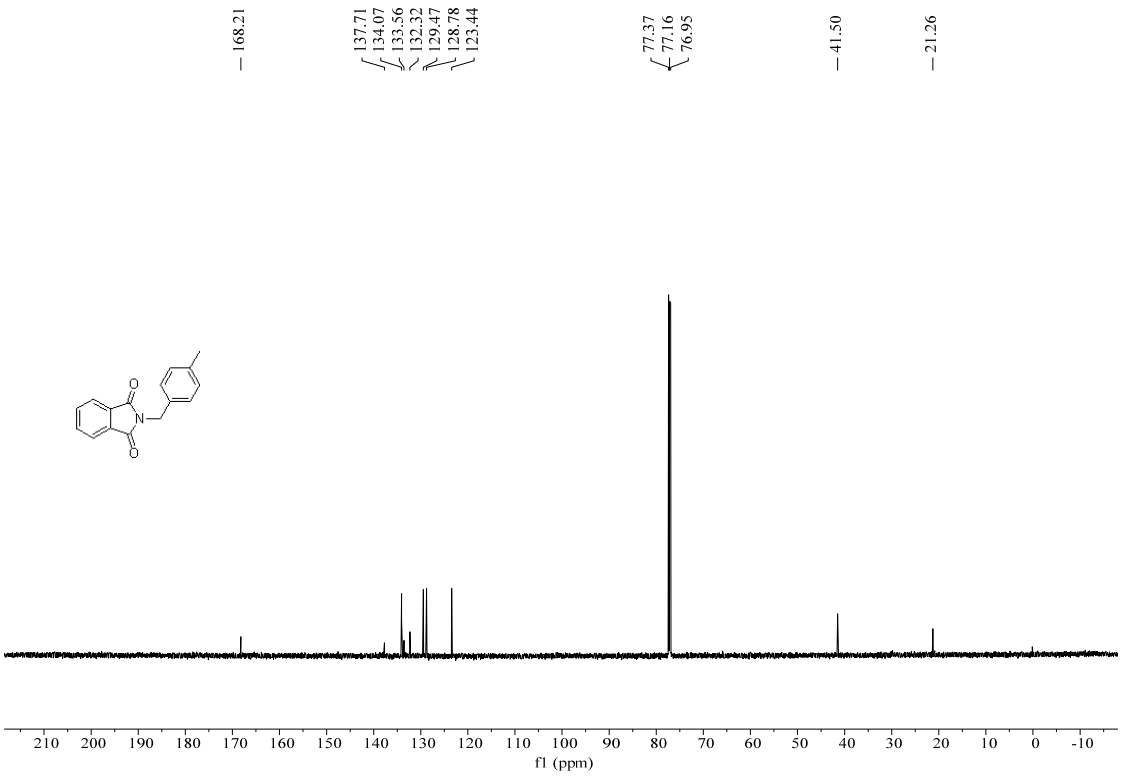
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f1 (ppm)

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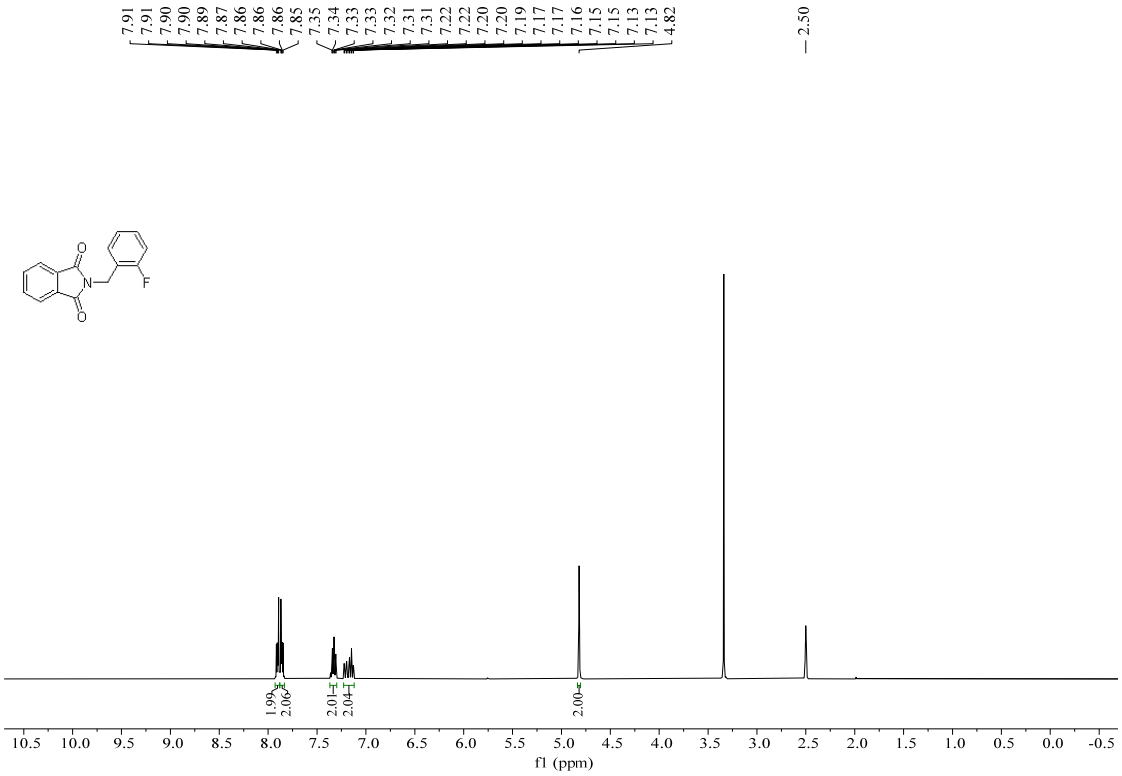
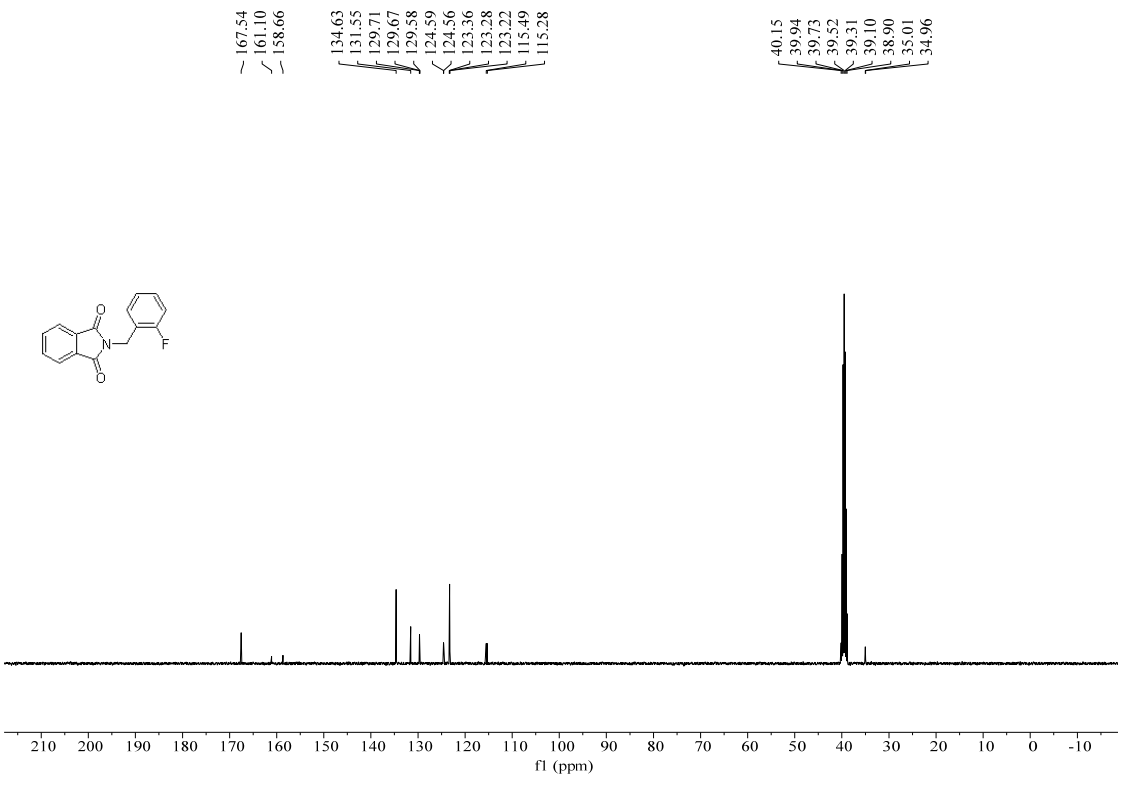

7.91
7.91
7.90
7.90
7.89
7.87
7.86
7.86
7.86
7.85
7.35
7.34
7.33
7.33
7.32
7.31
7.31
7.22
7.22
7.20
7.20
7.19
7.17
7.17
7.16
7.15
7.15
7.13
7.13
4.82
2.50
O
N
F
O
1.90
2.06
2.01
2.04
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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161.10
158.66
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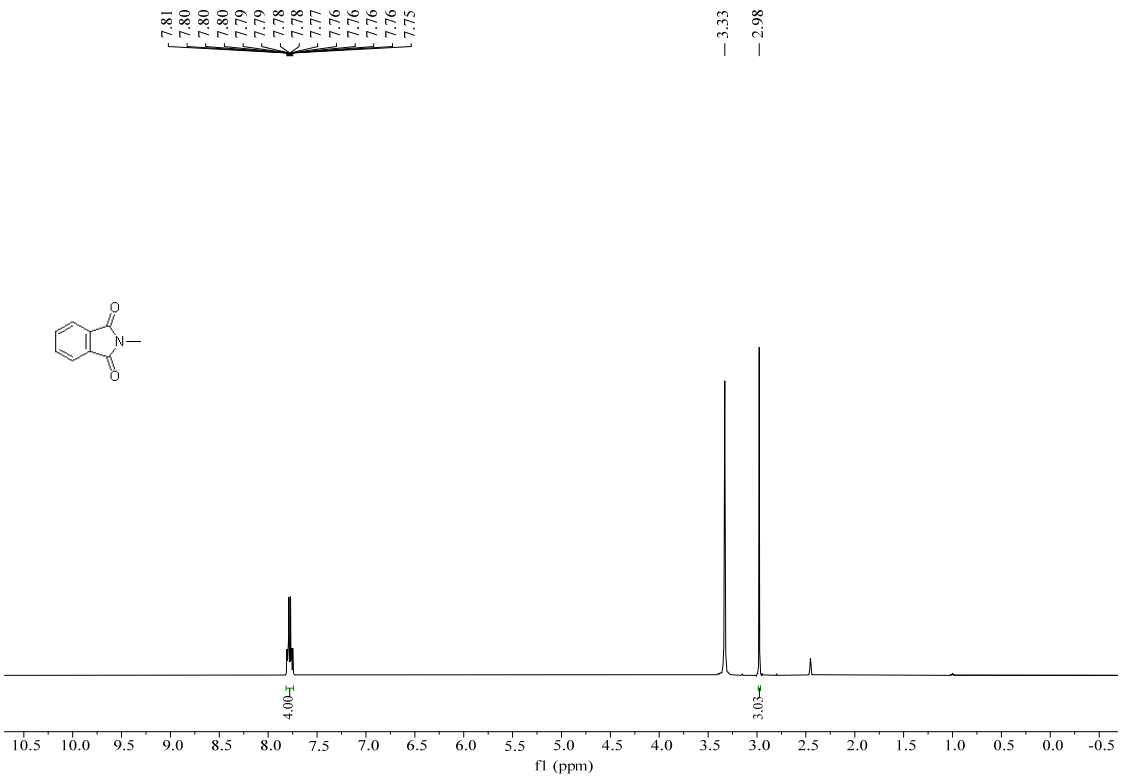
131.55
129.71
129.67
129.58
124.59
124.56
123.36
123.28
123.22
115.49
115.28
40.15
39.94
39.73
39.52
39.31
39.10
38.90
35.01
34.96
O
N
F
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

1af: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7.80
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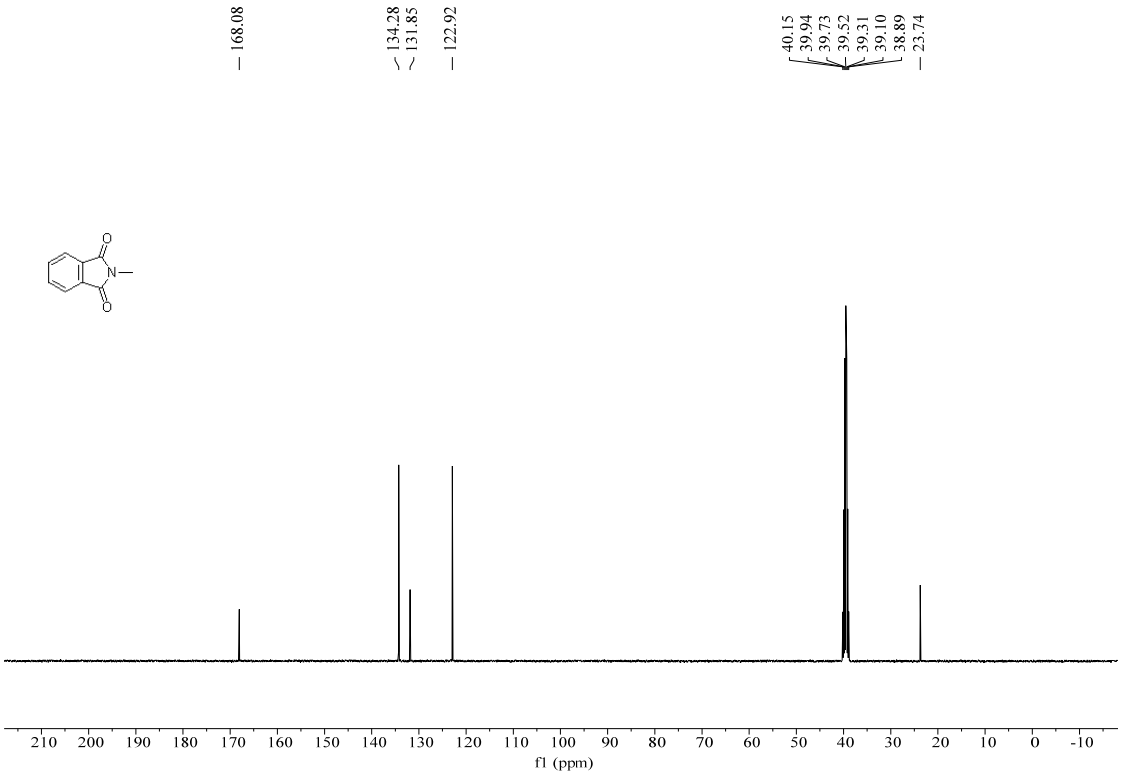
7.79
7.78
7.78
7.77
7.76
7.76
7.76
7.76
7.75
3.33
2.98
O
N
O
4.00
3.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


168.08
134.28
131.85
122.92
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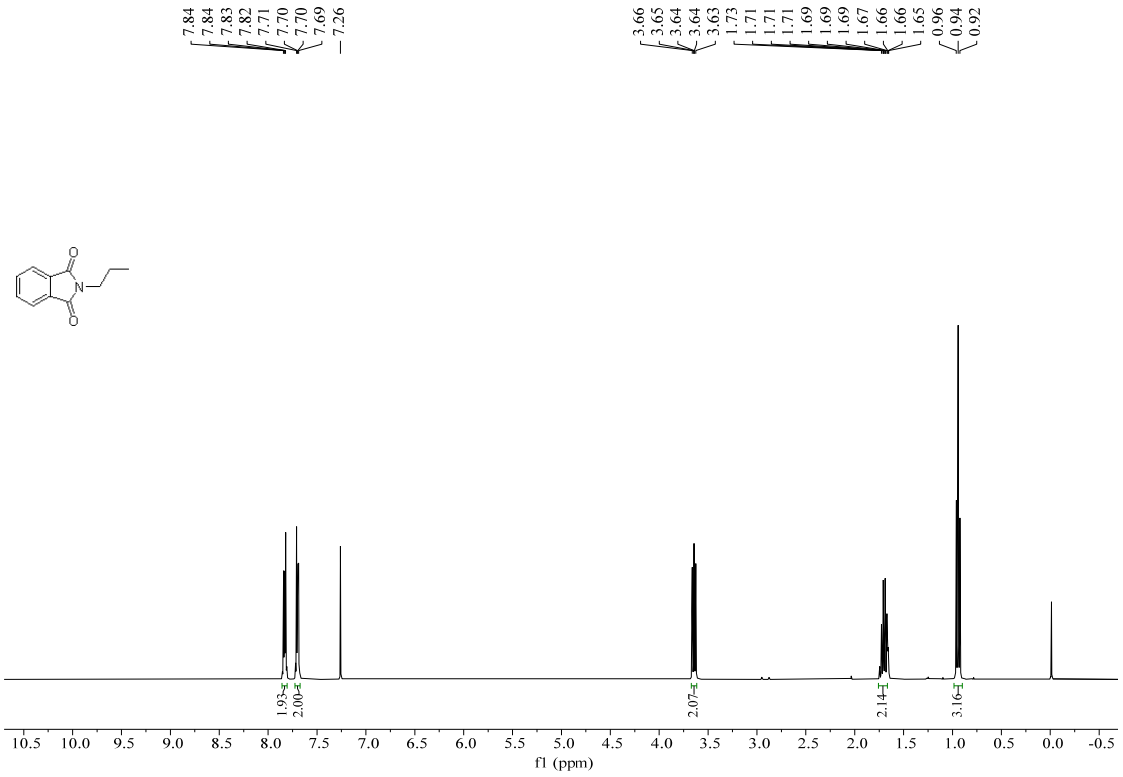
39.94
39.73
39.52
39.31
39.10
38.89
23.74
f1 (ppm)

1ag: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7.84
7.83
7.82
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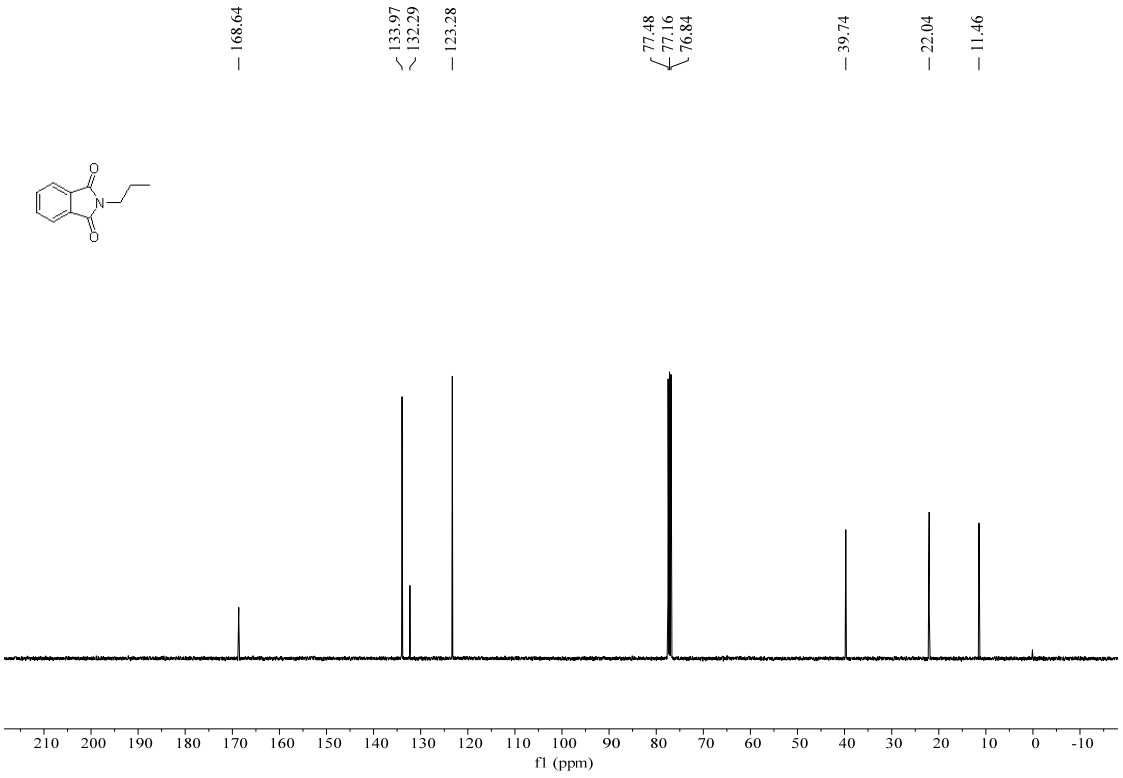
7.70
7.70
7.69
7.26
3.66
3.65
3.64
3.64
3.63
1.73
1.71
1.71
1.71
1.69
1.69
1.69
1.67
1.66
1.66
1.65
0.96
0.94
0.92
1.93
2.00
2.07
2.14
3.16
f1 (ppm)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133.97
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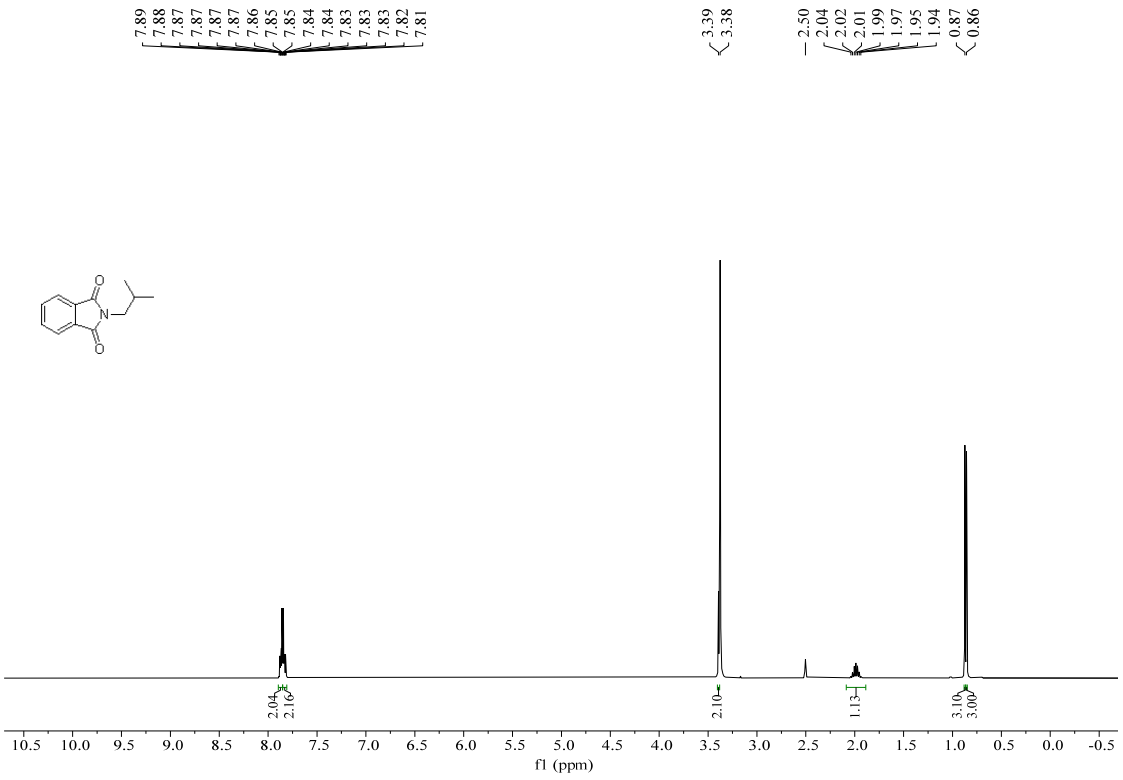
123.28
77.48
77.16
76.84
39.74
22.04
11.46
f1 (ppm)

1ah: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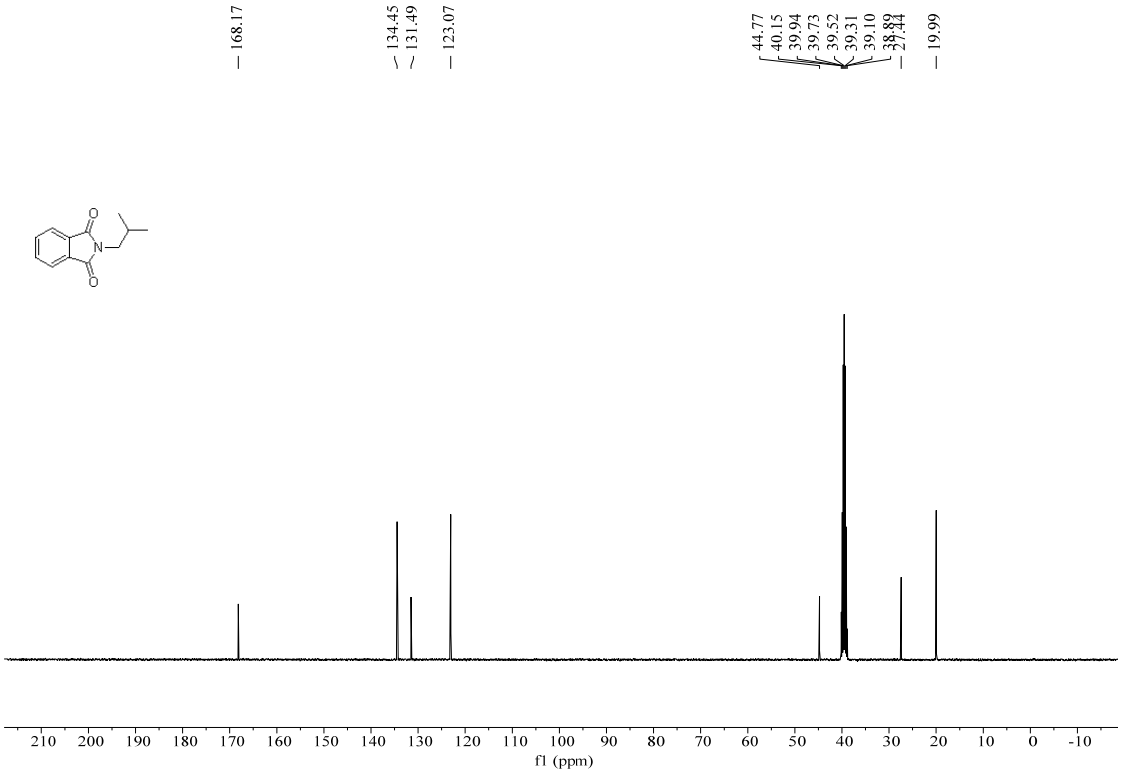
7.87
7.87
7.87
7.87
7.86
7.85
7.85
7.84
7.84
7.83
7.83
7.83
7.82
7.81
3.39
3.38
2.50
2.04
2.02
2.01
1.99
1.97
1.95
1.94
0.87
0.86
2.04
2.16
2.10
1.13
3.10
3.00
f1 (ppm)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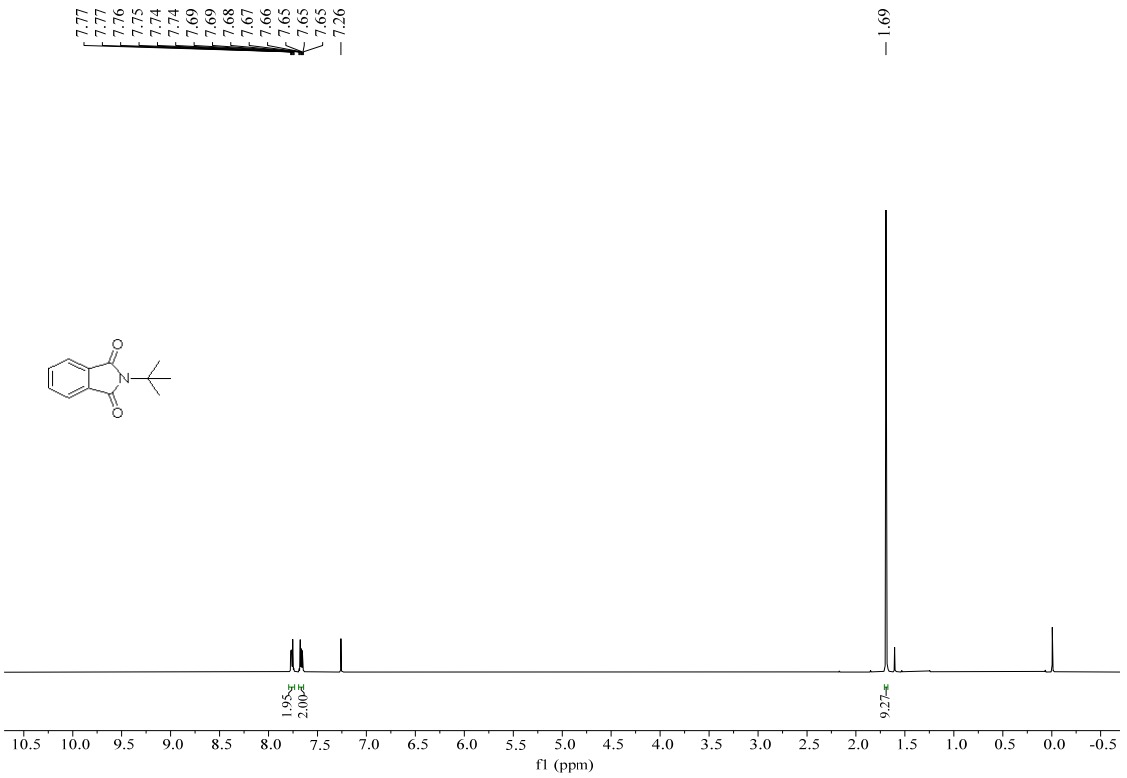
134.45
131.49
123.07
44.77
40.15
39.94
39.73
39.52
39.31
39.10
38.89
27.44
19.99
O
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

1ai: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7.76
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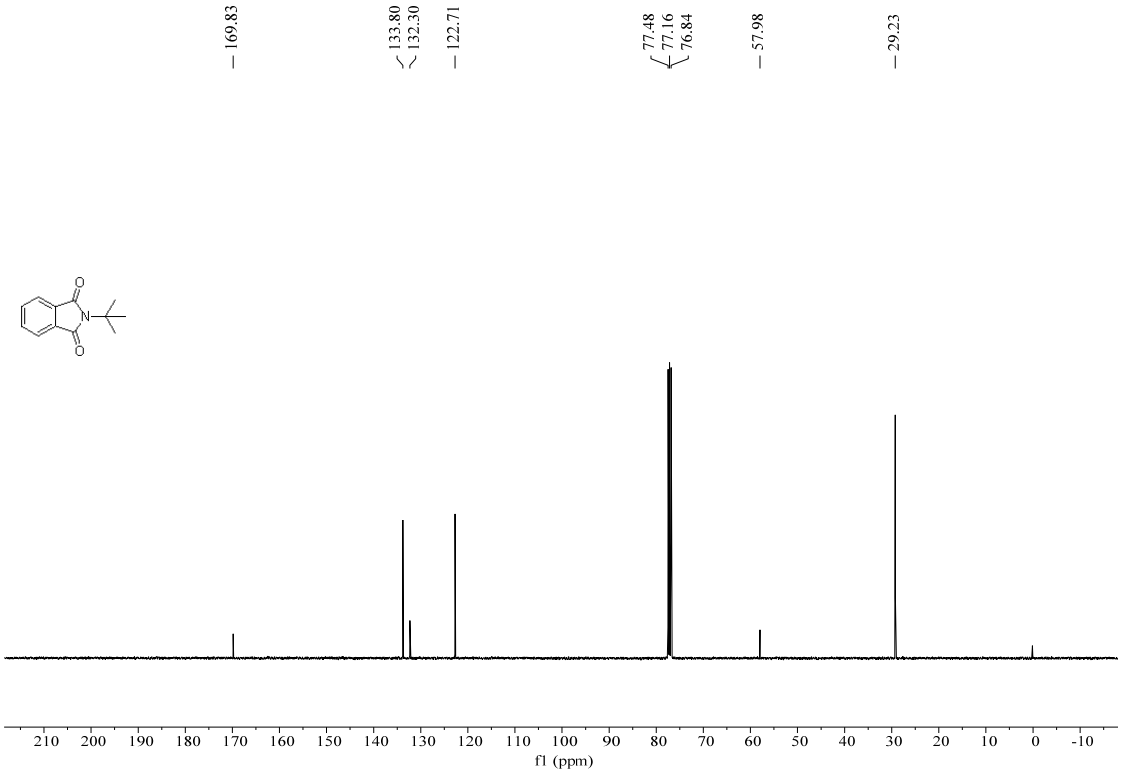
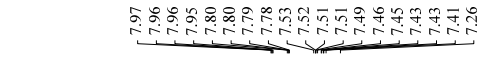
7.74
7.74
7.69
7.69
7.68
7.67
7.66
7.65
7.65
7.26
1.69
1.95
2.00
9.27
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


169.83
133.80
132.30
122.71
77.48
77.16
76.84
57.98
29.23
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

1aj: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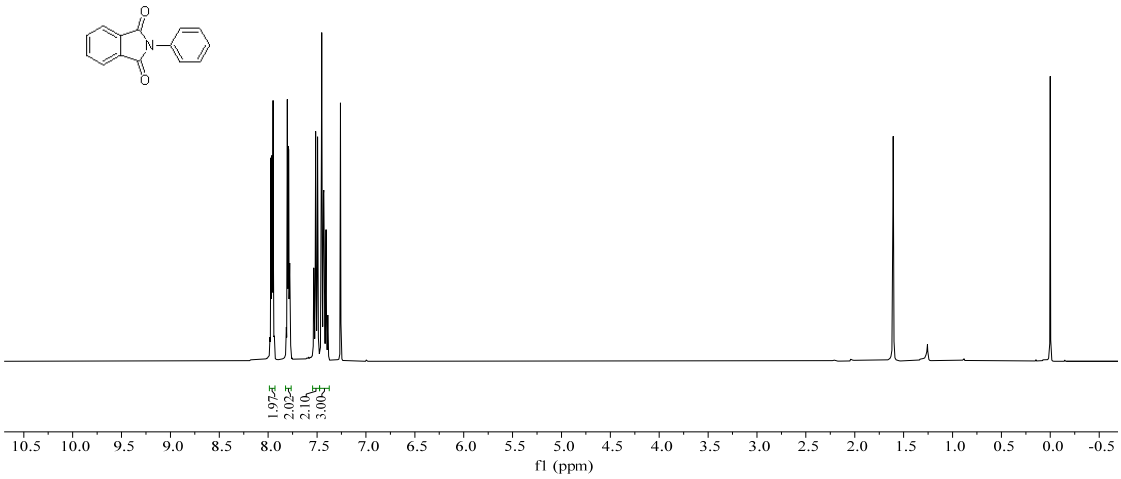
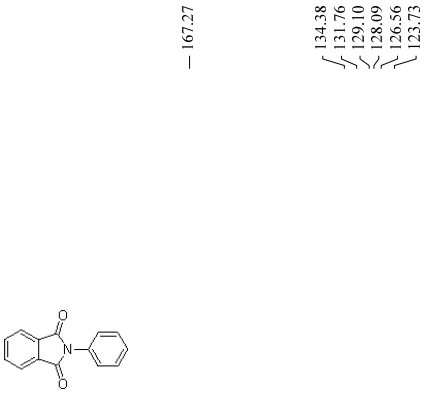
7.96
7.96
7.95
7.80
7.80
7.79
7.78
7.53
7.52
7.51
7.51
7.49
7.46
7.45
7.43
7.43
7.41
7.26


1.97
2.02
2.10
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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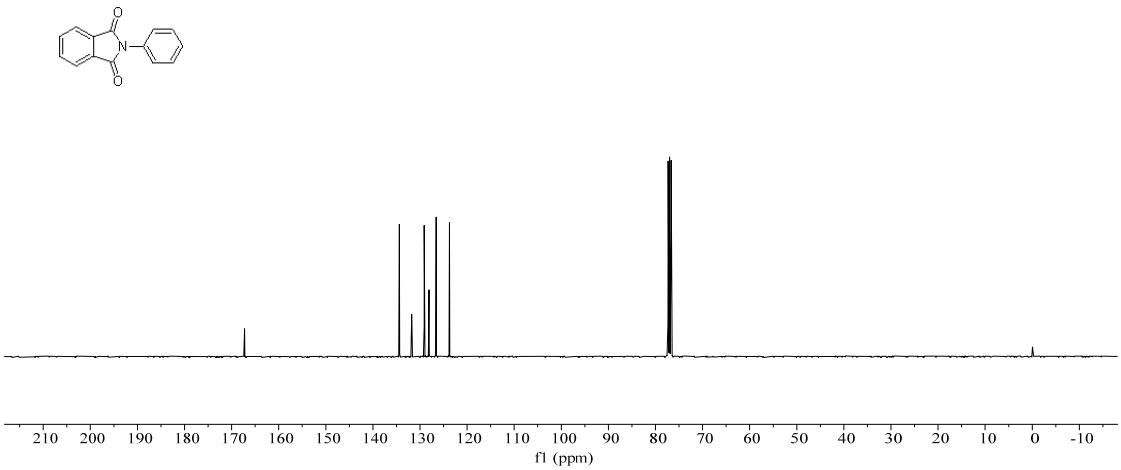
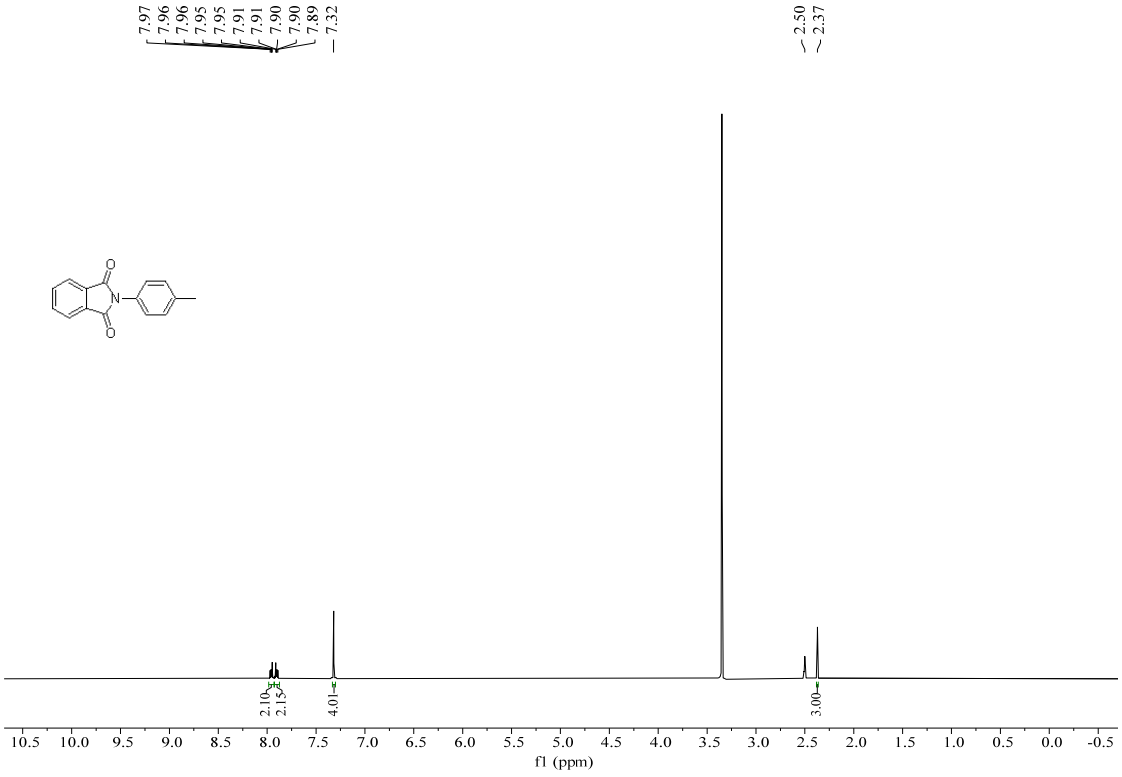
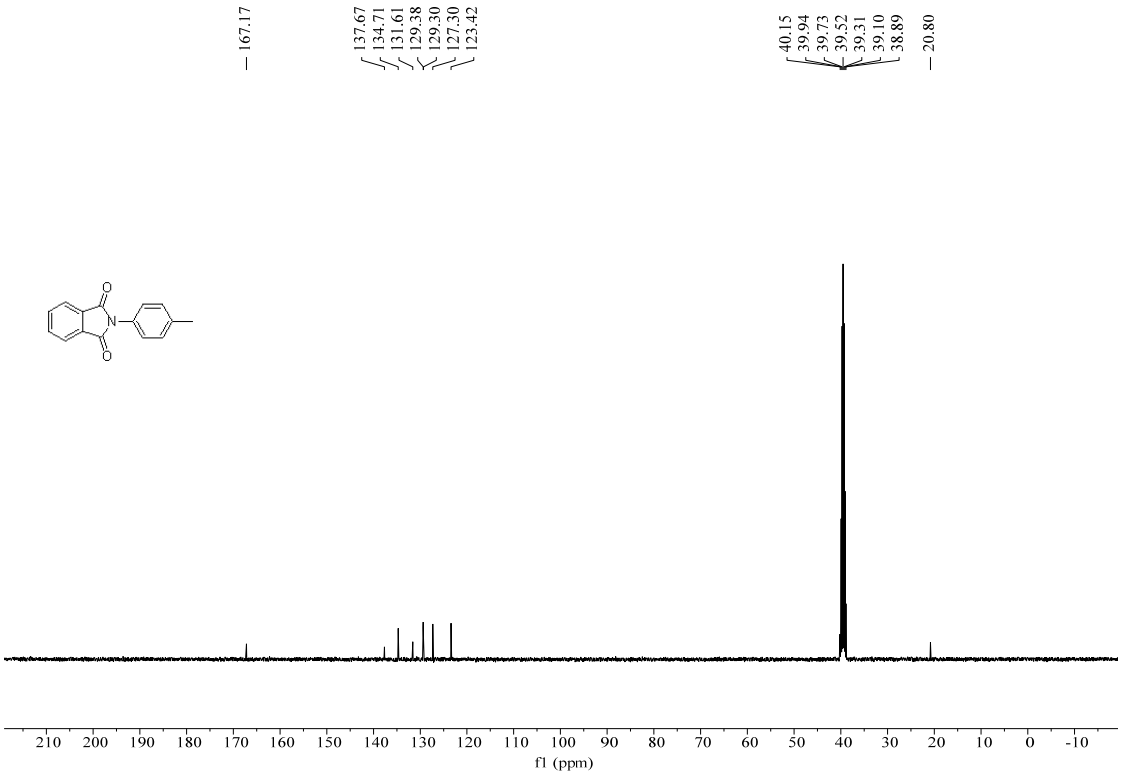
134.38
131.76
129.10
128.09
126.56
123.73

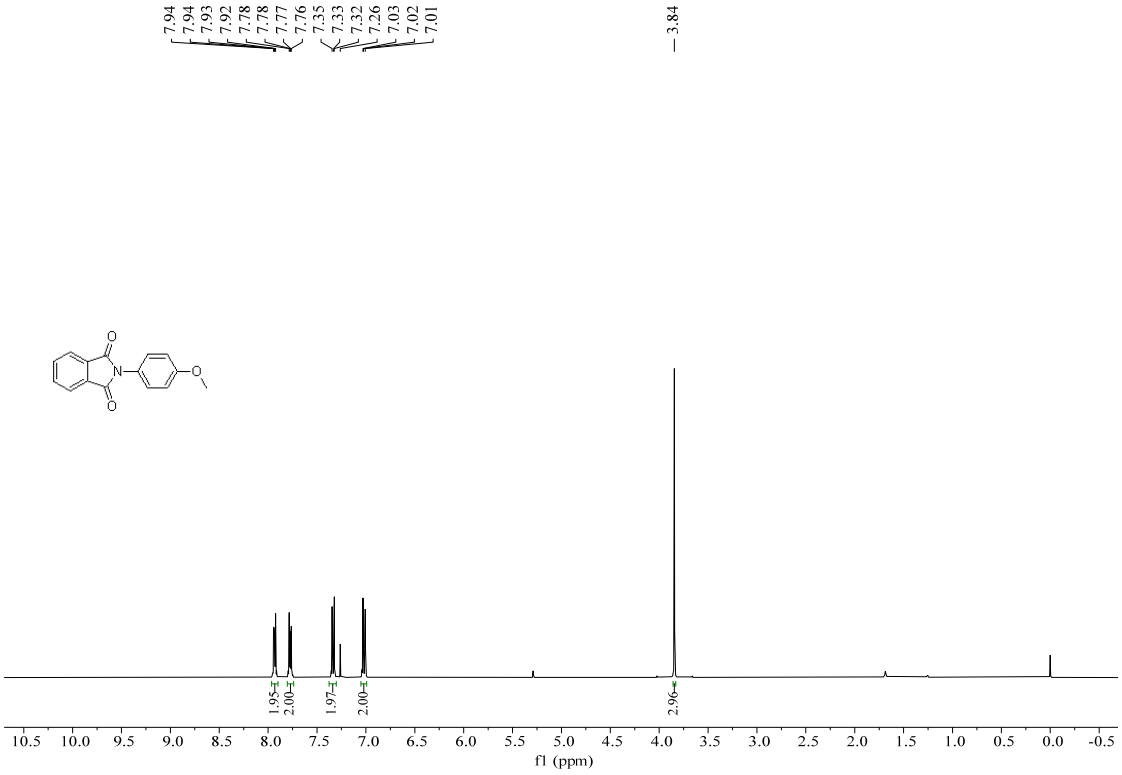

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

1ak:


7.97
7.96
7.96
7.95
7.95
7.91
7.91
7.90
7.90
7.89
7.32
2.50
2.37
O
N
O
2.10
2.15
4.01
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


167.17
137.67
134.71
131.61
129.38
129.30
127.30
123.42
40.15
39.94
39.73
39.52
39.31
39.10
38.89
20.80
f1 (ppm)

1al:


7.94
7.94
7.93
7.92
7.78
7.78
7.77
7.76
7.35
7.33
7.32
7.26
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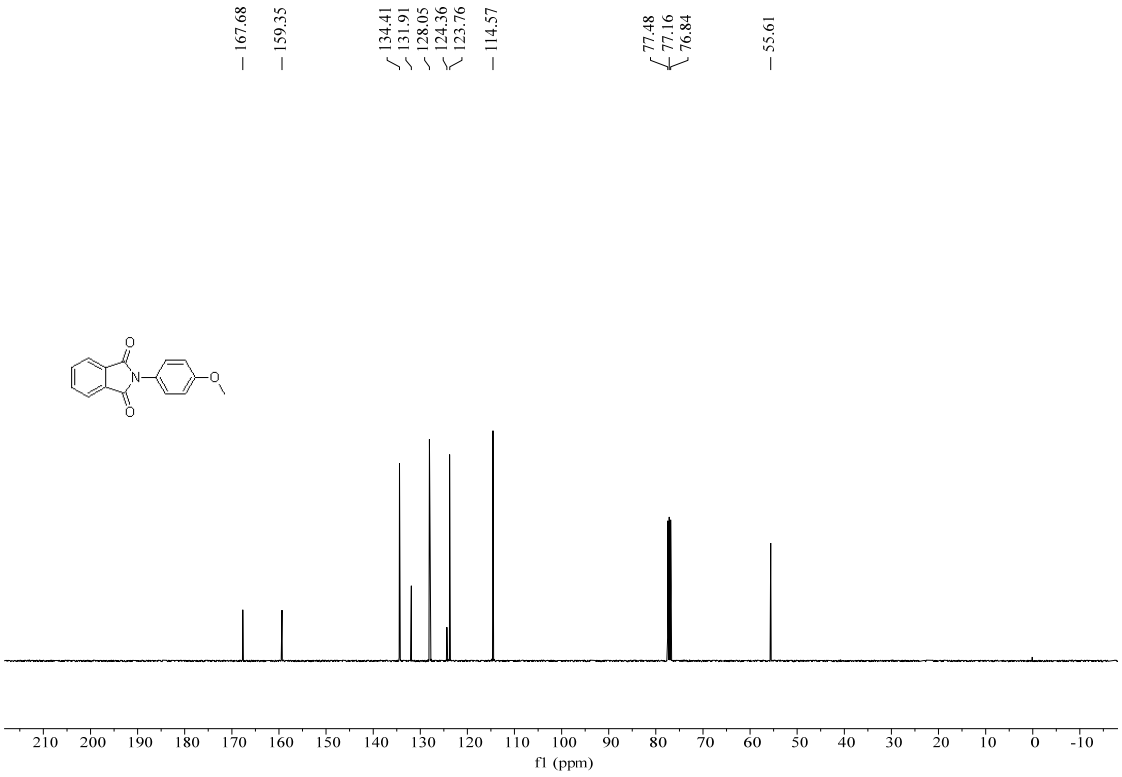
7.02
7.01
3.84
1.95
2.00
1.97
2.00
2.96
f1 (ppm)


167.68
159.35
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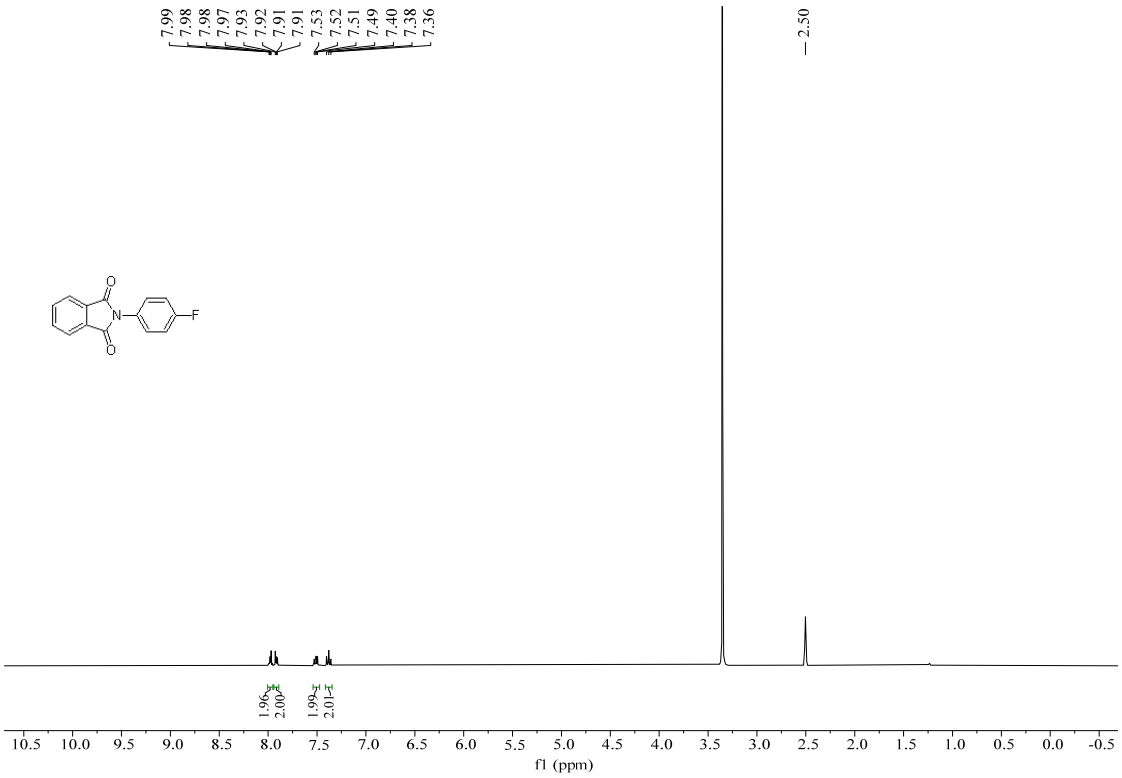
131.91
128.05
124.36
123.76
114.57
77.48
77.16
76.84
55.61
O
N
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

1am: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7.97
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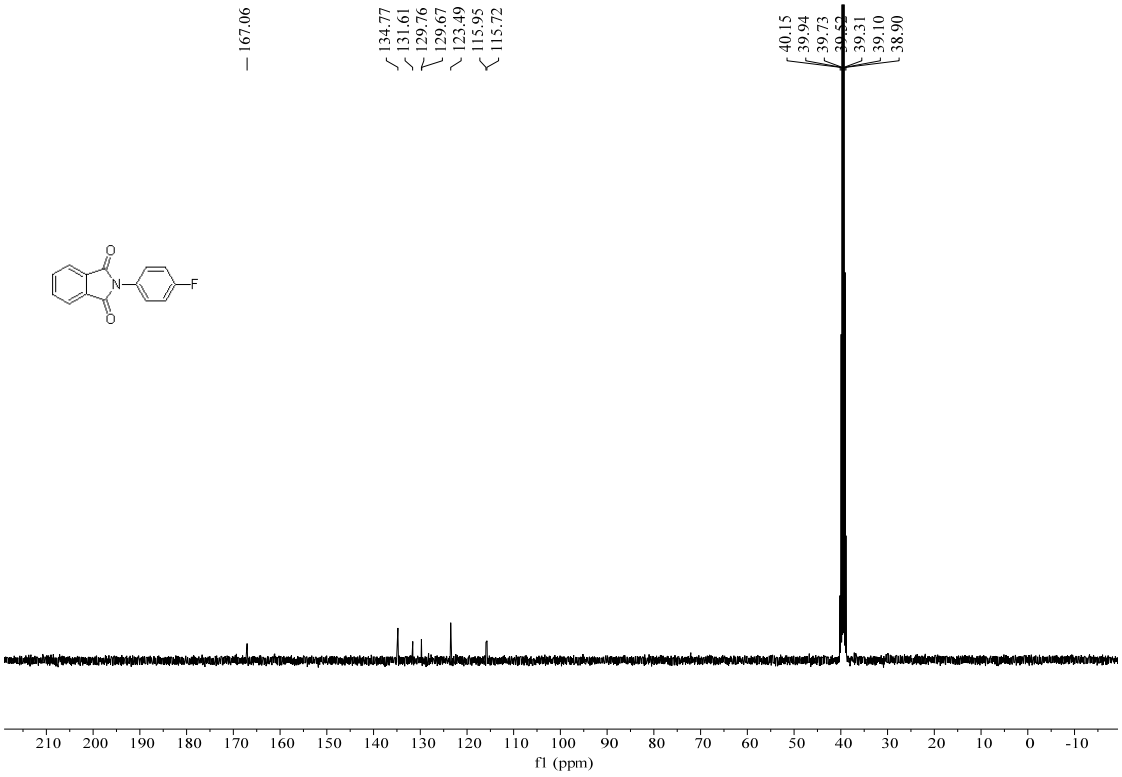
7.92
7.91
7.91
7.53
7.52
7.51
7.49
7.40
7.38
7.36
2.50
O
N
F
O
1.96
2.00
1.90
2.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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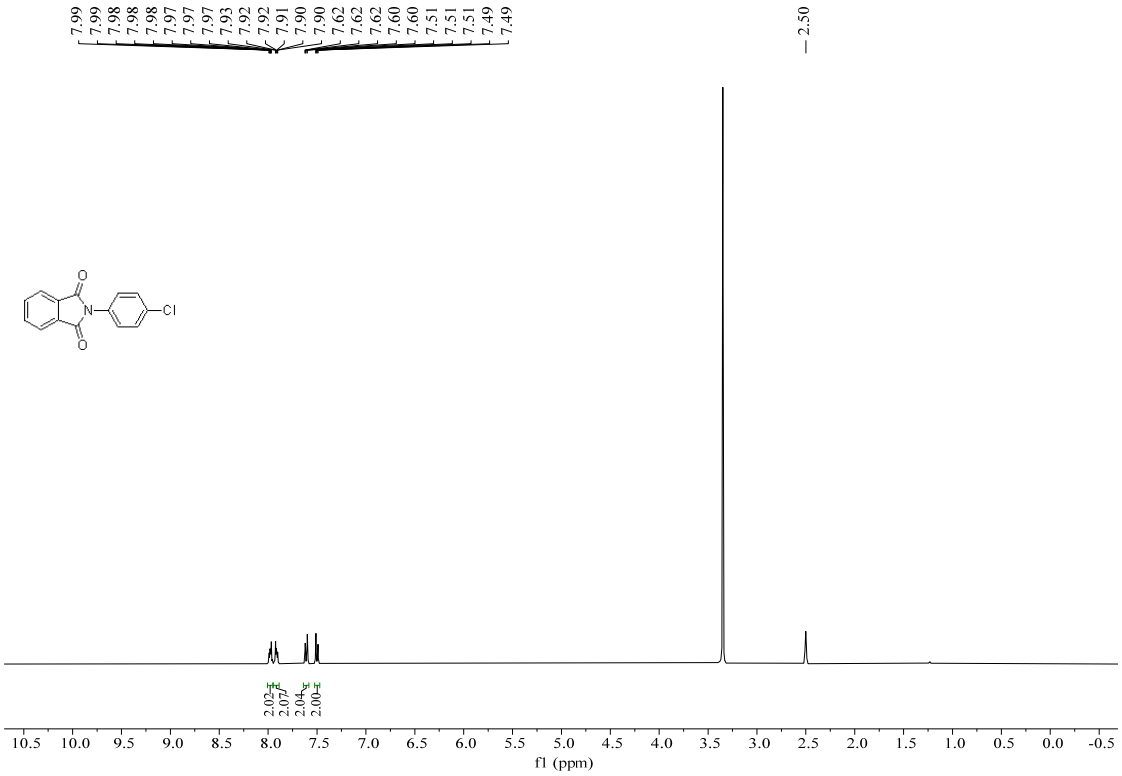
131.61
129.76
129.67
123.49
115.95
115.72
40.15
39.94
39.73
39.52
39.31
39.10
38.90
O
N
F
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

1an: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7.99
7.98
7.98
7.98
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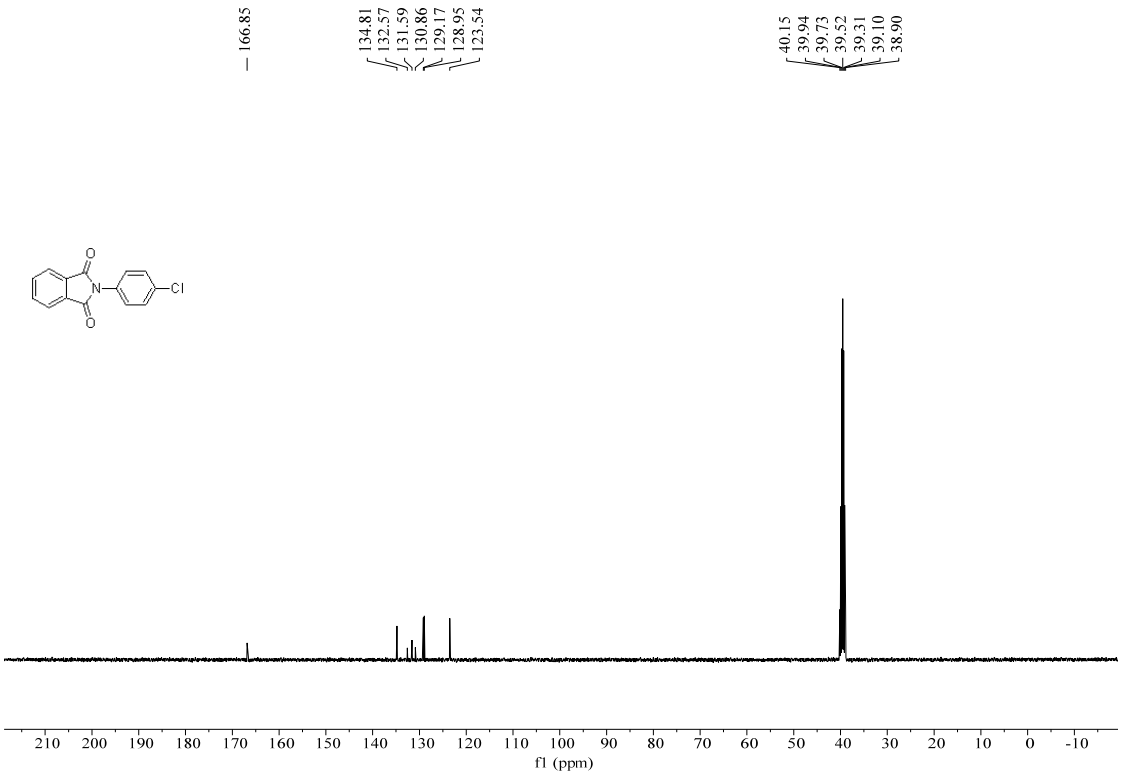
7.97
7.93
7.92
7.92
7.91
7.90
7.90
7.62
7.62
7.62
7.60
7.60
7.51
7.51
7.51
7.49
7.49
2.50
O
N
O
Cl
2.02
2.07
2.04
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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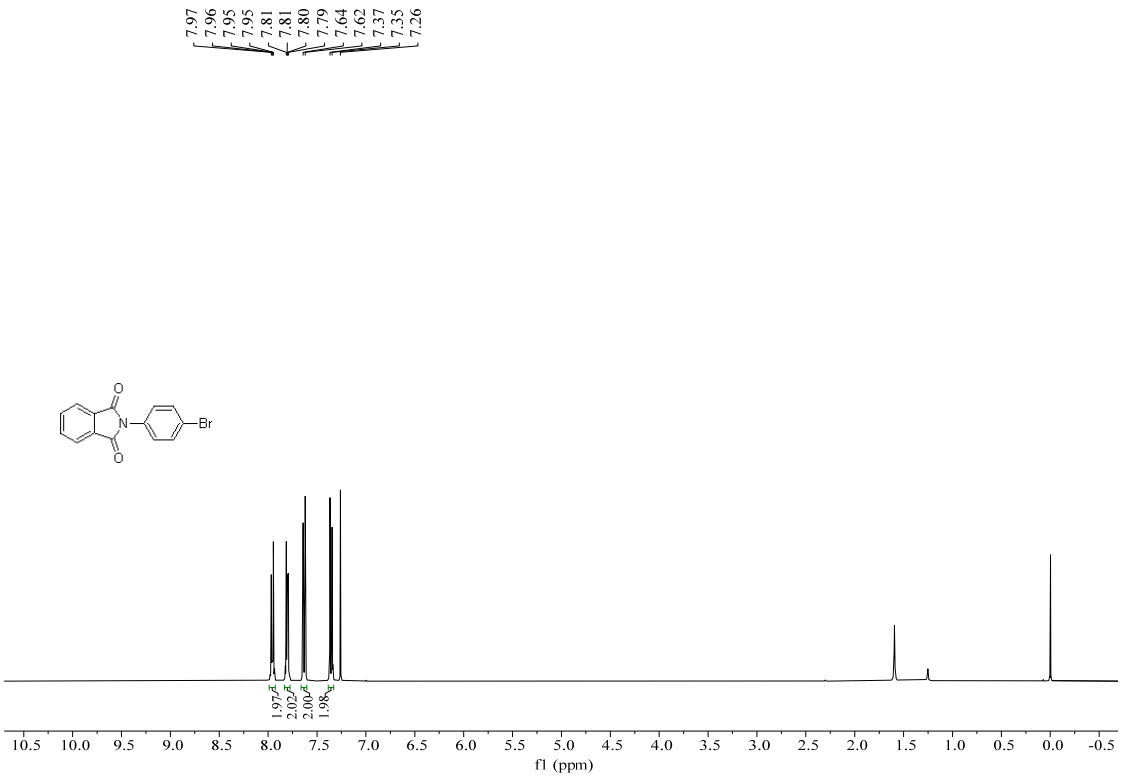
131.59
130.86
129.17
128.95
123.54
40.15
39.94
39.73
39.52
39.31
39.10
38.90
O
N
O
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

1ao: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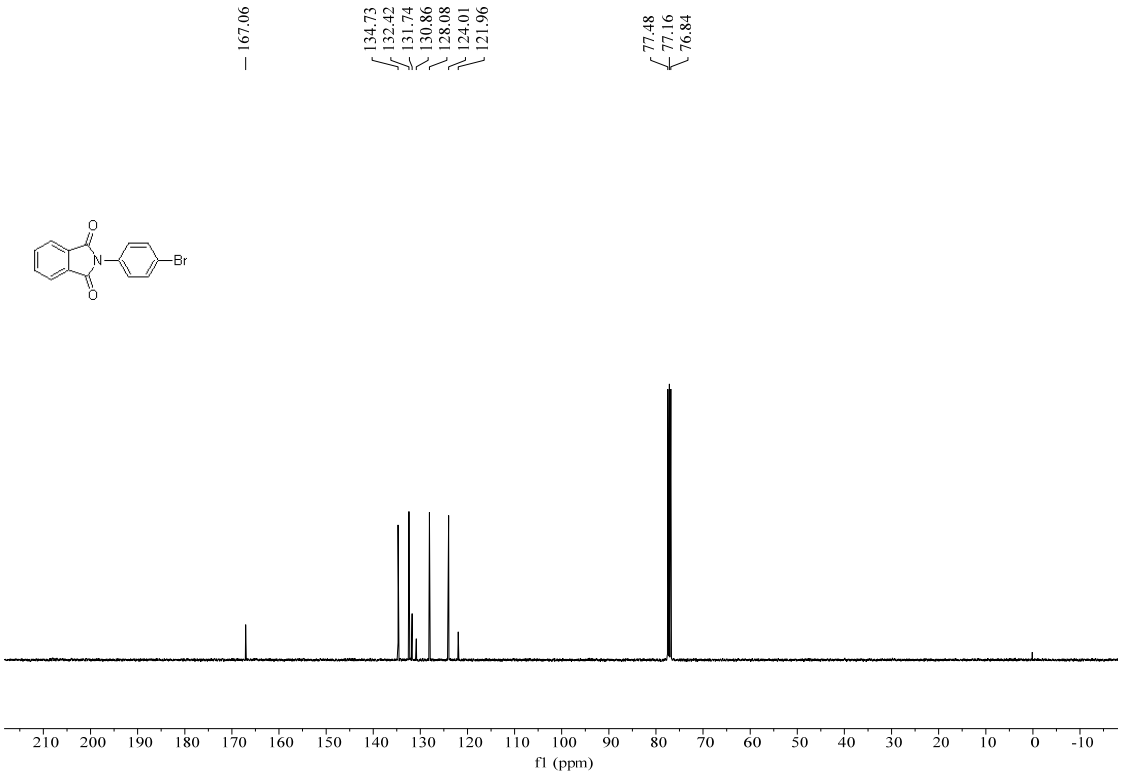
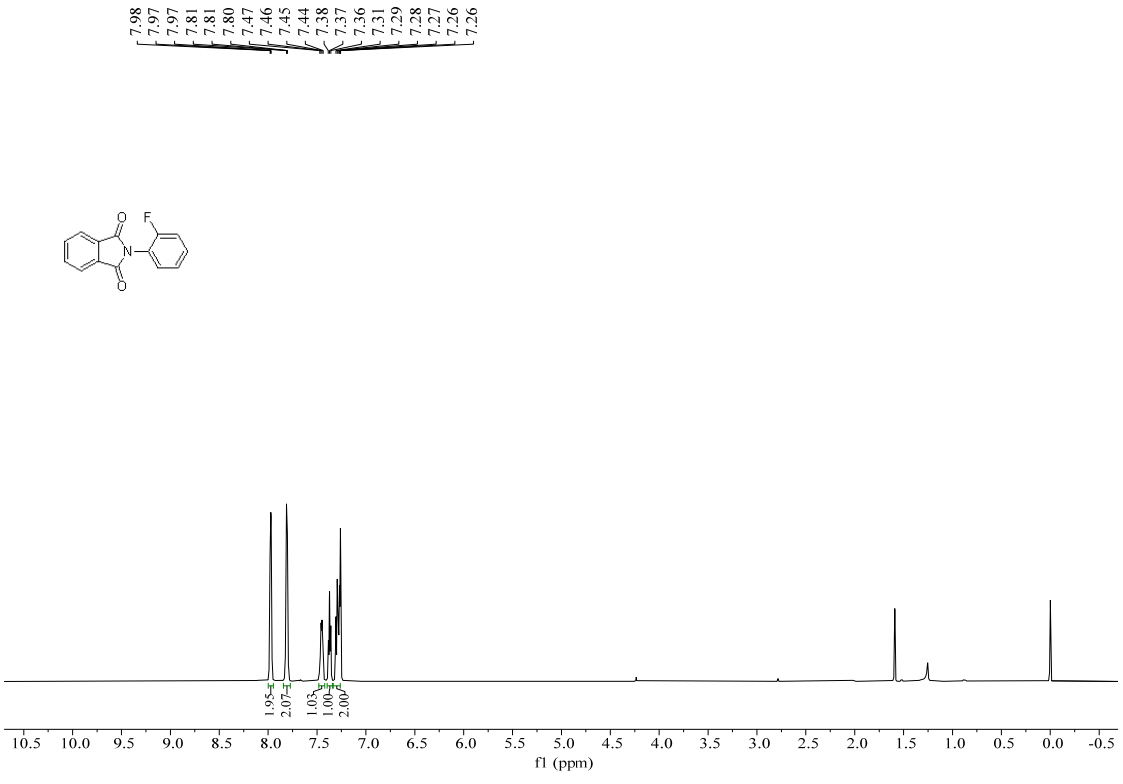
7.96
7.95
7.95
7.81
7.81
7.80
7.79
7.64
7.62
7.37
7.35
7.26
O
N
Br
O
1.97
2.02
2.00
1.98
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


167.06
134.73
132.42
131.74
130.86
128.08
124.01
121.96
77.48
77.16
76.84
Br
f1 (ppm)

1ap: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7.97
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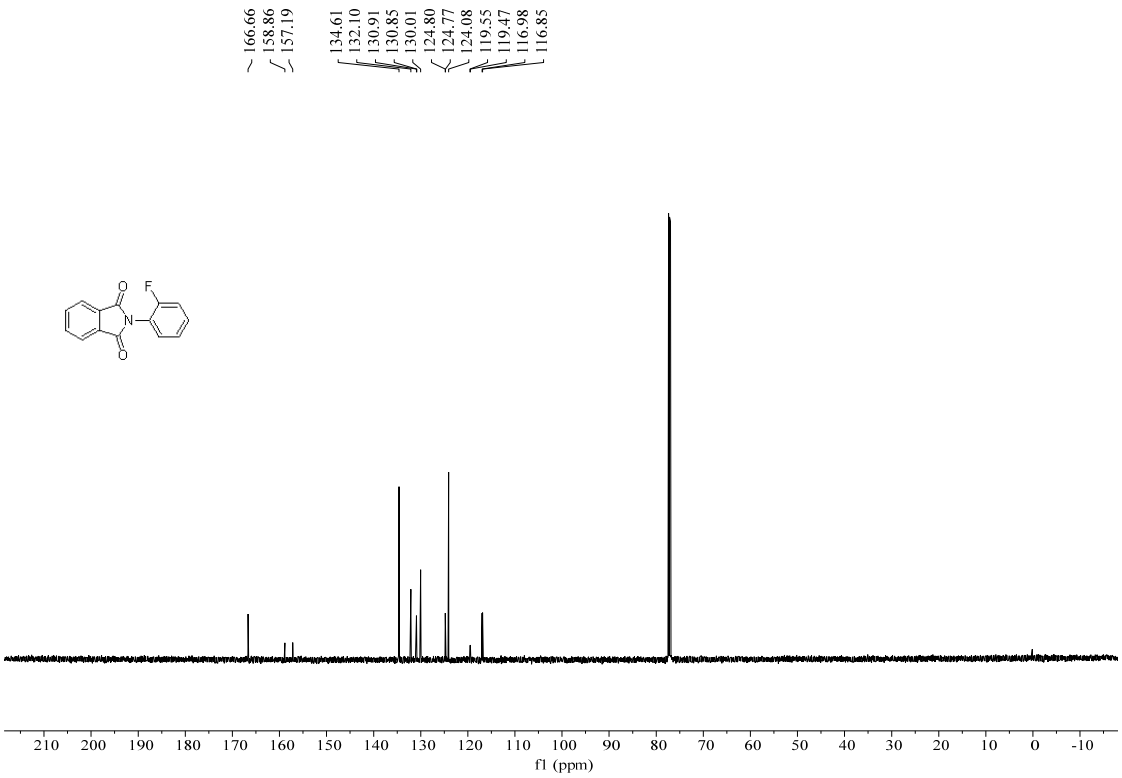
7.81
7.80
7.47
7.46
7.45
7.44
7.38
7.37
7.36
7.31
7.29
7.28
7.27
7.26
7.26
F
1.95
2.07
1.03
1.00
2.00
f1 (ppm)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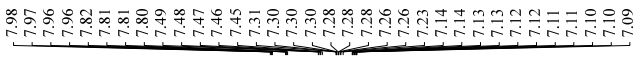
130.91
130.85
130.01
124.80
124.77
124.08
119.55
119.47
116.98
116.85
O
F
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

1aq:


7.98
7.97
7.96
7.96
7.82
7.81
7.81
7.80
7.49
7.48
7.47
7.46
7.45
7.31
7.30
7.30
7.30
7.28
7.28
7.28
7.26
7.26
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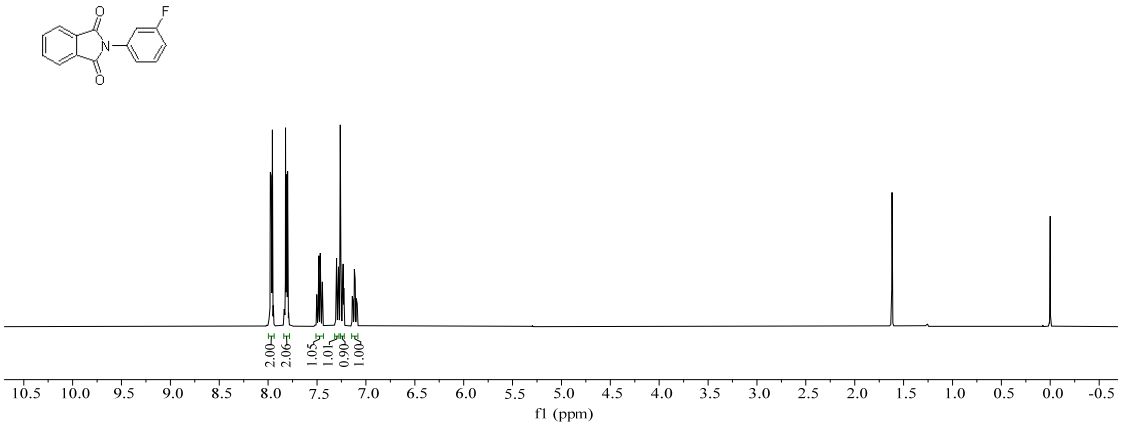
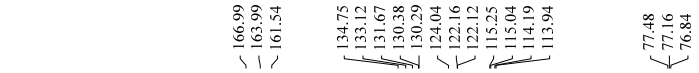
7.13
7.13
7.12
7.12
7.11
7.11
7.10
7.10
7.09


O
F
N
O
2.00
2.06
1.05
1.01
0.90
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


166.99
163.99
161.54
134.75
133.12
131.67
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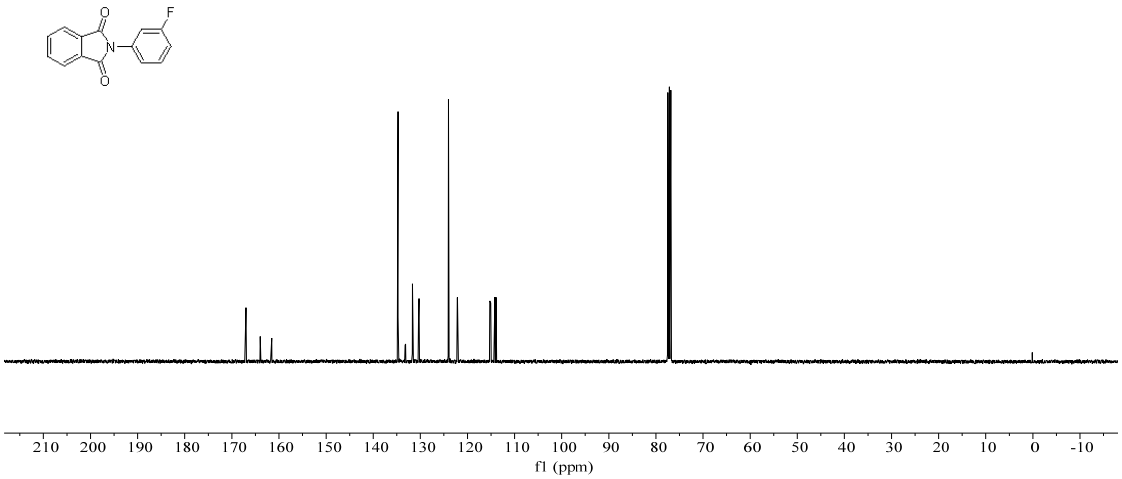
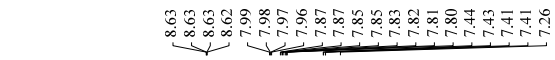
130.29
124.04
122.16
122.12
115.25
115.04
114.19
113.94
77.48
77.16
76.84


O
F
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

1ar:


8.63
8.63
8.63
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7.97
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7.85
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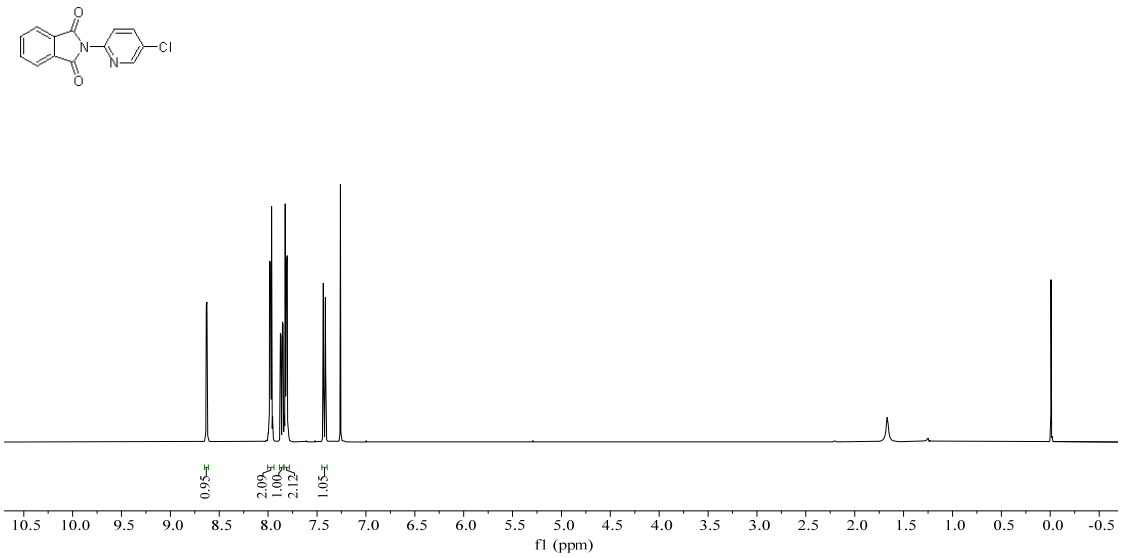
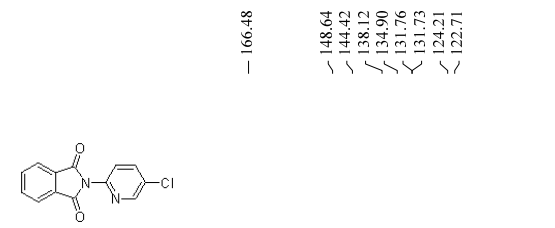
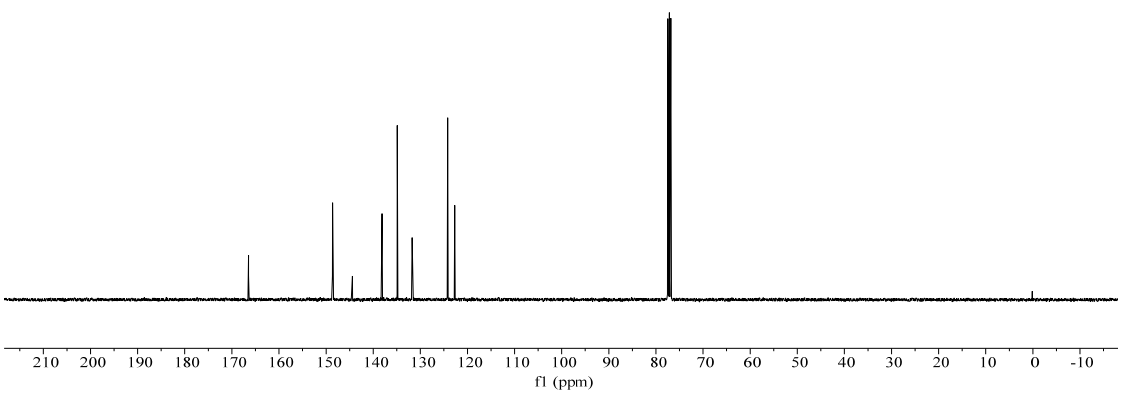
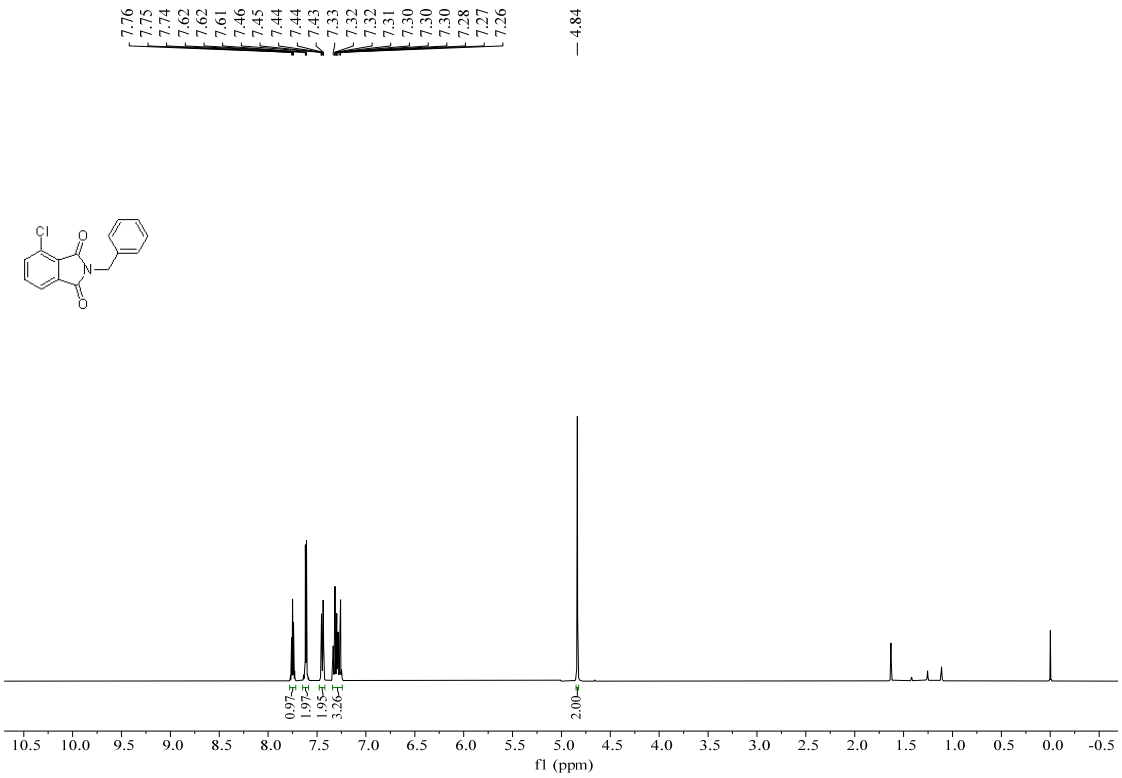
7.80
7.44
7.43
7.41
7.41
7.26

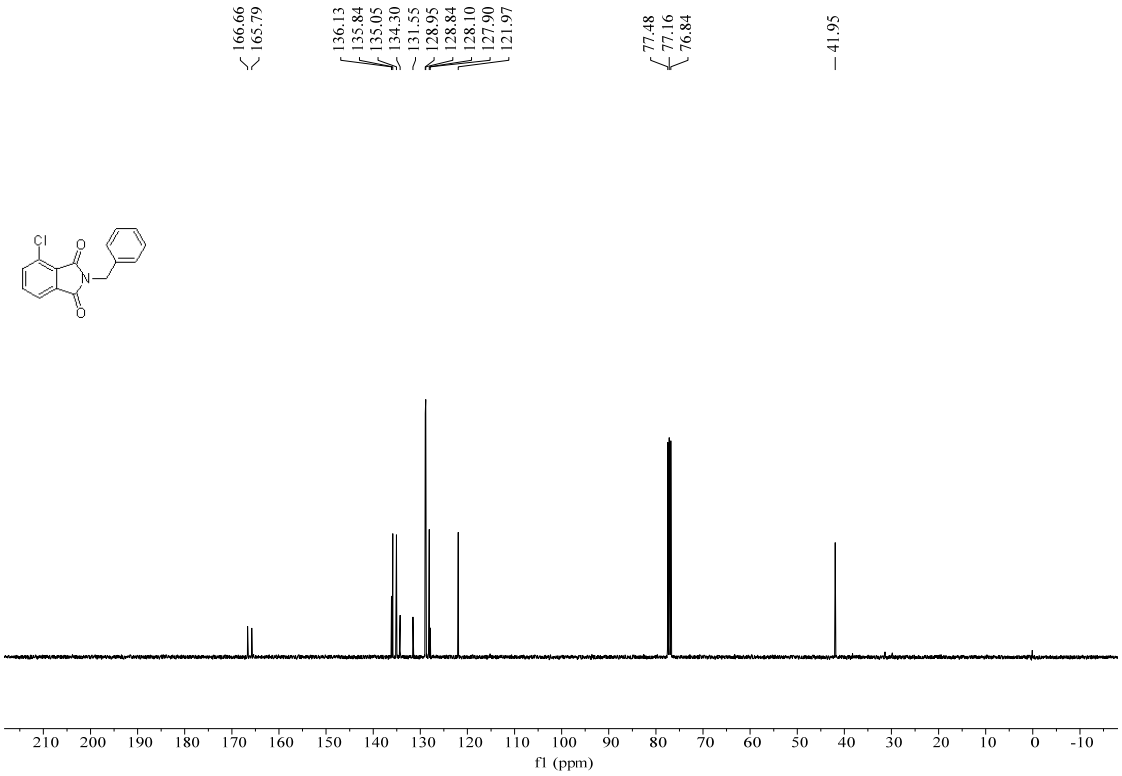

O
N
Cl
N
O
0.95
2.09
1.00
2.12
1.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


166.48
148.64
144.42
138.12
134.90
131.76
131.73
124.21
122.71
77.48
77.16
76.84
O
N
Cl
N
O

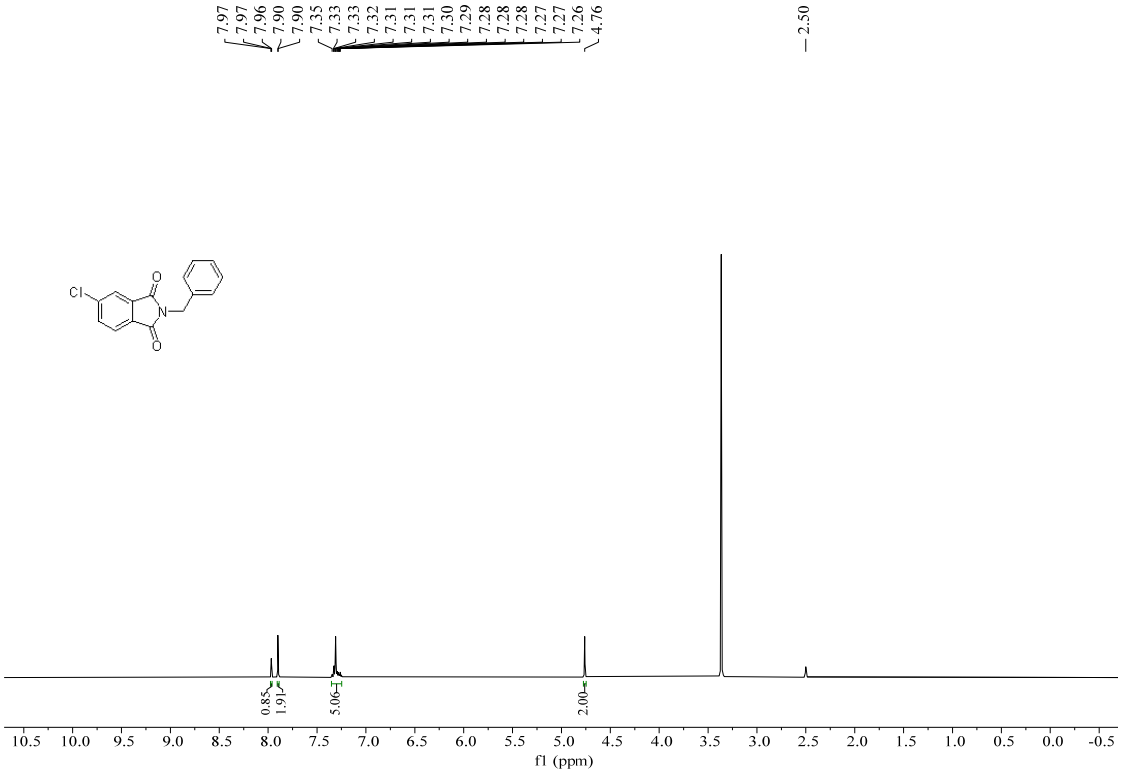

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

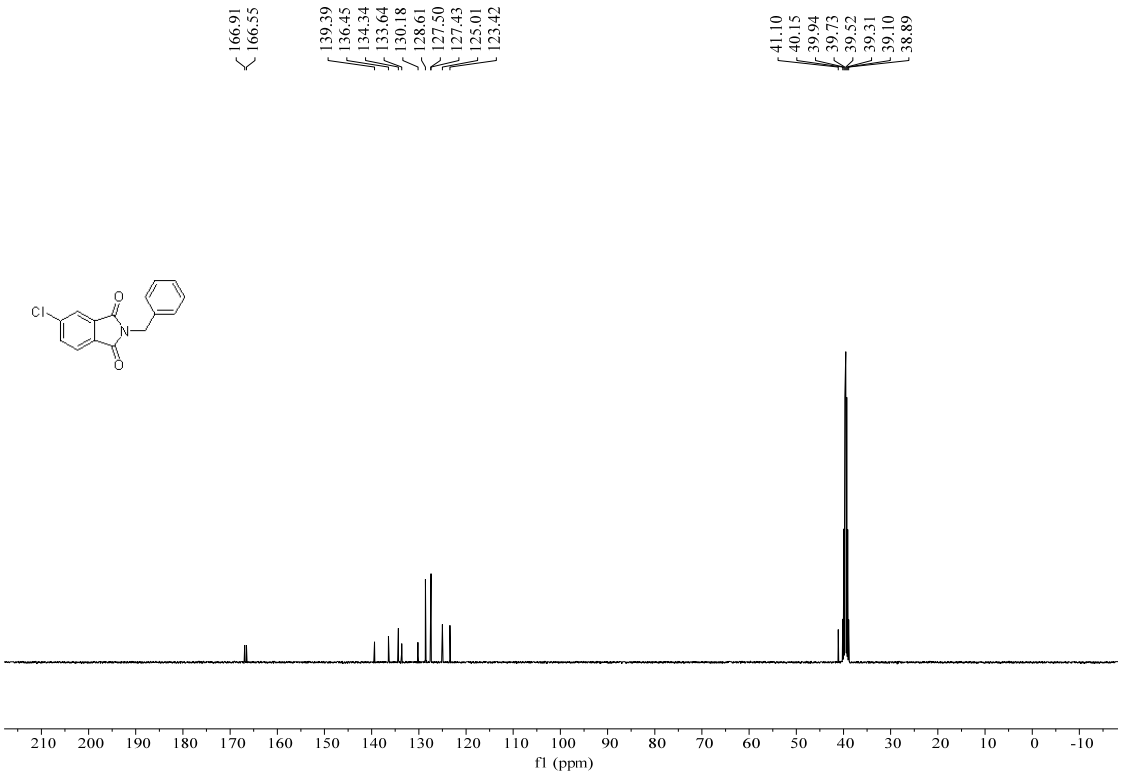
1ba:


7.76
7.75
7.74
7.62
7.62
7.61
7.46
7.45
7.44
7.44
7.43
7.33
7.32
7.32
7.31
7.30
7.30
7.30
7.28
7.27
7.26
4.84
Cl
O
N
O
0.97
1.97
1.95
3.26
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

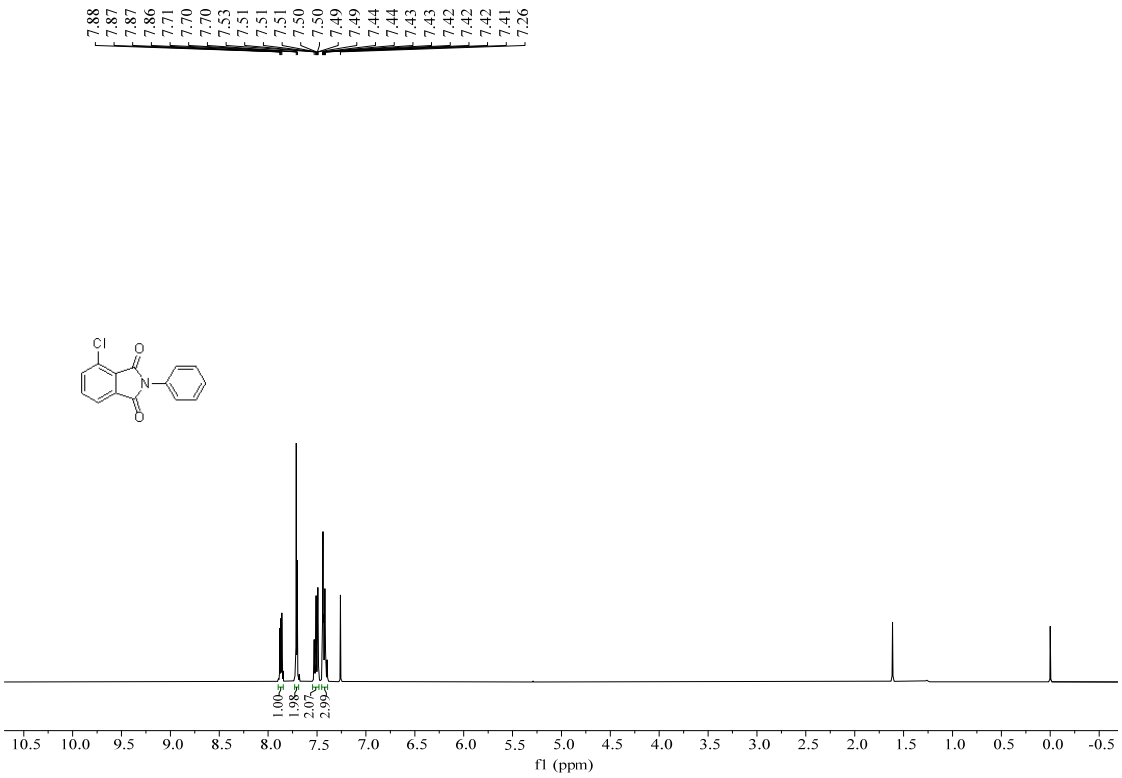

166.66
165.79
136.13
135.84
135.05
134.30
131.55
128.95
128.84
128.10
127.90
121.97
77.48
77.16
76.84
41.95
Cl
O
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

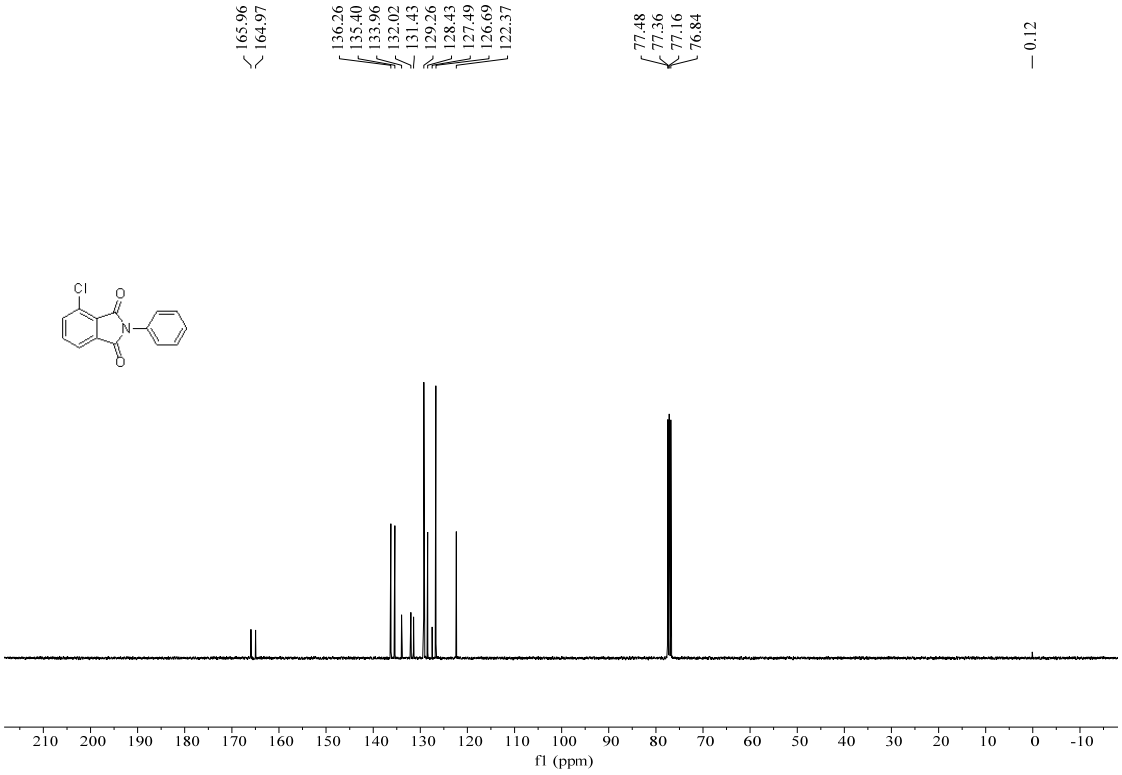
1ca:


7.97
7.97
7.96
7.90
7.90
7.35
7.33
7.33
7.32
7.31
7.31
7.31
7.30
7.29
7.28
7.28
7.28
7.27
7.27
7.27
7.26
4.76
2.50
Cl
O
N
O
0.85
1.91
5.06
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

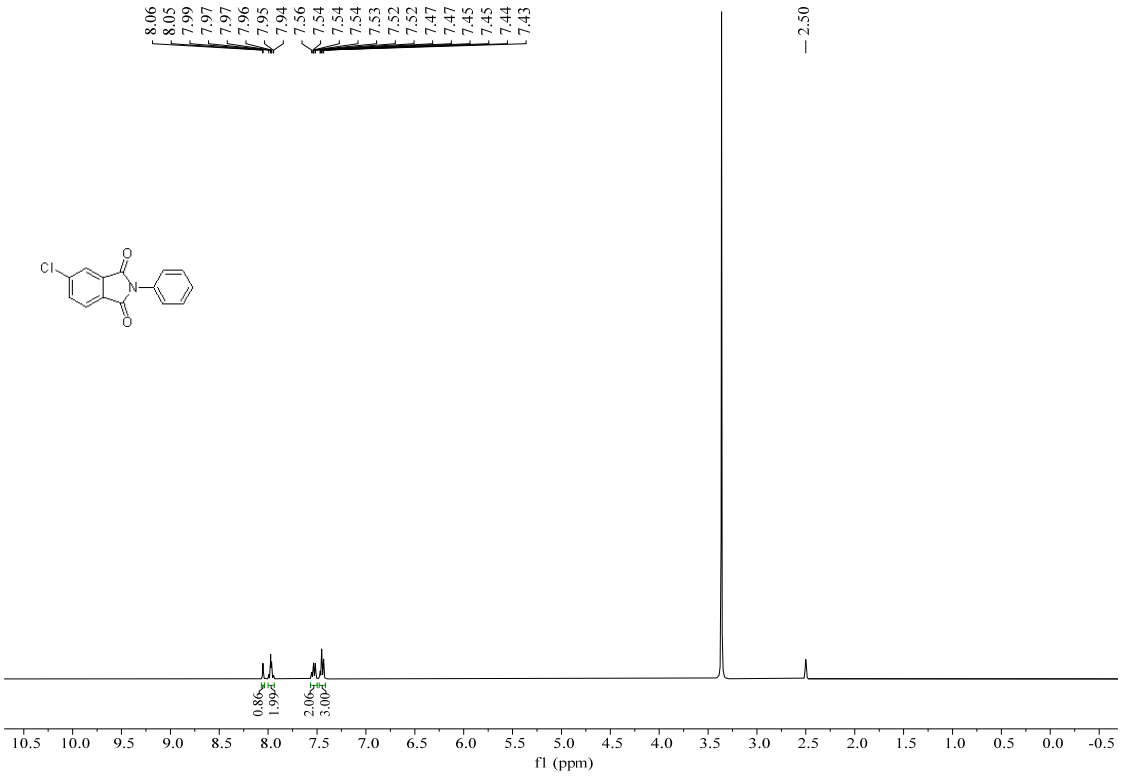

166.91
166.55
139.39
136.45
134.34
133.64
130.18
128.61
127.50
127.43
125.01
123.42
41.10
40.15
39.94
39.73
39.52
39.31
39.10
38.89
Cl
O
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

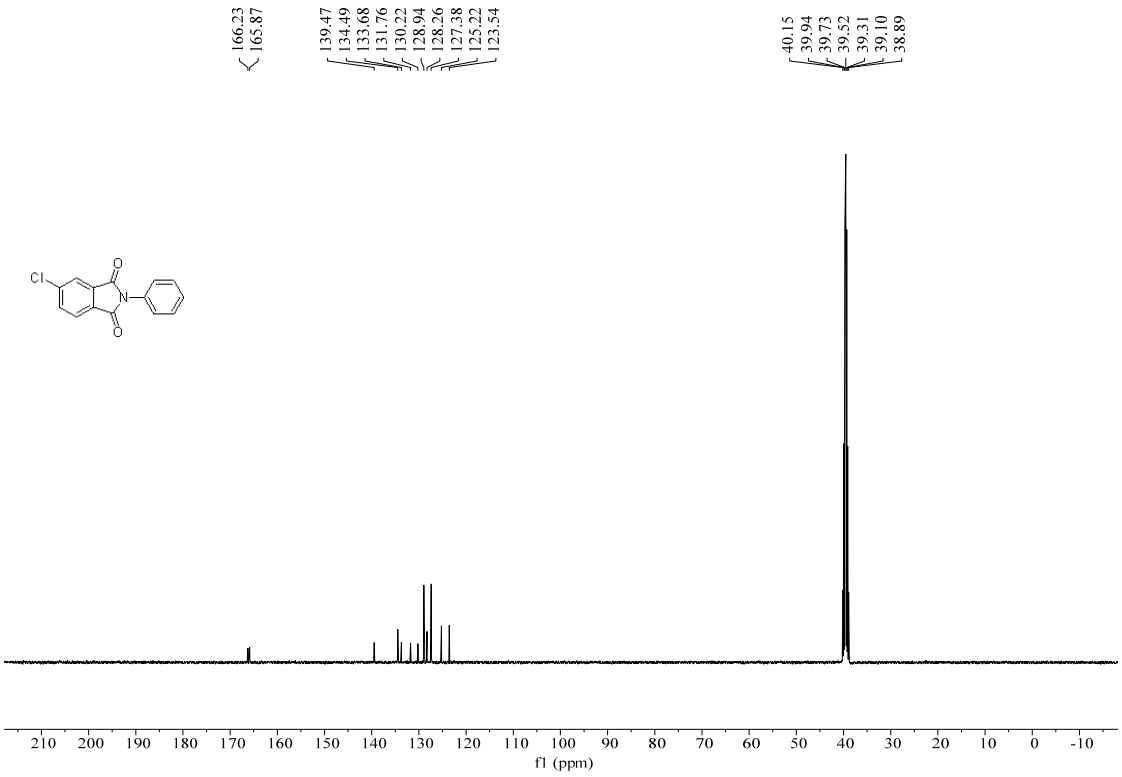
1bj:


7.88
7.87
7.87
7.86
7.71
7.70
7.70
7.53
7.51
7.51
7.51
7.50
7.50
7.49
7.49
7.44
7.44
7.43
7.43
7.42
7.42
7.42
7.41
7.26
Cl
O
N
O
1.00
1.98
2.07
2.99
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


165.96
164.97
136.26
135.40
133.96
132.02
131.43
129.26
128.43
127.49
126.69
122.37
77.48
77.36
77.16
76.84
0.12
Cl
O
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

1cj:


8.06
8.05
7.99
7.97
7.97
7.96
7.95
7.94
7.56
7.54
7.54
7.54
7.53
7.52
7.52
7.47
7.47
7.45
7.45
7.44
7.43
2.50
Cl
O
N
O
0.86
1.99
2.06
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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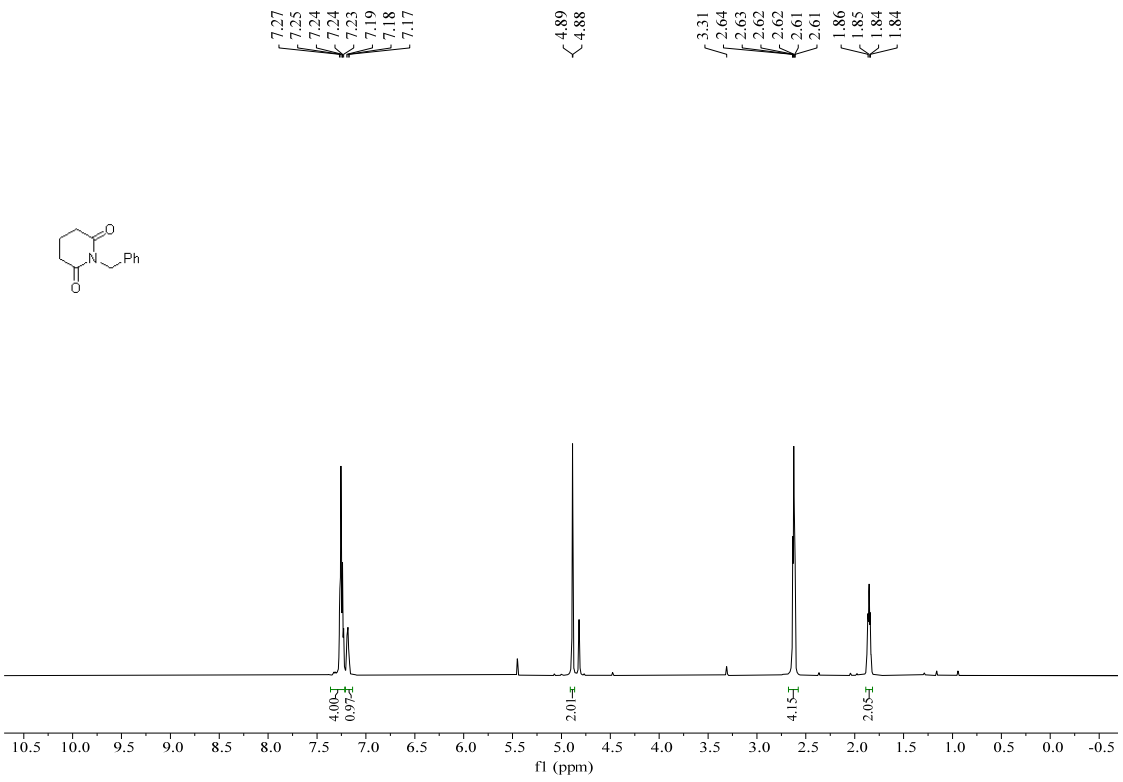
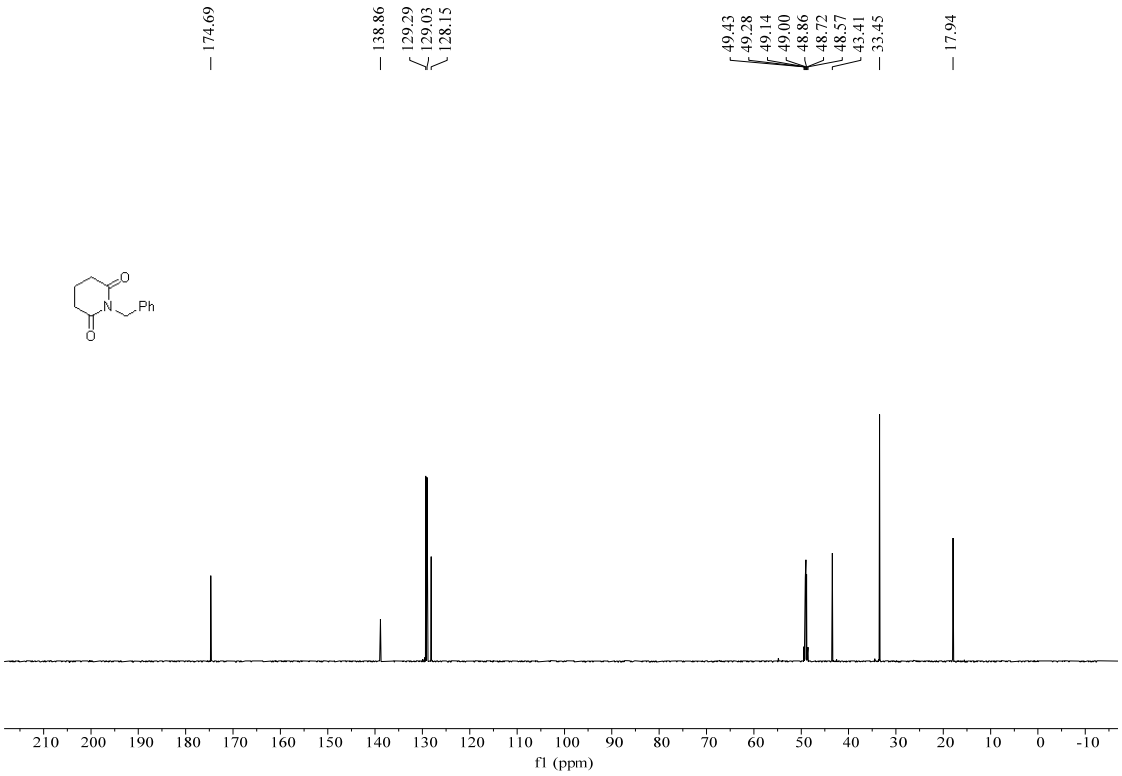
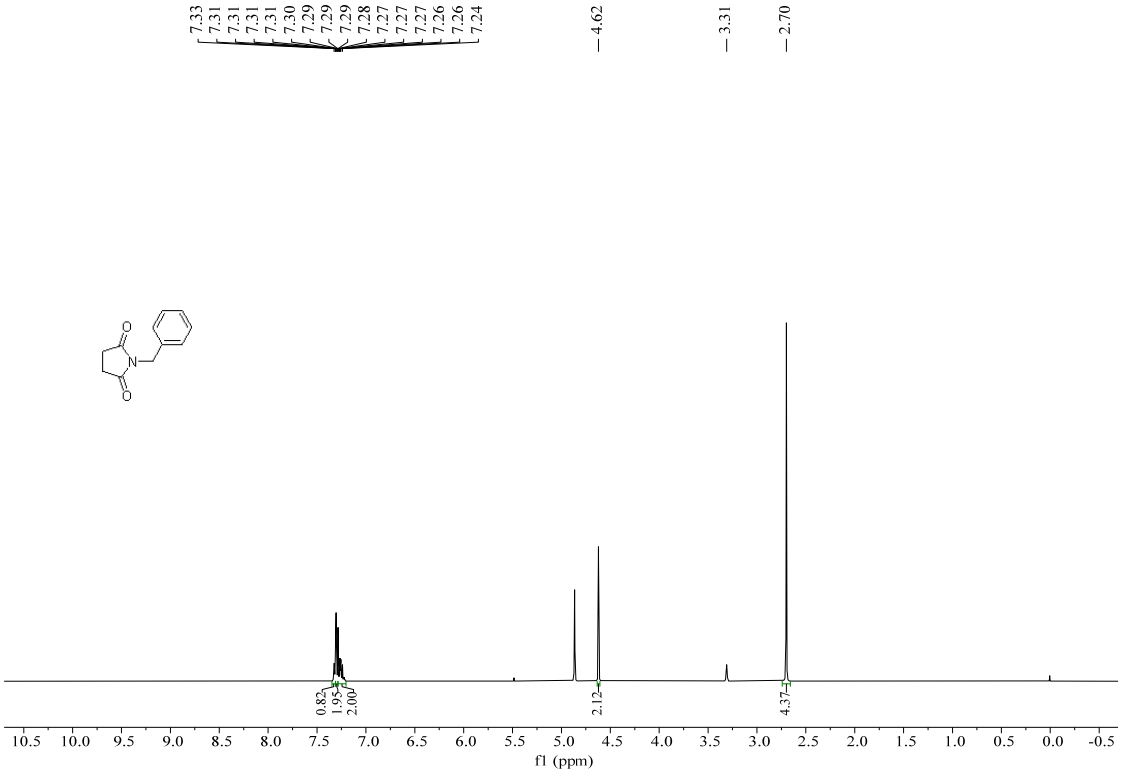
165.87
139.47
134.49
133.68
131.76
130.22
128.94
128.26
127.38
125.22
123.54
40.15
39.94
39.73
39.52
39.31
39.10
38.89
Cl
O
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

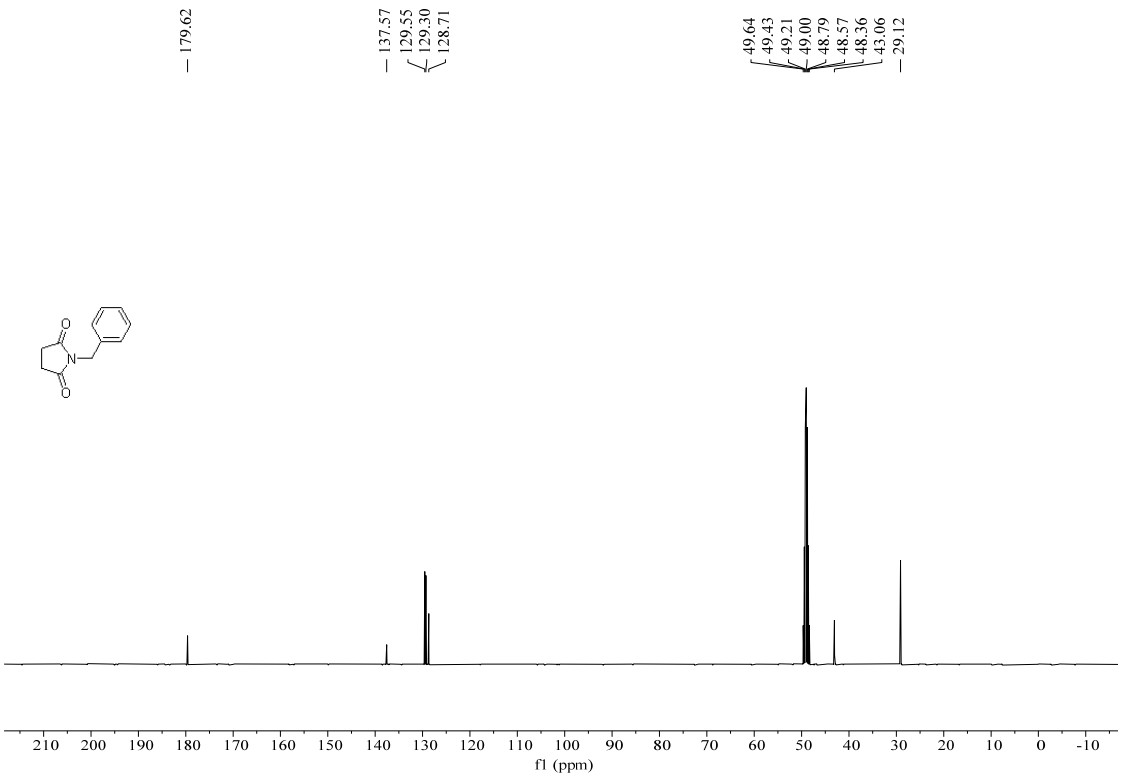
1da:


7.27
7.25
7.24
7.24
7.23
7.19
7.18
7.17
4.89
4.88
3.31
2.64
2.63
2.62
2.62
2.61
2.61
1.86
1.85
1.84
1.84
O
N
Ph
O
4.00
0.97
2.01
4.15
2.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

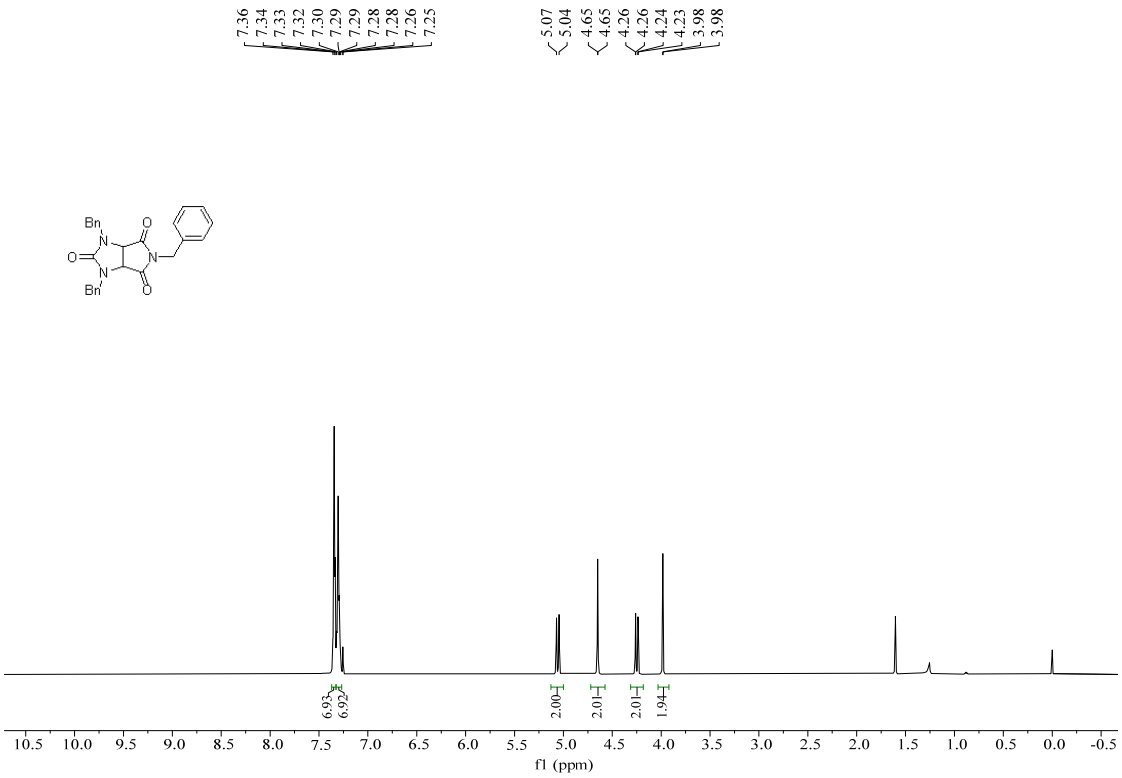

174.69
138.86
129.29
129.03
128.15
49.43
49.28
49.14
49.00
48.86
48.72
48.57
43.41
33.45
17.94
O
N
Ph
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

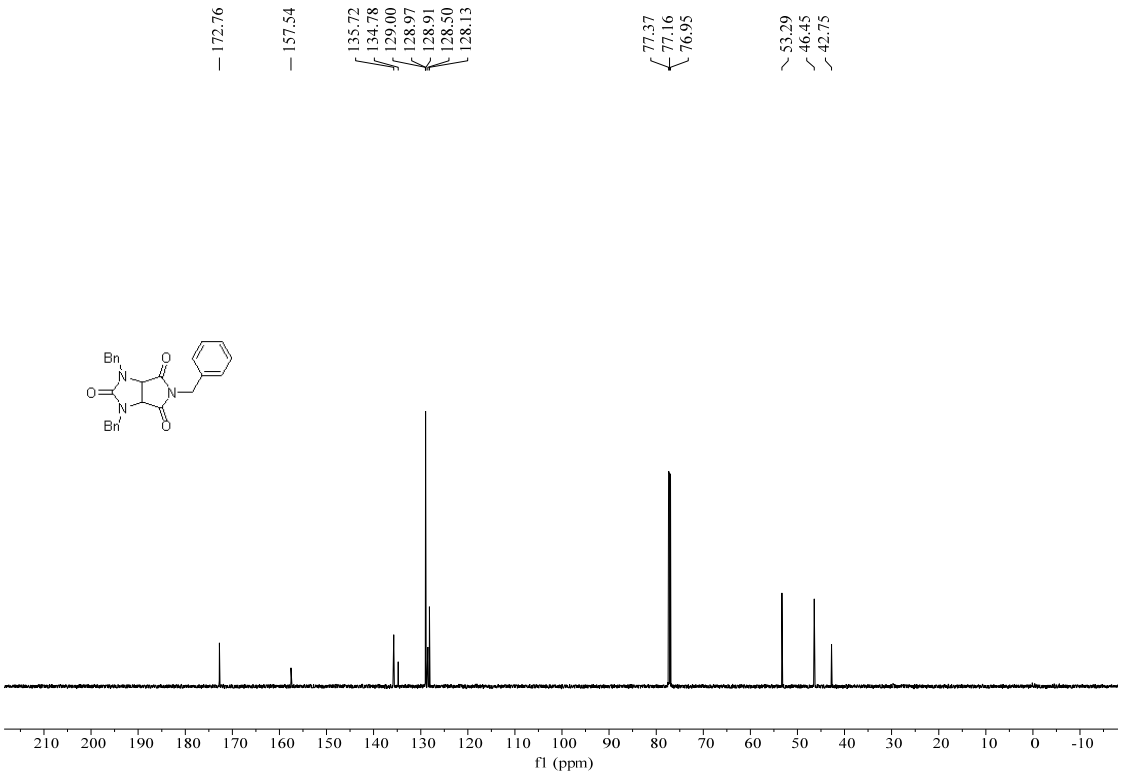
1ea:


7.33
7.31
7.31
7.31
7.31
7.30
7.29
7.29
7.29
7.28
7.27
7.27
7.27
7.26
7.26
7.24
4.62
3.31
2.70
O
N
O
0.83
1.95
2.00
2.12
4.37
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

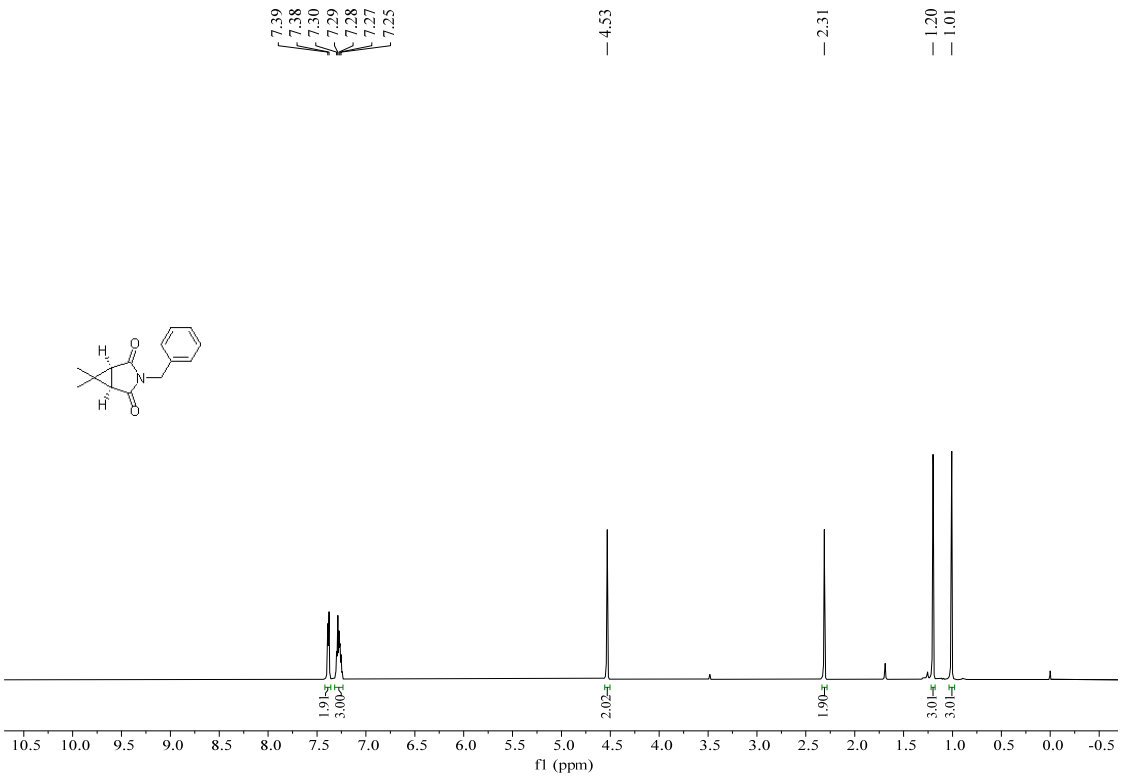

179.62
137.57
129.55
129.30
128.71
49.64
49.43
49.21
49.00
48.79
48.57
48.36
43.06
29.12
O
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

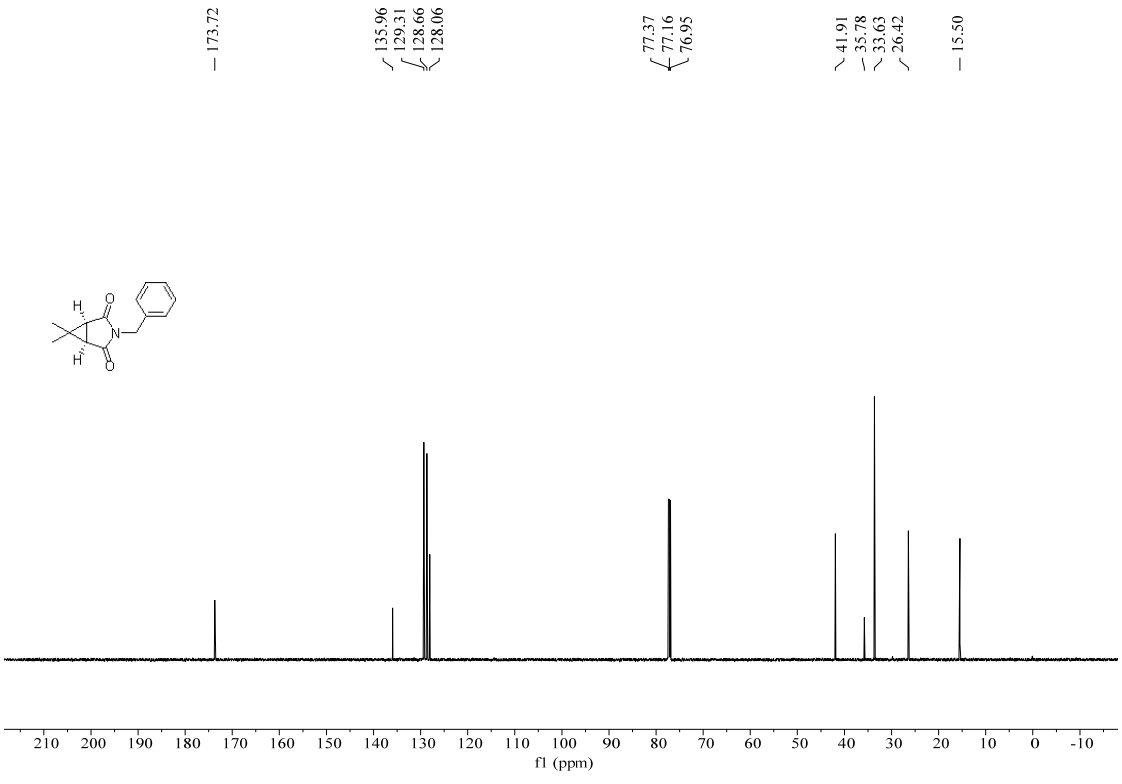
1fa:


7.36
7.34
7.33
7.32
7.30
7.29
7.29
7.28
7.28
7.26
7.25
5.07
5.04
4.65
4.65
4.26
4.26
4.24
4.23
3.98
3.98
Bn
Bn
6.93
6.92
2.00
2.01
2.01
1.94
f1 (ppm)

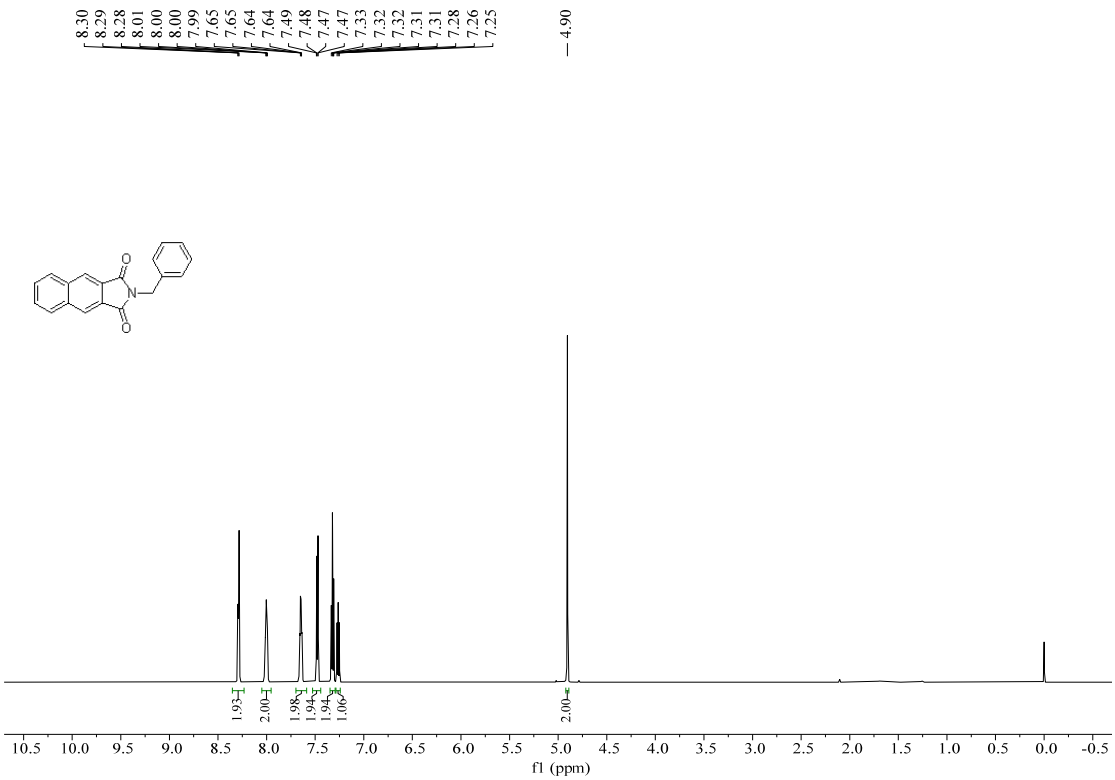

172.76
157.54
135.72
134.78
129.00
128.97
128.91
128.50
128.13
77.37
77.16
76.95
53.29
46.45
42.75
Bn
Bn
f1 (ppm)

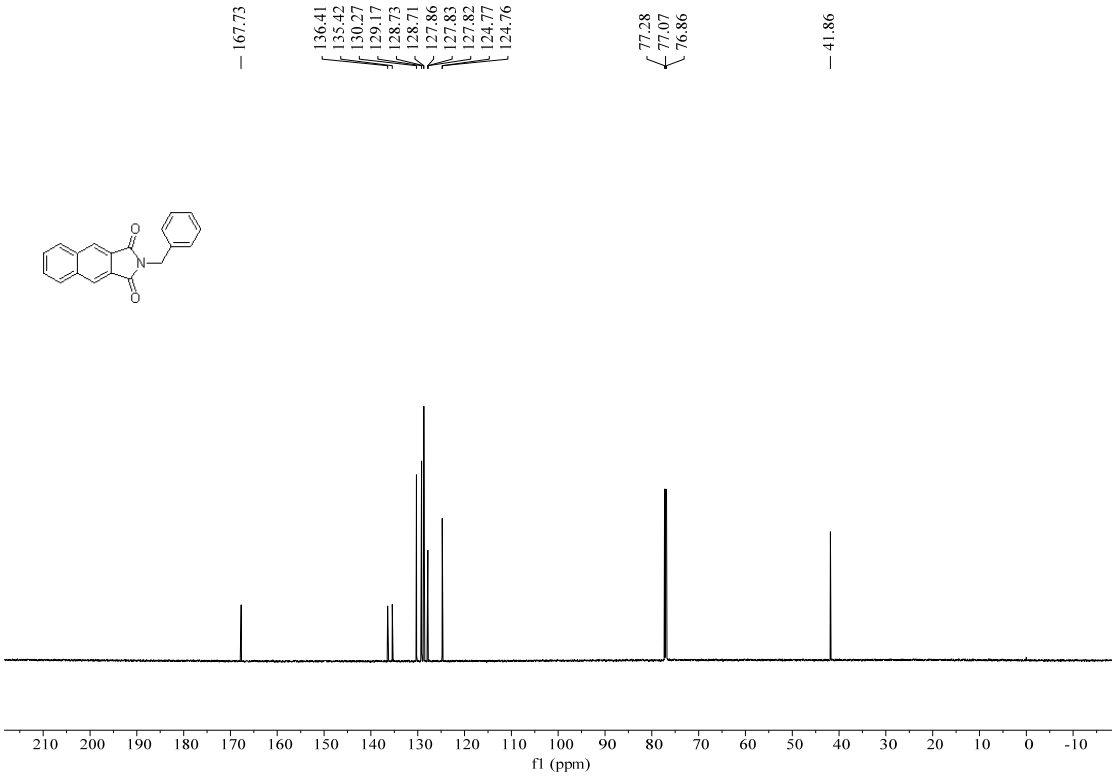
1ga:


7.39
7.38
7.30
7.29
7.28
7.27
7.25
4.53
2.31
1.20
1.01
1.91
3.00
2.02
1.90
3.01
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

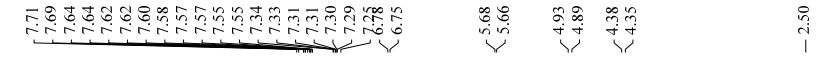

173.72
135.96
129.31
128.66
128.06
77.37
77.16
76.95
41.91
35.78
33.63
26.42
15.50
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

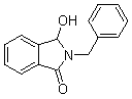
1ha:

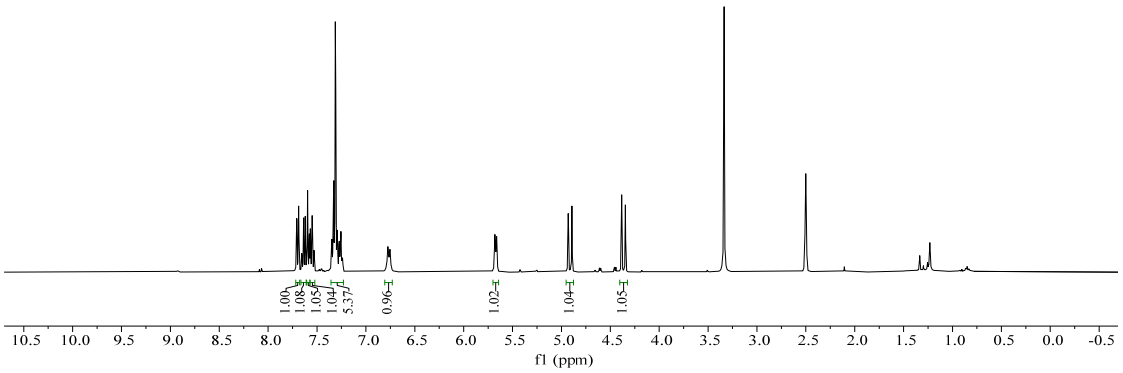

8.30
8.29
8.28
8.01
8.00
8.00
7.99
7.65
7.65
7.64
7.64
7.49
7.48
7.47
7.47
7.33
7.32
7.32
7.31
7.31
7.28
7.26
7.25
4.90
1.93
2.00
1.98
1.94
1.94
1.06
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

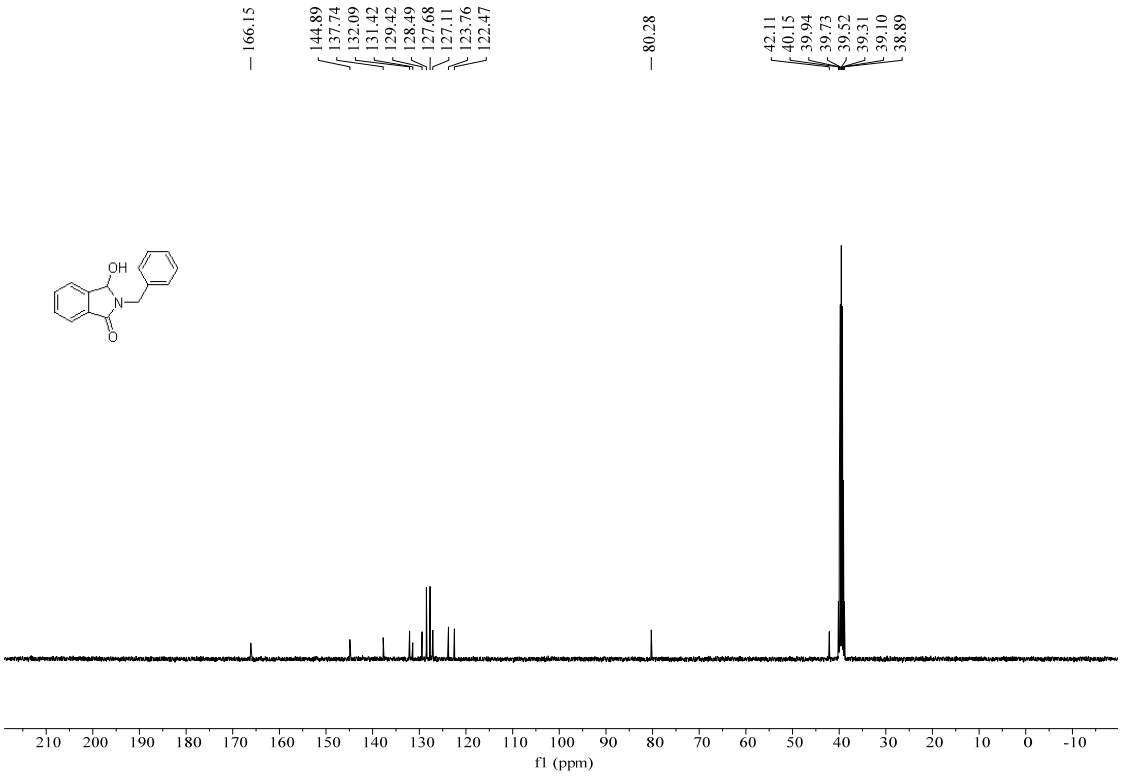

167.73
136.41
135.42
130.27
129.17
128.73
128.71
127.86
127.83
127.82
124.77
124.76
77.28
77.07
76.86
41.86
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2aa:

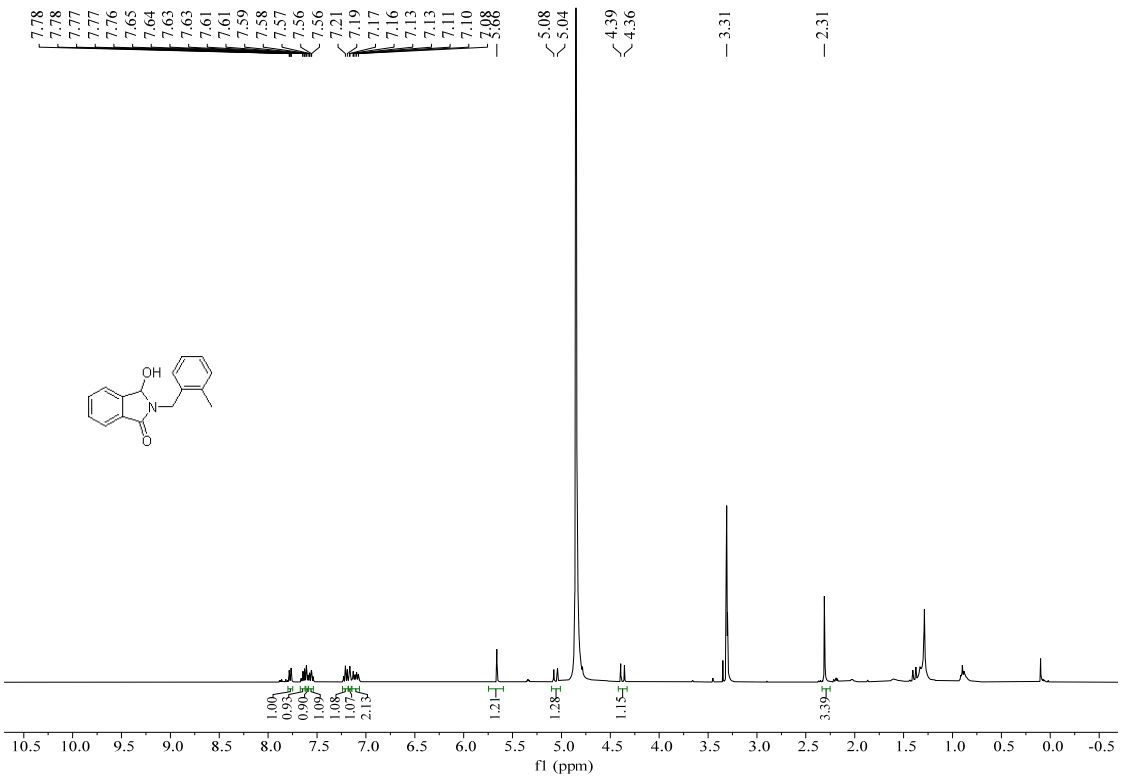

7.71
7.69
7.64
7.64
7.62
7.62
7.60
7.58
7.57
7.57
7.55
7.55
7.34
7.33
7.31
7.31
7.30
7.29
6.78
6.75
5.68
5.66
4.93
4.89
4.38
4.35
2.50


OH
N
O


1.00
1.08
1.05
1.04
5.37
0.96
1.02
1.04
1.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


166.15
144.89
137.74
132.09
131.42
129.42
128.49
127.68
127.11
123.76
122.47
80.28
42.11
40.15
39.94
39.73
39.52
39.31
39.10
38.89
OH
N
O
f1 (ppm)

2ab: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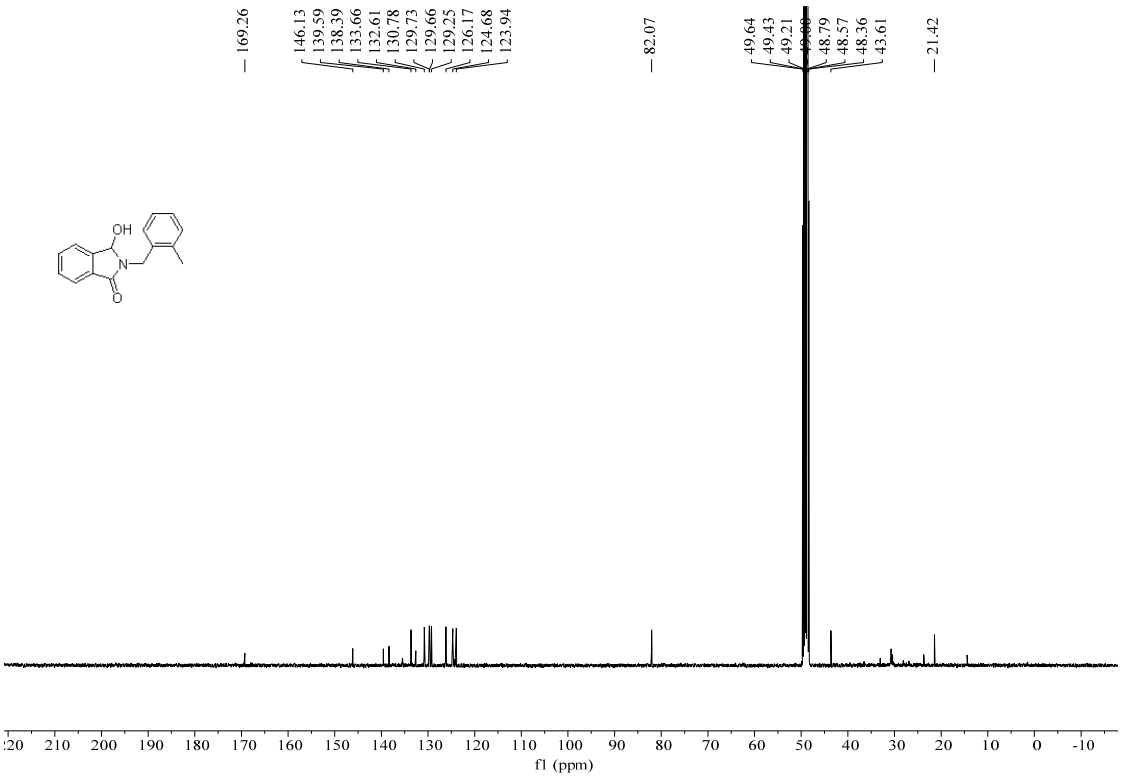
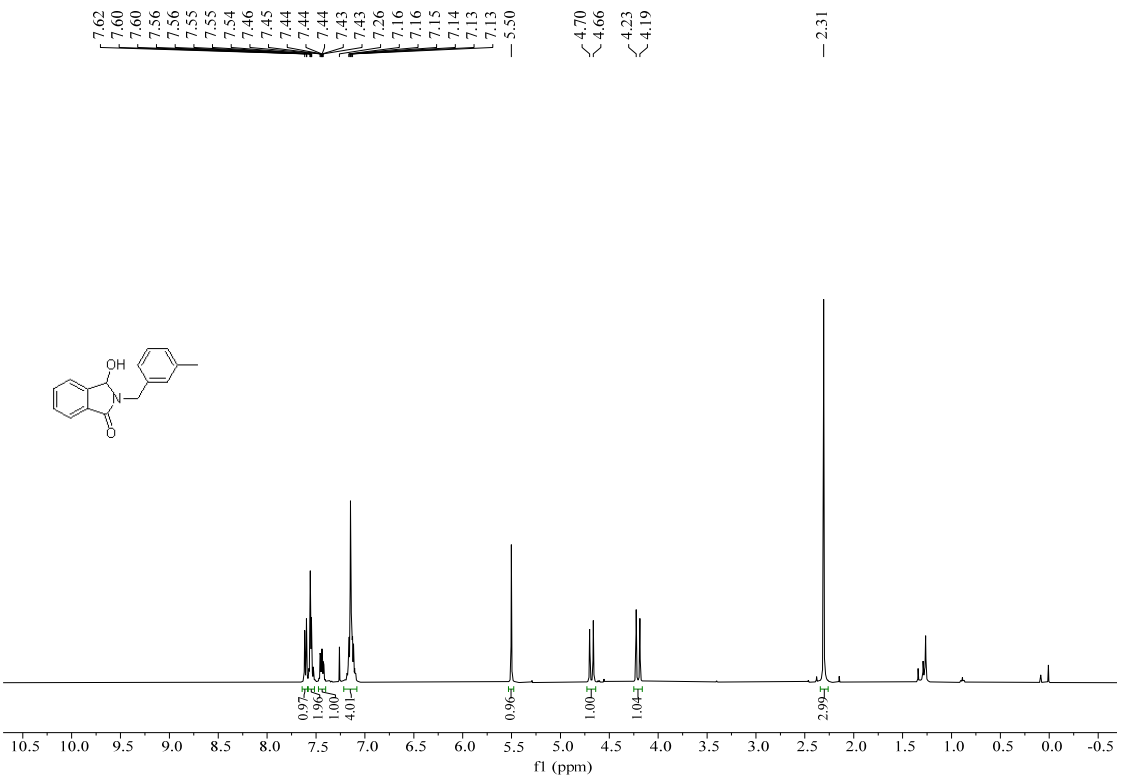
7.78
7.77
7.77
7.77
7.76
7.65
7.64
7.63
7.63
7.61
7.61
7.59
7.58
7.57
7.56
7.56
7.21
7.19
7.17
7.16
7.13
7.13
7.11
7.10
7.08
5.66
5.08
5.04
4.39
4.36
3.31
2.31
OH
N
O
1.00
0.93
0.90
1.09
1.08
1.07
2.13
1.21
1.28
1.15
3.39
f1 (ppm)


169.26
146.13
139.59
138.39
133.66
132.61
130.78
129.73
129.66
129.25
126.17
124.68
123.94
82.07
49.64
49.43
49.21
48.79
48.57
48.36
43.61
21.42
OH
N
O
f1 (ppm)

2ac:


7.62
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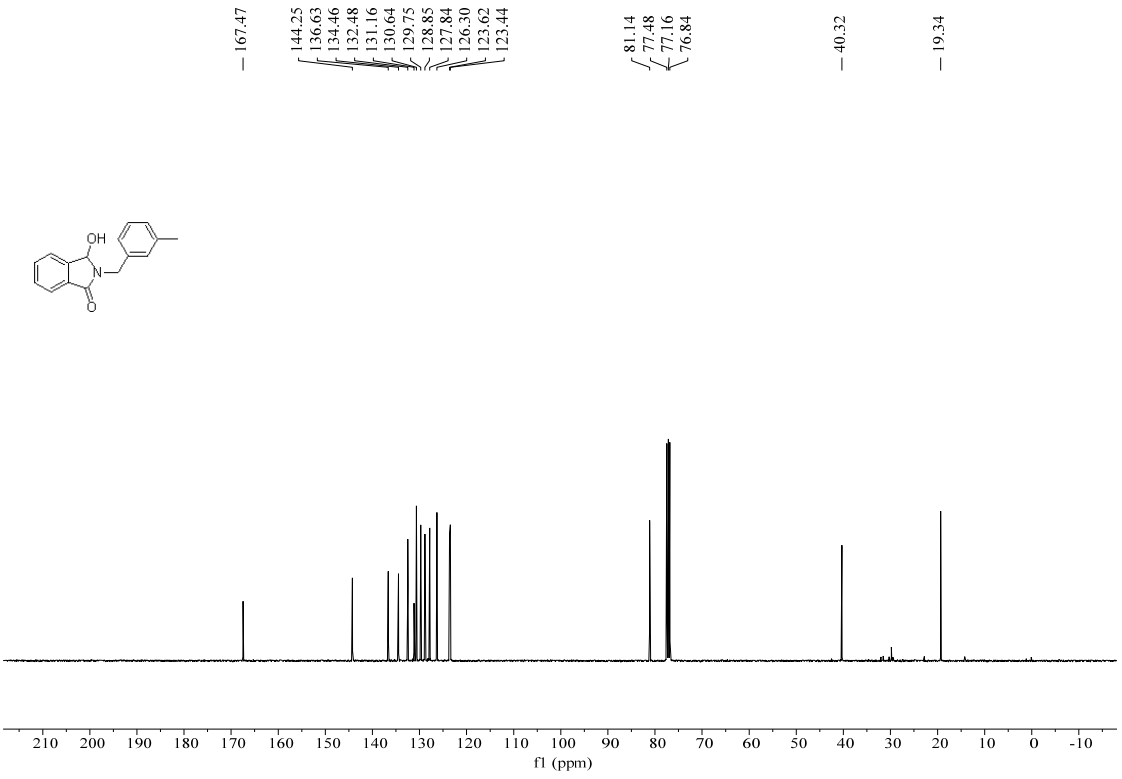
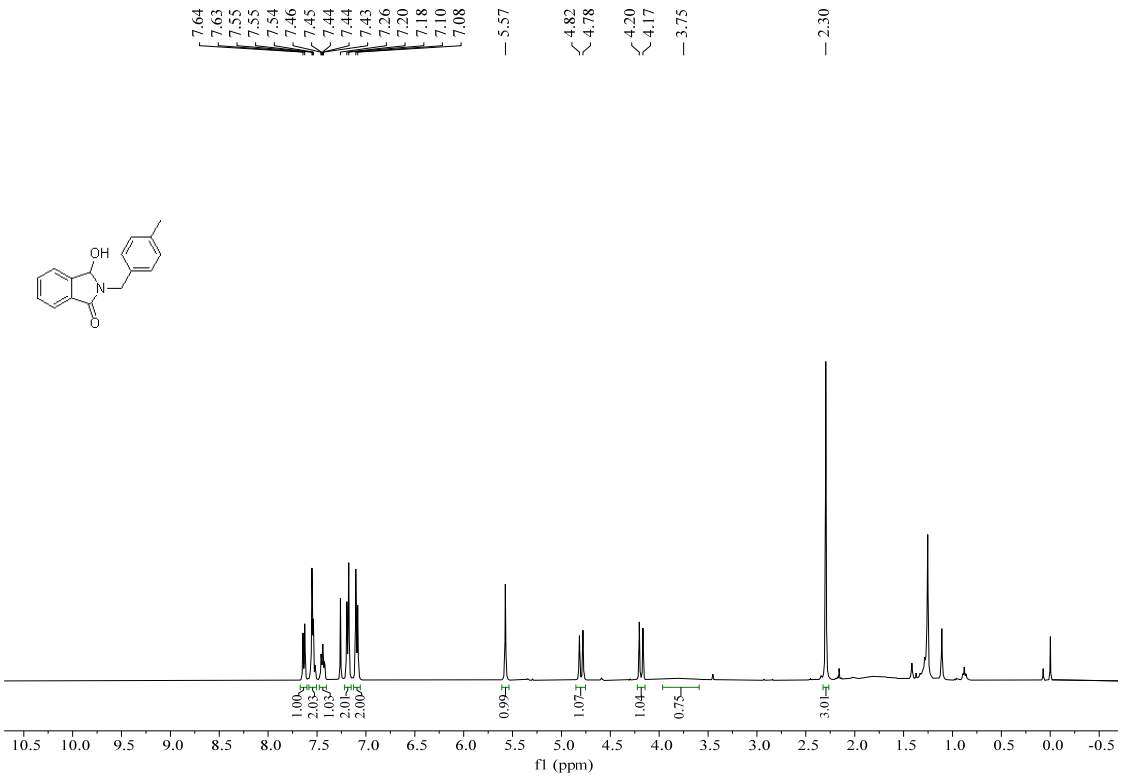
7.60
7.56
7.56
7.55
7.55
7.54
7.46
7.45
7.44
7.44
7.44
7.43
7.43
7.26
7.16
7.16
7.15
7.14
7.13
7.13
5.50
4.70
4.66
4.23
4.19
2.31
OH
N
O
0.97
1.96
1.00
4.01
0.96
1.00
1.04
2.99
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


167.47
144.25
136.63
134.46
132.48
131.16
130.64
129.75
128.85
127.84
126.30
123.62
123.44
81.14
77.48
77.16
76.84
40.32
19.34
OH
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2ad:


7.64
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7.55
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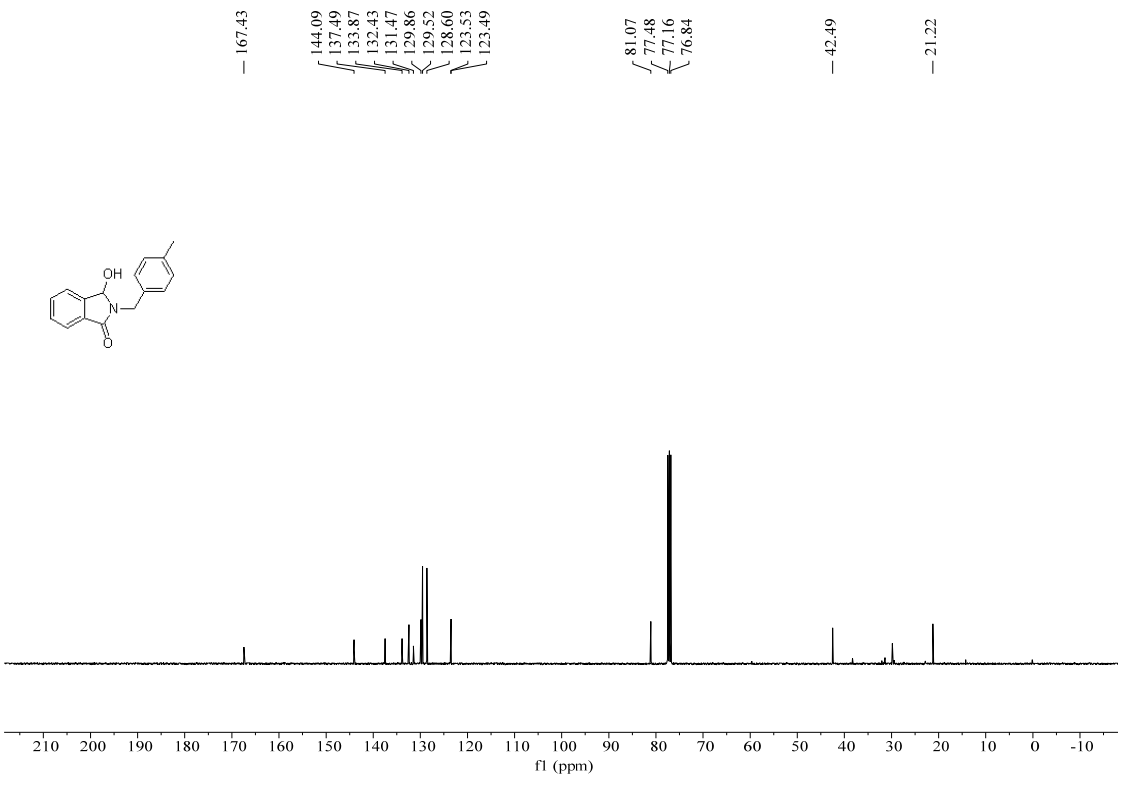
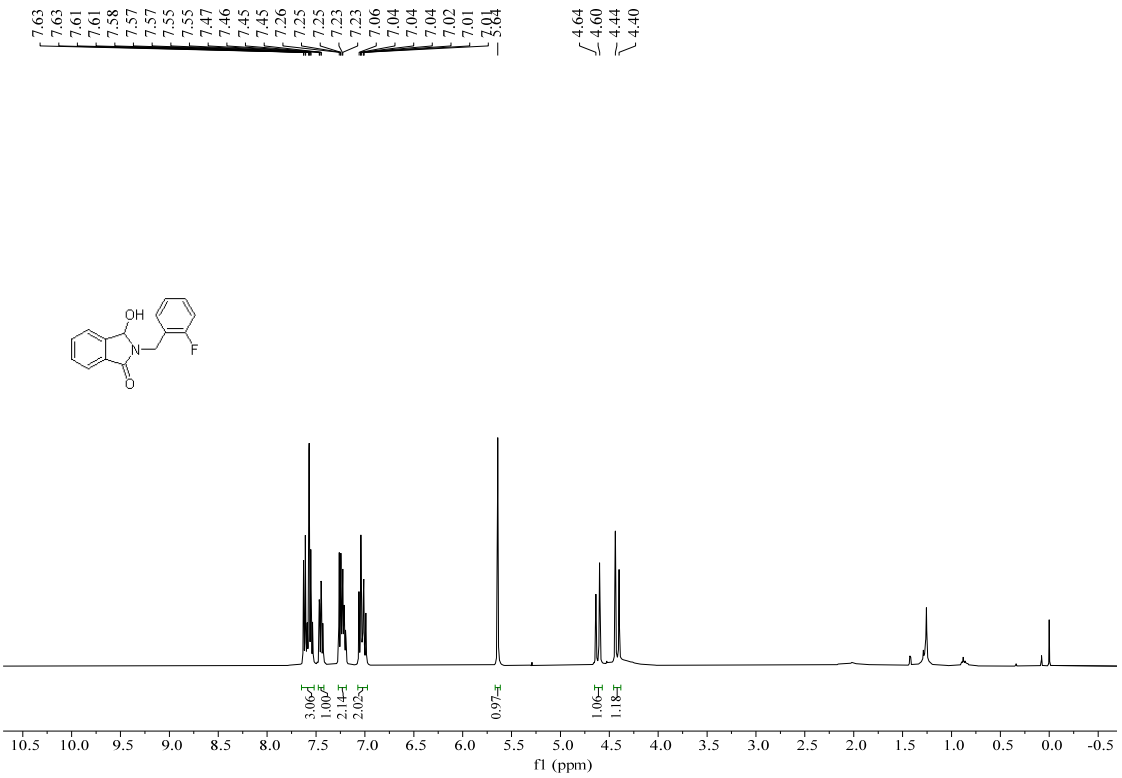
7.44
7.44
7.43
7.26
7.20
7.18
7.10
7.08
5.57
4.82
4.78
4.20
4.17
3.75
2.30
OH
N
O
1.00
2.05
1.03
2.01
2.00
0.99
1.07
1.04
0.75
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


167.43
144.09
137.49
133.87
132.43
131.47
129.86
129.52
128.60
123.53
123.49
81.07
77.48
77.16
76.84
42.49
21.22
OH
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2ae: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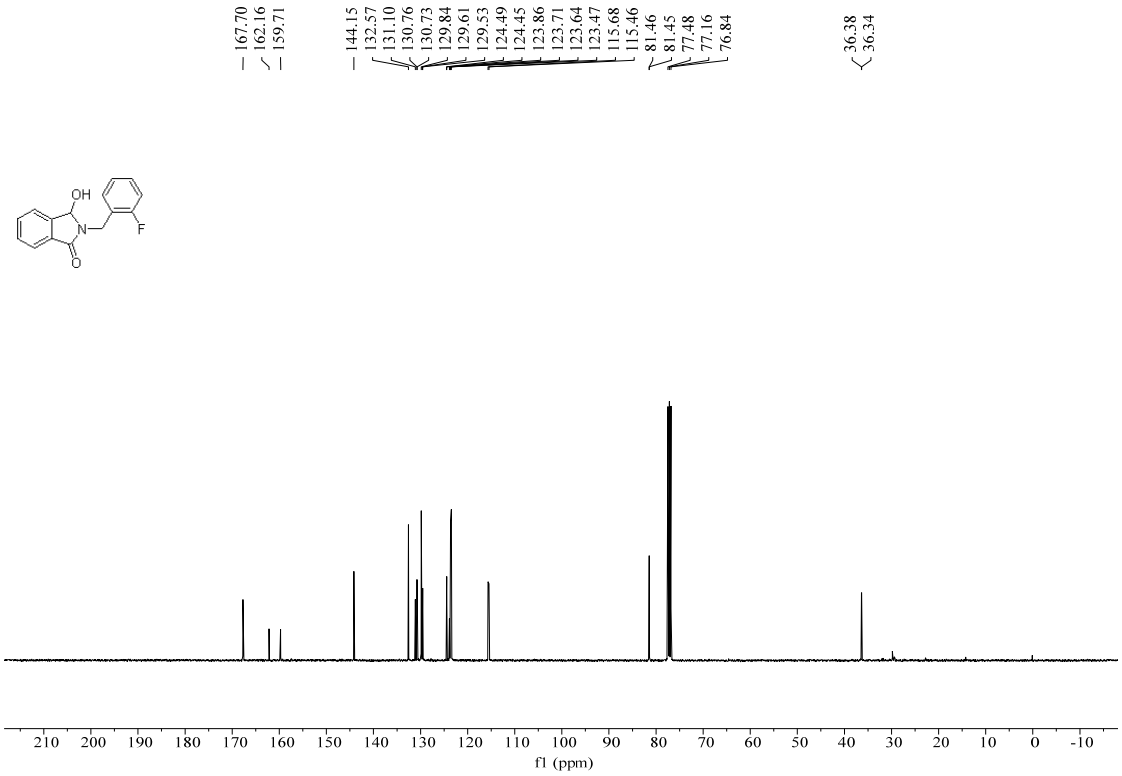
7.61
7.58
7.57
7.57
7.55
7.55
7.47
7.46
7.45
7.45
7.26
7.25
7.25
7.23
7.23
7.06
7.04
7.04
7.04
7.02
7.01
7.01
5.84
4.64
4.60
4.44
4.40
OH
N
O
F
3.06
1.00
2.14
2.02
0.97
1.06
1.18
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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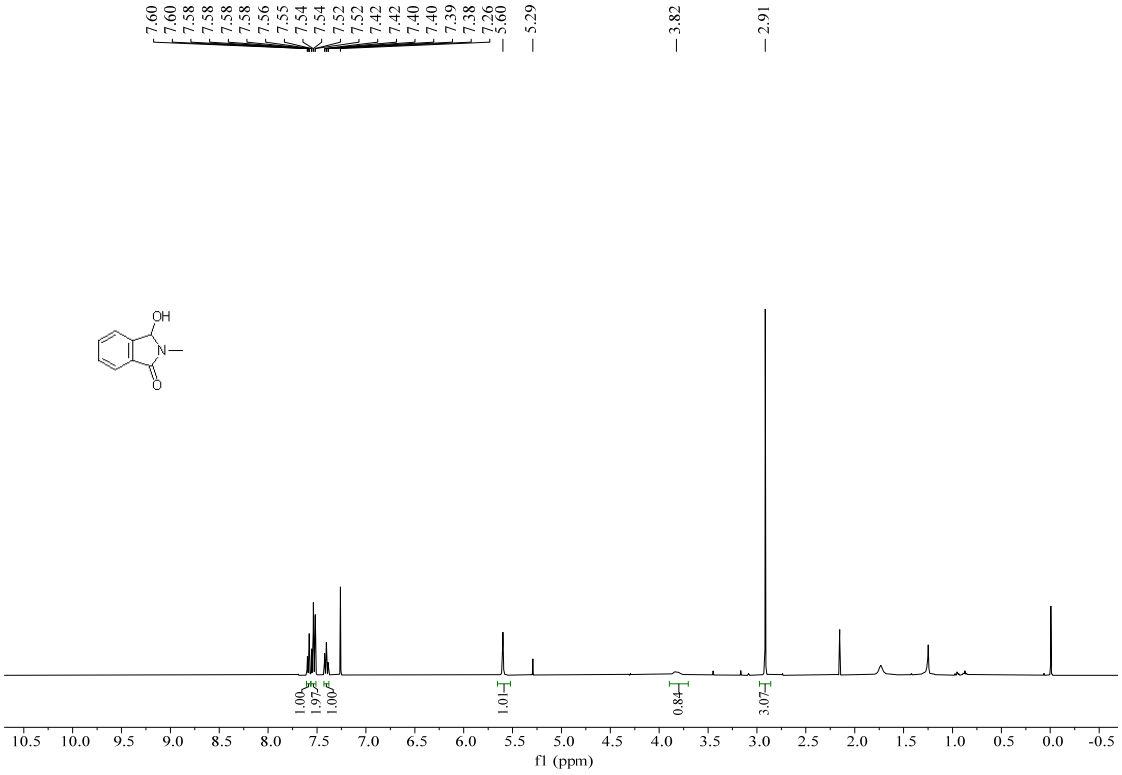
162.16
159.71
144.15
132.57
131.10
130.76
130.73
129.84
129.61
129.53
124.49
124.45
123.86
123.71
123.64
123.47
115.68
115.46
81.46
81.45
77.48
77.16
76.84
36.38
36.34
OH
N
F
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2af: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7.60
7.58
7.58
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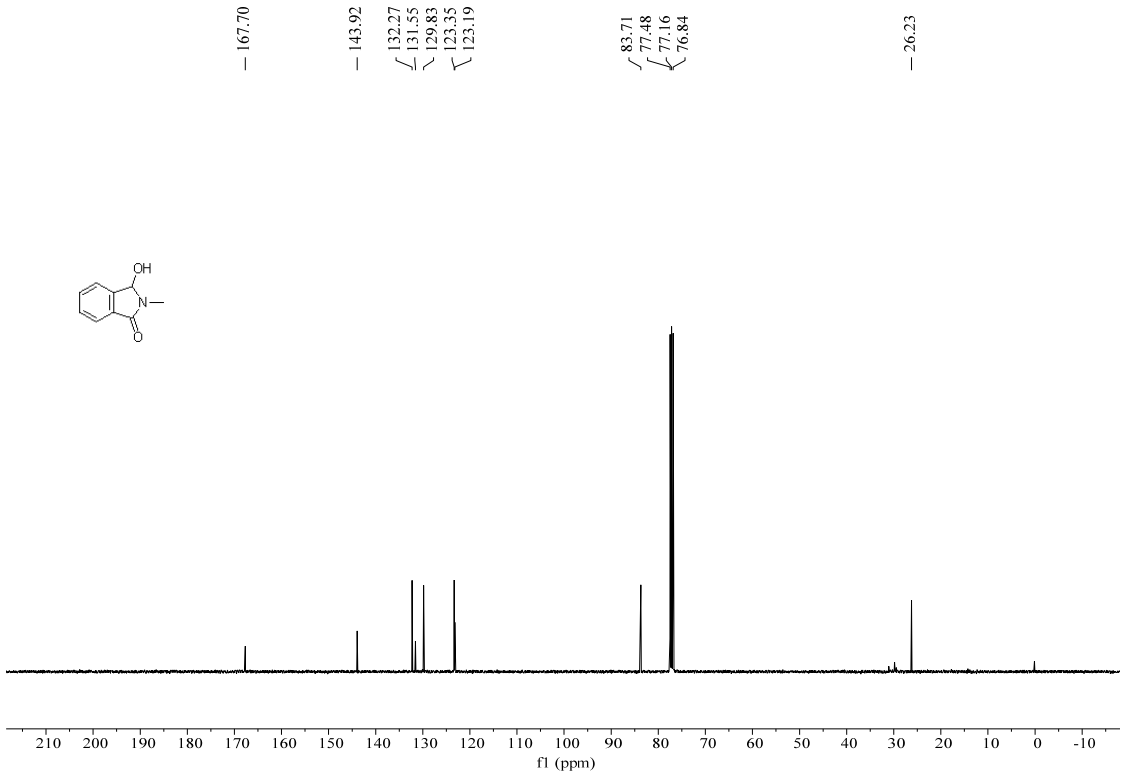
7.58
7.56
7.55
7.54
7.54
7.52
7.52
7.42
7.42
7.40
7.40
7.39
7.38
7.26
5.60
5.29
3.82
2.91
OH
N
O
1.00
1.97
1.00
1.01
0.84
3.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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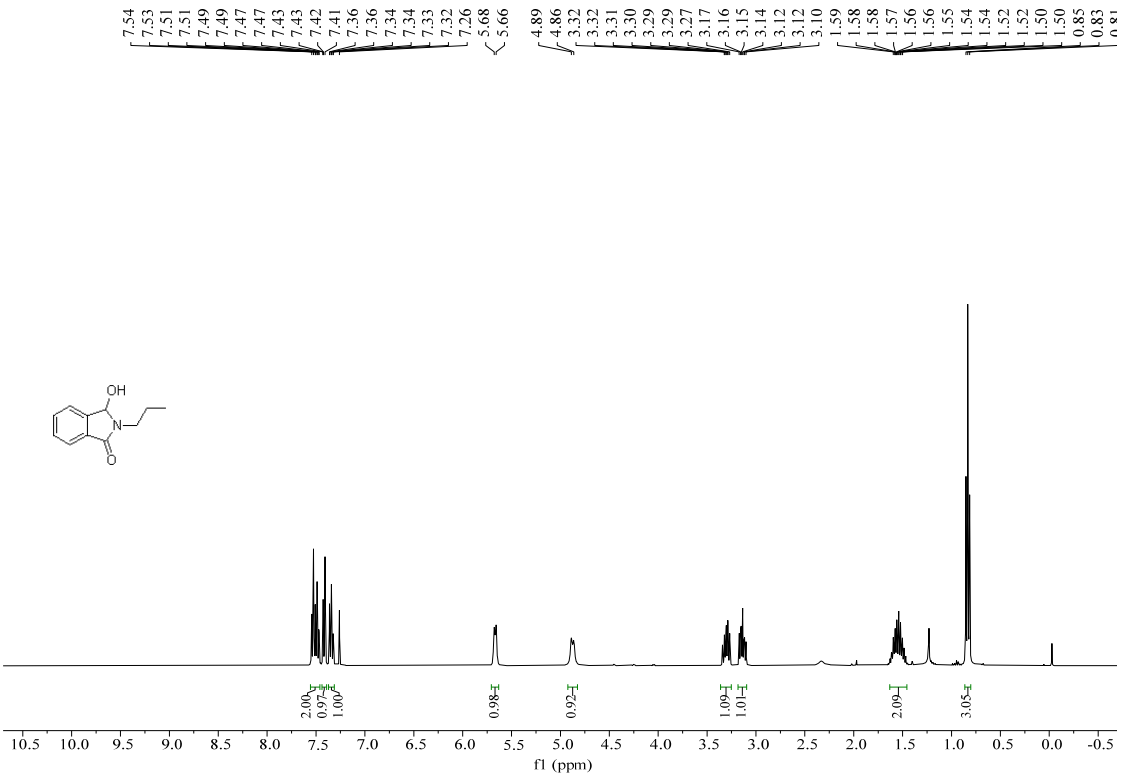
143.92
132.27
131.55
129.83
123.35
123.19
83.71
77.48
77.16
76.84
26.23
OH
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2ag: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7.47
7.47
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7.43
7.42
7.41
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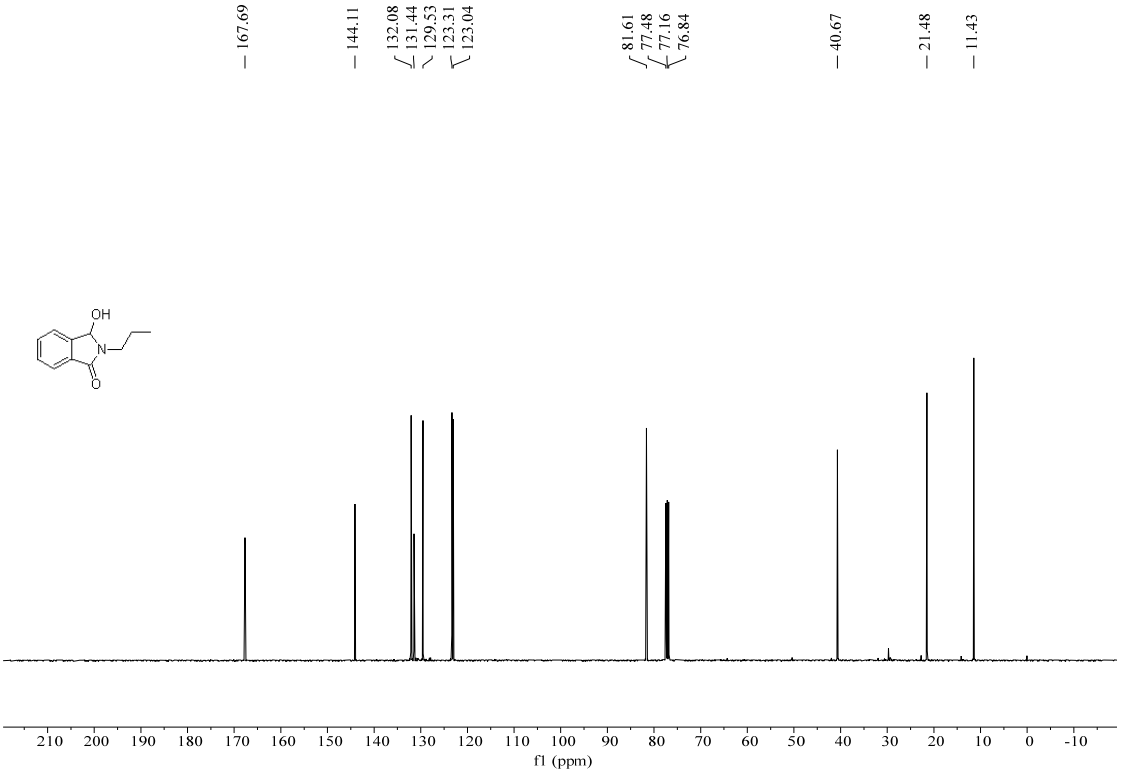
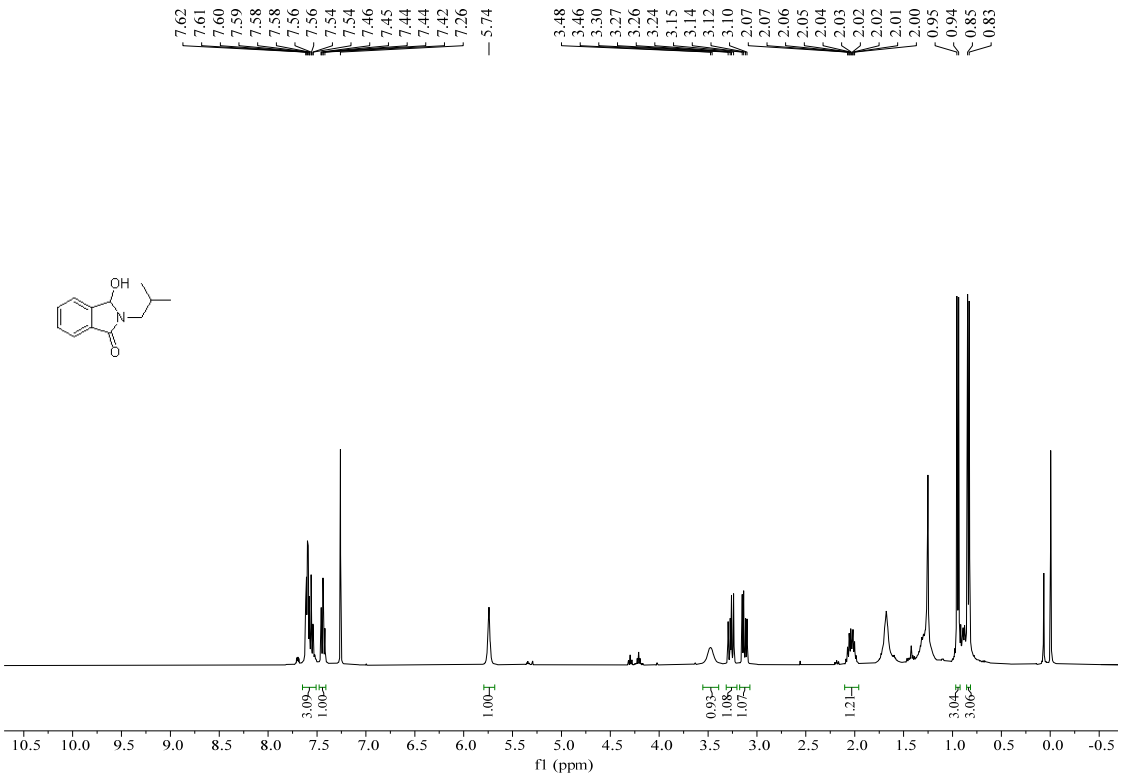
7.36
7.34
7.34
7.33
7.32
7.26
5.68
5.66
4.89
4.86
3.32
3.32
3.31
3.30
3.29
3.29
3.27
3.17
3.16
3.15
3.14
3.12
3.12
3.10
1.59
1.58
1.58
1.57
1.56
1.56
1.55
1.54
1.54
1.52
1.52
1.50
1.50
0.85
0.83
OH
N
O
2.00
0.97
1.00
0.98
0.92
1.09
1.01
2.09
3.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


167.69
144.11
132.08
131.44
129.53
123.31
123.04
81.61
77.48
77.16
76.84
40.67
21.48
11.43
OH
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2ah: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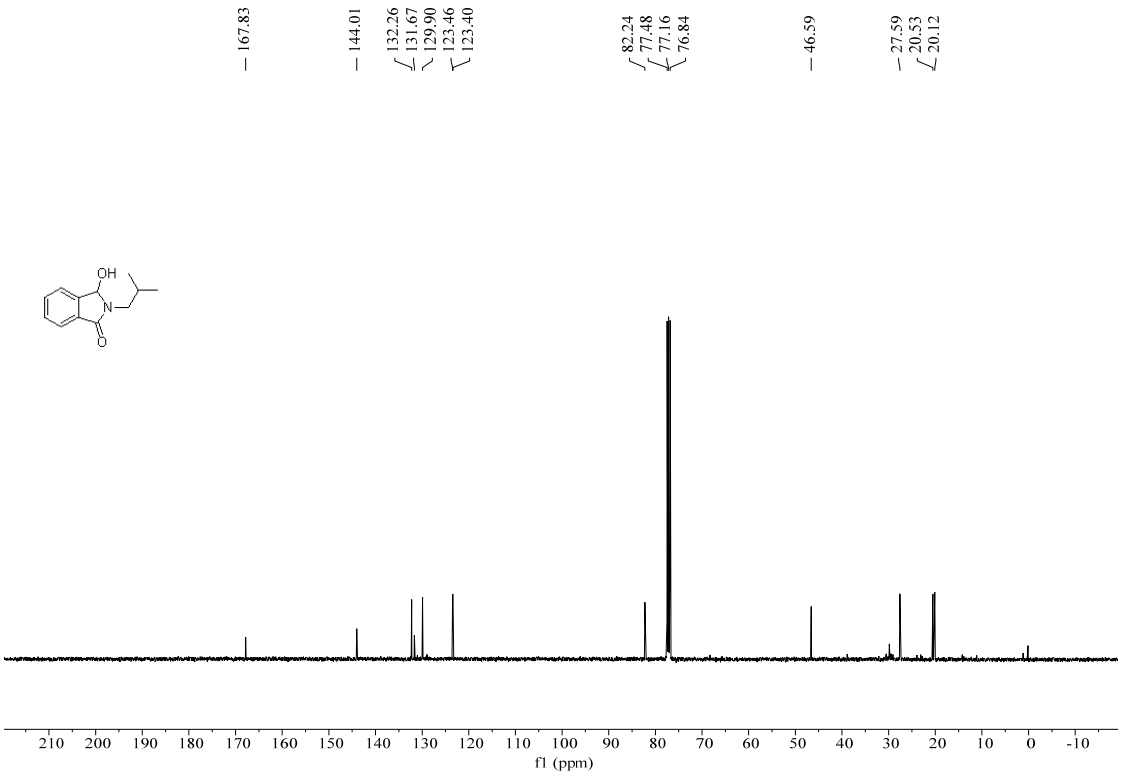
7.59
7.58
7.58
7.56
7.56
7.54
7.54
7.46
7.45
7.44
7.44
7.42
7.26
5.74
3.48
3.46
3.30
3.27
3.26
3.24
3.15
3.14
3.12
3.10
2.07
2.07
2.06
2.05
2.04
2.03
2.02
2.02
2.01
2.00
0.95
0.94
0.85
0.83
OH
N
O
3.09
1.00
1.00
0.93
1.08
1.07
1.21
3.04
3.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


167.83
144.01
132.26
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129.90
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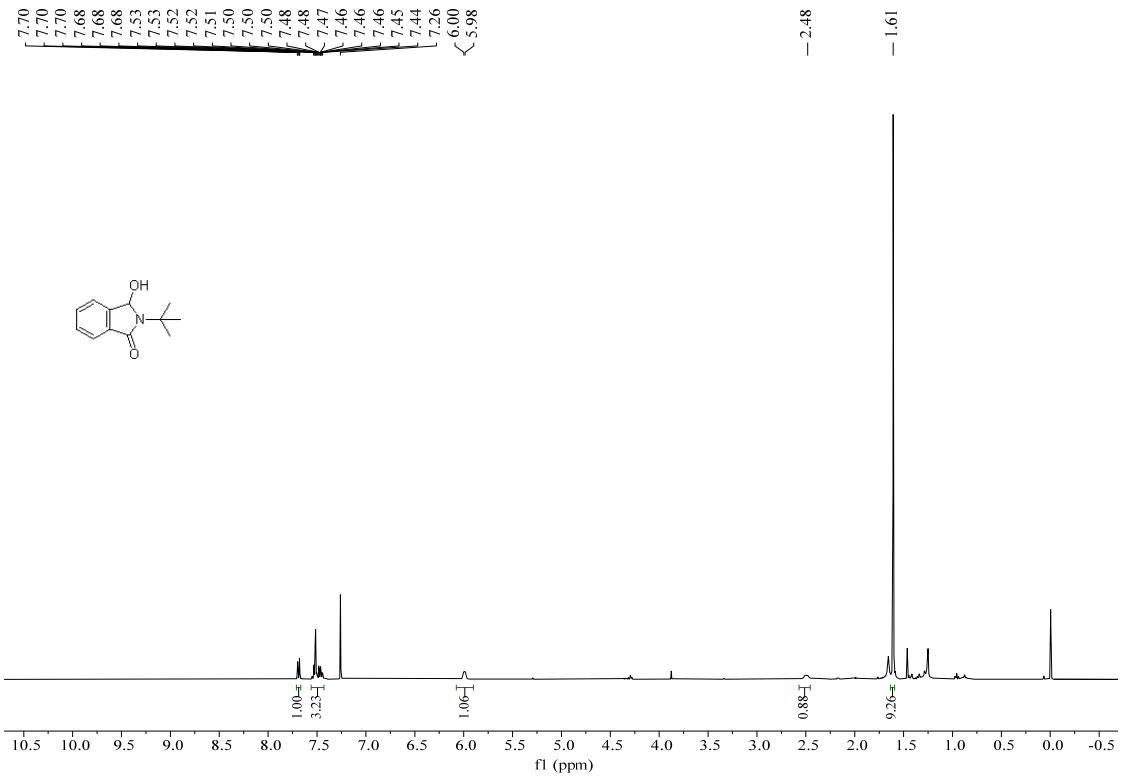
123.40
82.24
77.48
77.16
76.84
46.59
27.59
20.53
20.12
OH
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2ai: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7.70
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7.68
7.53
7.53
7.52
7.52
7.51
7.50
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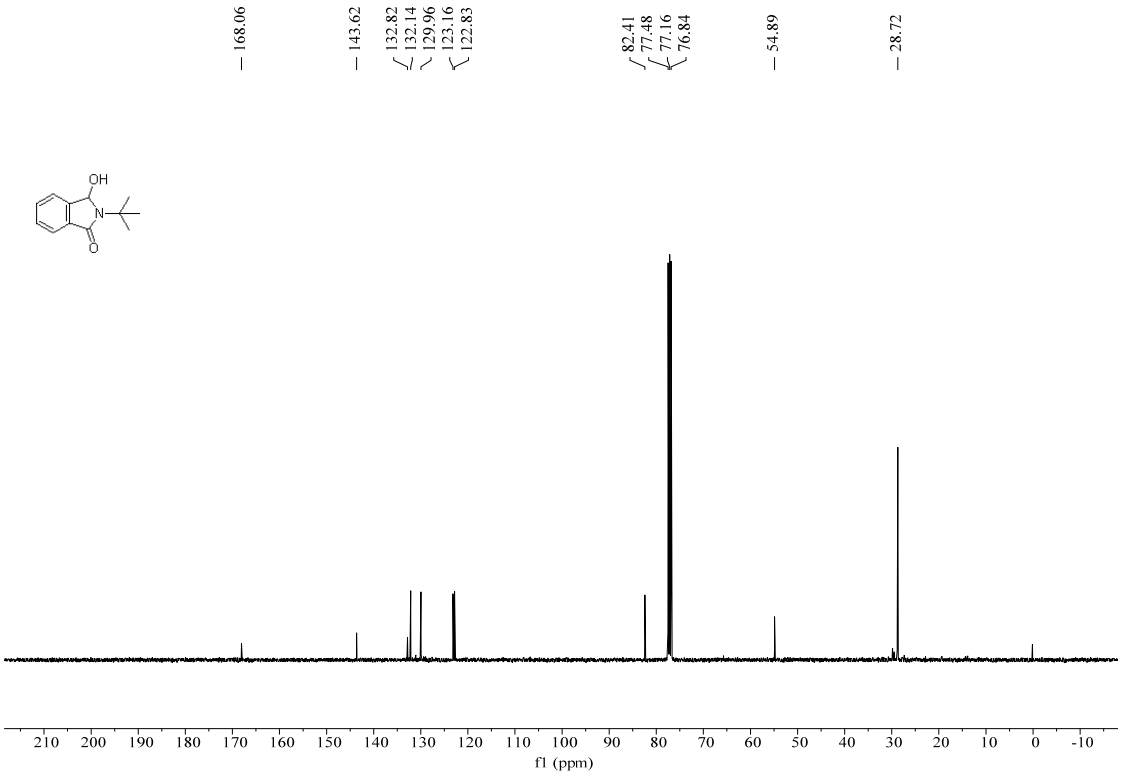
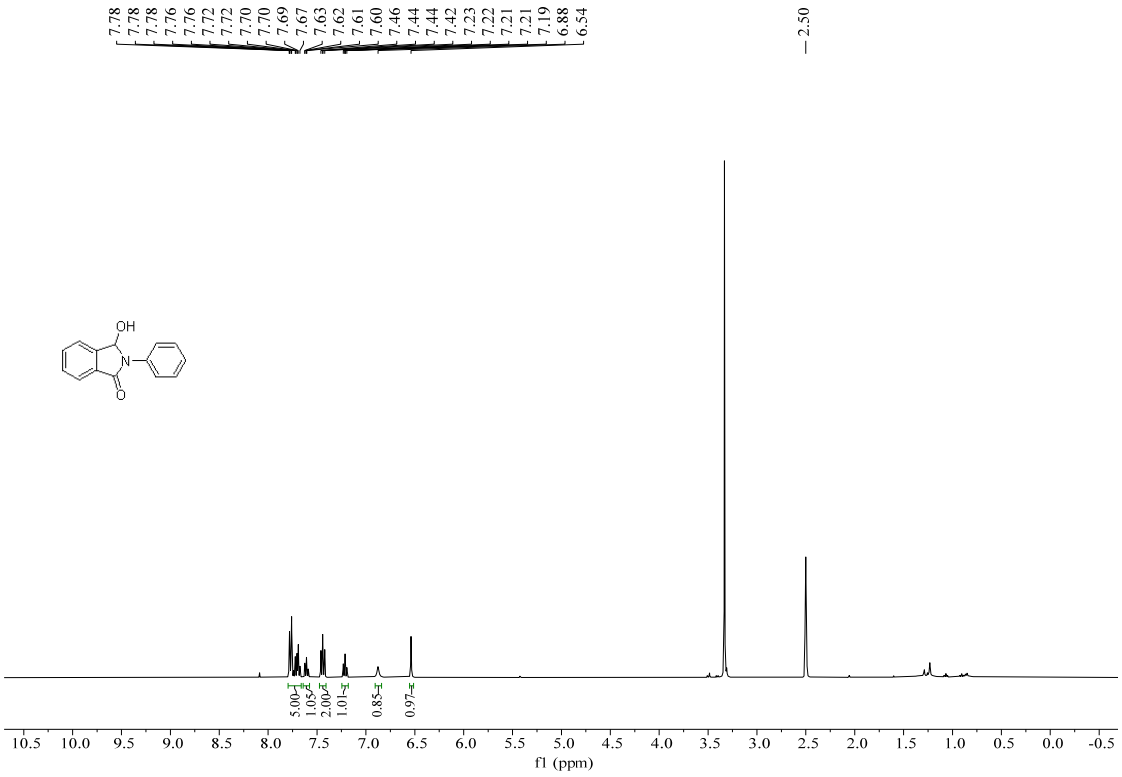
7.50
7.48
7.48
7.47
7.46
7.46
7.46
7.45
7.44
7.26
6.00
5.98
2.48
1.61
OH
N
O
1.00
3.23
1.06
0.88
9.26
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


168.06
143.62
132.82
132.14
129.96
123.16
122.83
82.41
77.48
77.16
76.84
54.89
28.72
OH
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2aj: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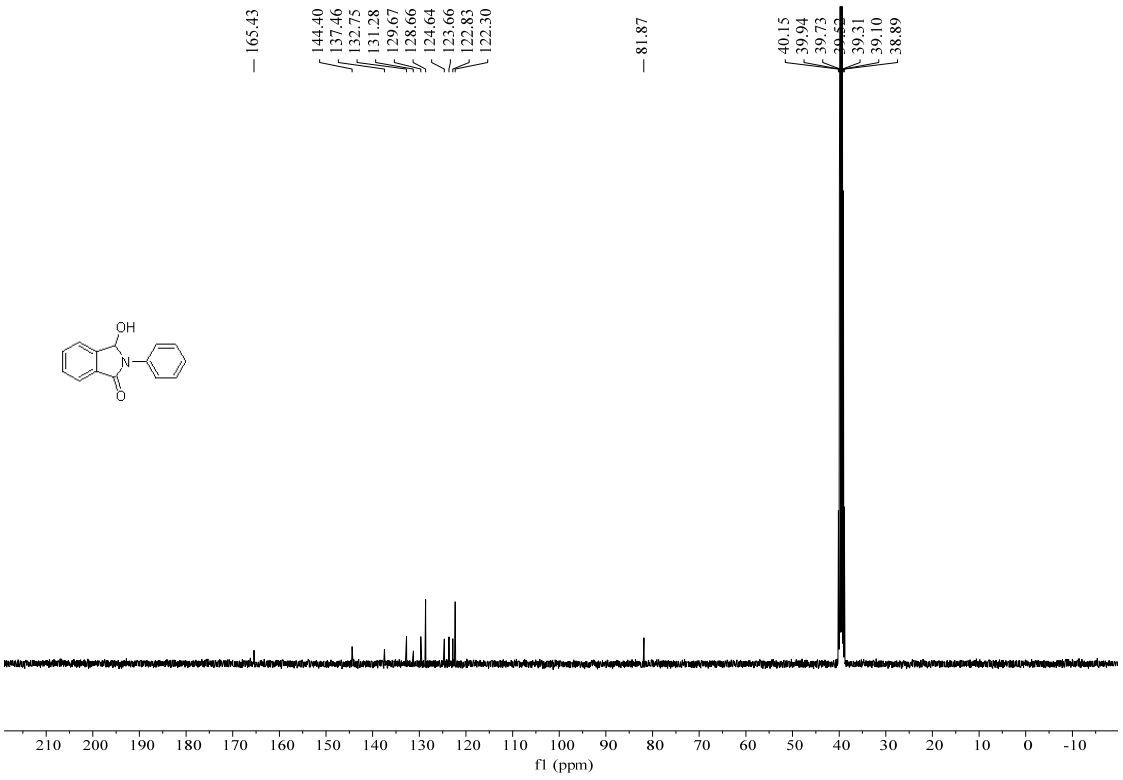
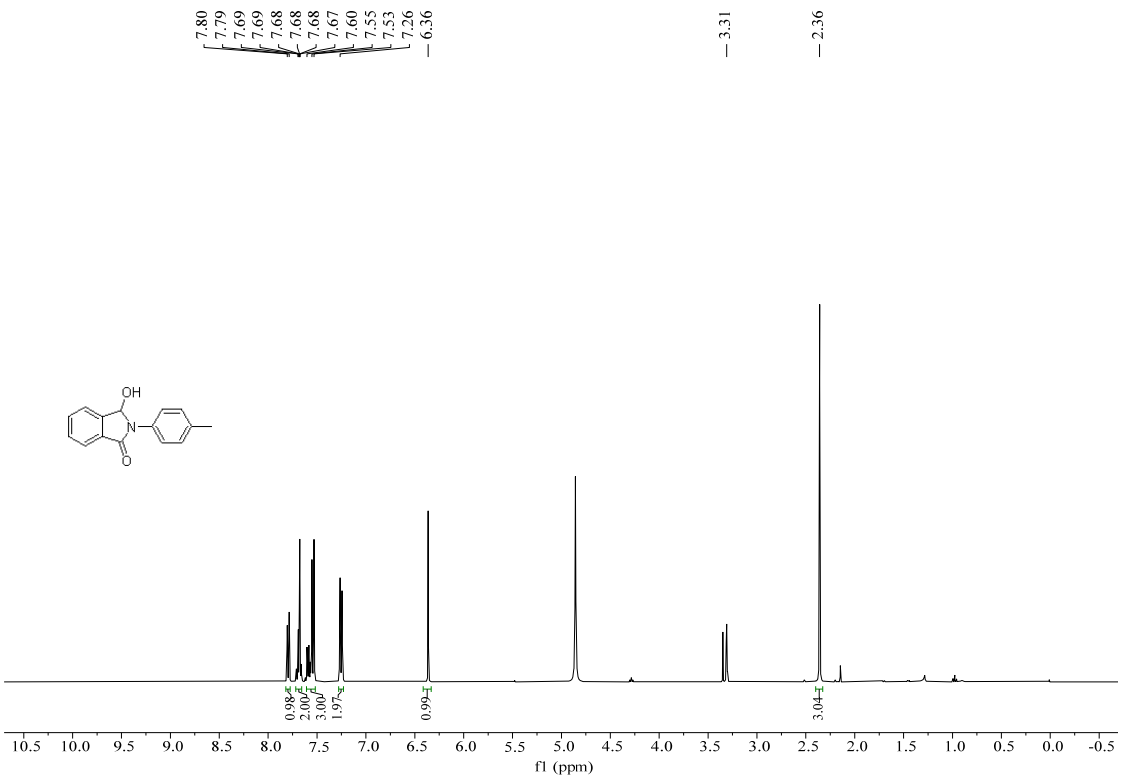
7.78
7.76
7.76
7.72
7.72
7.70
7.70
7.69
7.67
7.63
7.62
7.61
7.60
7.46
7.44
7.44
7.42
7.23
7.22
7.21
7.21
7.19
6.88
6.54
2.50
OH
N
O
5.00
1.05
2.00
1.01
0.85
0.97
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


165.43
144.40
137.46
132.75
131.28
129.67
128.66
124.64
123.66
122.83
122.30
81.87
40.15
39.94
39.73
39.52
39.31
39.10
38.89
OH
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2ak: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7.69
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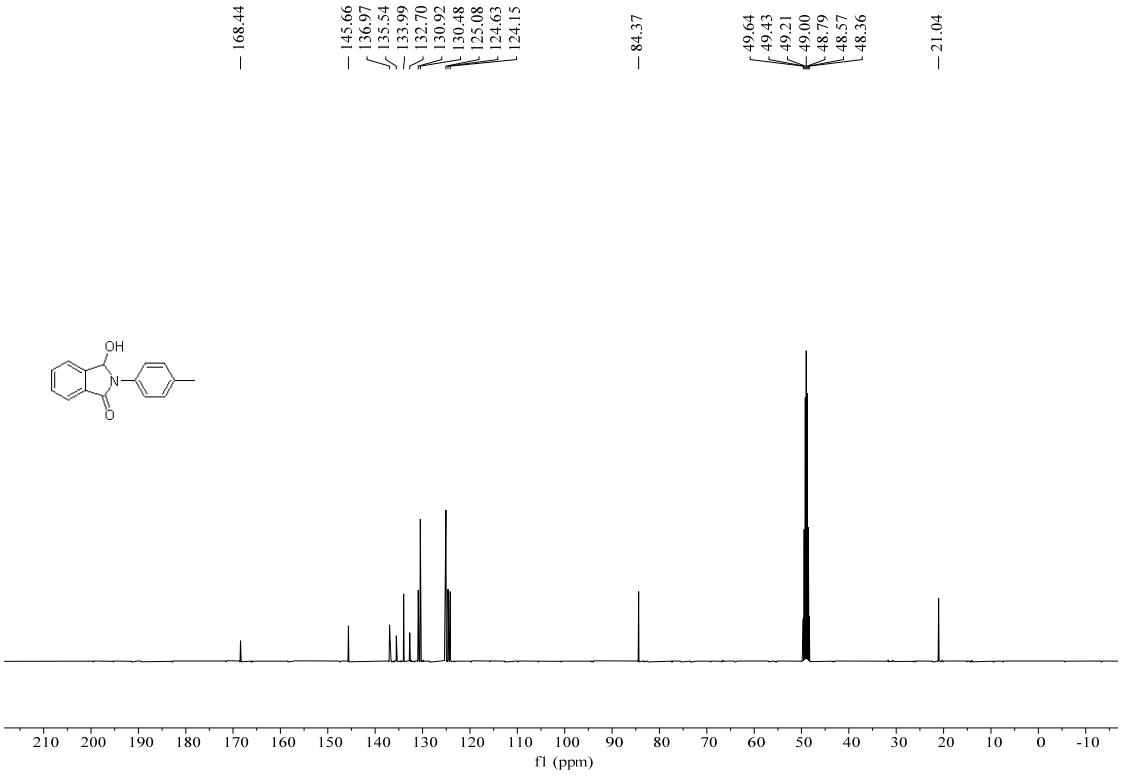
7.68
7.68
7.67
7.60
7.55
7.53
7.26
6.36
3.31
2.36
OH
N
O
0.98
2.00
3.00
1.97
0.99
3.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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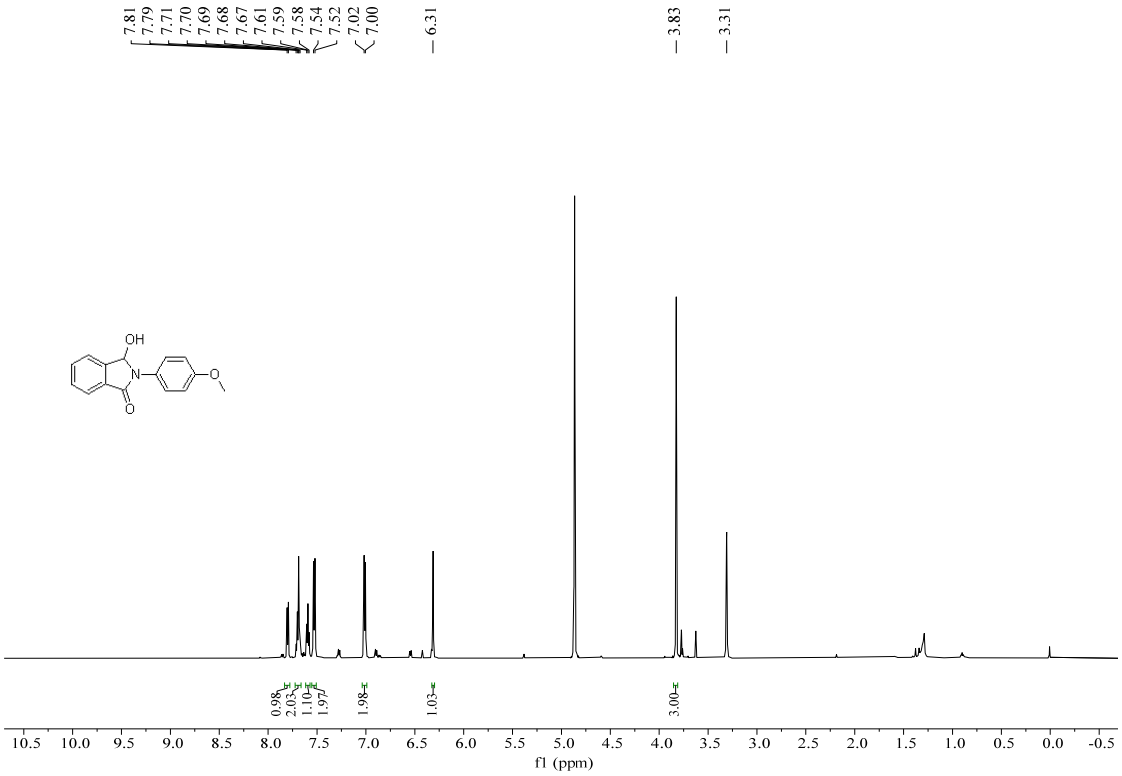
132.70
130.92
130.48
125.08
124.63
124.15
84.37
49.64
49.43
49.21
49.00
48.79
48.57
48.36
21.04
OH
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2al: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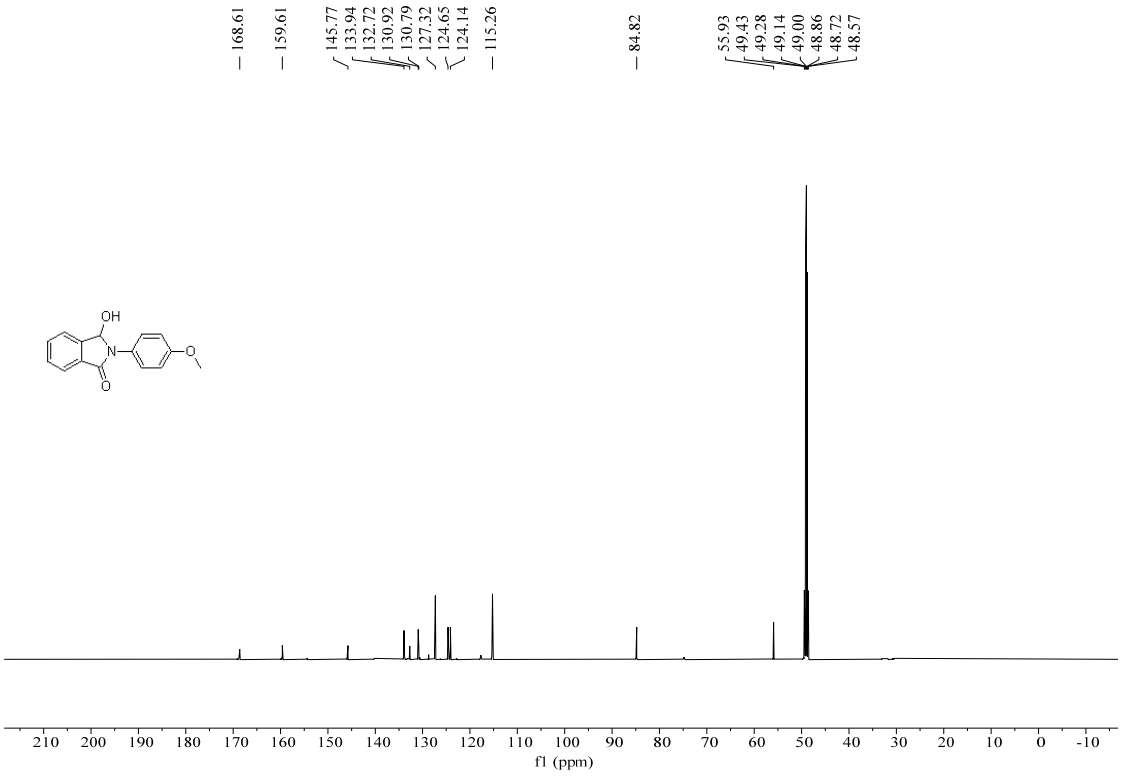
7.68
7.67
7.61
7.59
7.58
7.54
7.52
7.02
7.00
6.31
3.83
3.31
OH
N
O
O
0.98
2.03
1.10
1.97
1.98
1.03
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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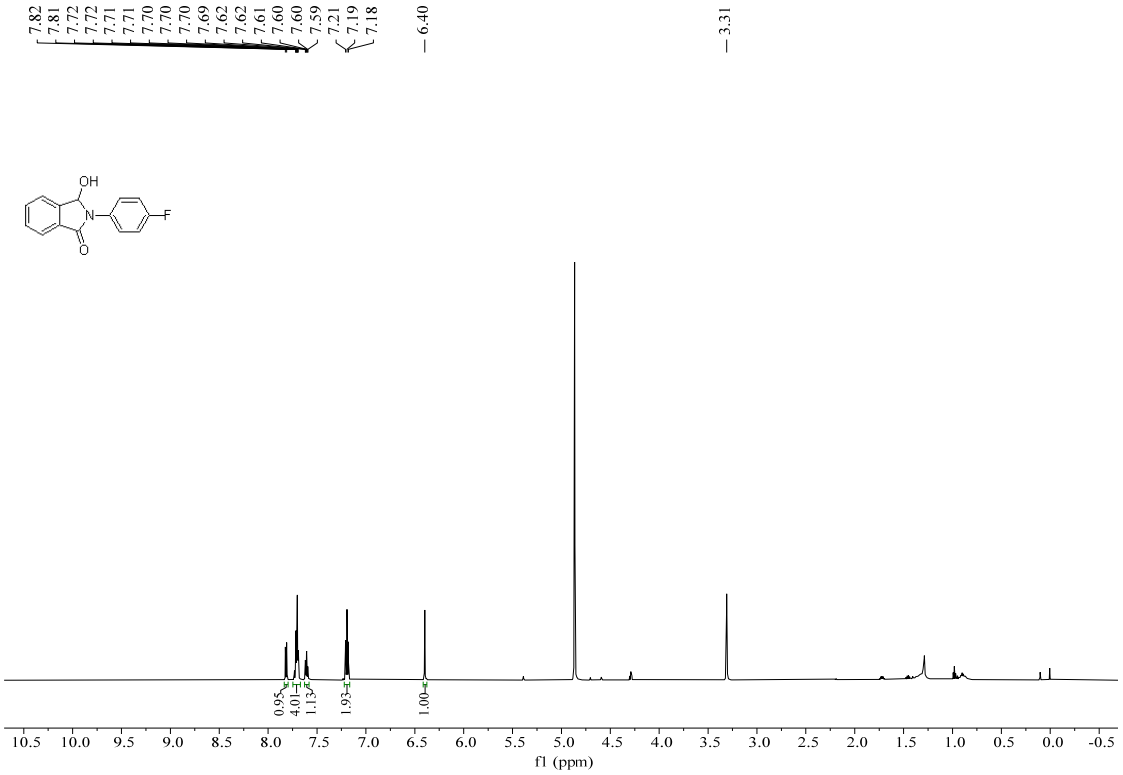
145.77
133.94
132.72
130.92
130.79
127.32
124.65
124.14
115.26
84.82
55.93
49.43
49.28
49.14
49.00
48.86
48.72
48.57
OH
N
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2am: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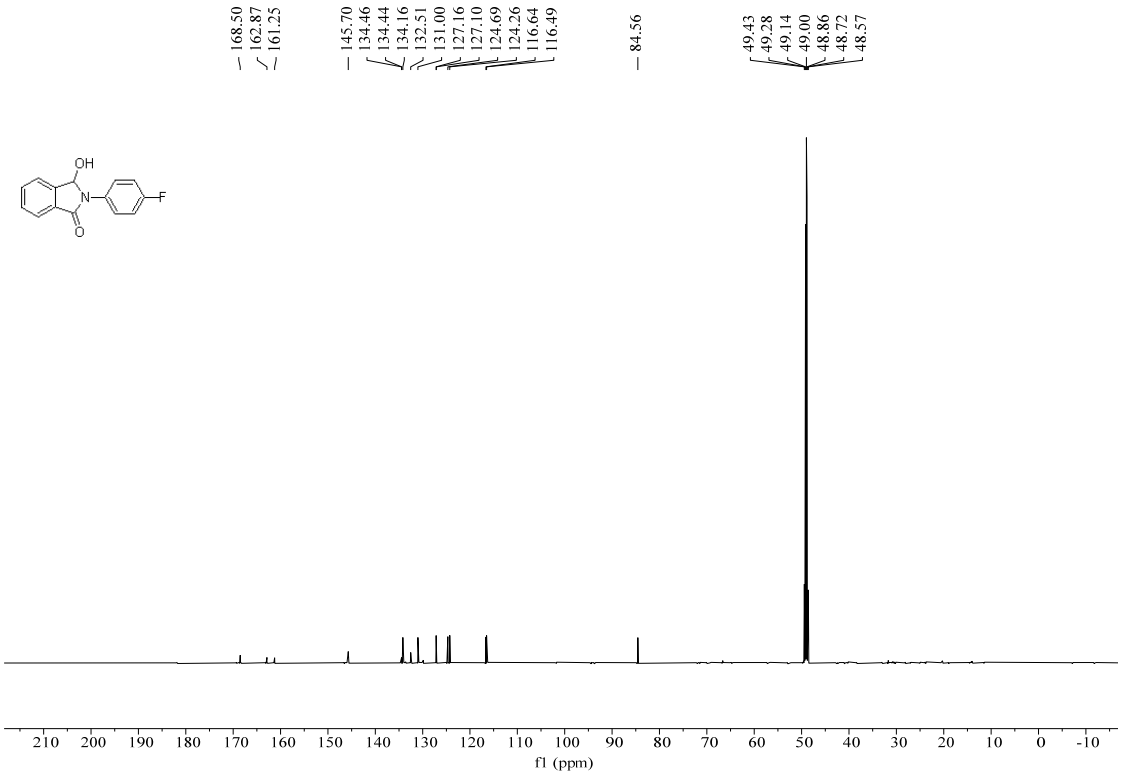
7.72
7.72
7.71
7.71
7.70
7.70
7.70
7.69
7.62
7.62
7.61
7.60
7.60
7.59
7.21
7.19
7.18
6.40
3.31
OH
N
F
O
0.95
4.01
1.13
1.93
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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134.46
134.44
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132.51
131.00
127.16
127.10
124.69
124.26
116.64
116.49
84.56
49.43
49.28
49.14
49.00
48.86
48.72
48.57
OH
N
F
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

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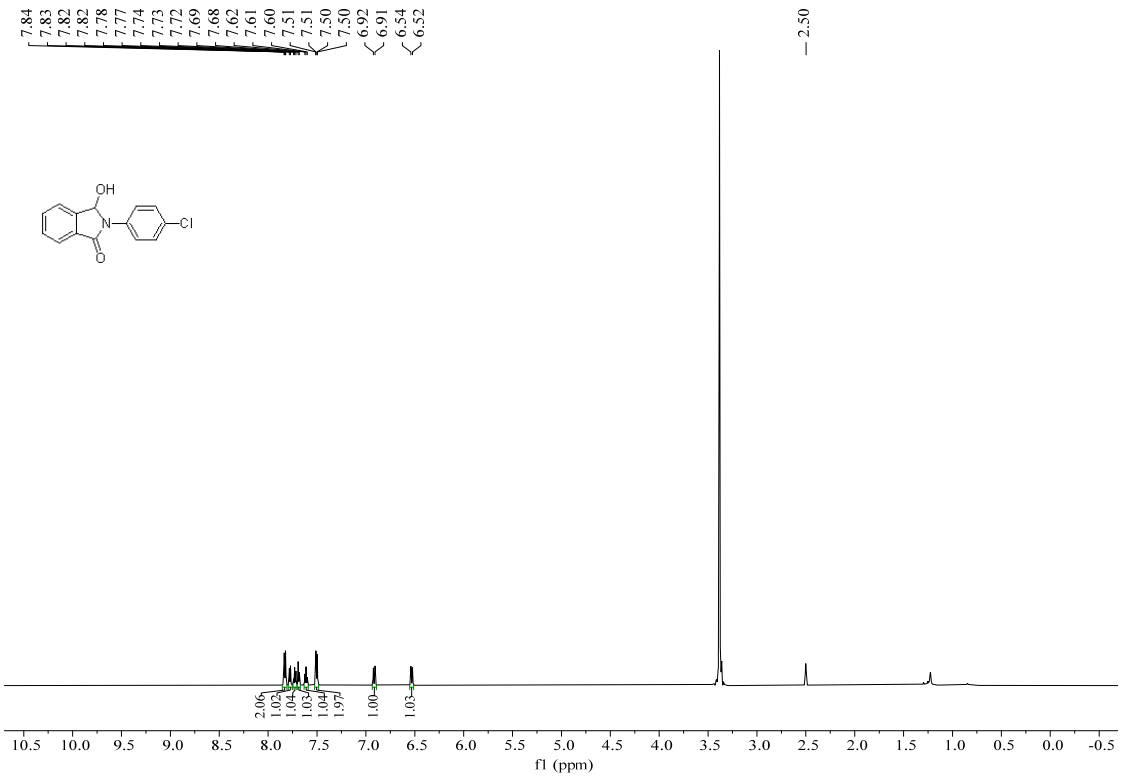
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7.77
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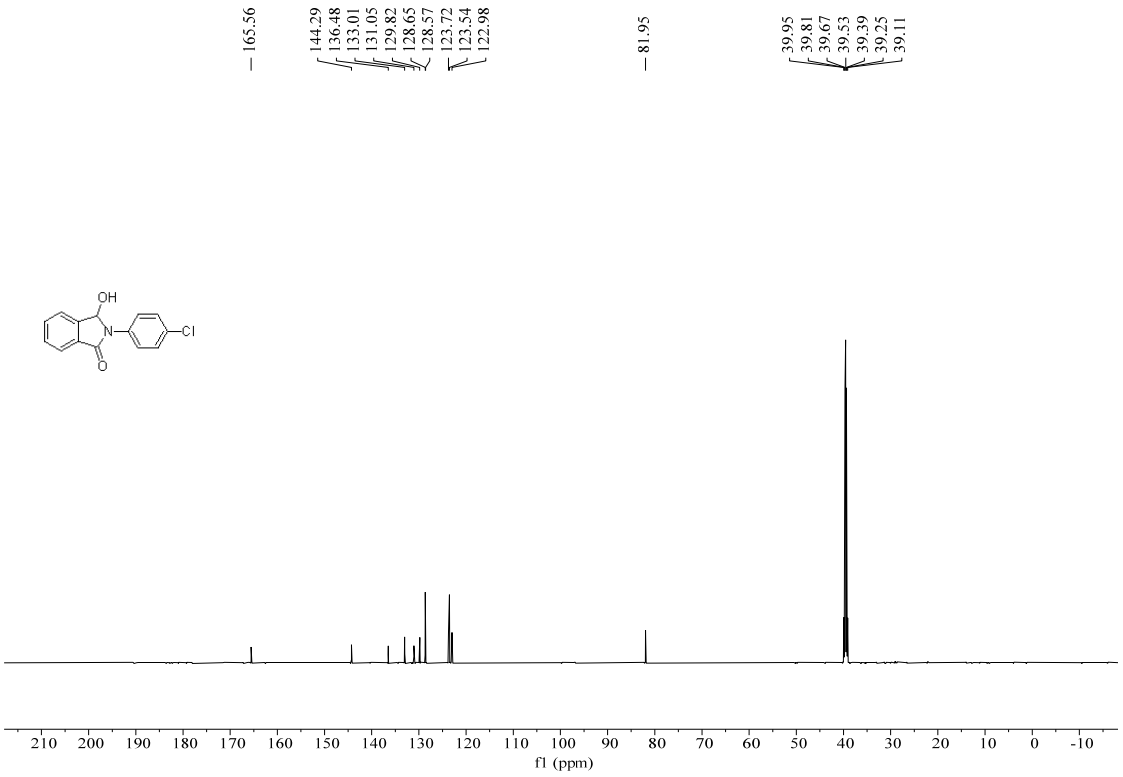
7.69
7.68
7.62
7.61
7.60
7.51
7.51
7.50
7.50
6.92
6.91
6.54
6.52
2.50
OH
N
Cl
O
2.06
1.02
1.04
1.03
1.04
1.97
1.00
1.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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133.01
131.05
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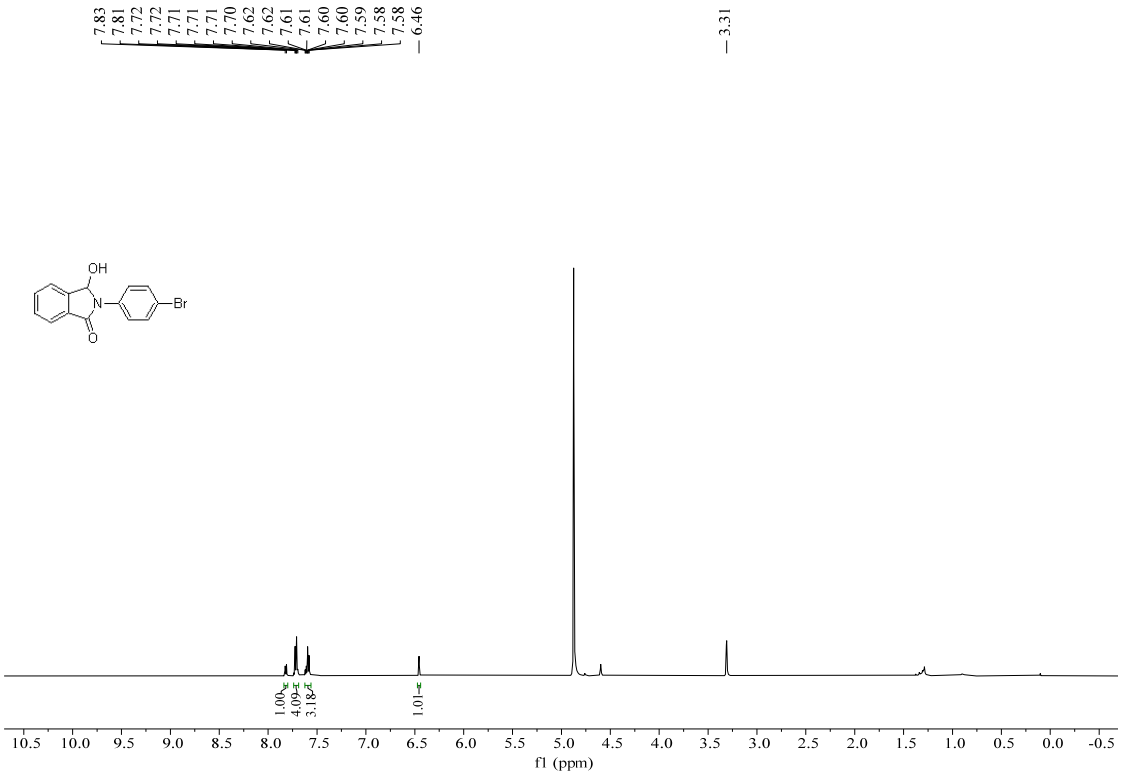
128.65
128.57
123.72
123.54
122.98
81.95
39.95
39.81
39.67
39.53
39.39
39.25
39.11
OH
N
Cl
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2ao: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7.81
7.72
7.72
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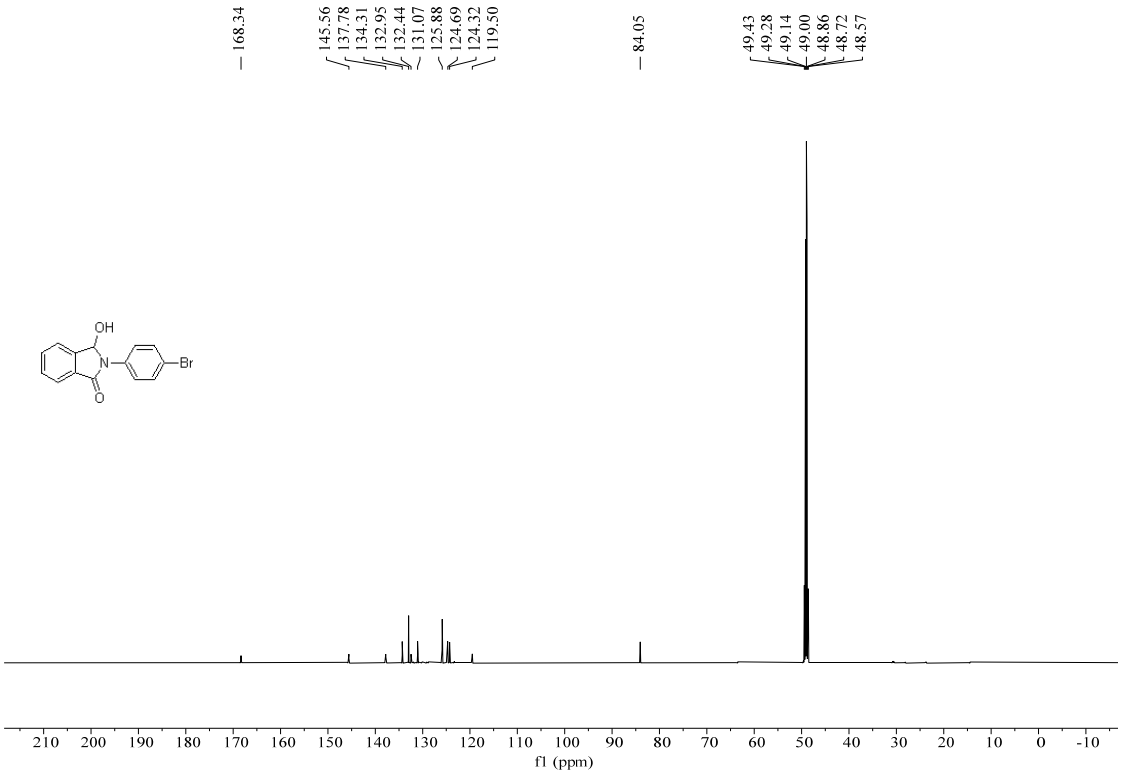
7.71
7.71
7.70
7.62
7.62
7.61
7.61
7.60
7.60
7.59
7.58
7.58
6.46
3.31
OH
N
Br
O
1.00
4.09
3.18
1.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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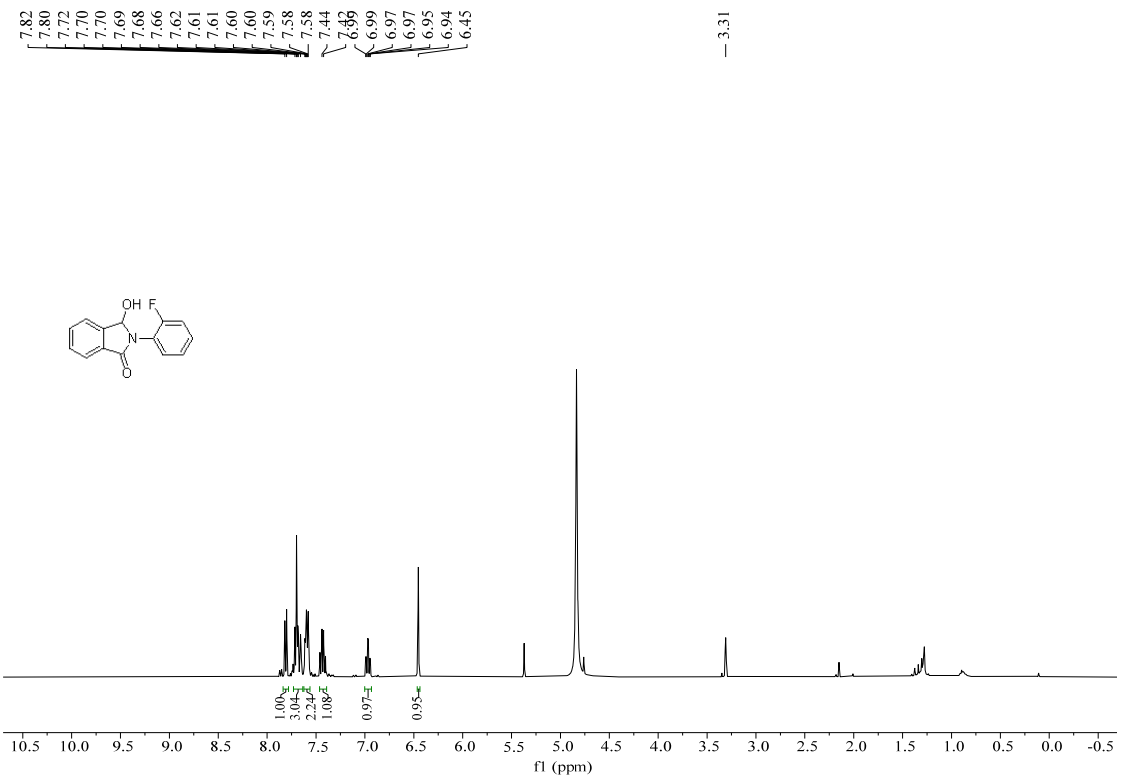
132.95
132.44
131.07
125.88
124.69
124.32
119.50
84.05
49.43
49.28
49.14
49.00
48.86
48.72
48.57
OH
N
Br
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2ap: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7.68
7.66
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7.61
7.61
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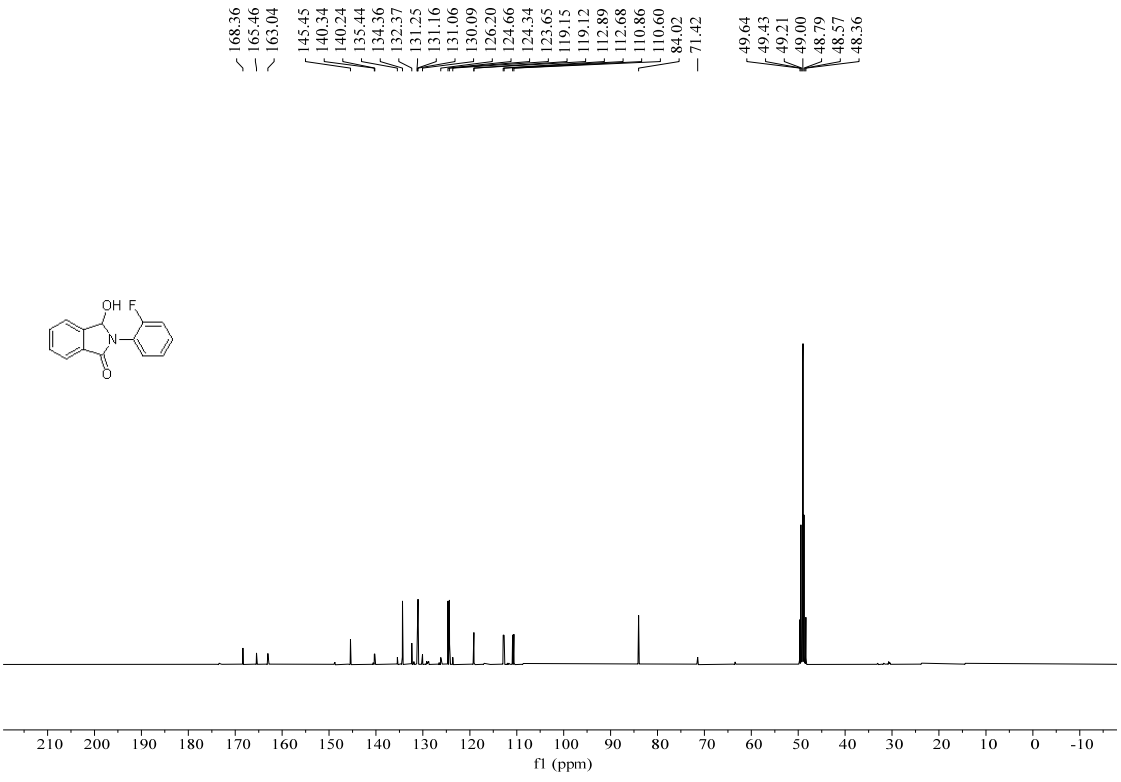
7.59
7.58
7.58
7.44
6.99
6.99
6.97
6.97
6.95
6.94
6.45
3.31
OH F
N
O
1.00
3.04
2.24
1.08
0.97
0.95
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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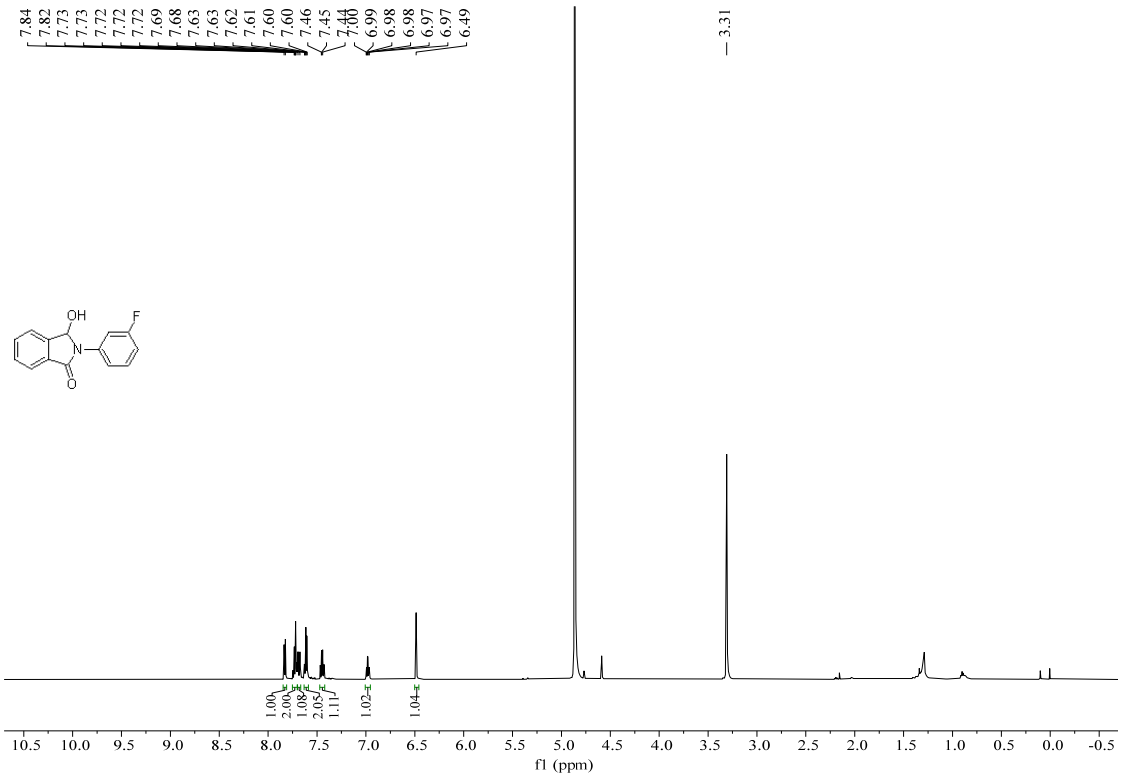
165.46
163.04
145.45
140.34
140.24
135.44
134.36
132.37
131.25
131.16
131.06
130.09
126.20
124.66
124.34
123.65
119.15
119.12
112.89
112.68
110.86
110.60
84.02
71.42
49.64
49.43
49.21
49.00
48.79
48.57
48.36
OH F
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2aq: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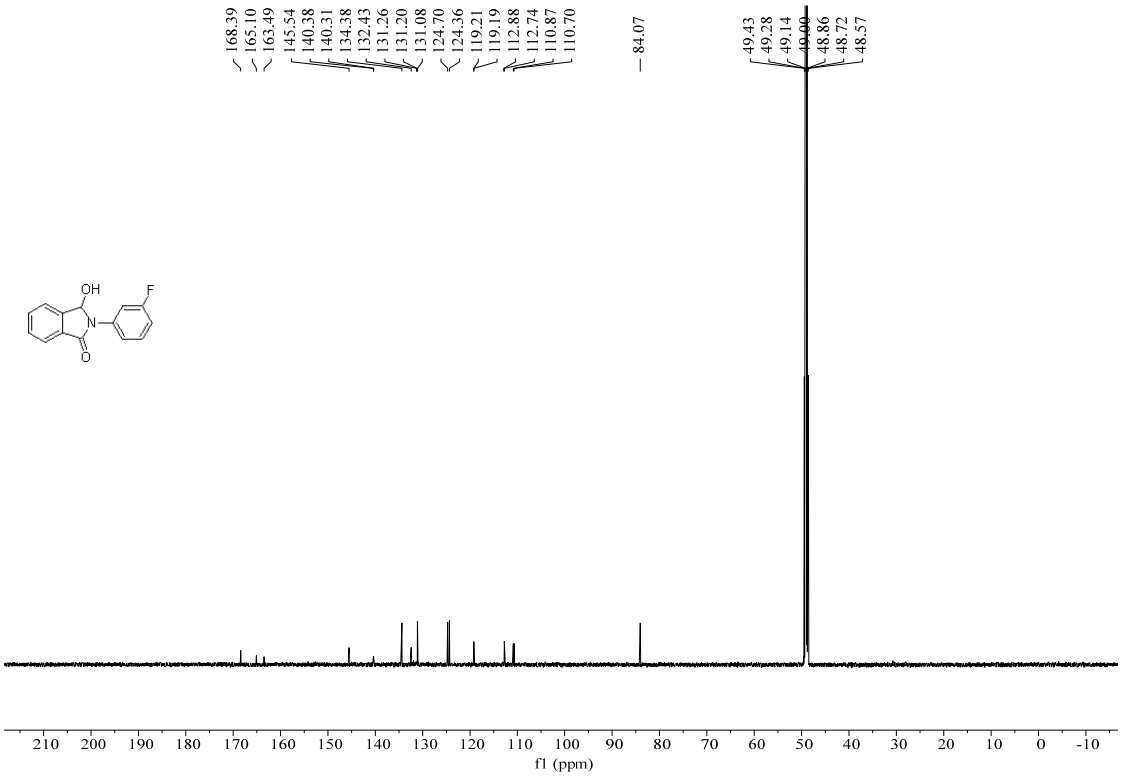
7.82
7.73
7.73
7.72
7.72
7.72
7.69
7.68
7.63
7.63
7.62
7.61
7.60
7.60
7.46
7.45
7.44
7.00
6.99
6.98
6.98
6.97
6.97
6.49
3.31
OH
F
N
O
1.00
2.06
1.08
2.05
1.11
1.02
1.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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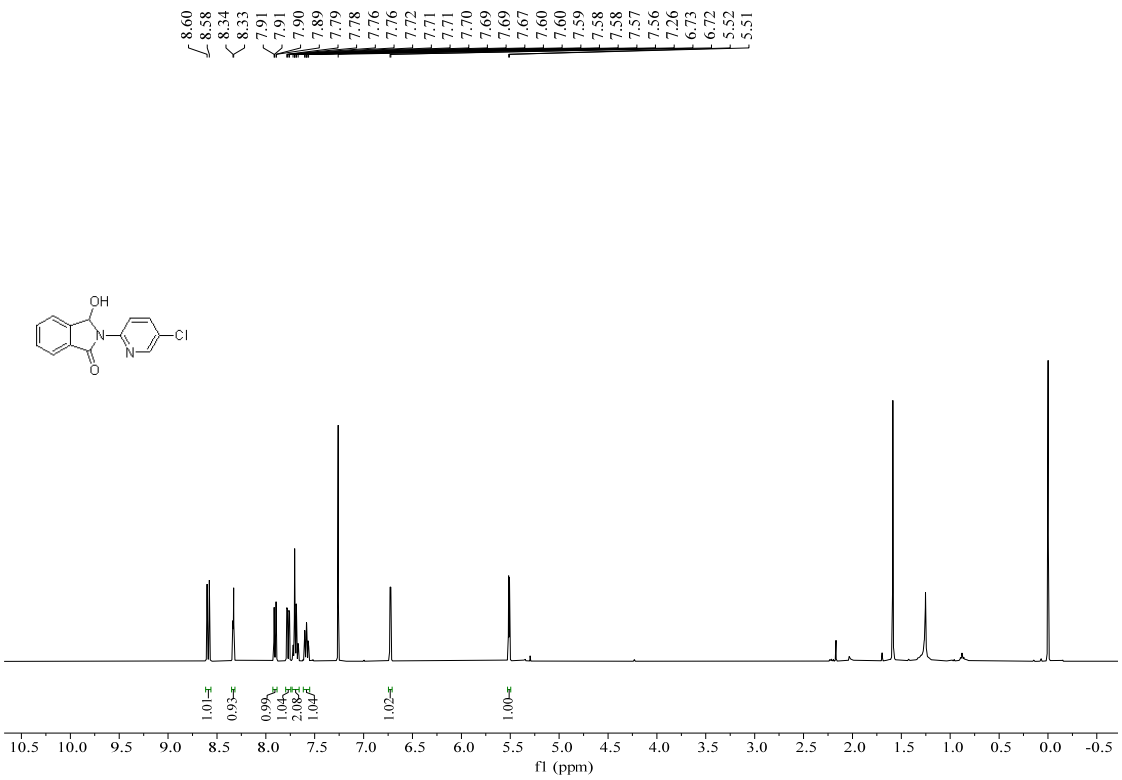
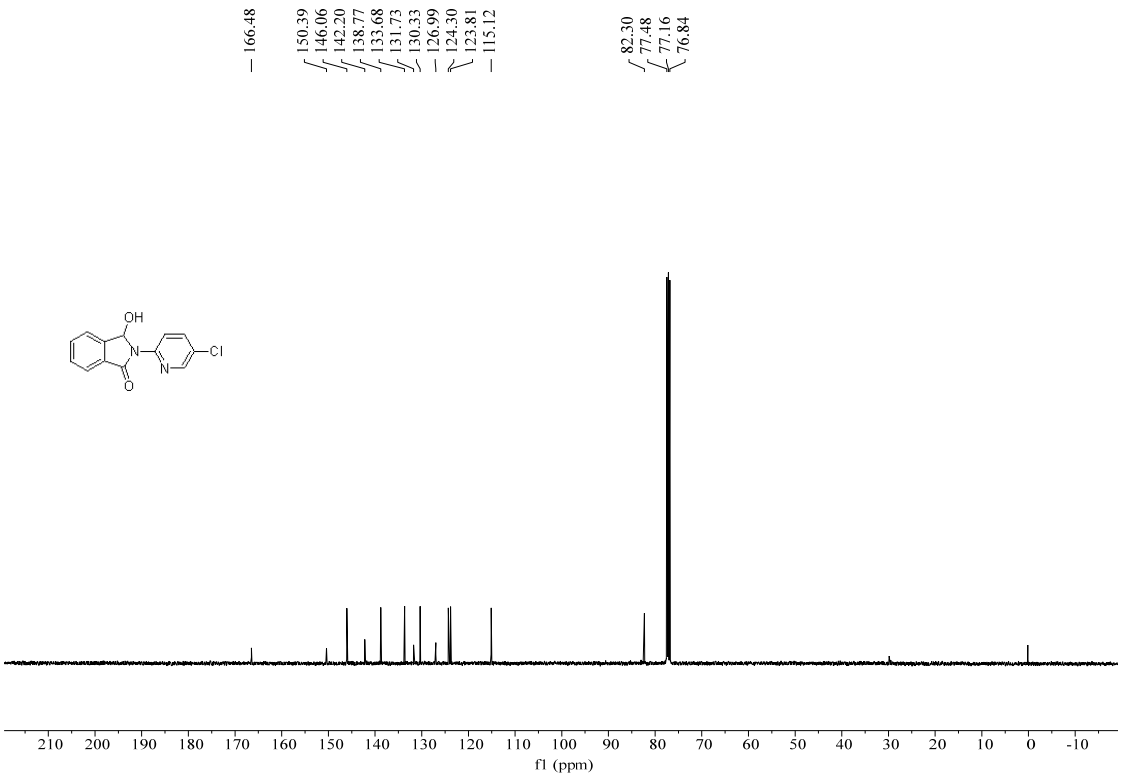
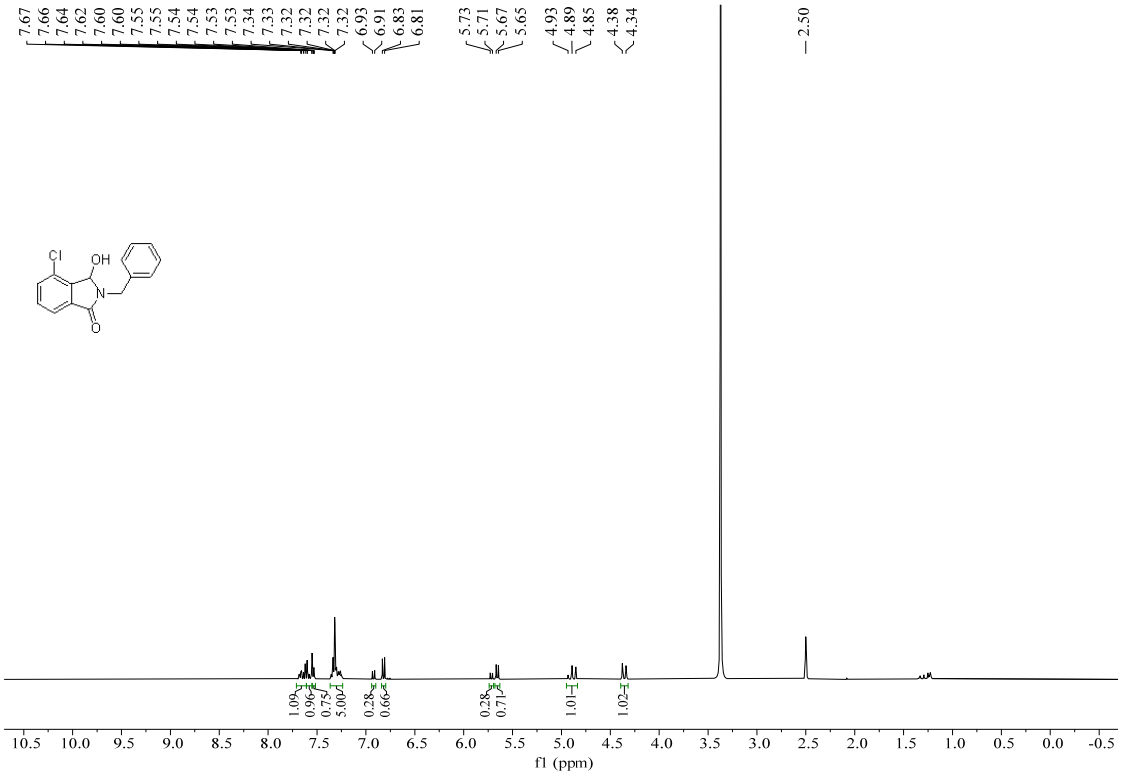
165.10
163.49
145.54
140.38
140.31
134.38
132.43
131.26
131.20
131.08
124.70
124.36
119.21
119.19
112.88
112.74
110.87
110.70
84.07
49.43
49.28
49.14
49.00
48.86
48.72
48.57
OH
F
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2ar:


8.60
8.58
8.34
8.33
7.91
7.91
7.90
7.89
7.79
7.78
7.76
7.76
7.72
7.71
7.71
7.70
7.69
7.69
7.67
7.60
7.60
7.59
7.58
7.58
7.57
7.56
7.26
6.73
6.72
5.52
5.51
OH
N
Cl
N
O
1.01
0.93
0.99
1.04
2.08
1.04
1.02
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


166.48
150.39
146.06
142.20
138.77
133.68
131.73
130.33
126.99
124.30
123.81
115.12
82.30
77.48
77.16
76.84
OH
N
Cl
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2ba: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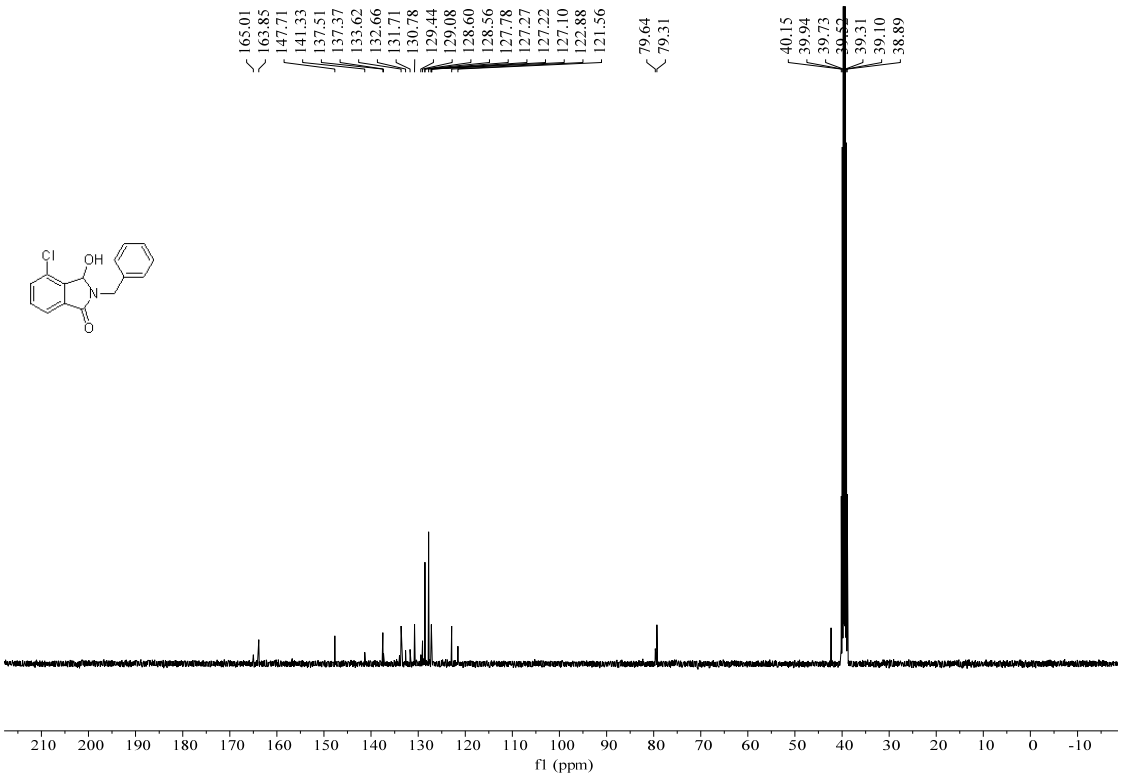
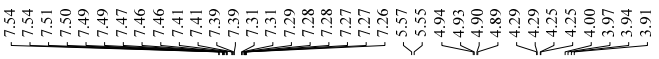
7.66
7.64
7.62
7.60
7.60
7.55
7.55
7.54
7.54
7.53
7.53
7.34
7.33
7.32
7.32
7.32
7.32
6.93
6.91
6.83
6.81
5.73
5.71
5.67
5.65
4.93
4.89
4.85
4.38
4.34
2.50
Cl
OH
N
O
1.09
0.96
0.75
5.00
0.28
0.66
0.28
0.71
1.01
1.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


165.01
163.85
147.71
141.33
137.51
137.37
133.62
132.66
131.71
130.78
129.44
129.08
128.60
128.56
127.78
127.27
127.22
127.10
122.88
121.56
79.64
79.31
40.15
39.94
39.73
39.52
39.31
39.10
38.89
Cl
OH
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2ca: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7.54
7.51
7.50
7.49
7.49
7.47
7.46
7.46
7.41
7.41
7.39
7.39
7.31
7.31
7.29
7.28
7.28
7.27
7.27
7.26
5.57
5.55
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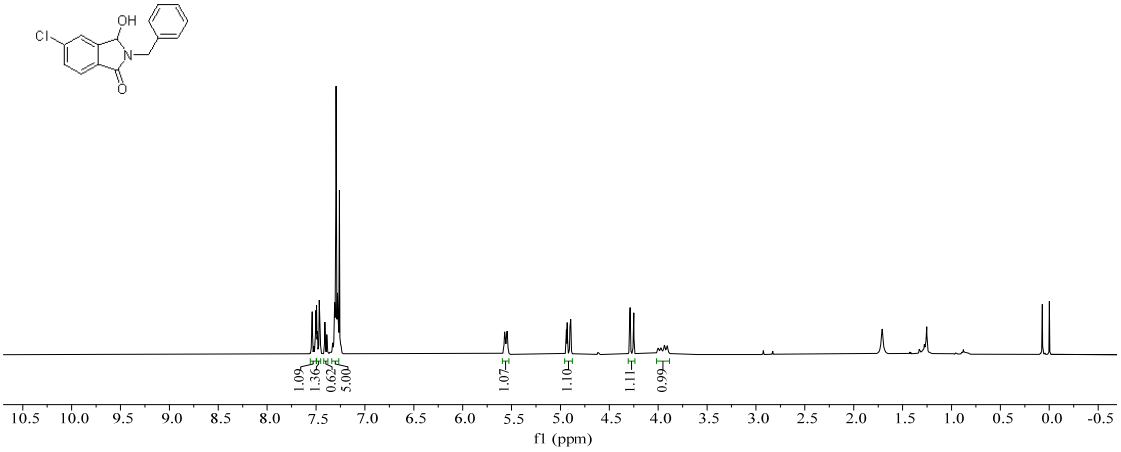
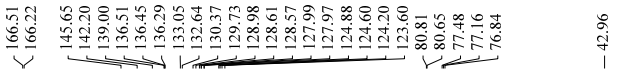
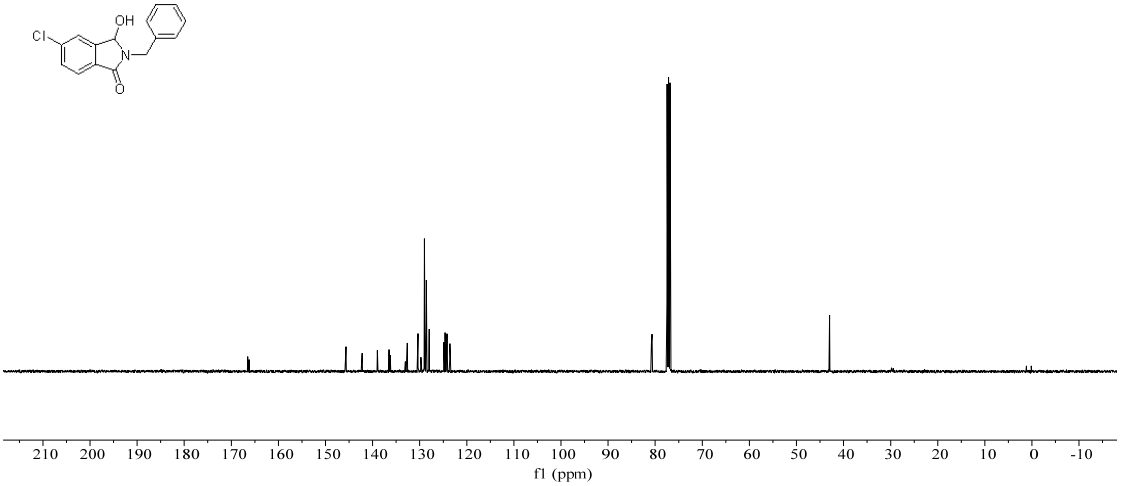
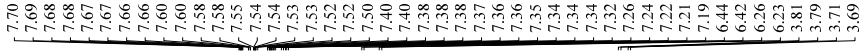
4.25
4.25
4.00
3.97
3.94
3.91


OH
Cl
N
O
1.09
1.36
0.62
5.00
1.07
1.10
1.11
0.99
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


166.51
166.22
145.65
142.20
139.00
136.51
136.45
136.29
133.05
132.64
130.37
129.73
128.98
128.61
128.57
127.99
127.97
124.88
124.60
124.20
123.60
80.81
80.65
77.48
77.16
76.84
42.96


OH
Cl
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2bj:


7.70
7.69
7.68
7.68
7.67
7.67
7.66
7.66
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7.60
7.58
7.58
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7.54
7.54
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7.53
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7.52
7.50
7.40
7.40
7.38
7.38
7.38
7.37
7.36
7.36
7.35
7.34
7.34
7.34
7.32
7.26
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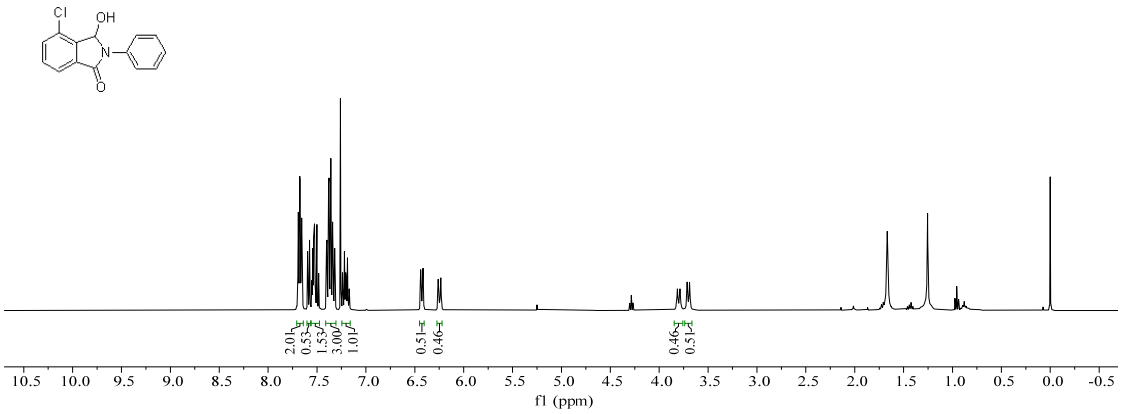
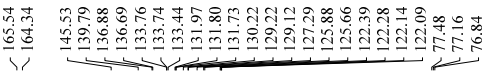
6.26
6.23
3.81
3.79
3.71
3.69


Cl
OH
N
O
2.01
0.53
1.52
3.00
1.01
0.51
0.46
0.46
0.51
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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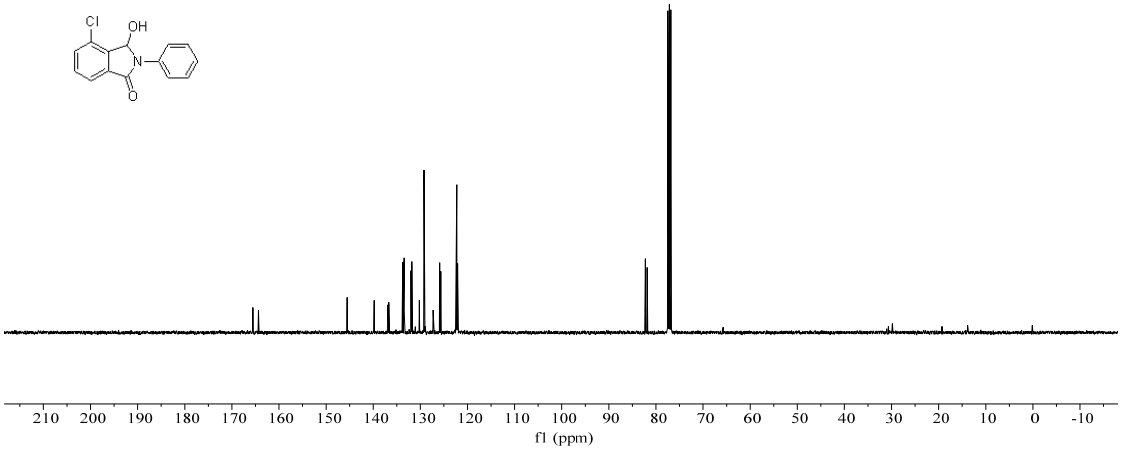
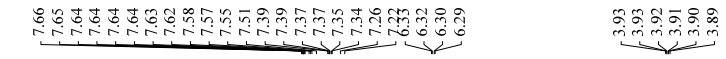
164.34
145.53
139.79
136.88
136.69
133.76
133.74
133.44
131.97
131.80
131.73
130.22
129.22
129.12
127.29
125.88
125.66
122.39
122.28
122.14
122.09
77.48
77.16
76.84


Cl
OH
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2cj: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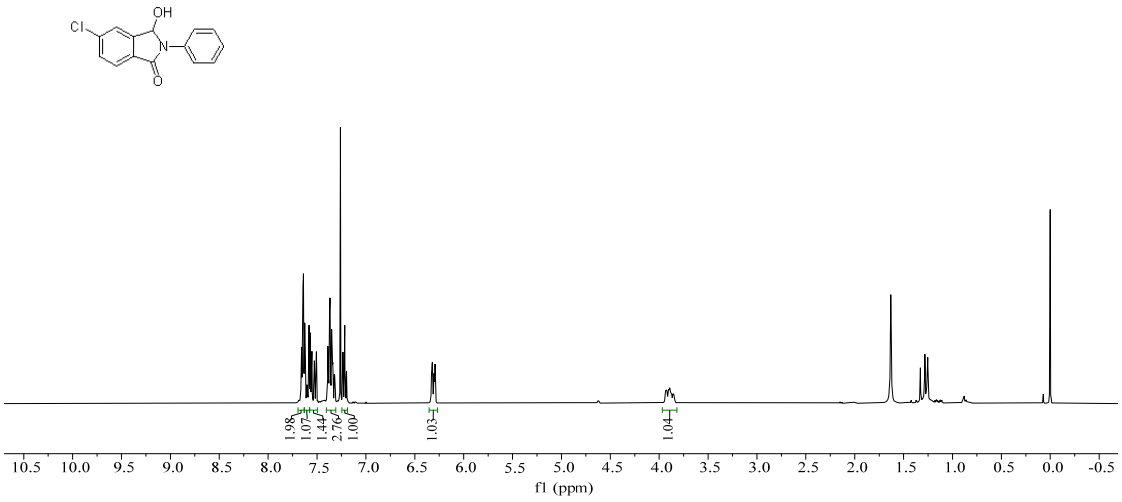
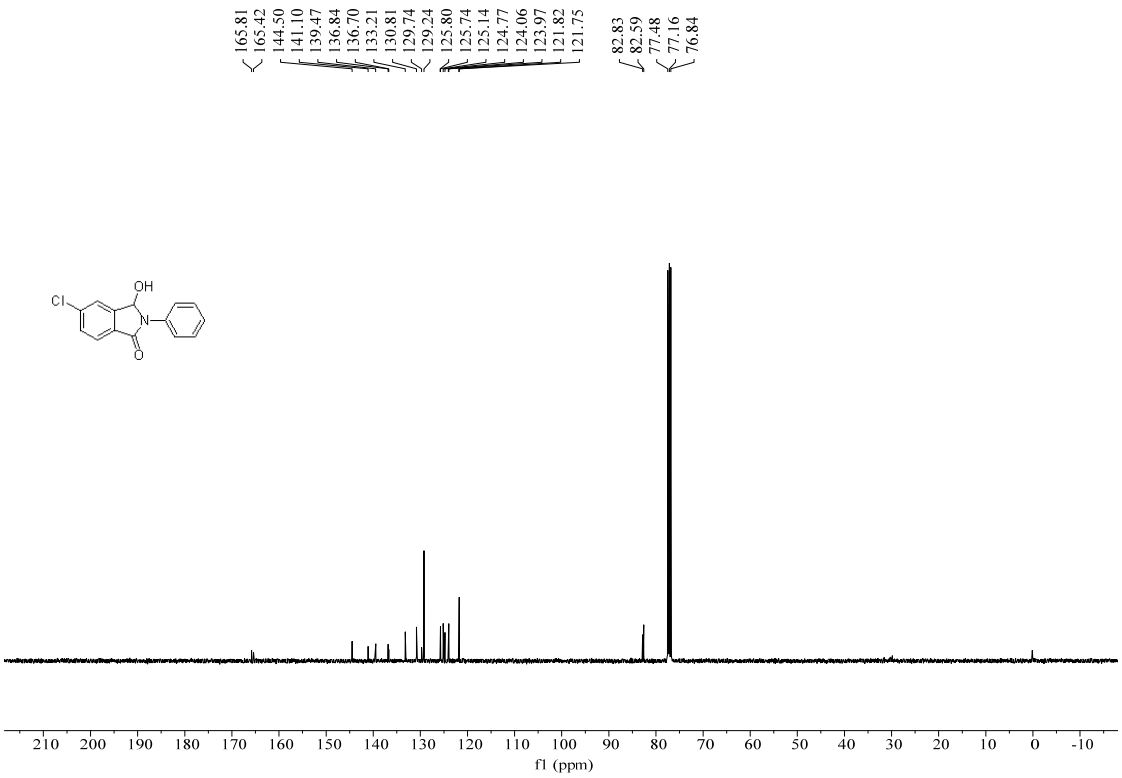
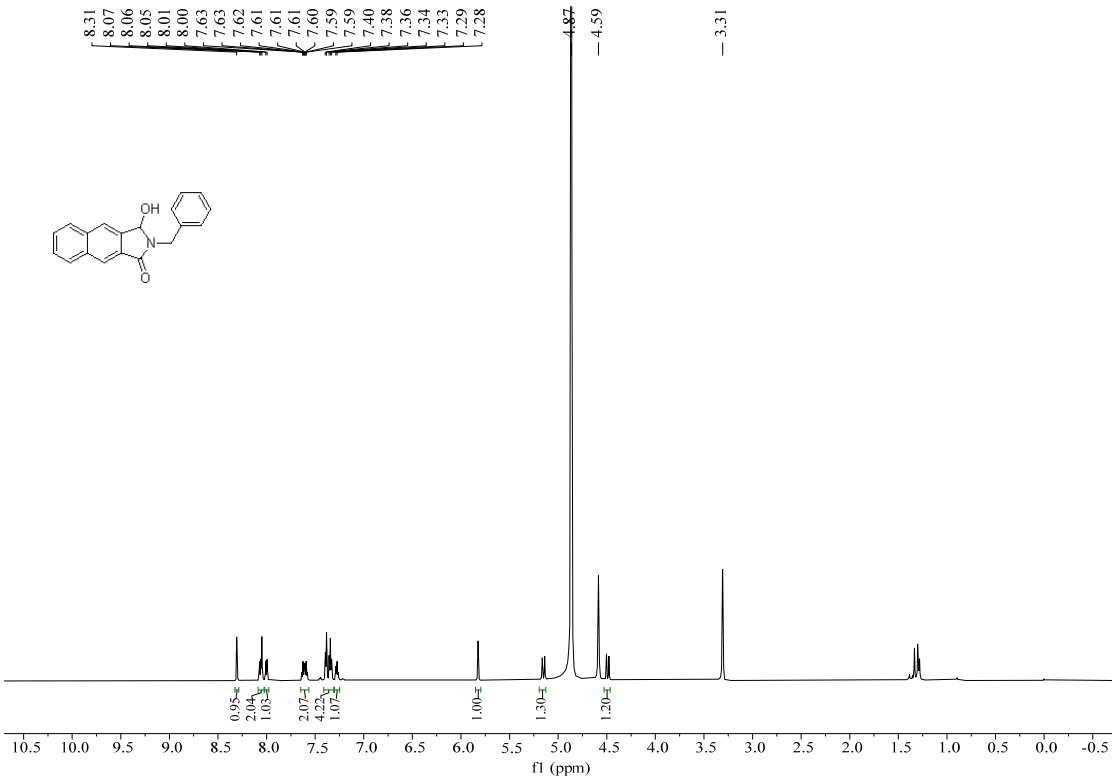
7.65
7.64
7.64
7.64
7.64
7.63
7.62
7.58
7.57
7.55
7.51
7.39
7.39
7.37
7.37
7.35
7.34
7.26
7.22
6.33
6.32
6.30
6.29
3.93
3.93
3.92
3.91
3.90
3.89


OH
Cl
N
O
1.98
1.07
1.44
2.76
1.00
1.03
1.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


165.81
165.42
144.50
141.10
139.47
136.84
136.70
133.21
130.81
129.74
129.24
125.80
125.74
125.14
124.77
124.06
123.97
121.82
121.75
82.83
82.59
77.48
77.16
76.84
Cl
OH
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

2ha:


8.31
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7.63
7.62
7.61
7.61
7.61
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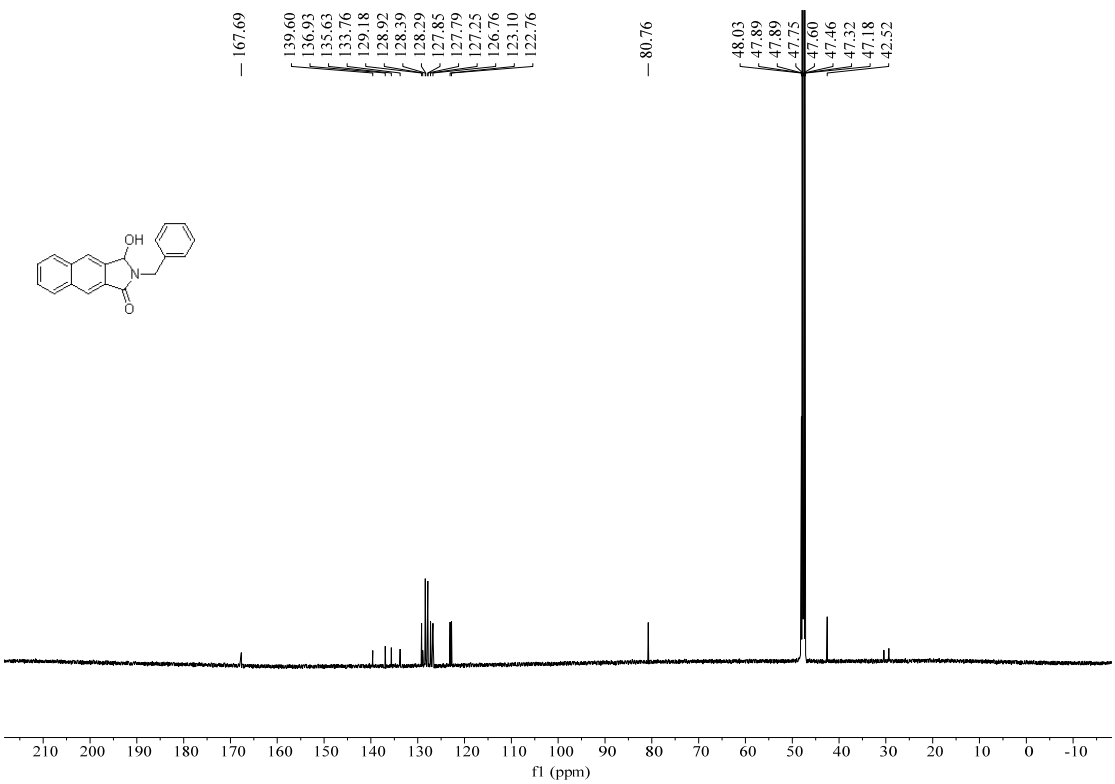
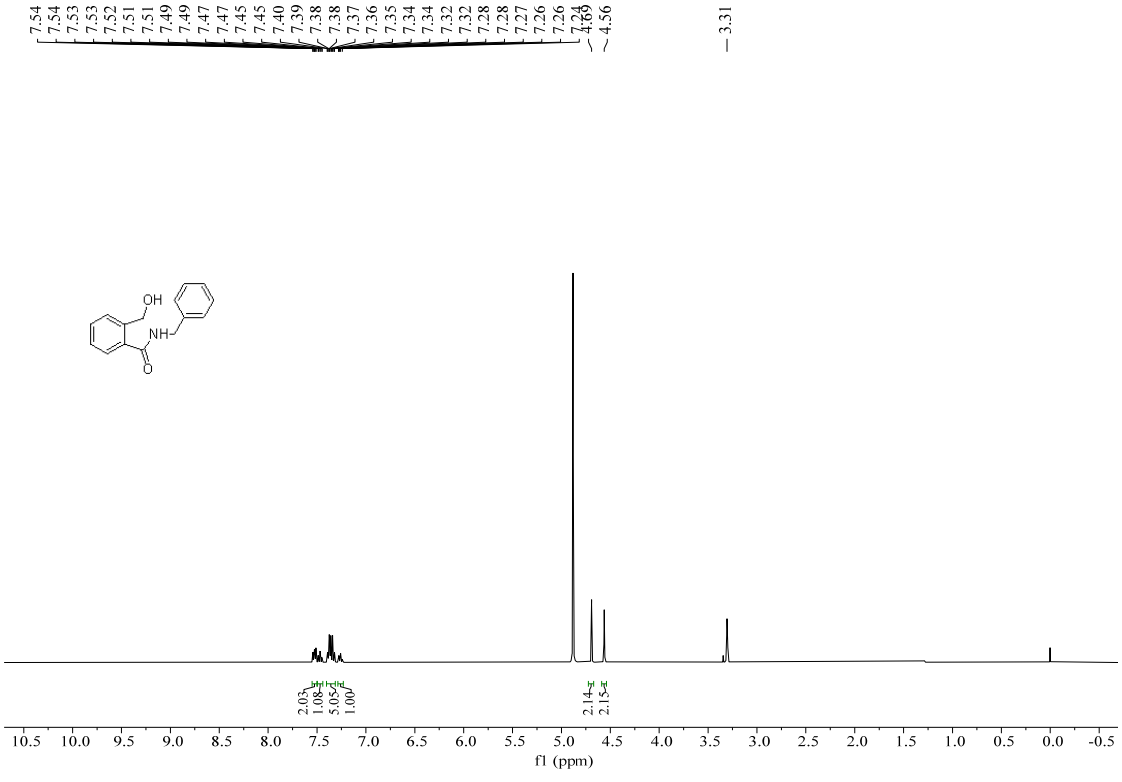
7.59
7.59
7.59
7.40
7.38
7.36
7.34
7.33
7.29
7.28
4.87
4.59
3.31
OH
N
O
0.95
2.04
1.03
2.07
4.22
1.07
1.00
1.30
1.20
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


167.69
139.60
136.93
135.63
133.76
129.18
128.92
128.39
128.29
127.85
127.79
127.25
126.76
123.10
122.76
80.76
48.03
47.89
47.89
47.75
47.60
47.46
47.32
47.18
42.52
OH
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3aa: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7.54
7.53
7.53
7.52
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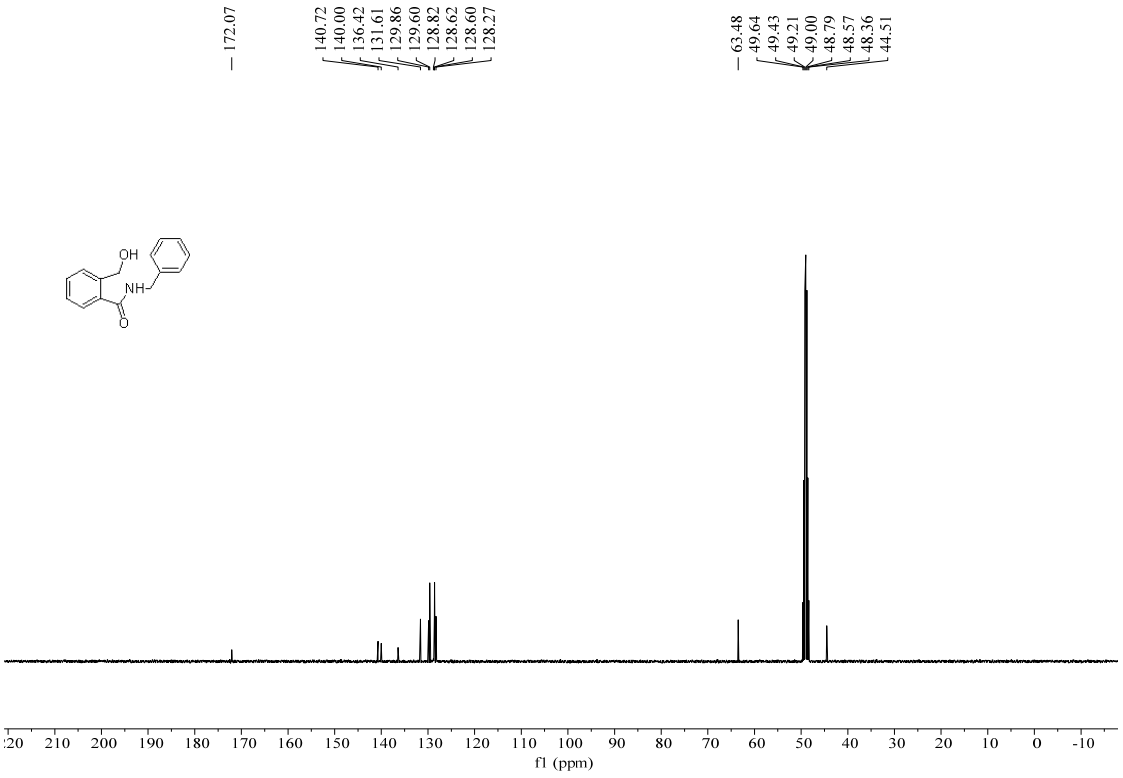
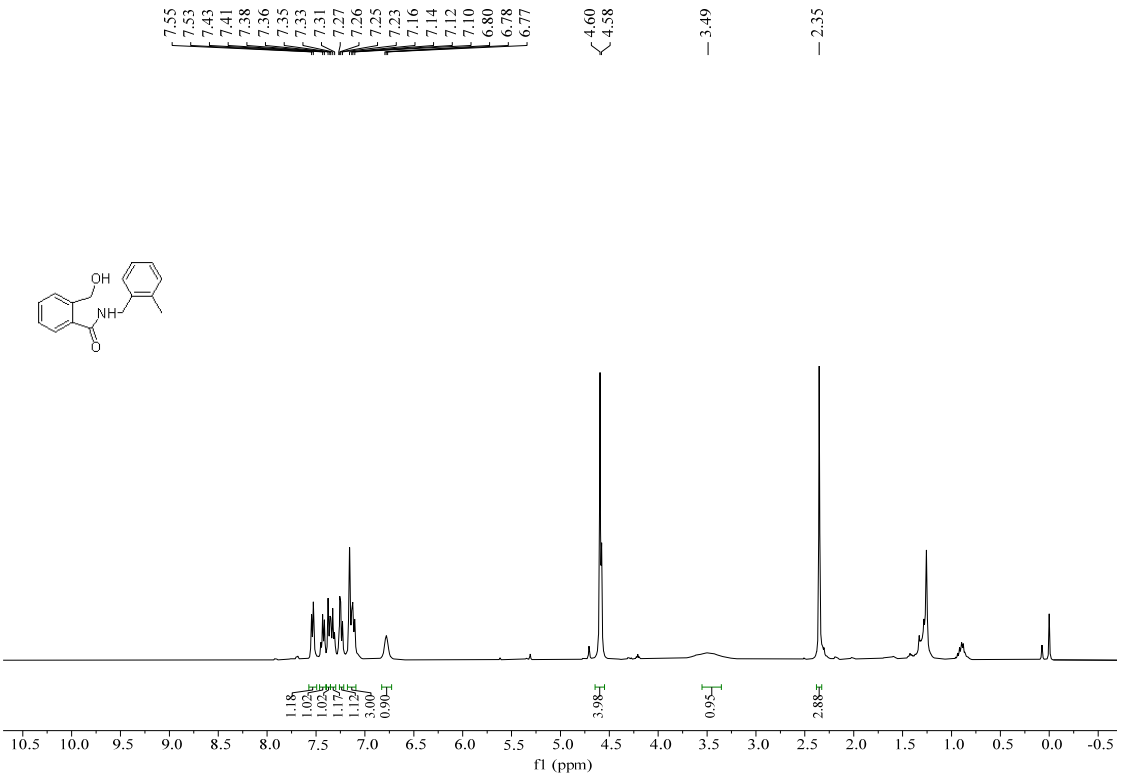
7.51
7.49
7.49
7.47
7.47
7.45
7.45
7.40
7.39
7.38
7.38
7.37
7.36
7.35
7.34
7.34
7.32
7.32
7.28
7.28
7.27
7.26
7.26
7.24
4.69
4.56
3.31
OH
NH
O
2.03
1.08
5.05
1.00
2.14
2.15
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


172.07
140.72
140.00
136.42
131.61
129.86
129.60
128.82
128.62
128.60
128.27
63.48
49.64
49.43
49.21
49.00
48.79
48.57
48.36
44.51
OH
NH
O
f1 (ppm)

3ab: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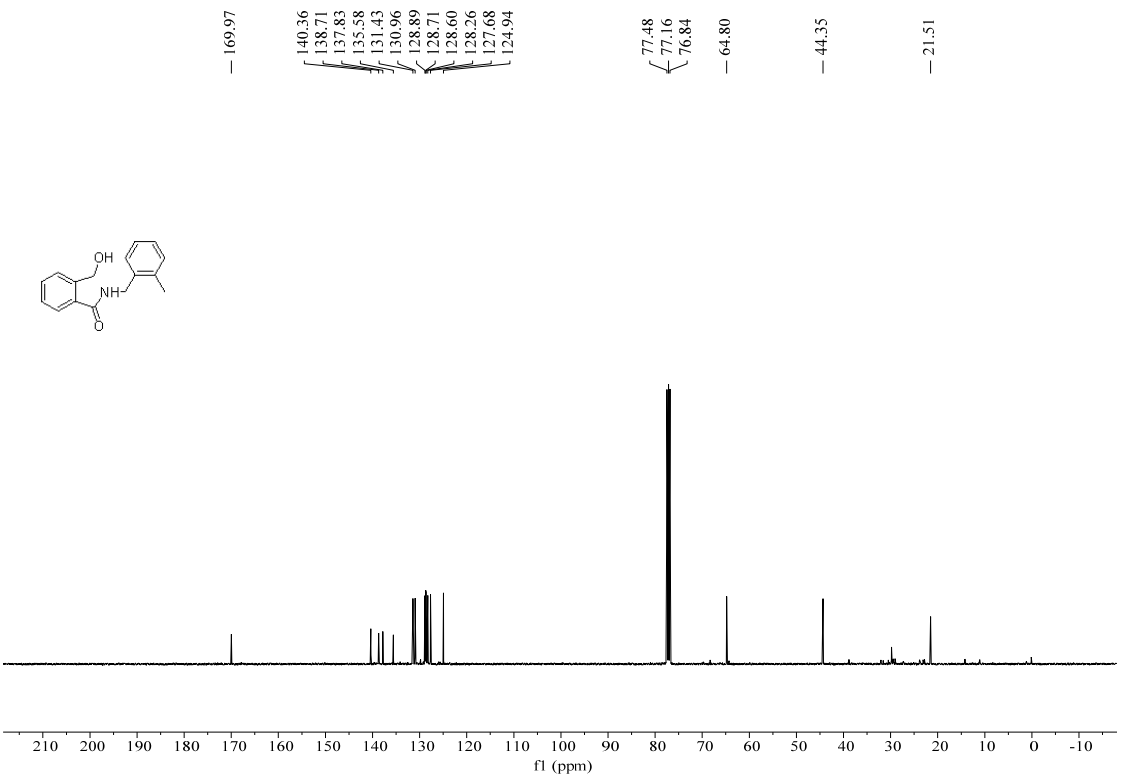
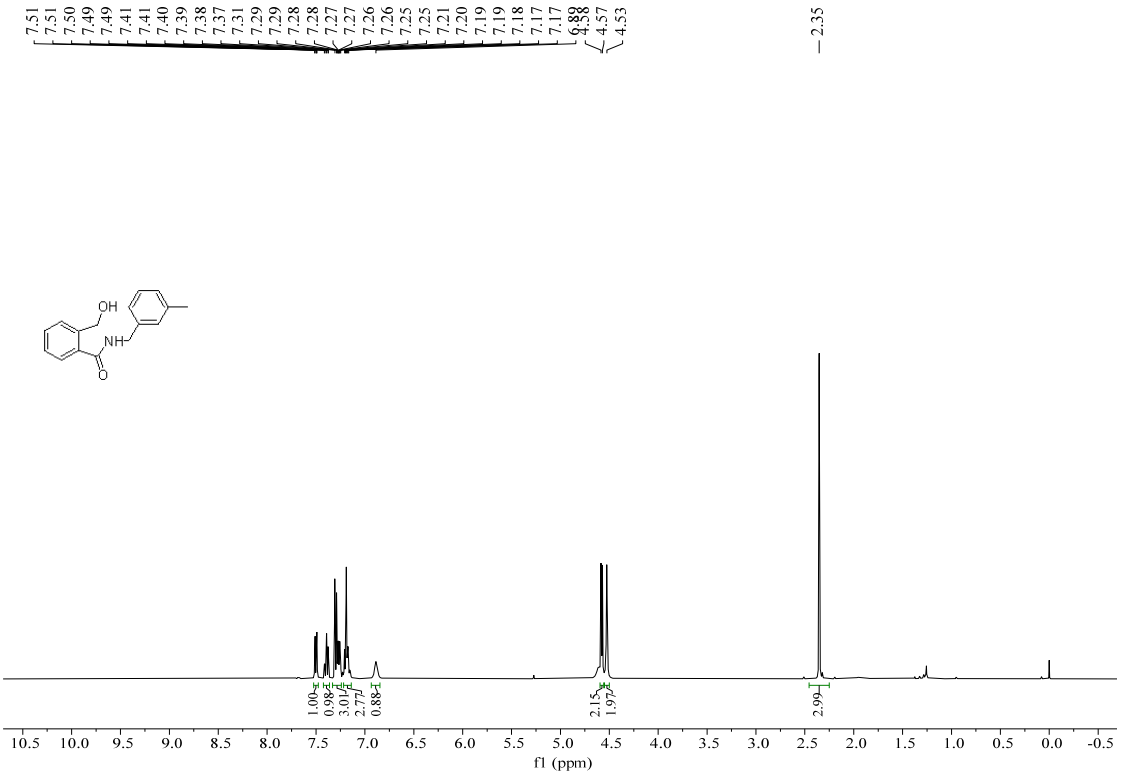
7.35
7.33
7.31
7.27
7.26
7.25
7.23
7.16
7.14
7.12
7.10
6.80
6.78
6.77
4.60
4.58
3.49
2.35
OH
NH
O
1.18
1.02
1.02
1.17
1.12
3.00
0.90
3.98
0.95
2.88
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


169.97
140.36
138.71
137.83
135.58
131.43
130.96
128.89
128.71
128.60
128.26
127.68
124.94
77.48
77.16
76.84
64.80
44.35
21.51
OH
NH
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3ac: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7.51
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7.49
7.41
7.41
7.40
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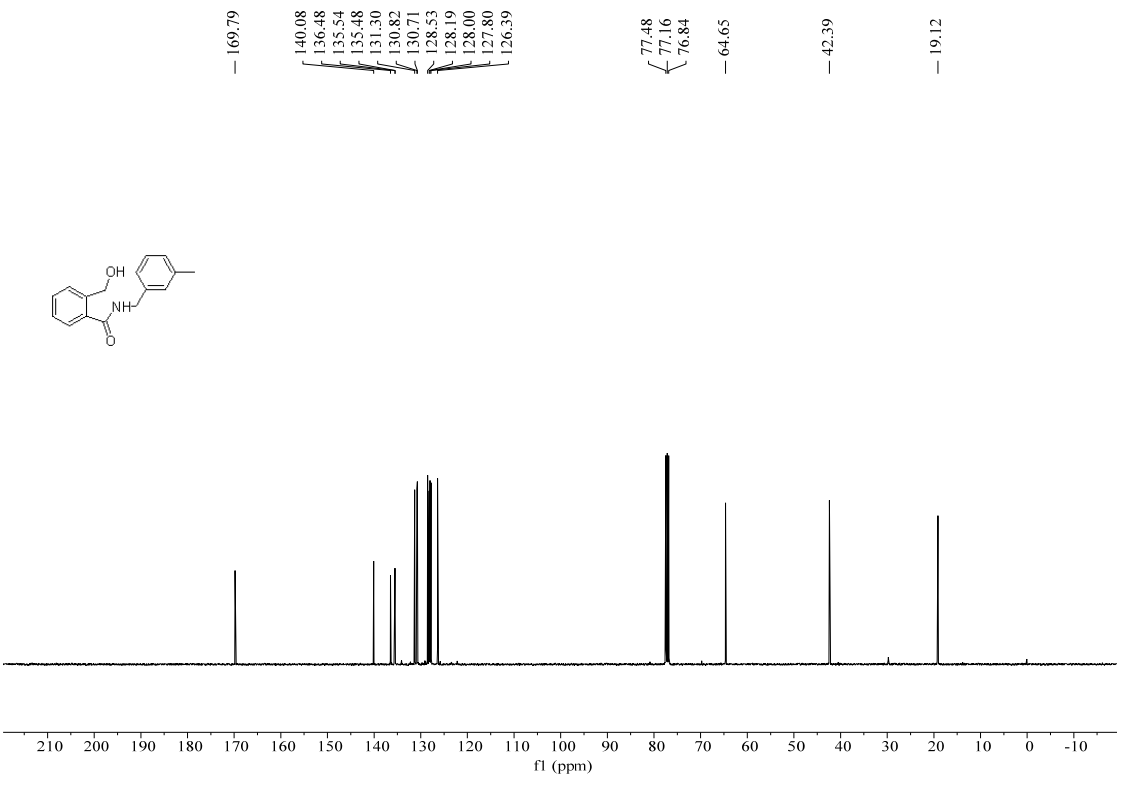
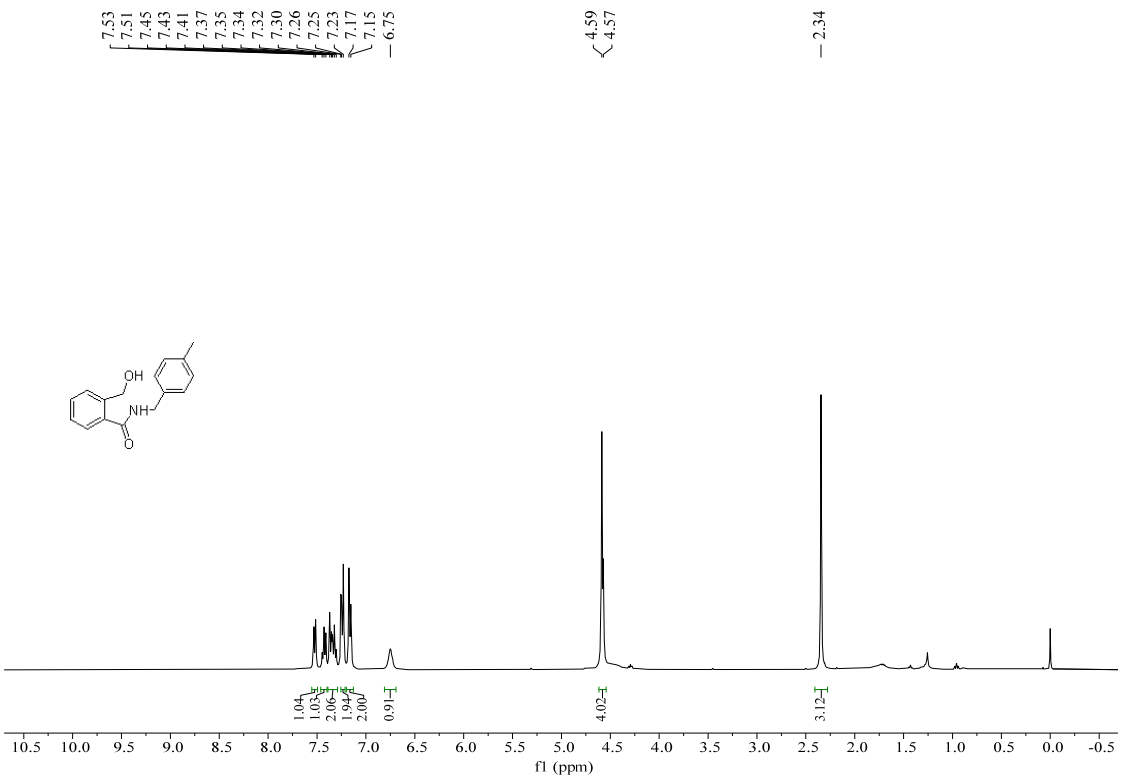
7.38
7.37
7.31
7.29
7.29
7.28
7.28
7.27
7.27
7.26
7.26
7.25
7.25
7.21
7.20
7.19
7.19
7.18
7.17
7.17
6.89
4.58
4.57
4.53
2.35
OH
NH
O
1.00
0.98
3.01
2.77
0.88
2.15
1.97
2.99
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


169.79
140.08
136.48
135.54
135.48
131.30
130.82
130.71
128.53
128.19
128.00
127.80
126.39
77.48
77.16
76.84
64.65
42.39
19.12
OH
NH
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3ad: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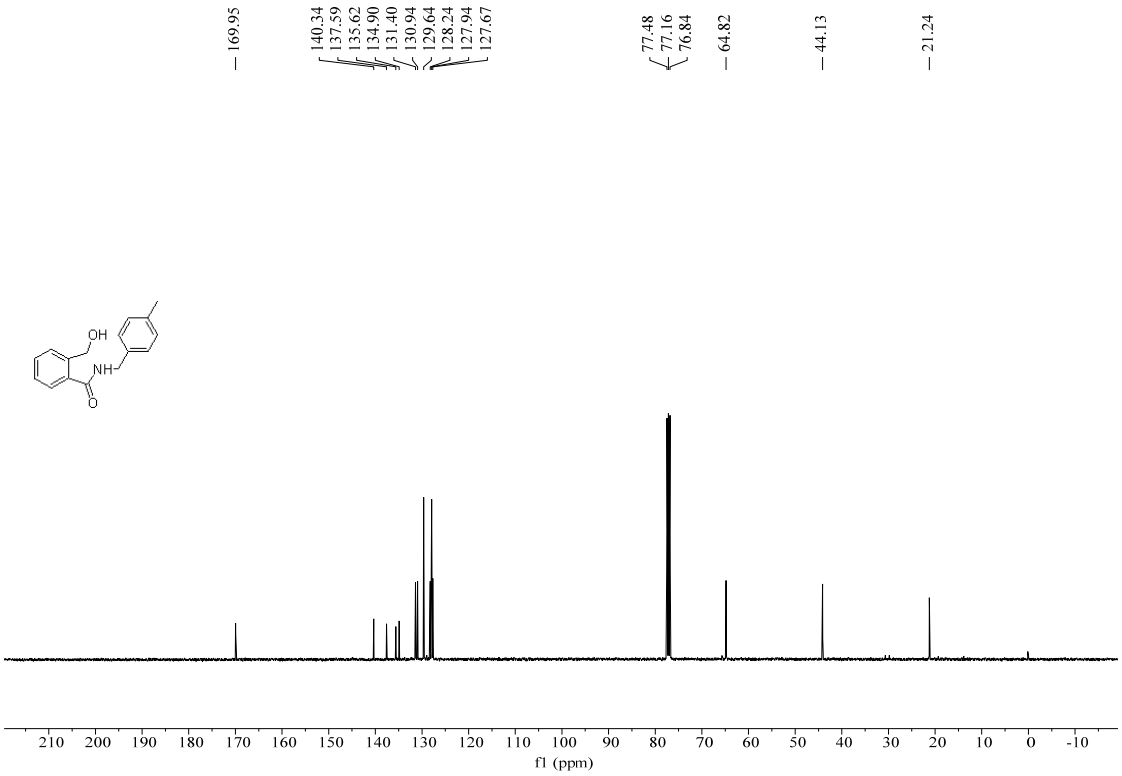
7.43
7.41
7.37
7.35
7.34
7.32
7.30
7.26
7.25
7.23
7.17
7.15
6.75
4.59
4.57
2.34
OH
NH
O
1.04
1.03
2.06
1.94
2.00
0.91
4.02
3.12
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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134.90
131.40
130.94
129.64
128.24
127.94
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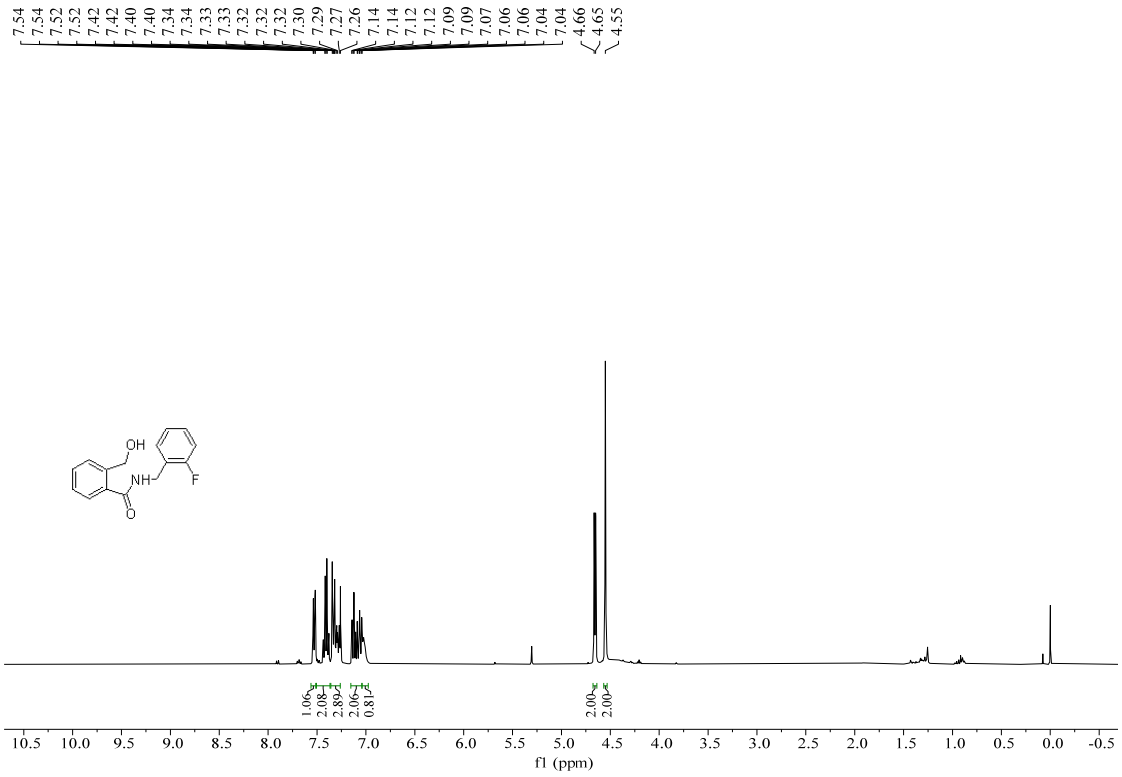
77.16
76.84
64.82
44.13
21.24
OH
NH
O
f1 (ppm)

3ae: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7.42
7.40
7.40
7.34
7.34
7.33
7.33
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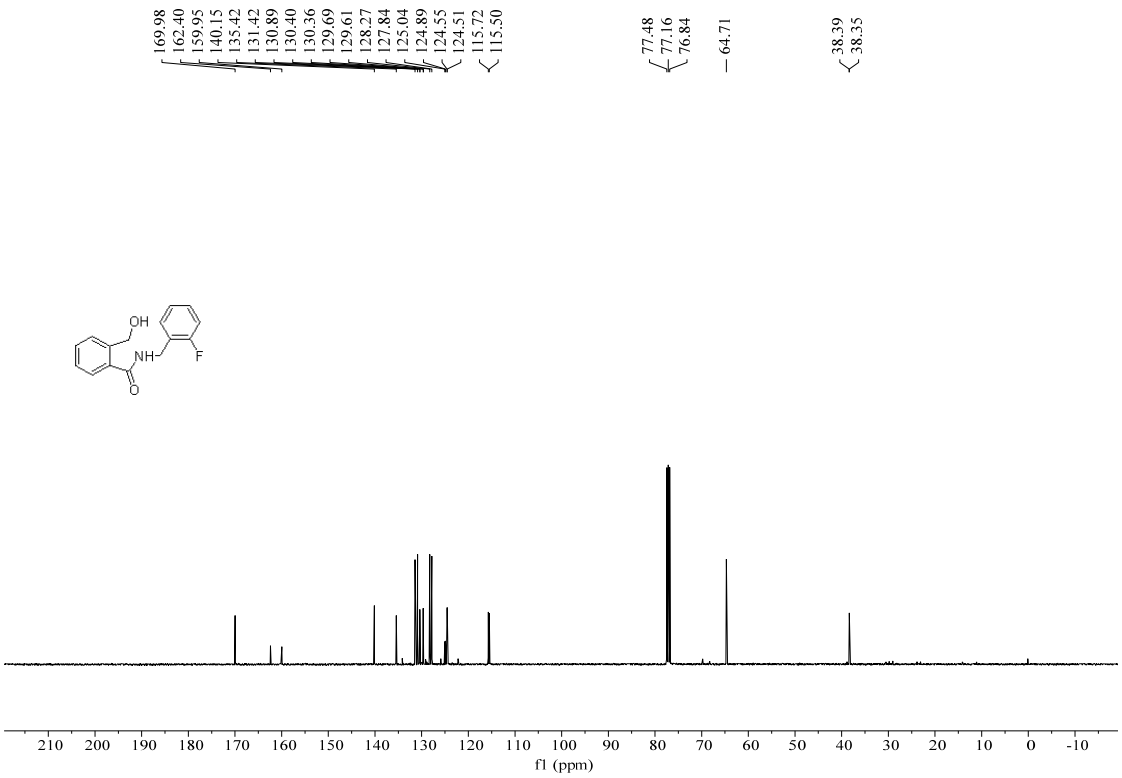
7.32
7.32
7.30
7.29
7.27
7.26
7.14
7.14
7.12
7.12
7.09
7.09
7.07
7.06
7.06
7.04
7.04
4.66
4.65
4.55
OH
NH
F
O
1.06
2.08
2.89
2.06
0.81
2.00
2.00
f1 (ppm)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162.40
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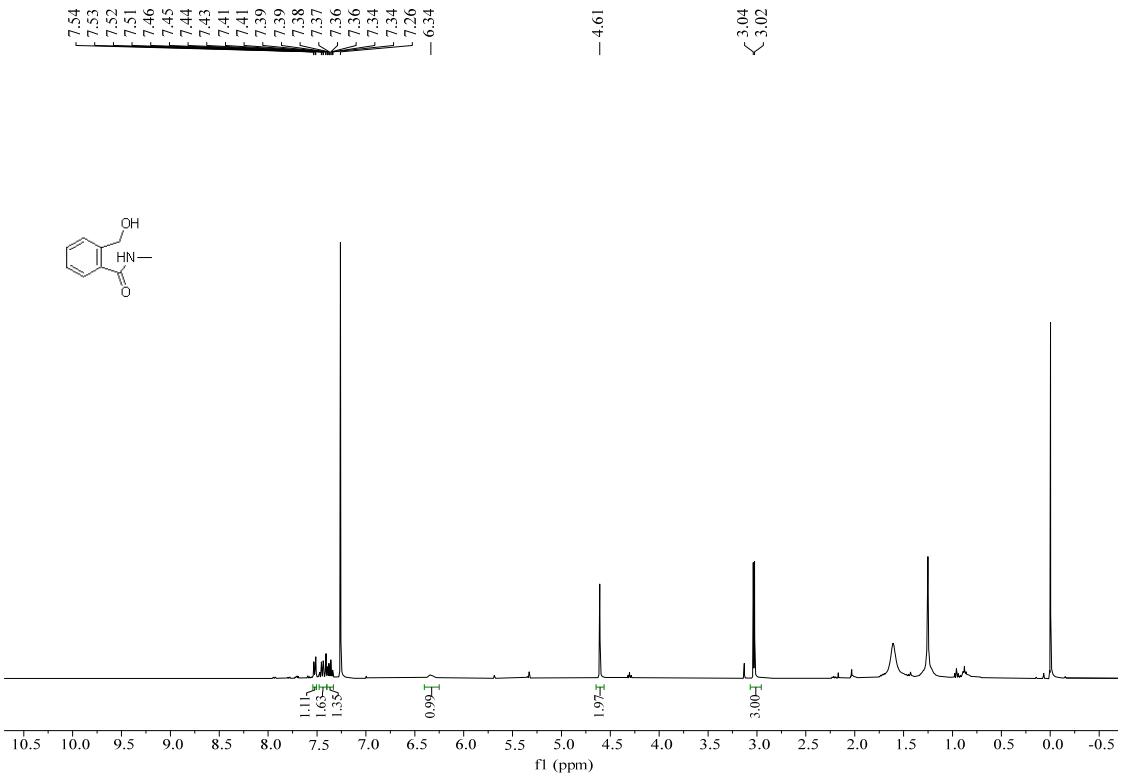
131.42
130.89
130.40
130.36
129.69
129.61
128.27
127.84
125.04
124.89
124.55
124.51
115.72
115.50
77.48
77.16
76.84
64.71
38.39
38.35
OH
NH
F
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3af: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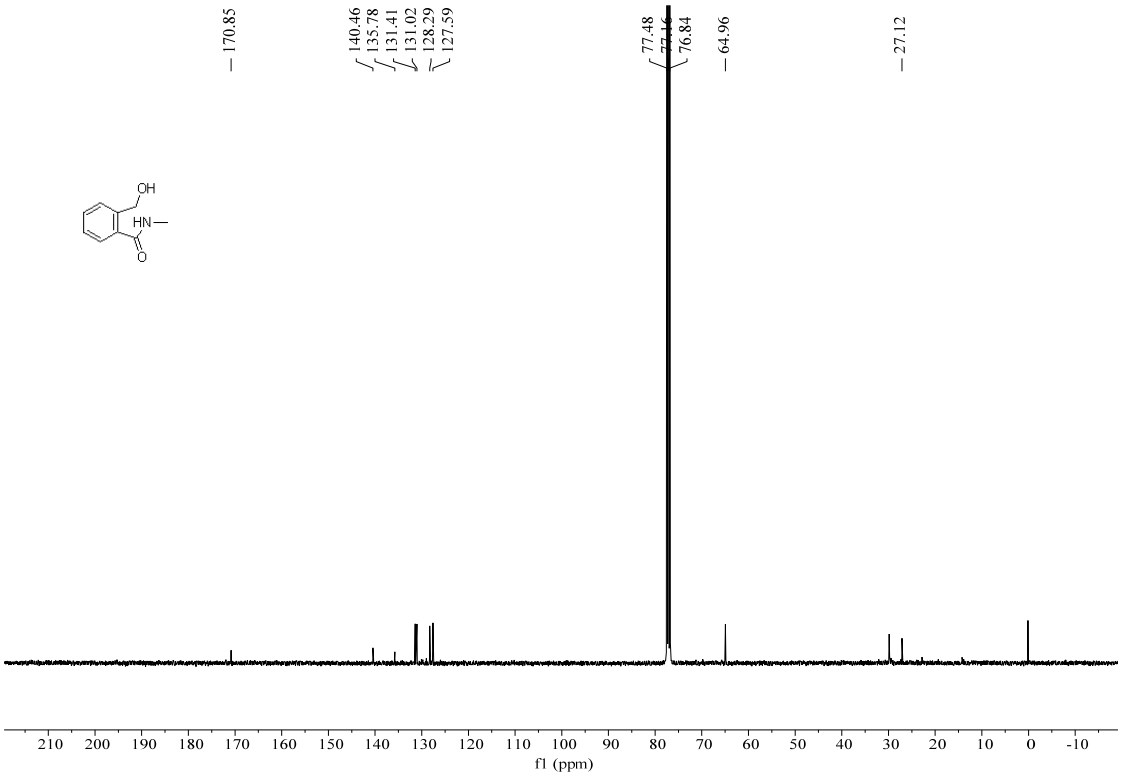
7.43
7.41
7.41
7.39
7.39
7.38
7.37
7.36
7.36
7.34
7.34
7.26
6.34
4.61
3.04
3.02
OH
HN
O
1.11
1.63
1.35
0.99
1.97
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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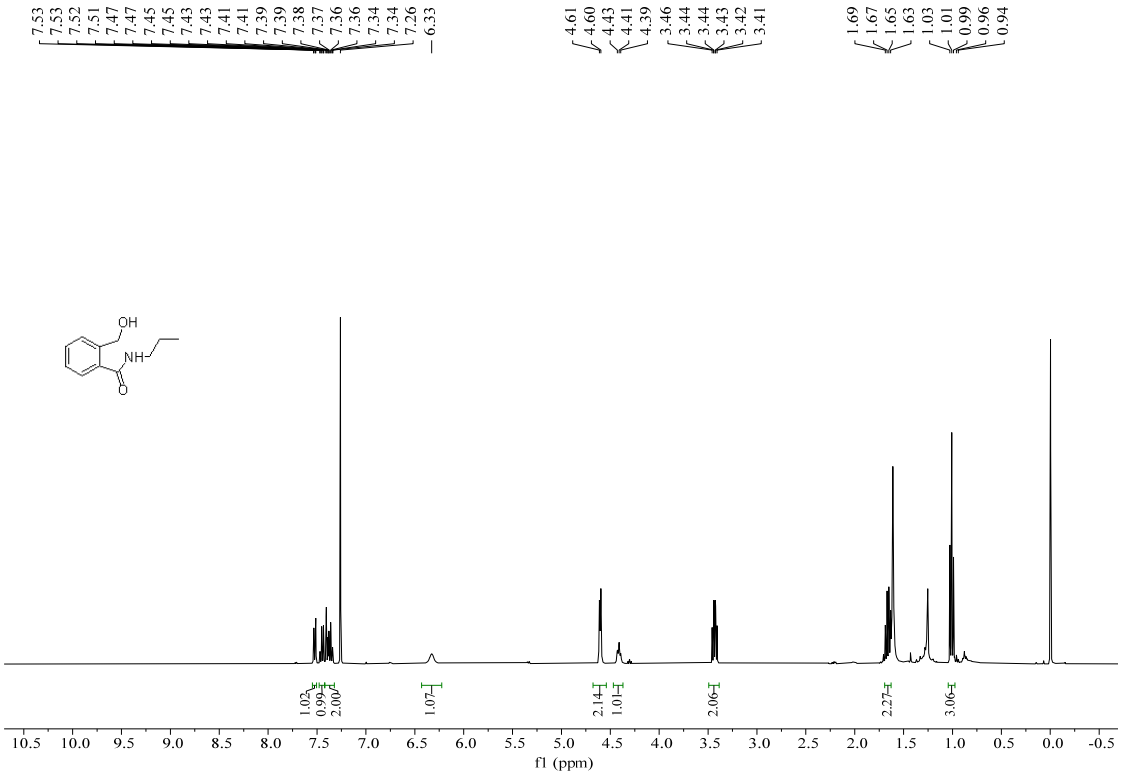
140.46
135.78
131.41
131.02
128.29
127.59
77.48
77.16
76.84
64.96
27.12
OH
HN
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3ag: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7.51
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7.47
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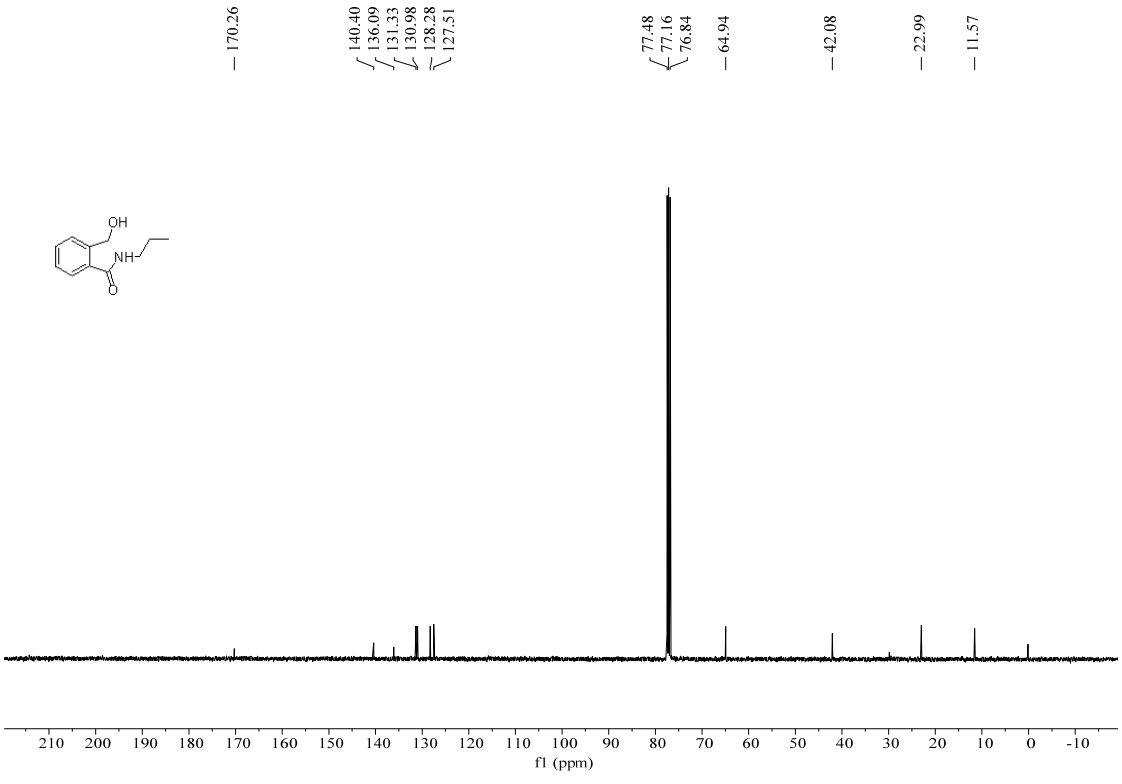
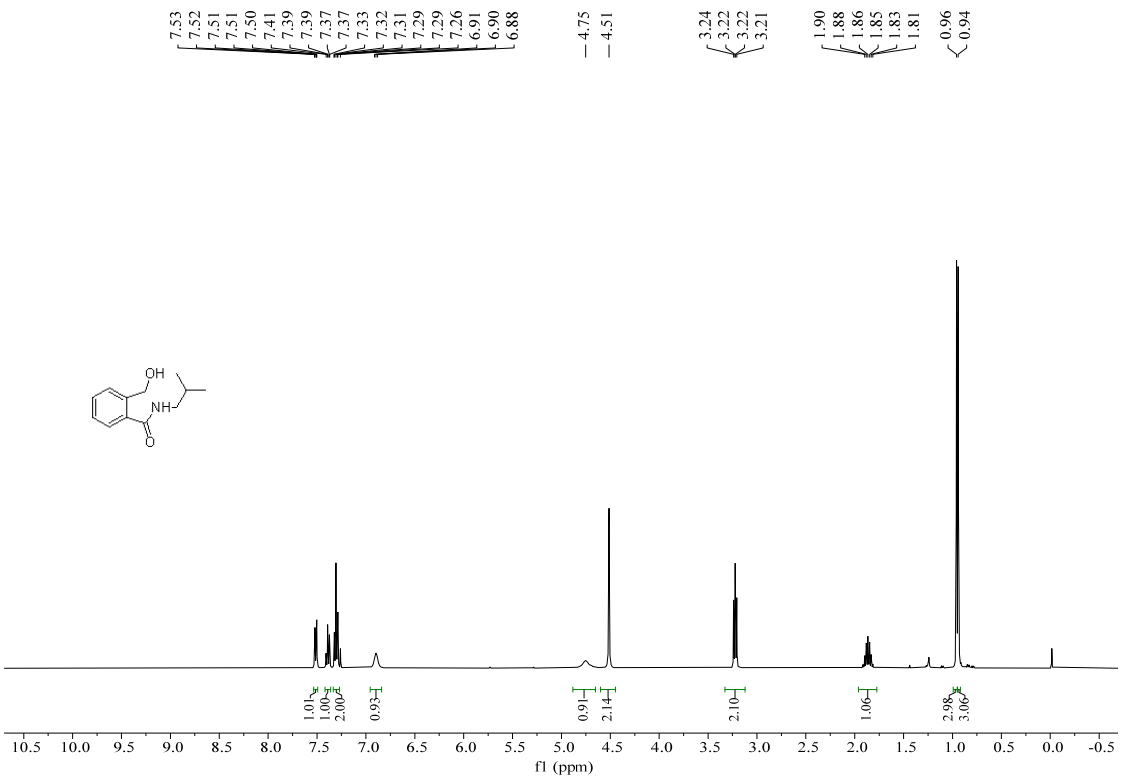
7.45
7.43
7.43
7.41
7.41
7.39
7.39
7.38
7.37
7.36
7.36
7.34
7.34
7.26
6.33
4.61
4.60
4.43
4.41
4.39
3.46
3.44
3.44
3.43
3.42
3.41
1.69
1.67
1.65
1.63
1.03
1.01
0.99
0.96
0.94
OH
NH
O
1.02
0.99
2.00
1.07
2.14
1.01
2.06
2.27
3.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


170.26
140.40
136.09
131.33
130.98
128.28
127.51
77.48
77.16
76.84
64.94
42.08
22.99
11.57
OH
NH
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3ah: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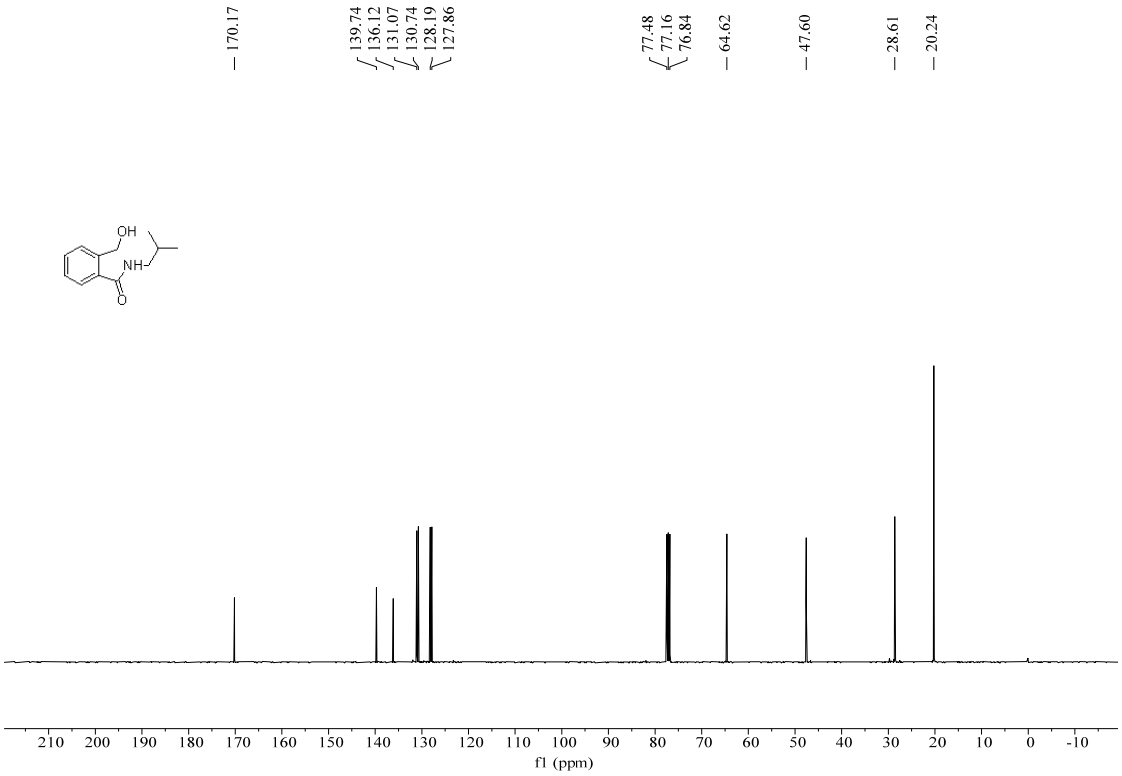
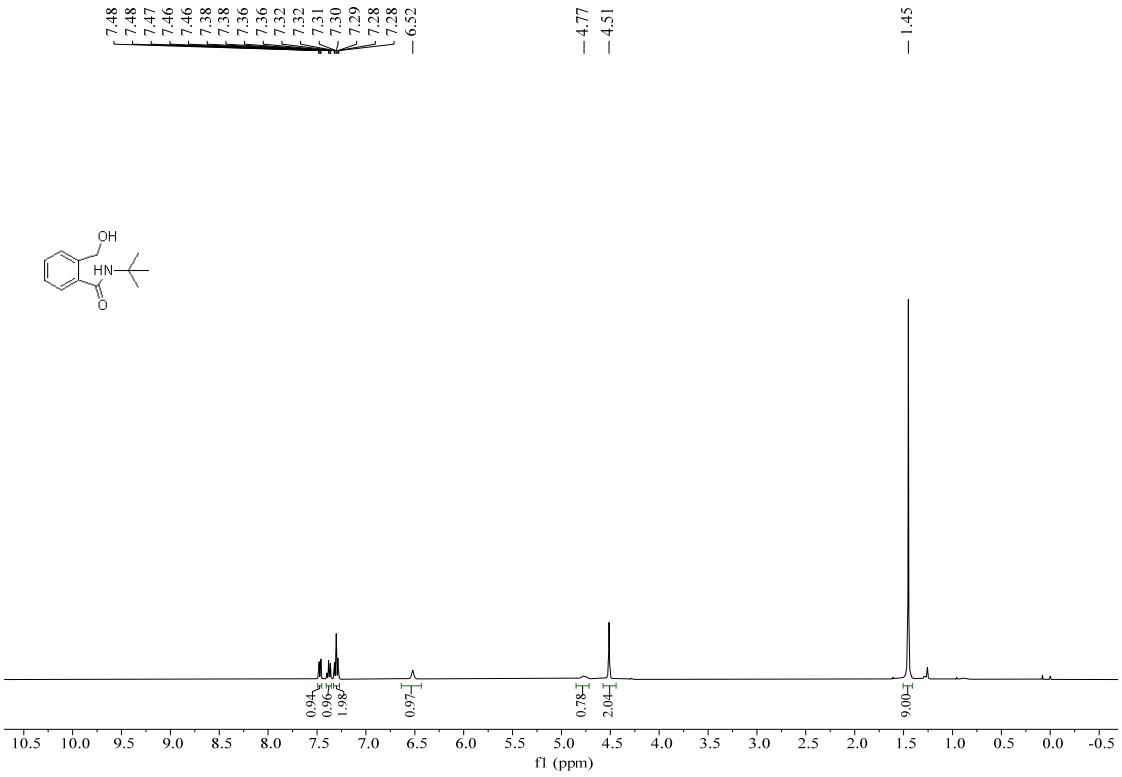
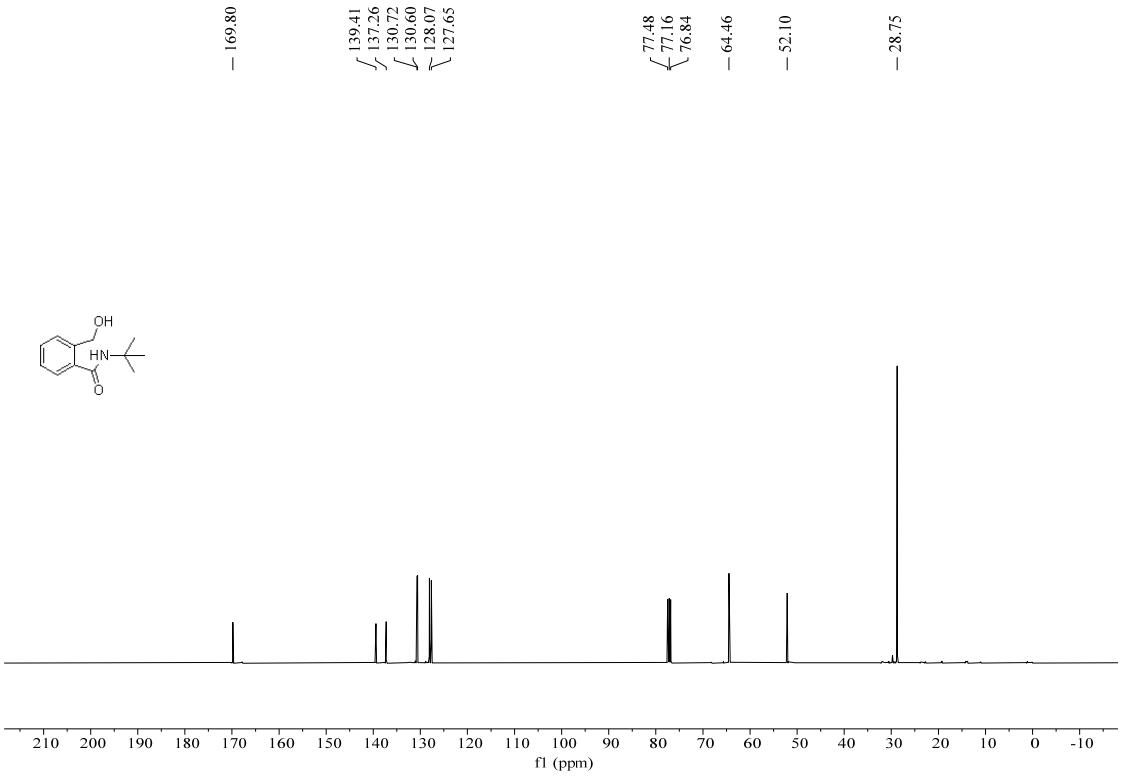
7.52
7.51
7.51
7.50
7.41
7.39
7.39
7.37
7.37
7.33
7.32
7.31
7.29
7.29
7.26
6.91
6.90
6.88
4.75
4.51
3.24
3.22
3.22
3.21
1.90
1.88
1.86
1.85
1.83
1.81
0.96
0.94
OH
NH
O
1.01
1.00
2.00
0.93
0.91
2.14
2.10
1.06
2.98
3.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

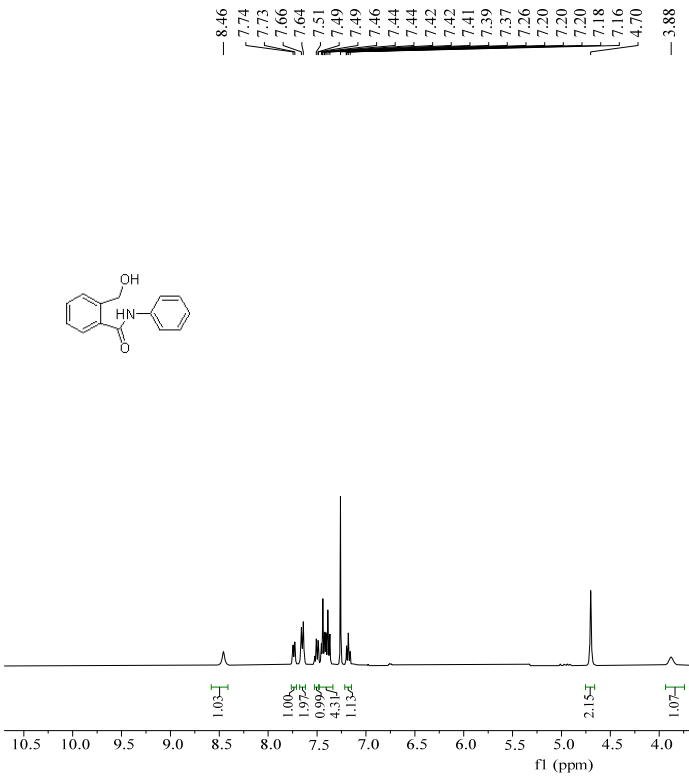

170.17
139.74
136.12
131.07
130.74
128.19
127.86
77.48
77.16
76.84
64.62
47.60
28.61
20.24
OH
NH
O
f1 (ppm)

3ai:


7.48
7.48
7.47
7.46
7.46
7.38
7.38
7.36
7.36
7.32
7.32
7.31
7.30
7.29
7.28
7.28
6.52
4.77
4.51
1.45
OH
HN
O
0.94
0.96
1.98
0.97
0.78
2.04
9.00
f1 (ppm)


169.80
139.41
137.26
130.72
130.60
128.07
127.65
77.48
77.16
76.84
64.46
52.10
28.75
OH
HN
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3aj: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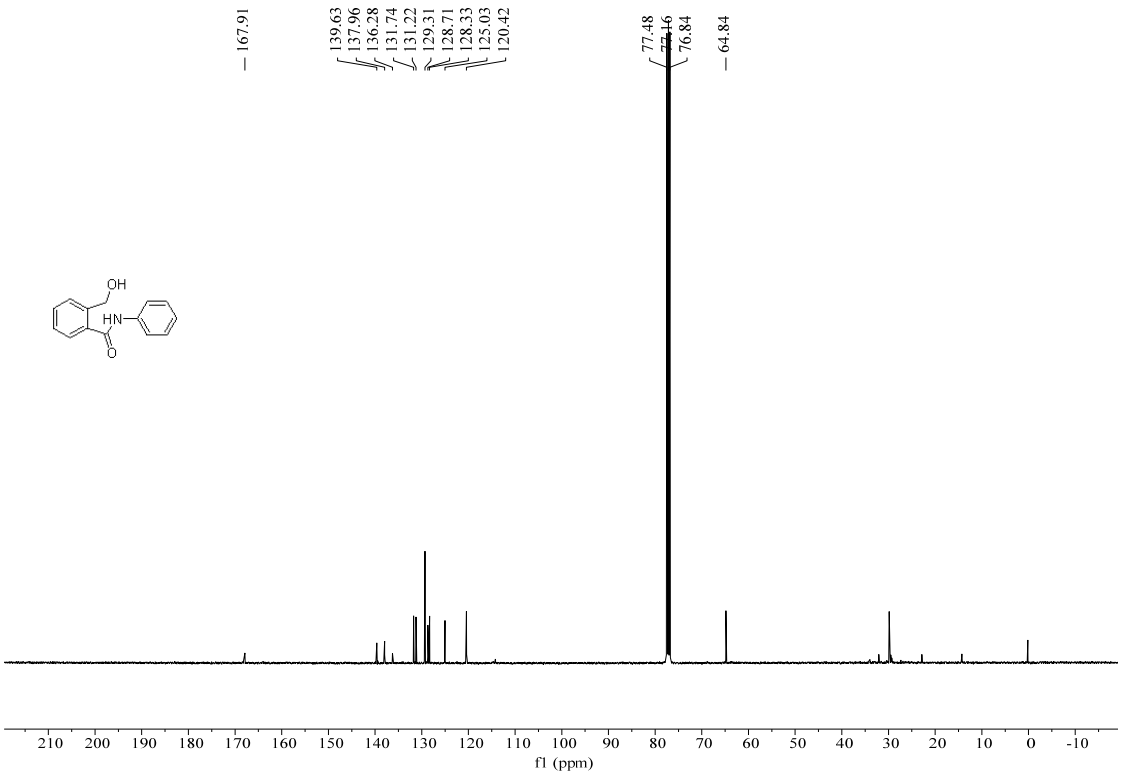
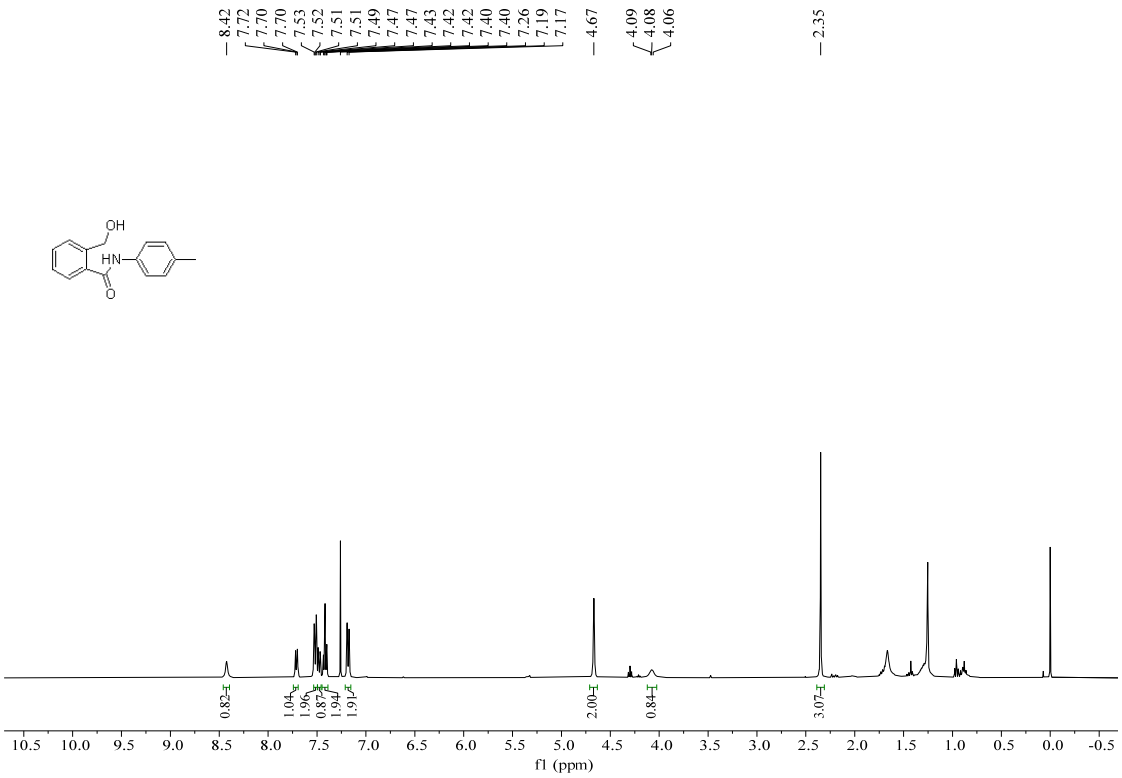
7.74
7.73
7.66
7.64
7.51
7.49
7.49
7.46
7.44
7.44
7.42
7.42
7.41
7.39
7.37
7.26
7.20
7.20
7.20
7.18
7.16
4.70
3.88
OH
HN
O
1.03
1.00
1.97
0.99
4.31
1.13
2.15
1.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


167.91
139.63
137.96
136.28
131.74
131.22
129.31
128.71
128.33
125.03
120.42
77.48
77.16
76.84
64.84
OH
HN
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3ak: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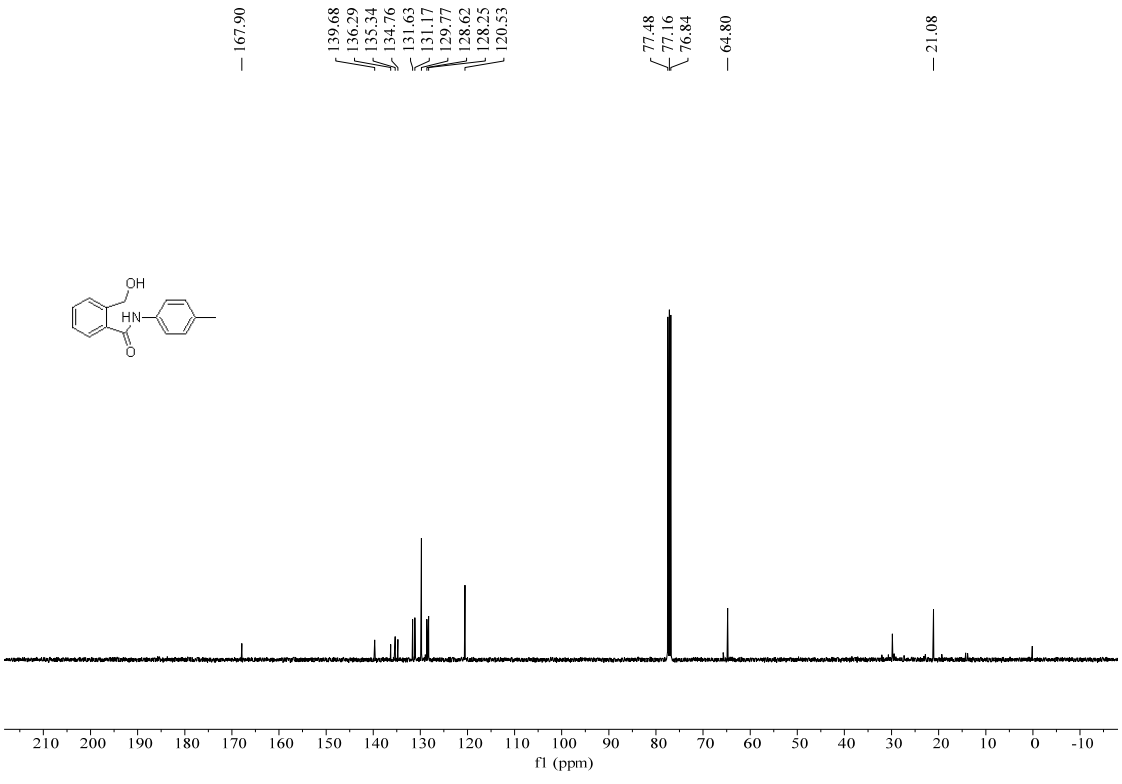
7.72
7.70
7.70
7.53
7.52
7.51
7.51
7.49
7.47
7.47
7.43
7.42
7.42
7.40
7.40
7.26
7.19
7.17
4.67
4.09
4.08
4.06
2.35
OH
HN
O
0.82
1.04
1.96
0.87
1.94
1.91
2.00
0.84
3.07
fl (ppm)


167.90
139.68
136.29
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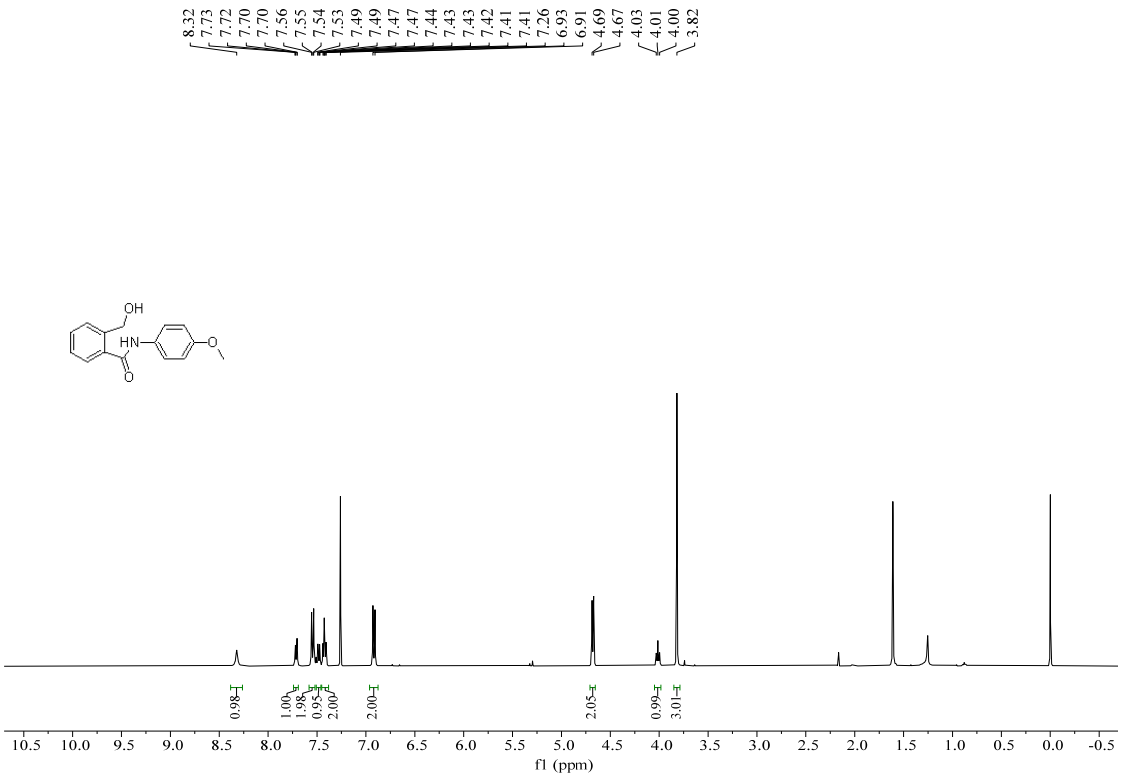
134.76
131.63
131.17
129.77
128.62
128.25
120.53
77.48
77.16
76.84
64.80
21.08
OH
HN
O
fl (ppm)

3al: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7.72
7.70
7.70
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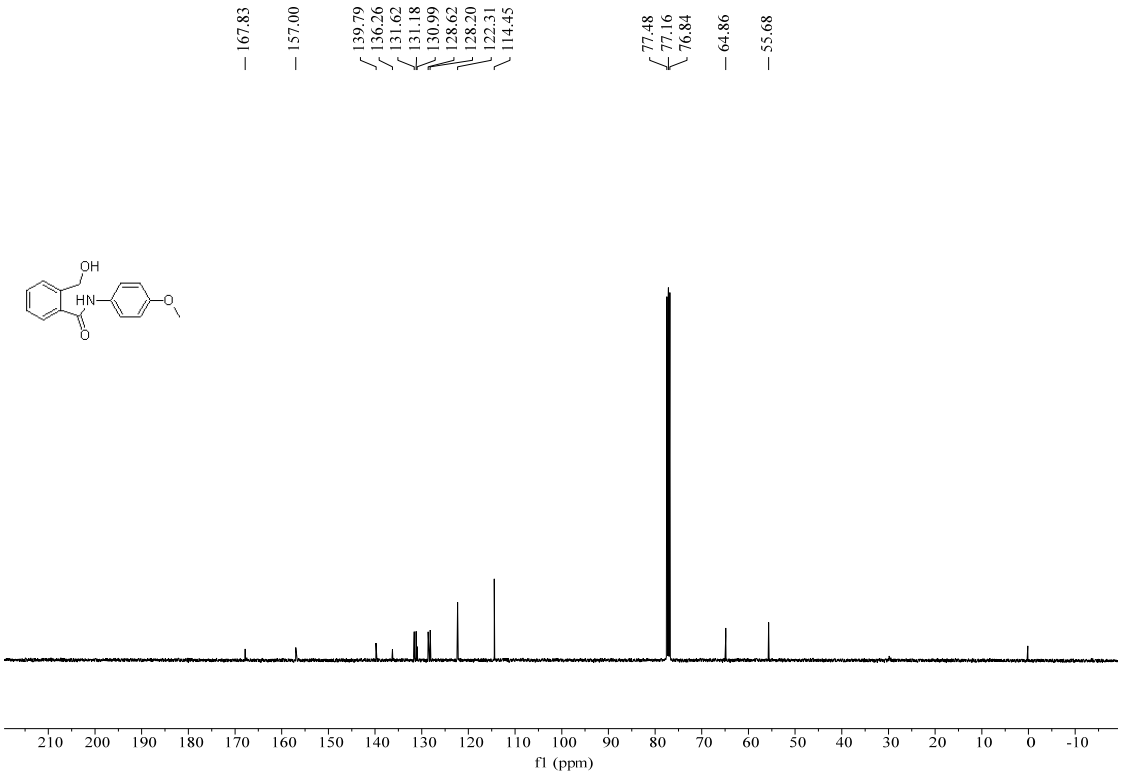
7.55
7.54
7.53
7.49
7.49
7.47
7.47
7.44
7.43
7.43
7.42
7.41
7.41
7.26
6.93
6.91
4.69
4.67
4.03
4.01
4.00
3.82
OH
HN
O
O
0.98
1.00
1.98
0.95
2.00
2.00
2.05
0.99
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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157.00
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136.26
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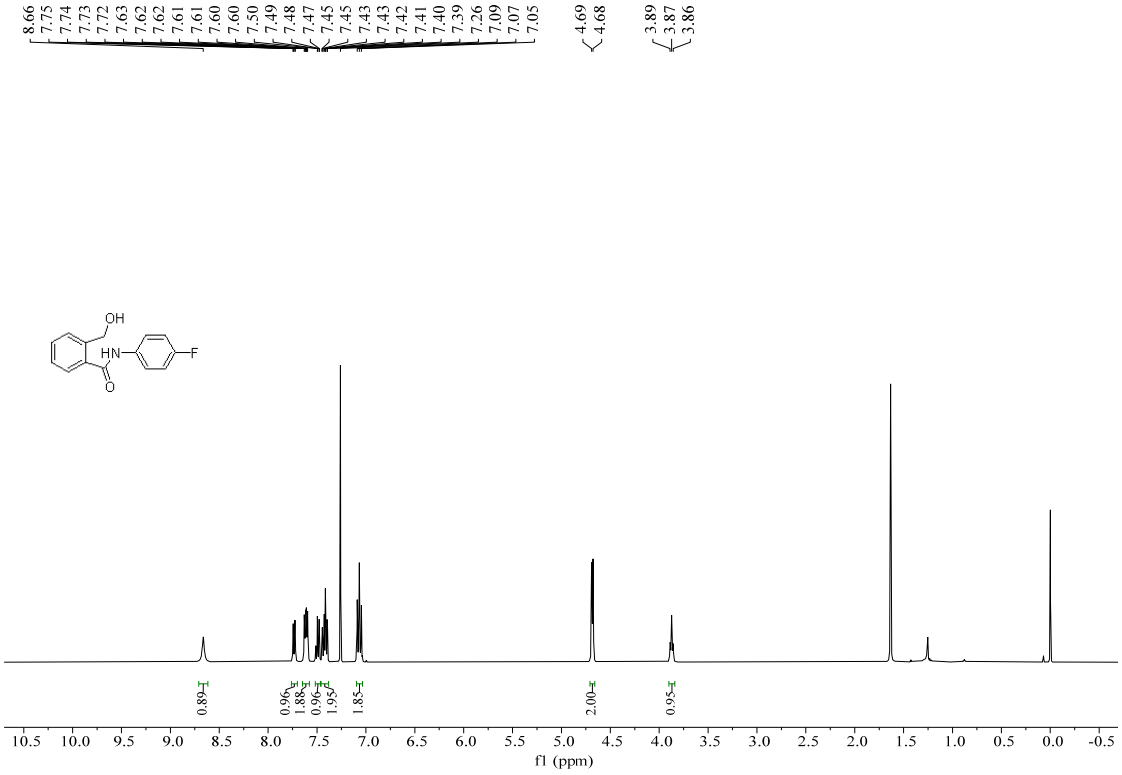
131.18
130.99
128.62
128.20
122.31
114.45
77.48
77.16
76.84
64.86
55.68
OH
HN
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3am: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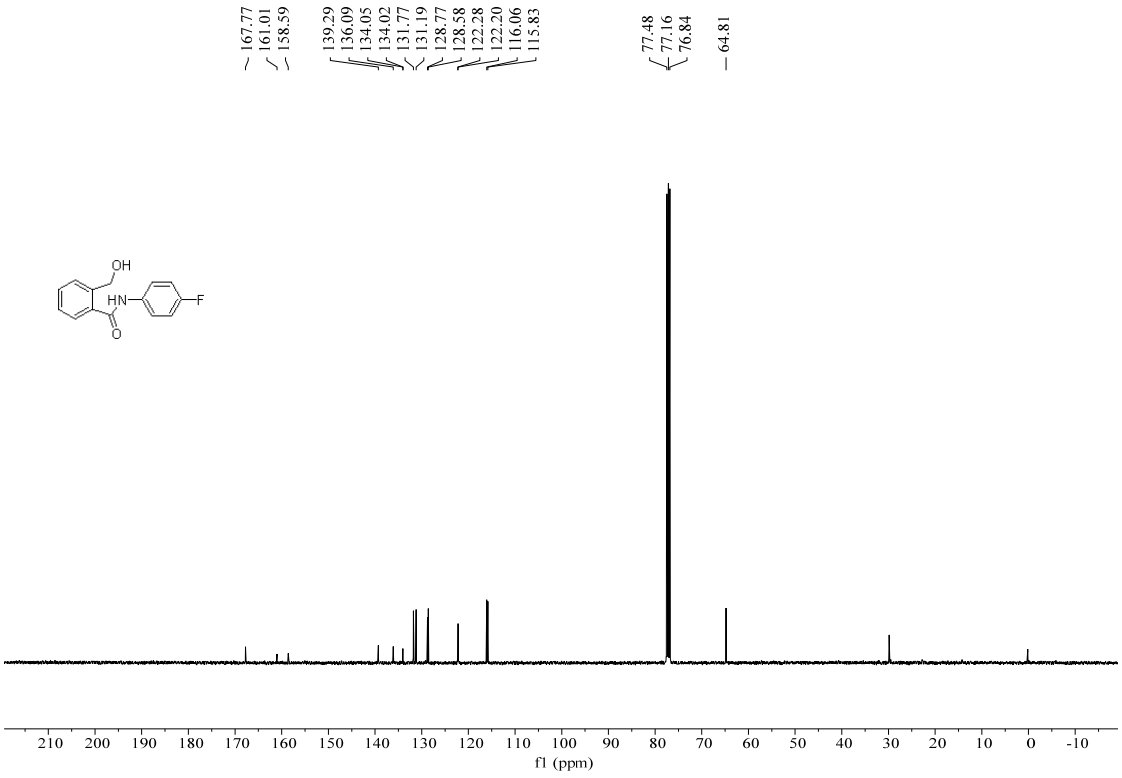
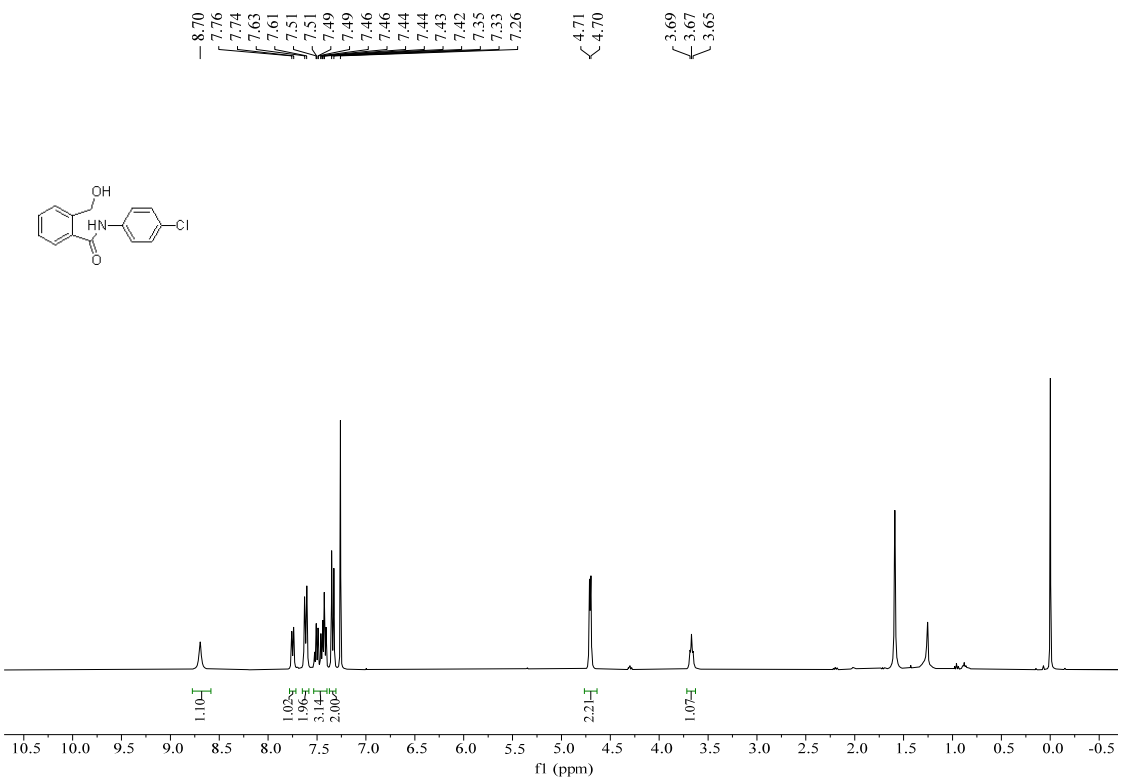
7.75
7.74
7.73
7.72
7.63
7.62
7.62
7.61
7.61
7.60
7.60
7.50
7.49
7.48
7.47
7.45
7.45
7.43
7.43
7.42
7.41
7.40
7.39
7.26
7.09
7.07
7.05
4.69
4.68
3.89
3.87
3.86
OH
HN
F
O
0.89
0.96
1.88
0.96
1.95
1.85
2.00
0.95
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


167.77
161.01
158.59
139.29
136.09
134.05
134.02
131.77
131.19
128.77
128.58
122.28
122.20
116.06
115.83
77.48
77.16
76.84
64.81
OH
HN
F
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3an: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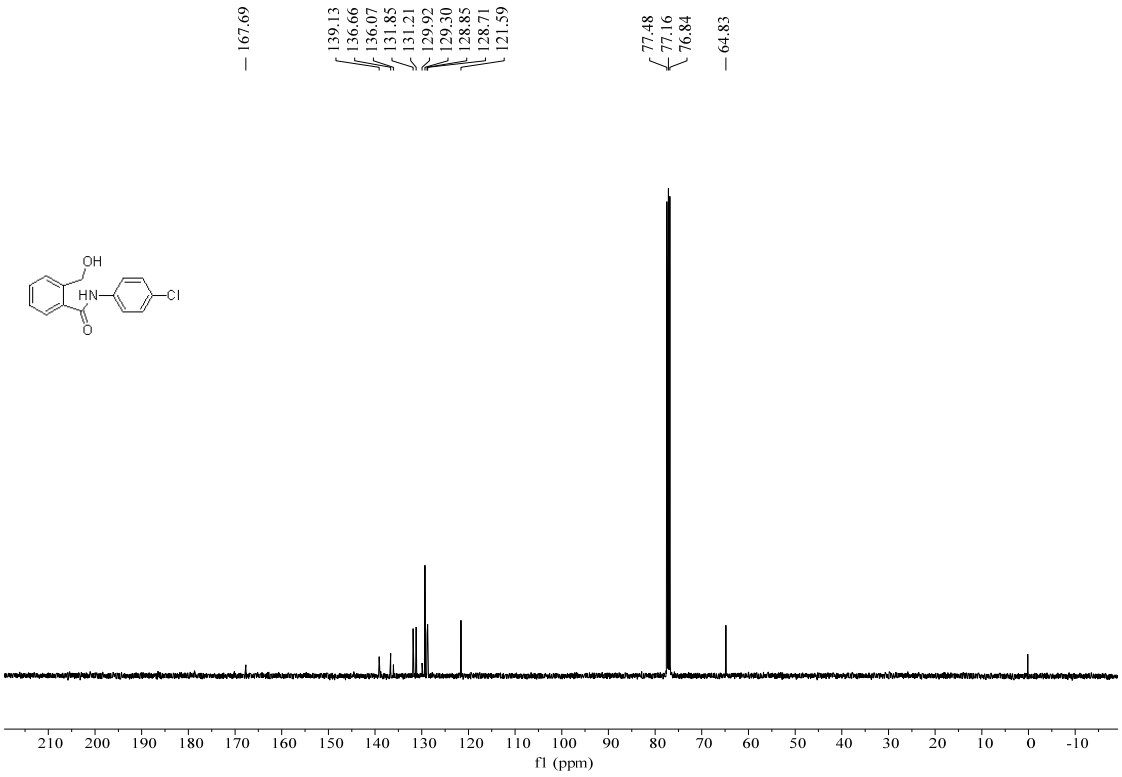
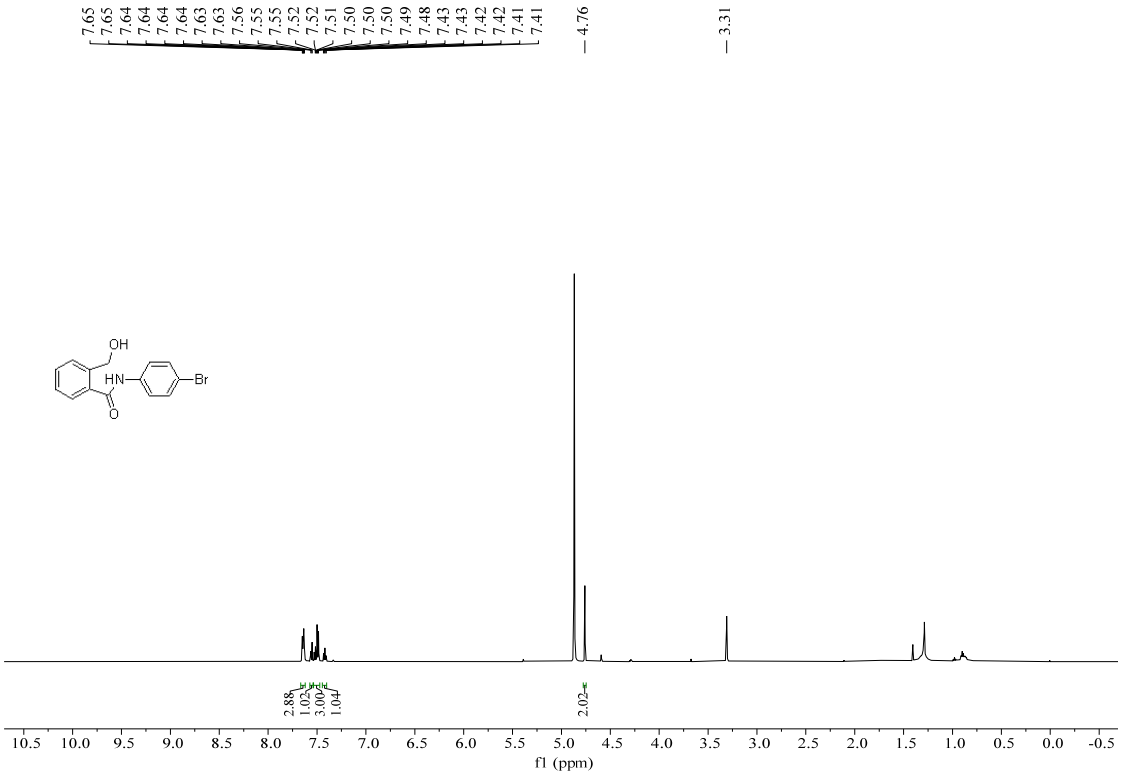
7.61
7.51
7.51
7.49
7.49
7.46
7.46
7.44
7.44
7.43
7.42
7.35
7.33
7.26
4.71
4.70
3.69
3.67
3.65
OH
HN
Cl
O
1.10
1.02
1.96
3.14
2.00
2.21
1.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


167.69
139.13
136.66
136.07
131.85
131.21
129.92
129.30
128.85
128.71
121.59
77.48
77.16
76.84
64.83
OH
HN
Cl
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3ao: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7.65
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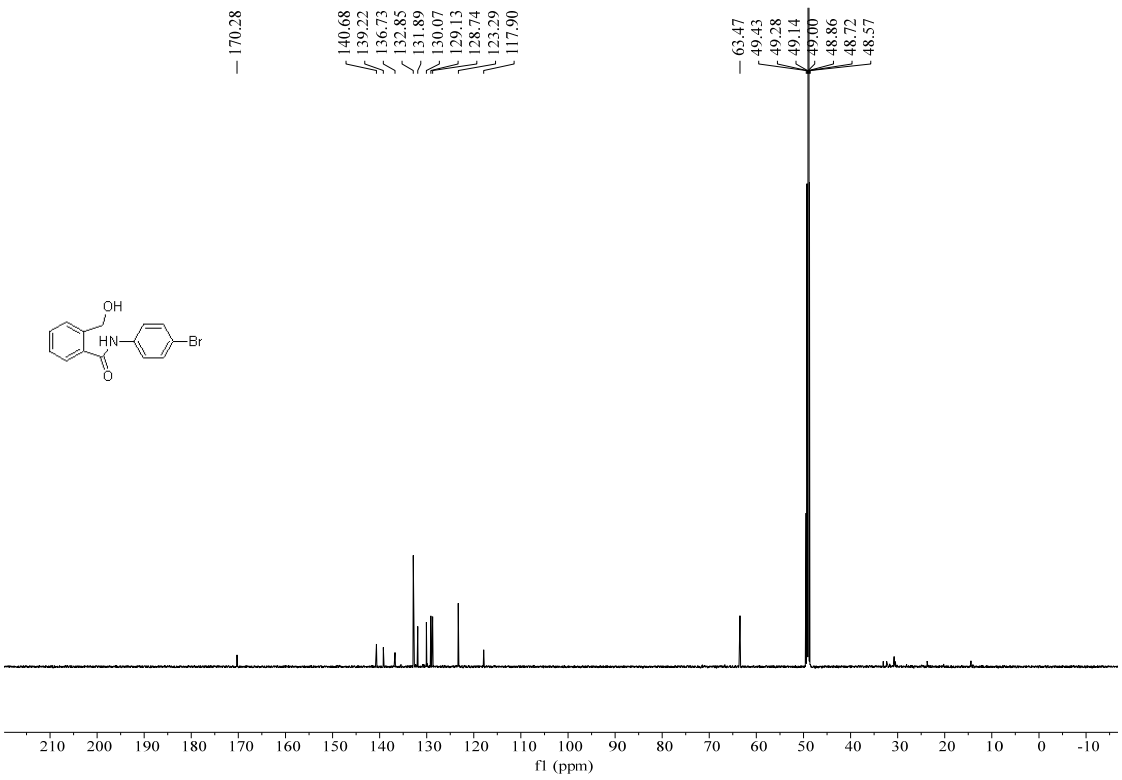
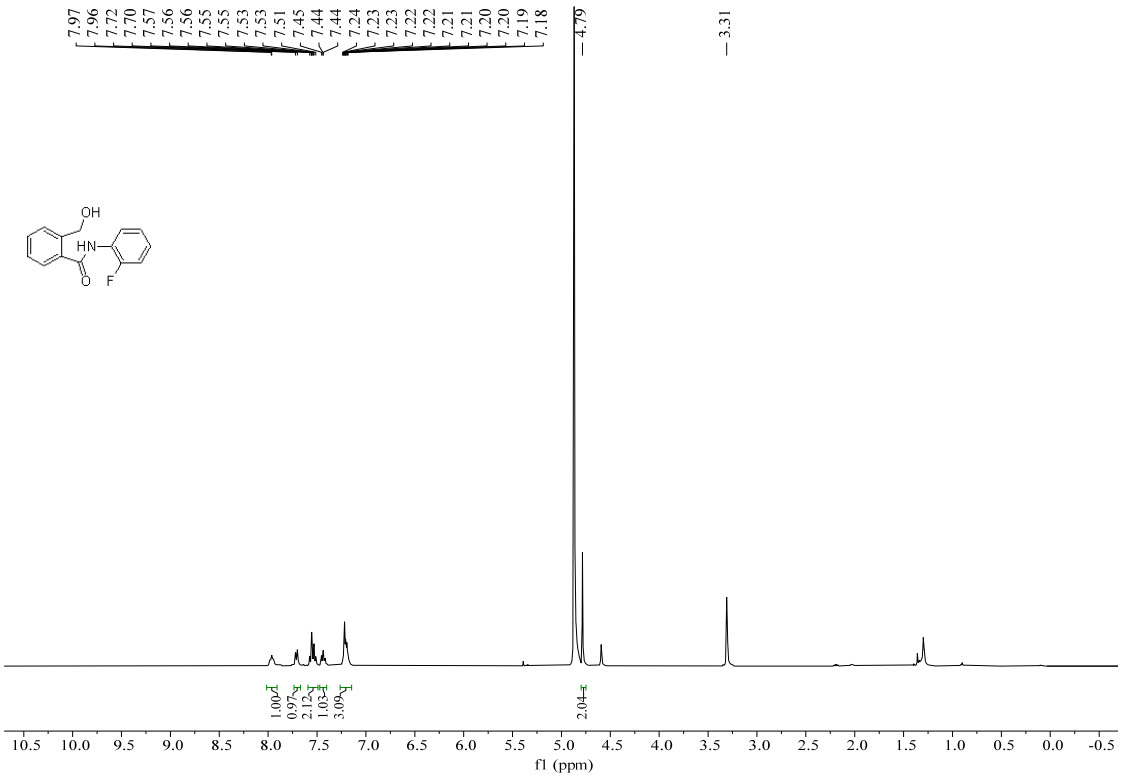
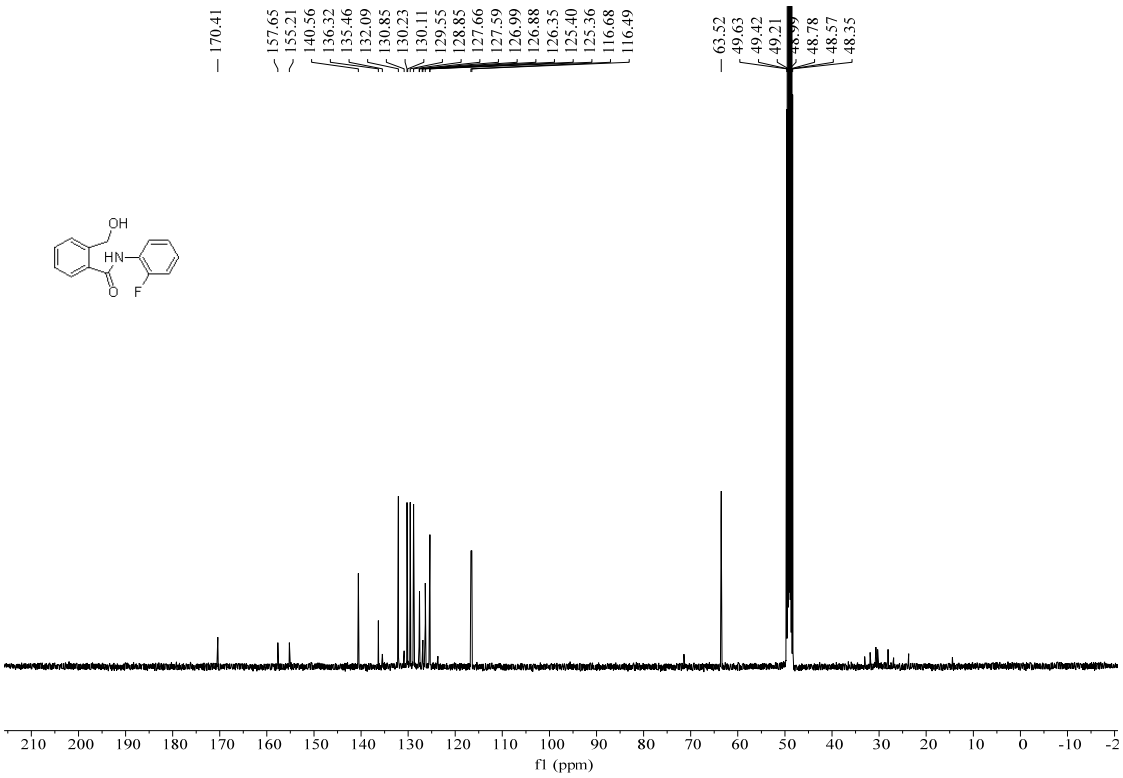
7.64
7.64
7.64
7.63
7.63
7.56
7.55
7.55
7.52
7.52
7.51
7.50
7.50
7.50
7.49
7.48
7.43
7.43
7.42
7.42
7.41
7.41
4.76
3.31
OH
HN
Br
O
2.88
1.02
3.00
1.04
2.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

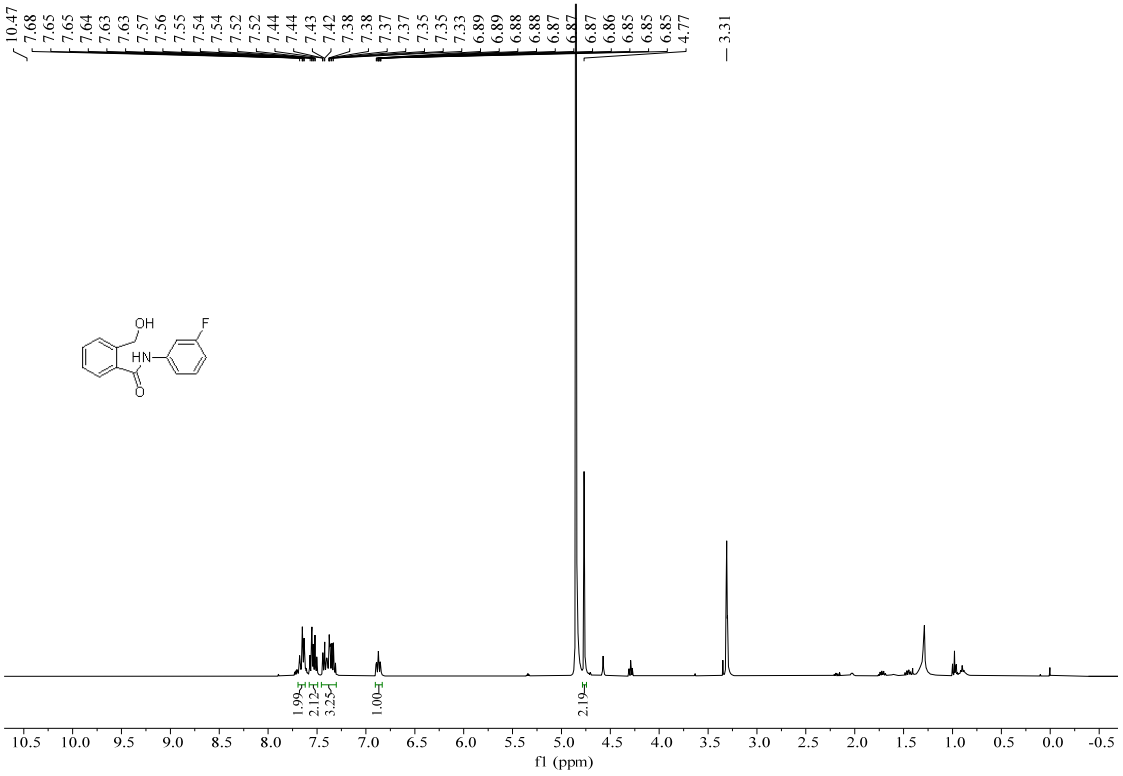

170.28
140.68
139.22
136.73
132.85
131.89
130.07
129.13
128.74
123.29
117.90
63.47
49.43
49.28
49.14
49.00
48.86
48.72
48.57
OH
HN
Br
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

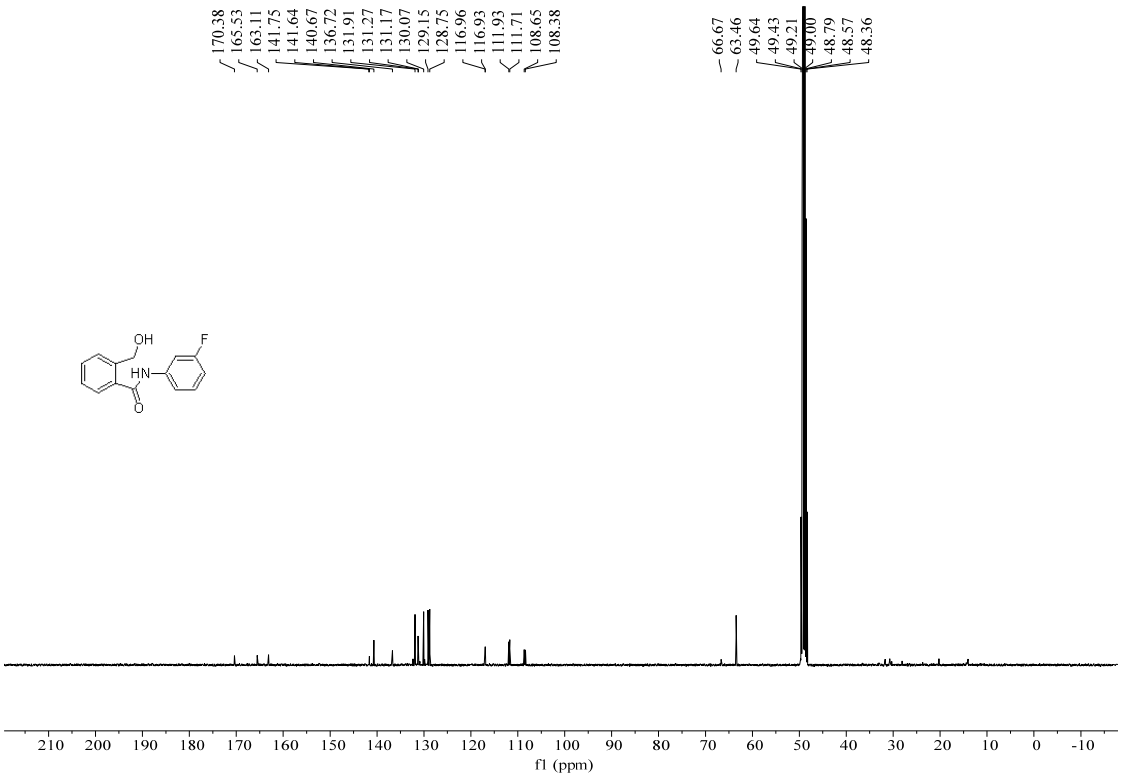
3ap:


7.97
7.96
7.72
7.70
7.57
7.56
7.56
7.55
7.55
7.53
7.53
7.51
7.45
7.44
7.44
7.24
7.23
7.23
7.22
7.22
7.21
7.21
7.20
7.20
7.19
7.18
4.79
3.31
OH
HN
O
F
1.00
0.97
2.12
1.03
3.09
2.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

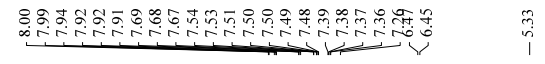

170.41
157.65
155.21
140.56
136.32
135.46
132.09
130.85
130.23
130.11
129.55
128.85
127.66
127.59
126.99
126.88
126.35
125.40
125.36
116.68
116.49
63.52
49.63
49.42
49.21
48.99
48.78
48.57
48.35
OH
HN
O
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (ppm)

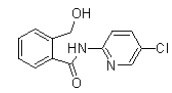
3aq:

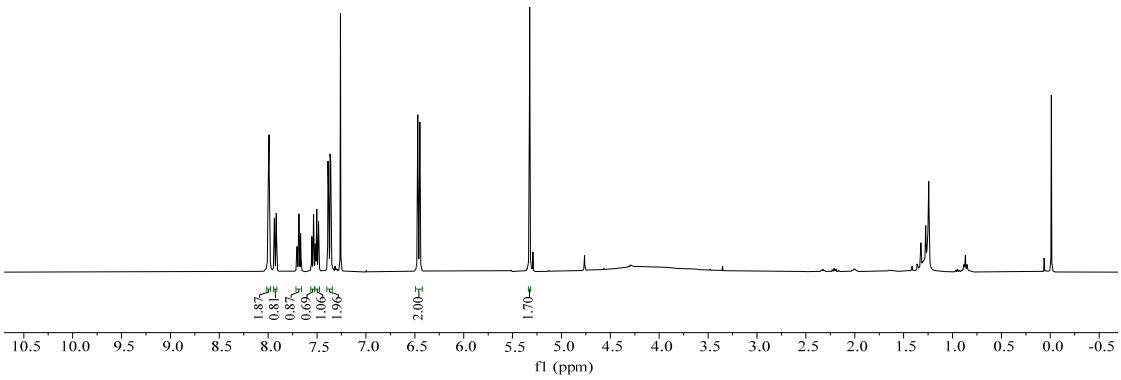

10.47
7.68
7.65
7.65
7.64
7.63
7.63
7.57
7.56
7.55
7.54
7.54
7.52
7.52
7.44
7.44
7.43
7.42
7.38
7.38
7.37
7.37
7.35
7.35
7.33
6.89
6.89
6.88
6.88
6.87
6.87
6.87
6.86
6.85
6.85
6.85
4.77
3.31
OH
HN
O
F
1.99
2.12
3.25
1.00
2.19
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

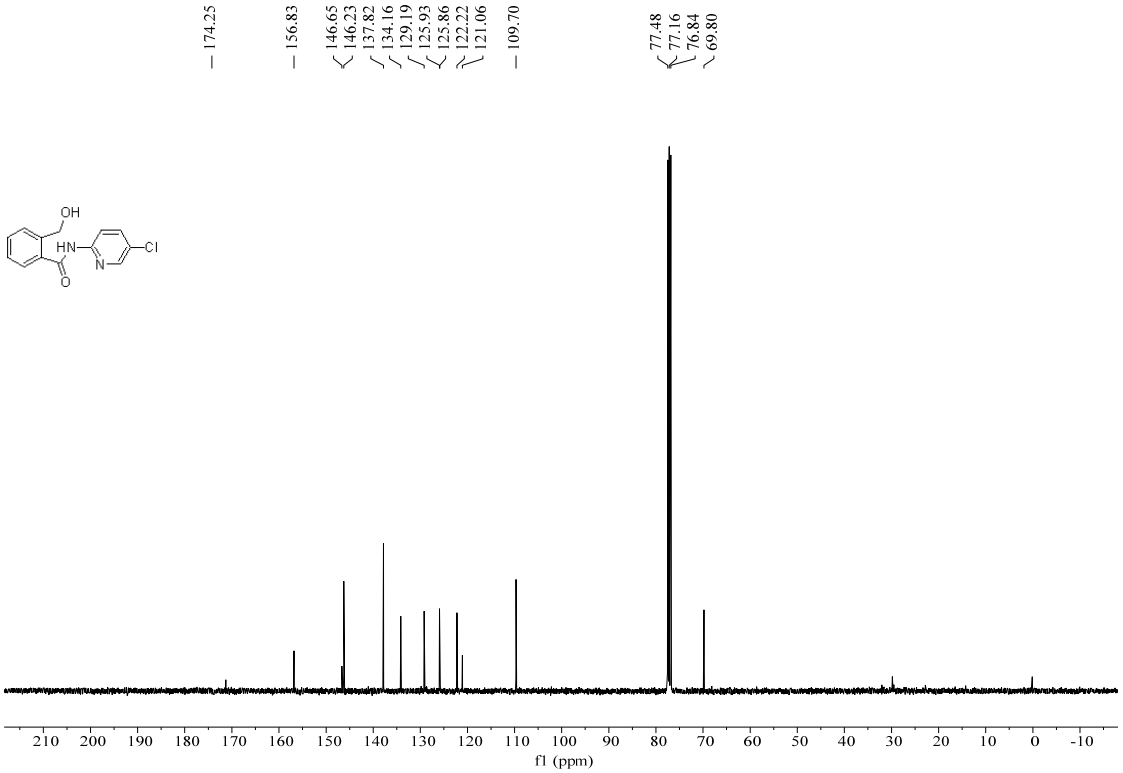

170.38
165.53
163.11
141.75
141.64
140.67
136.72
131.91
131.27
131.17
130.07
129.15
128.75
116.96
116.93
111.93
111.71
108.65
108.38
66.67
63.46
49.64
49.43
49.21
49.00
48.79
48.57
48.36
OH
F
HN
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3ar:

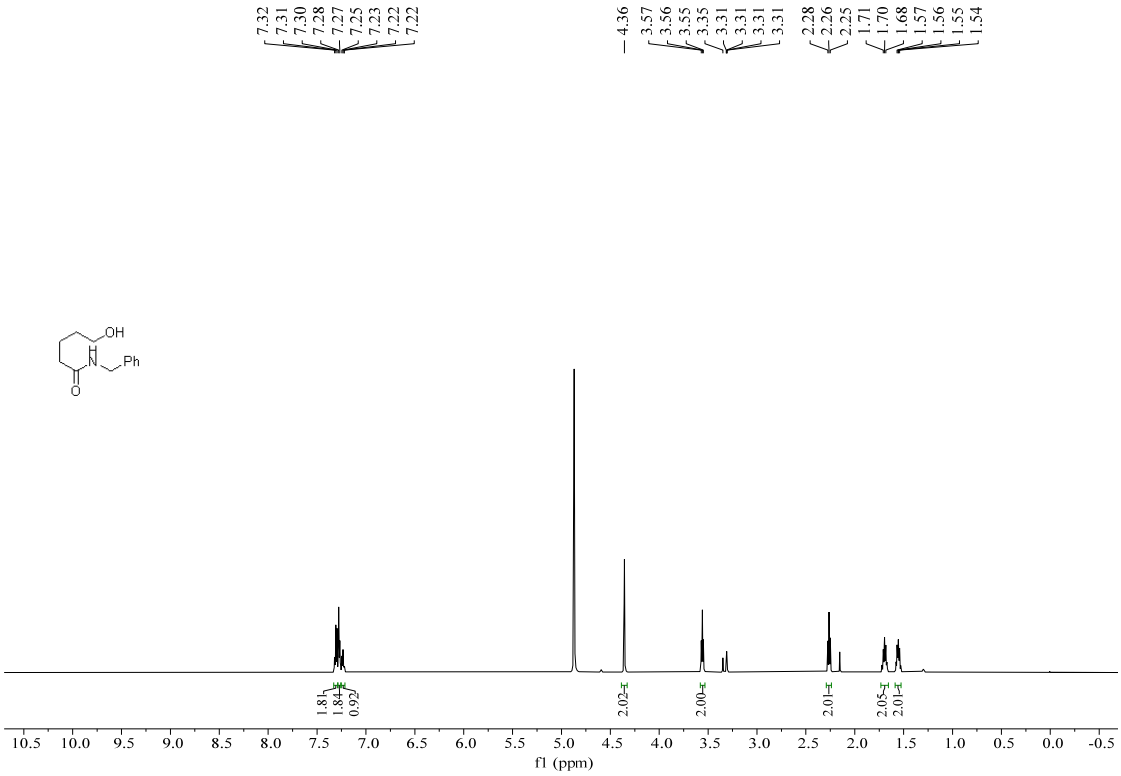

8.00
7.99
7.94
7.92
7.92
7.91
7.69
7.68
7.67
7.54
7.53
7.51
7.50
7.50
7.49
7.48
7.39
7.38
7.37
7.36
7.26
6.47
6.45
5.33


OH
HN
Cl
N
O


1.87
0.81
0.87
0.69
1.06
1.96
2.00
1.70
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


174.25
156.83
146.65
146.23
137.82
134.16
129.19
125.93
125.86
122.22
121.06
109.70
77.48
77.16
76.84
69.80
OH
HN
Cl
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3da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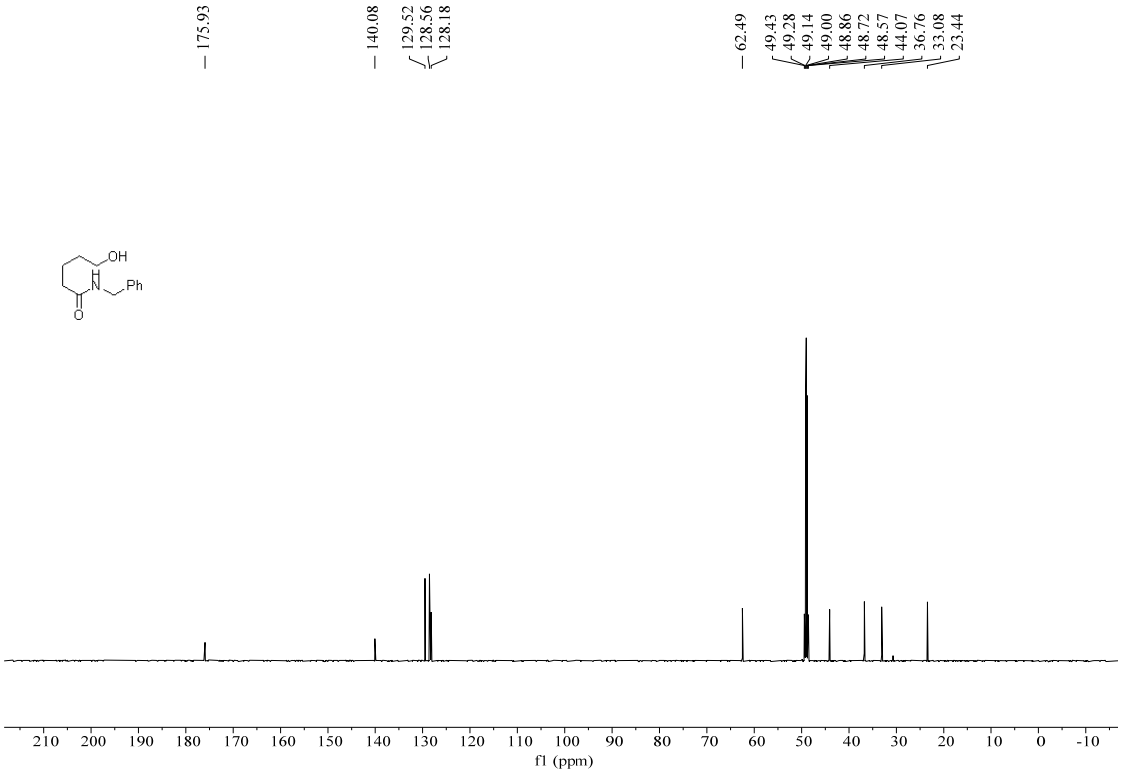
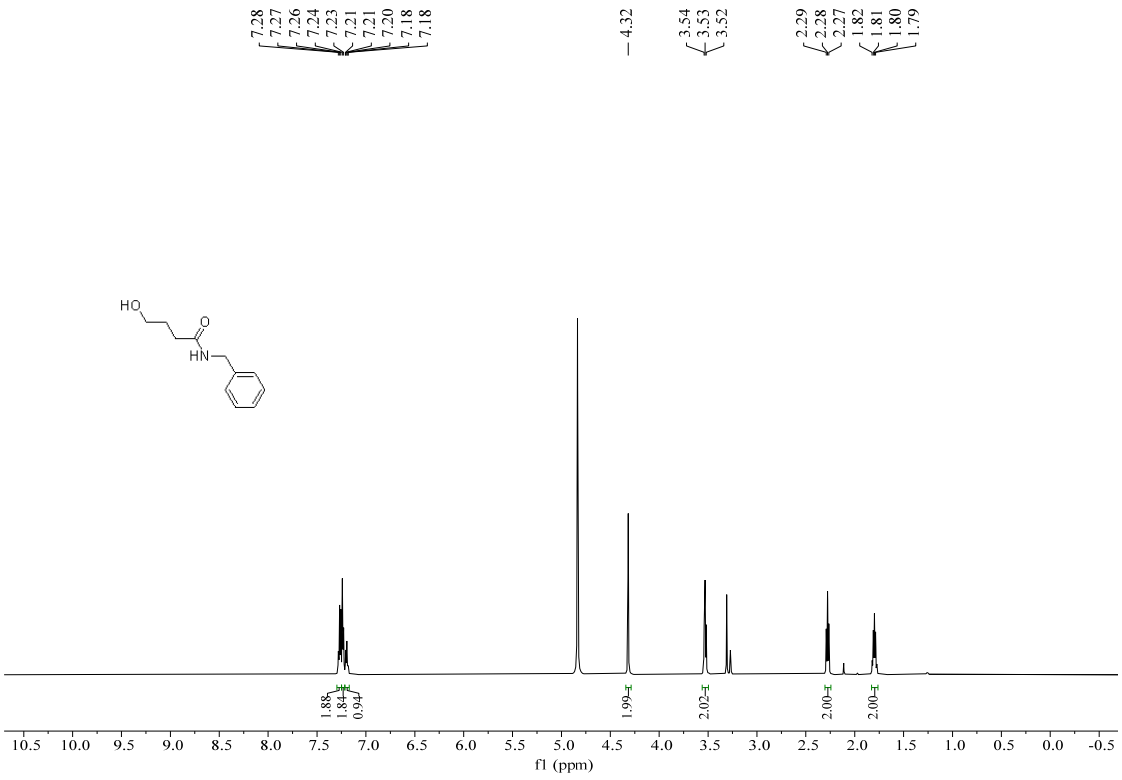
7.31
7.30
7.28
7.27
7.25
7.23
7.22
7.22
4.36
3.57
3.56
3.55
3.35
3.31
3.31
3.31
3.31
2.28
2.26
2.25
1.71
1.70
1.68
1.57
1.56
1.55
1.54
OH
N
H
Ph
O
1.81
1.84
0.92
2.02
2.00
2.01
2.05
2.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


175.93
140.08
129.52
128.56
128.18
62.49
49.43
49.28
49.14
49.00
48.86
48.72
48.57
44.07
36.76
33.08
23.44
OH
N
H
Ph
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3ea: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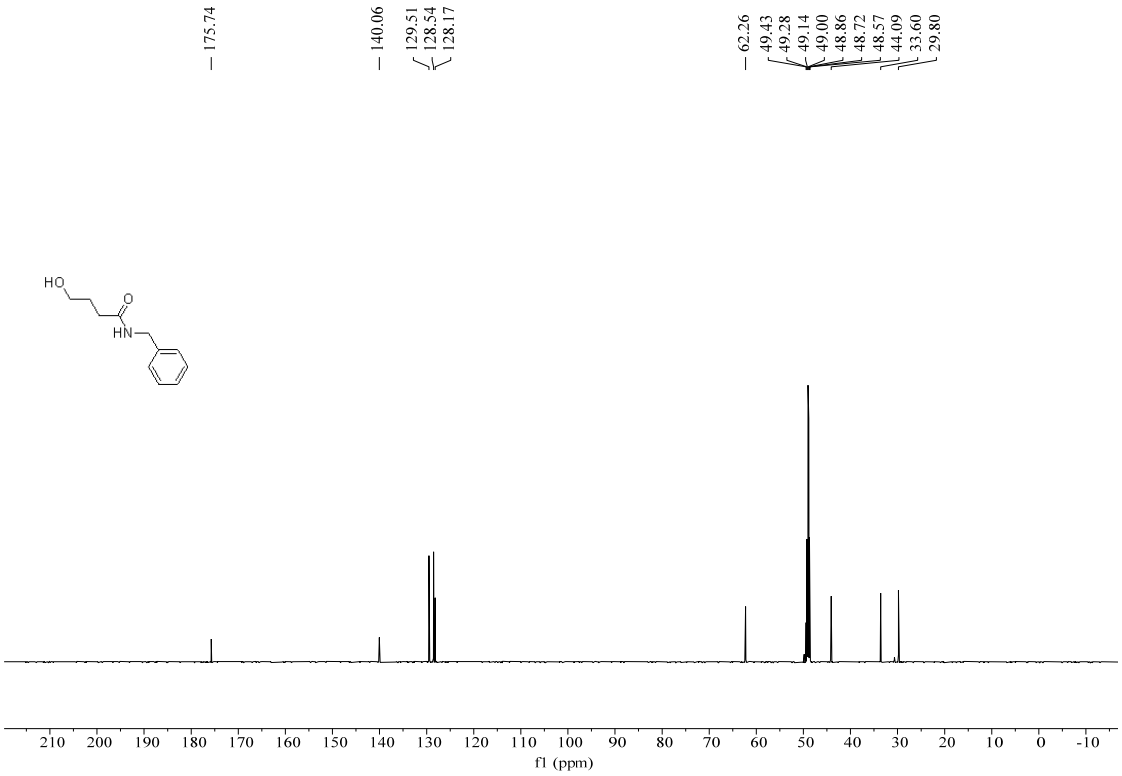
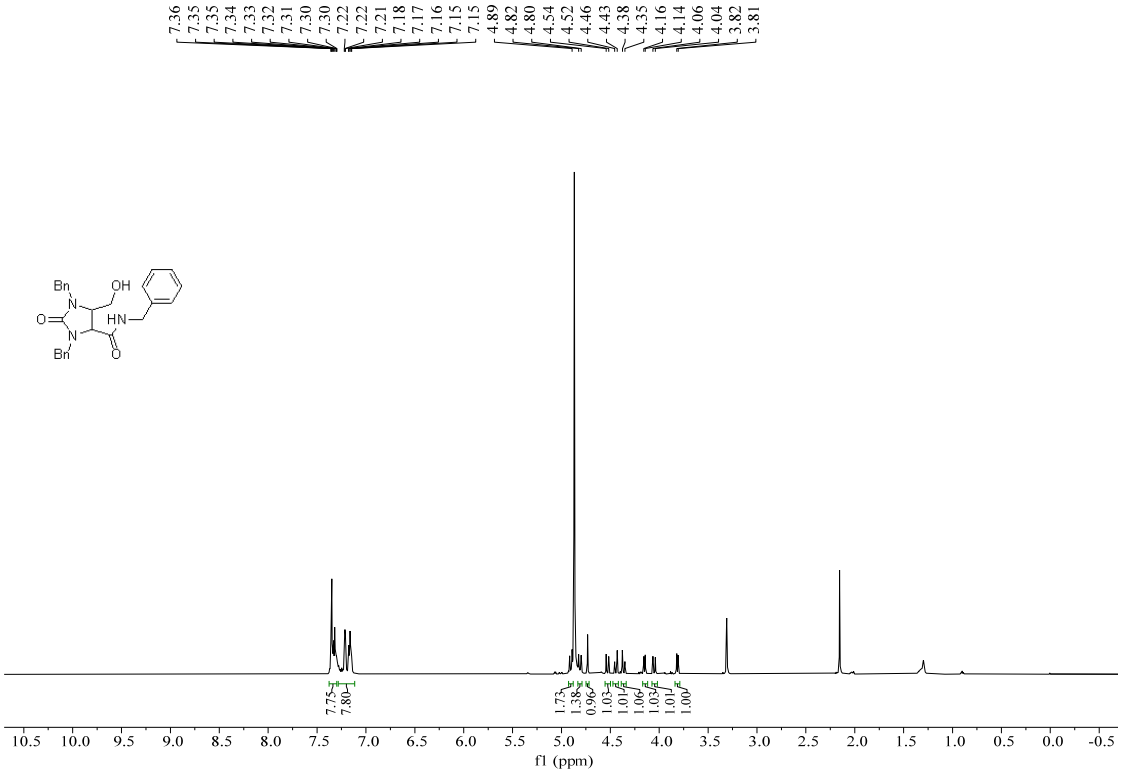
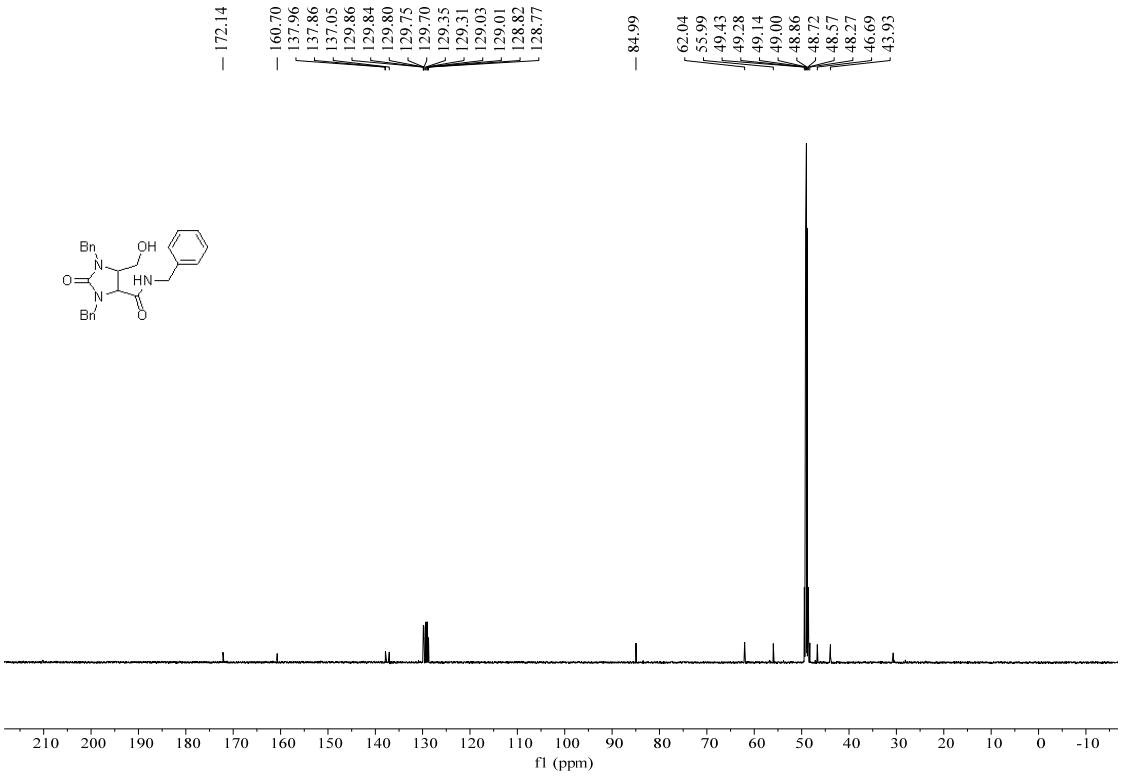
7.27
7.26
7.24
7.23
7.21
7.21
7.20
7.18
7.18
4.32
3.54
3.53
3.52
2.29
2.28
2.27
1.82
1.81
1.80
1.79
HO
O
HN
1.88
1.84
0.94
1.99
2.02
2.00
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

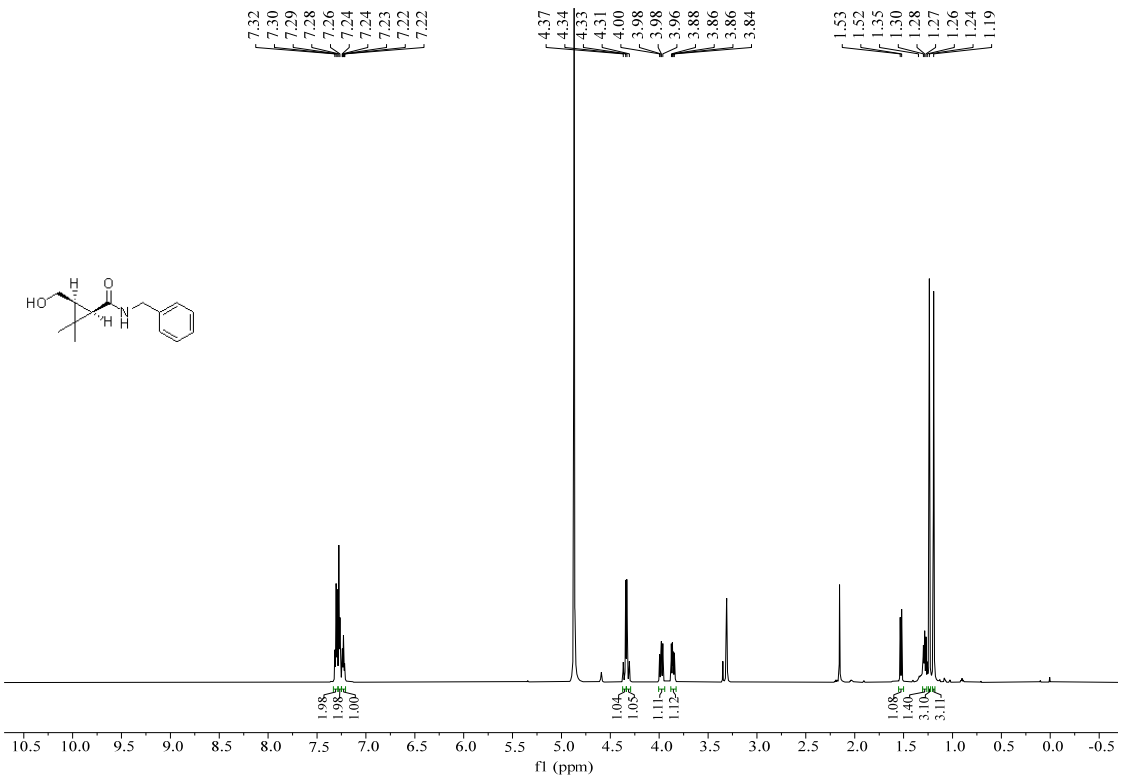

175.74
140.06
129.51
128.54
128.17
62.26
49.43
49.28
49.14
49.00
48.86
48.72
48.57
44.09
33.60
29.80
HO
O
HN
f1 (ppm)

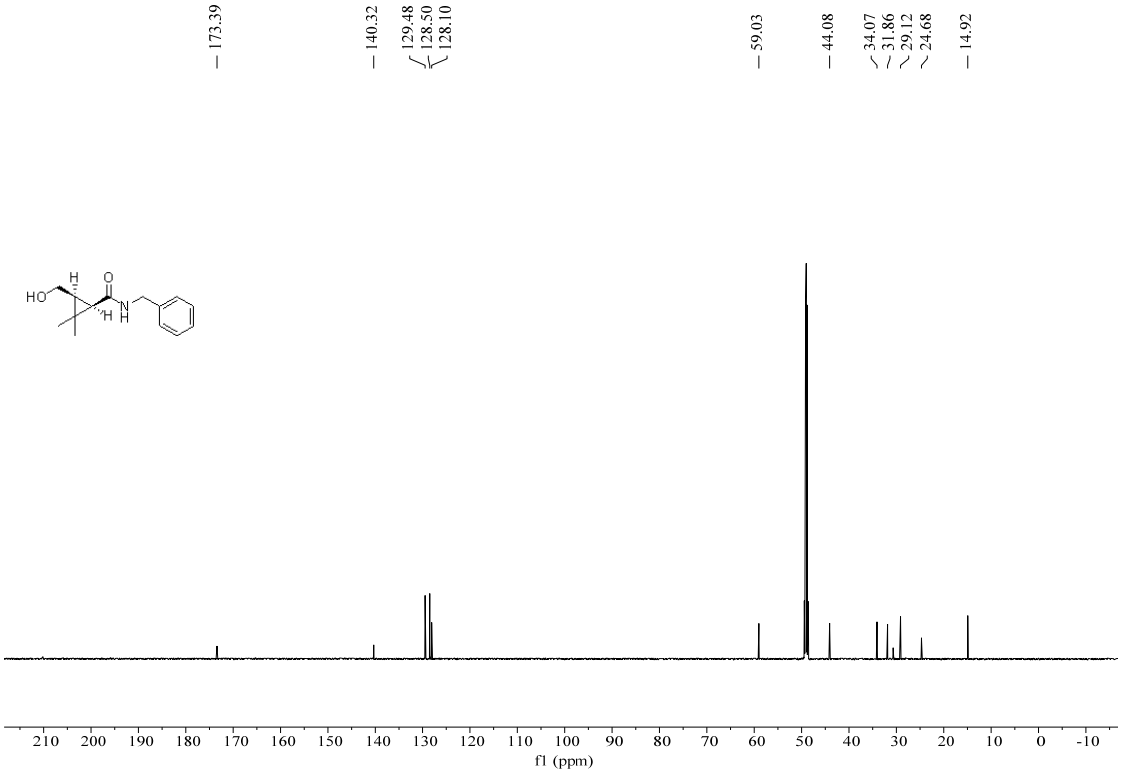
3fa:


7.36
7.35
7.35
7.34
7.33
7.32
7.31
7.30
7.30
7.22
7.22
7.21
7.18
7.17
7.16
7.15
7.15
4.89
4.82
4.80
4.54
4.52
4.46
4.43
4.38
4.35
4.16
4.14
4.06
4.04
3.82
3.81
Bn
OH
HN
O
Bn
7.75
7.80
1.73
1.38
0.96
1.03
1.01
1.06
1.03
1.01
1.00
f1 (ppm)

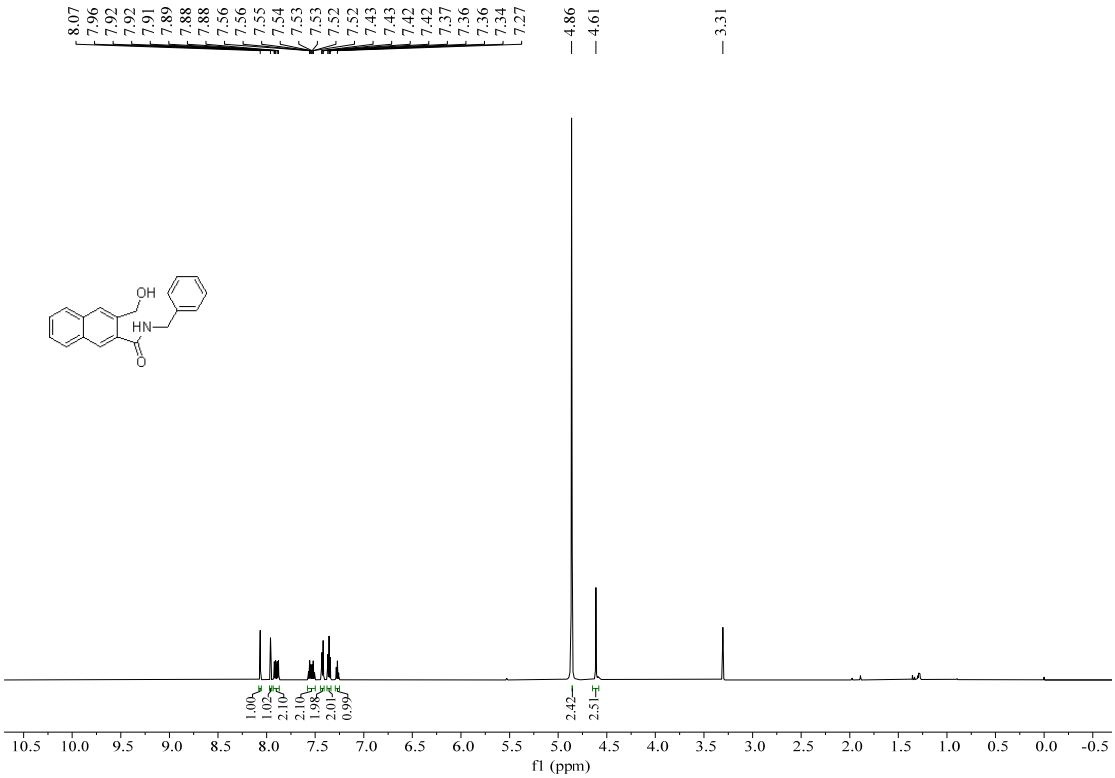

172.14
160.70
137.96
137.86
137.05
129.86
129.84
129.80
129.75
129.70
129.35
129.31
129.03
129.01
128.82
128.77
84.99
62.04
55.99
49.43
49.28
49.14
49.00
48.86
48.72
48.57
48.27
46.69
43.93
Bn
OH
N
O
HN
N
Bn
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3ga:


7.32
7.30
7.29
7.28
7.26
7.24
7.24
7.23
7.22
7.22
4.37
4.34
4.33
4.31
4.00
3.98
3.98
3.96
3.88
3.86
3.86
3.84
1.53
1.52
1.35
1.30
1.28
1.27
1.26
1.24
1.19
HO
H
O
N
H
1.98
1.98
1.00
1.04
1.05
1.11
1.12
1.08
1.40
3.10
3.11
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


173.39
140.32
129.48
128.50
128.10
59.03
44.08
34.07
31.86
29.12
24.68
14.92
HO
H
O
N
H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3ha:


8.07
7.96
7.92
7.92
7.91
7.89
7.88
7.88
7.56
7.56
7.55
7.54
7.53
7.53
7.52
7.52
7.43
7.43
7.42
7.42
7.37
7.36
7.34
7.27
4.86
4.61
3.31
OH
HN
O
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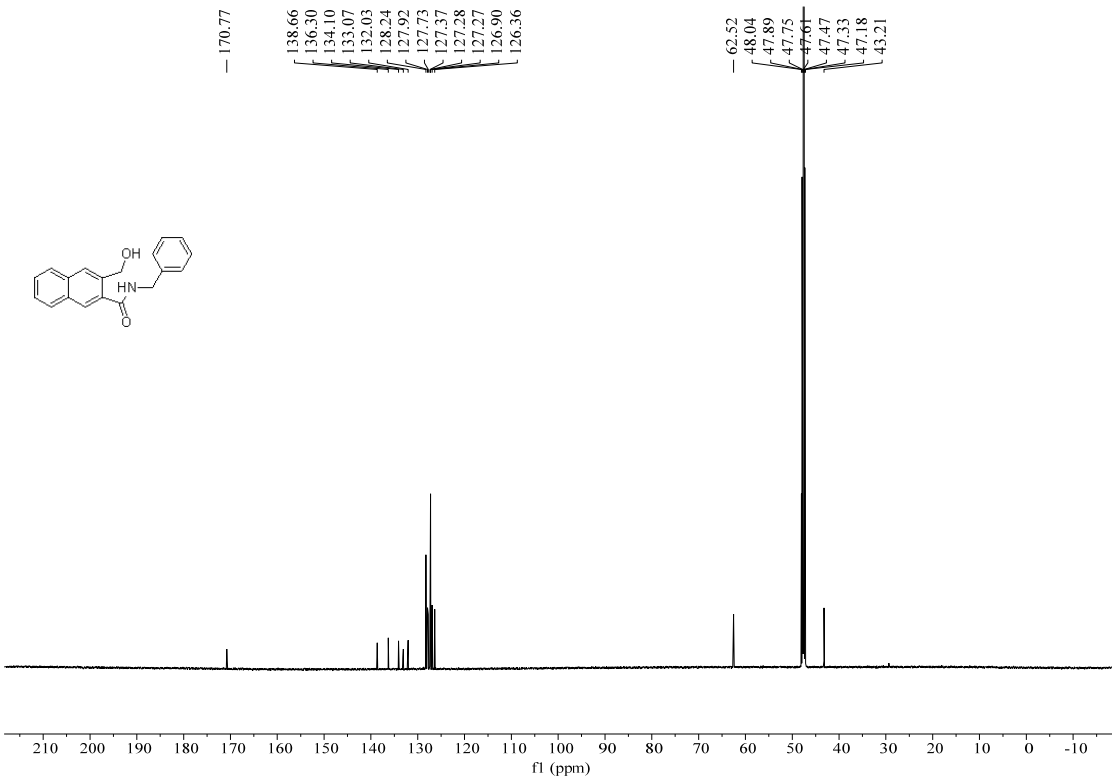
1.02
2.10
2.10
1.98
2.01
0.99
2.42
2.51
f1 (ppm)


170.77
138.66
136.30
134.10
133.07
132.03
128.24
127.92
127.73
127.37
127.28
127.27
126.90
126.36
62.52
48.04
47.89
47.75
47.61
47.47
47.33
47.18
43.21
OH
HN
O
f1 (ppm)