Experimental section

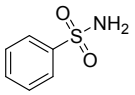
General comments

All reactions were carried out under air. Reactions were monitored by TLC analysis (pre-coated silica gel plates with fluorescent indicator UV254, 0.2 mm) and visualized with 254 nm UV light. Chemicals were purchased from Aldrich, Alfa-Asar, TCI and unless otherwise noted were used without further purification. All compounds were characterized by ^{1}H NMR and ^{13}C NMR spectroscopy and recorded on Bruker AV 300 and AV 400 spectrometers. Gas-chromatography-mass-analysis was performed using an Agilent HP-5890 with an Agilent HP-5973 Mass Selective Detector (EI) and an HP-5-capillary column using helium as a carrier gas.

General procedure for the synthesis of benzenesulfonamide

Benzenethiol (1 mmol), I_2 (20 mol%) were added in a 25 mL tube equipped with a stirring bar. 1 mL of acetonitrile, 5 equiv. of NH_3 (25% NH_3 in H_2O) and 5 equiv. of TBHP (70 wt. % in H_2O) were injected by syringe. After that, closed the tube and heated up to 100 ℃ for 16 h. When the reaction completed, cool the reaction mixture to room temperature. The reaction was quenched with distilled water and the solution was extracted with ethyl acetate. The crude product was purified by column chromatography (ethyl acetate/pentane = 1:4).

Benzenesulfonamide

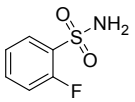


^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.97 – 7.91 (m, 2H), 7.63 (d, *J* = 1.3 Hz, 0H), 7.62 – 7.49 (m, 3H), 4.83 (s, 2H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 132.82, 129.16, 126.43.

GC-MS (EI, 70ev): m/z (%) = 77 (M+, 100), 157 (44), 141 (26), 94 (16), 93 (42), 51 (45), 50 (15).

2-Fluorobenzenesulfonamide

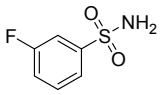


^{1}H NMR (300 MHz, DMSO-d_6) δ 7.81 (td, *J* = 7.7, 1.8 Hz, 1H), 7.67 (dddd, *J* = 8.3, 7.4, 5.1, 1.8 Hz, 3H), 7.49 – 7.31 (m, 2H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 158.03 (d, *J* = 252.3 Hz), 134.49 (d, *J* = 8.3 Hz), 131.49 (d, *J* = 14.2 Hz), 128.35, 124.54 (d, *J* = 3.9 Hz), 116.96 (d, *J* = 21.0 Hz).

GC-MS (EI, 70ev): m/z (%) = 95 (M+, 100), 175 (49), 159 (42), 112 (41), 111 (45), 75 (50), 69 (12) , 64 (15), 50 (10).

3-Fluorobenzenesulfonamide

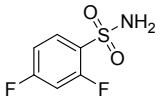


^{1}H NMR (300 MHz, DMSO-d_6) δ 7.71 – 7.57 (m, 3H), 7.55 – 7.43 (m, 3H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 163.19, 146.12 (d, *J* = 6.5 Hz), 131.37 (d, *J* = 8.1 Hz), 121.75 (d, *J* = 3.2 Hz), 118.89 (d, *J* = 21.1 Hz), 112.63 (d, *J* = 24.1 Hz).

GC-MS (EI, 70ev): m/z (%) = 95 (M+, 100), 175 (30), 159 (14), 112 (14), 111 (50), 75 (36).

2,4-Difluorobenzenesulfonamide

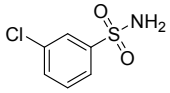


^{1}H NMR (300 MHz, DMSO-d_6) δ 7.86 (td, *J* = 8.7, 6.4 Hz, 1H), 7.73 (s, 2H), 7.52 (ddd, *J* = 10.6, 9.2, 2.5 Hz, 1H), 7.26 (dddd, *J* = 8.8, 8.3, 2.5, 1.1 Hz, 1H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 130.28 (d, *J* = 10.4 Hz), 128.48, 128.24 , 111.91 (d, *J* = 3.9 Hz), 111.62 (d, *J* = 3.6 Hz), 106.68 – 104.83 (m).

GC-MS (EI, 70ev): m/z (%) = 113 (M+, 100), 193 (57), 177 (68), 130 (49), 129 (63), 101 (19), 64 (20), 63 (57).

3-Chlorobenzenesulfonamide

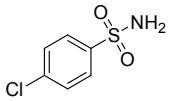


^{1}H NMR (300 MHz, DMSO-d_6) δ 7.84 (ddd, *J* = 2.2, 1.7, 0.5 Hz, 1H), 7.78 (ddd, *J* = 7.6, 1.7, 1.2 Hz, 1H), 7.70 (ddd, *J* = 8.0, 2.1, 1.3 Hz, 1H), 7.62 (ddd, *J* = 8.0, 7.6, 0.5 Hz, 1H), 7.52 (s, 2H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 145.86, 133.44, 131.73, 131.09, 125.35, 124.21.

GC-MS (EI, 70ev): m/z (%) = 111 (M+, 100), 193 (14), 191 (37), 175 (16), 129 (24), 128 (16), 127 (71), 113 (32), 76 (11), 75 (59), 74 (16), 64 (11), 50 (20).

4-Chlorobenzenesulfonamide

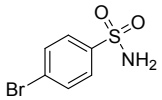


^{1}H NMR (300 MHz, DMSO-d_6) δ 7.91 – 7.78 (m, 2H), 7.72 – 7.60 (m, 2H), 7.48 (s, 2H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 142.92, 136.51, 129.03, 127.55.

GC-MS (EI, 70ev): m/z (%) = 111 (M+, 100), 193 (14), 191 (39), 177 (15), 175 (40) 129 (10), 128 (29), 127 (27), 113 (31), 76 (11), 75 (56), 74 (17), 64 (10), 50 (21).

4-Bromobenzenesulfonamide

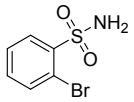


^{1}H NMR (300 MHz, DMSO-d_6) δ 7.83 – 7.78 (m, 1H), 7.78 – 7.73 (m, 1H), 7.48 (s, 1H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 143.32, 131.96, 127.67, 125.39.

GC-MS (EI, 70ev): m/z (%) = 155 (M+, 100), 237 (53), 235 (51), 221 (40), 219 (40) 174 (33), 173 (35), 172 (35), 171 (35), 157 (97), 76 (76), 75 (86), 74 (41), 65 (16), 64 (21), 63 (11), 51 (10), 50 (64).

2-Bromobenzenesulfonamide

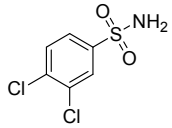


^{1}H NMR (300 MHz, DMSO-d_6) δ 8.06 – 7.97 (m, 1H), 7.83 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.63 – 7.44 (m, 4H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 142.62, 134.94, 133.30, 129.07, 127.93, 118.80.

GC-MS (EI, 70ev): m/z (%) = 155 (M+, 100), 237 (64), 235 (63), 221 (18), 219 (18) 174 (48), 173 (40), 172 (50), 171 (40), 157 (99), 156 (18), 108 (19), 92 (51), 80 (10), 77 (15), 76 (85), 75 (94), 74 (42), 65 (26), 64 (36), 63 (13), 51 (14), 50 (73).

3,4-Dichlorobenzenesulfonamide

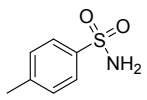


^{1}H NMR (300 MHz, DMSO-d_6) δ 8.01 (d, *J* = 2.1 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.77 (ddd, *J* = 8.4, 2.1, 0.5 Hz, 1H), 7.60 (s, 2H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 144.27, 134.73, 131.70, 131.43, 127.54, 125.76.

GC-MS (EI, 70ev): m/z (%) = 145 (M+, 100), 227 (30), 225 (44), 211 (24), 209 (35), 164 (18), 163 (36) , 162 (28), 161 (56), 149 (11), 147 (63), 111 (22) , 110 (15), 109 (58), 84 (13), 75 (38), 74 (46), 73 (13), 64 (19) , 50 (10).

4-Methylbenzenesulfonamide

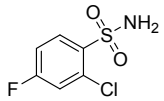


^{1}H NMR (300 MHz, DMSO-d_6) δ 7.81 – 7.57 (m, 2H), 7.42 – 7.32 (m, 1H), 7.29 (s, 2H), 2.37 (s, 3H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 141.82, 141.36, 129.25, 125.57, 20.87.

GC-MS (EI, 70ev): m/z (%) = 91 (M+, 100), 171 (37), 155 (32), 108 (14), 107 (23), 89 (10), 65 (30) , 63 (11), 39 (11).

2-Chloro-4-fluorobenzenesulfonamide

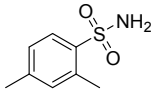


^{1}H NMR (300 MHz, DMSO-d_6) δ 8.04 (dd, *J* = 8.9, 6.0 Hz, 1H), 7.72 – 7.64 (m, 3H), 7.41 (ddd, *J* = 8.9, 8.2, 2.6 Hz, 1H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 163.28 (d, *J* = 253.3 Hz), 137.71 (d, *J* = 3.6 Hz), 132.09 (d, *J* = 11.5 Hz), 131.19 (d, *J* = 9.9 Hz), 118.89 (d, *J* = 25.8 Hz), 114.51 (d, *J* = 21.7 Hz).

GC-MS (EI, 70ev): m/z (%) = 129 (M+, 100), 211 (19), 209 (50), 195 (17), 193 (47), 148 (18), 147 (21) , 146 (56), 145 (53), 131 (33), 117 (10), 109 (26) , 94 (27), 93 (29), 74 (19), 64 (23), 50 (12).

2,4-Dimethylbenzenesulfonamide

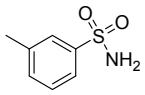


^{1}H NMR (300 MHz, DMSO-d_6) δ 7.74 (d, *J* = 7.9 Hz, 1H), 7.30 (s, 2H), 7.22 – 7.07 (m, 2H), 2.56 (s, 3H), 2.32 (s, 3H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 141.73, 139.41, 135.65, 132.63, 127.12, 126.29, 20.61, 19.70.

GC-MS (EI, 70ev): m/z (%) = 104 (M+, 100), 185 (23), 151 (10), 120 (36), 103 (23), 105 (62), 91 (11) , 79 (24), 78 (29), 77 (41), 51 (12), 39 (10).

3-Methylbenzenesulfonamide

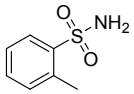


^{1}H NMR (300 MHz, DMSO-d_6) δ 7.72 – 7.57 (m, 2H), 7.50 – 7.37 (m, 2H), 7.31 (s, 2H), 2.39 (s, 3H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 144.00, 138.45, 132.30, 128.76, 125.81, 122.69, 20.84.

GC-MS (EI, 70ev): m/z (%) = 91 (M+, 100), 171 (30), 155 (12), 107 (28), 106 (30), 89 (11), 65 (33), 63 (12), 39 (13).

2-Methylbenzenesulfonamide

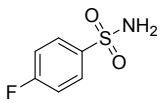


^{1}H NMR (300 MHz, DMSO-d_6) δ 7.87 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.55 – 7.44 (m, 1H), 7.44 – 7.28 (m, 4H), 2.60 (s, 3H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 142.07, 135.80, 132.11, 131.78, 126.92, 125.97, 19.79.

GC-MS (EI, 70ev): m/z (%) = 90 (M+, 100), 171 (21), 137 (17), 107 (13), 106 (69), 89 (35), 77 (12) , 65 (40), 63 (18), 51 (10), 39 (16).

4-Fluorobenzenesulfonamide

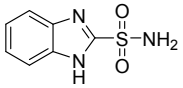


^{1}H NMR (300 MHz, DMSO-d_6) δ 7.95 – 7.82 (m, 2H), 7.52 – 7.32 (m, 4H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 163.63 (d, J = 249.8 Hz), 140.52 (d, J = 3.1 Hz), 128.49 (d, J = 9.6 Hz), 115.96 (d, J = 22.7 Hz).

GC-MS (EI, 70ev): m/z (%) = 95 (M+, 100), 175 (38), 159 (47), 112 (17), 111 (18), 75 (35).

1*H*-benzo[*d*]imidazole-2-sulfonamide

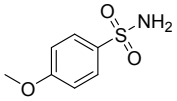


^{1}H NMR (300 MHz, DMSO-d_6) δ 13.46 (s, 1H), 8.05 (s, 2H), 7.75 (d, *J* = 7.9 Hz, 1H), 7.56 (d, *J* = 7.9 Hz, 1H), 7.43 – 7.25 (m, 2H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 151.59, 141.90, 133.61, 124.61, 122.89, 120.13, 112.64.

HRMS(ESI): calcd. for $[C_7H_7N_3O_2S + H]^+$: 198.03317; fond: 198.03356.

4-Methoxybenzenesulfonamide

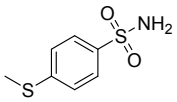


^{1}H NMR (300 MHz, DMSO-d_6) δ 7.82 – 7.70 (m, 2H), 7.22 (s, 2H), 7.15 – 7.03 (m, 2H), 3.82 (s, 3H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 161.57, 136.12, 127.62, 113.95, 55.54.

GC-MS (EI, 70ev): m/z (%) = 171 (M+, 100), 187 (81), 123 (33), 107 (53), 92 (50), 77 (77), 64 (36), 63 (30), 50 (12).

4-(Methylthio)benzenesulfonamide

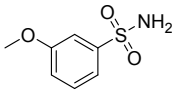


^{1}H NMR (300 MHz, DMSO-d_6) δ 7.78 – 7.67 (m, 2H), 7.50 – 7.36 (m, 2H), 7.32 (s, 2H), 2.53 (s, 3H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 143.47, 140.07, 126.05, 125.17, 14.08.

GC-MS (EI, 70ev): m/z (%) = 203 (M+, 100), 187 (34), 140 (14), 139 (40), 124 (11), 123 (39), 108 (23) , 79 (23), 77 (20), 69 (16), 63 (12), 50 (11) , 45 (38).

3-Methoxybenzenesulfonamide

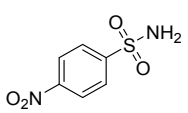


^{1}H NMR (300 MHz, DMSO-d_6) δ 7.49 (t, *J* = 7.9 Hz, 1H), 7.43 – 7.32 (m, 4H), 7.17 (ddd, *J* = 8.1, 2.6, 1.1 Hz, 1H), 3.82 (s, 3H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 159.19, 145.31, 130.10, 117.57, 110.72, 55.49.

GC-MS (EI, 70ev): m/z (%) = 108 (M+, 100), 187 (95), 107 (100), 95 (10), 94 (18), 93 (22), 92 (75) , 80 (19), 78 (10), 77 (99), 76 (15), 64 (51) , 63 (43), 51 (10), 50 (15).

4-Nitrobenzenesulfonamide

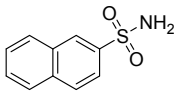


^{1}H NMR (300 MHz, DMSO-d_6) δ 8.66 – 8.27 (m, 1H), 8.25 – 7.94 (m, 1H), 7.74 (s, 1H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 149.33, 149.13, 127.17, 124.40.

GC-MS (EI, 70ev): m/z (%) = 138 (M+, 100), 202 (76), 186 (37), 156 (16), 139 (41), 122 (46), 109 (24) , 108 (36), 92 (33), 80 (20), 76 (61), 75 (99) , 74 (41), 65 (22), 64 (55), 63 (26), 51 (12), 50 (65), 39 (12), 30 (15).

Naphthalene-2-sulfonamide

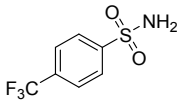


^{1}H NMR (300 MHz, DMSO-d_6) δ 8.50 – 8.39 (m, 1H), 8.18 – 8.08 (m, 2H), 8.07 – 7.99 (m, 1H), 7.89 (dd, *J* = 8.7, 1.9 Hz, 1H), 7.74 – 7.60 (m, 2H), 7.47 (s, 3H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 141.11, 133.82, 131.63, 129.00, 128.35, 127.74, 127.44, 125.64, 122.04.

GC-MS (EI, 70ev): m/z (%) = 127 (M+, 100), 207 (55), 144 (14), 143 (46), 128 (12), 126 (27), 115 (26) , 77 (12).

4-(Trifluoromethyl)benzenesulfonamide

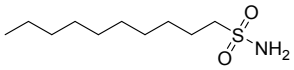


^{1}H NMR (300 MHz, DMSO-d_6) δ 8.10 – 8.01 (m, 1H), 8.01 – 7.92 (m, 1H), 7.64 (s, 1H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 147.75, 131.66 (q, *J* = 32.2 Hz), 126.57, 126.19 (q, *J* = 3.8 Hz), 123.52 (d, *J* = 272.6 Hz).

GC-MS (EI, 70ev): m/z (%) = 145 (M+, 100), 225 (26), 209 (14), 206 (10), 162 (20), 125 (14), 95 (16) , 75 (15).

Decane-1-sulfonamide



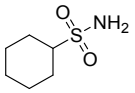
^{1}H NMR (300 MHz, DMSO-d_6) δ 6.71 (s, 2H), 2.99 – 2.87 (m, 2H), 1.67 (tt, *J* = 7.9, 6.1 Hz, 2H), 1.44 – 1.20 (m, 15H), 0.92 – 0.80 (m, 3H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 54.37, 31.27, 28.91, 28.77, 28.67, 28.59, 27.58, 23.47, 22.07, 13.90.

GC-MS (EI, 70ev): m/z (%) = 82 (M+, 100), 140 (62), 112 (42), 111 (37), 108 (34), 98 (30), 97 (59), 95 (15), 85 (21), 84 (58), 83 (68), 71 (28), 70 (67), 69 (71), 68 (28), 67(14), 64(10), 57(63), 56(64), 55(69), 54(11), 44(13), 43(66), 42(36), 41(71), 39(20).

HRMS(ESI): calcd. for $[C_{10}H_{23}NO_2S - H]^-$: 220:13767; fond: 220:13777.

Cyclohexanesulfonamide

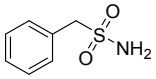


^{1}H NMR (300 MHz, DMSO-d_6) δ 6.62 (s, 2H), 2.74 (tt, *J* = 11.6, 3.5 Hz, 1H), 2.13 – 1.94 (m, 2H), 1.79 (dt, *J* = 12.6, 3.2 Hz, 2H), 1.63 (dqd, *J* = 12.4, 3.1, 1.4 Hz, 1H), 1.42 – 0.99 (m, 5H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 61.26, 26.28, 24.90, 24.52.

GC-MS (EI, 70ev): m/z (%) = 55 (M+, 100), 84 (33), 83 (98), 82 (50), 81 (21), 79 (12), 67 (43), 56 (24), 54 (19), 53 (16), 43 (11), 41 (88), 39 (34).

Phenylmethanesulfonamide

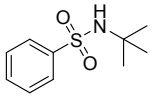


^{1}H NMR (300 MHz, DMSO-d_6) δ 7.46 – 7.28 (m, 5H), 6.85 (s, 2H), 4.27 (s, 2H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 130.73, 128.23, 127.84, 60.16.

GC-MS (EI, 70ev): m/z (%) = 91 (M+, 100), 65 (15).

N-(*tert*-Butyl)benzenesulfonamide



^{1}H NMR (300 MHz, DMSO-d_6) δ 7.90 – 7.78 (m, 2H), 7.64 – 7.48 (m, 3H), 1.08 (s, 9H).

^{13}C NMR (75 MHz, DMSO-d_6) δ 144.23, 131.75, 128.88, 126.18, 53.16, 29.69.

HRMS(ESI): calcd. for $[C_{10}H_{15}NO_2S + Na]^+$: 236.07157; fond: 236.07166.

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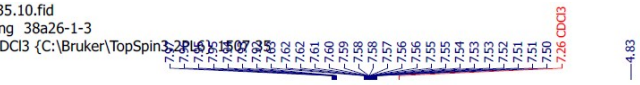
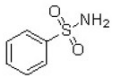
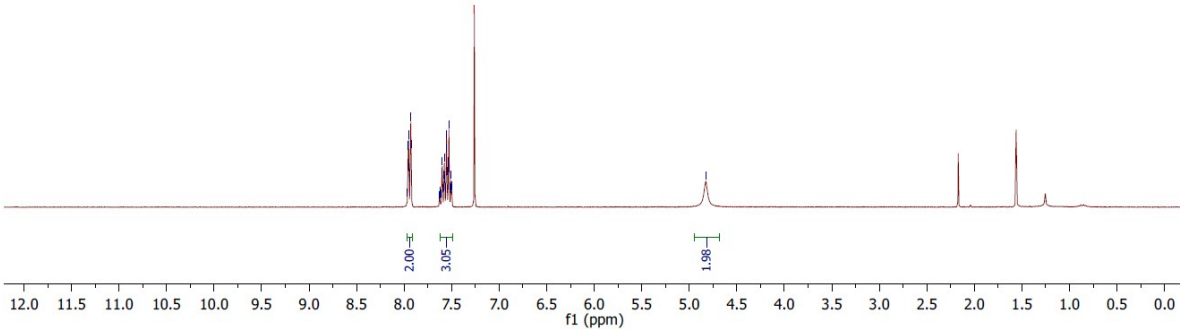
Jian-Bo Feng 38a26-1-3
PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1507 35







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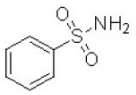

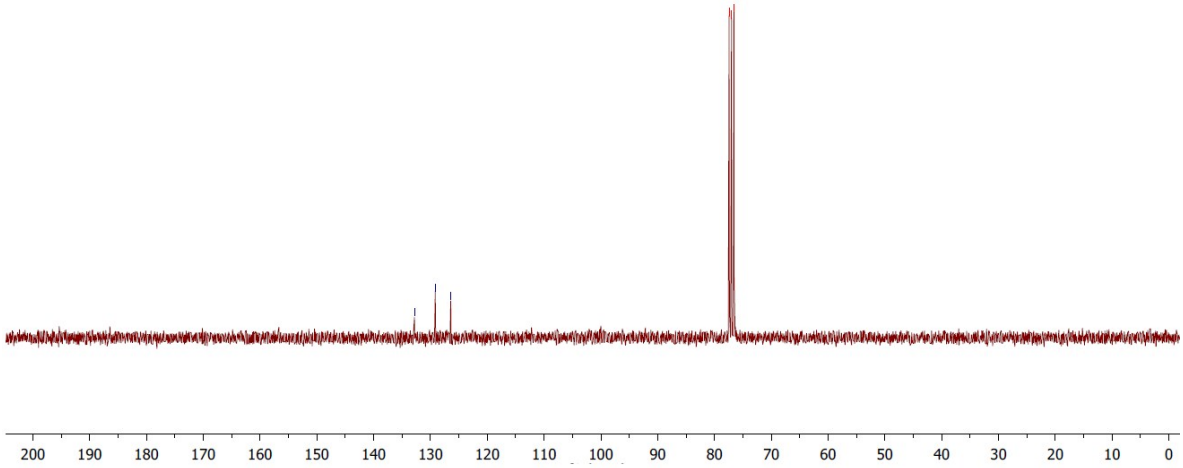

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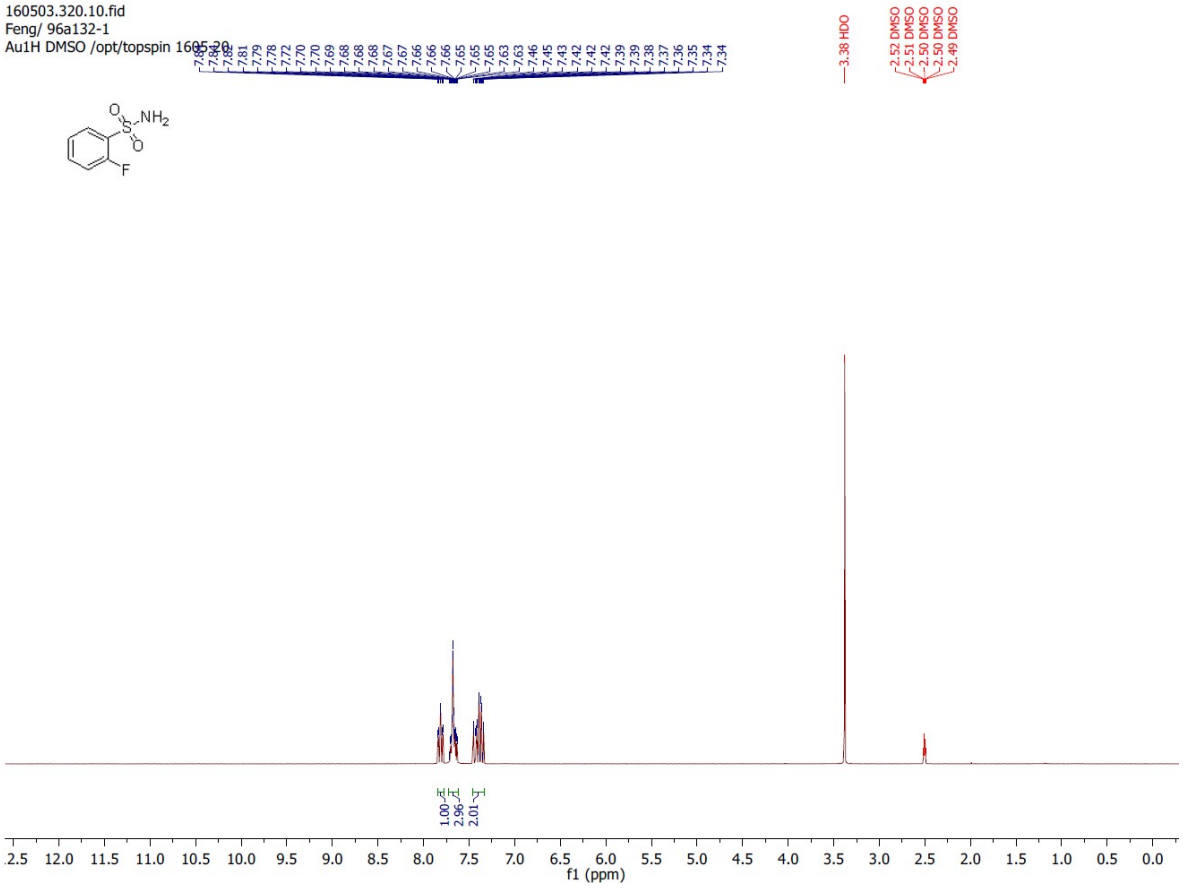
Feng/ 96a132-1
Au1H DMSO /opt/topspin 1605 20



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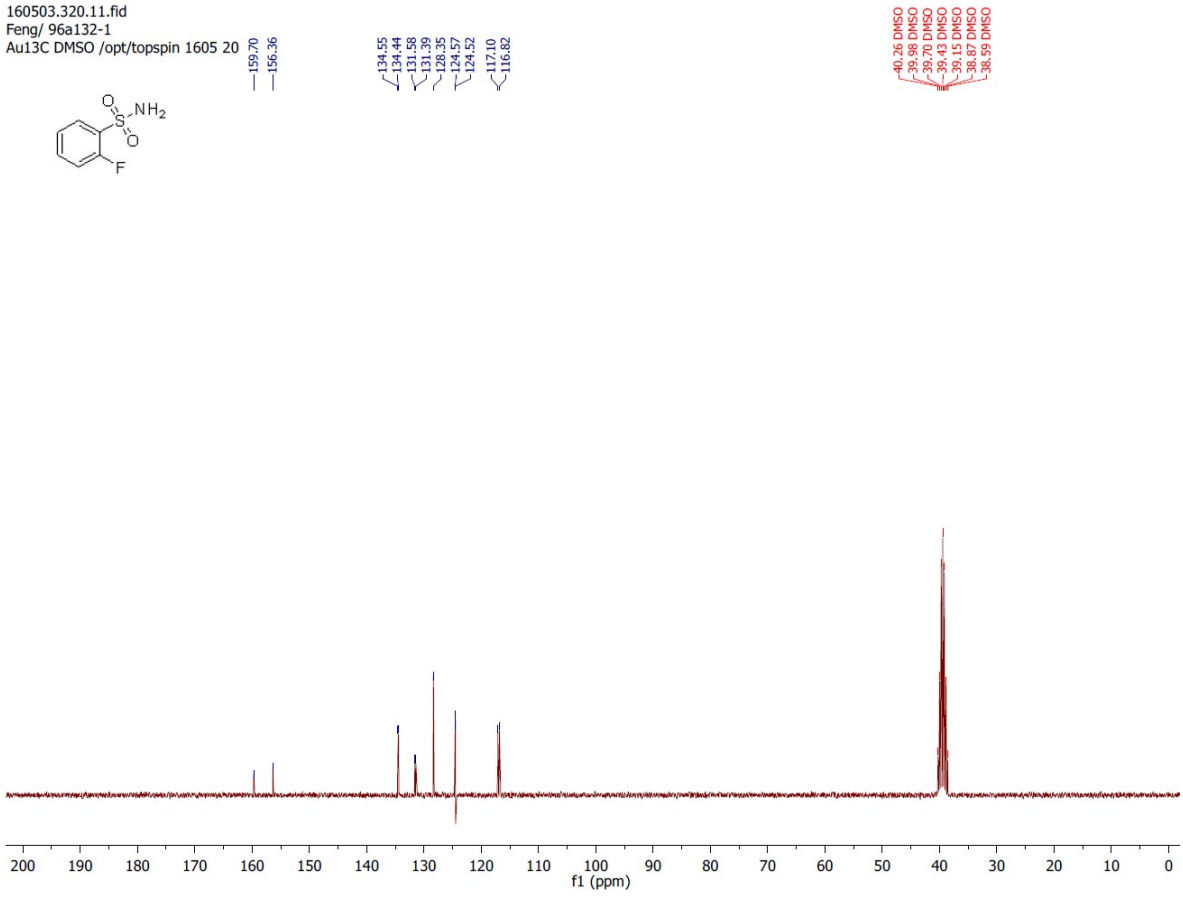
Au13C DMSO /opt/topspin 1605 20



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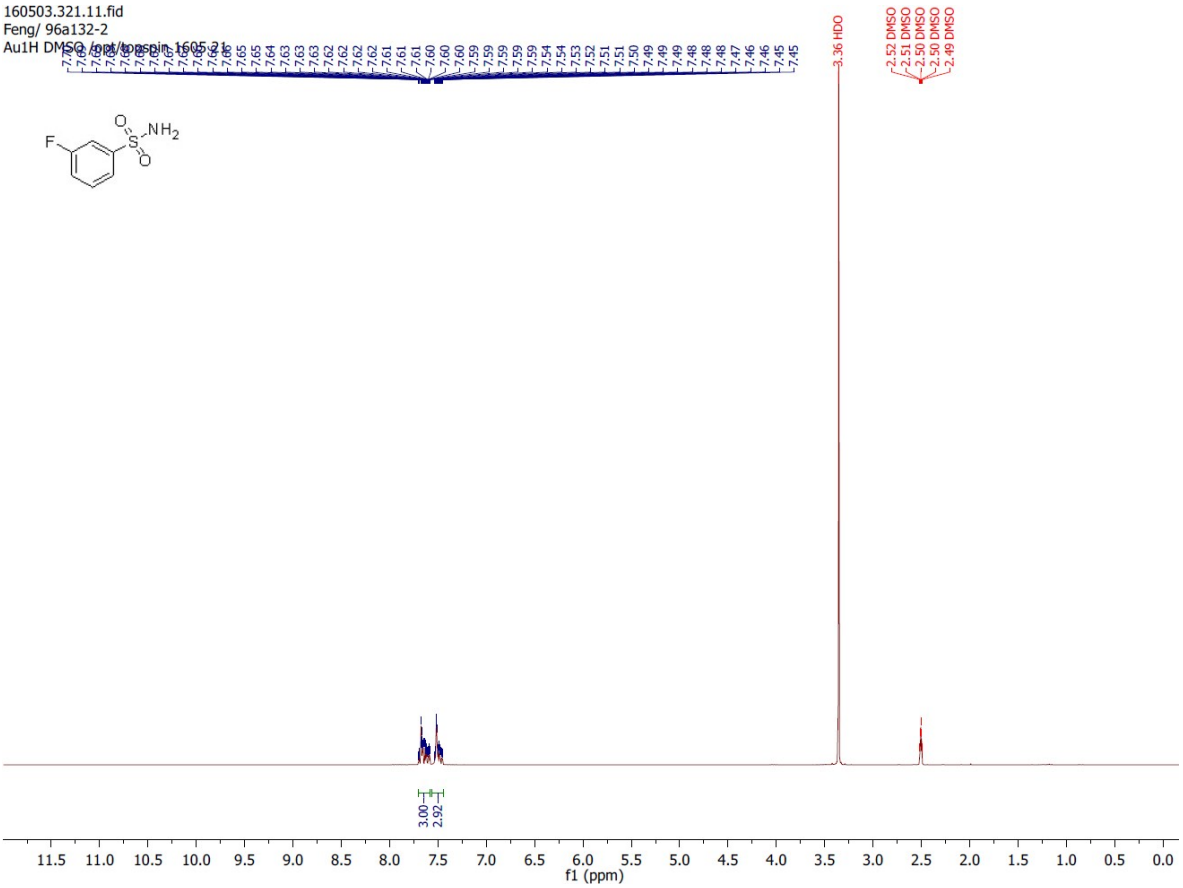

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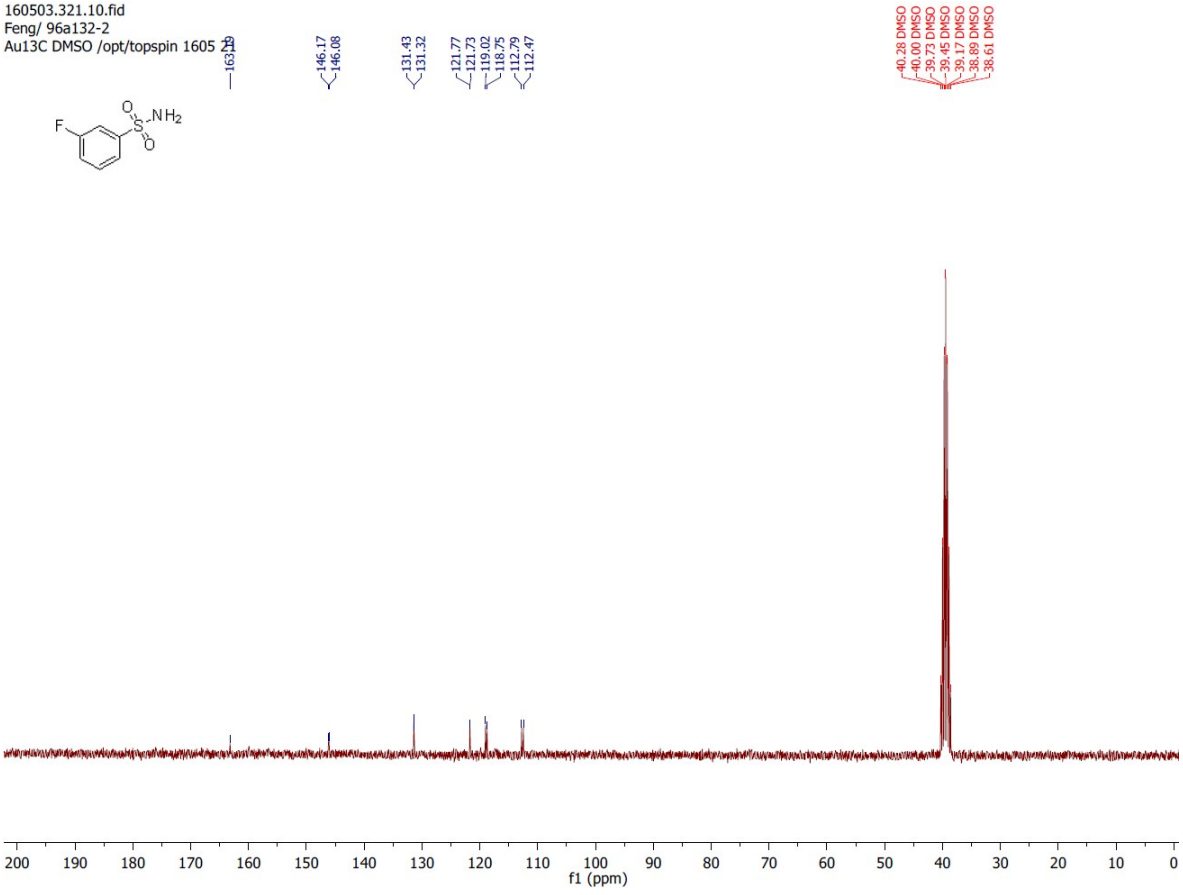

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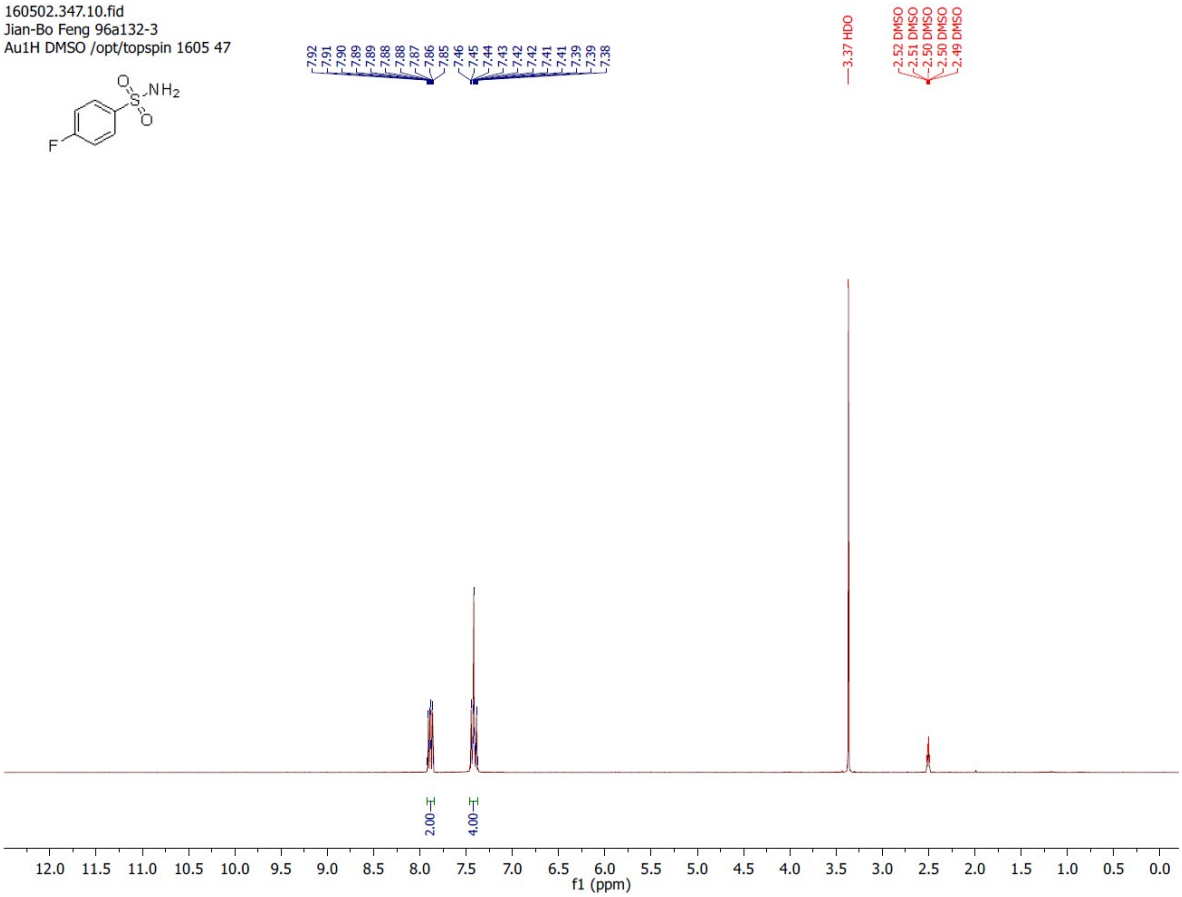

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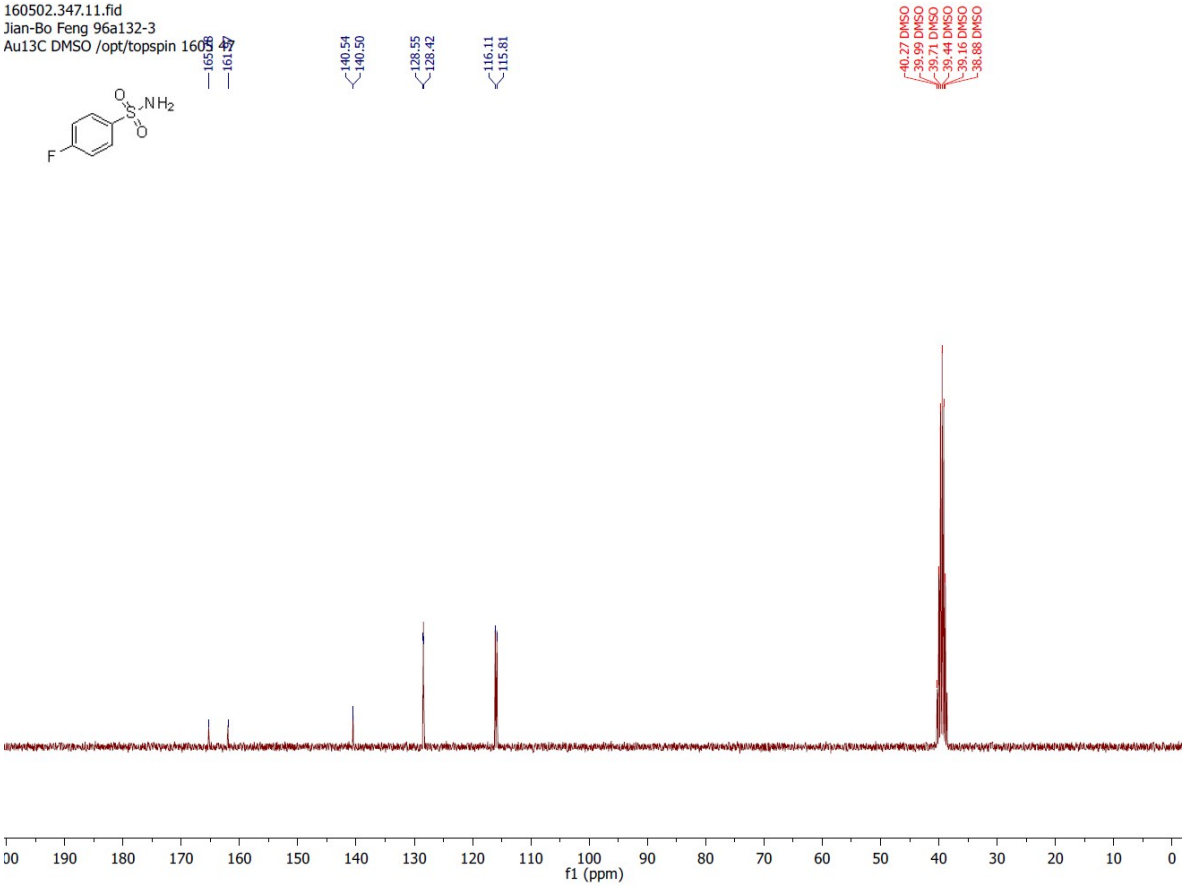
Au13C DMSO /opt/topspin 1605 47



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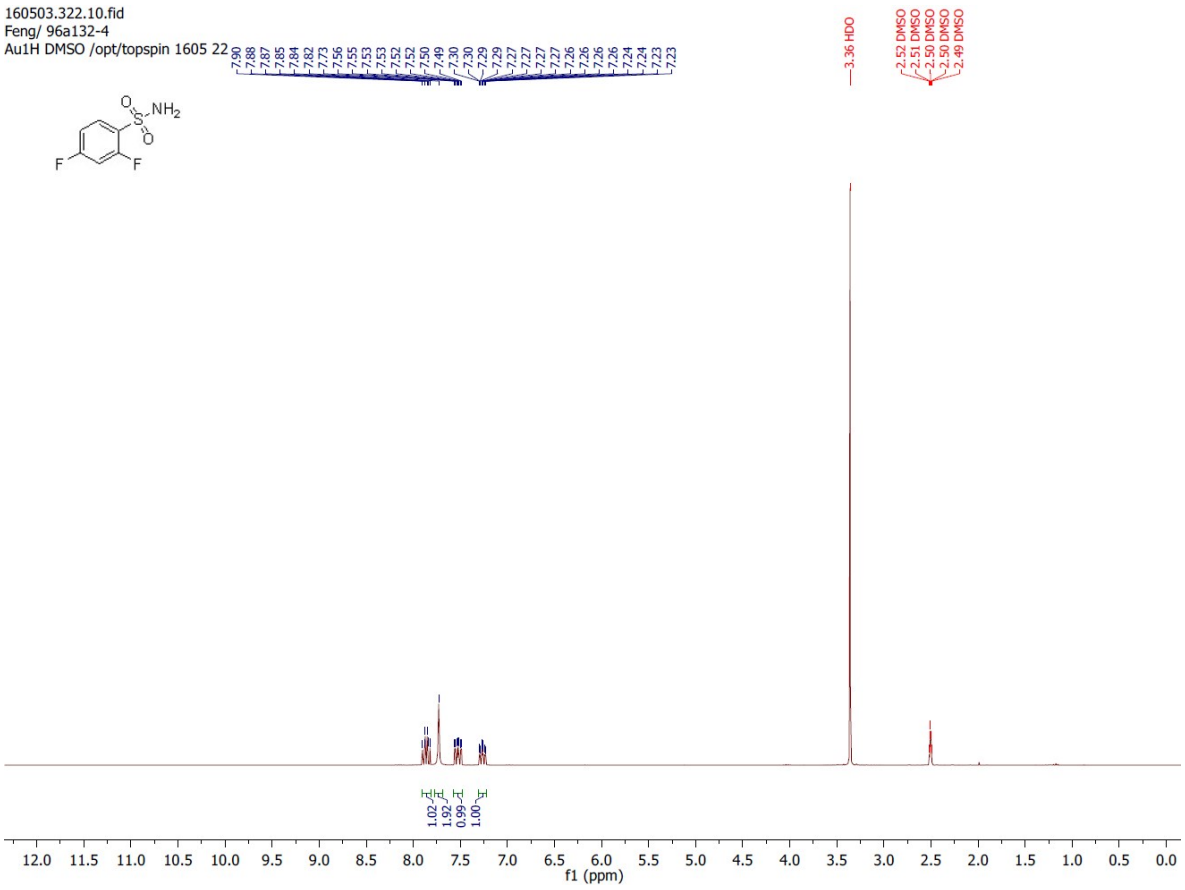

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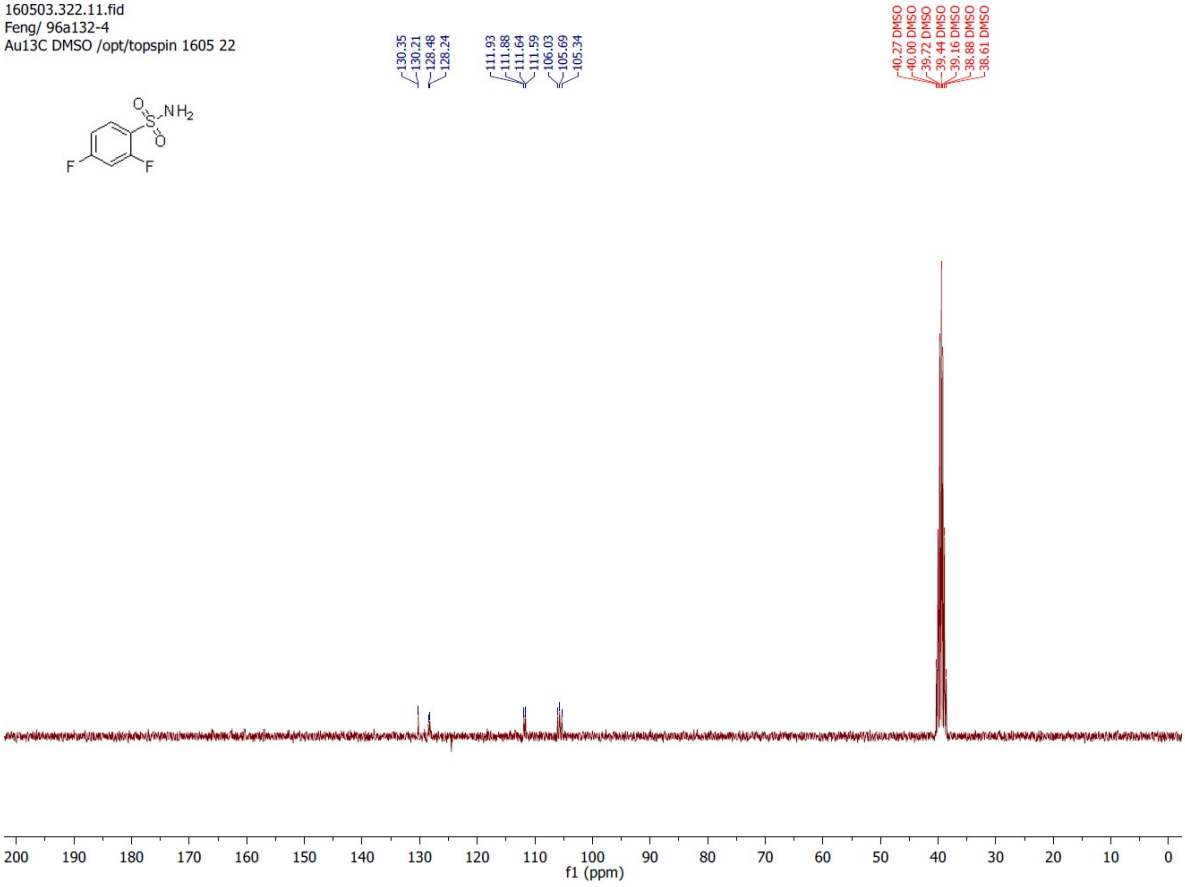

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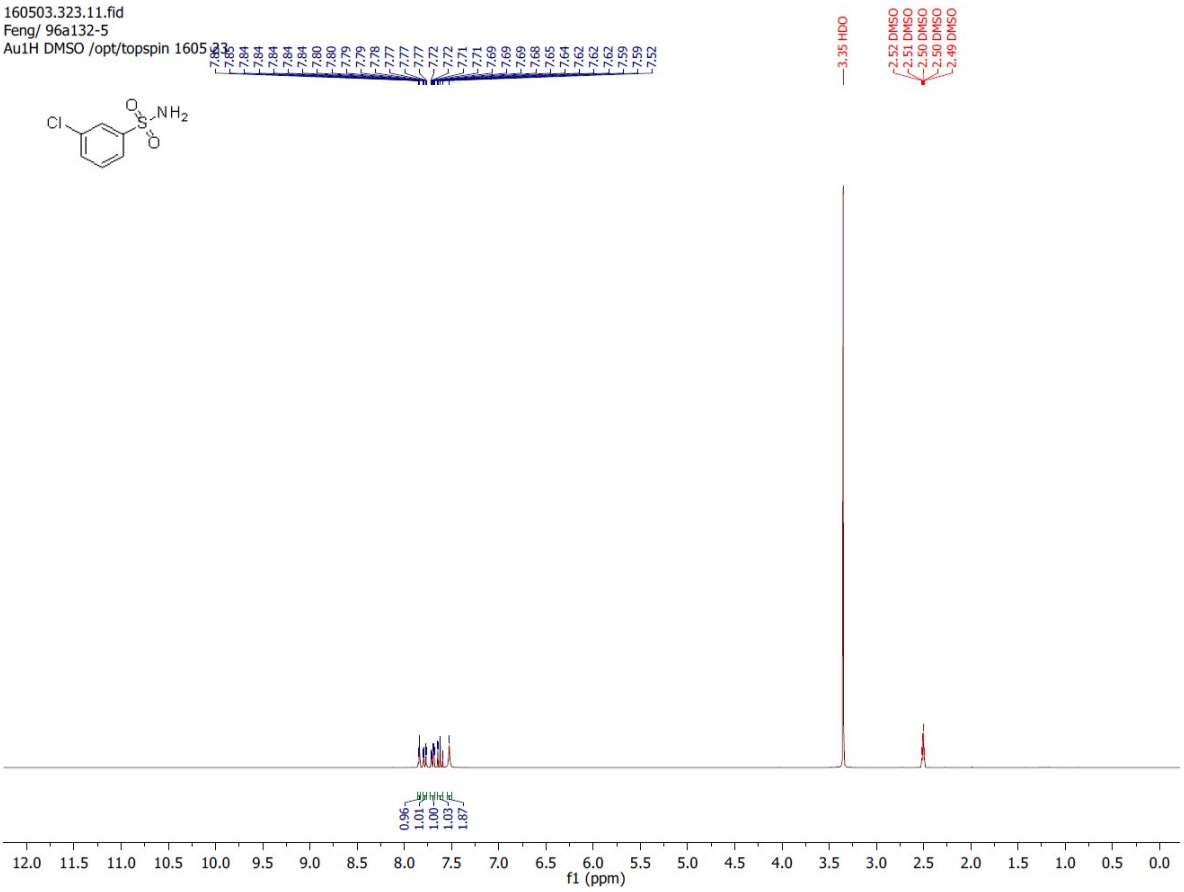

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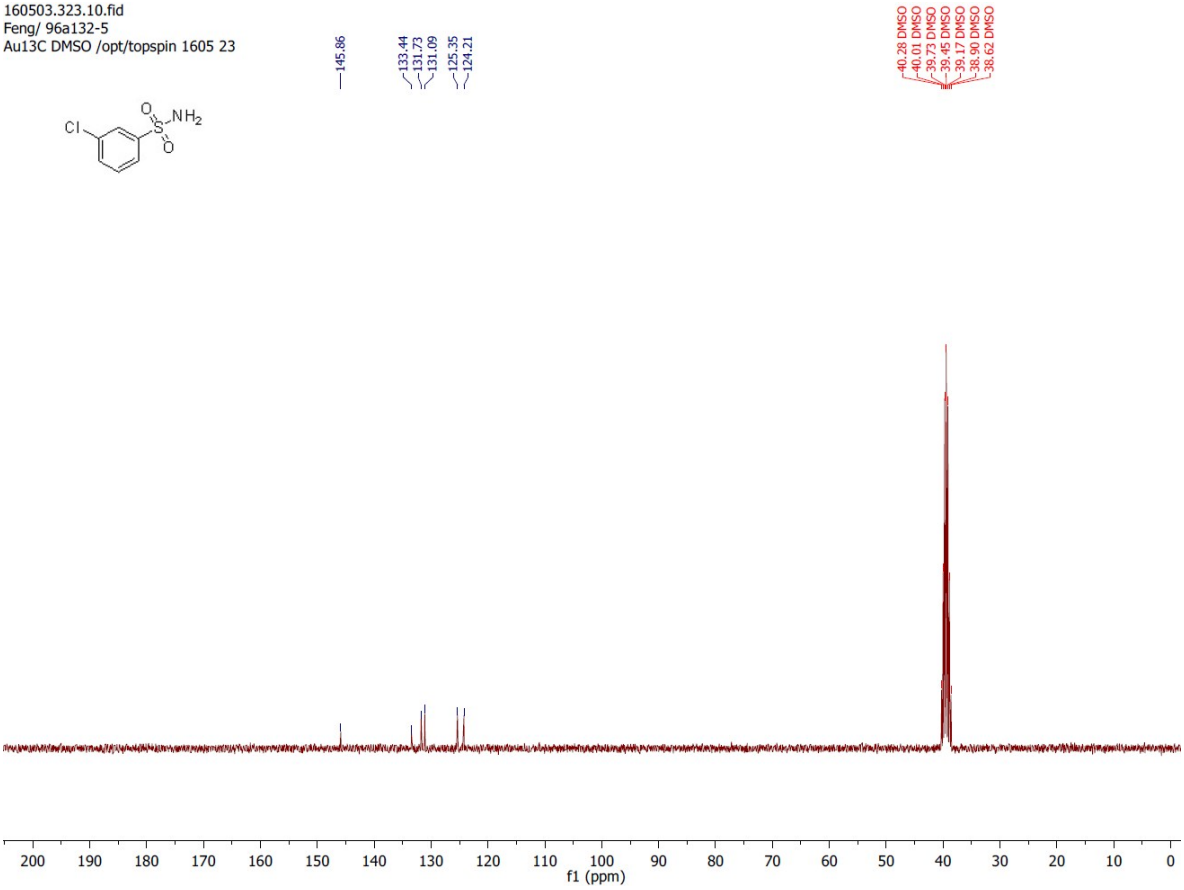

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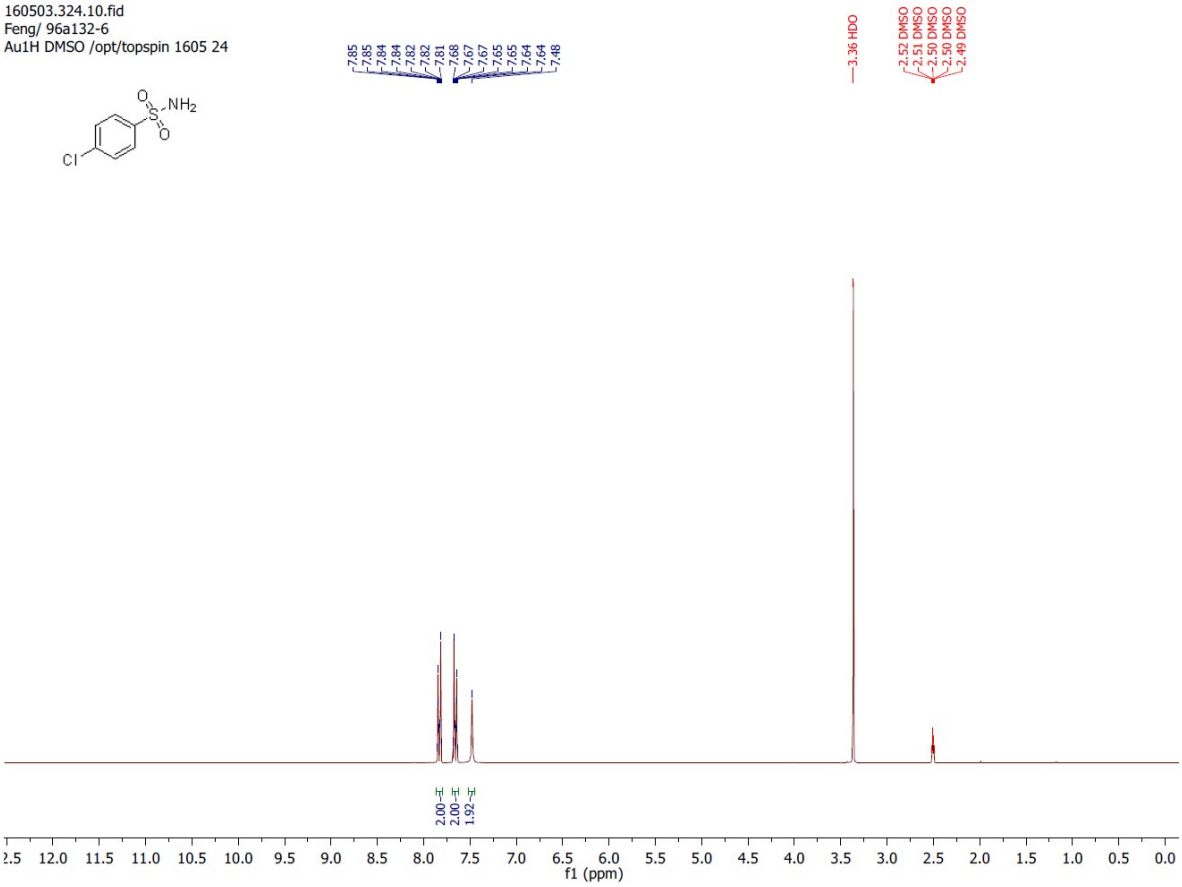

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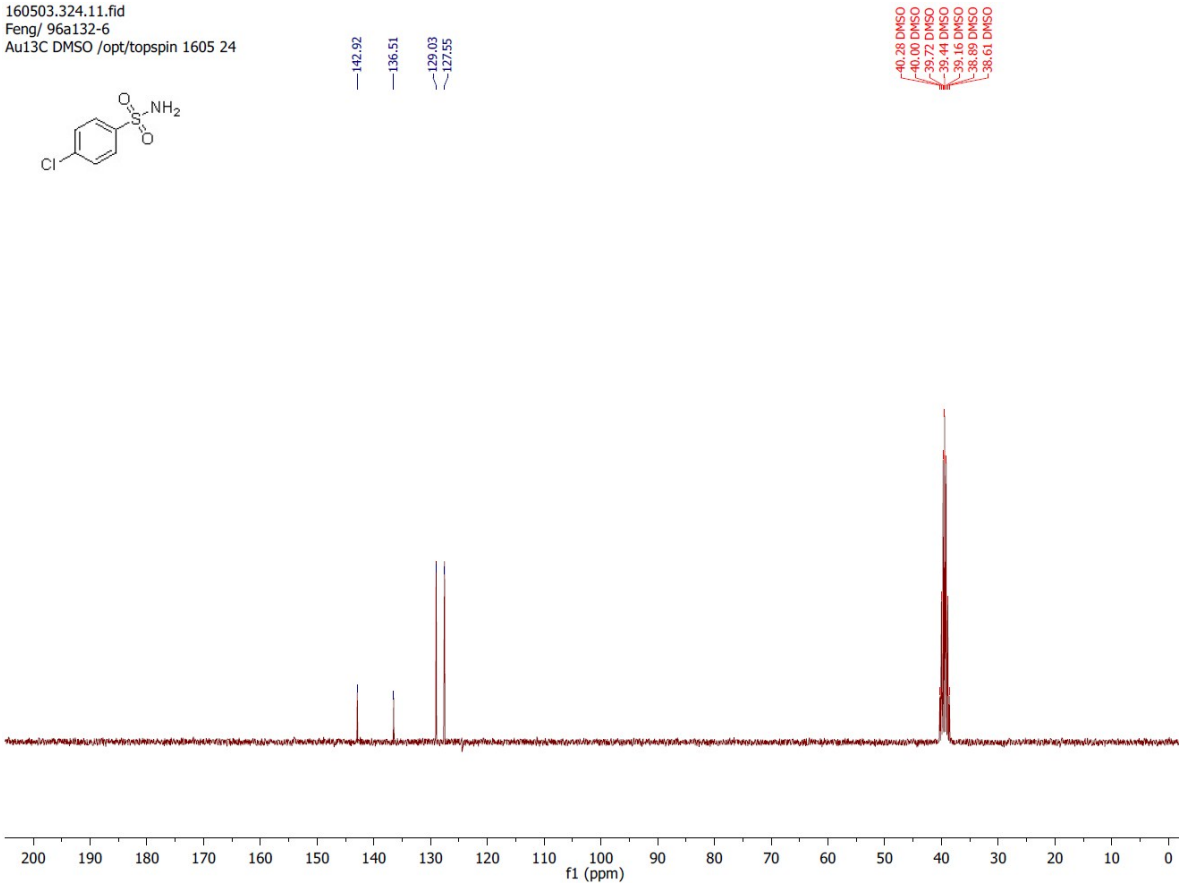

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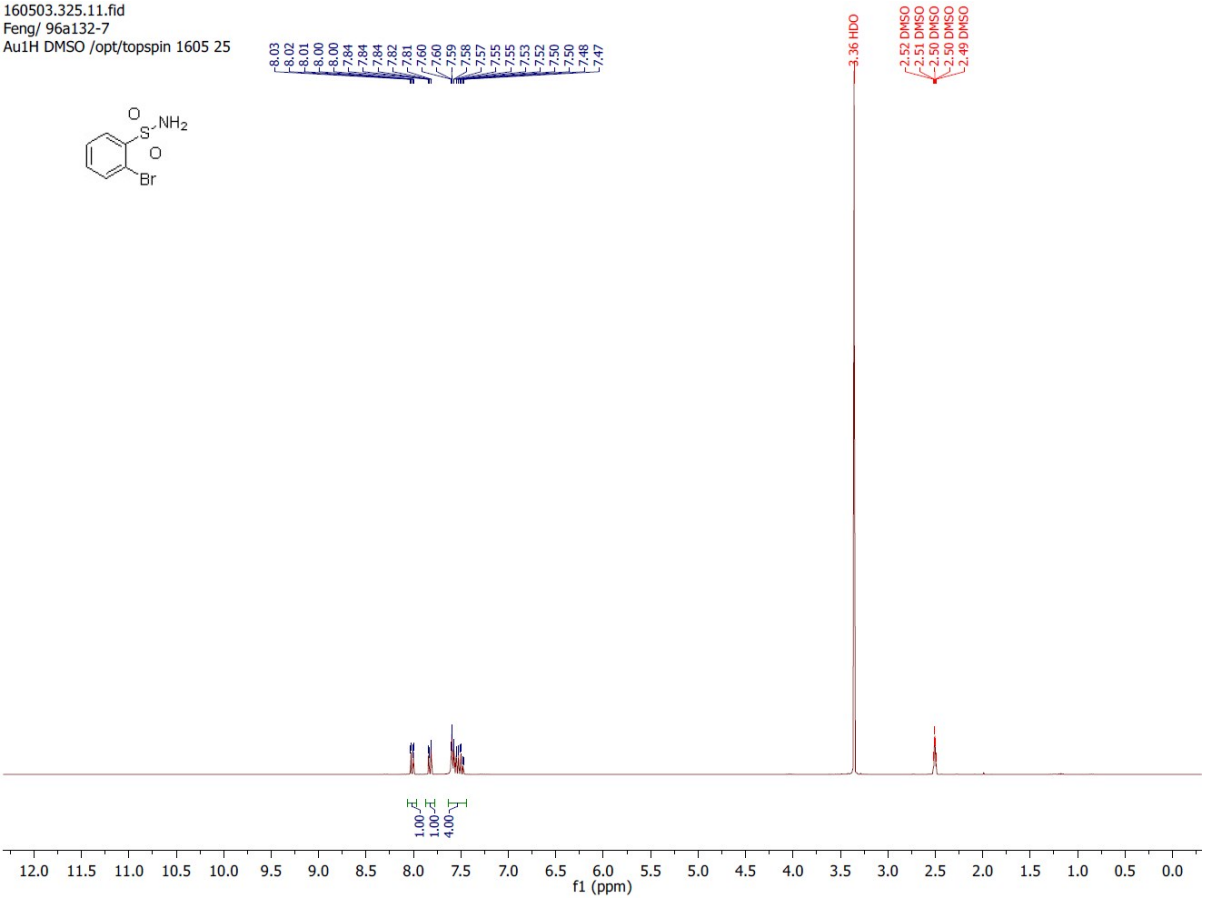

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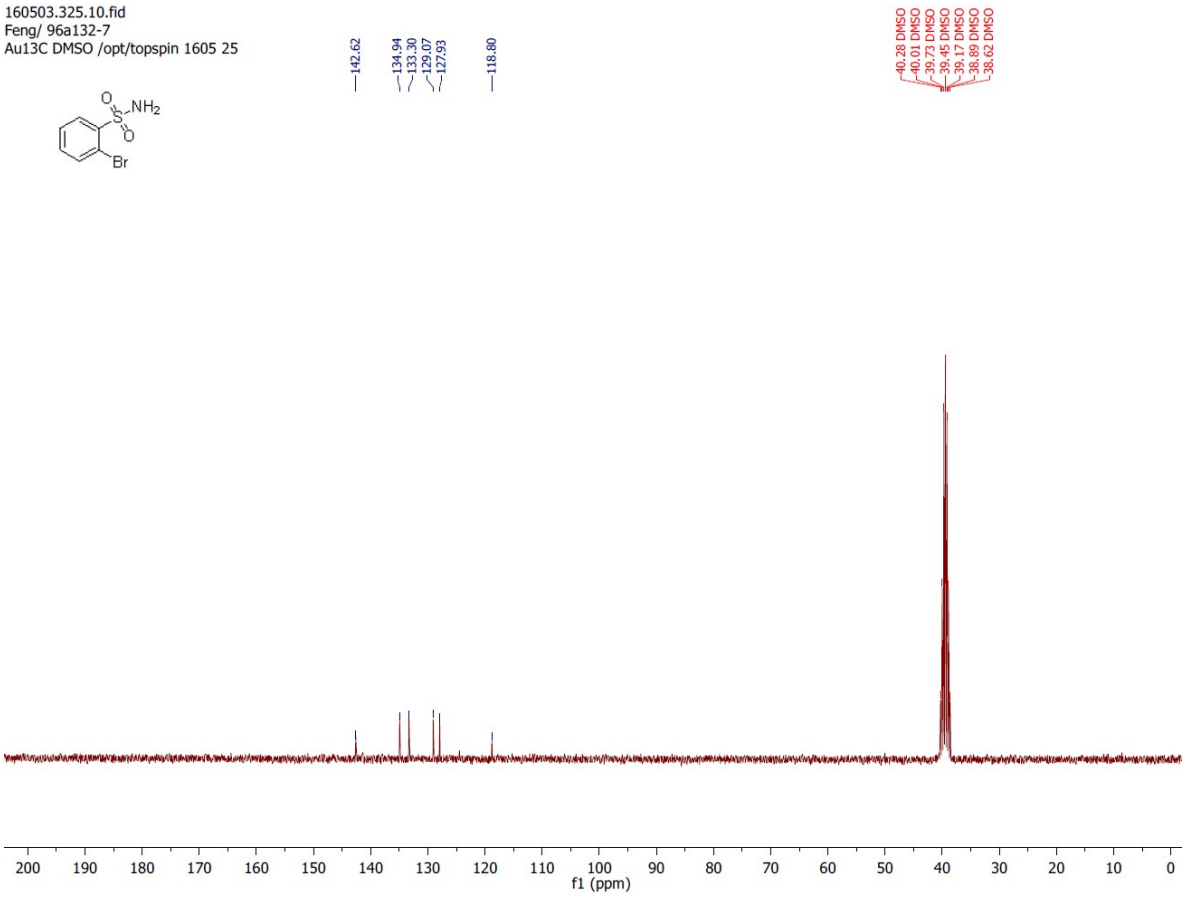

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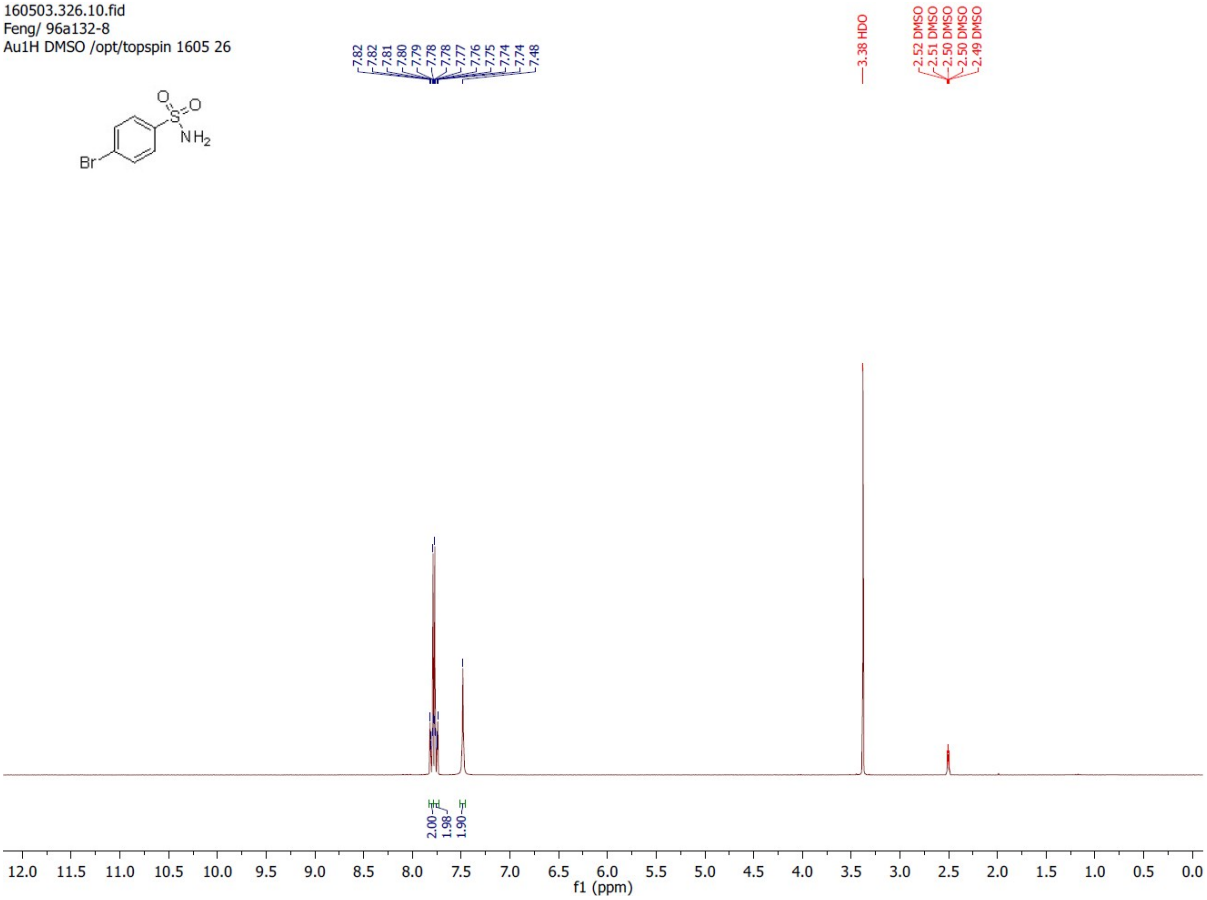

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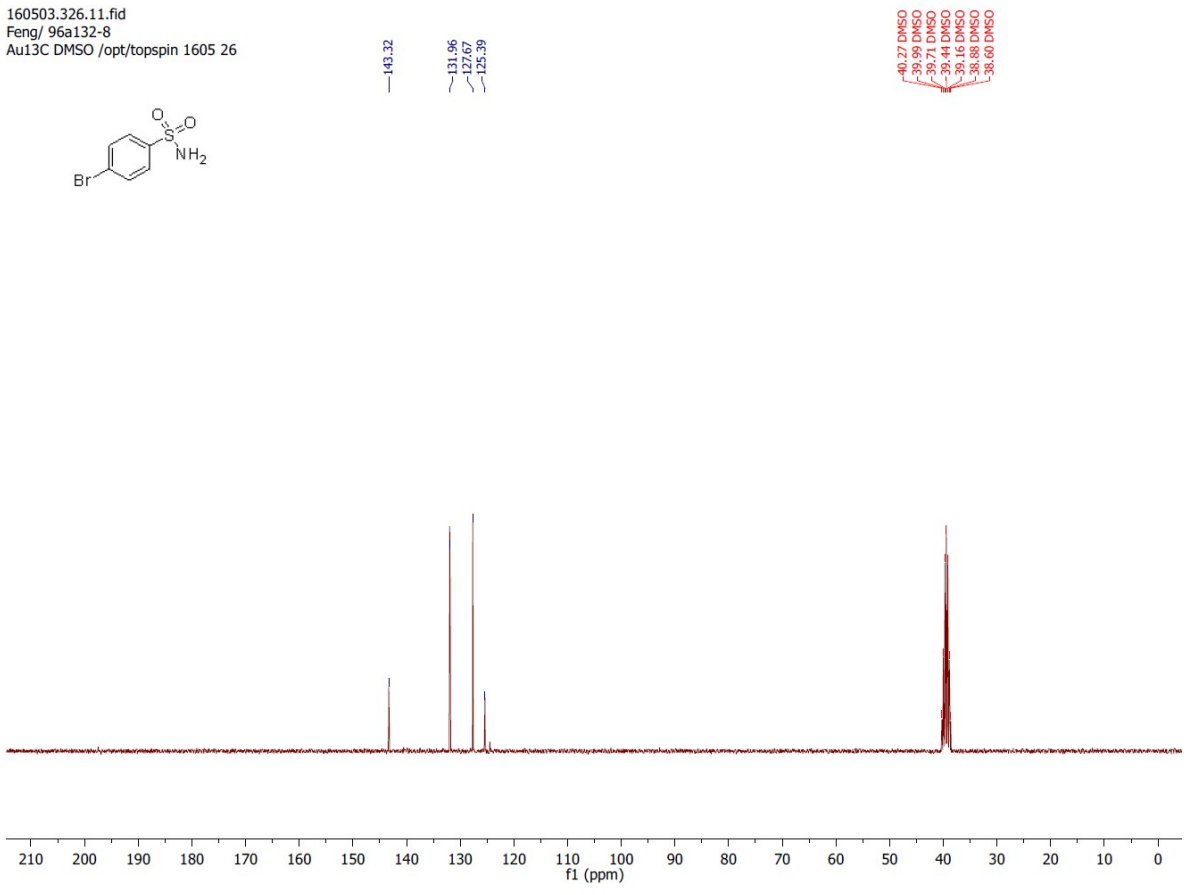

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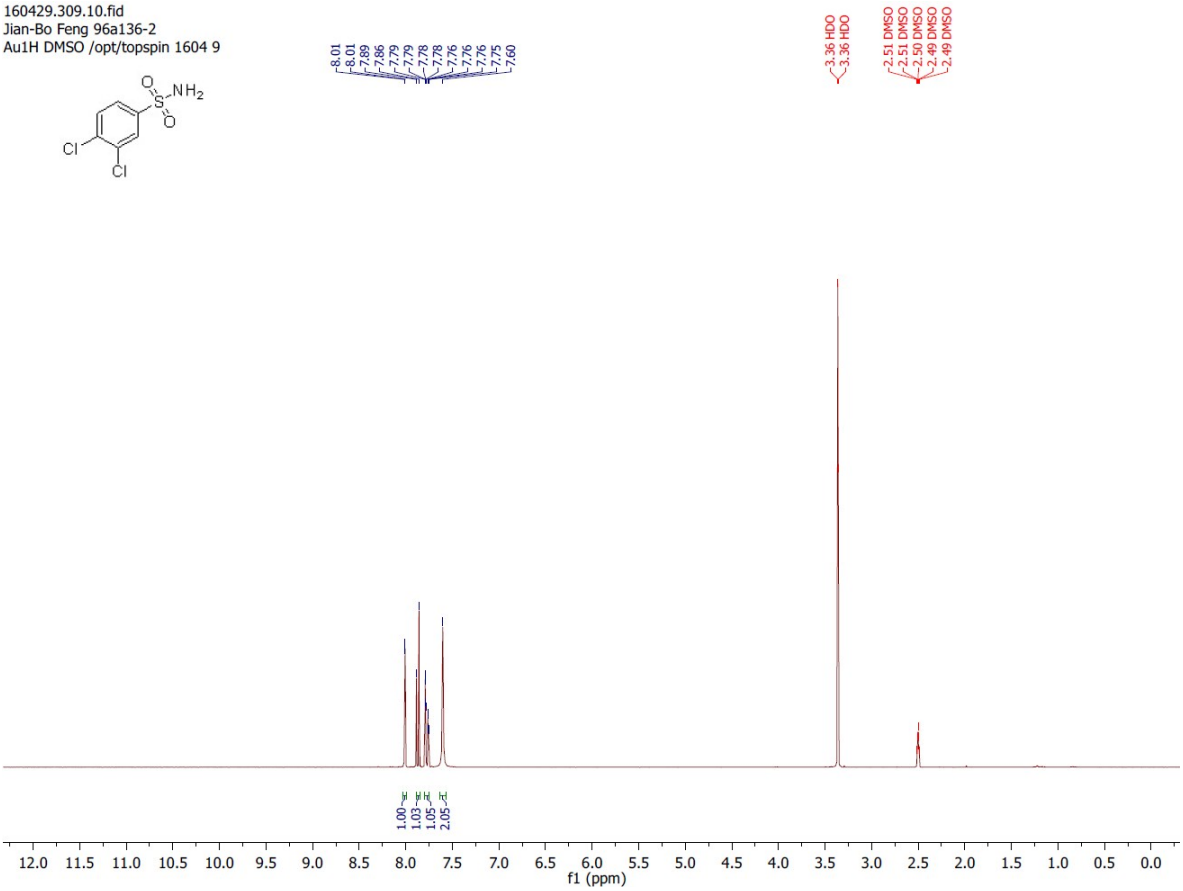

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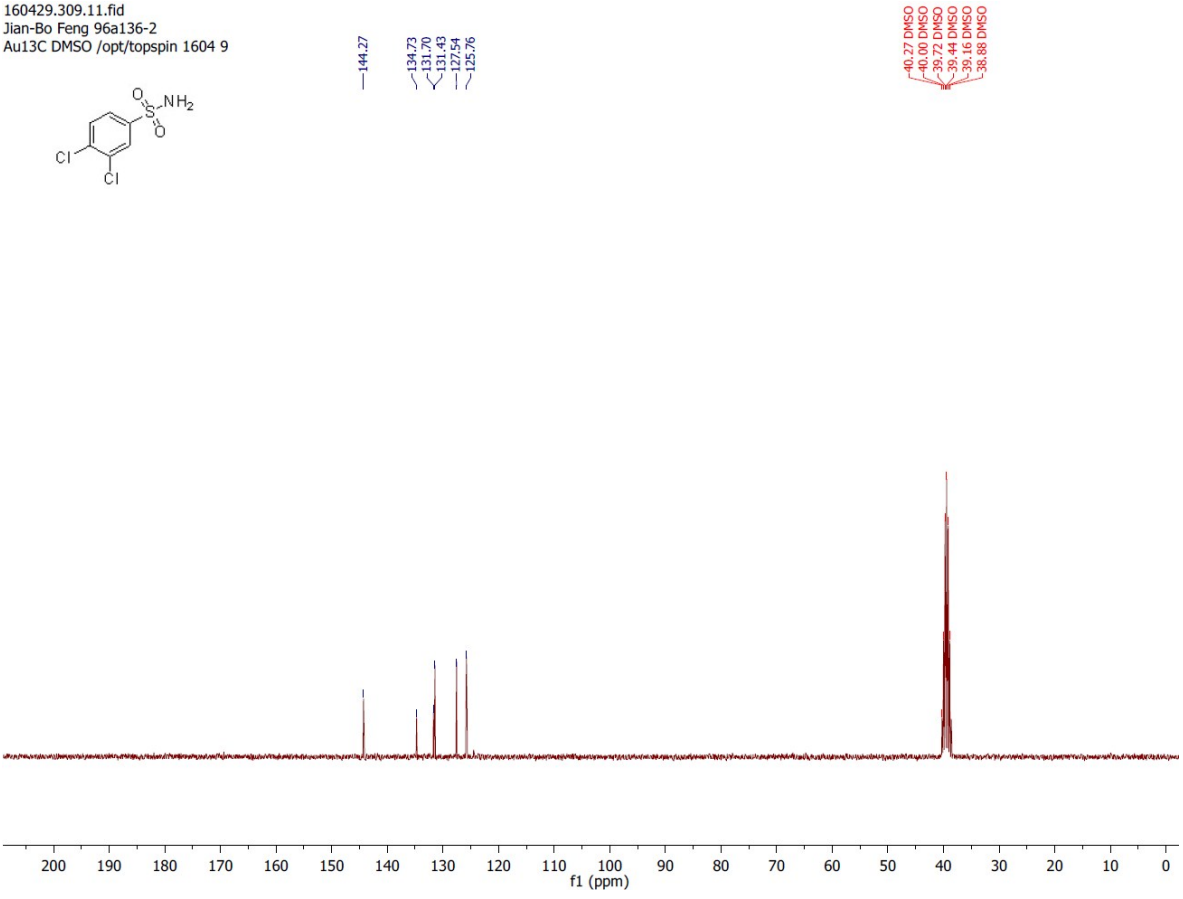

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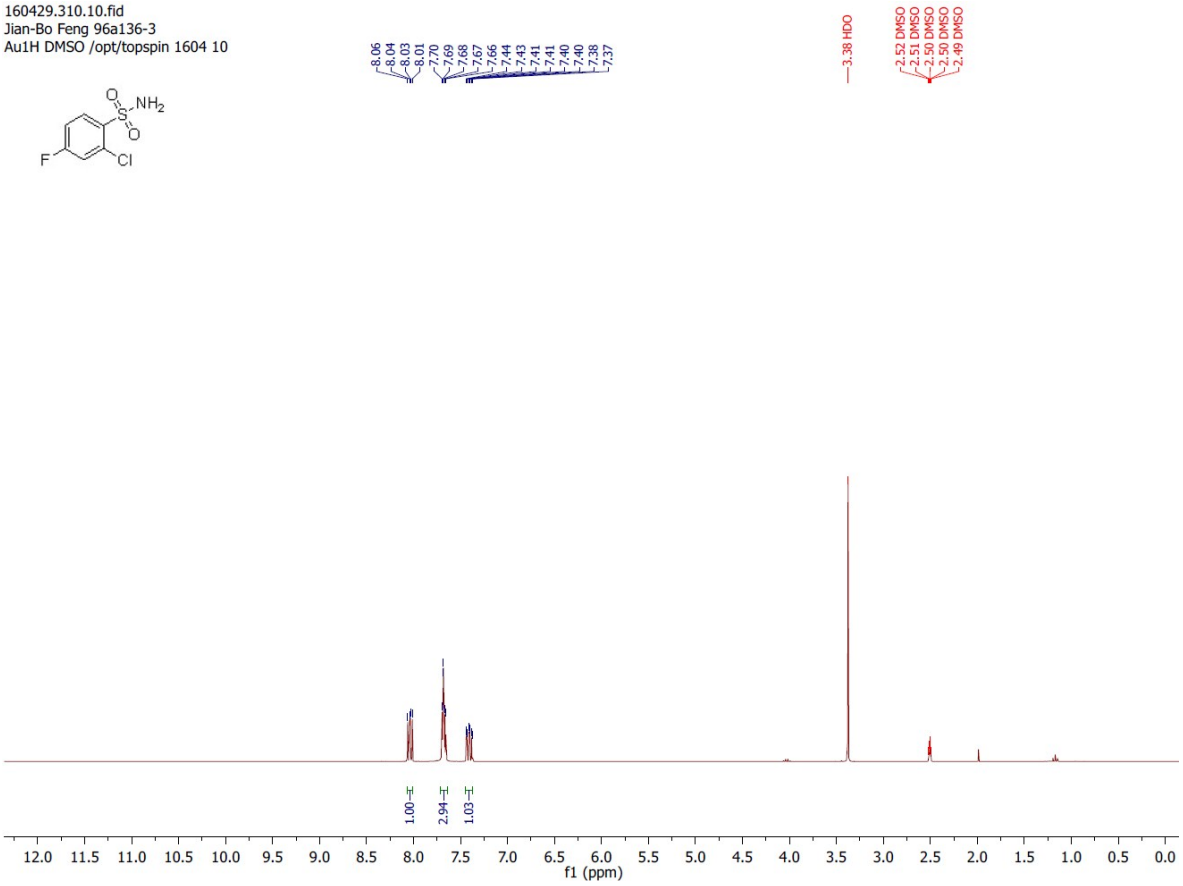

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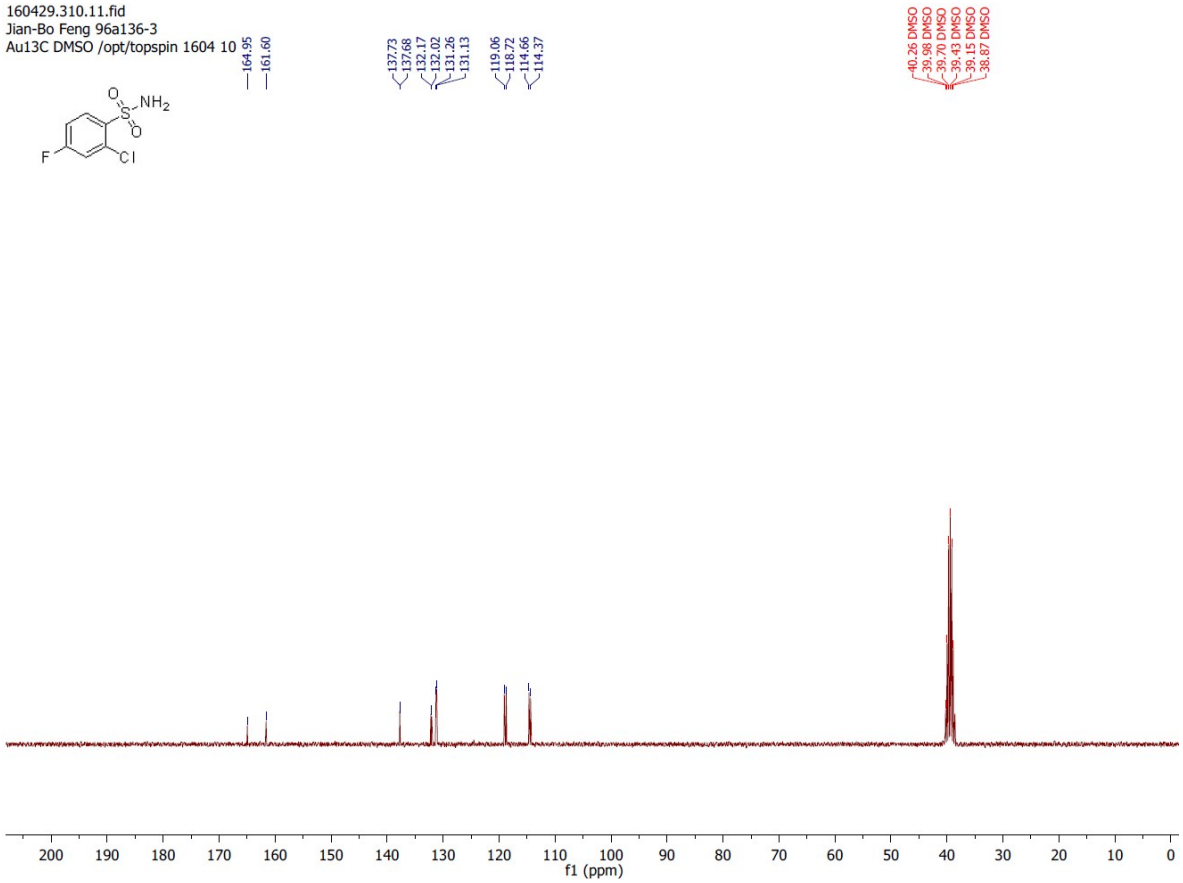

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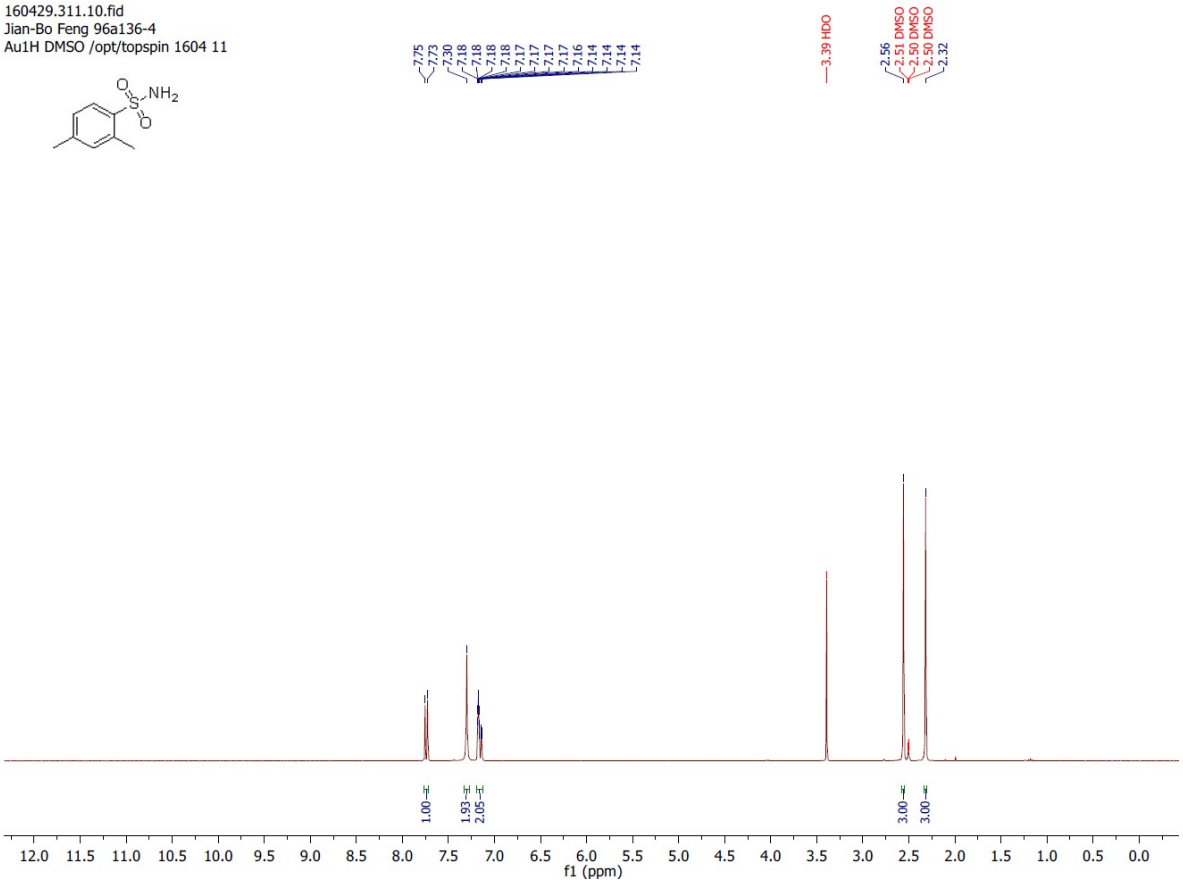

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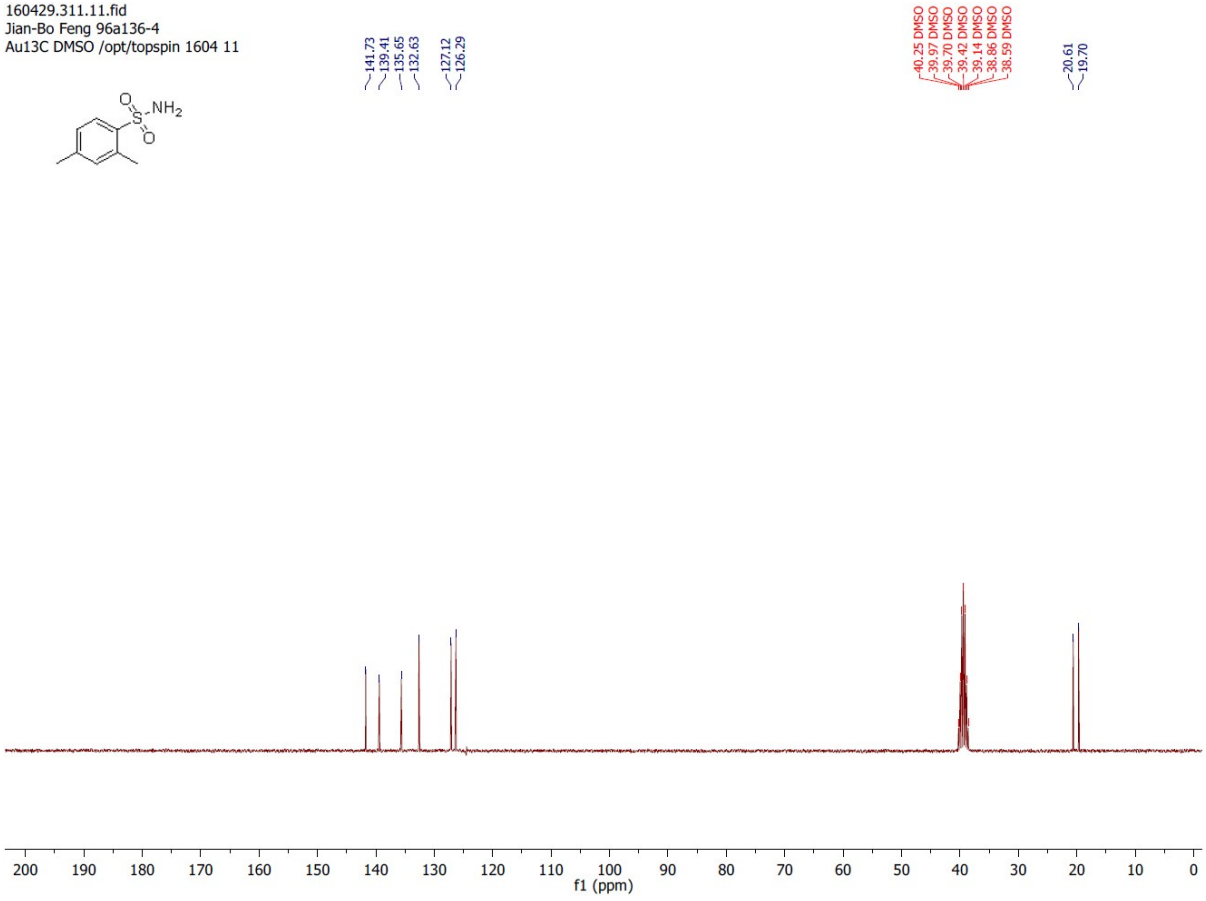

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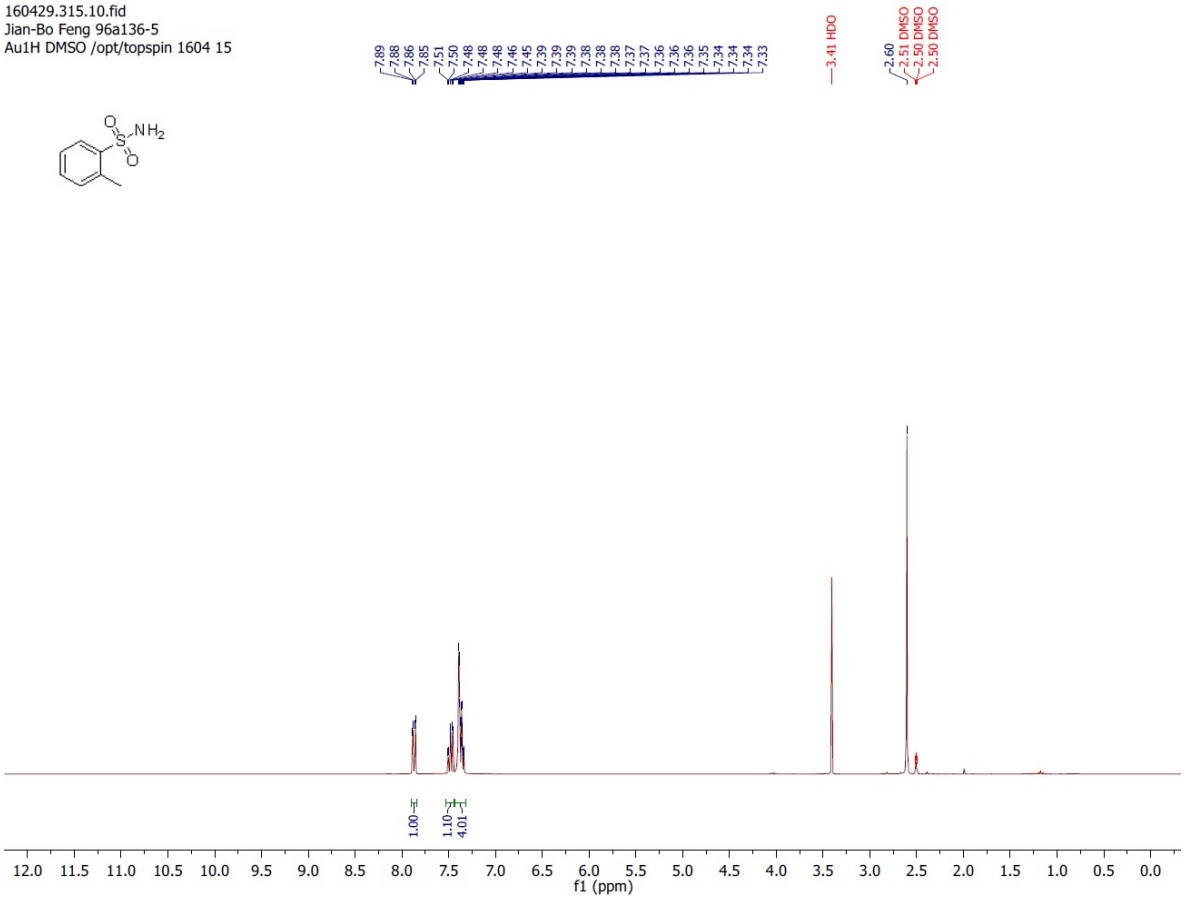

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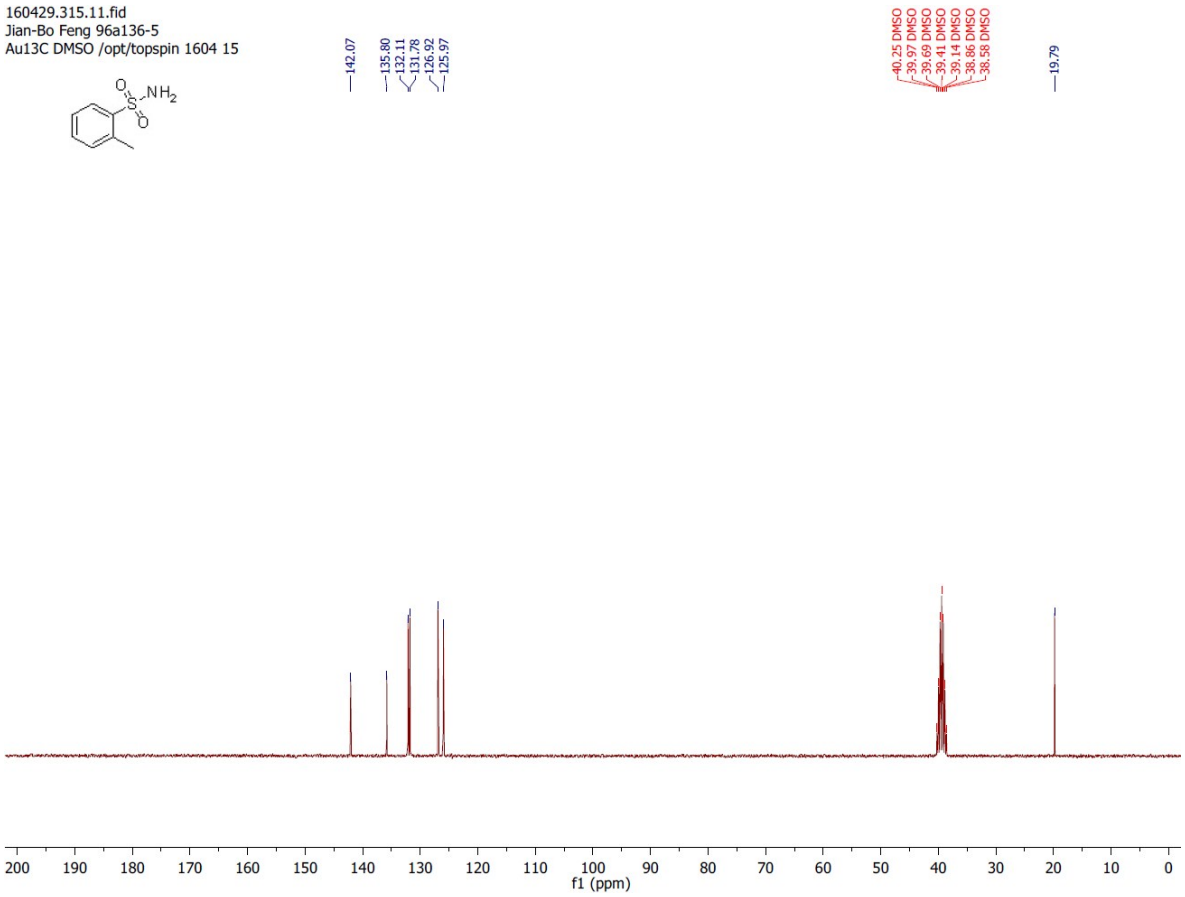
Au13C DMSO /opt/topspin 1604 15



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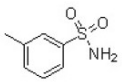

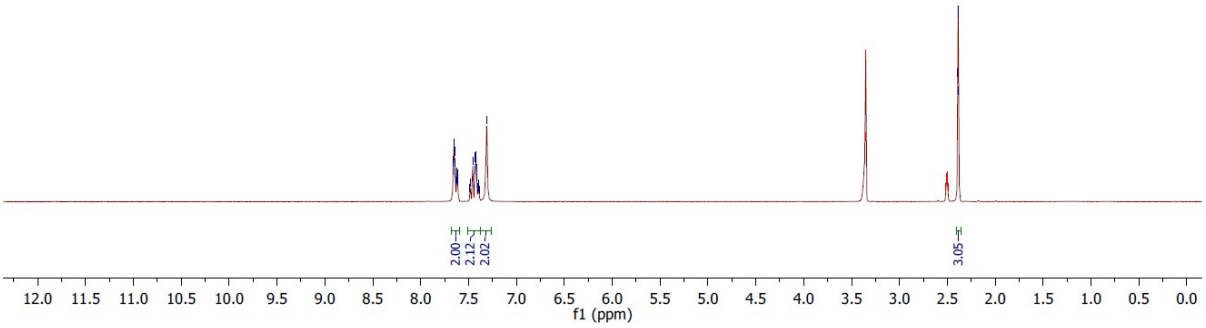

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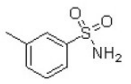
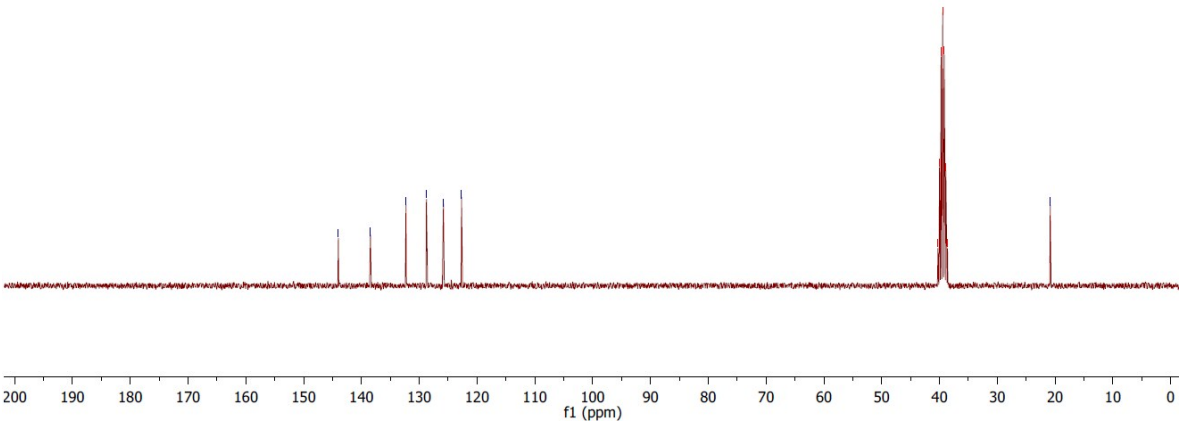
Au13C DMSO /opt/topspin 1604 13





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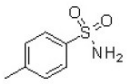
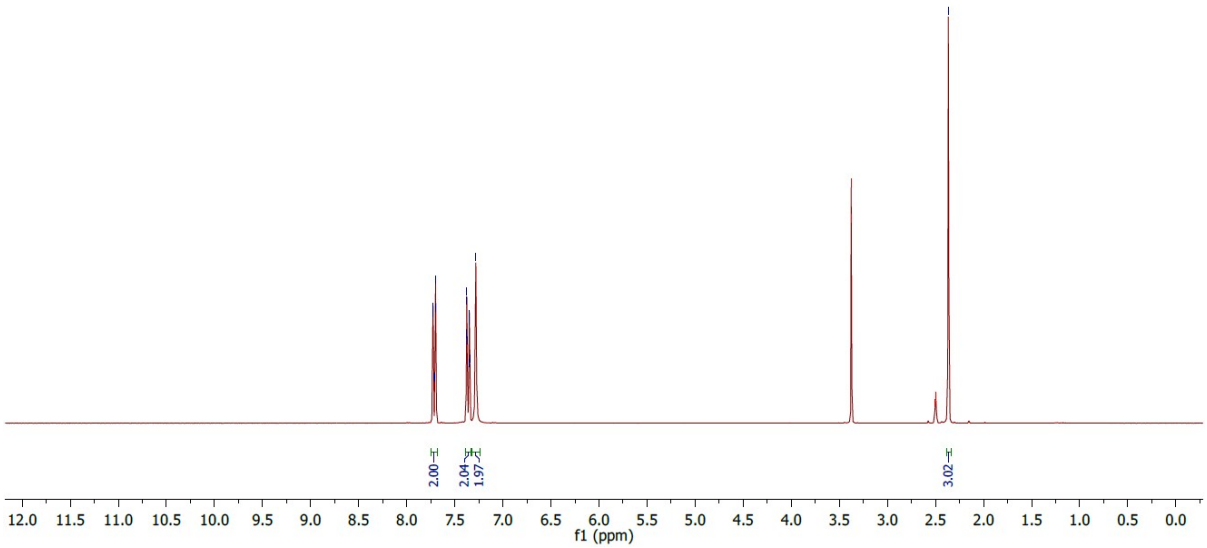
Au1H DMSO /opt/topspin 1604 14





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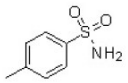

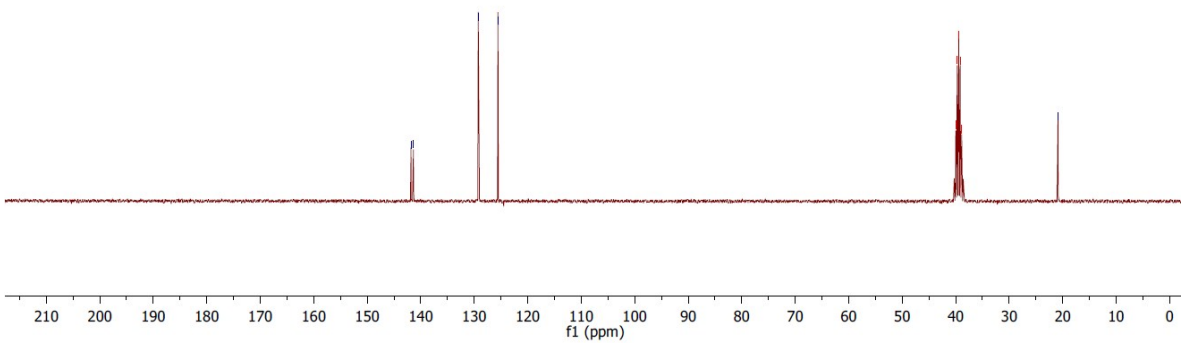

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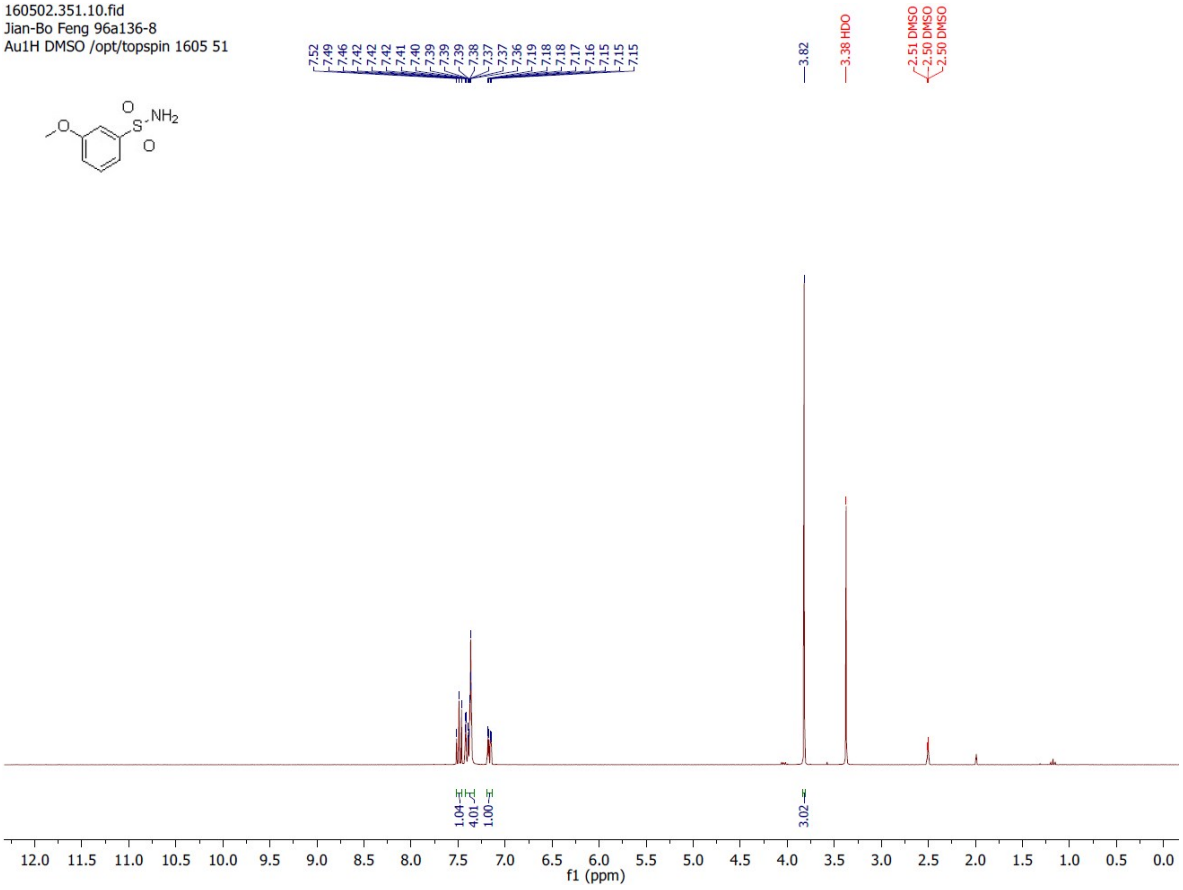

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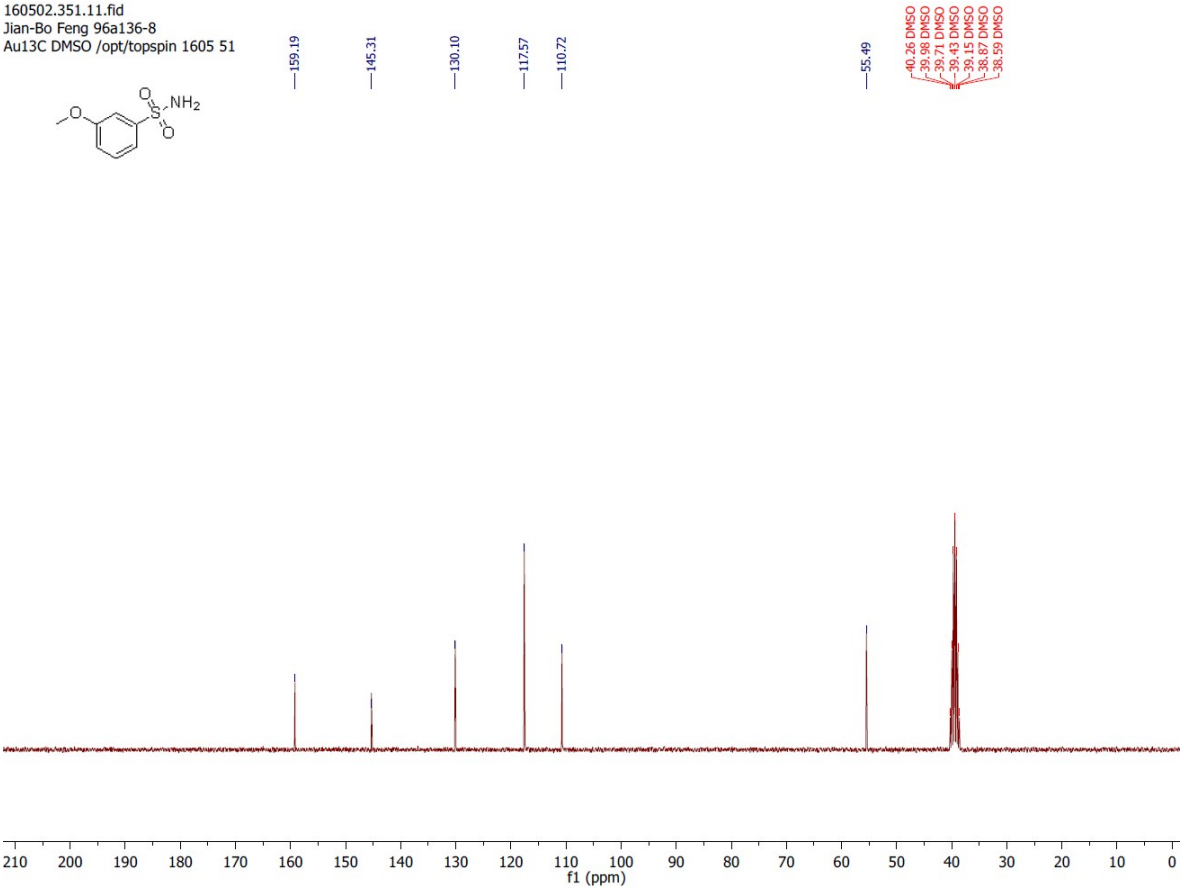

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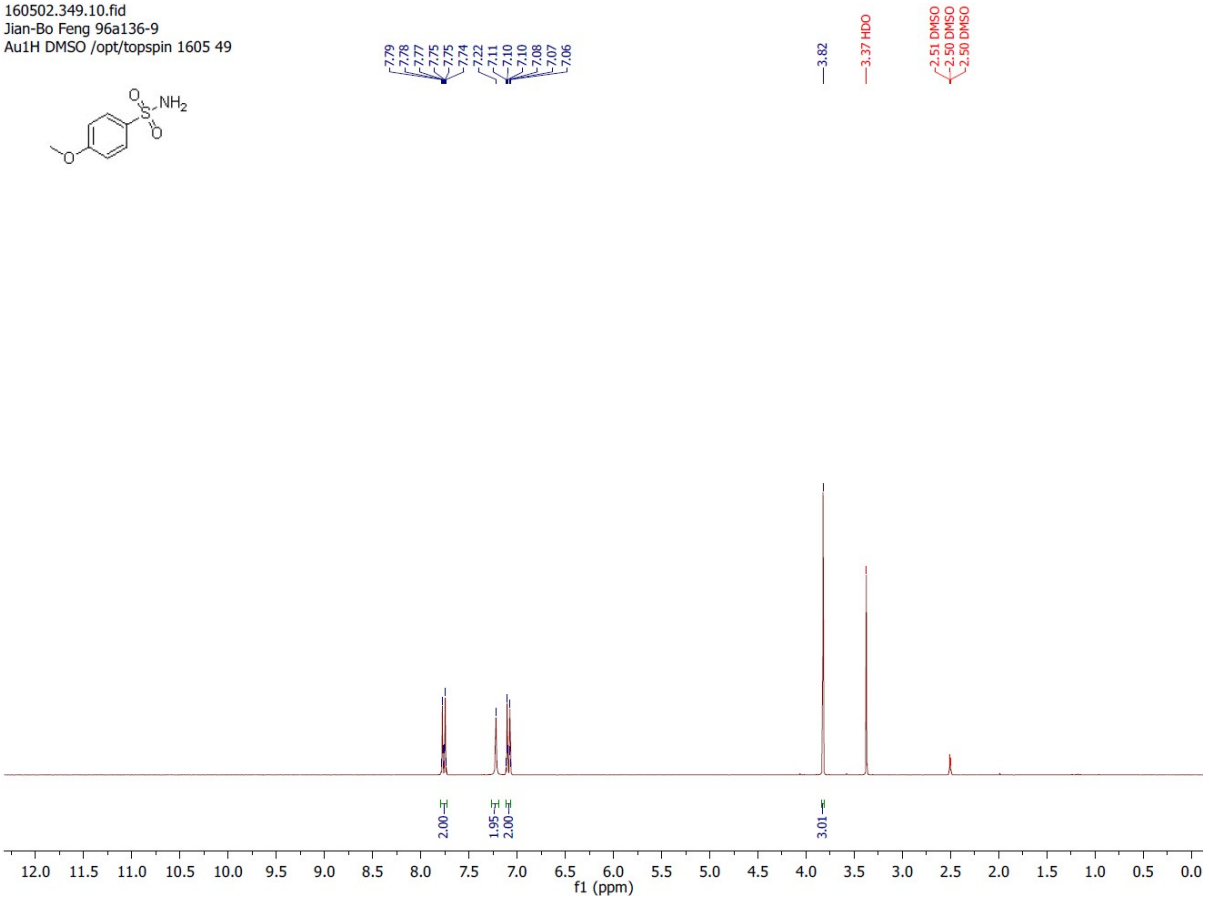

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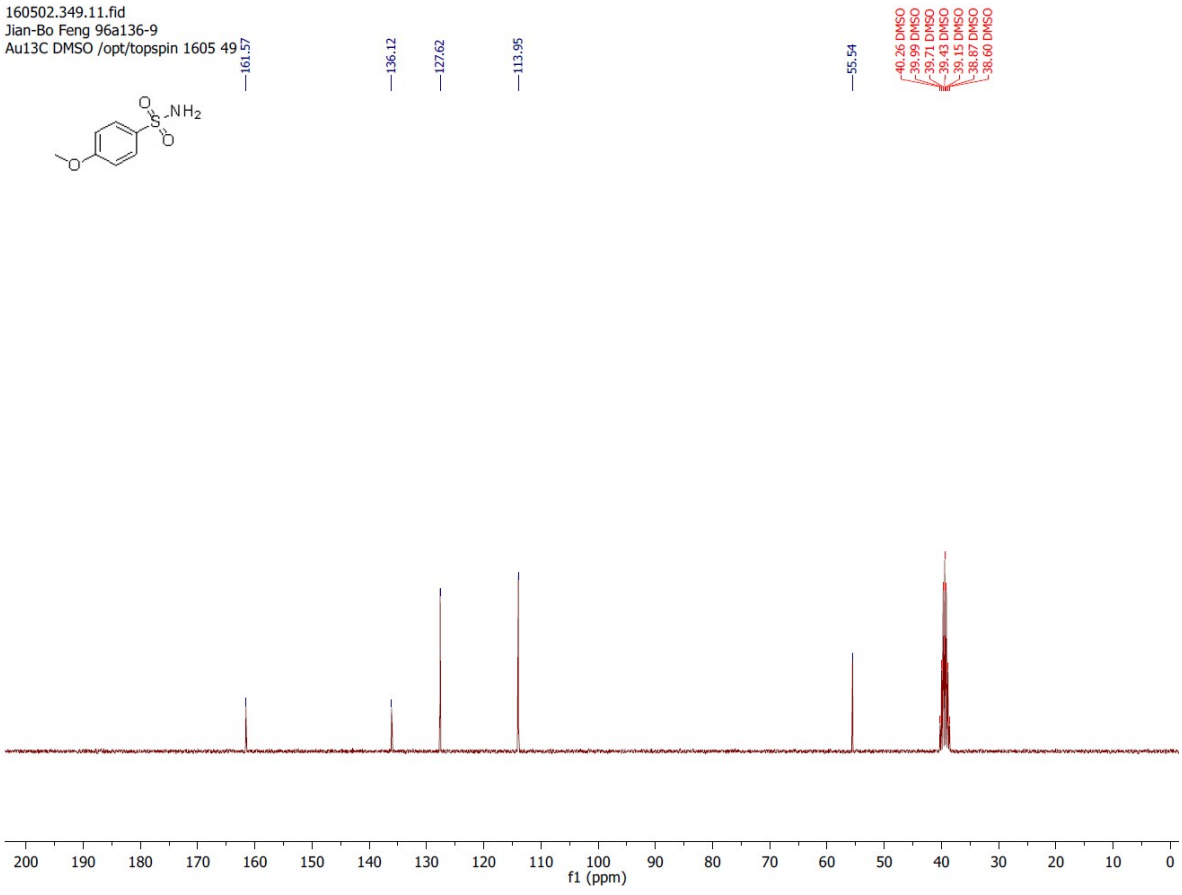

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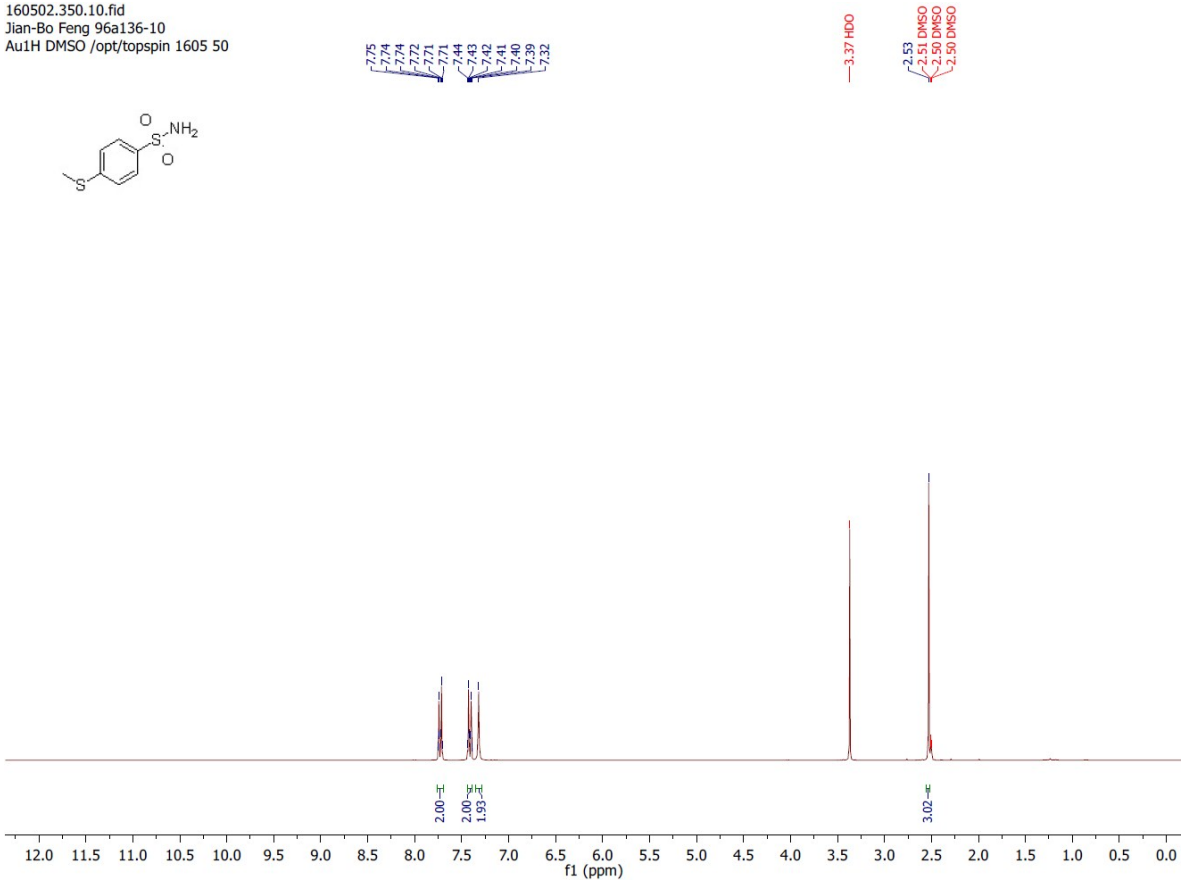

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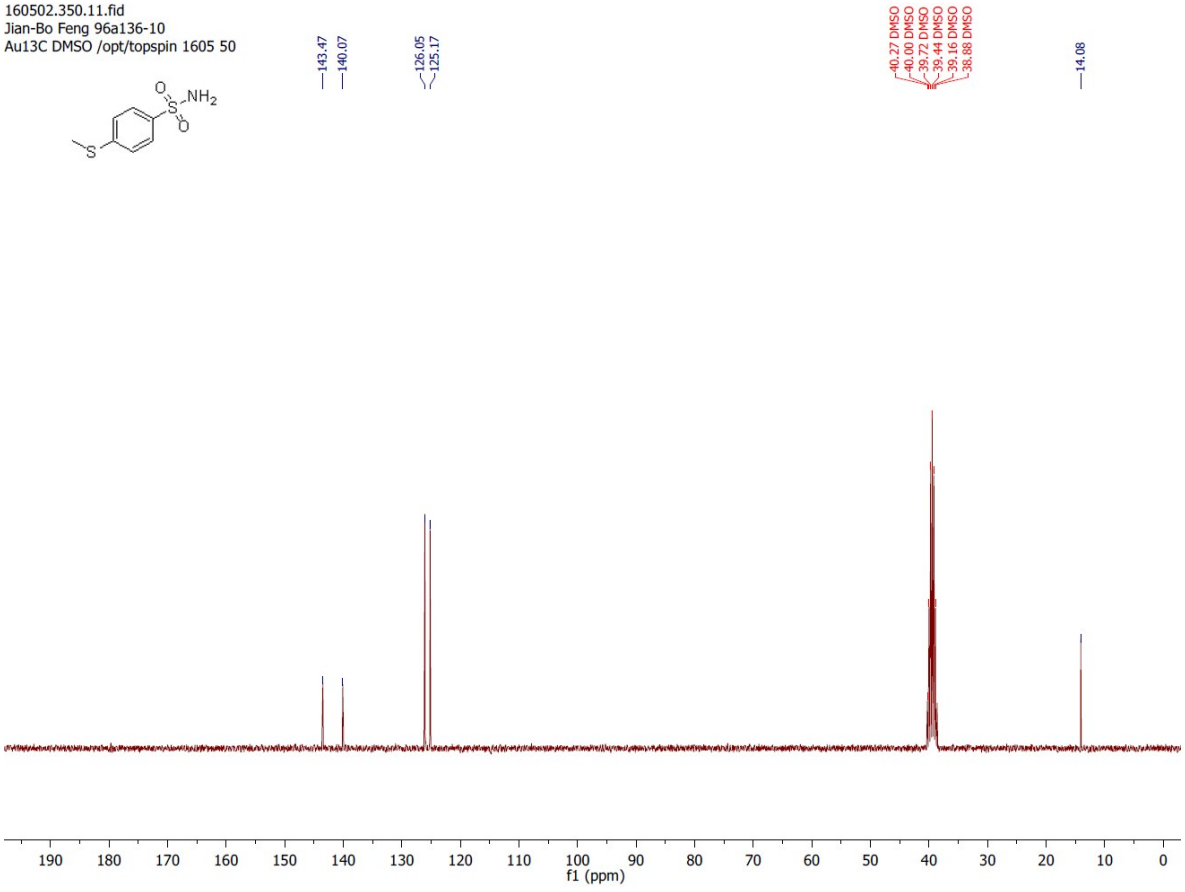

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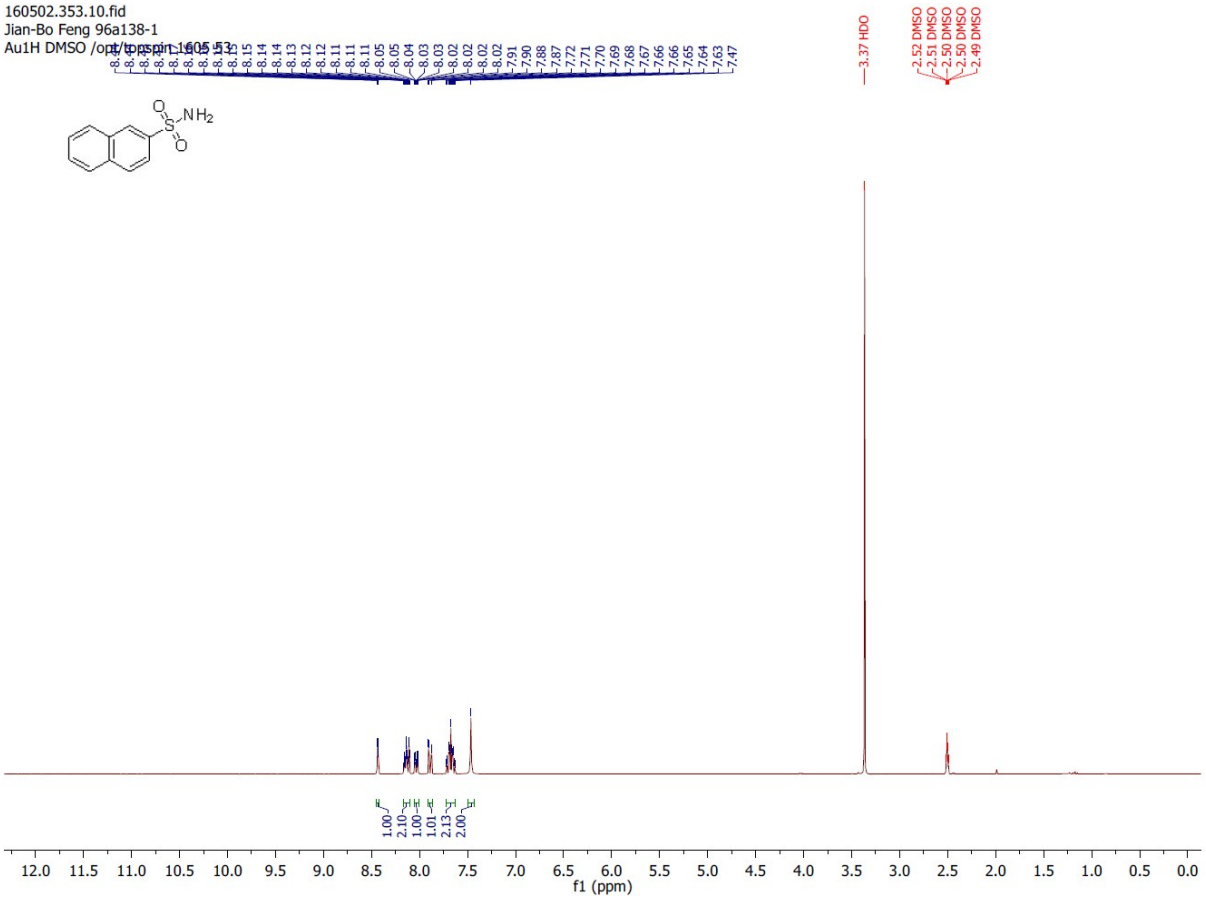
Jian-Bo Feng 96a138-1
Au1H DMSO /opt/topspin 1605 53



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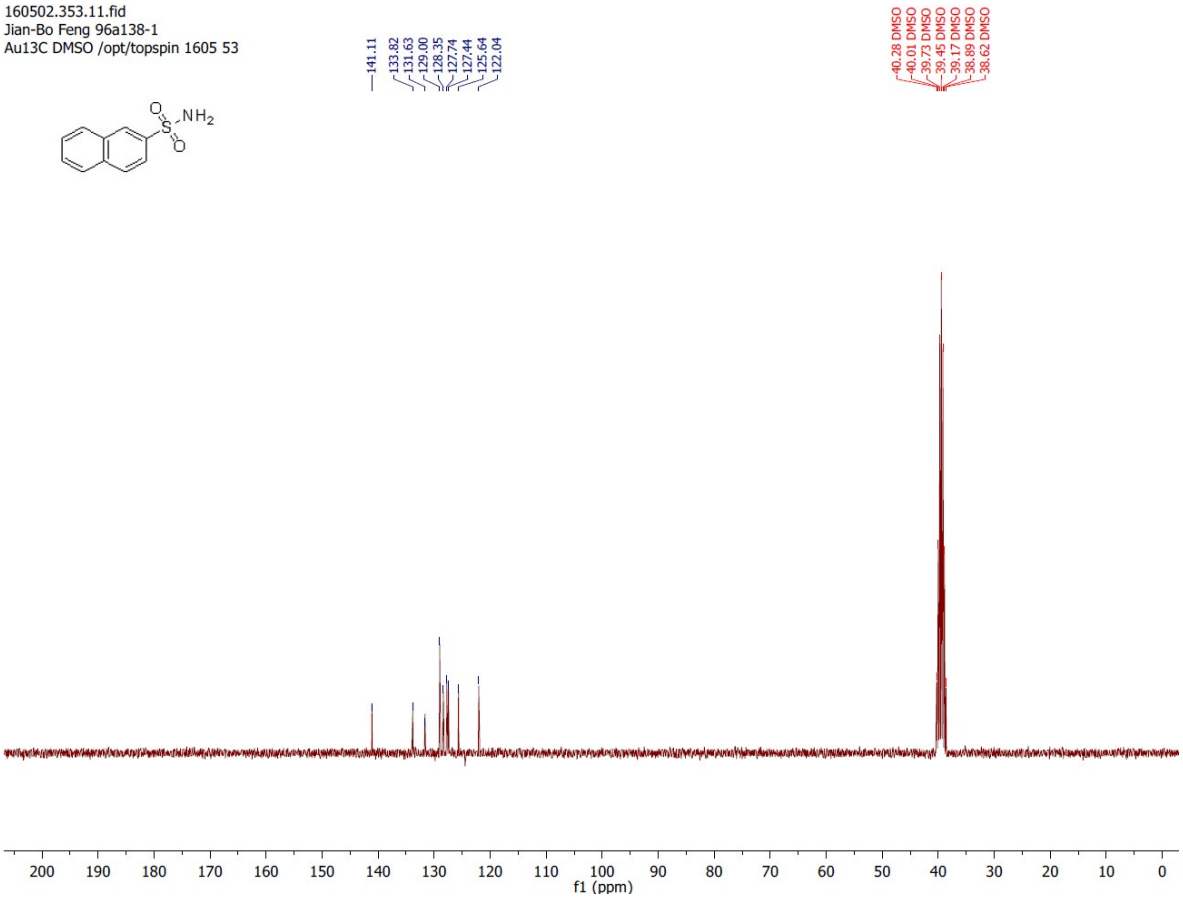
Au13C DMSO /opt/topspin 1605 53



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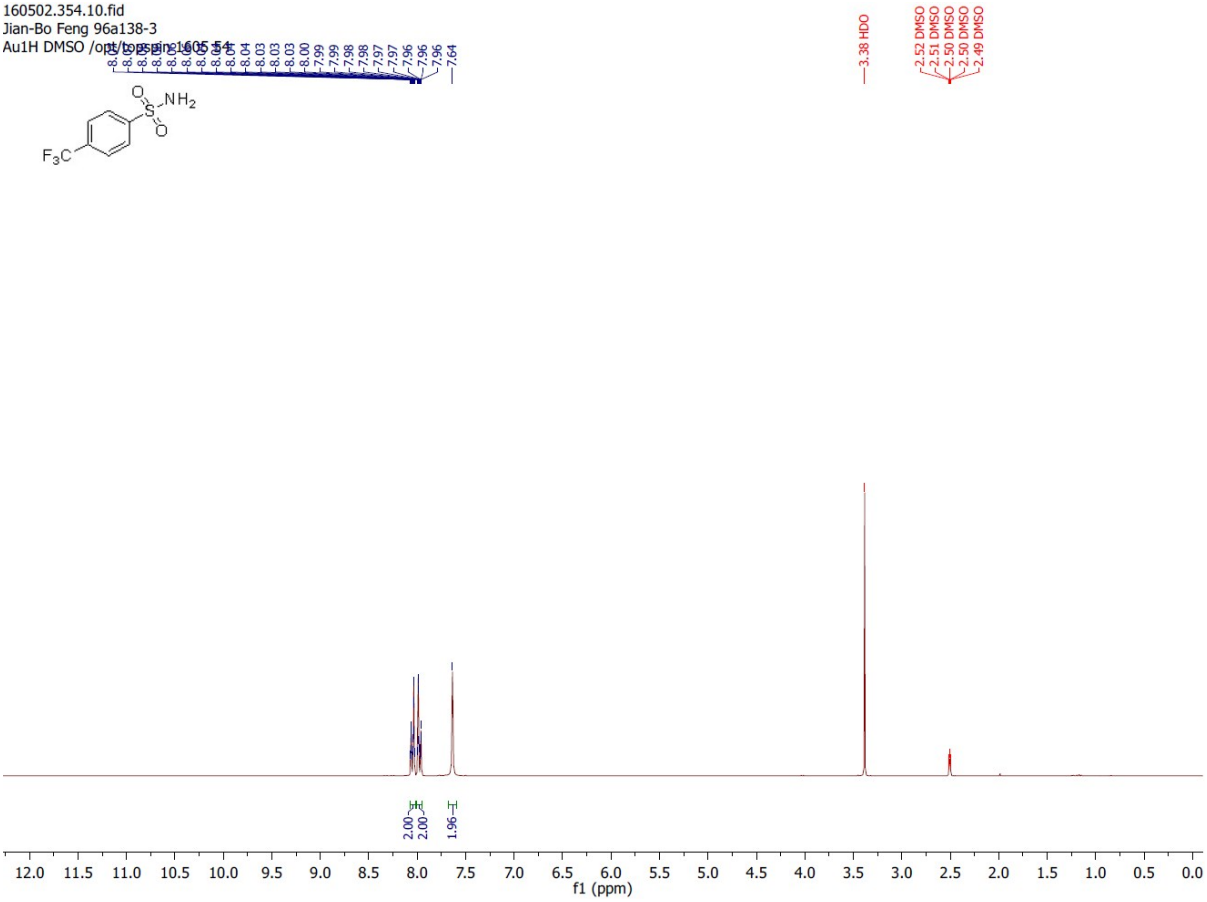
Jian-Bo Feng 96a138-3
Au1H DMSO /opt/topspin 1605 54



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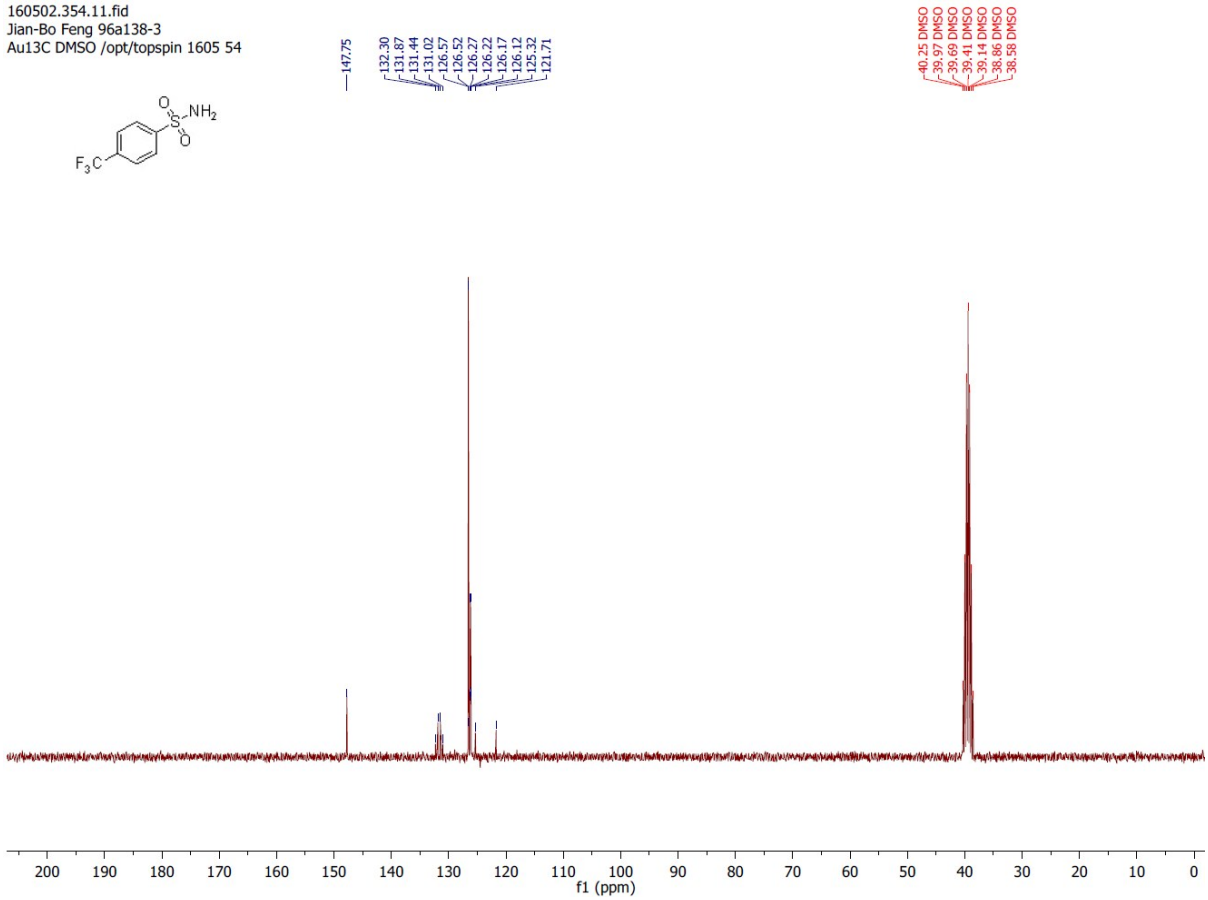

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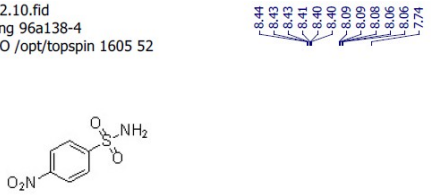
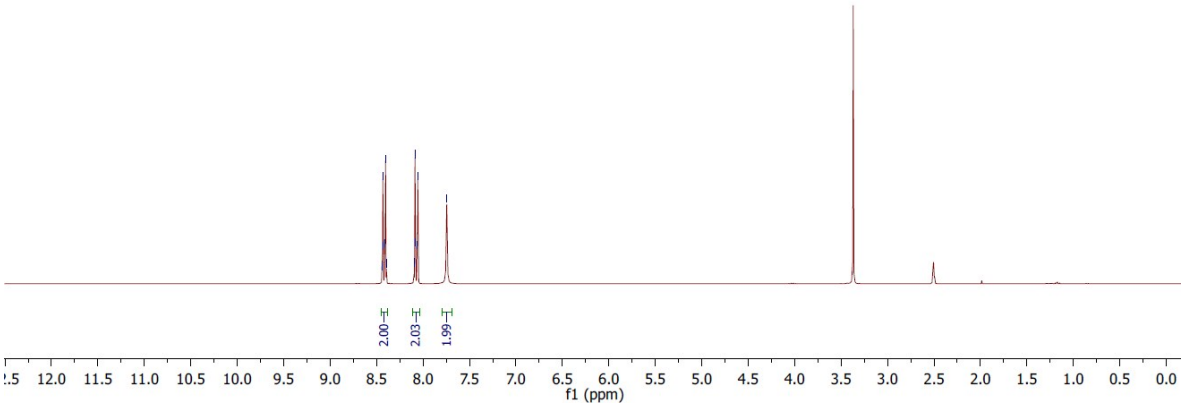
Au1H DMSO /opt/topspin 1605 52





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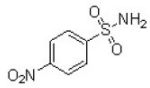

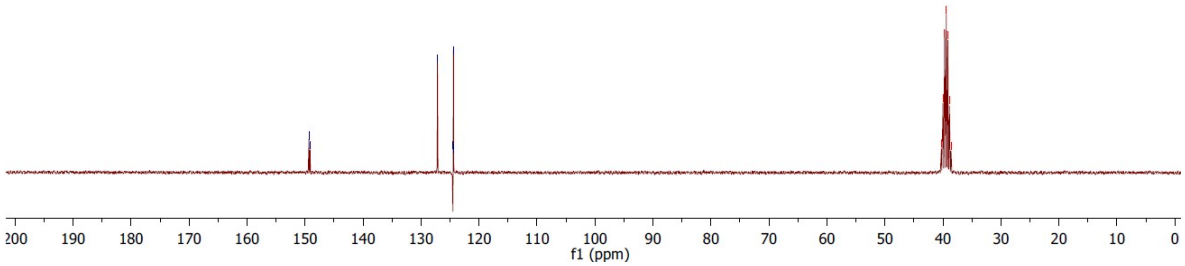

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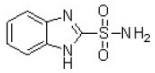
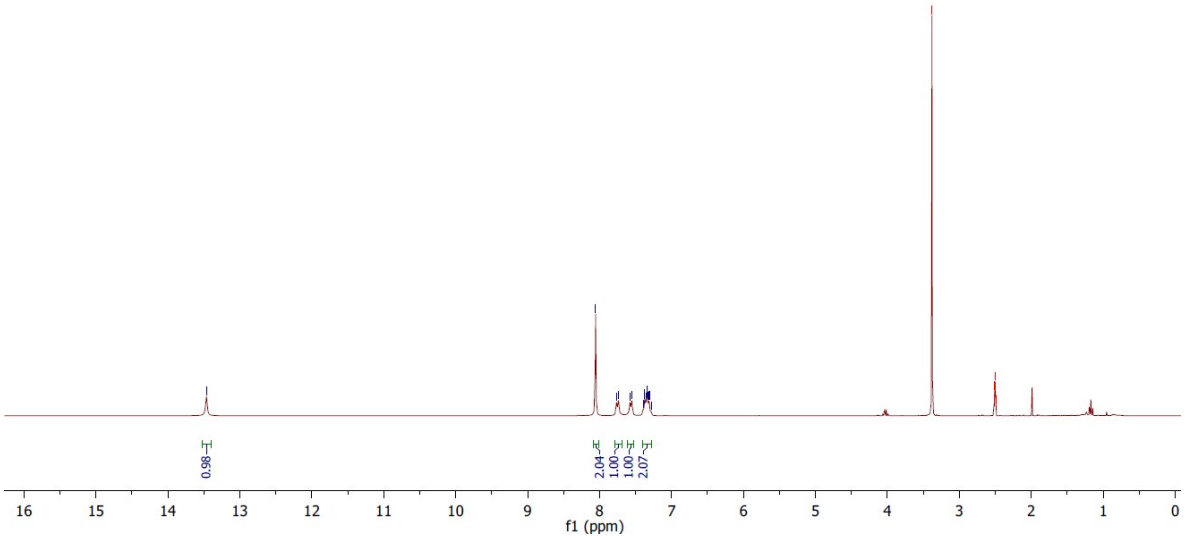
Au1H DMSO /opt/topspin 1605 48





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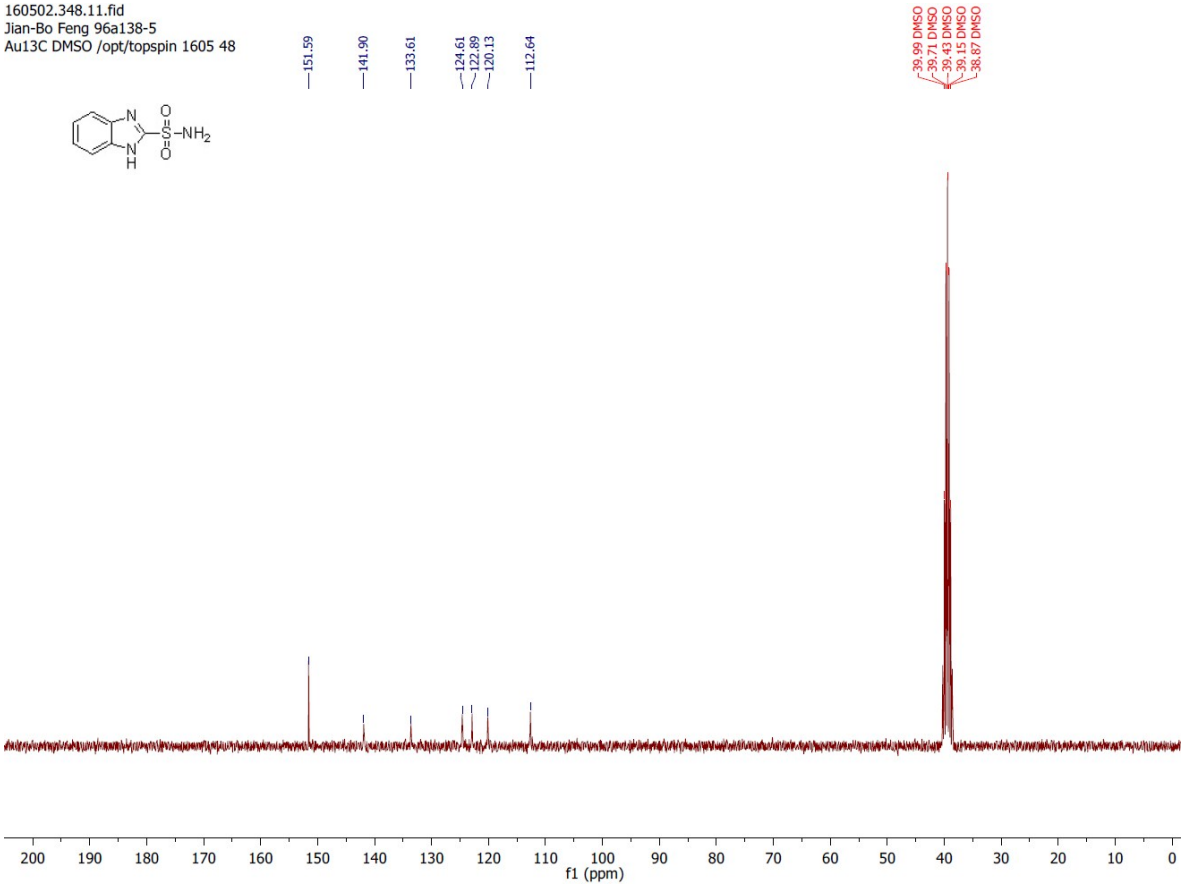

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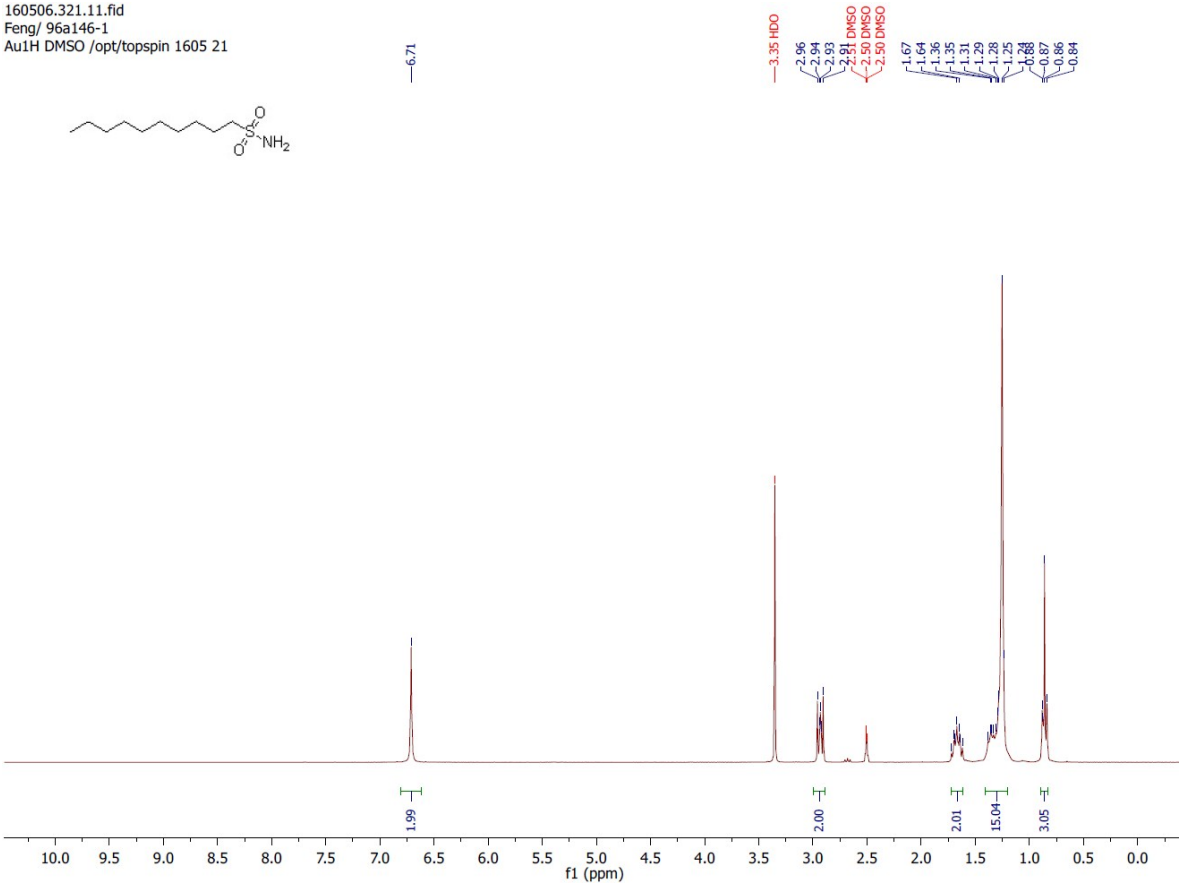
Au1H DMSO /opt/topspin 1605 21



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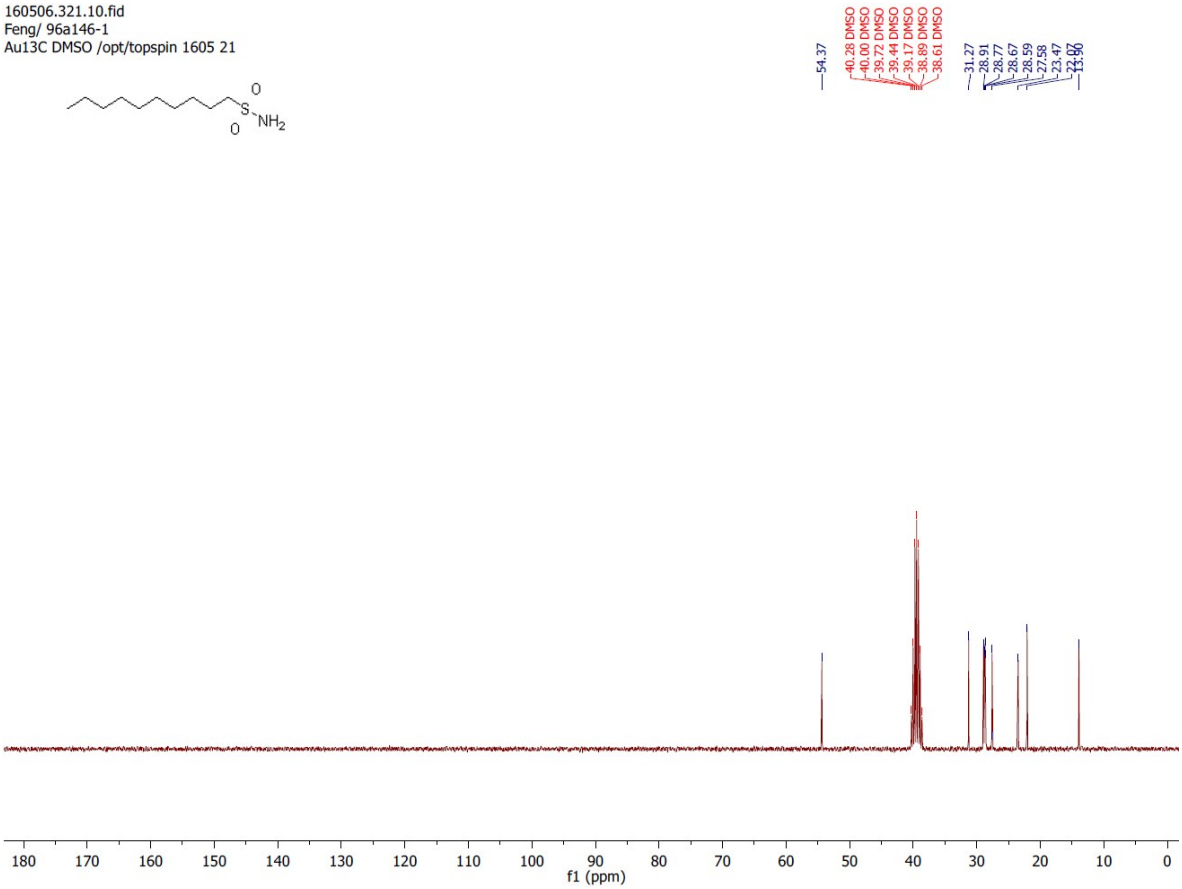

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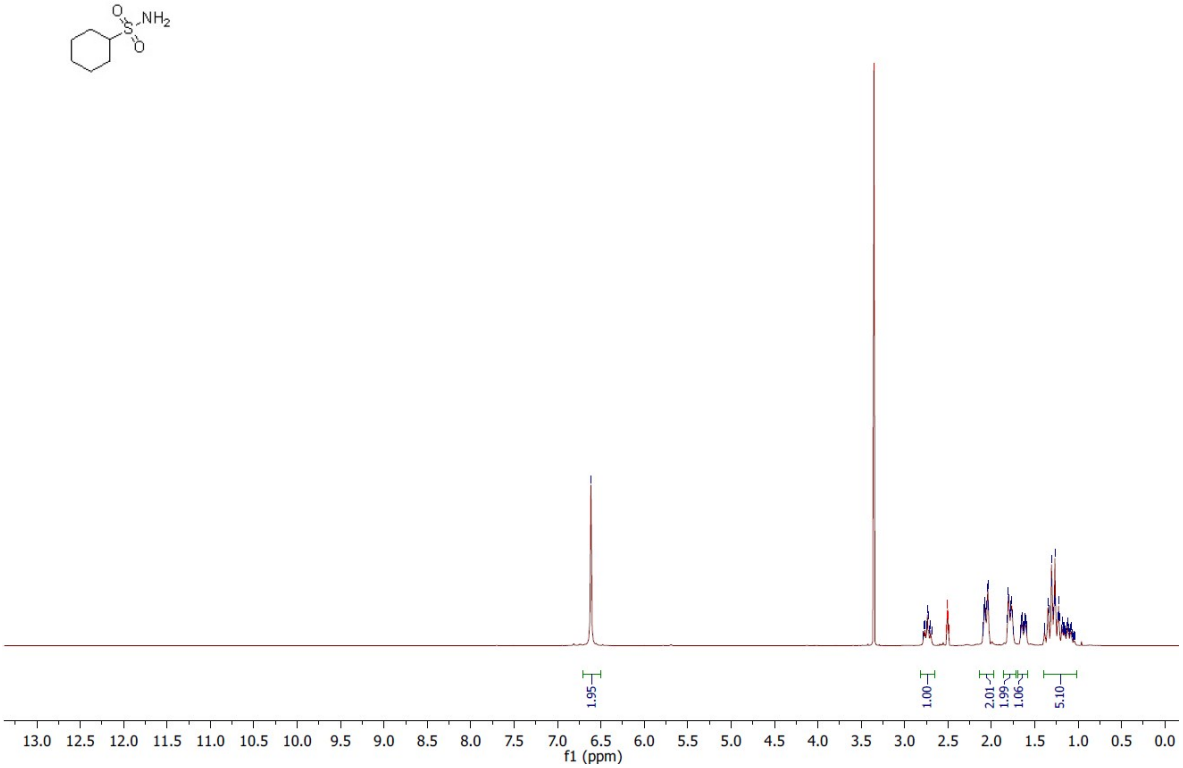

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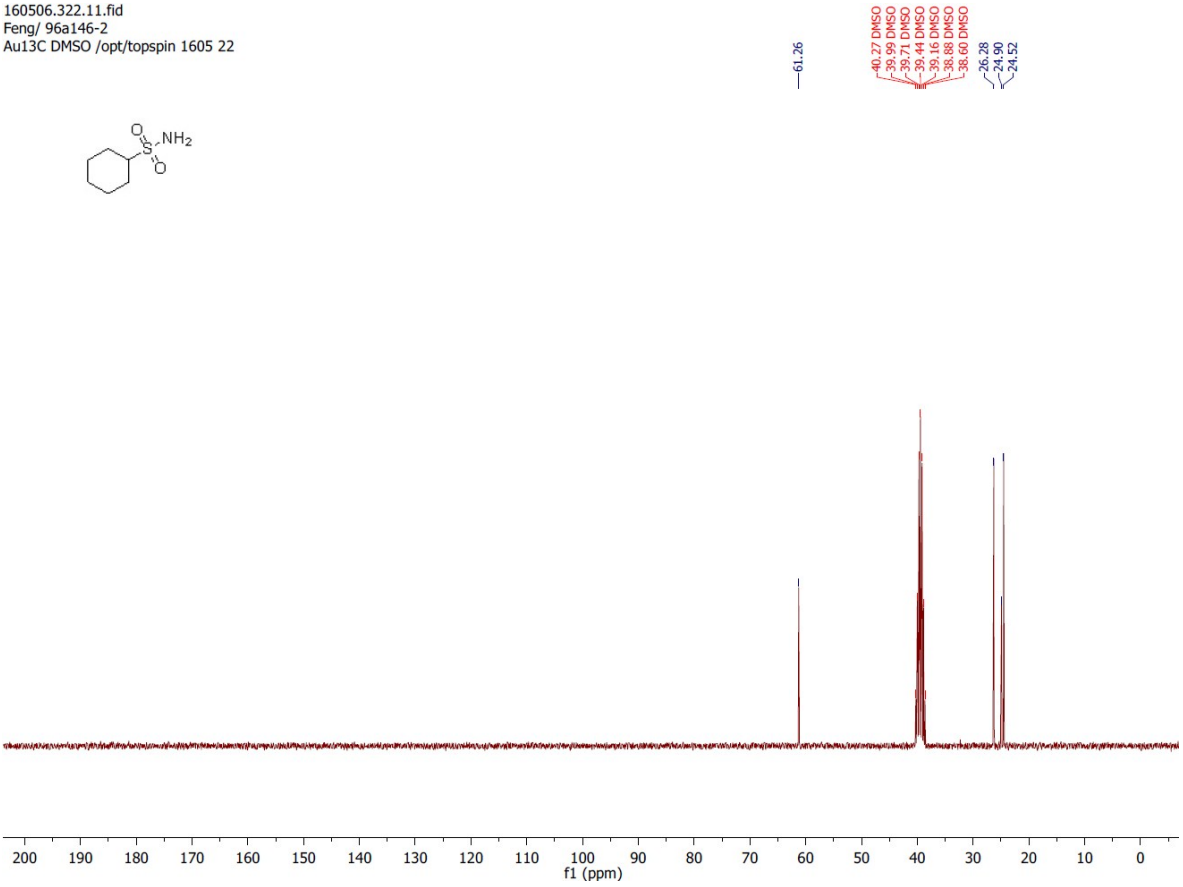

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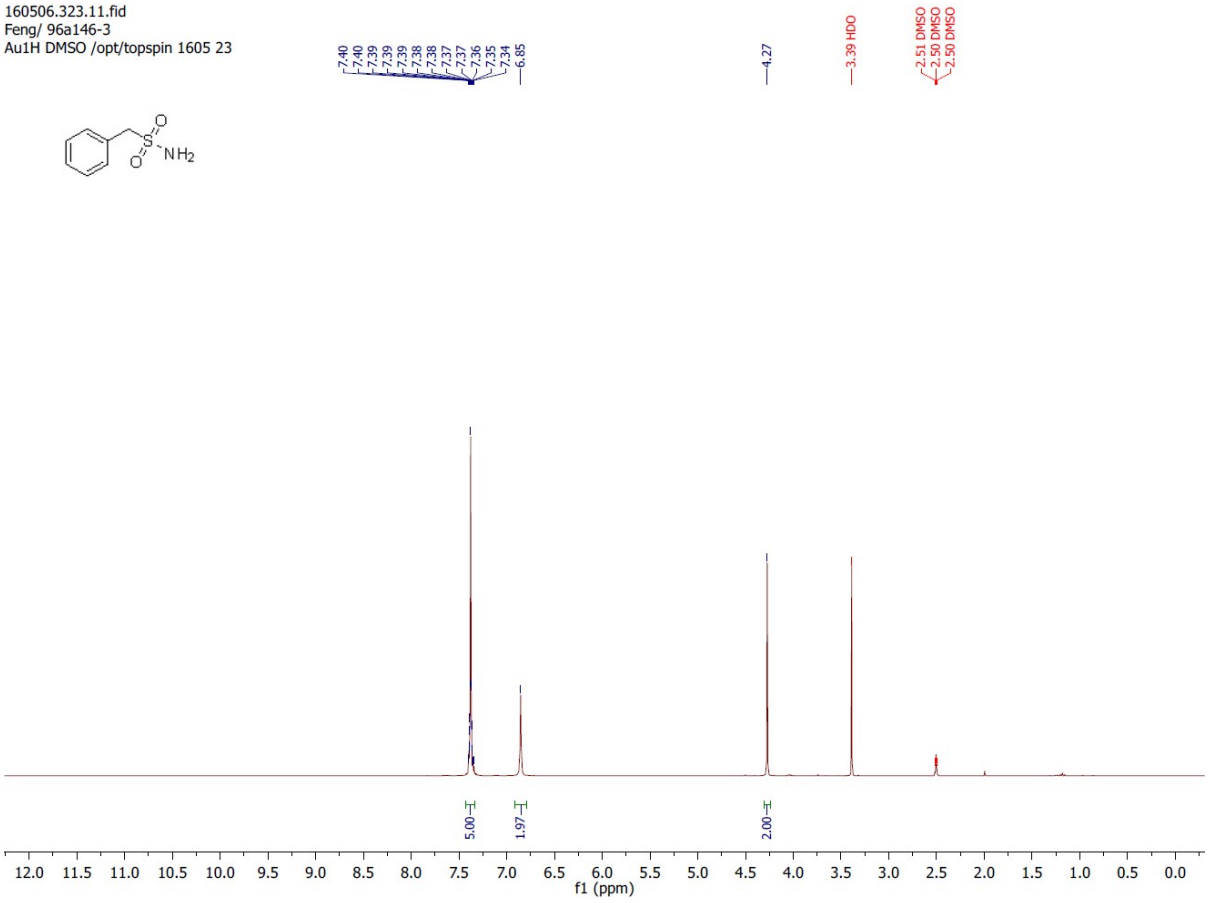

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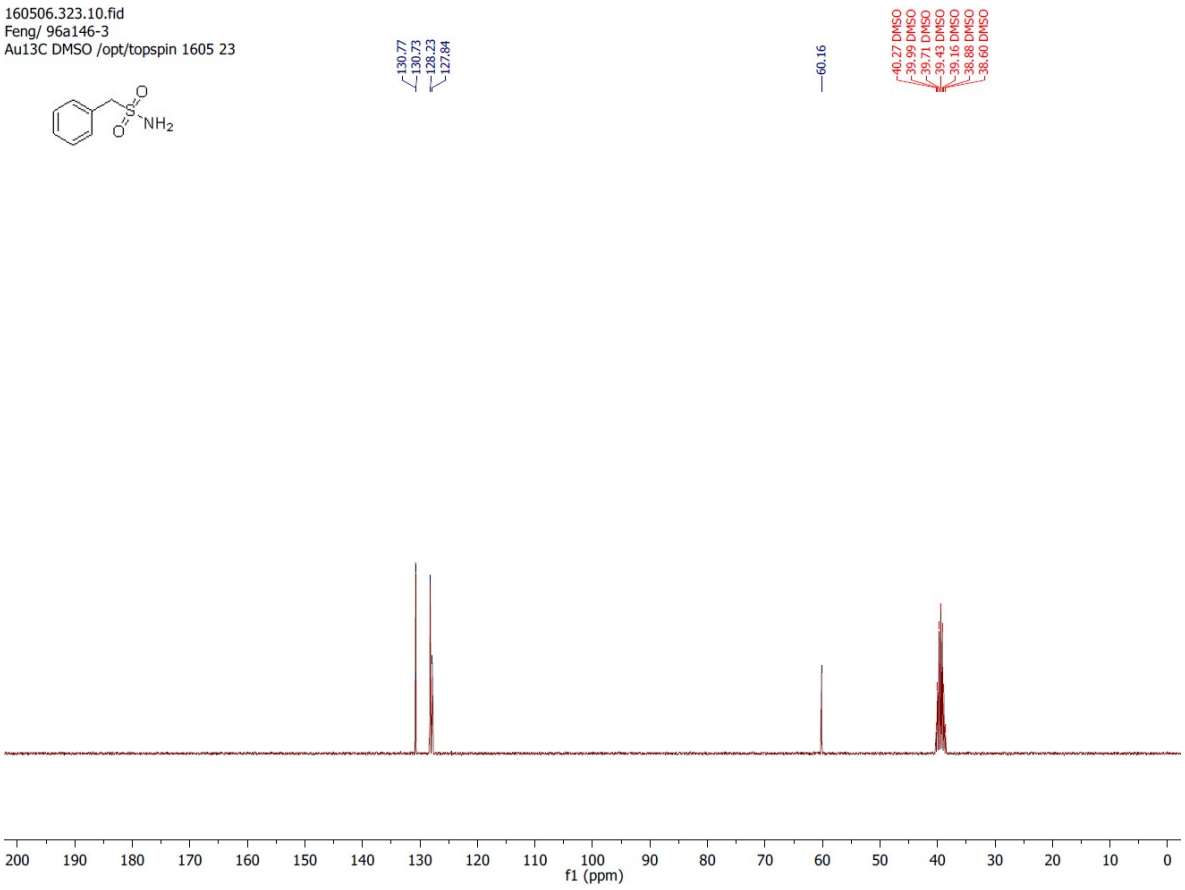

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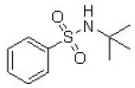
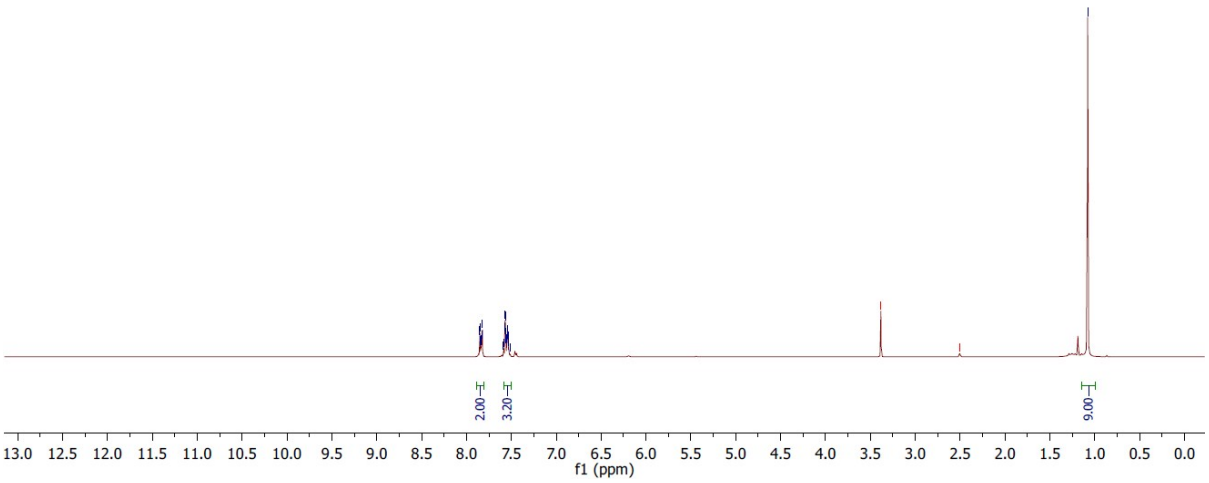
Jian-Bo Feng 96a151
Au1H DMSO /opt/topspin 1605 18





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