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Supporting Information

A General Palladium-Catalyzed Hiyama Cross-Coupling Reaction of Aryl and Heteroaryl Chlorides

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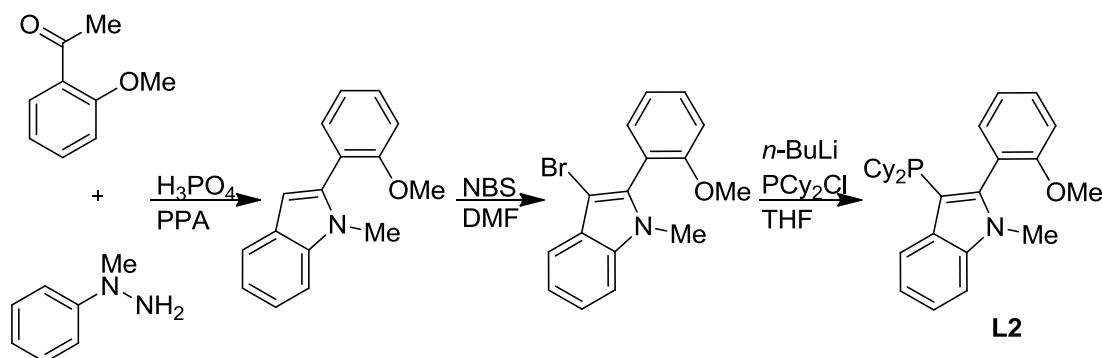
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1. General considerations

Unless otherwise noted, all reagents were purchased from commercial suppliers and used without purification. All Hiyama cross-coupling reactions were performed in resealable screw cap Schlenk tube (approx. 15 mL volume) in the presence of Teflon-coated magnetic stirrer bar (4 mm×10 mm). A blast shield was applied to all close-capped reactions. Toluene and tetrahydrofuran (THF) were distilled from sodium and sodium benzophenone ketyl under nitrogen, respectively.¹ Indolylphosphine ligand **L1**, **L3** and **L4** were prepared according to the reported procedures.² Ligands **L5** – **L10** were purchased from commercial suppliers. Tetrabutylammonium fluoride trihydrate (TBAF•3H₂O) was purchased from Aldrich, Acros and Fluka. The tetrabutylammonium fluoride trihydrate (TBAF•3H₂O) may be subjected to further purification depending on the receiving quality. KF and CsF were purchased from Aldrich. Aryl silanes except for trimethoxy(*o*-tolyl)silane, triethoxy(4-fluorophenyl)silane, (4-(*tert*-butyl)phenyl)triethoxysilane, 1-methyl-5-(triethoxysilyl)-1*H*-indole and tri(methoxy-*d*₃)phenylsilane were purchased from commercial suppliers and used directly. Trimethoxy(*o*-tolyl)silane, triethoxy(4-fluorophenyl)silane, (4-(*tert*-butyl)phenyl)triethoxysilane, 1-methyl-5-(triethoxysilyl)-1*H*-indole and tri(methoxy-*d*₃)phenylsilane were synthesized according to the reported procedures.³ New bottle of *n*-butyllithium was used (*Note*: since the concentration of *n*-BuLi may vary, we recommend performing a titration prior to use). Thin layer chromatography was performed on pre-coated silica gel 60 F₂₅₄ plates. Silica gel (Merck, 70-230 and 230-400 mesh) was used for column chromatography. Melting points were recorded on an uncorrected Büchi Melting Point B-545 instrument. NMR spectra were recorded on a Bruker spectrometer (400 MHz for ¹H, 100 MHz for ¹³C, 376 MHz for ¹⁹F and 162 MHz for ³¹P). Spectra were referenced internally to the residual proton resonance in CDCl₃ (δ 7.26 ppm) as the internal standard. Chemical shifts (δ) were reported as part per million (ppm) in δ scale downfield from TMS. ¹³C NMR spectra were referenced to CDCl₃ (δ 77.0 ppm, the middle peak). ¹⁹F NMR chemical shifts were determined relative to CFC₃ as the external standard and low field is positive. ³¹P NMR spectra were referenced to 85% H₃PO₄ externally. Coupling constants (*J*) were reported in Hertz (Hz). Mass spectra (EI-MS and ES-MS) were recorded on a HP 5989B Mass Spectrometer. High-resolution mass spectra (HRMS) were obtained on a Bruker APEX 47e FTICR mass spectrometer (ESI-MS). GC-MS analysis was conducted on a HP 5973 GCD system using a HP5MS column (30 m × 0.25 mm). The products described in GC yield were accorded to the authentic

samples/dodecane calibration standard from HP 6890 GC-FID system. All yields reported refer to isolated yield of compounds estimated to be greater than 95% purity as determined by capillary gas chromatography (GC) or ^1H NMR. Compounds described in the literature were characterized by comparison of their ^1H , ^{13}C and/or ^{19}F NMR spectra to the previously reported data. The procedures in this section are representative, and thus the yields may differ from those reported in tables.

2. Preparation of indolylphosphine ligand L2



Indolylphosphine ligand L2 was prepared according to the reported procedures without modification.²

3-(Dicyclohexylphosphino)-2-(2-methoxyphenyl)-1-methyl-1-*H*-indole (L2)

3-Bromo-2-(2-methoxyphenyl)-1-methyl-1*H*-indole (10 mmol), *n*-BuLi (11 mmol) and chlorodicyclohexylphosphine (12 mmol) in THF (25 ml) were given white solid product (3.1 g, 71%). ^1H NMR (400 MHz, C_6D_6) δ 1.02-1.39 (m, 10H), 1.50-2.01 (m, 10H), 2.31-2.37 (m, 1H), 2.47-2.54 (m, 1H), 3.09 (s, 3H), 3.23 (s, 3H), 7.09-7.13 (m, 1H), 7.14-7.16 (m, 1H), 7.22-7.26 (m, 2H), 7.44 (d, J = 7.4 Hz, 1H), 8.07 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, C_6D_6) δ 27.2, 27.3, 29.9, 30.2, 30.3, 30.8, 30.9, 31.8, 32.0, 32.2, 32.4, 33.9, 34.0, 34.5, 34.7, 54.5, 104.5, 104.7, 109.7, 110.4, 119.7, 119.9, 121.3, 121.5, 122.1, 129.8, 130.9, 131.0, 134.01, 134.04, 138.3, 146.5, 146.9, 158.2; ^{31}P NMR (162 MHz, C_6D_6) δ -17.87; MS (EI): m/z (relative intensity) 433.3 (M^+ , 5), 402.3 (100), 320 (10), 268.1 (30).

3. General procedure for initial ligand and reaction conditions screening

An array of stock solutions of Pd metal sources (0.010 mmol) with ligand (Pd:L = 1:4) in freshly distilled THF (4.0 mL) were initially prepared with continuously stirring at room temperature for 1 min. An array of Schlenk tubes were charged with magnetic stirrer bar (4

mm x 10 mm) and were evacuated and backfilled with nitrogen (3 cycles). The stock solutions (0.40 mL, 0.20 mol% Pd) were added by syringe to the array of Schlenk tubes respectively. The solvent in Schlenk tubes were removed under reduced pressure. The Schlenk tubes were charged with bases and were again evacuated and backfilled with nitrogen (3 cycles). The Schlenk tubes were then added with trimethoxyphenylsilane (0.19 mL, 1.0 mmol) via autopipette. The reaction mixtures were allowed stir for 1 min and 2-chlorotoluene (59 μ L, 0.50 mmol) was added to each Schlenk tubes via autopipette. This batch of Schlenk tube was resealed and magnetically stirred in a preheated 110 °C oil bath for 3 h. The reactions were allowed to reach room temperature. Ethyl acetate (~8 mL), dodecane (113 μ L, internal standard) and water (~2 mL) were added. The organic layer was subjected to GC analysis. The GC yield was previously calibrated by authentic sample/dodecane calibration curve.

4. General procedure for palladium-catalyzed Hiyama coupling of aryl chlorides

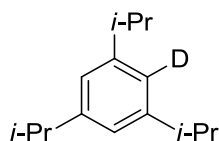
Pd(OAc)₂ (2.3 mg, 0.010 mmol) with ligand **L2** (17.3 mg, 0.040 mmol) in freshly distilled 10 mL THF (0.2 mol% Pd per 1 mL stock solution) were initially prepared with continuously stirring at room temperature for 1 min. Schlenk tube was charged with magnetic stirrer bar (4 mm x 10 mm) and was evacuated and backfilled with nitrogen (3 cycles). The corresponding volume of stock solution was added by syringe to the tube. The solvent was removed under reduced pressure. TBAF•3H₂O (0.32 g, 1.0 mmol) and solid aryl chlorides (0.50 mmol) was added to the tube which was again evacuated and backfilled with nitrogen (3 cycles). Trimethoxyphenylsilane (0.19 mL, 1.0 mmol) was then added to the tube via autopipette and the reaction mixture was allowed stir for 1 min. Liquid aryl chlorides (0.50 mmol) was added to the tube via autopipette. Acetic acid or water and/or toluene (0.50-1.0 mL) were then added via autopipette and syringe respectively (if needed, as indicated in Table 2 and 4). The tube was resealed and magnetically stirred in a preheated 110 °C oil bath for 3 h. The reaction was allowed to reach room temperature. Ethyl acetate (~8 mL), water (~2 mL) were added. The organic layers were combined and concentrated. The crude products were purified by column chromatography on silica gel (230-400 mesh).

5. General procedure for large-scale Hiyama coupling of aryl chlorides

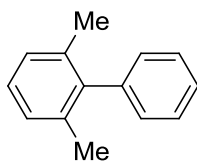
$\text{Pd}(\text{OAc})_2$ (23 mg, 0.10 mmol) and ligand **L1** (0.173 g, 0.40 mmol) were loaded to a 250 mL Schlenk flask (with a glass stopcock and 24/29 joint with hooks) which equipped with a magnetic stirrer bar (30 mm x 6 mm) and fitted with septum. The flask was carefully evacuated and backfilled with nitrogen for three cycles. Precomplexation was accomplished by adding 10 mL freshly distilled THF in to the flask and the solution was allowed to stir at room temperature for 1 min. The solvent was removed under reduced pressure. $\text{TBAF} \cdot 3\text{H}_2\text{O}$ (63 g, 0.20 mol) was quickly charged to the flask which was evacuated and backfilled with nitrogen for other three cycles. Trimethoxyphenylsilane (38 mL, 0.20 mol) was then added to the tube by syringe and the reaction mixture was allowed to stir for 10 min. 3-chlorotoluene (11.8 mL, 0.10 mol) was added to the flask by syringe and allowed to stir for another 5 min. The septum was replaced with a 24/29 stopper with hooks which was then fixed with wire to the flask. The stopcock was closed and the flask was placed in a preheated 110 °C oil bath for 3 h (CAUTION! A BLAST SHIELD HAS TO BE APPLIED!). The reaction was allowed to reach room temperature. Ethyl acetate and water were added to the flask and the mixture was transferred to separating funnel and subjected to extraction. The organic layers were combined and concentrated. The crude product was filtered through a pad of silica gel (10 cm x 20 cm, 230-400 mesh) and eluted with hexane to yield the pure 3-methylbiphenyl (16.6 g, 99%).

6. Characterization data for coupling products

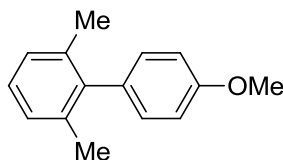
Benzene-*d*, 2,4,6-tris(1-methylethyl)- (Scheme 1)



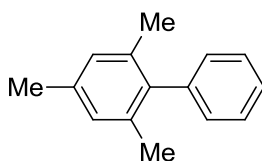
Eluents (Hexane, R_f 0.50) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 1.36 (d, J = 6.8 Hz, 18H), 2.93-3.03 (m, 3H), 7.02 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 24.1, 34.2, 34.3, 122.1, 148.6, 148.7; MS (EI): m/z (relative intensity) 205.2 (M^+ , 27), 190.1 (100), 162.1 (51), 106.0 (20), 92.0 (11); HRMS: calcd. for $\text{C}_{15}\text{H}_{24}\text{D}^+$: 206.2019, found 206.2016.

2,6-Dimethyl-1,1'-biphenyl (Table 3, entry 1-2)^{2a}

Eluents (Hexane, R_f 0.55) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 2.11 (s, 6H), 7.17-7.26 (m, 5H), 7.40 (t, J = 7.4 Hz, 1H), 7.49 (t, J = 7.4 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 20.8, 126.6, 127.0, 127.2, 128.4, 129.0, 136.0, 141.0, 141.8; MS (EI): m/z (relative intensity) 182.0 (M^+ , 72), 167.0 (100), 152.0 (30), 115.0 (21), 77.0 (15).

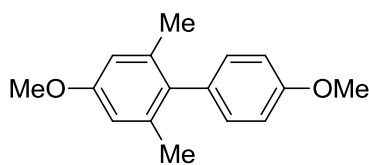
4'-Methoxy-2,6-dimethyl-1,1'-biphenyl (Table 3, entry 3)⁴

Eluents (DCM: Hexane = 1: 10, R_f 0.30) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 2.11 (s, 3H), 3.91 (s, 3H), 7.01-7.05 (m, 2H), 7.11-7.23 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3) δ 20.8, 55., 113.7, 126.8, 127.2, 130.0, 133.3, 136.4, 141.5, 158.2; MS (EI): m/z (relative intensity) 212.2 (M^+ , 100), 197.1 (34), 181.1 (26), 165.1 (28), 153.1 (22).

2,4,6-Trimethyl-1,1'-biphenyl (Table 3, entry 4-5)⁵

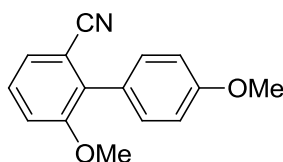
Eluents (Hexane, R_f 0.55) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 2.07 (s, 6H), 2.40 (s, 3H), 7.01 (s, 2H), 7.20 (d, J = 7.8 Hz, 2H), 7.38 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 20.7, 21.0, 126.5, 128.0, 128.3, 129.3, 135.9, 136.5, 139.0, 141.1; MS (EI): m/z (relative intensity) 196.1 (M^+ , 100), 165.0 (66), 141.0 (7), 115.0 (15), 89.0 (13).

4,4'-Dimethoxy-2,6-dimethyl-1,1'-biphenyl (Table 3, entry 6)

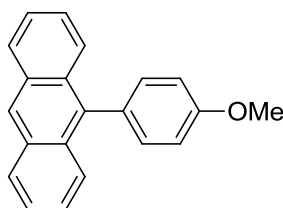


Eluents (DCM: Hexane= 1: 10, R_f 0.20) was used for flash column chromatography. White solid; m.p.=114.7-117.2 ; ^1H NMR (400 MHz, CDCl_3) δ 2.07 (s, 3H), 3.85 (s, 3H), 3.88 (s, 3H), 6.71 (s, 2H), 6.99 (d, J = 8.4 Hz, 2H), 7.09 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 21.1, 55.0, 55.1, 112.5, 113.7, 127.7, 130.6, 133.0, 134.1, 137.8, 158.1; MS (EI): m/z (relative intensity) 242.2 (M^+ , 100), 227.1 (22), 199.1 (7), 184.1 (4), 152.1 (4); HRMS: calcd. for $\text{C}_{16}\text{H}_{18}\text{O}_2^+$: 242.1301, found 242.1301.

4',6-Dimethoxy-[1,1'-biphenyl]-2-carbonitrile (Table 3, entry 7)

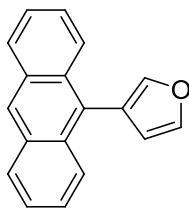


Eluents (Ethyl acetate: Hexane= 1: 9, R_f 0.20) was used for flash column chromatography. White solid; m.p.= 89.1-92.1; ^1H NMR (400 MHz, CDCl_3) δ 3.79 (s, 3H), 3.86 (s, 3H), 7.00 (d, J = 8.8 Hz, 2H), 7.17 (d, J = 8.0 Hz, 1H), 7.32-7.40 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 55.1, 55.9, 113.6, 113.7, 115.2, 118.4, 125.0, 126.2, 128.7, 131.2, 134.3, 156.9, 159.6; MS (EI): m/z (relative intensity) 239.1 (M^+ , 100), 224.1 (29), 209.1 (19), 193.1 (12), 153.1 (12); HRMS: calcd. for $\text{C}_{15}\text{H}_{14}\text{NO}_2^+$: 240.1019, found 240.1020.

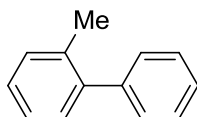
9-(4-Methoxyphenyl)anthracene (Table 3, entry 8)⁶

Eluents (Hexane, R_f 0.40) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 3.98 (s, 3H), 7.17 (d, J = 8.6 Hz, 2H), 7.39-7.43 (m, 4H), 7.51 (t, J = 8.4 Hz, 2H), 7.80 (d, J = 8.8 Hz, 2H), 8.08 (d, J = 8.8 Hz, 2H), 8.52 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 55.3, 113.8, 125.0, 125.2, 126.3, 126.9, 128.3, 130.5, 130.8, 131.4, 132.3, 136.8, 159.0; MS (EI): m/z (relative intensity) 284.1 (M^+ , 100), 269.1 (16), 239.1 (36), 119.6 (12).

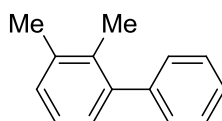
3-(Anthracen-9-yl)furan (Table 3, entry 9)



Eluents (Hexane, R_f 0.40) was used for flash column chromatography. Yellow gel; ^1H NMR (400 MHz, CDCl_3) δ 6.71 (s, 1H), 7.46–7.55 (m, 4H), 7.705–7.709 (m, 1H), 7.796–8.804 (m, 1H), 8.06–8.09 (m, 4H), 8.51 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 114.1, 121.4, 125.1, 125.5, 126.5, 126.9, 127.5, 128.4, 130.9, 131.3, 141.9, 143.0; MS (EI): m/z (relative intensity) 244.1 (M^+ , 100), 215.1 (75), 189.1 (7), 106.7 (7); HRMS: calcd. for $\text{C}_{18}\text{H}_{12}\text{O}^+$: 244.0883, found 244.0883.

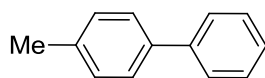
2-Methyl-1,1'-biphenyl (Table 4, entry 1)^{2a}

Eluents (Hexane, R_f 0.55) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 2.36 (s, 3H), 7.32–7.36 (m, 4H), 7.40–7.43 (m, 3H), 7.47–7.51 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 20.4, 125.7, 126.7, 127.2, 128.0, 129.2, 129.8, 130.3, 135.3, 141.9, 142.0; MS (EI): m/z (relative intensity) 168.1 (M^+ , 100), 153.0 (40), 139.0 (8), 115.0 (14), 77.0 (4).

2,3-Dimethyl-1,1'-biphenyl (Table 4, entry 2)⁷

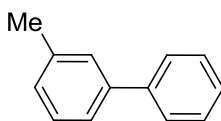
Eluents (Hexane, R_f 0.50) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 2.55 (s, 3H), 2.44 (s, 3H), 7.18–7.27 (m, 3H), 7.39–7.44 (m, 3H), 7.49 (t, J = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 16.9, 20.7, 125.2, 126.6, 127.6, 128.8, 129.4, 134.0, 137.1, 142.2, 142.6; MS (EI): m/z (relative intensity) 182.1 (M^+ , 95), 167.1 (100), 152.0 (26), 128.0 (8), 76.0 (8).

4-Methyl-1,1'-biphenyl (Table 4, entry 3)^{2a}^{Error! Bookmark not defined.}



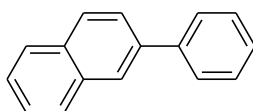
Eluents (Hexane, R_f 0.50) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 2.48 (s, 3H), 7.33 (d, J = 7.6 Hz, 2H), 7.40 (t, J = 7.6 Hz, 1H), 7.50 (t, J = 7.6 Hz, 2H), 7.58 (d, J = 8.0 Hz, 2H), 7.66 (d, J = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 21.1, 126.9, 127.0, 128.7, 129.4, 137.0, 138.3, 141.1; MS (EI): m/z (relative intensity) 168.0 (M^+ , 100), 139.0 (8), 115.0 (15), 91.0 (6), 62.9 (9).

3-Methyl-1,1'-biphenyl (Table 4, entry 4)⁸



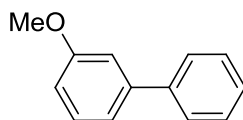
Eluents (Hexane, R_f 0.50) was used for flash column chromatography. ^1H NMR (400MHz, CDCl_3) δ 2.48 (s, 3H), 7.29 (d, J = 7.6 Hz, 1H), 7.46 (t, J = 7.6 Hz, 2H), 7.52–7.57 (m, 4H), 7.72 (d, J = 7.8 Hz, 2H); ^{13}C NMR (100MHz, CDCl_3) δ 21.5, 124.2, 127.1, 127.2, 127.9, 128.0, 128.6, 128.7, 138.3, 141.2, 141.3; MS (EI): m/z (relative intensity) 168.1 (M^+ , 100), 152.0 (23), 139.0 (5), 115.0 (8), 89.0 (4).

2-Phenylnaphthalene (Table 4, entry 5)⁹



Eluents (Hexane, R_f 0.50) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 2.48 (s, 3H), 7.47–7.51 (m, 1H), 7.57–7.63 (m, 4H), 7.82–7.87 (m, 3H), 7.96–8.02 (m, 3H), 8.16 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 125.5, 125.7, 125.9, 126.2, 127.3, 127.4, 127.6, 128.2, 128.4, 128.8, 132.6, 133.6, 138.5, 141.1; MS (EI): m/z (relative intensity) 204.1 (M^+ , 100), 176.0 (3), 152.1 (3), 126.0 (3), 101.0 (7).

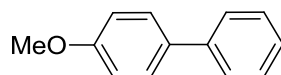
3-Methoxy-1,1'-biphenyl (Table 4, entry 6)¹⁰



Eluents (Ethyl acetate: Hexane = 1: 50, R_f 0.40) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 3.96 (s, 3H), 7.03 (d, J = 8.2 Hz, 1H), 7.29 (s, 1H), 7.33 (d, J =

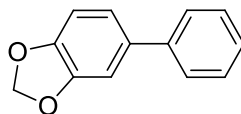
8.0 Hz, 1H), 7.46–7.50 (m, 2H), 7.56 (t, J = 7.6 Hz, 2H), 7.73. (d, J = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 55.1, 112.6, 112.8, 119.6, 127.1, 127.3, 128.7, 129.7, 141.0, 142.7, 159.9; MS (EI): m/z (relative intensity) 184.0 (M^+ , 100), 154.1 (28), 141.0 (51), 115.0 (92), 76.1 (17).

4-Methoxy-1,1'-biphenyl (Table 4, entry 7)^{2a}



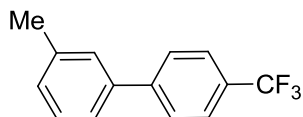
Eluents (Ethyl acetate: Hexane = 1: 20, R_f = 0.50) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 3.90 (s, 3H), 7.05 (d, J = 8.8 Hz, 2H), 7.38 (t, J = 7.6 Hz, 1H), 7.49 (t, J = 7.6 Hz, 1H), 7.59–7.65 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 55.2, 114.2, 126.6, 126.7, 128.1, 128.7, 133.7, 140.8, 159.1; MS (EI): m/z (relative intensity) 184.0 (M^+ , 100), 169.0 (47), 141.0 (57), 115.0 (52), 89.1 (7).

5-Phenylbenzo[d][1,3]dioxole (Table 4, entry 8)⁹



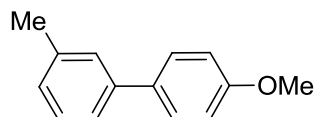
Eluents (Ethyl acetate: Hexane = 1: 9, R_f = 0.40) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 6.03 (s, 3H), 6.94 (d, J = 8.0 Hz, 1H), 7.11–7.15 (m, 2H), 7.37 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.6 Hz, 2H), 7.58 (d, J = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 101.0, 107.6, 108.5, 120.5, 126.8, 126.9, 128.7, 135.5, 140.8, 147.0, 148.0; MS (EI): m/z (relative intensity) 198.0 (M^+ , 100), 139.0 (44), 115.0 (4), 98.8 (4), 77.0 (2).

3-Methyl-4'-(trifluoromethyl)-1,1'-biphenyl (Table 4, entry 9-10)¹¹



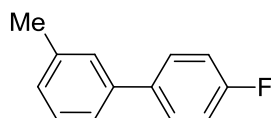
Eluents (Hexane, R_f = 0.50) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 2.48 (s, 3H), 7.26 (d, J = 7.4 Hz, 1H), 7.38–7.45 (m, 3H), 7.72 (s, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 21.5, 124.36 (q, J = 270 Hz), 124.37, 125.6 (q, J = 4.0 Hz), 127.4, 128.0, 128.88, 128.92, 129.2 (q, J = 32 Hz), 138.6, 139.8, 144.9; ^{19}F NMR (376 MHz, CDCl_3) δ -62.3; MS (EI): m/z (relative intensity) 236.0 (M^+ , 100), 217.1 (13), 165.0 (45), 152.0 (16), 91.1 (6).

4'-Methoxy-3-methyl-1,1'-biphenyl (Table 4, entry 11-12)¹²



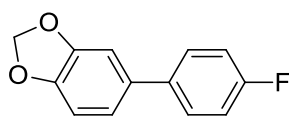
Eluents (Ethyl acetate: Hexane= 1: 50, R_f = 0.50) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 2.47 (s, 3H), 3.89 (s, 3H), 7.03 (d, J = 8.8 Hz, 2H), 7.19 (d, J = 7.6 Hz, 1H), 7.37 (t, J = 7.4 Hz, 1H), 7.41–7.44 (m, 2H), 7.59 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 21.5, 55.2, 114.1, 123.8, 127.4, 127.5, 128.1, 128.6, 133.8, 138.2, 140.8, 159.0; MS (EI): m/z (relative intensity) 198.1 (M^+ , 100), 183.0 (51), 155.0 (40), 128.0 (16), 89.0 (4).

4'-Fluoro-3-methyl-1,1'-biphenyl (Table 4, entry 13)¹³



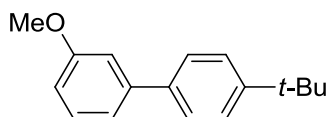
Eluents (Hexane, R_f = 0.50) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 2.48 (s, 3H), 7.14-7.24 (m, 3H), 7.36-7.42 (m, 3H), 7.56-7.61 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 21.5, 115.5 (d, J = 21.0 Hz), 124.1, 127.8, 128.0, 128.6 (d, J = 8.0 Hz), 128.7, 137.4 (d, J = 3.0 Hz), 138.4, 140.2, 162.4 (d, J = 245.0 Hz); ^{19}F NMR (376 MHz, CDCl_3) δ -115.9; MS (EI): m/z (relative intensity) 186.1 (M^+ , 100), 165.1 (26), 133.1 (5), 91.2 (4).

5-(4-Fluorophenyl)benzo[d][1,3]dioxole (Table 4, entry 14)¹⁴



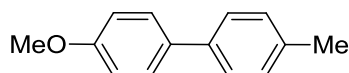
Eluents (Ethyl acetate: Hexane= 1: 9, R_f = 0.50) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 6.00 (s, 2H), 6.88 (d, J = 7.92 Hz, 1H), 7.01 (d, J = 8.08 Hz, 1H), 7.03 (s, 1H), 7.08-7.13 (m, 2H), 7.45-7.48 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 101.1, 107.4, 108.4, 115.5 (d, J = 21.0 Hz), 120.3, 128.3 (d, J = 8.0 Hz), 134.5, 137.0 (d, J = 3.0 Hz), 146.9, 148.0, 162.1 (d, J = 244.0 Hz); ^{19}F NMR (376 MHz, CDCl_3) δ -116.1; MS (EI): m/z (relative intensity) 216.1 (M^+ , 100), 157.1 (47), 138.1 (3), 107.8 (4).

4'-(*tert*-Butyl)-3-methoxy-1,1'-biphenyl (Table 4, entry 15)¹⁵



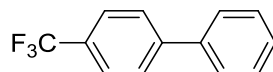
Eluents (Ethyl acetate: Hexane= 1: 9, R_f 0.50) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 1.45 (s, 9H), 3.92 (s, 3H), 6.96 (d, J = 8.2 Hz, 1H), 7.23 (s, 1H), 7.27 (d, J = 7.68 Hz, 1H), 7.42 (t, J = 7.88 Hz, 1H), 7.55 (d, J = 8.44 Hz, 2H), 7.63 (d, J = 8.44 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 31.3, 34.5, 55.2, 112.3, 112.7, 119.5, 125.6, 126.8, 129.6, 138.1, 142.6, 150.4, 159.9; MS (EI): m/z (relative intensity) 240.2 (M^+ , 42), 225.2 (100), 197.1 (13), 165.1 (8).

4-Methoxy-4'-methyl-1,1'-biphenyl (Table 4, entry 16)¹⁰



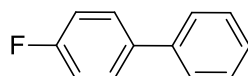
Eluents (Ethyl acetate: Hexane= 1: 9, R_f 0.40) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 2.46 (s, 3H), 3.90 (s, 3H), 7.04 (d, J = 8.4 Hz, 2H), 7.30 (d, J = 7.6 Hz, 2H), 7.53 (d, J = 6.4 Hz, 2H), 7.59 (d, J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 21.0, 55.3, 114.2, 126.6, 127.9, 129.4, 133.7, 136.3, 138.0, 158.9; MS (EI): m/z (relative intensity) 198.1 (M^+ , 100), 183.1 (61), 155.0 (45), 128.0 (19), 77.1 (6).

4-(Trifluoromethyl)-1,1'-biphenyl (Table 4, entry 17)¹⁶



Eluents (Hexane, R_f 0.60) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 7.46 (d, J = 7.2 Hz, 1H), 7.52 (t, J = 7.6 Hz, 2H), 7.64 (d, J = 7.6 Hz, 2H), 7.71-7.75 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 124.3 (q, J = 270.0 Hz), 125.7 (q, J = 4.0 Hz), 127.3, 127.4, 128.1, 129.0, 129.3 (q, J = 33.0 Hz), 139.7, 144.7; ^{19}F NMR (376 MHz, CDCl_3) δ -62.3; MS (EI): m/z (relative intensity) 222.1 (M^+ , 100), 201.0 (12), 172.0 (4), 152.0 (24), 75.0 (3).

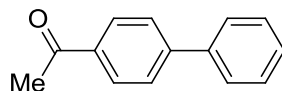
4-Fluoro-1,1'-biphenyl (Table 4, entry 18)¹⁶



Eluents (Hexane, R_f 0.50) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 7.14 (t, J = 8.6 Hz, 2H), 7.36 (t, J = 7.4 Hz, 1H), 7.45 (t, J = 7.4 Hz, 2H), 7.55-7.57 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 115.6 (d, J = 22.0 Hz), 126.9, 127.2, 128.6 (d, J = 8.0

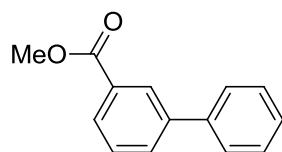
Hz), 128.8, 137.3 (d, $J = 3.0$ Hz), 140.2, 162.4 (d, $J = 244.0$ Hz); ^{19}F NMR (376 MHz, CDCl_3) δ -115.7; MS (EI): m/z (relative intensity) 172.0 (M^+ , 100), 146.0 (6), 120.0 (3), 74.0 (4), 51.0 (3).

1-([1,1'-Biphenyl]-4-yl)ethanone (Table 4, entry 19-20)¹⁷



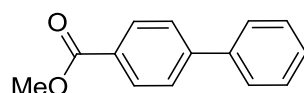
Eluents (Ethyl acetate: Hexane= 1: 9, $R_f = 0.40$) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 2.63 (s, 3H), 7.41 (t, $J = 7.4$ Hz, 1H), 7.47 (t, $J = 7.4$ Hz, 2H), 7.63 (d, $J = 7.2$ Hz, 2H), 7.68 (d, $J = 8.4$ Hz, 2H), 8.03 (d, $J = 8.4$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 26.5, 127.0, 127.1, 128.1, 128.8, 128.9, 135.7, 139.7, 145.6, 197.6; MS (EI): m/z (relative intensity) 196.0 (M^+ , 43), 181.0 (100), 152.0 (65), 126.9 (6), 76.0 (10).

Methyl [1,1'-biphenyl]-3-carboxylate (Table 4, entry 21-25)¹⁸



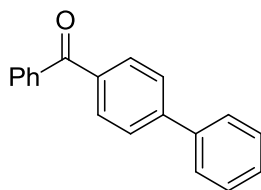
Eluents (Ethyl acetate: Hexane= 1: 9, $R_f = 0.50$) was used for flash column chromatography.; ^1H NMR (400 MHz, CDCl_3) δ 3.96 (s, 3H), 7.39 (t, $J = 7.2$ Hz, 1H), 7.46-7.54 (m, 3H), 7.64 (d, $J = 7.2$ Hz, 2H), 7.80 (d, $J = 7.6$ Hz, 1H), 8.04 (d, $J = 7.6$ Hz, 1H), 8.31 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 52.1, 127.1, 127.7, 128.2, 128.3, 128.8, 128.9, 130.6, 131.5, 140.0, 141.4, 167.0 ; MS (EI): m/z (relative intensity) 212.0 (M^+ , 87), 196.0 (8), 181.0 (100), 152.0 (92), 76.0 (19).

Methyl [1,1'-biphenyl]-4-carboxylate (Table 4, entry 26-29)¹⁰



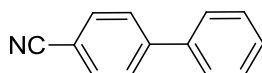
Eluents (Ethyl acetate: Hexane= 1: 9, $R_f = 0.40$) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 3.95 (s, 3H), 7.40 (t, $J = 7.2$ Hz, 1H), 7.47 (t, $J = 7.4$ Hz, 2H), 7.62-7.67 (m, 4H), 8.13 (d, $J = 8.4$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 51.9, 126.9, 127.1, 128.0, 128.7, 128.8, 130.0, 139.8, 145.4, 166.8; MS (EI): m/z (relative intensity) 212.1 (M^+ , 72), 181.0 (100), 152.0 (56), 126.0 (5), 76.0 (9).

[1,1'-Biphenyl]-4-yl(phenyl)methanone (Table 4, entry 30)¹⁰



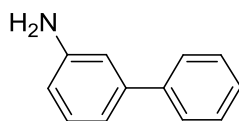
Eluents (Ethyl acetate: Hexane= 1: 4, R_f 0.50) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 7.43 (d, J = 7.2 Hz, 1H), 7.47-7.53 (m, 4H), 7.58-7.63 (m, 1H), 7.67 (d, J = 8.0 Hz, 2H), 7.72 (d, J = 8.4 Hz, 2H), 7.82-7.86 (m, 2H), 7.92 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 126.8, 127.1, 128.1, 128.2, 128.8, 129.9, 130.6, 132.2, 136.1, 137.6, 139.8, 145.0, 196.2; MS (EI): m/z (relative intensity) 258.1 (M^+ , 75), 181.0 (100), 152.0 (64), 105.0 (24), 77.0 (40).

[1,1'-Biphenyl]-4-carbonitrile (Table 4, entry 31)¹⁹

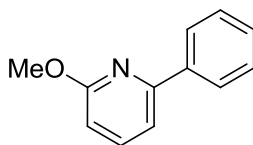


Eluents (Ethyl acetate: Hexane= 1: 4, R_f 0.50) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 7.41-7.45 (m, 1H), 7.49 (t, J = 7.4 Hz, 2H), 7.59-7.61 (m, 2H), 7.67-7.73 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 110.8, 118.8, 127.1, 127.6, 128.6, 129.0, 132.5, 139.0, 145.5; MS (EI): m/z (relative intensity) 179.1 (M^+ , 100), 151.0 (14), 126.0 (3), 100.0 (2), 76.0 (6).

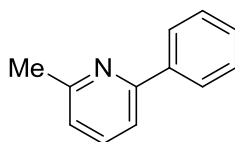
[1,1'-Biphenyl]-3-amine (Table 4, entry 32)²⁰



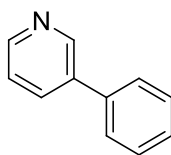
Eluents (Ethyl acetate: Hexane= 1: 2, R_f 0.60) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 3.62 (s, 2H), 6.71 (d, J = 7.2 Hz, 1H), 6.94 (s, 1H), 7.04 (d, J = 7.6 Hz, 1H), 7.27 (t, J = 7.6 Hz, 2H), 7.37 (t, J = 7.2 Hz, 1H), 7.46 (t, J = 7.6 Hz, 2H), 7.61 (d, J = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 113.8, 114.0, 117.6, 127.0, 127.1, 128.6, 129.6, 141.3, 142.4, 146.6; MS (EI): m/z (relative intensity) 169.0 (M^+ , 100), 141.0 (11), 115.0 (11), 89.0 (4), 71.6 (3).

2-Methoxy-6-phenylpyridine (Table 5, entry 1)²¹

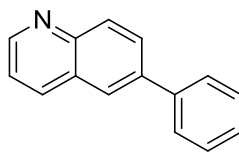
Eluents (Ethyl acetate: Hexane= 3: 7, R_f 0.50) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 4.09 (s, 3H), 6.74 (d, J = 8.0 Hz, 1H), 7.37 (d, J = 7.6 Hz, 1H), 7.44 (t, J = 7.2 Hz, 1H), 7.51 (t, J = 7.4 Hz, 2H), 7.64 (t, J = 7.8 Hz, 1H), 8.11 (d, J = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 53.1, 109.2, 112.7, 126.6, 128.5, 128.8, 139.0, 139.1, 154.6, 163.7; MS (EI): m/z (relative intensity) 184.0 (M^+ , 100), 154.0 (60), 127.0 (10), 102.0 (6), 77.0 (8).

2-Methyl-6-phenylpyridine (Table 5, entry 2)¹⁰

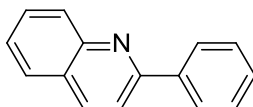
Eluents (Ethyl acetate: Hexane= 1: 4, R_f 0.50) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 2.65 (s, 3H), 7.08 (d, J = 7.6 Hz, 1H), 7.42 (t, J = 7.2 Hz, 1H), 7.47-7.52 (m, 3H), 7.61 (t, J = 7.6 Hz, 1H), 8.02 (d, J = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 24.6, 117.5, 121.4, 126.9, 128.5, 128.6, 136.7, 139.6, 156.8, 158.2; MS (EI): m/z (relative intensity) 169.1 (M^+ , 100), 154.0 (8), 127.0 (6), 115.0 (5), 77.0 (6).

3-Phenylpyridine (Table 5, entry 3)¹⁰

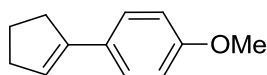
Eluents (Ethyl acetate: Hexane= 1: 2, R_f 0.40) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 7.32-7.35 (m, 1H), 7.37-7.41 (m, 1H), 7.46 (t, J = 7.4 Hz, 2H), 7.56 (d, J = 7.2 Hz, 2H), 7.85 (d, J = 7.6 Hz, 1H), 8.58 (d, J = 3.6 Hz, 1H), 8.85 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 123.4, 127.0, 128.0, 129.0, 134.2, 136.5, 137.7, 148.2, 148.3; MS (EI): m/z (relative intensity) 155.1 (M^+ , 100), 127.0 (16), 102.0 (14), 76.0 (7), 51.0 (9).

6-Phenylquinoline (Table 5, entry 4)²²

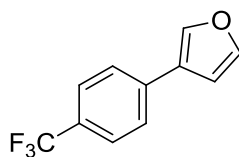
Eluents (Ethyl acetate: Hexane= 1: 4, R_f 0.25) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 7.35-7.41 (m, 2H), 7.48 (t, J = 7.6 Hz, 2H), 7.69 (d, J = 7.6 Hz, 2H), 7.95-7.97 (m, 2H), 8.13-8.19 (m, 2H), 8.89-8.91 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 121.3, 125.3, 127.3, 127.6, 128.3, 128.8, 129.0, 129.7, 136.1, 139.1, 140.1, 147.5, 150.2; MS (EI): m/z (relative intensity) 205.1 (M^+ , 100), 176.0 (12), 151.0 (6), 102.1 (8), 76.0 (5).

2-Phenylquinoline (Table 5, entry 5)²³

Eluents (Ethyl acetate: Hexane= 1: 2, R_f 0.30) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 7.47-7.57 (m, 4H), 7.75 (t, J = 7.8 Hz, 1H), 7.81 (d, J = 8.0 Hz, 1H), 7.85 (d, J = 8.8 Hz, 1H), 7.17-8.24 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 118.9, 126.2, 127.1, 127.4, 127.5, 128.7, 129.2, 129.5, 129.6, 136.7, 139.5, 148.2, 157.2; MS (EI): m/z (relative intensity) 205.1 (M^+ , 100), 176.0 (6), 151.0 (3), 102.1 (6), 75.0 (4).

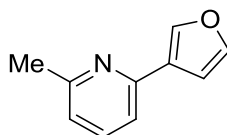
1-Cyclopentenyl-4-methoxybenzene (Table 5, entry 6)^{2b}

Eluents (Hexane, R_f 0.30) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 1.99-2.07 (m, 2H), 2.51-2.56 (m, 2H), 2.67-2.72 (m, 2H), 3.82 (s, 3H), 6.06-6.08 (m, 1H), 6.87 (d, J = 8.8 Hz, 2H), 7.40 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 23.4, 33.2, 33.3, 55.2, 113.6, 123.9, 126.7, 129.7, 141.8, 158.6 ; MS (EI): m/z (relative intensity) 174.1 (M^+ , 100), 159.0 (37), 143.1 (54), 128.0 (35), 91.0 (20).

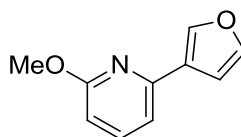
3-(4-(Trifluoromethyl)phenyl)furan (Table 6, entry 1)²⁴

Eluents (Ethyl acetate: Hexane= 1: 20, R_f = 0.80) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 6.73 (d, J = 0.8 Hz, 1H), 7.52 (dd, J =1.6 Hz, 1.6 Hz, 1H), 7.58 (d, J = 8.0 Hz, 2H), 7.63 (d, J = 8.4 Hz, 2H), 7.80 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ ; ^{19}F NMR (376 MHz, CDCl_3) δ -62.5; MS (EI): m/z (relative intensity) 212.0 (M^+ , 100), 183.0 (40), 164.0 (15), 133.0 (29), 115.0 (76).

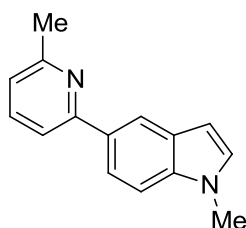
2-(Furan-3-yl)-6-methylpyridine (Table 6, entry 2)



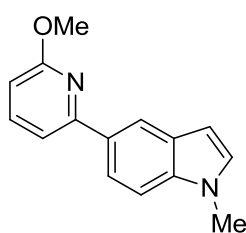
Eluents (Ethyl acetate: Hexane= 1: 9, R_f = 0.35) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 2.56 (s, 3H), 6.88 (d, J = 1.2 Hz, 1H), 6.99 (d, J = 7.6 Hz, 1H), 7.24 (d, J = 7.6 Hz, 1H), 7.47 (dd, J = 1.8 Hz, 1.6 Hz, 1H), 7.54 (t, J = 7.6 Hz, 1H), 8.02 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 24.5, 108.7, 117.1, 121.2, 127.2, 136.7, 141.1, 143.6, 151.1, 158.4 ; MS (EI): m/z (relative intensity) 159.0 (M^+ , 100), 130.0 (100), 118.0 (4), 103.0 (13), 77.0 (17); HRMS: calcd. for $\text{C}_{10}\text{H}_{10}\text{NO}^+$: 160.0757, found 160.0757.

2-(Furan-3-yl)-6-methoxypyridine (Table 6, entry 3)²⁵

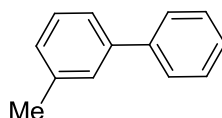
Eluents (Ethyl acetate: Hexane= 1: 9, R_f = 0.50) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 3.98 (s, 3H), 6.61 (d, J = 8.4 Hz, 1H), 6.87 (d, J = 0.8 Hz, 1H), 7.03 (d, J = 7.2 Hz, 1H), 7.48 (dd, J = 1.6 Hz, 1.6 Hz, 1H), 7.54 (t, J = 8.0 Hz, 1H), 8.03 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 53.1, 108.5, 108.6, 112.4, 127.0, 138.9, 141.2, 143.6, 149.2, 163.7; MS (EI): m/z (relative intensity) 175.0 (M^+ , 100), 146.0 (32), 117.0 (49), 90.0 (26), 77.0 (10).

1-Methyl-5-(6-methylpyridin-2-yl)-1*H*-indole (Table 6, entry 4)

Eluents (Ethyl acetate: Hexane= 1: 9, R_f 0.45) was used for flash column chromatography. Yellow solid; m.p.= 129.9-132.2; ^1H NMR (400 MHz, CDCl_3) δ 2.65 (s, 3H), 3.82 (s, 3H), 6.57 (d, J = 2.8 Hz, 1H), 7.03-7.08 (m, 2H), 7.39 (d, J = 8.8 Hz, 1H), 7.56-7.63 (m, 2H), 7.91 (d, J = 8.8 Hz, 1H), 8.27 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 24.8, 32.9, 101.8, 109.3, 117.4, 119.7, 120.5, 121.0, 128.8, 129.4, 131.4, 136.7, 137.2, 158.0, 158.3; MS (EI): m/z (relative intensity) 222.1 (M^+ , 100), 206.1 (6), 180.1 (5), 155.0 (5), 111.0 (3); HRMS: calcd. for $\text{C}_{15}\text{H}_{15}\text{N}_2^+$: 223.1230, found 223.1231.

5-(6-Methoxypyridin-2-yl)-1-methyl-1*H*-indole (Table 6, entry 5)

Eluents (Ethyl acetate: Hexane= 1: 9, R_f 0.30) was used for flash column chromatography. Yellow solid; m.p.= 117.3-120.8; ^1H NMR (400 MHz, CDCl_3) δ 3.83 (s, 3H), 4.09 (s, 3H), 6.58 (d, J = 2.8 Hz, 1H), 6.64 (d, J = 8.0 Hz, 1H), 7.08 (d, J = 2.8 Hz, 1H), 7.37-7.41 (m, 2H), 7.62 (t, J = 8.0 Hz, 1H), 7.98 (d, J = 8.8 Hz, 1H); 8.35 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 32.9, 53.2, 101.8, 107.7, 109.2, 112.4, 119.5, 120.8, 128.8, 129.5, 130.7, 139.0, 163.6; MS (EI): m/z (relative intensity) 238.1 (M^+ , 100), 207.1 (31), 192.0 (11), 155.0 (8), 103.1 (6); HRMS: calcd. for $\text{C}_{15}\text{H}_{15}\text{N}_2\text{O}^+$: 239.1179, found 239.1181.

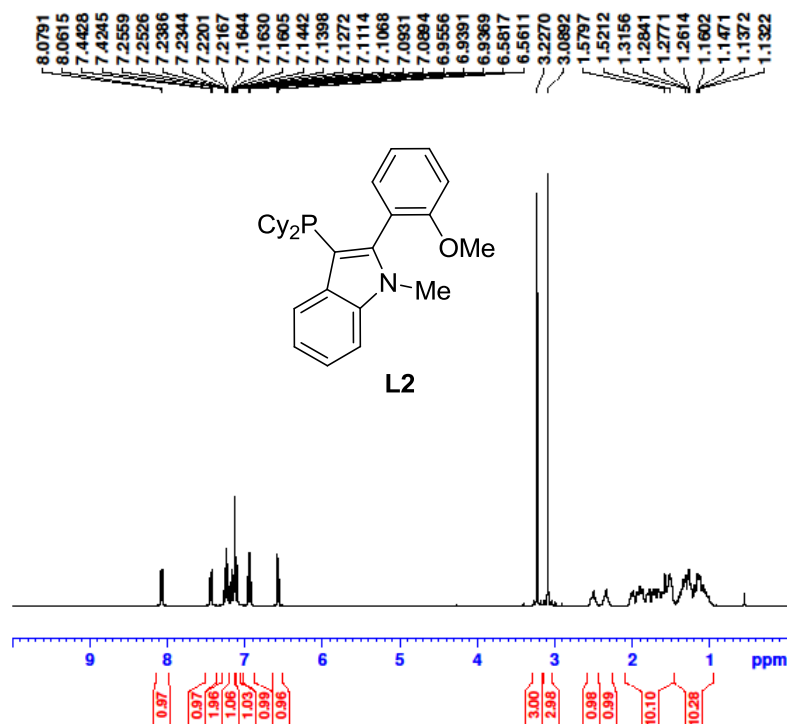
3-Methyl-1,1'-biphenyl (Scheme 3)⁸

Eluents (Hexane, R_f 0.50) was used for flash column chromatography. ^1H NMR (400 MHz, CDCl_3) δ 2.68 (s, 3H), 7.43 (d, J = 7.6 Hz, 1H), 7.59 (t, J = 7.6 Hz, 2H), 7.67–7.70 (m, 4H), 7.87 (d, J = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 21.4, 124.2, 127.1, 127.8, 127.9,

128.4, 128.60, 128.62, 138.2, 141.2, 141.3; MS (EI): m/z (relative intensity) 168.1 (M^+ , 100), 152.0 (26), 115.0 (10), 82.8 (5), 63.0 (5).

7. ^1H , ^{13}C , ^{19}F , ^{31}P NMR, MS and HRMS spectra

N-Me 3-PCy2 2-(2-methoxyphenyl)indole



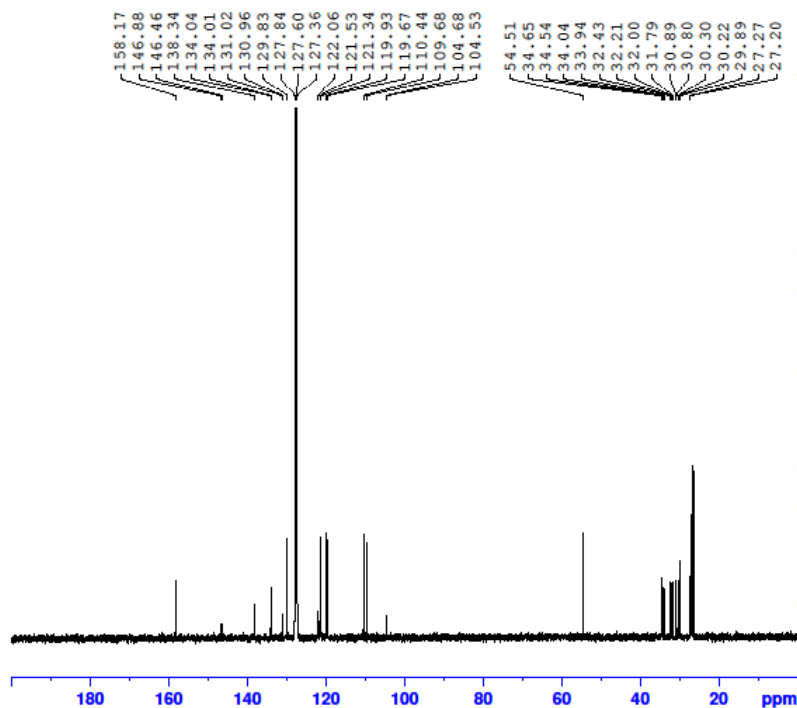
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NAME      test
EXPNO     149
PROCNO    1
Date_     20141113
Time      10.13
INSTRUM   spect
PROBHD    5 mm F4BBO BB-
PULPROG   zgpg30
TD         32768
SOLVENT   CDCl3
NS         32
DS         2
SWH        8012.820 Hz
FIDRES     0.244532 Hz
AQ         2.0447731 sec
RG         36
DW         62.400 usec
DE         6.30 usec
TE         298.4 K
D1         1.00000000 sec
D11        1
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         14.70 usec
PL1        0.00 dB
PL1W       11.88122272 W
SFO1       400.1318007 MHz
SI         32768
SF         400.1300098 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

```

N-Me 3-PCy2 2-(2-methoxyphenyl)indole



```

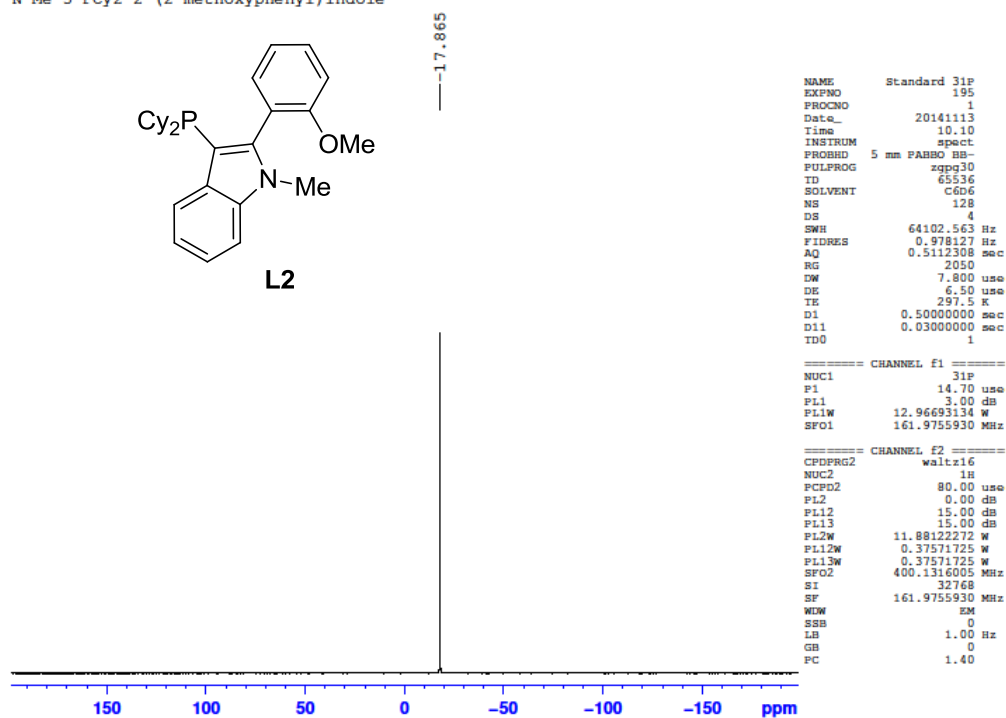
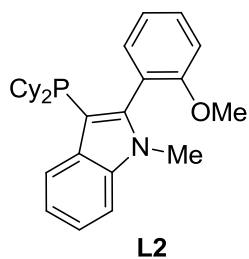
NAME      test-C
EXPNO     93
PROCNO    1
Date_     20141113
Time      10.18
INSTRUM   spect
PROBHD    5 mm F4BBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         81
DS         2
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         322
DW         20.800 usec
DE         6.50 usec
TE         298.5 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         9.50 usec
PL1        2.00 dB
PL1W       58.52175522 W
SFO1       100.6228298 MHz

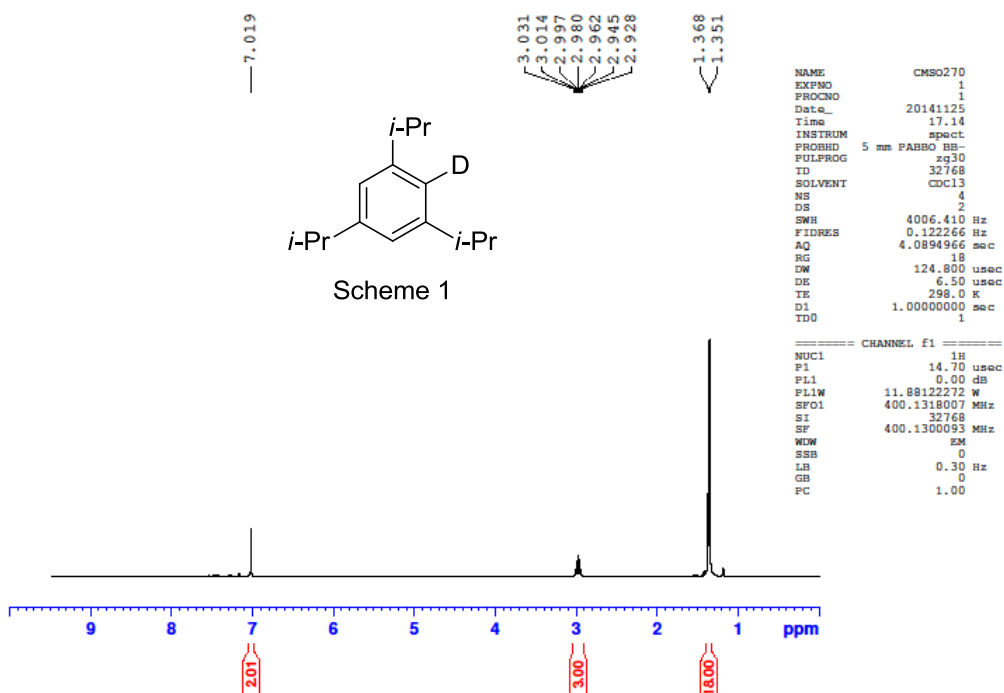
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2        0.00 dB
PL12       15.00 dB
PL13       15.00 dB
PL2W       11.88122272 W
PL12W      0.37571725 W
PL13W      0.37571725 W
SFO2       400.1324008 MHz
SI         32768
SF         100.6127780 MHz
WDW        EM
SSB        0
LB         1.50 Hz
GB         0
PC         1.40

```

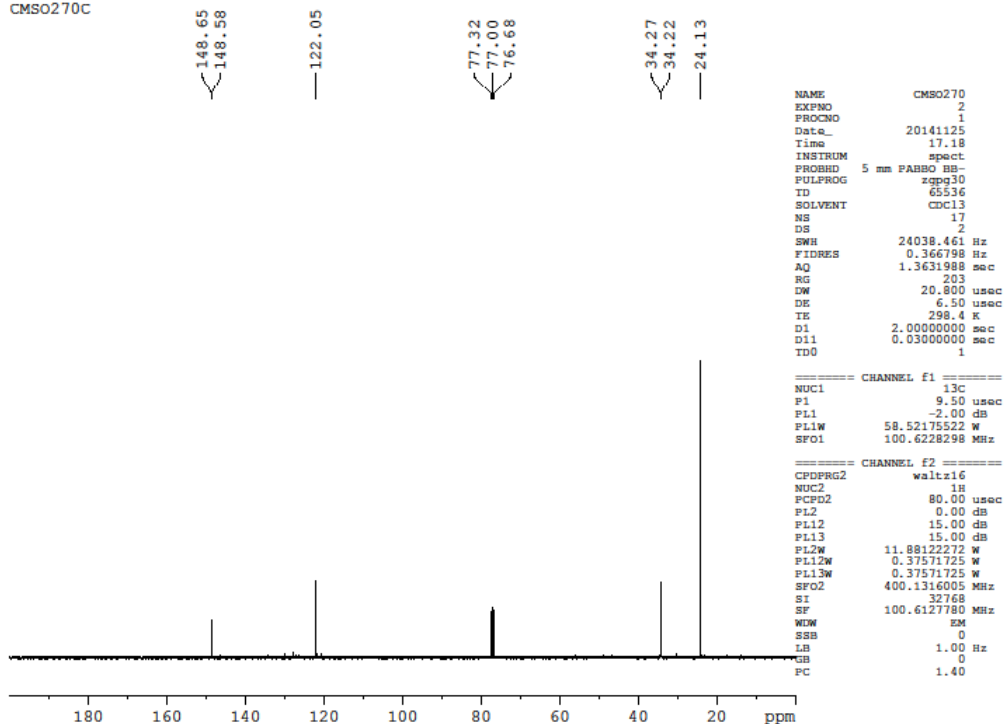
N-Me 3-PCy2 2-(2-methoxyphenyl)indole



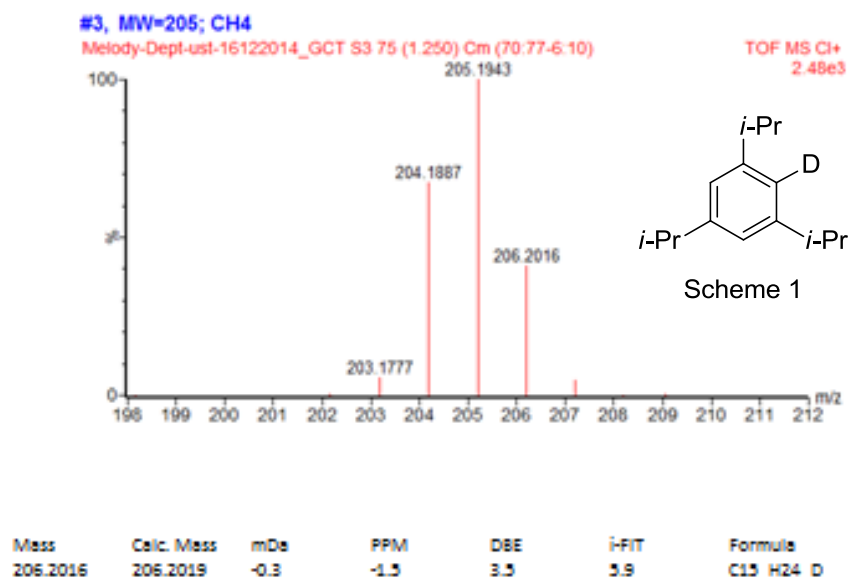
CMSO270H



CMSO270C



HS



CMS0177H

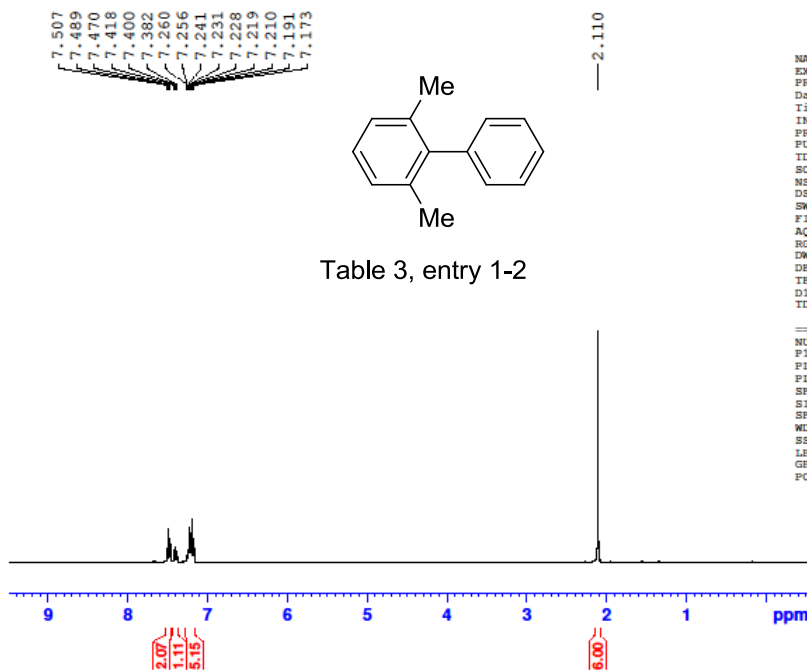


Table 3, entry 1-2

```

NAME          CMS0177
EXPNO         1
PROCNO        1
Date_         20141106
Time          13.08
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            2
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            25.4
DW            124.800 usec
DE            6.50 usec
TE            297.4 K
D1            1.0000000 sec
TD0           1

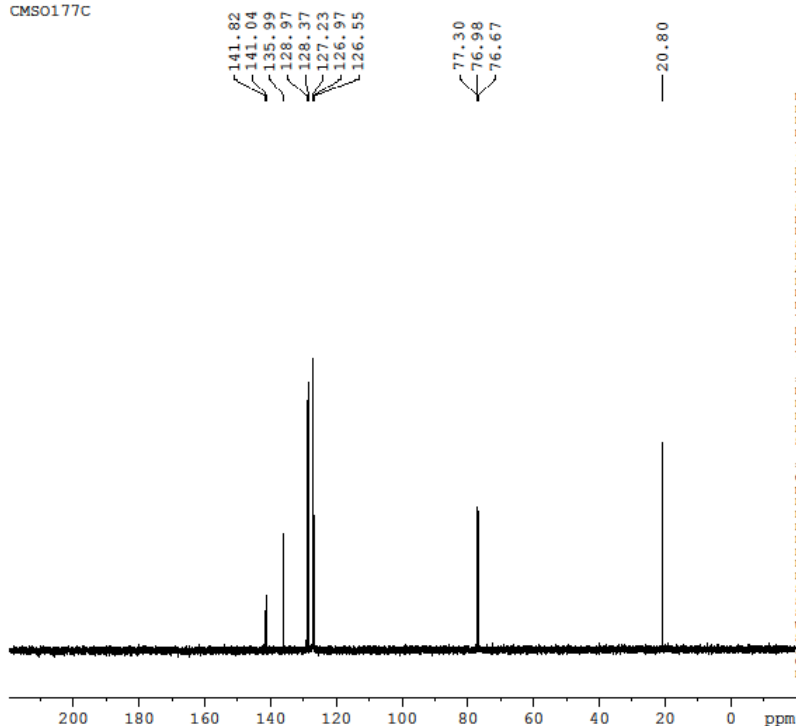
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```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300097 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

CMS0177C



```

NAME          CMS0177
EXPNO         2
PROCNO        1
Date_         20141106
Time          13.09
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            13
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            297.7 K
D1            2.0000000 sec
D11           0.03000000 sec
TD0           1

```

```

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

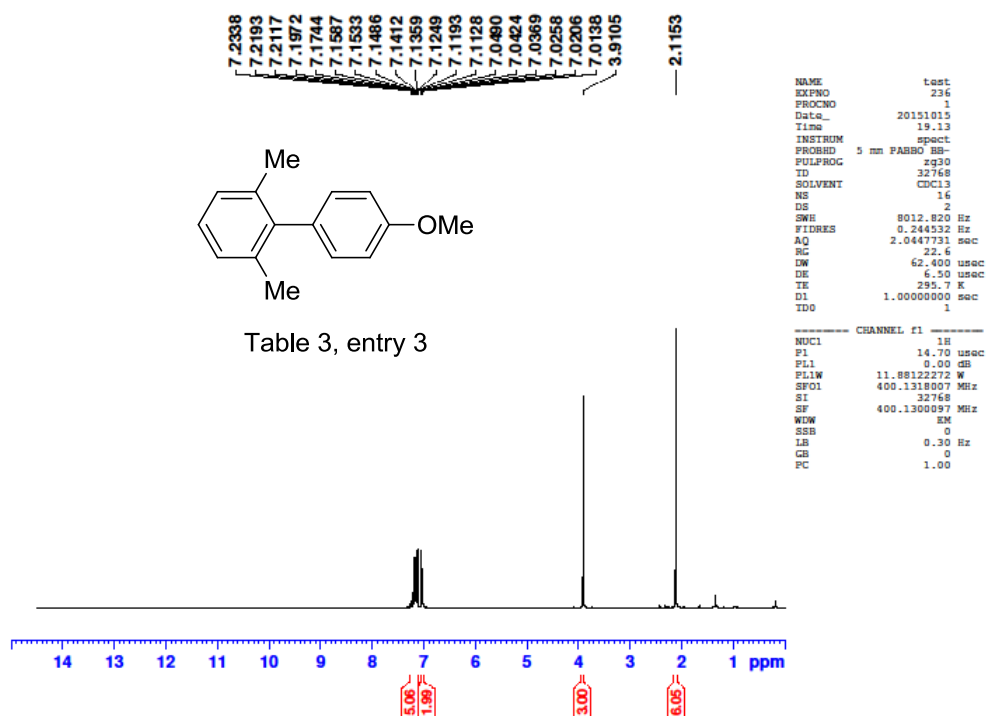
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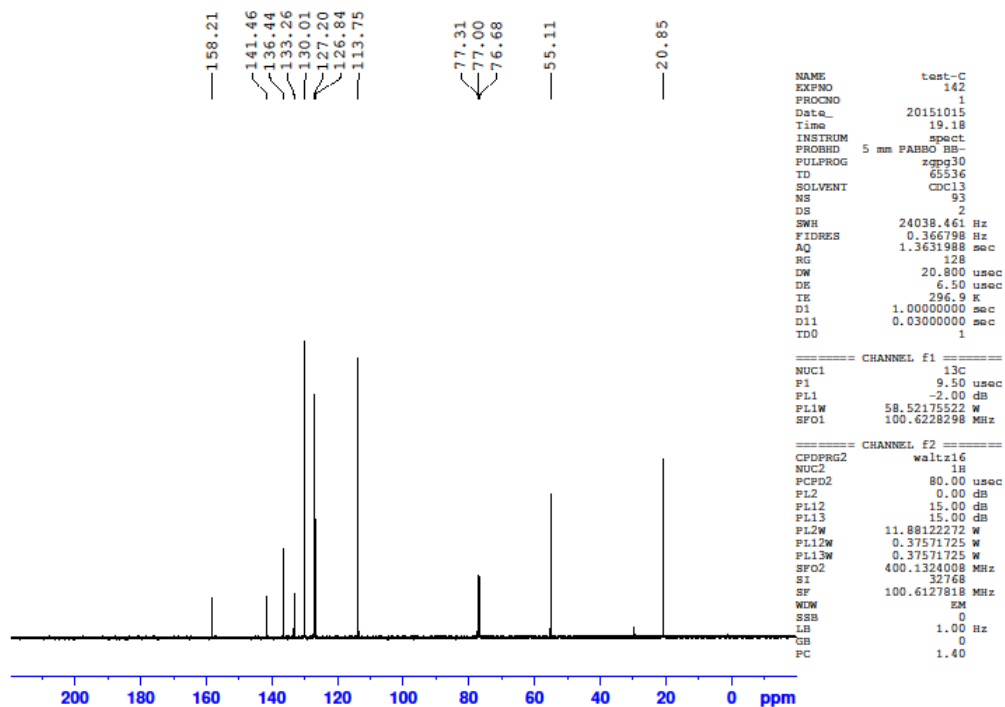
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127817 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```

cms0330



cms0330



CMS0175H

7.489
7.471
7.452
7.400
7.382
7.363
7.216
7.213
7.195
7.011

— 2.399
— 2.073

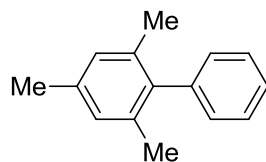
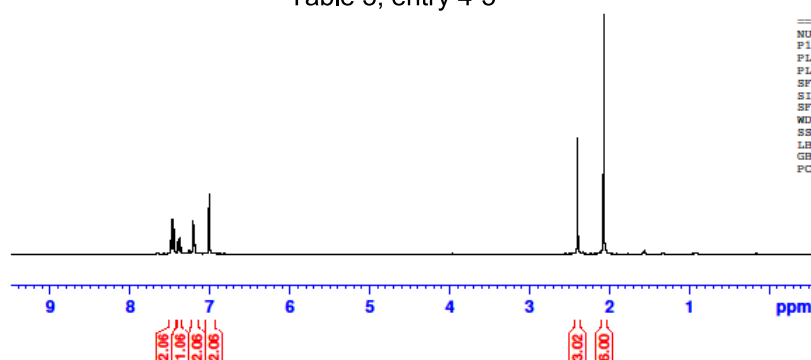


Table 3, entry 4-5



```

NAME          CMS0175
EXPNO         1
PROCNO        1
Date_         20141106
Time          12.43
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            2
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            25.4
DW            124.800 usec
DE            6.50 usec
TE            300.0 K
D1            1.0000000 sec
TD0           1

```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300100 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

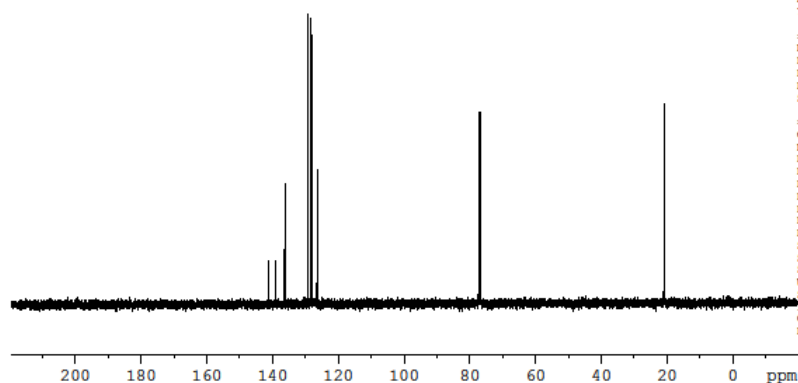
```

CMS0175C

141.05
139.02
136.50
135.52
129.25
128.32
128.01
126.46

77.31
76.99
76.67

20.99
20.70



```

NAME          CMS0175
EXPNO         2
PROCNO        1
Date_         20141106
Time          12.45
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            13
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            297.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

```

```

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127799 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```

CMSO332H

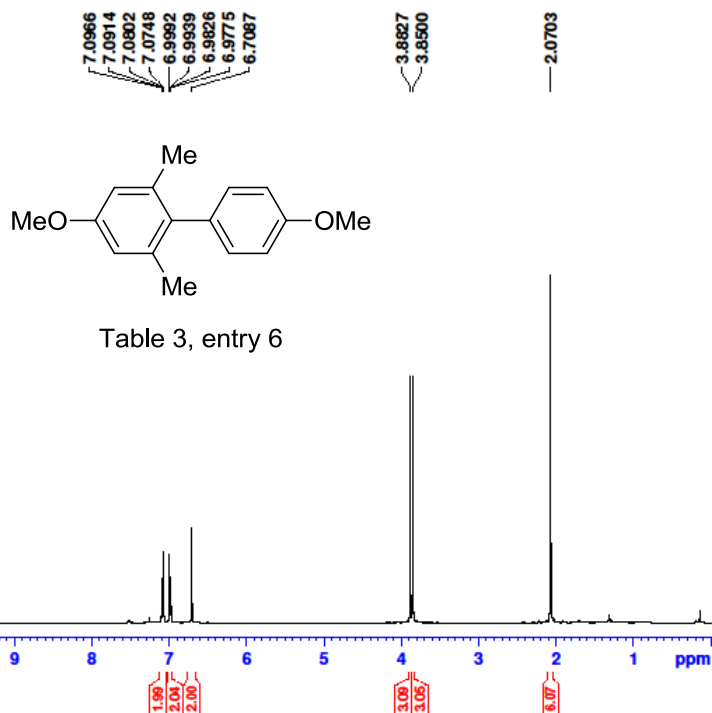


Table 3, entry 6

```

NAME      CMSO332
EXPNO     1
PROCNO    1
Date_     20151015
Time      14.08
INSTRUM    spect
PROBHD     5 mm F4BBO BB-
PULPROG    zgpg30
TD         32768
SOLVENT    CDCl3
NS         16
DS         2
SWH         8012.820 Hz
FIDRES     0.244532 Hz
AQ         2.0447731 sec
RG          25.4
DW         62.400 usec
DE         6.30 usec
TE         296.1 K
D1         1.00000000 sec
D11        1
D10        1

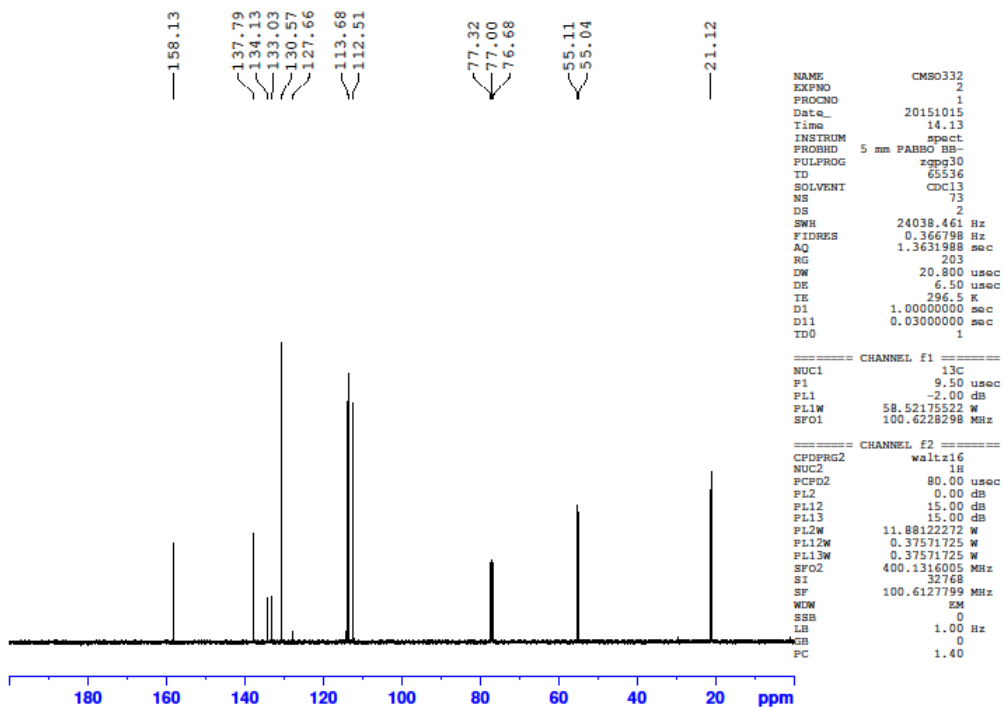
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```

===== CHANNEL f1 =====
NUC1       1H
P1         14.70 usec
PL1        0.00 dB
PL1W       11.88122272 W
SFO1       400.1324008 MHz
SI         32768
SF         400.1300095 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

```

CMSO332C



```

NAME      CMSO332
EXPNO     2
PROCNO    1
Date_     20151015
Time      14.13
INSTRUM    spect
PROBHD     5 mm F4BBO BB-
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         73
DS         2
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG          203
DW         20.800 usec
DE         6.50 usec
TE         296.5 K
D1         1.00000000 sec
D11        0.03000000 sec
D10        1

```

```

===== CHANNEL f1 =====
NUC1       13C
P1         9.50 usec
PL1        -2.00 dB
PL1W       58.52175522 W
SFO1       100.6228298 MHz

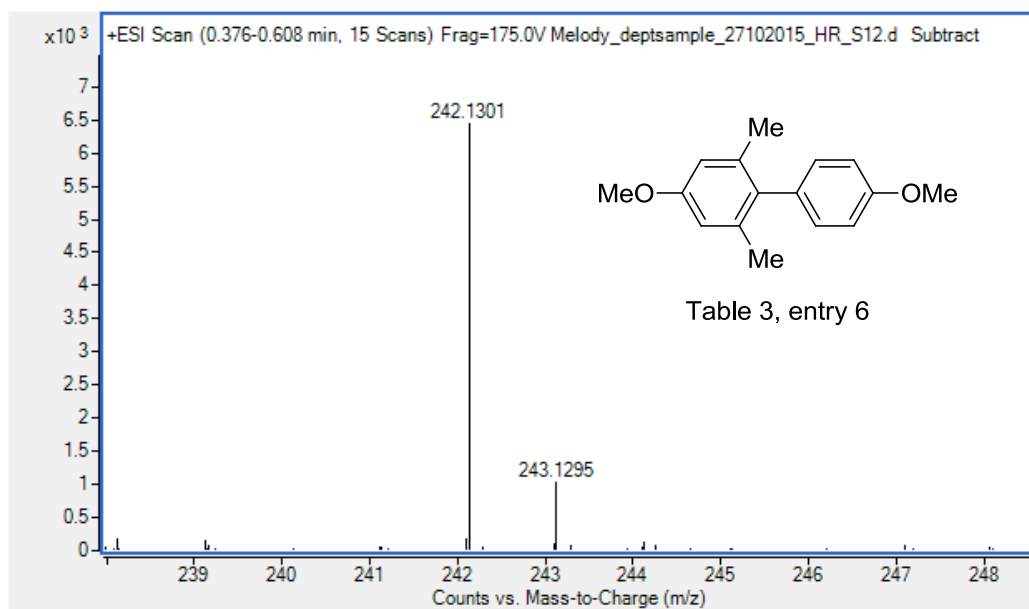
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```

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        0.00 dB
PL12       15.00 dB
PL13       15.00 dB
PL2W       11.88122272 W
PL12W      0.37571725 W
PL13W      0.37571725 W
SFO2       400.1316005 MHz
SI         32768
SF         100.6127799 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```

HS



CMSO335H

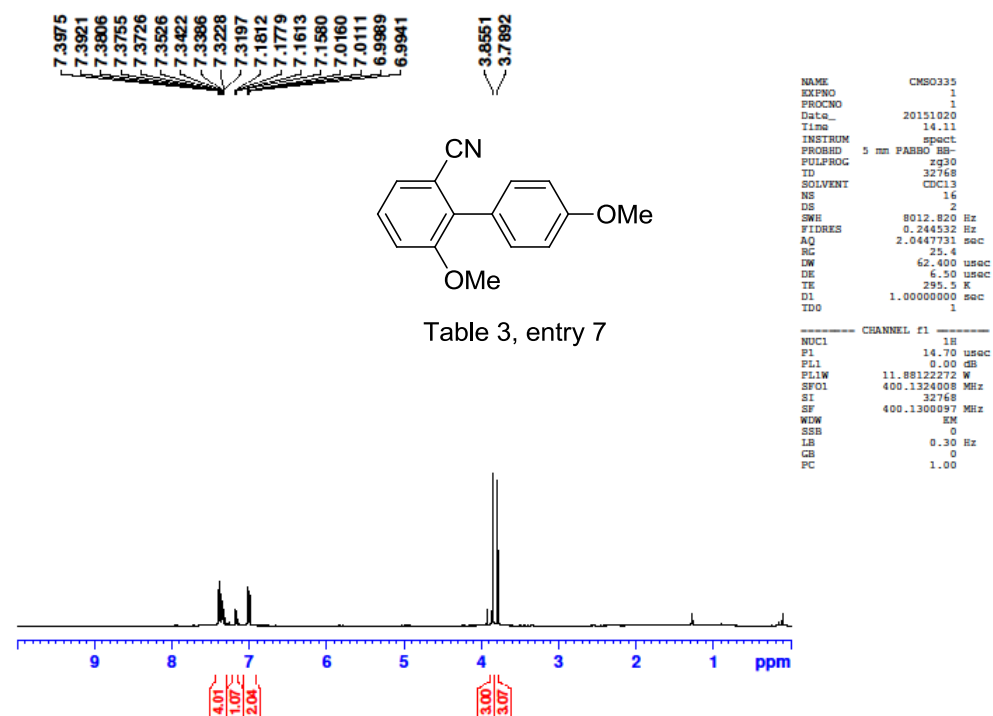
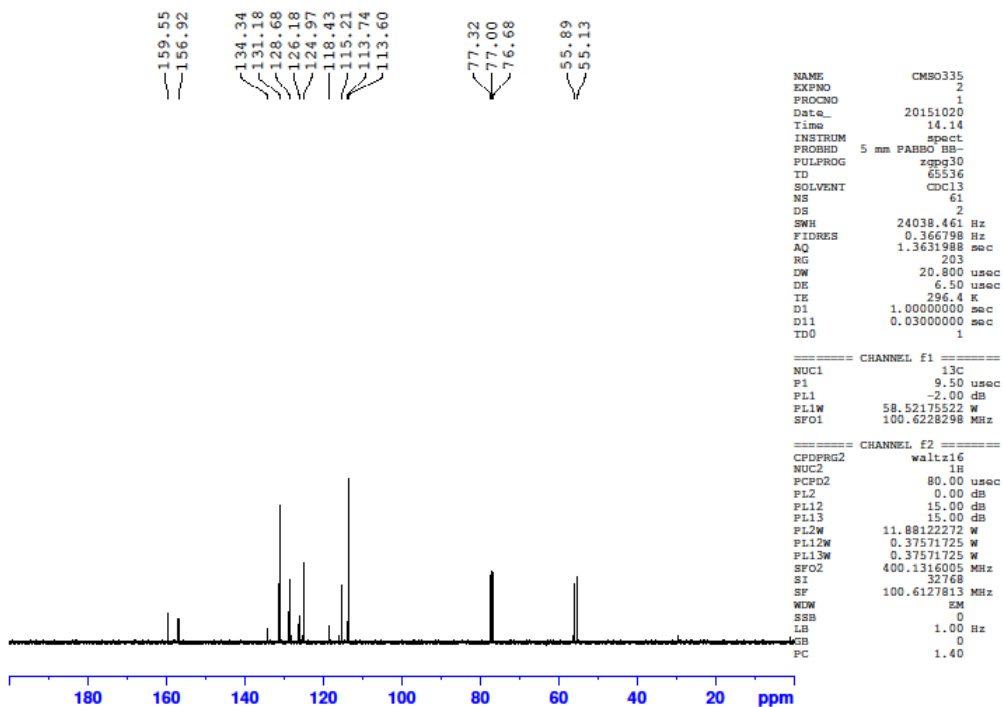
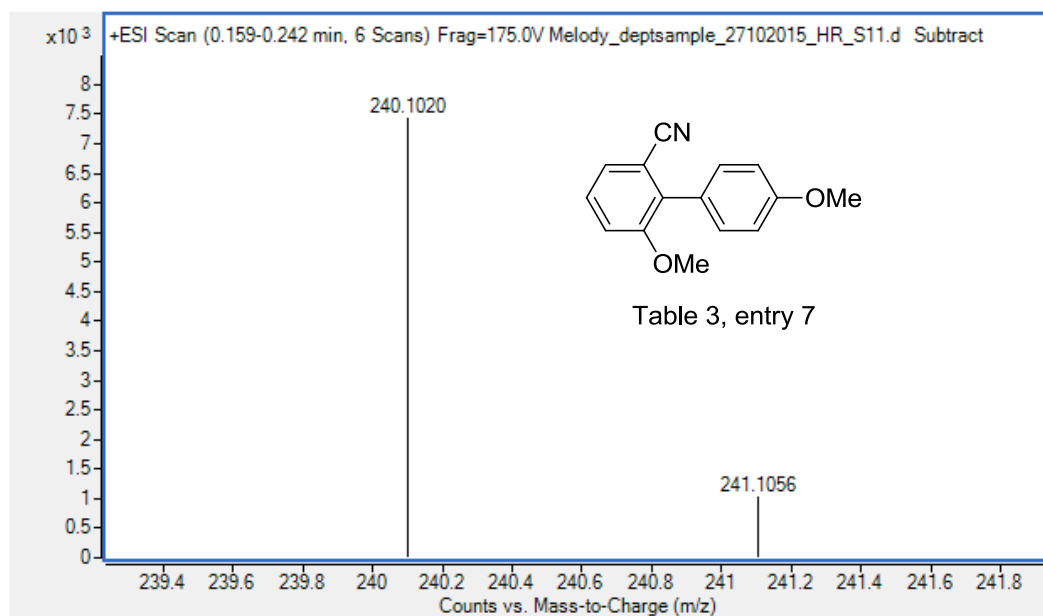


Table 3, entry 7

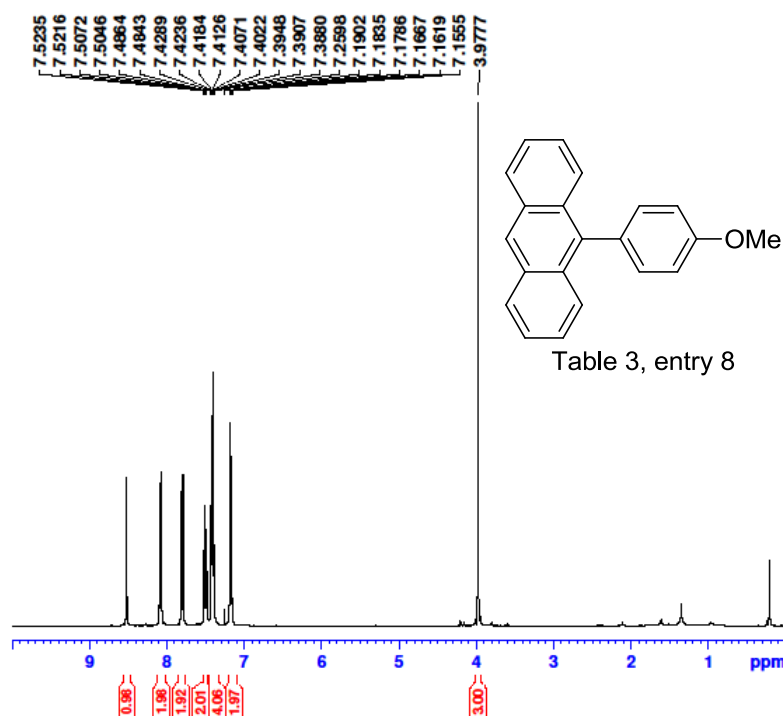
CMSO335C



HS



CMSO314H



```

NAME      CMSO314
EXPNO     1
PROCNO    1
Date_     20151020
Time      14.06
INSTRUM    spect
PROBHD     5 mm F4BBO BB-
PULPROG    zgpg30
TD         32768
SOLVENT    CDCl3
NS         16
DS         2
SWH        8012.820 Hz
FIDRES     0.244532 Hz
AQ         2.0447731 sec
RG         25.4
DW         62.400 usec
DE         6.30 usec
TE         295.5 K
D1         1.00000000 sec
D11        1
TD0        1

```

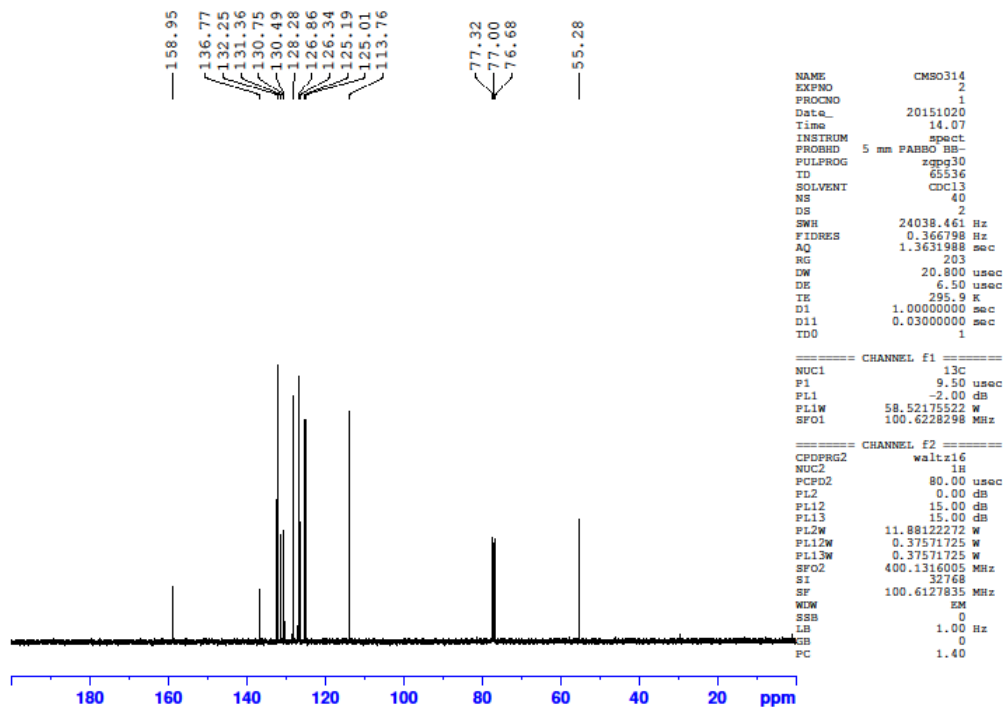
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===== CHANNEL f1 =====
NUC1       1H
P1         14.70 usec
PL1        0.00 dB
PL1W       11.88122272 W
SFO1       400.1324008 MHz
SI         32768
SF         400.1300095 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

```

Table 3, entry 8

CMSO314C



```

NAME      CMSO314
EXPNO     2
PROCNO    1
Date_     20151020
Time      14.07
INSTRUM    spect
PROBHD     5 mm F4BBO BB-
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         40
DS         2
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         203
DW         20.800 usec
DE         6.50 usec
TE         295.9 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1

```

```

===== CHANNEL f1 =====
NUC1       13C
P1         9.50 usec
PL1        -2.00 dB
PL1W       58.52175522 W
SFO1       100.6228298 MHz

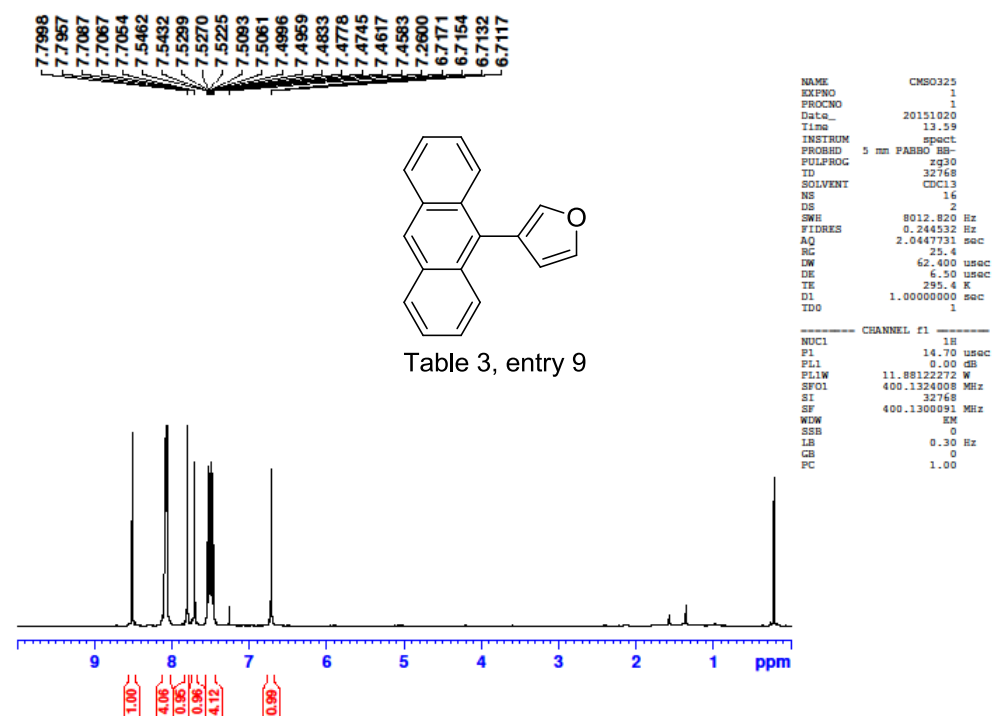
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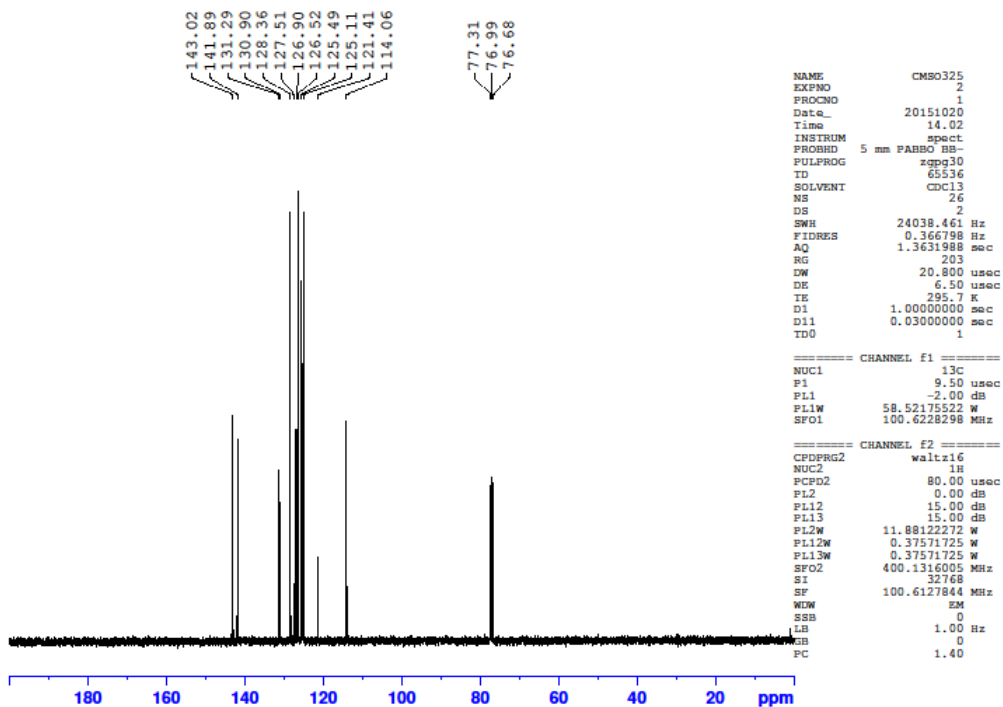
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        0.00 dB
PL12       15.00 dB
PL13       15.00 dB
PL2W       11.88122272 W
PL12W      0.37571725 W
PL13W      0.37571725 W
SFO2       400.1316005 MHz
SI         32768
SF         100.6127835 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```

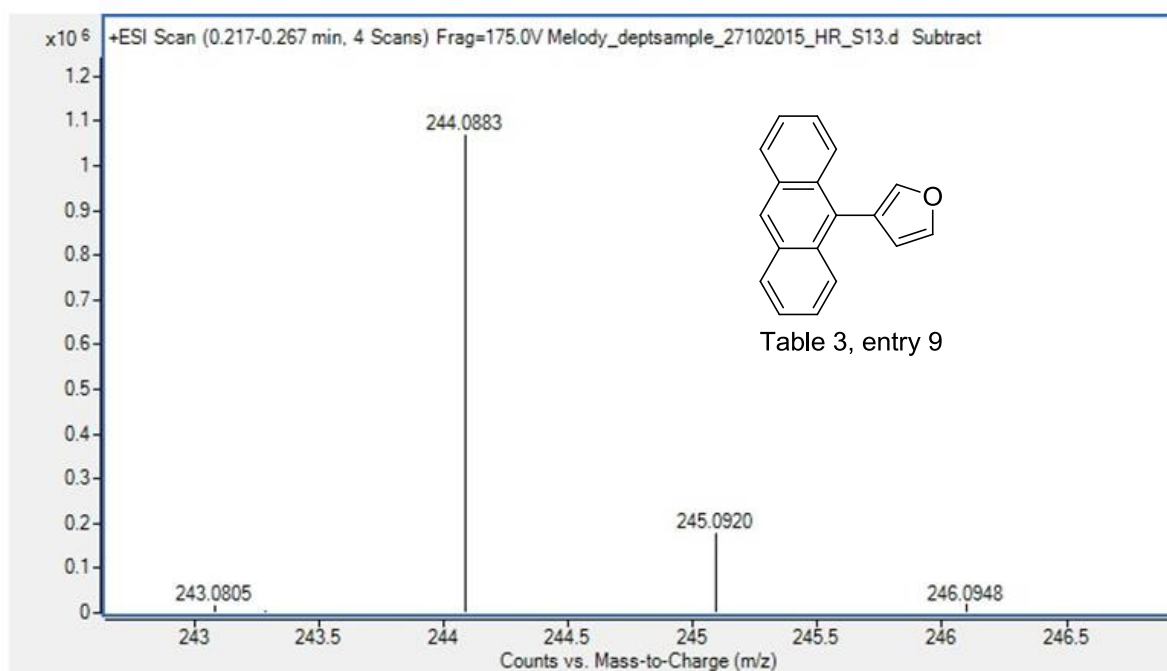

CMSO325H

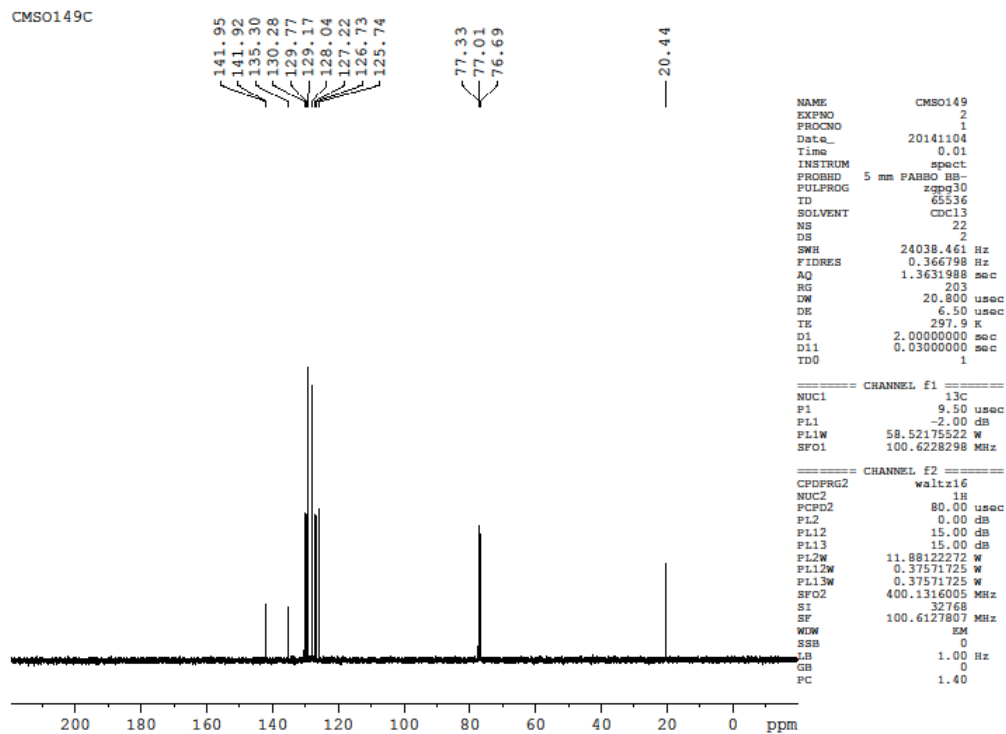
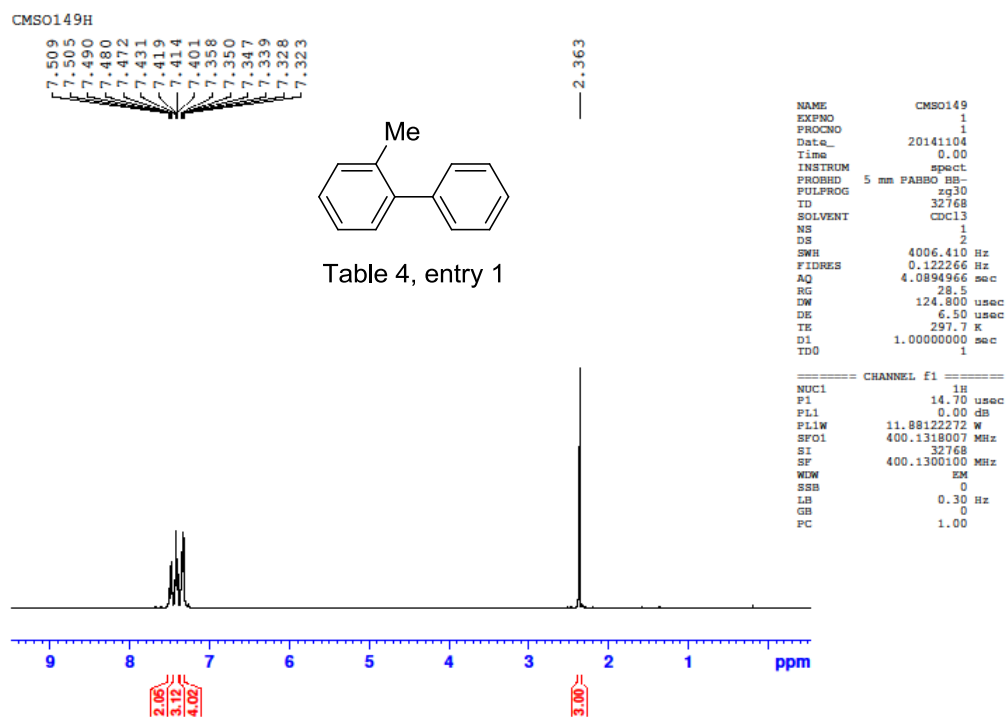


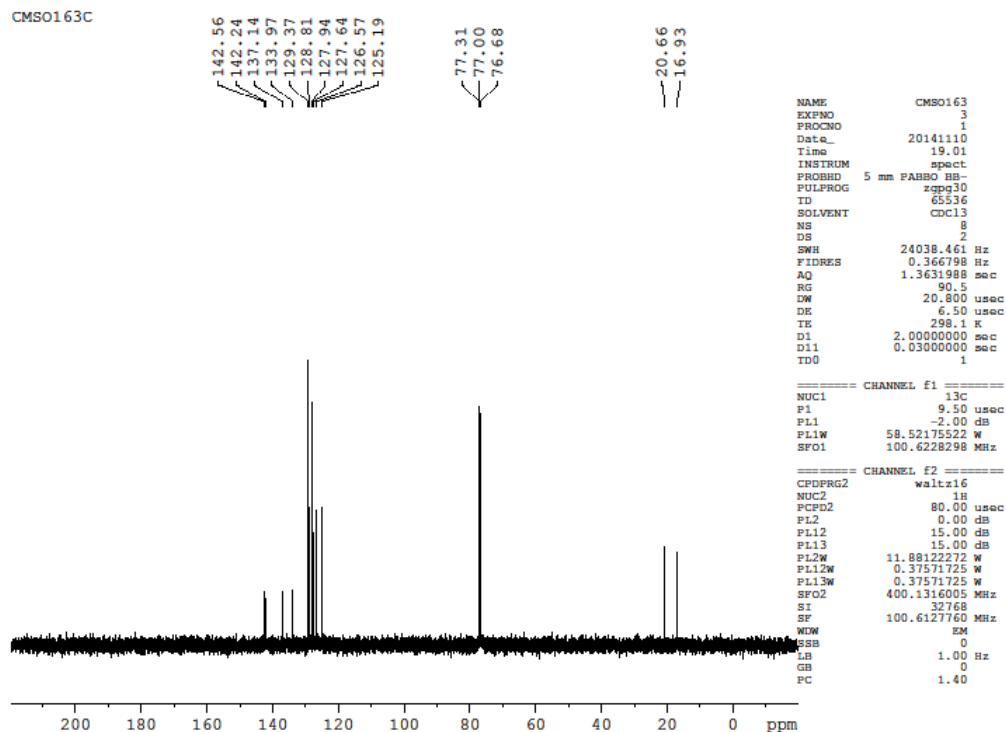
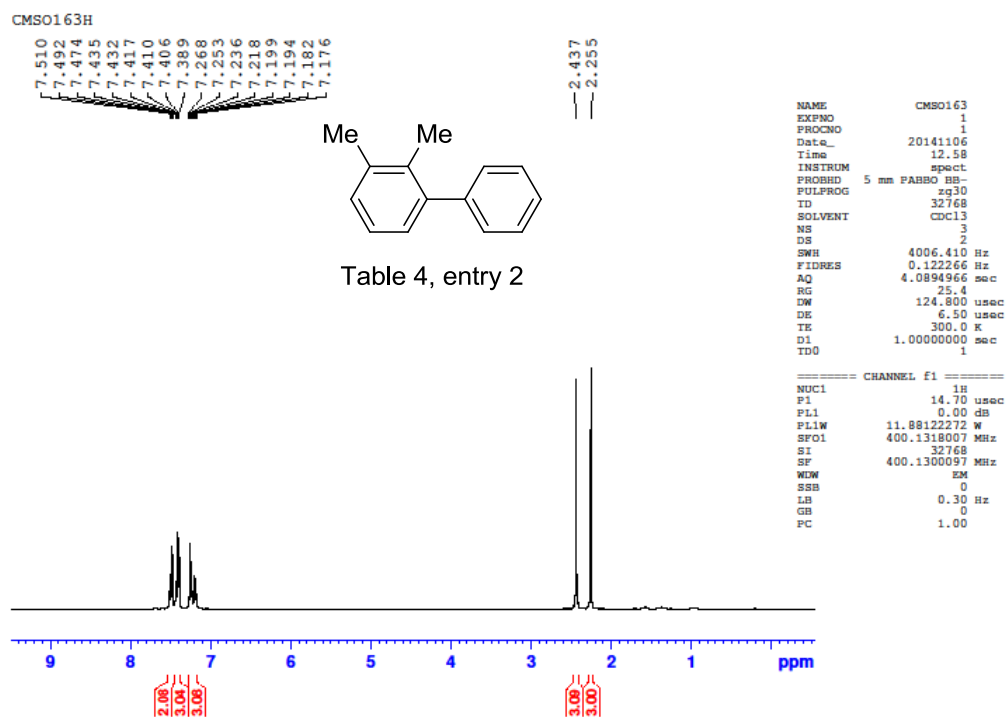
CMSO325C



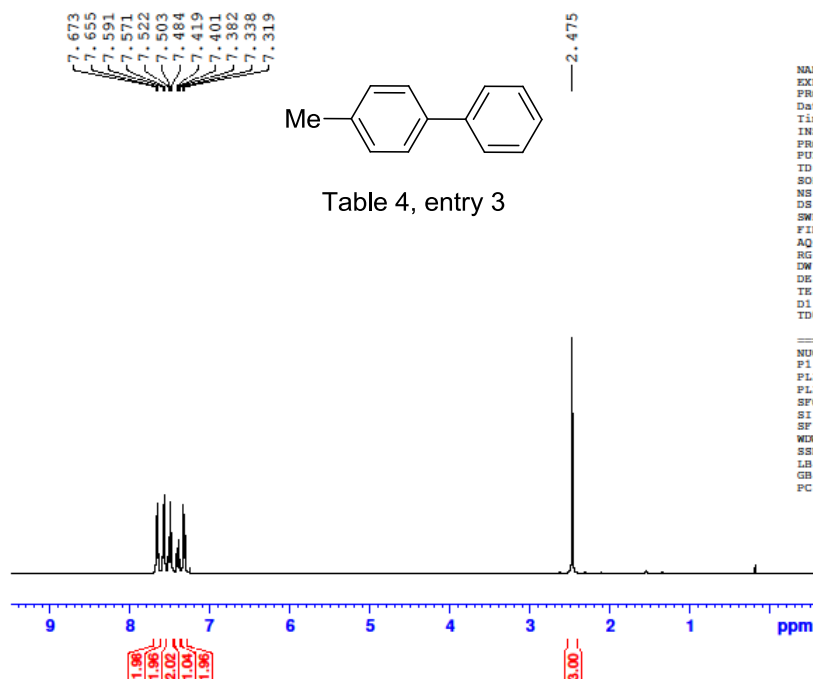
HS







CMS0128H



```

NAME          CMS0128
EXPNO         1
PROCNO        1
Date_         20141101
Time          2.29
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            12
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            25.4
DW            124.800 usec
DE            6.50 usec
TE            297.4 K
D1            1.0000000 sec
TD0           1

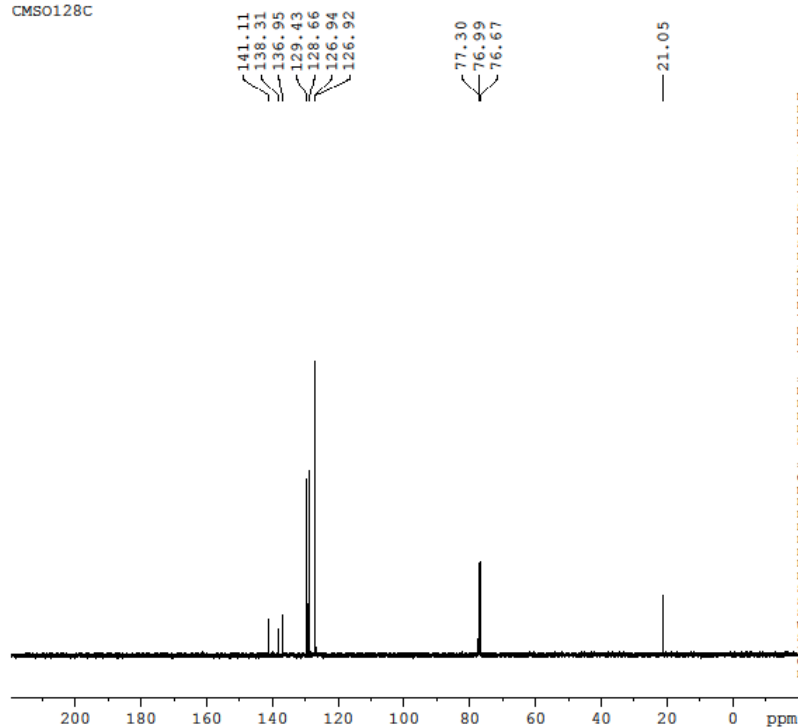
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300100 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

CMS0128C



```

NAME          CMS0128
EXPNO         2
PROCNO        1
Date_         20141101
Time          2.32
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

```

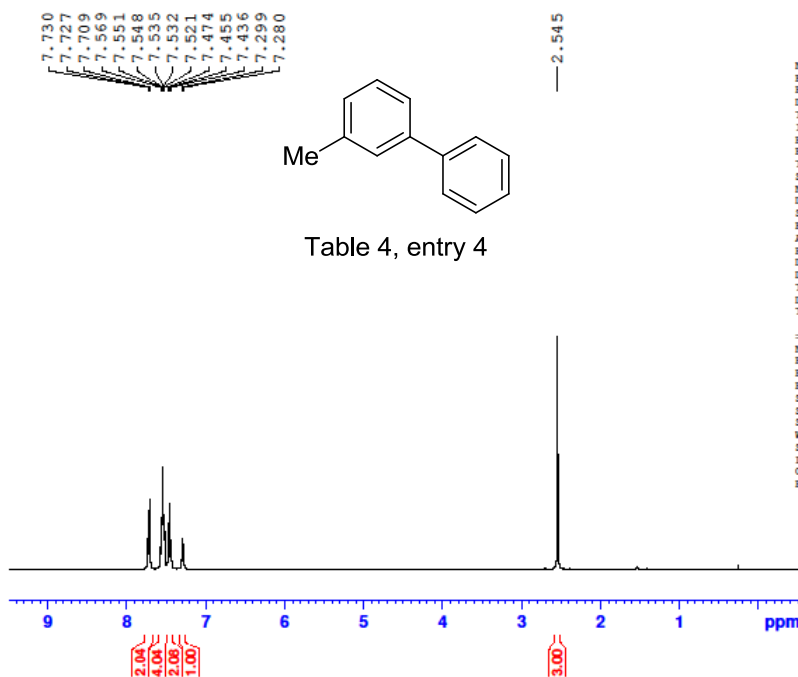
```

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127835 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```

CMS0138H



```

NAME          CMS0138
EXPNO         1
PROCNO        1
Date_         20141103
Time          12.07
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            4
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            25.4
DW            124.800 usec
DE            6.50 usec
TE            297.7 K
D1            1.0000000 sec
D11           1
TD0           1

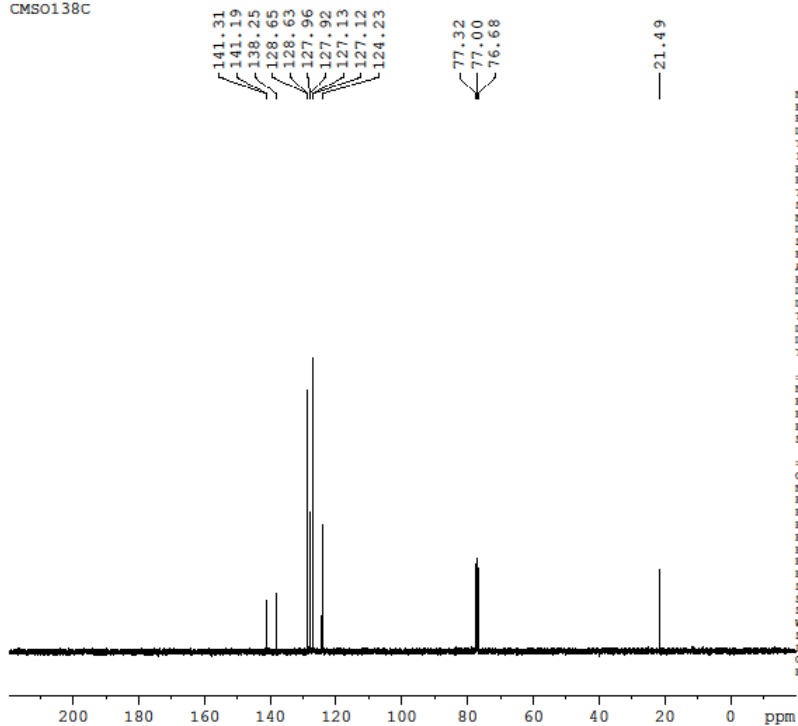
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300097 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

CMS0138C



```

NAME          CMS0138
EXPNO         2
PROCNO        1
Date_         20141103
Time          12.09
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            298.0 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1

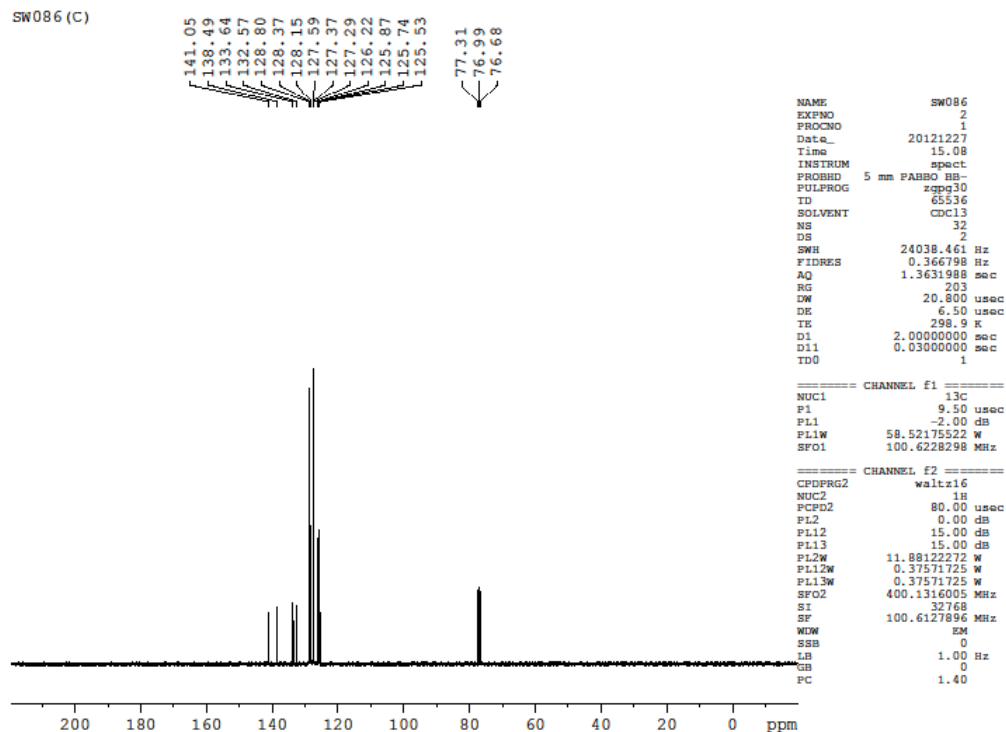
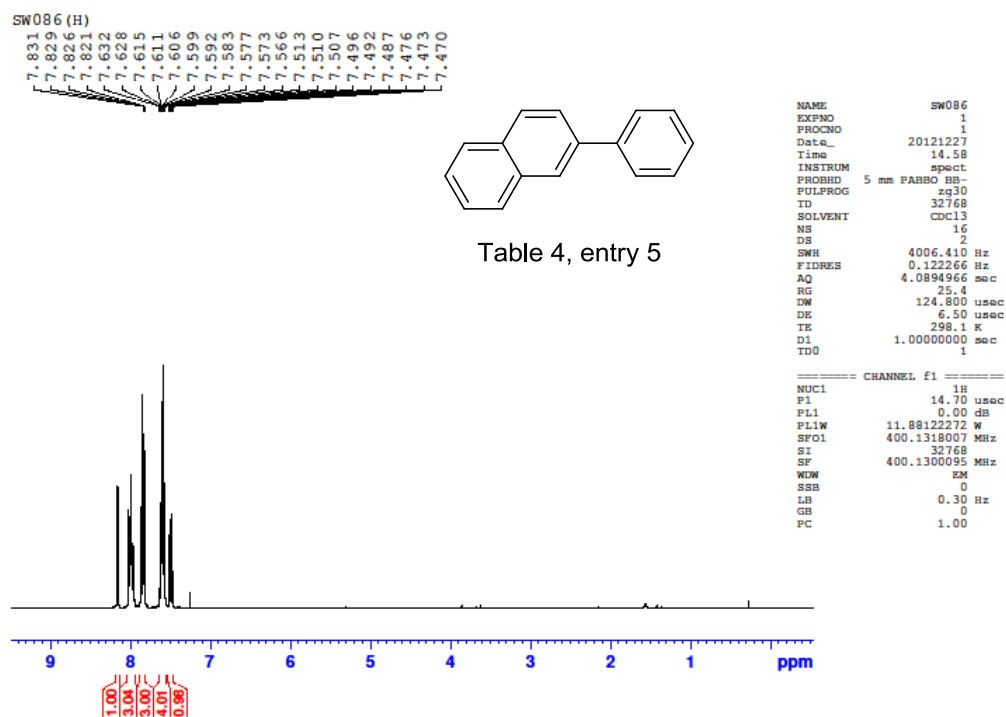
```

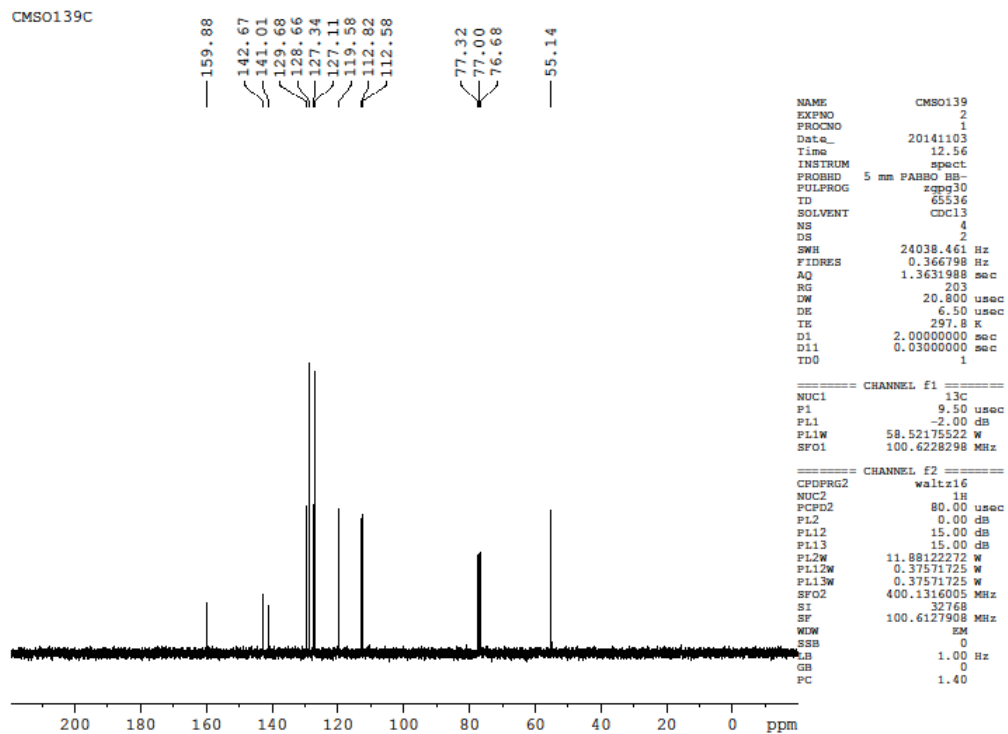
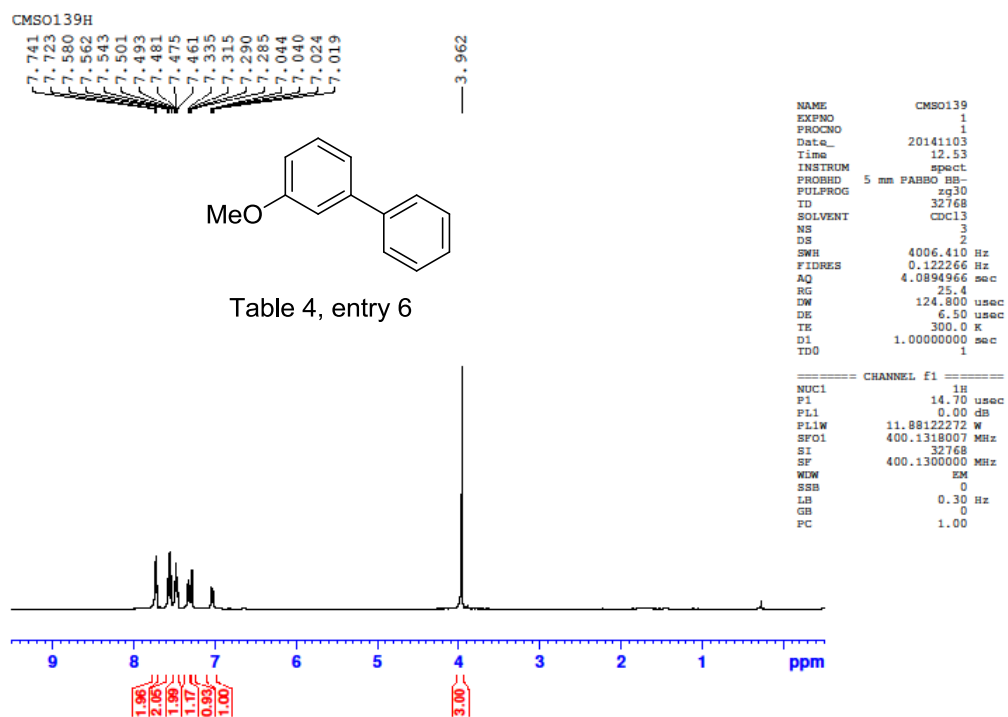
```

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127882 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```





CMS0127H

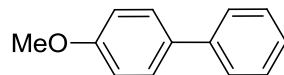
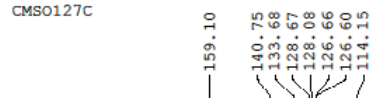


Table 4, entry 7

NAME CMS0127
EXPNO 1
PROCNO 1
Date_ 20141101
Time 2.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4006.410 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 25.4
DW 124.800 usec
DE 6.50 usec
TE 297.5 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1318007 MHz
SI 32768
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CMS0127C



NAME CMS0127
EXPNO 2
PROCNO 1
Date_ 20141101
Time 2.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127849 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CMS0141H

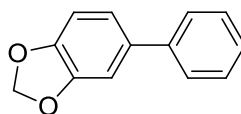


Table 4, entry 8

```

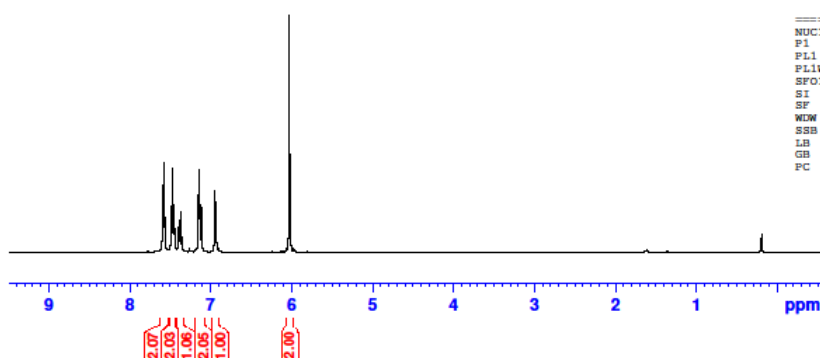
NAME          CMS0141
EXPNO         1
PROCNO        1
Date_         20141103
Time          12.59
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            2
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            25.4
DW            124.800 usec
DE            6.50 usec
TE            297.8 K
D1            1.0000000 sec
TD0           1

```

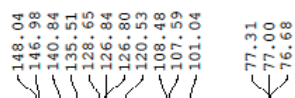
```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300095 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```



CMS0141C



```

NAME          CMS0141
EXPNO         2
PROCNO        1
Date_         20141103
Time          13.00
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            6
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            298.1 K
D1            2.0000000 sec
D11           0.03000000 sec
TD0           1

```

```

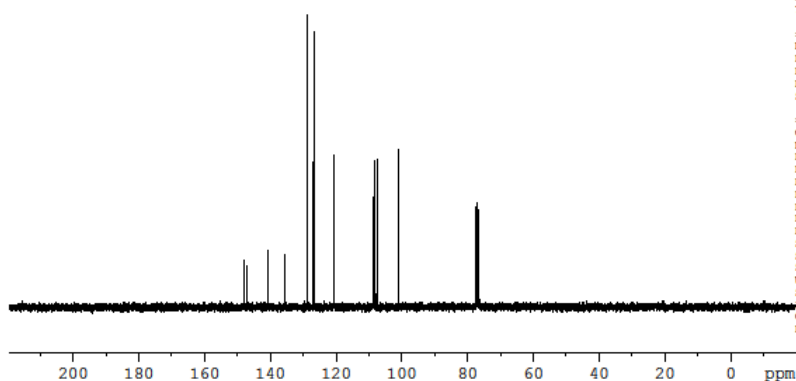
===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

```

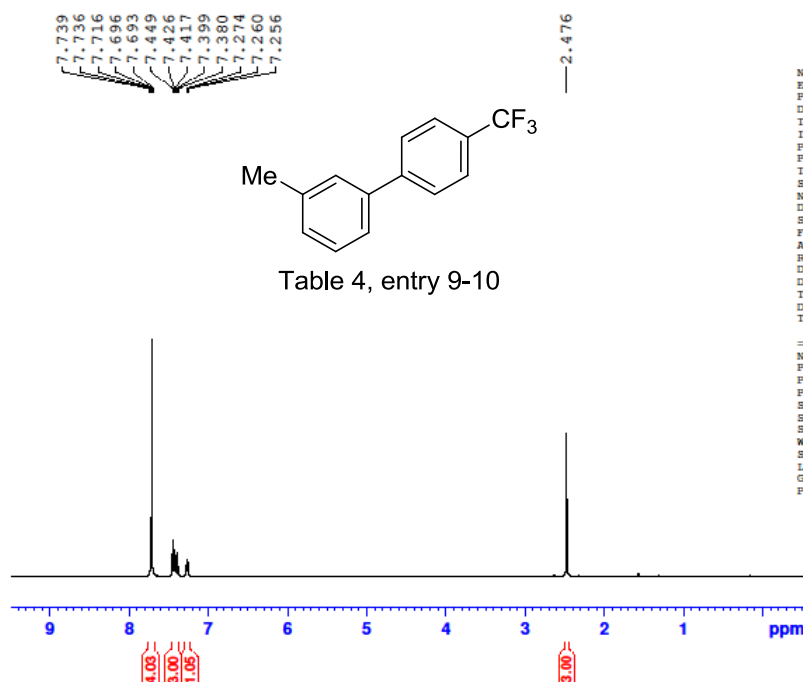
```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127859 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```



CMS0157H



```

NAME          CMS0157
EXPNO         1
PROCNO        1
Date_         20141106
Time          13.38
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            9
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            25.4
DW            124.800 usec
DE            6.50 usec
TE            297.3 K
D1            1.00000000 sec
D11           1
TD0           1

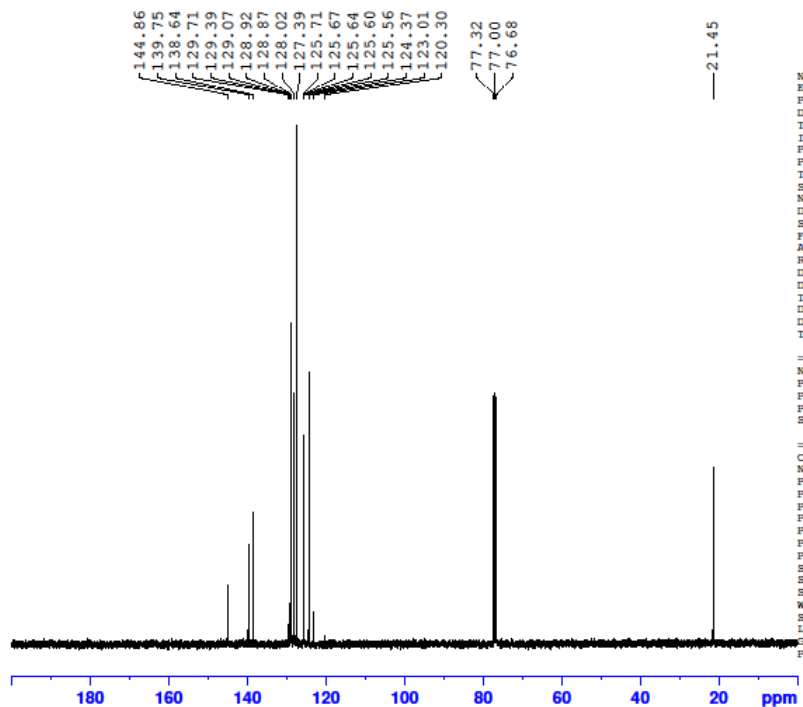
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300096 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

CMS0157C



```

NAME          CMS0157
EXPNO         2
PROCNO        1
Date_         20141106
Time          13.44
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            64
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            298.7 K
D1            2.00000000 sec
D11           0.03000000 sec
D11           1
TD0           1

```

```

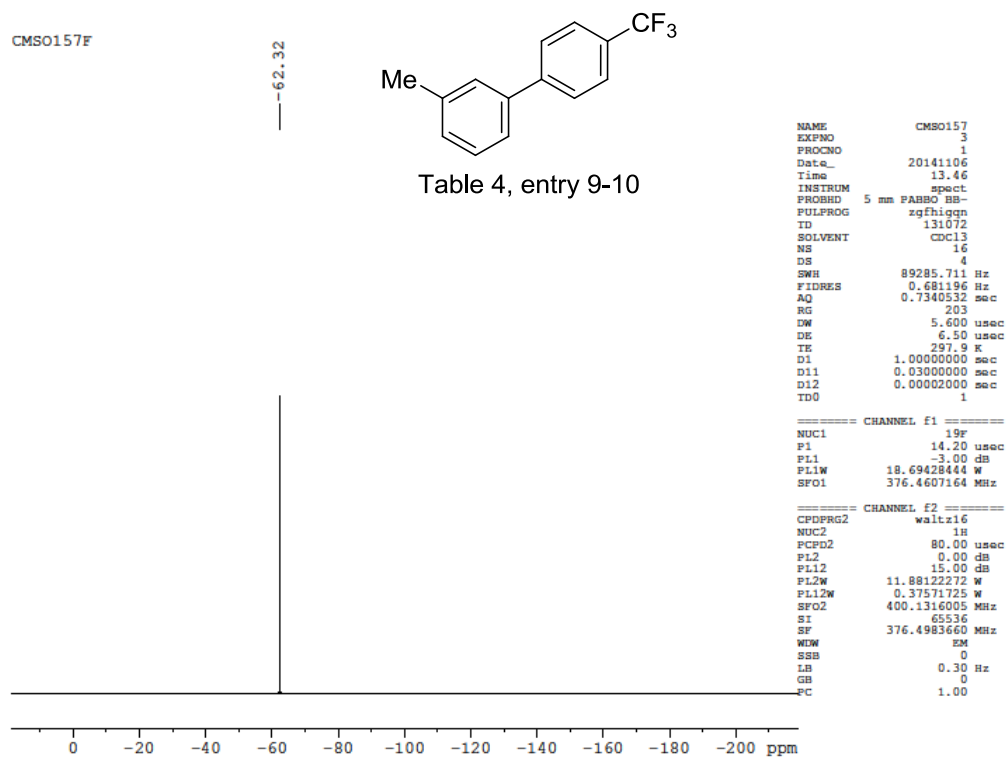
===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

```

```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127739 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```



CMS0156H

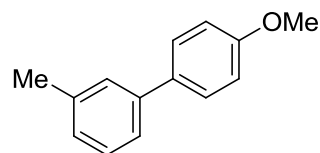
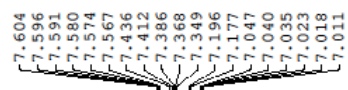
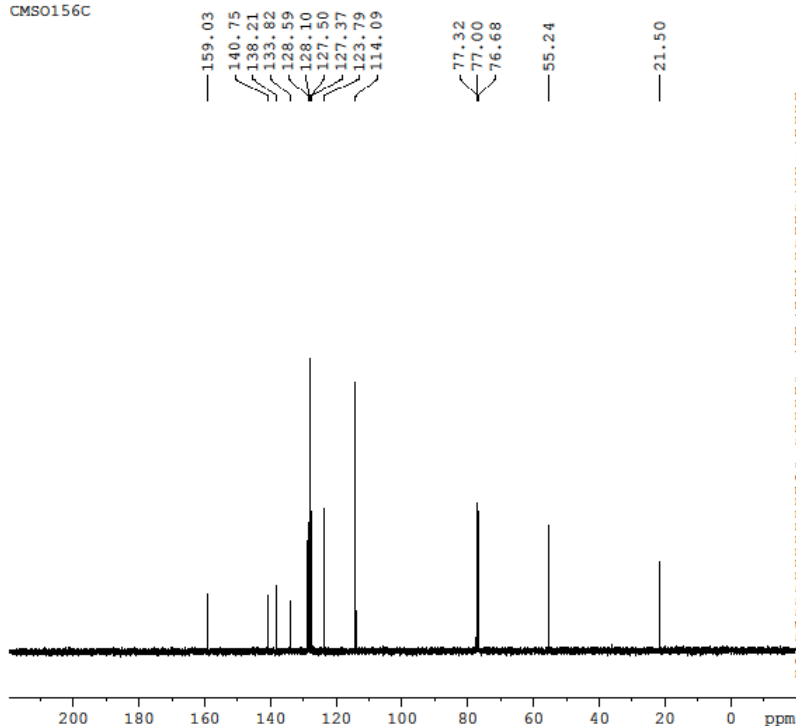


Table 4, entry 11-12

NAME CMS0156
 EXPNO 1
 PROCNO 1
 Date_ 20141106
 Time 13.32
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 10
 DS 2
 SWH 4006.410 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 25.4
 DW 124.800 usec
 DE 6.50 usec
 TE 297.3 K
 D1 1.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.70 usec
 PL1 0.00 dB
 PL1W 11.88122272 W
 SFO1 400.1318007 MHz
 SI 32768
 SF 400.1300096 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

CMS0156C

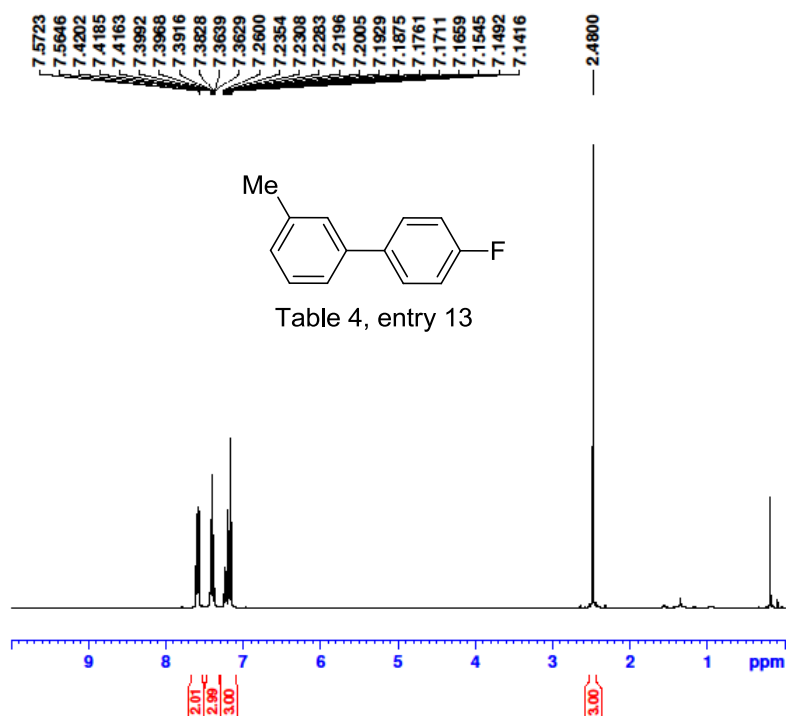


NAME CMS0156
 EXPNO 2
 PROCNO 1
 Date_ 20141106
 Time 13.34
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 17
 DS 2
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.50 usec
 PL1 -2.00 dB
 PL1W 58.52175522 W
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.00 dB
 PL13 15.00 dB
 PL2W 11.88122272 W
 PL12W 0.37571725 W
 PL13W 0.37571725 W
 SFO2 400.1316005 MHz
 SI 32768
 SF 100.6127819 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

CMSO352H



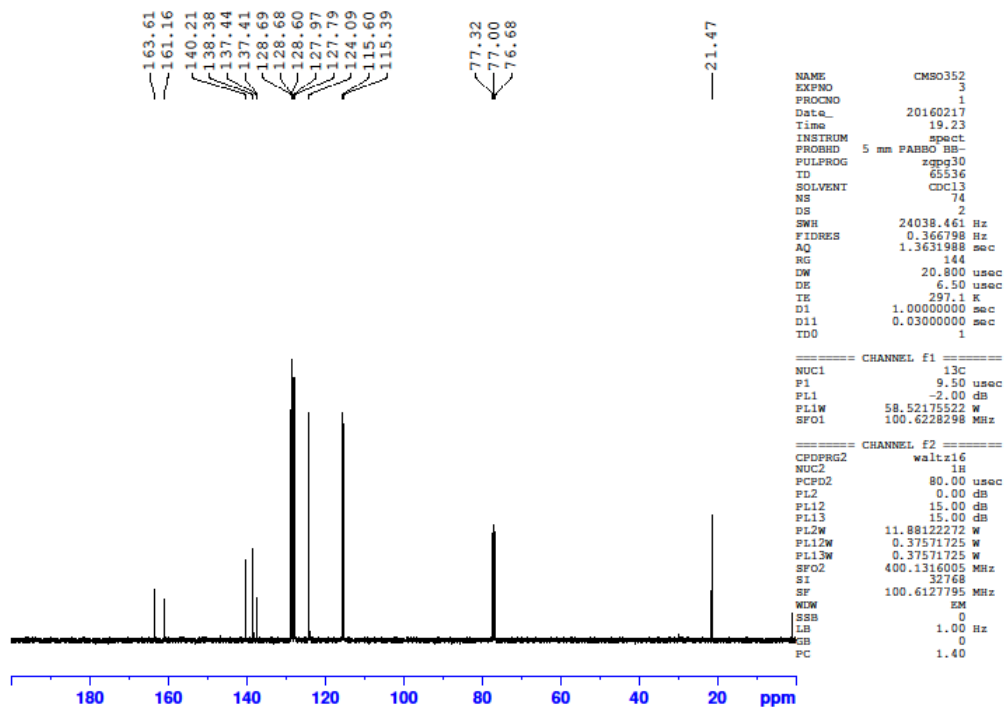
```

NAME      CMSO352
EXPNO     1
PROCNO    1
Date_     20160217
Time      19.14
INSTRUM   spect
PROBHD    5 mm F4BBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8012.820 Hz
FIDRES     0.244532 Hz
AQ         2.0447731 sec
RG         25.4
DW         62.400 usec
DE         6.30 usec
TE         296.3 K
D1         1.00000000 sec
D11        1
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         14.70 usec
PL1        0.00 dB
PL1W       11.88122272 W
SFO1       400.1324008 MHz
SI         32768
SF         400.1300095 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

```

CMSO352C



```

NAME      CMSO352
EXPNO     3
PROCNO    1
Date_     20160217
Time      19.23
INSTRUM   spect
PROBHD    5 mm F4BBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         74
DS         2
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         144
DW         20.800 usec
DE         6.50 usec
TE         297.1 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         9.50 usec
PL1        -2.00 dB
PL1W       58.52175522 W
SFO1       100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2        0.00 dB
PL12      15.00 dB
PL13      15.00 dB
PL2W       11.88122272 W
PL12W     0.37571725 W
PL13W     0.37571725 W
SFO2       400.1316005 MHz
SI         32768
SF         100.6127795 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```

CMSO352F

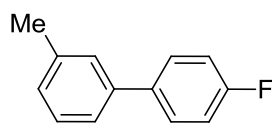
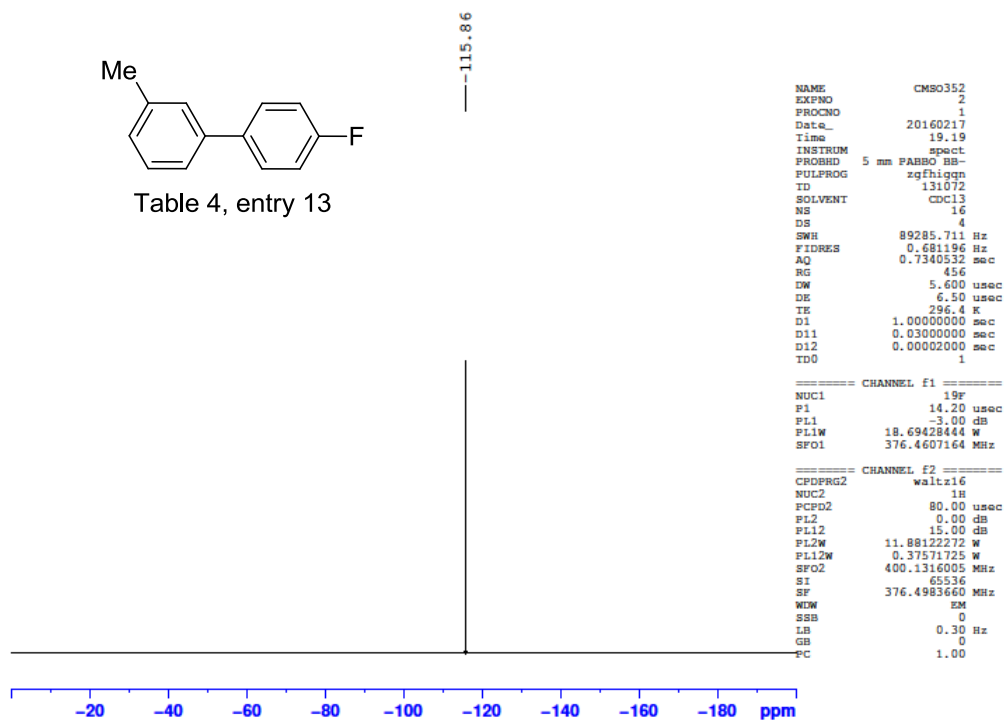
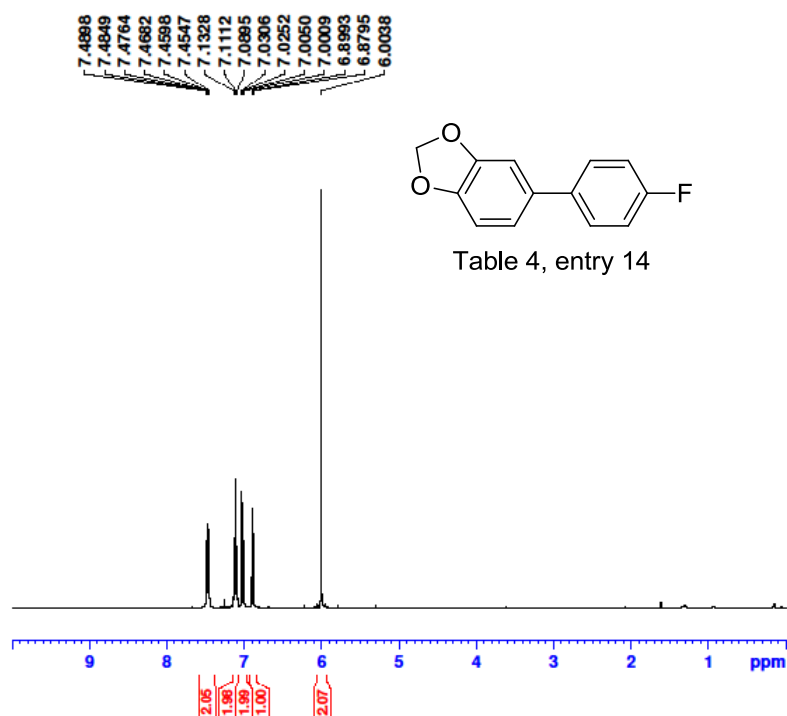


Table 4, entry 13



CMSO354H



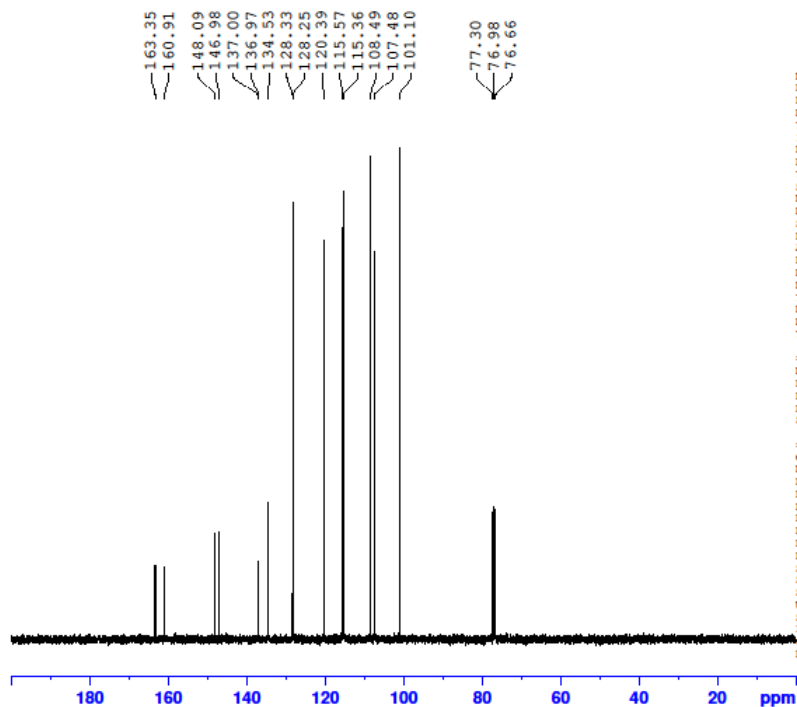
```

NAME          CMSO354
EXPNO         1
PROCNO        1
Date_         20160217
Time          18.52
INSTRUM       spect
PROBHD        5 mm F4BBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           8012.820 Hz
FIDRES        0.244532 Hz
AQ            2.0447731 sec
RG            25.4
DW            62.400 usec
DE            6.30 usec
TE            296.4 K
D1            1.00000000 sec
D11           1
D10           1

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1324008 MHz
SI            32768
SF            400.1300088 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

CMSO354C



```

NAME          CMSO354
EXPNO         2
PROCNO        1
Date_         20160217
Time          18.57
INSTRUM       spect
PROBHD        5 mm F4BBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            67
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            128
DW            20.800 usec
DE            6.50 usec
TE            297.4 K
D1            1.00000000 sec
D11           0.03000000 sec
D10           1

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127808 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```


CMSO354F

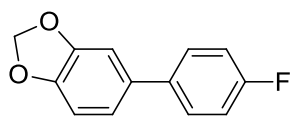
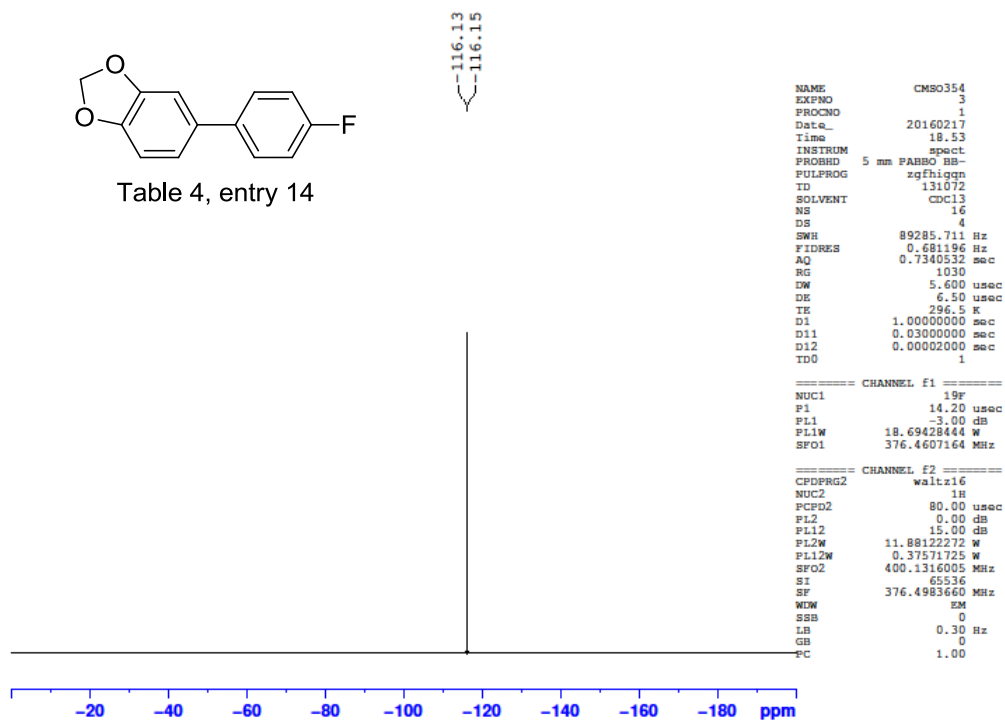
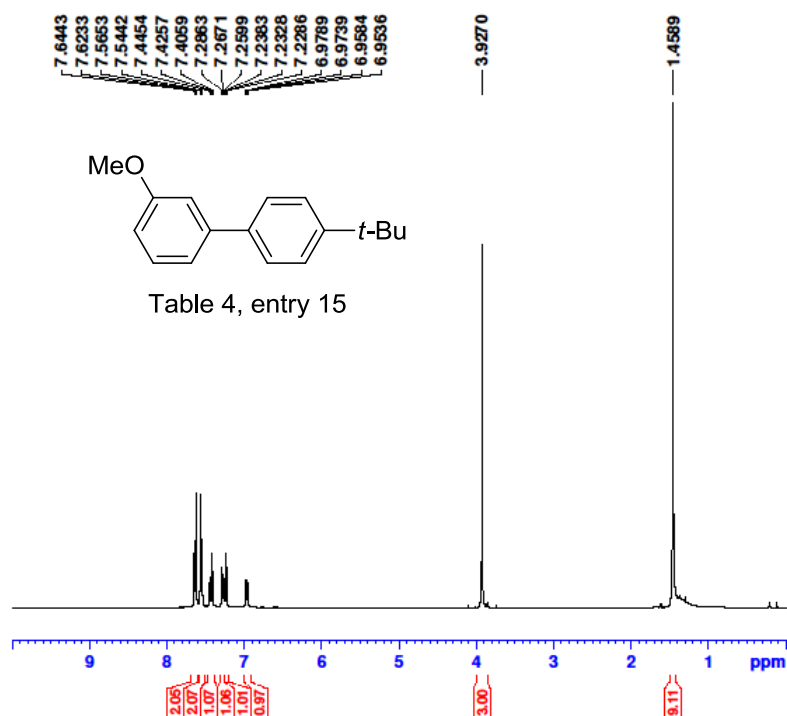


Table 4, entry 14



CMSO353H



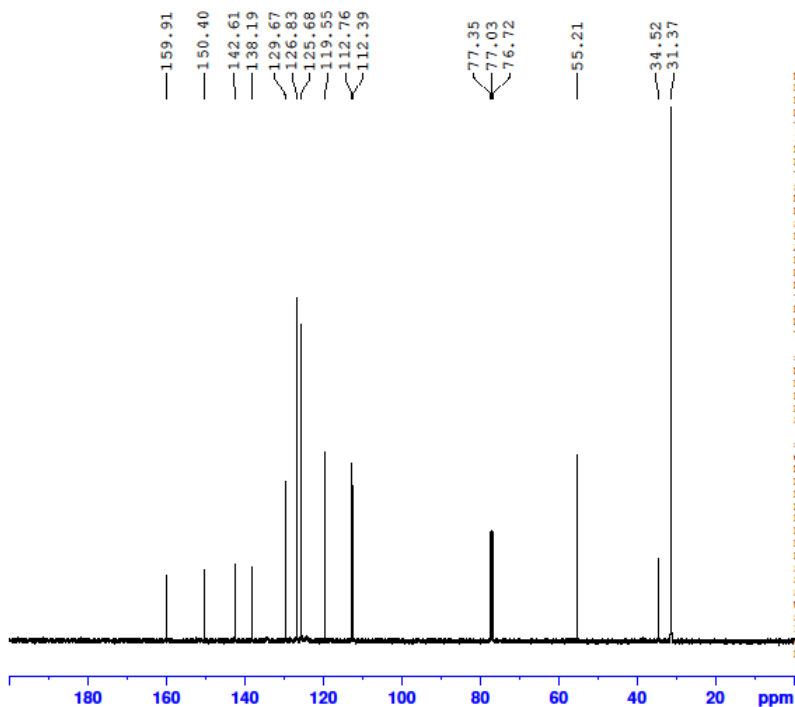
```

NAME          CMSO353
EXPNO         1
PROCNO        1
Date_         20160217
Time         19.28
INSTRUM       spect
PROBHD        5 mm F4BBO BB-
PULPROG       zgpg30
ID            32768
SOLVENT       CDCl3
NS            15
DS            2
SWH           8012.820 Hz
FIDRES       0.244532 Hz
AQ           2.0447731 sec
RG            25.4
DW           62.400 usec
DE           6.30 usec
TE           296.5 K
D1           1.00000000 sec
D11          1
TD0          1

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W         11.88122272 W
SFO1         400.1324008 MHz
SI            32768
SF           400.1300095 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

CMSO353C



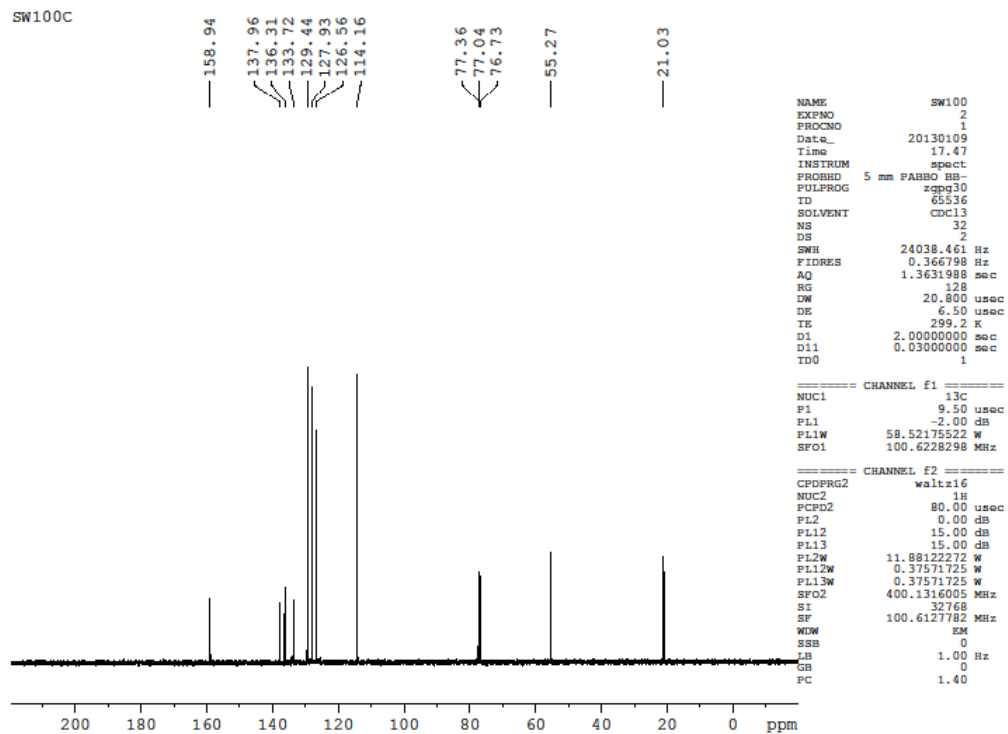
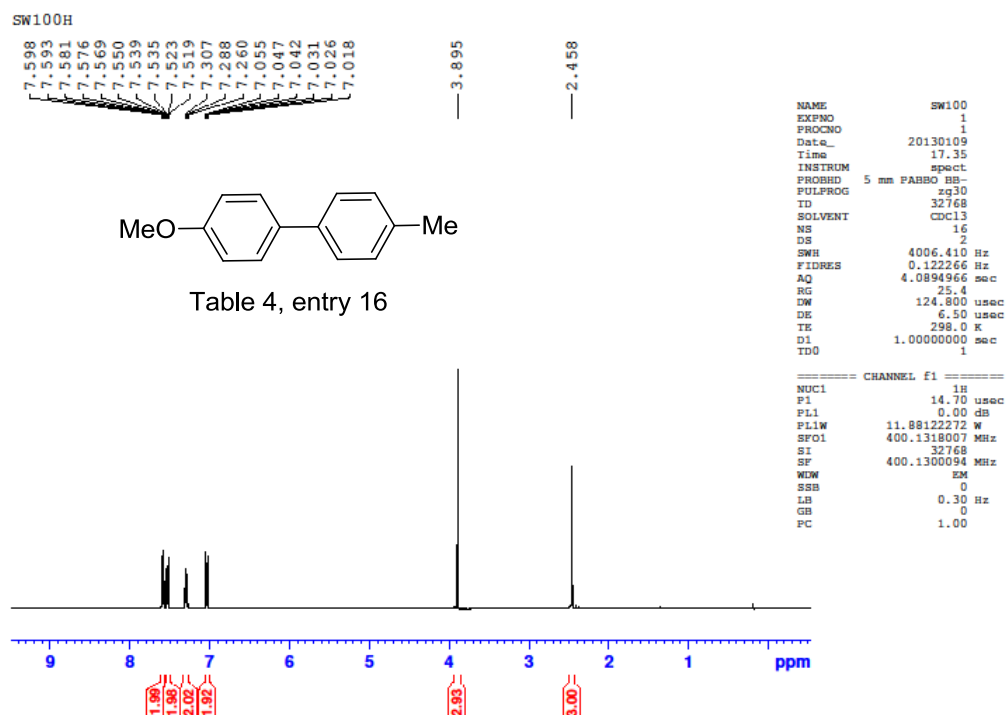
```

NAME          CMSO353
EXPNO         2
PROCNO        1
Date_         20160217
Time         19.31
INSTRUM       spect
PROBHD        5 mm F4BBO BB-
PULPROG       zgpg30
ID            65536
SOLVENT       CDCl3
NS            64
DS            2
SWH           24038.461 Hz
FIDRES       0.366798 Hz
AQ           1.3631988 sec
RG            144
DW           20.800 usec
DE           6.50 usec
TE           297.3 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0          1

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W         58.52175522 W
SFO1         100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12         15.00 dB
PL13         15.00 dB
PL2W         11.88122272 W
PL12W        0.37571725 W
PL13W        0.37571725 W
SFO2         400.1316005 MHz
SI            32768
SF           100.6127795 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```



CMS0123H

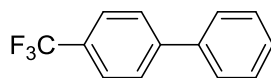


Table 4, entry 17

```

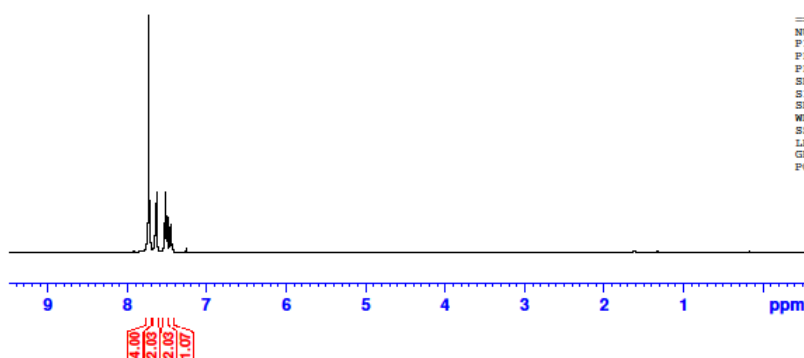
NAME          CMS0123
EXPNO         1
PROCNO        1
Date_         20141103
Time          12.21
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            2
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            45.2
DW            124.800 usec
DE            6.50 usec
TE            297.8 K
D1            1.0000000 sec
TD0           1

```

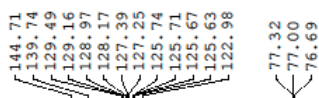
```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300097 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```



CMS0123C



```

NAME          CMS0123
EXPNO         2
PROCNO        1
Date_         20141103
Time          12.22
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            17
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            298.4 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1

```

```

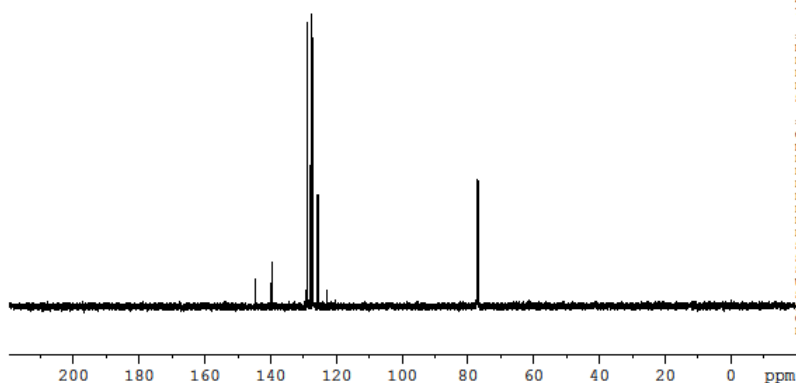
===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

```

```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127751 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```



CMS0123F

-62.33

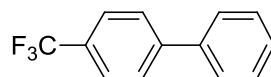
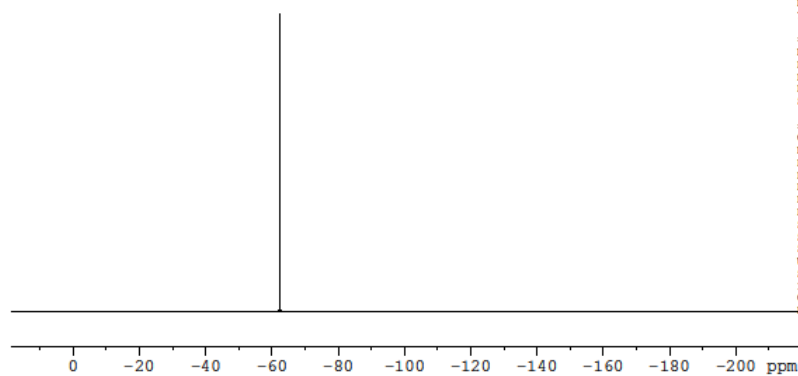


Table 4, entry 17



```

NAME          CMS0123
EXPNO         3
PROCNO        1
Date_         20141103
Time         12.24
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            131072
SOLVENT       CDCl3
NS            7
DS            4
SWH           89285.711 Hz
FIDRES        0.681196 Hz
AQ            0.7340532 sec
RG            203
DW            5.600 usec
DE            6.50 usec
TE            298.0 K
D1            1.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
TD0           1

===== CHANNEL f1 =====
NUC1           19F
P1            14.20 usec
PL1            3.00 dB
PL1W          18.69428444 W
SFO1          376.4607164 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2          80.00 usec
PL2            0.00 dB
PL12          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
SFO2          400.1316005 MHz
SI            65536
SF            376.4983660 MHz
WDW            EM
SSB            0
LB            0.30 Hz
GB            0
PC            1.00

```

CMS0140H

7.574
7.562
7.552
7.545
7.466
7.448
7.428
7.375
7.357
7.339
7.259
7.160
7.138
7.121
7.117

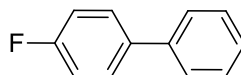
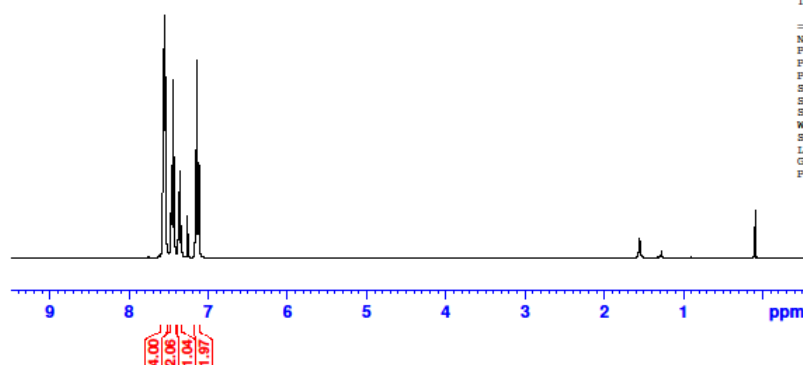


Table 4, entry 18



```

NAME          CMS0140
EXPNO         4
PROCNO        1
Date_         20141107
Time          0.25
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            2
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            25.4
DW            124.800 usec
DE            6.50 usec
TE            300.0 K
D1            1.0000000 sec
TD0           1

```

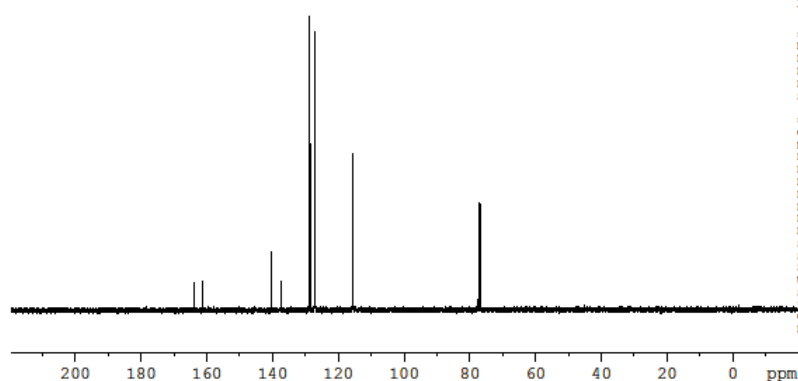
```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300101 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

CMS0140C

163.66
161.22
140.21
137.31
137.28
128.79
128.68
128.60
127.22
127.13
126.98
115.68
115.46
77.32
77.01
76.69



```

NAME          CMS0140
EXPNO         3
PROCNO        1
Date_         20141103
Time          23.38
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            23
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            297.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

```

```

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127802 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```

CMS0140F

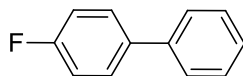
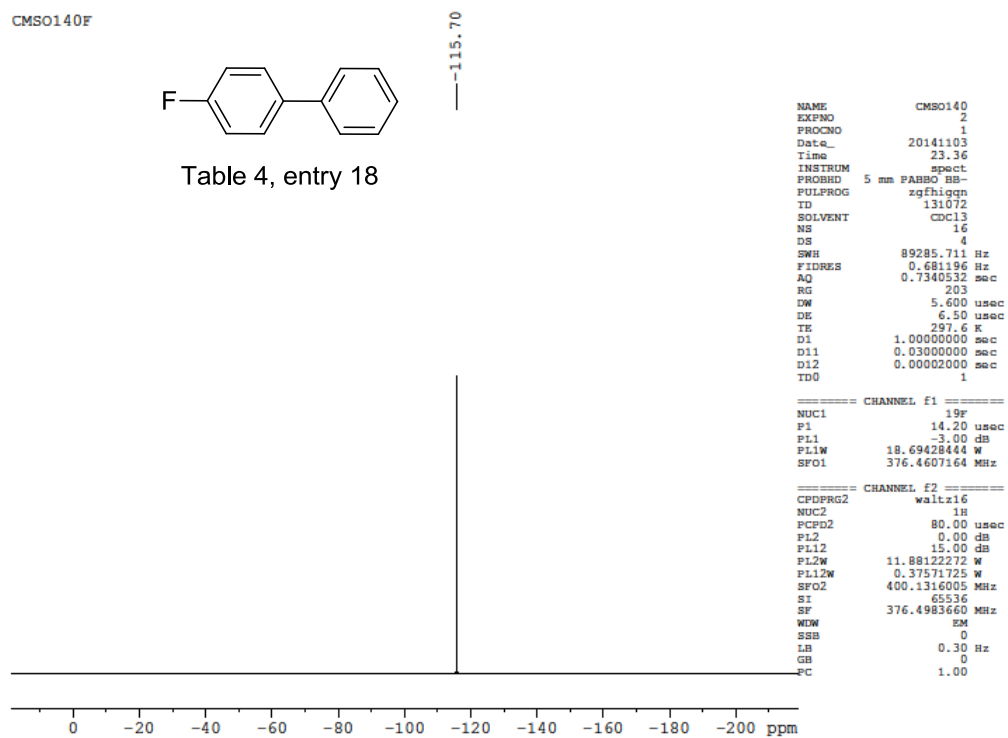


Table 4, entry 18



CMS0134H

8.042
8.021
7.691
7.670
7.637
7.619
7.492
7.474
7.455
7.423
7.405
7.386

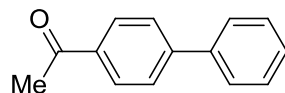
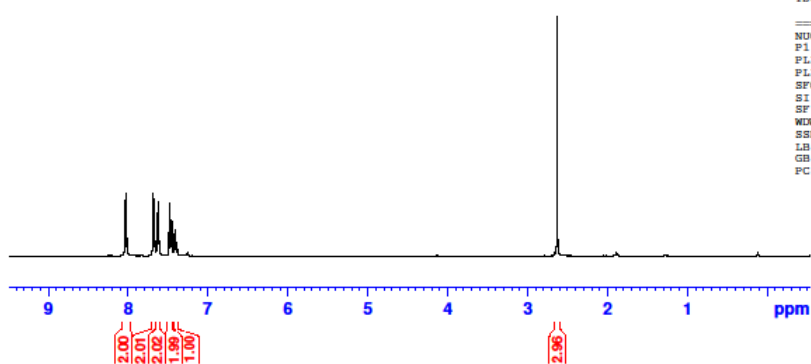


Table 4, entry 19-20

2.631



NAME CMS0134
EXFNO 1
PROCNO 1
Date_ 20141103
Time 12.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 2
DS 2
SWH 4006.410 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 25.4
DW 124.800 usec
DE 6.50 usec
TE 297.8 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1318007 MHz
SI 32768
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

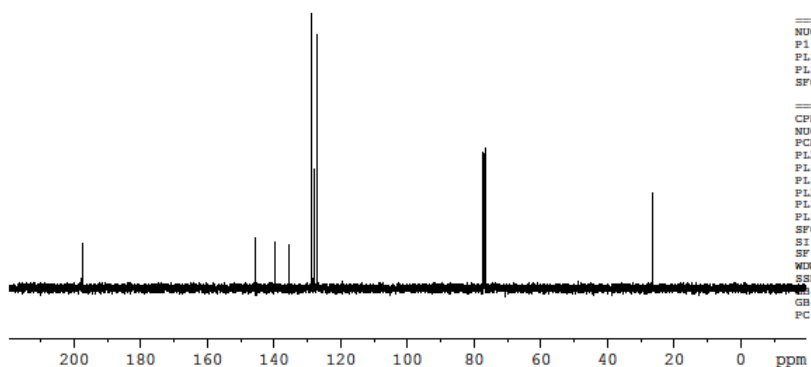
CMS0134C

197.62

145.61
139.71
135.71
128.85
128.80
128.13
127.14
127.08

77.31
77.00
76.68

26.53



NAME CMS0134
EXFNO 2
PROCNO 1
Date_ 20141103
Time 12.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127838 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CMS0135H

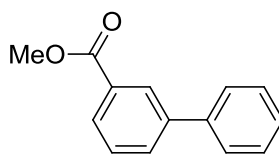
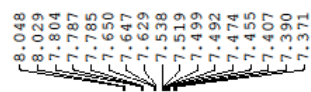
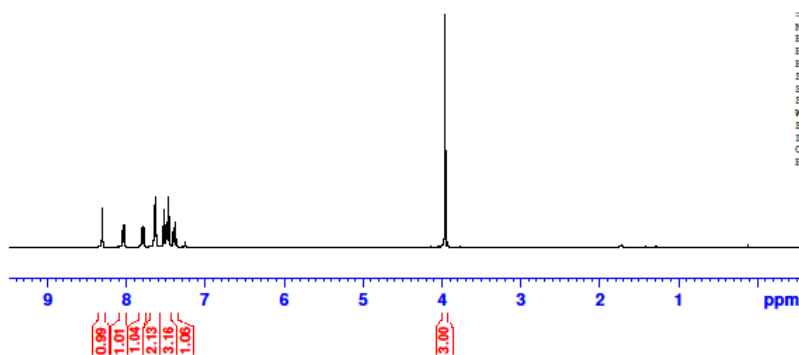


Table 4, entry 21-25



```

NAME          CMS0135
EXPNO         1
PROCNO        1
Date_         20141103
Time          12.17
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            2
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            45.2
DW           124.800 usec
DE            6.50 usec
TE            297.7 K
D1            1.0000000 sec
TD0           1

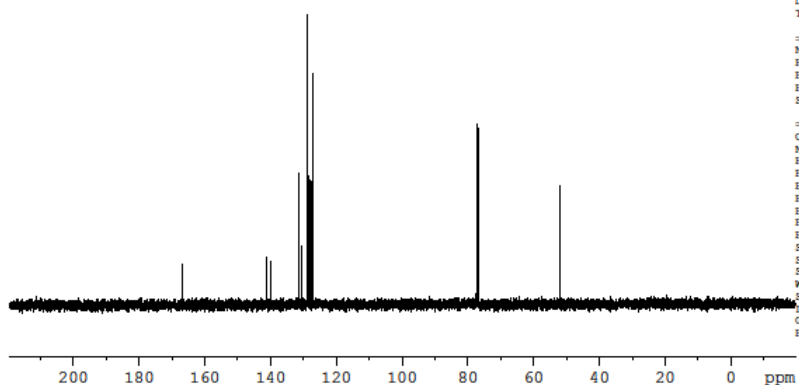
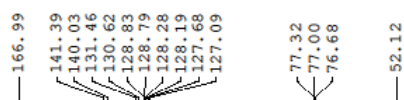
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300096 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

CMS0135C



```

NAME          CMS0135
EXPNO         2
PROCNO        1
Date_         20141103
Time          12.18
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW           20.800 usec
DE            6.50 usec
TE            298.1 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1

```

```

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

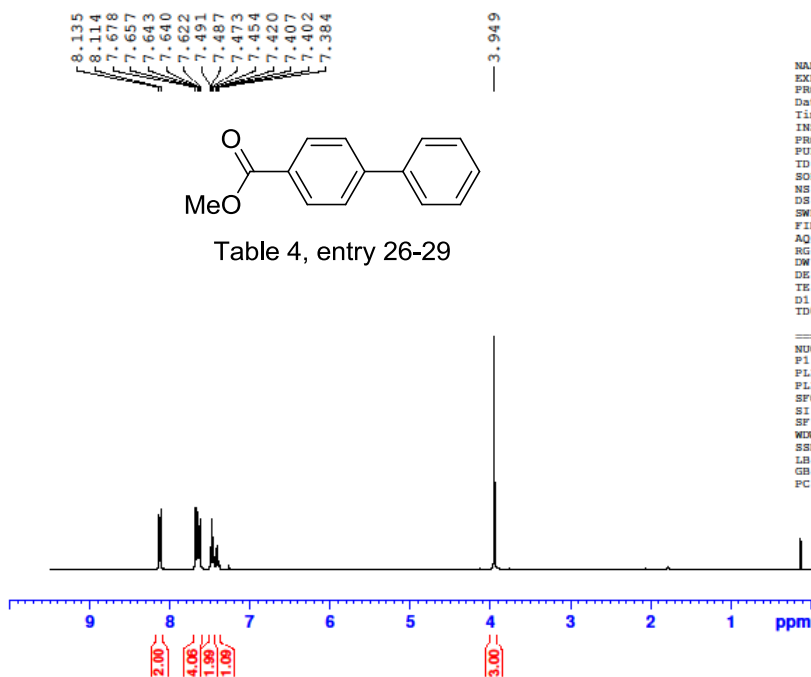
```

```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127786 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```

CMS0136H



```

NAME          CMS0136
EXPNO         1
PROCNO        1
Date_         20141103
Time          12.34
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            4
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            25.4
DW            124.800 usec
DE            6.50 usec
TE            297.8 K
D1            1.0000000 sec
TD0           1

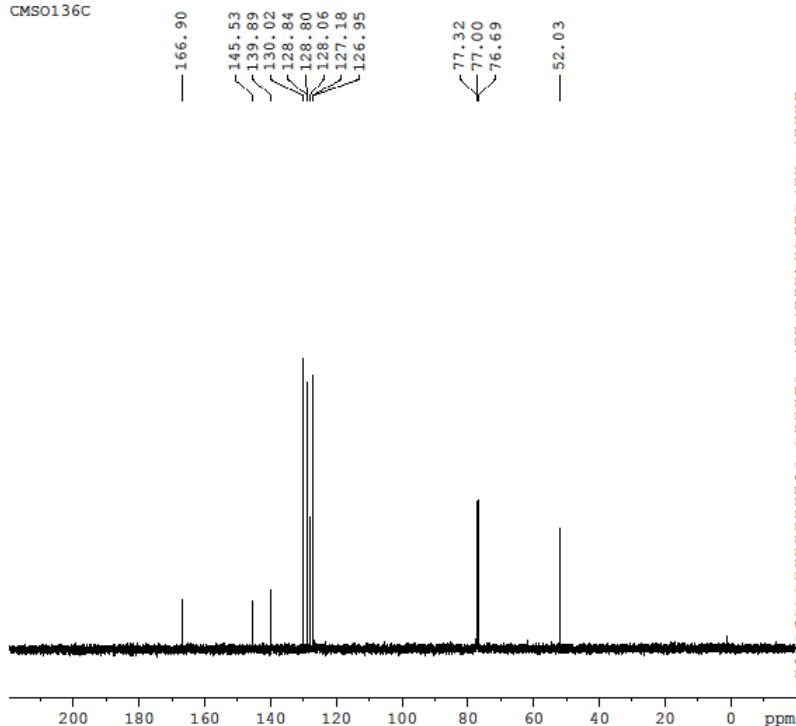
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300096 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

CMS0136C



```

NAME          CMS0136
EXPNO         2
PROCNO        1
Date_         20141103
Time          12.35
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            7
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

```

```

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

```

```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127803 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```

CMS0169H

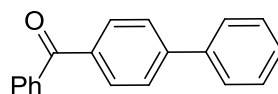


Table 4, entry 30

```

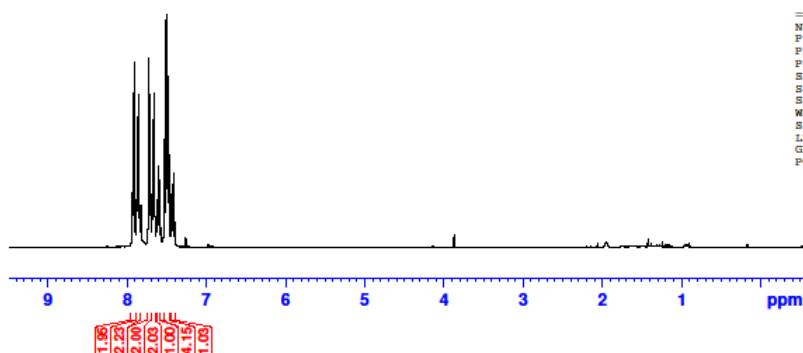
NAME          CMS0169
EXPNO         1
PROCNO        1
Date_         20141106
Time          14.06
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            9
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            25.4
DW            124.800 usec
DE            6.50 usec
TE            300.0 K
D1            1.0000000 sec
TD0           1

```

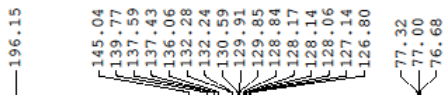
```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300093 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```



CMS0169C



```

NAME          CMS0169
EXPNO         2
PROCNO        1
Date_         20141106
Time          14.09
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            24
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            298.2 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1

```

```

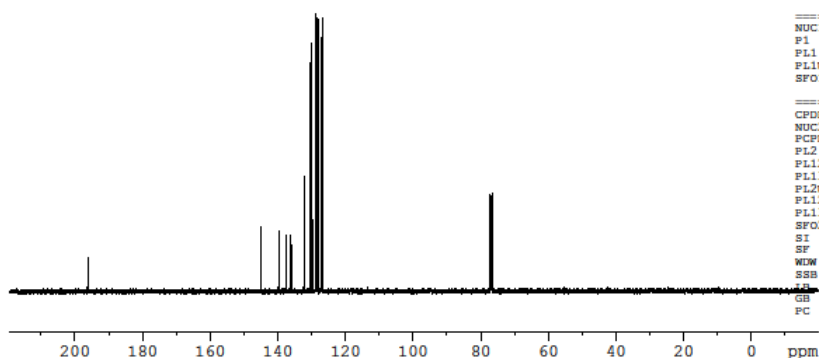
===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

```

```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127895 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```



CMS0168H

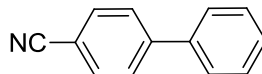
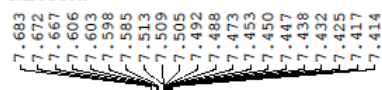


Table 4, entry 31

```

NAME          CMS0168
EXPNO         1
PROCNO        1
Date_         20141106
Time          14.02
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            9
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            25.4
DW            124.800 usec
DE            6.50 usec
TE            297.4 K
D1            1.0000000 sec
TD0           1

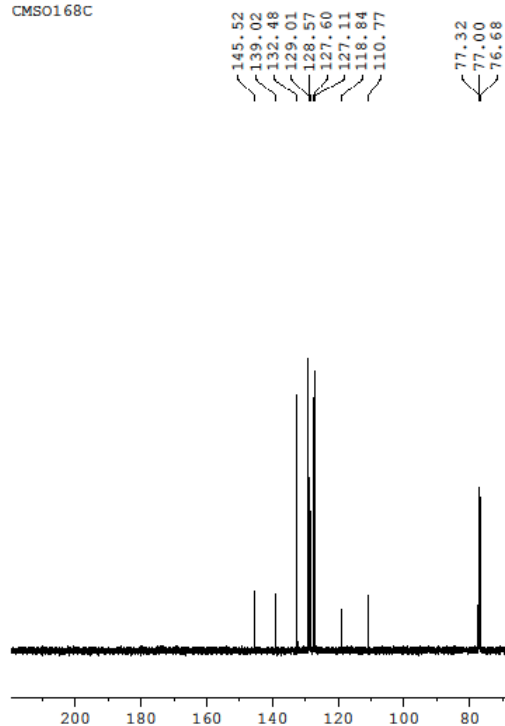
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300098 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

CMS0168C



```

NAME          CMS0168
EXPNO         2
PROCNO        1
Date_         20141106
Time          14.04
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            19
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            298.1 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1

```

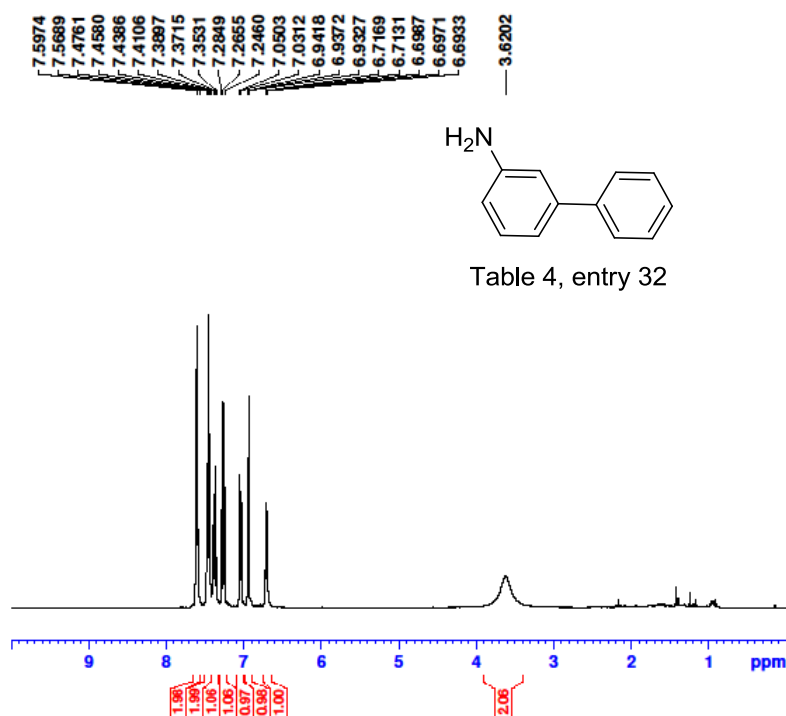
```

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127832 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```

CMS0145H



```

NAME          CMS0145
EXPNO         1
PROCNO        1
Date_         20141106
Time          13.15
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            4
DS            2
SWH           6393.862 Hz
FIDRES        0.190125 Hz
AQ            2.5623076 sec
RG            40.3
DW            78.200 usec
DE            6.30 usec
TE            297.4 K
D1            1.00000000 sec
D11           1
D10           1

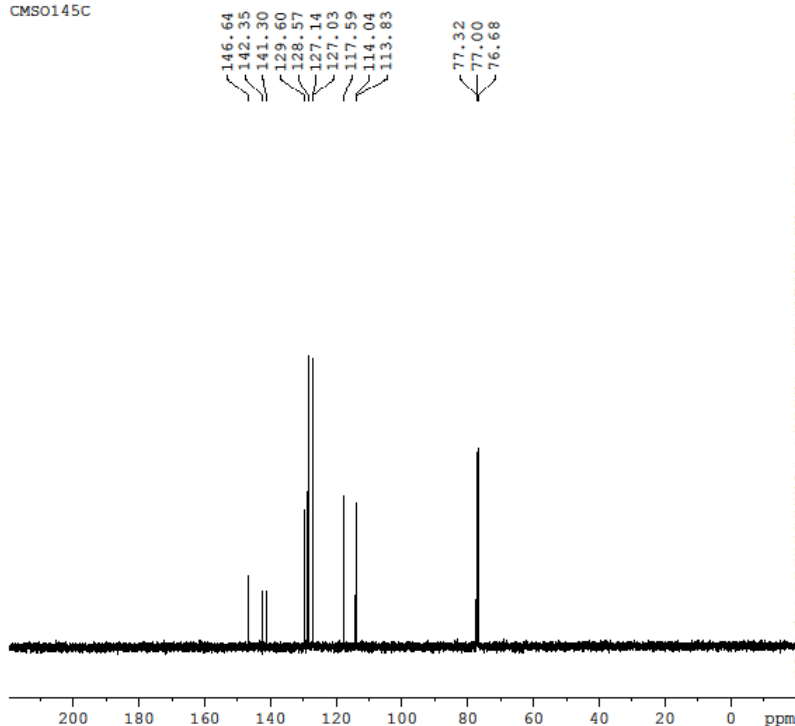
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300098 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

CMS0145C



```

NAME          CMS0145
EXPNO         2
PROCNO        1
Date_         20141106
Time          13.16
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            18
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
D10           1

```

```

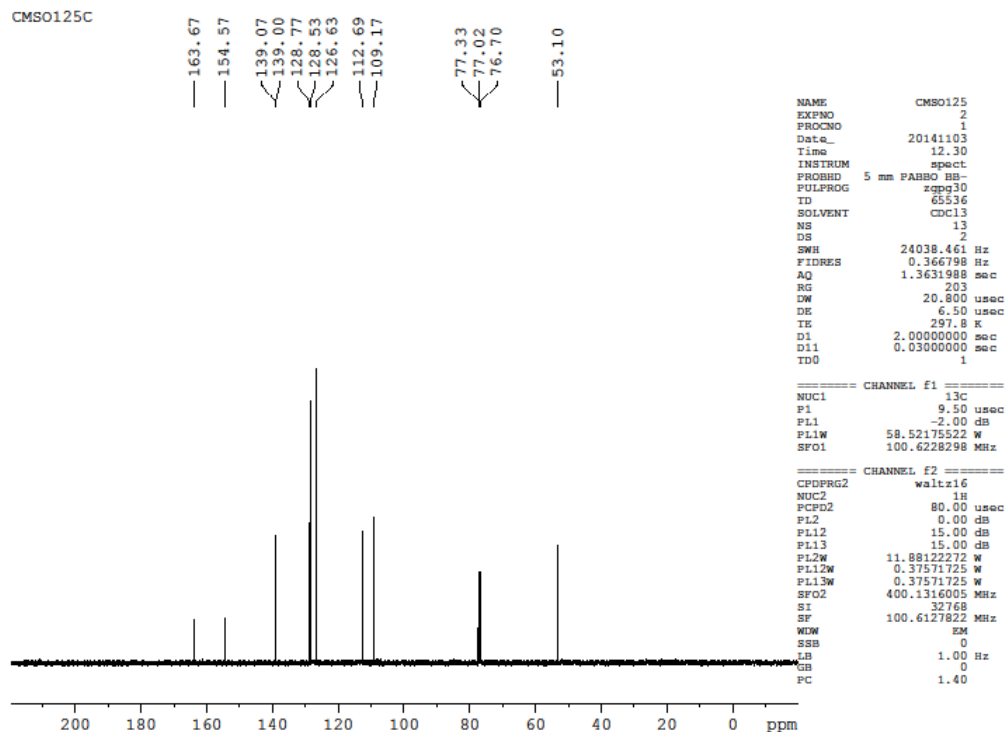
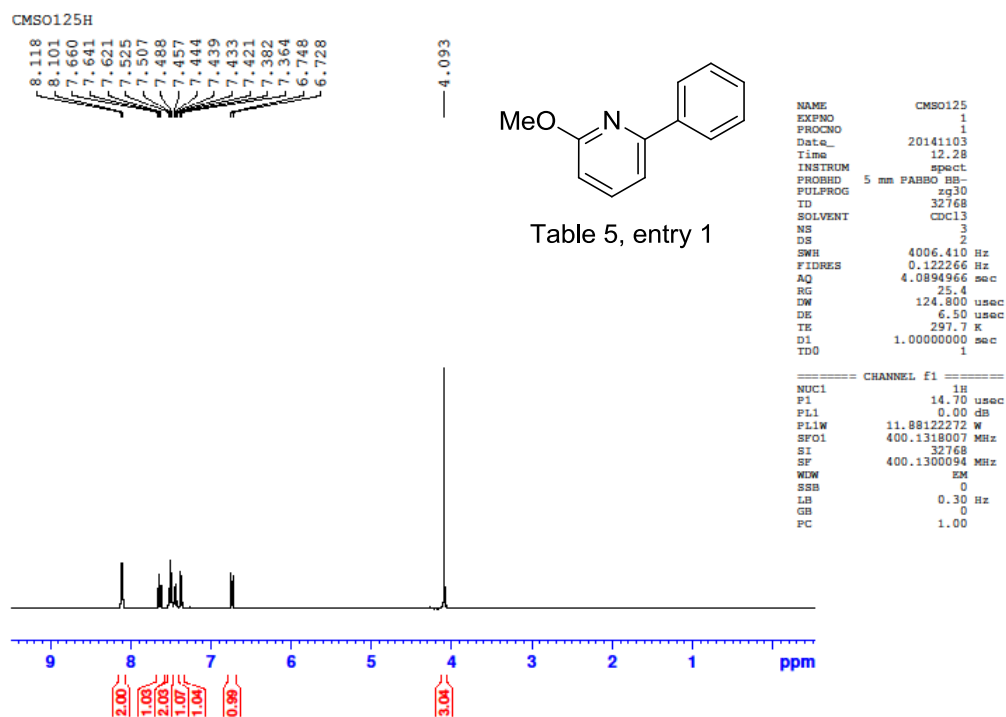
===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

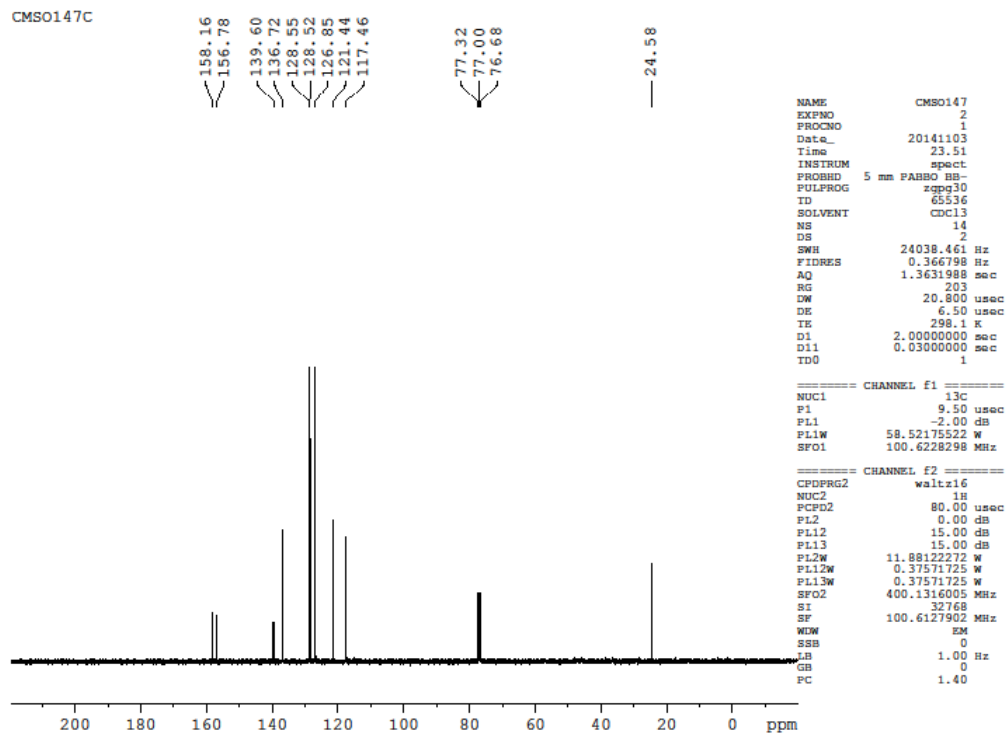
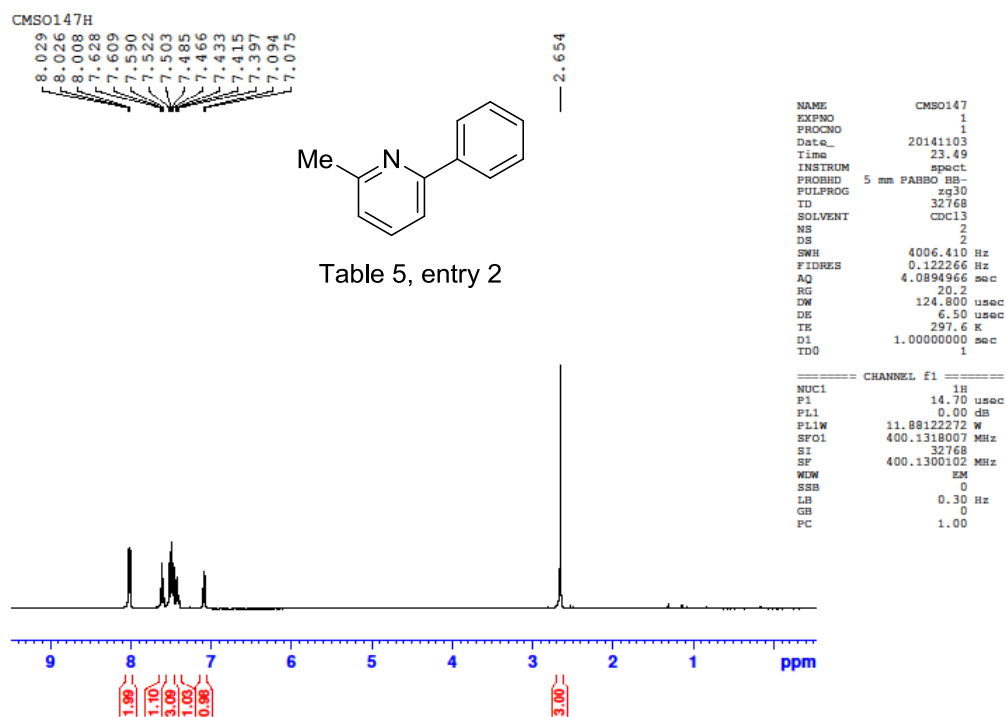
```

```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127831 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```





CMS0148H

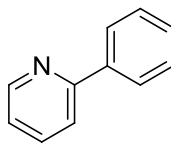
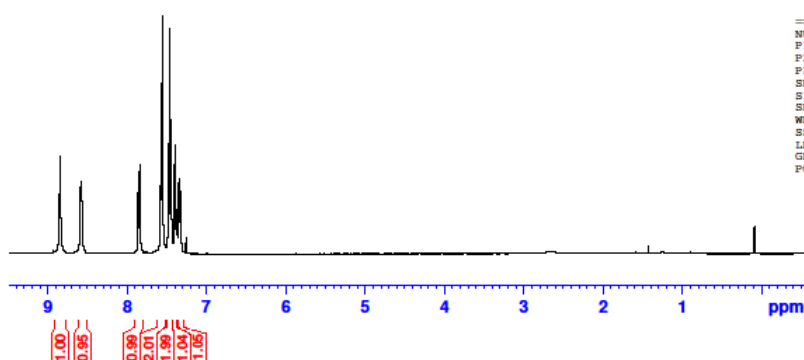


Table 5, entry 3



```

NAME          CMS0148
EXPNO         1
PROCNO        1
Date_         20141103
Time          23.56
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            2
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            45.2
DW            124.800 usec
DE            6.50 usec
TE            297.7 K
D1            1.0000000 sec
TD0           1

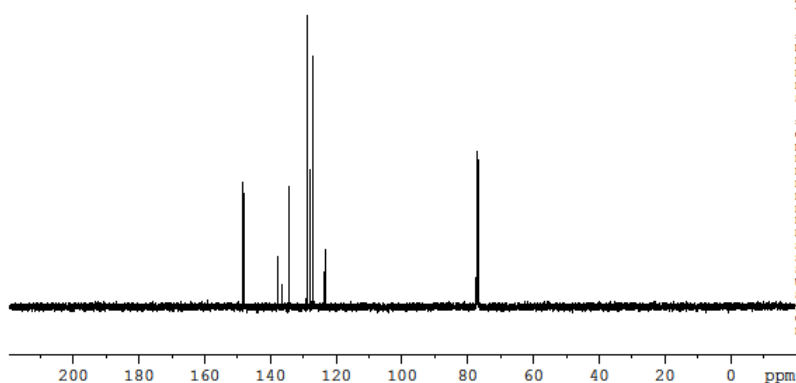
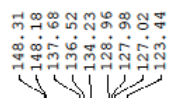
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300102 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

CMS0148C



```

NAME          CMS0148
EXPNO         2
PROCNO        1
Date_         20141103
Time          23.57
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            14
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            298.2 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1

```

```

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

```

```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127826 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```


CMS0155H

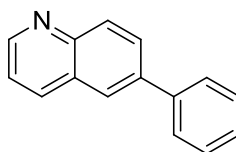
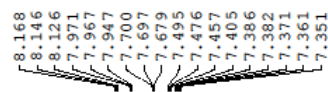


Table 5, entry 4

```

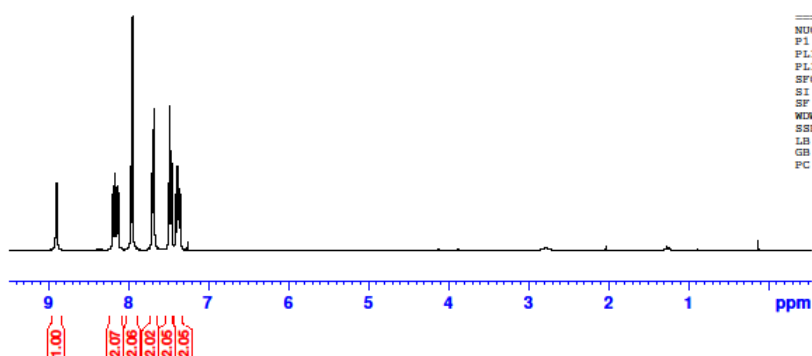
NAME          CMS0155
EXPNO         1
PROCNO        1
Date_         20141106
Time          12.48
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            2
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            25.4
DW            124.800 usec
DE            6.50 usec
TE            300.0 K
D1            1.0000000 sec
TD0           1

```

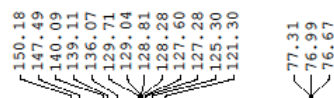
```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300098 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```



CMS0155C



```

NAME          CMS0155
EXPNO         2
PROCNO        1
Date_         20141106
Time          12.49
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            15
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            297.8 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1

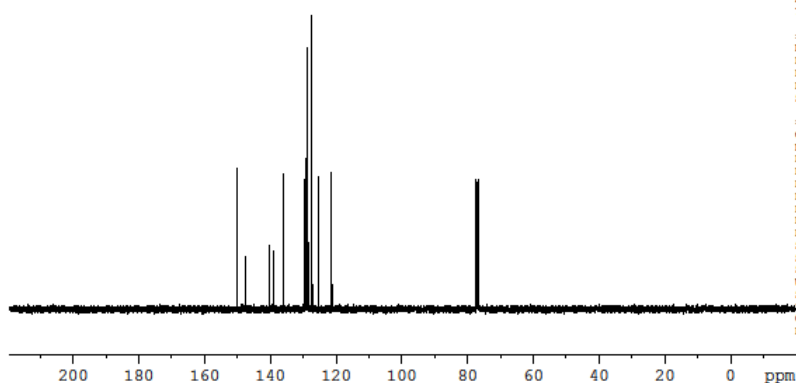
```

```

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127873 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```



CMS0162H

8.183
8.169
7.864
7.842
7.820
7.800
7.765
7.763
7.745
7.727
7.724
7.571
7.553
7.534
7.528
7.506
7.487
7.469

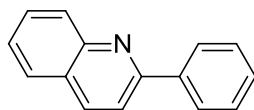
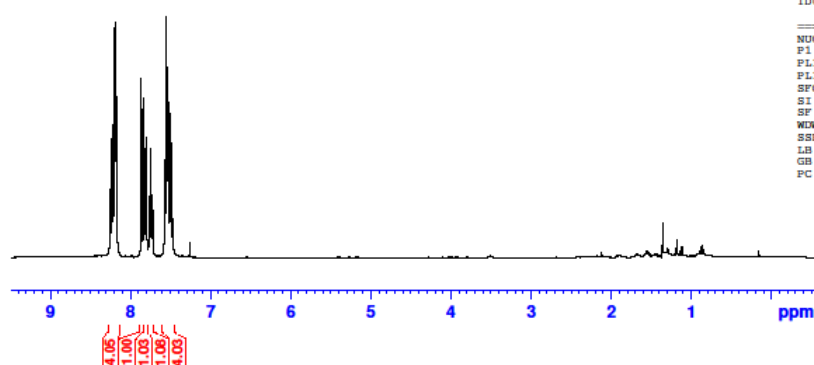


Table 5, entry 5



NAME CMS0162
EXFNO 2
PROCNO 1
Date_ 20141107
Time 0.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 2
SWH 4006.410 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 25.4
DW 124.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

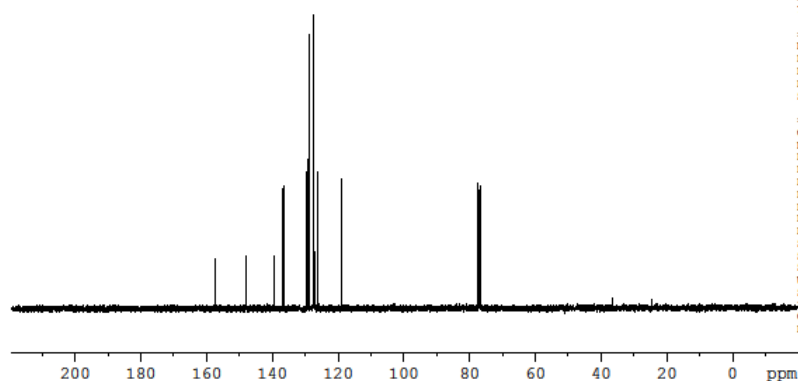
===== CHANNEL f1 =====
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1318007 MHz
SI 32768
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CMS0162C

157.23
148.15
139.54
136.67
129.59
129.55
129.22
128.73
127.88
127.36
127.06
126.16
118.89

77.32
77.00
76.68

— 36.56
— 24.58



NAME CMS0162
EXFNO 3
PROCNO 1
Date_ 20141107
Time 0.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 19
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127859 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CMS0170H

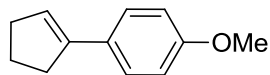
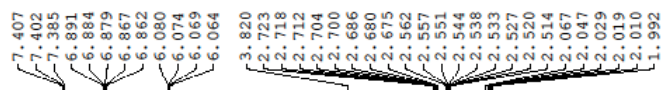
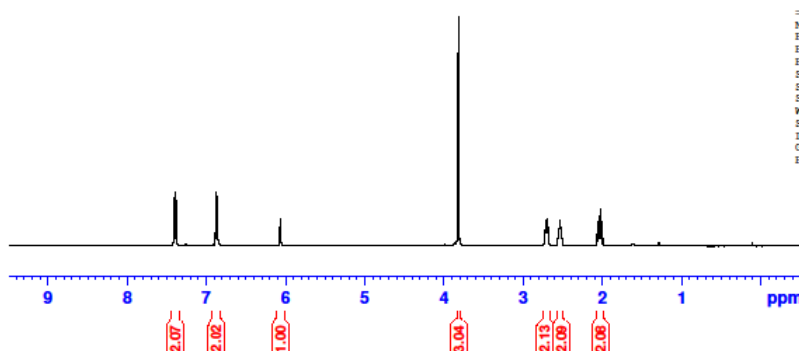


Table 5, entry 6



```

NAME          CMS0170
EXPNO         1
PROCNO        1
Date_         20141106
Time          13.55
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            13
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            25.4
DW            124.800 usec
DE            6.50 usec
TE            297.4 K
D1            1.0000000 sec
D11           1
TD0           1

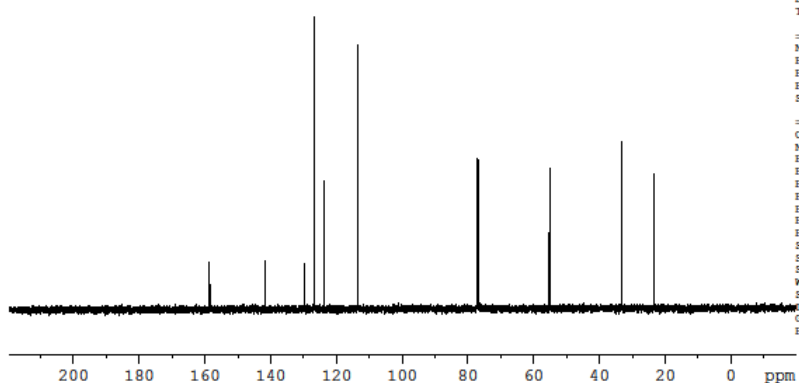
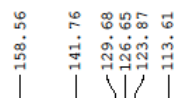
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300093 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

CMS0170C



```

NAME          CMS0170
EXPNO         2
PROCNO        1
Date_         20141106
Time          13.58
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            25
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            298.1 K
D1            2.0000000 sec
D11           0.0300000 sec
D111          1
TD0           1

```

```

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

```

```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL12W         11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127752 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```

CMSO206H

7.800
7.643
7.622
7.592
7.572
7.522
7.518
7.514
6.729
6.727

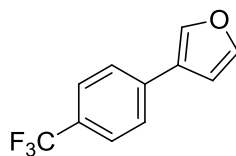
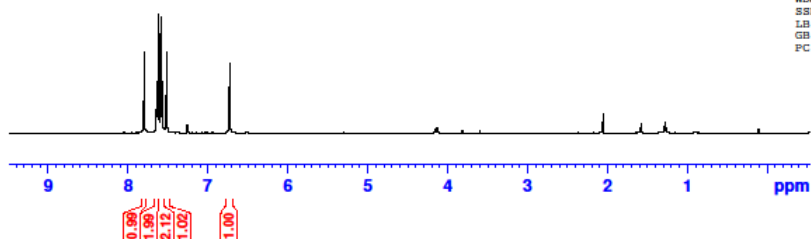


Table 6, entry 1



```

NAME          CMSO206
EXPNO         1
PROCNO        1
Date_         20141111
Time          19.52
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            8
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            64
DW            124.800 usec
DE            6.50 usec
TE            297.4 K
D1            1.0000000 sec
D11           1
TD0           1

```

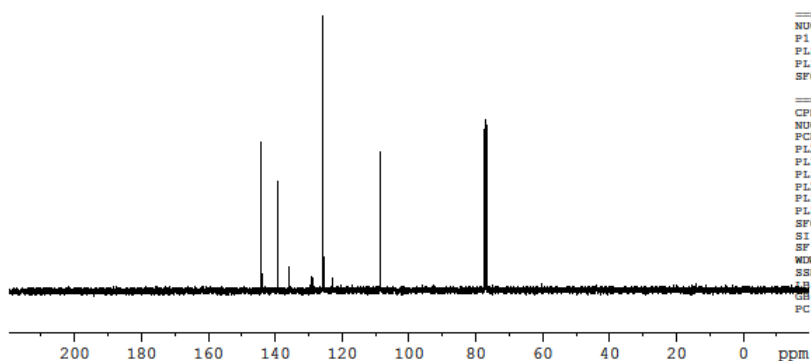
```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300098 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

CMSO206C

144.10
139.34
136.02
129.40
129.07
128.75
125.92
125.81
125.77
125.74
125.70
125.56
125.37
122.86
108.61
92.83
77.32
77.00
76.68
60.38



```

NAME          CMSO206
EXPNO         2
PROCNO        1
Date_         20141111
Time          19.56
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            22
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

```

```

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

```

```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127722 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```

CMSO206F

-62.18

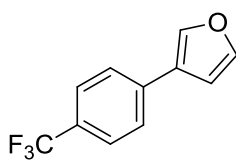
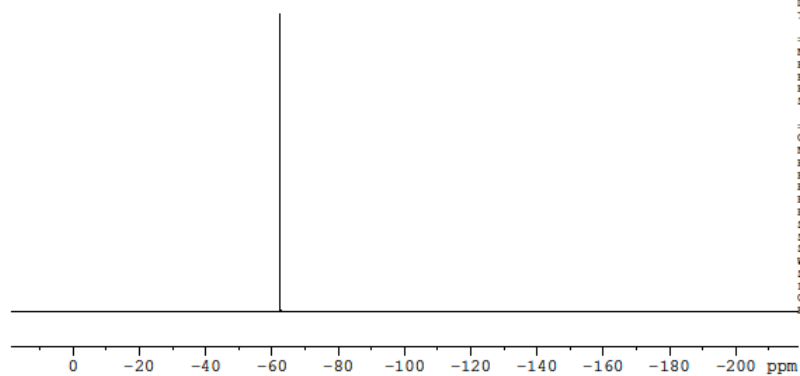


Table 6, entry 1



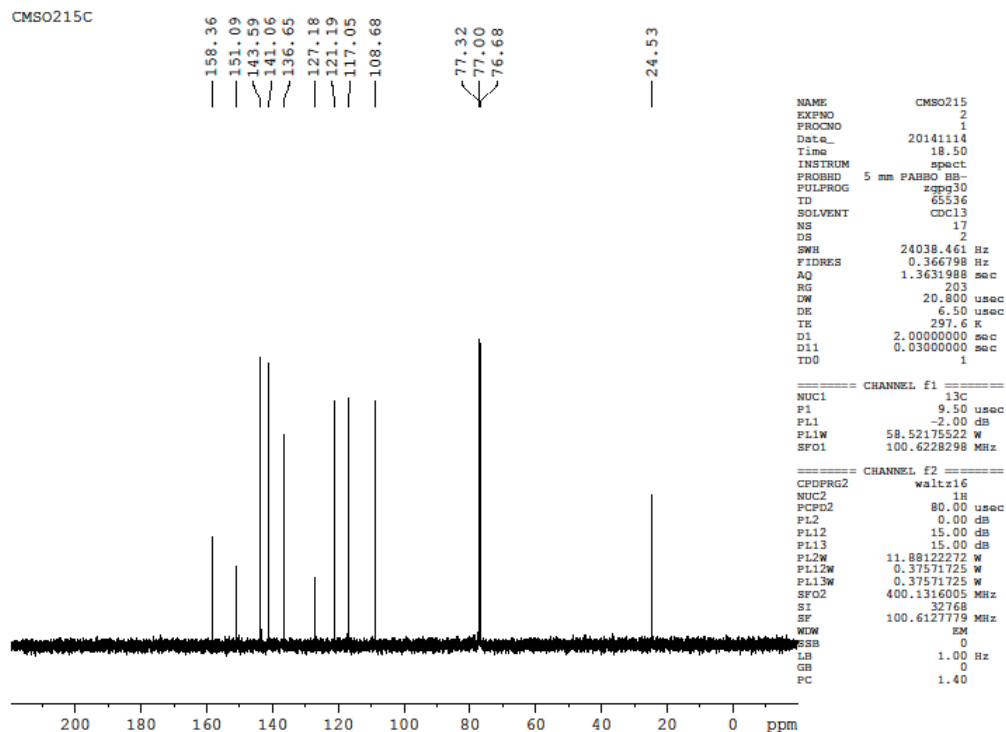
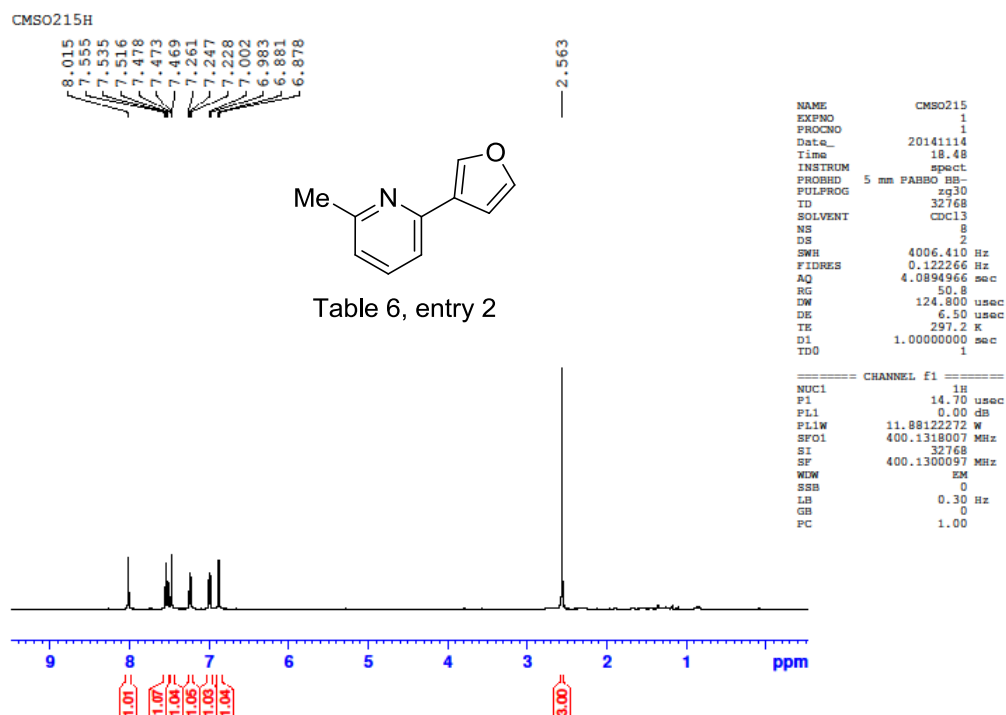
```

NAME          CMSO206
EXPNO         3
PROCNO        1
Date_         20141111
Time         19.59
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            131072
SOLVENT       CDCl3
NS            16
DS            4
SWH           89285.711 Hz
FIDRES        0.681196 Hz
AQ            0.7340532 sec
RG            203
DW            5.600 usec
DE            6.50 usec
TE            297.7 K
D1            1.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
TD0           1

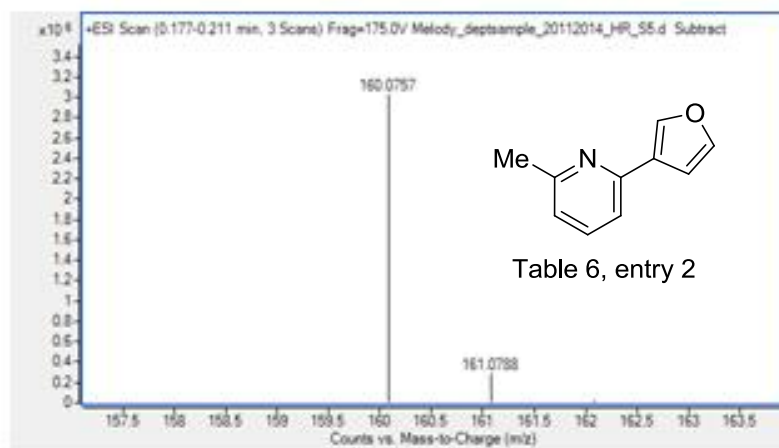
===== CHANNEL f1 =====
NUC1           19F
P1            14.20 usec
PL1           -3.00 dB
PL1W          18.69428444 W
SFO1          376.4607164 MHz

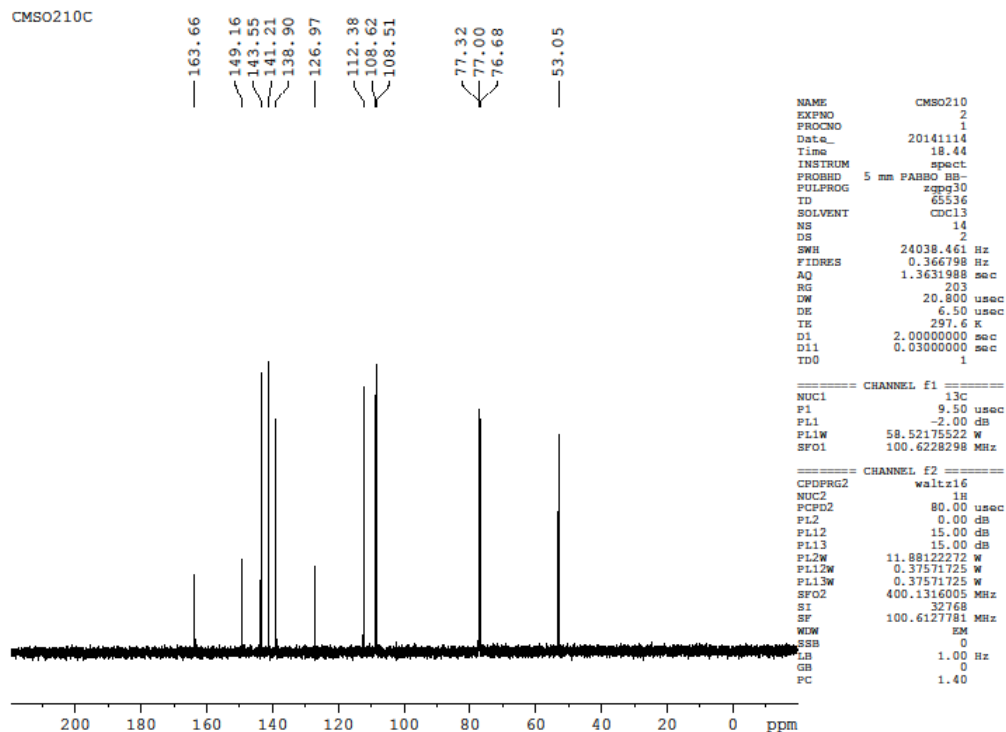
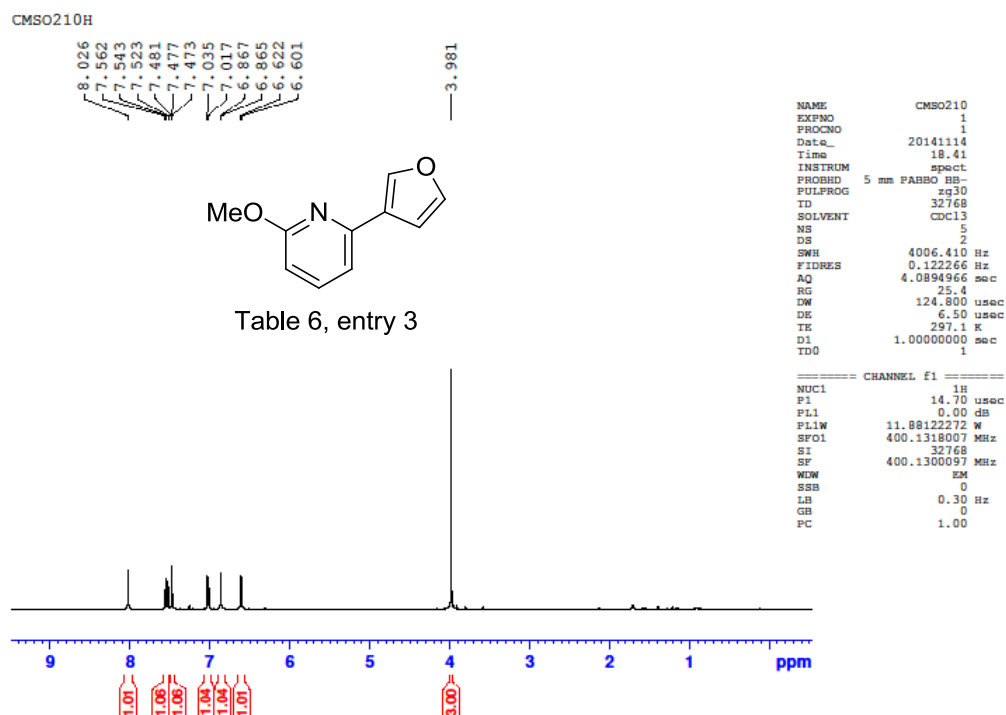
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2          80.00 usec
PL2            0.00 dB
PL12          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
SFO2          400.1316005 MHz
SI            65536
SF            376.4983660 MHz
WDW            EM
SSB            0
LB            0.30 Hz
GB            0
PC            1.00

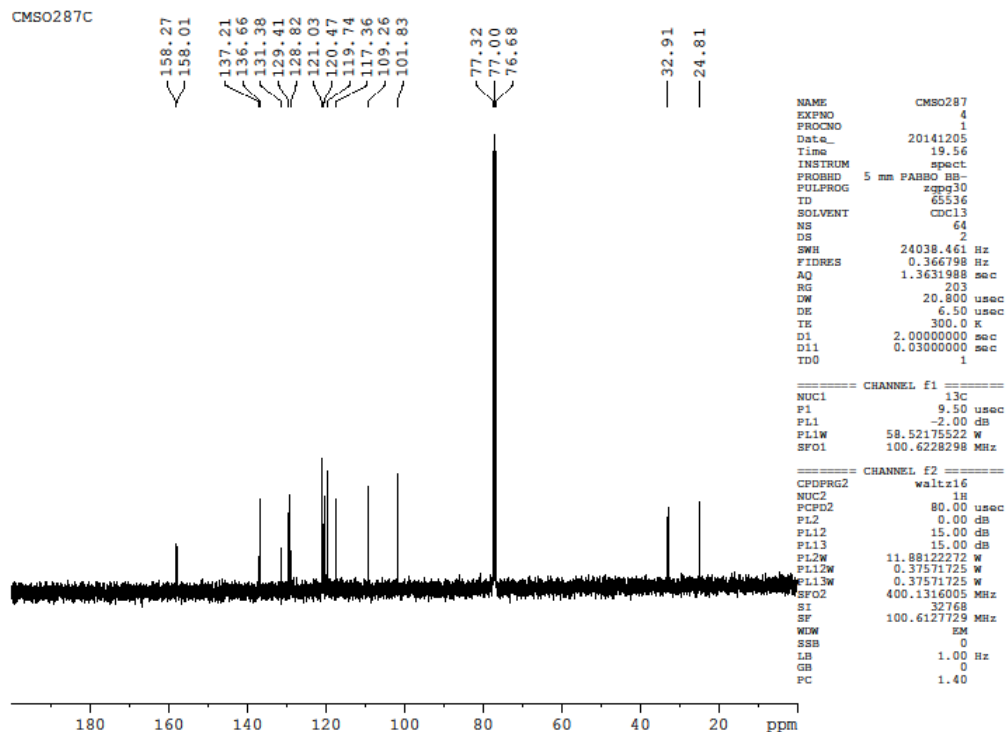
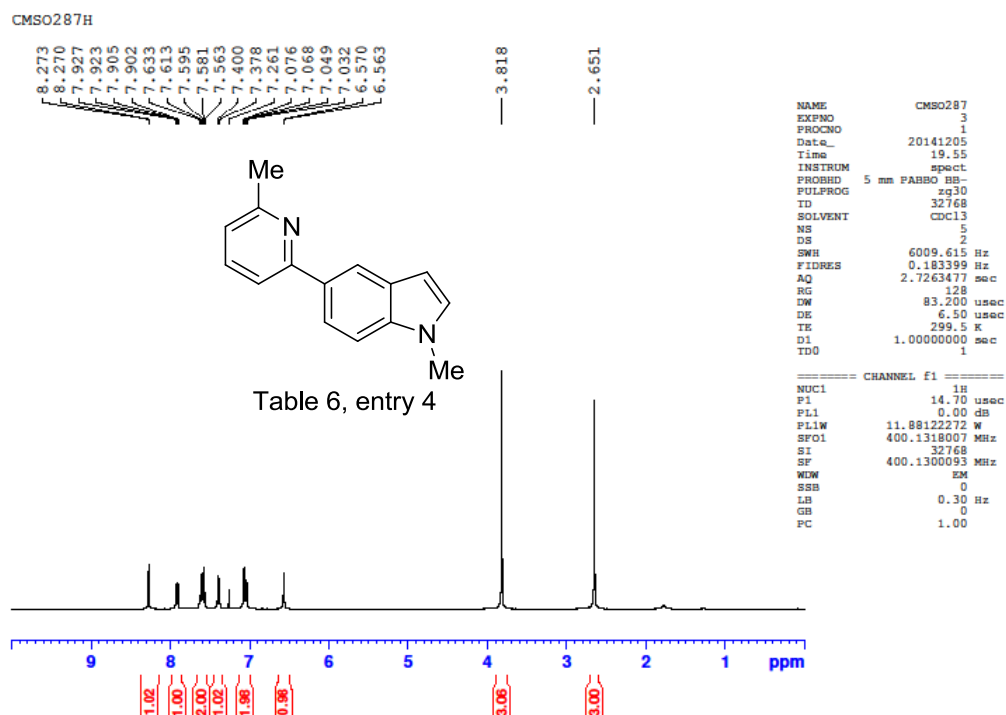
```



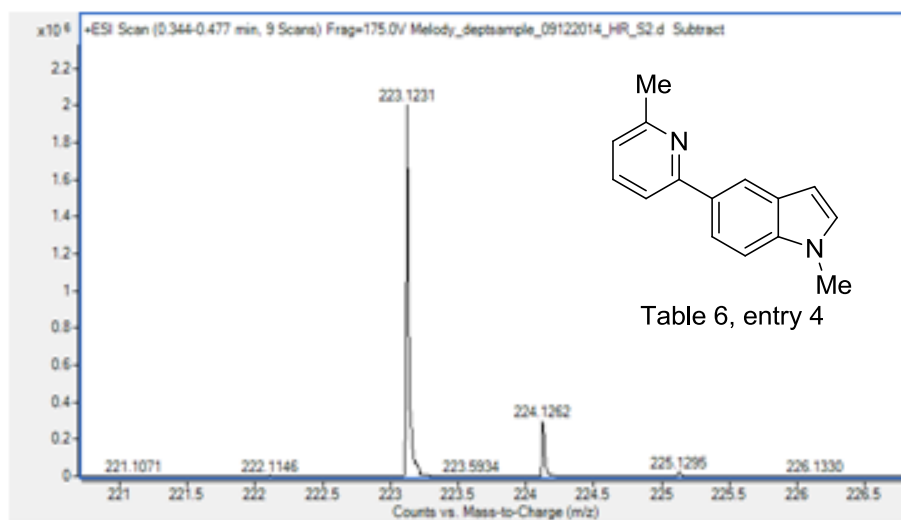
HS



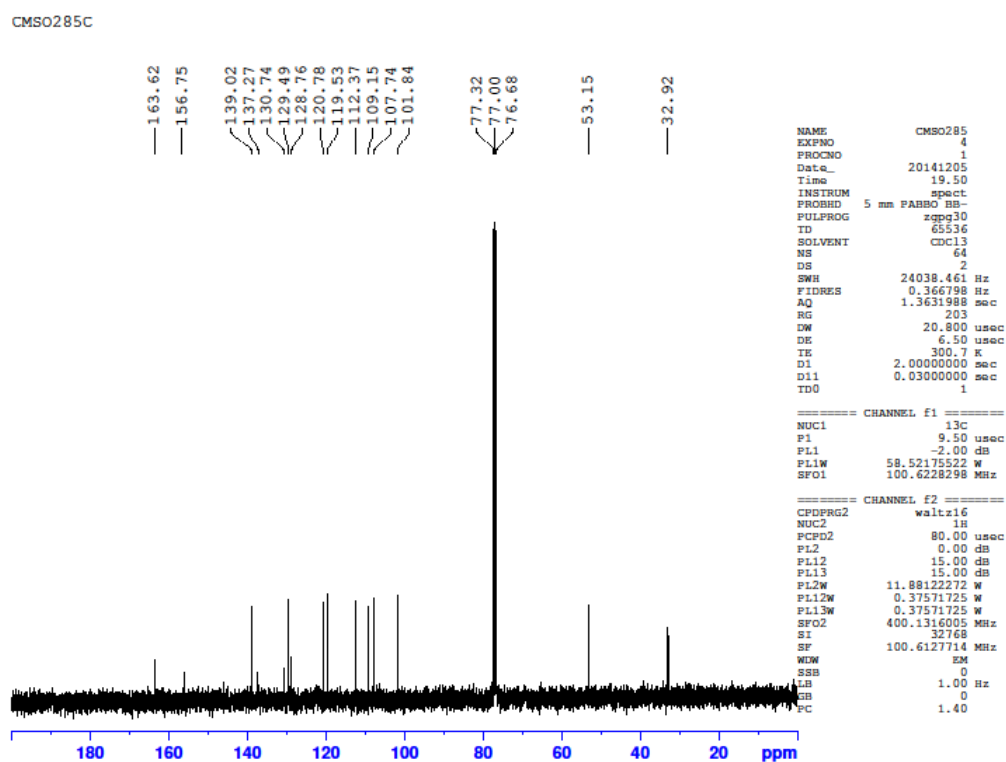
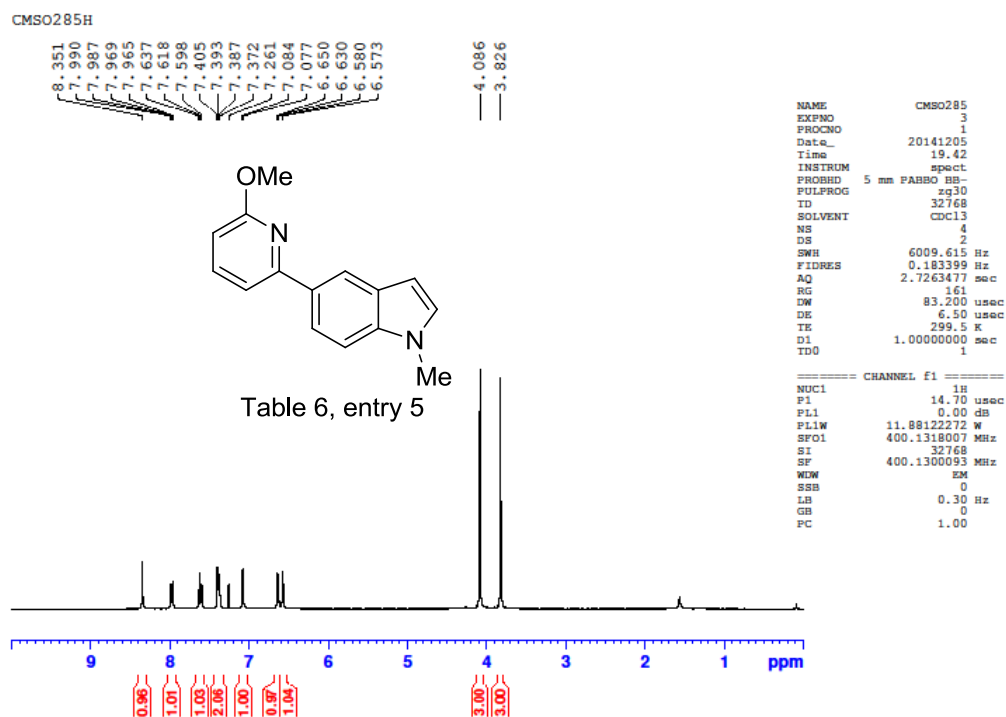




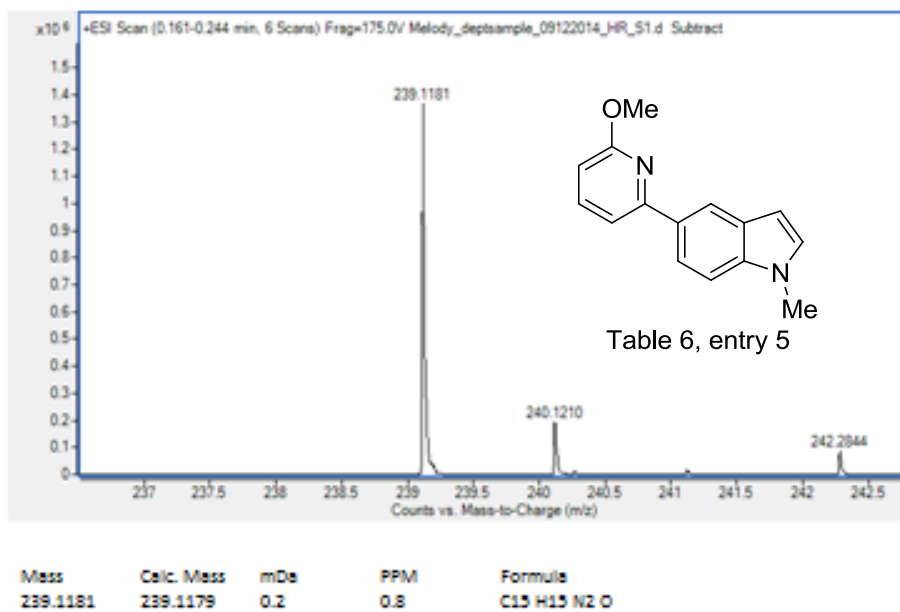
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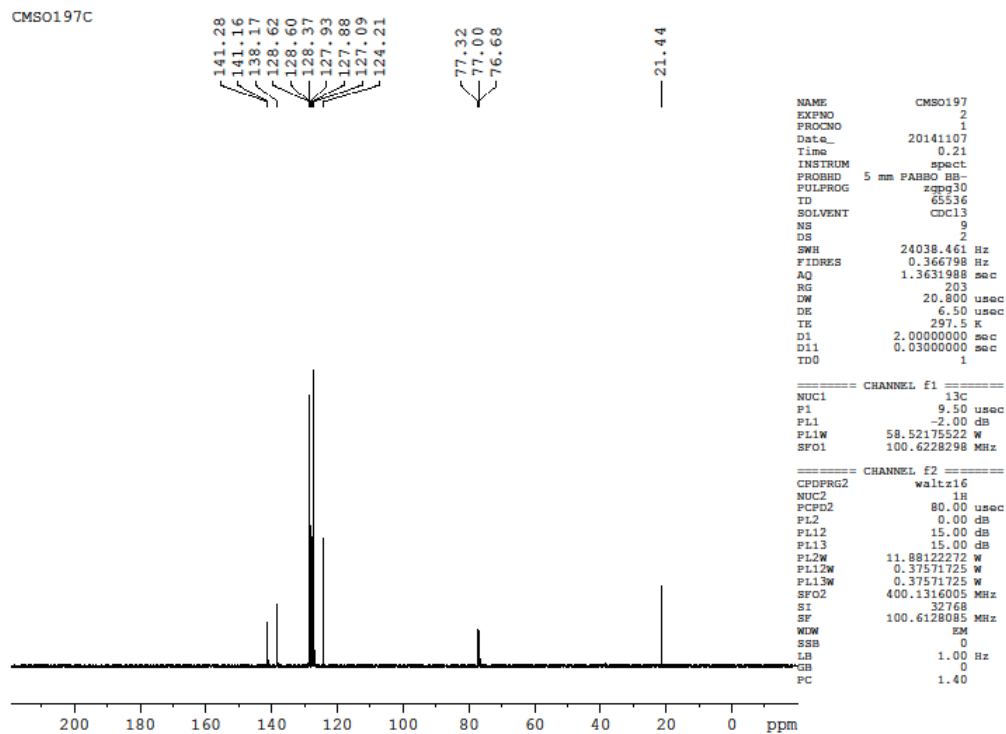
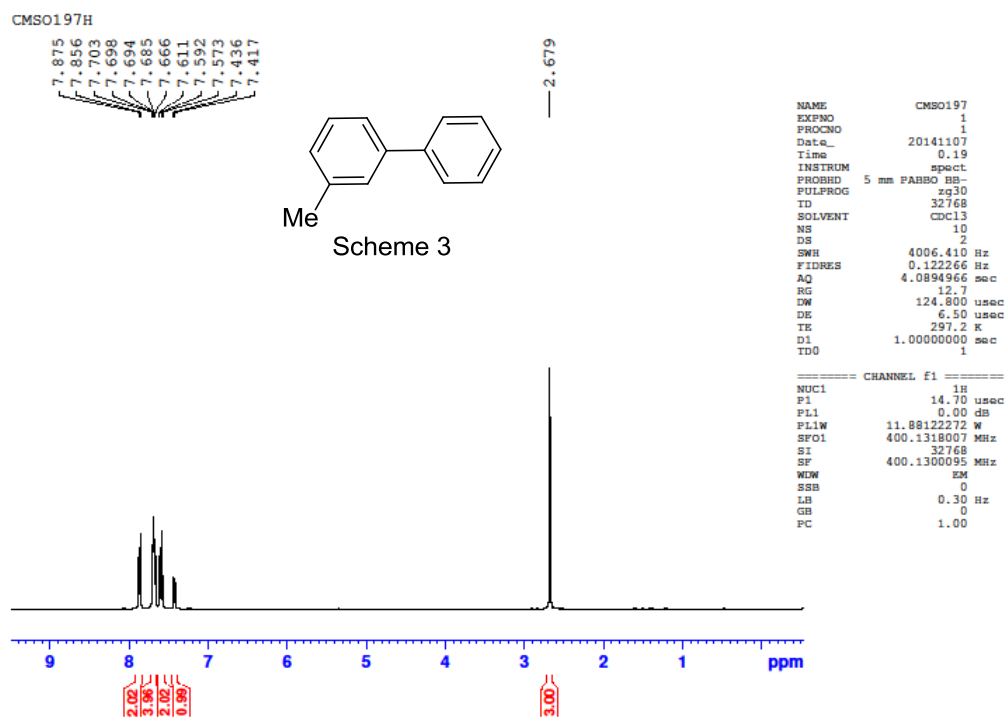


Mass	Calc. Mass	mDa	PPM	Formula
223.1231	223.1230	0.1	0.4	C15 H15 N2



HS





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