Protecting group-free use of alcohols as carbon electrophiles in atom efficient aluminium triflate-catalysed dehydrative nucleophilic displacement reactions

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Note on the order of presentation of experimental data. Experimental methods and analytical data are presented in the order in which the compounds are presented in the main text. In instances where a particular substrate is the product of a set of reactions that have not been presented in the main text, the synthetic procedure leading to that substrate is presented *ahead* of the data for that substrate. In this way, some numbers appear out of place, but the logical order of the chemistry is maintained.

Experimental

General Methods. Reactions were performed in oven-dried glassware under an atmosphere of argon. Reagents were used as supplied from commercial sources. Mass spectra were recorded on a double focusing sector instrument.

General procedure for the $Al(OTf)_3$ catalysed nucleophilic substitution of benzhydrol

To a mixture of benzhydrol (0.200 g, 1.09 mmol) and $Al(OTf)_3$ (5 mg, 1 mol %) in nitroethane (2 mL) was added 1 equivalent of the appropriate nucleophile. The mixture was stirred for 1 hour at 70 °C and the reaction quenched by the addition of saturated aqueous sodium bicarbonate (5 mL). The reaction mixture was extracted with Et_2O (3 × 5 mL), and the combined organic layers washed with water (2 × 5 mL) and dried over magnesium sulphate. The mixture was concentrated under reduced pressure and the residue purified by flash silica column chromatography using the eluents given below (for TLC analysis).

1,1'-Oxybis(ethane-1,1-diyl)dibenzene (2)[1]

244 mg, 1.08 mmol, >98%, clear oil, diastereomeric mixture (bold font and normal font represent each diastereomer); TLC: 0.89 (4:1 hexane/EtOAc); ^{1}H NMR: (400 MHz, $CDCl_3$) δ_H: 7.30–7.12 (m, 10H), 4.45 (q, 2H, *J* = 6.6 Hz), **4.17 (q, 2H, *J* = 6.6 Hz)**, 1.39 (d, 6H, *J* = 6.6 Hz), 1.31 **(d, 6H, *J* = 6.6 Hz)**; ^{13}C NMR: (100 MHz, $CDCl_3$) δ_C: 144.2, **144.1**, 128.4, **128.2**, 127.3, **127.1**, 126.3, **126.2**, 74.6, **74.4**, 24.7, **23.0**; IR: ν_{max} (ATR, cm^{-1}) 3027, 2973, 2927, 1492, 1450, 1281, 1086, 759, 697, 425; EIMS (*m/z*): 105 (100%); ESI-HRMS: Calculated for $[M]^+$ $C_{16}H_{18}O$, 226.1358; found, 226.1335.

Ethoxymethylenedibenzene (4a)[2]

227 mg, 1.07 mmol, 98%, clear oil; TLC: 0.86 (4:1 hexane/EtOAc); ^{1}H NMR: (400 MHz, $CDCl_3$) δ_H: 7.40 (d, 4H, *J* = 7.2 Hz), 7.35 (t, 4H, *J* = 7.2 Hz), 7.30–7.25 (m, 2H), 5.40 (s, 1H), 3.56 (q, 2H, *J* = 7.2 Hz), 1.31 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 142.5, 128.3, 127.2, 126.9, 83.4, 64.4, 15.2; IR: ν_{max} (ATR, cm^{-1}) 3027, 2974, 2866, 1493, 1452, 1093, 1072, 739, 696, 414; EIMS (*m/z*): 212 ($[M]^+$, 20%), 168 (20%), 167 (30%), 166 (20%),

136 (20%), 105 (20%); ESI-HRMS: Calculated for $[M]^+$ $C_{15}H_{16}O$, 212.1201; found, 212.1188.

Allyloxymethylenedibenzene (4b)[3]

230 mg, 1.03 mmol, 94%, clear oil; TLC: 0.89 (4:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.34–7.22 (m, 10H), 5.98 (ddt, 1H, *J* = 17.3, 10.4, 5.7 Hz), 5.43 (s, 1H), 5.31 (dq, 1H, *J* = 17.3, 1.8 Hz), 5.20 (dq, 1H, *J* = 10.4, 1.6 Hz), 4.02 (dt, 2H, *J* = 5.7, 1.5 Hz); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 142.2, 134.8, 128.4, 127.4, 127.0, 116.9, 82.6, 69.7; IR: ν_{max} (ATR, cm^{-1}) 3028, 1725, 1658, 1449, 1276, 1027, 919, 696, 638, 464; EIMS (*m/z*): 224 ($[M]^+$, 10%), 182 (80%), 168 (80%), 167 (100%), 165 (90%), 152 (70%), 147 (70%), 105 (90%); ESI-HRMS: Calculated for $[M]^+$ $C_{16}H_{16}O$, 224.1201; found, 224.1197.

Prop-2-ynyloxymethylenedibenzene (4c)[4]

240 mg, 1.08 mmol, >98%, clear oil; TLC: 0.78 (4:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.51 (d, 4H, *J* = 7.6 Hz), 7.45 (t, 4H, *J* = 7.4 Hz), 7.37 (t, 2H, *J* = 7.2 Hz), 5.82 (s, 1H), 4.28 (d, 2H, *J* = 2.4 Hz), 2.56 (t, 1H, *J* = 2.0 Hz); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 141.1, 128.3, 127.6, 127.1, 81.5, 79.6, 74.6, 55.6; IR: ν_{max} (ATR, cm^{-1}) 3288, 3028, 2855, 1493, 1452, 1259, 1065, 1026, 740, 696, 578, 468; EIMS (*m/z*): 222 ($[M]^+$, 10%), 182 (60%), 168 (30%) 167 (90%), 166 (80%), 152 (50%), 145 (90%), 115 (30%), 105 (100%); ESI-HRMS: Calculated for $[M]^+$ $C_{16}H_{14}O$, 222.1045; found, 222.1028.

3-Benzhydrylpentane-2,4-dione (4d)[5]

279 mg, 1.05 mmol, 96%, white solid; Mp: 111–113 °C; TLC: 0.33 (8:1 hexane/EtOAc); ^{1}H NMR: (400 MHz, $CDCl_3$) δ_H: 7.27 (d, 4H, *J* = 7.2 Hz), 7.24 (t, 4H, *J* = 7.6 Hz), 7.14 (t, 2H, *J* = 6.8 Hz), 4.89 (d, 1H, *J* = 12.4 Hz), 4.71 (d, 1H, *J* = 12.4 Hz), 1.98 (s, 6H); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 202.7, 141.1, 128.7, 127.6, 126.8, 74.2, 51.0, 29.5; IR: ν_{max} (ATR, cm^{-1}) 2160, 2031, 1692, 1355, 1183, 1153, 756, 699, 539, 510, 416; EIMS (*m/z*): 266 ($[M]^+$, 5%), 223 (50%), 167 (45%), 165 (50%); ESI-HRMS: Calculated for $[M]^+$ $C_{18}H_{18}O_2$, 266.1307; found 266.1325.

Ethyl-2-benzhydryl-3-oxobutanoate (4e)[5]

281 mg, 0.948 mmol, 87%, white solid; Mp: 84–86 °C; TLC: 0.35 (4:1 hexane/EtOAc); ^{1}H NMR: (400 MHz, $CDCl_3$) δ_H: 7.28–7.21 (m, 8H), 7.14–7.16 (m, 2H), 4.99 (d, 1H, *J* = 12.0 Hz), 4.27 (d, 1H, *J* = 12.0 Hz), 3.96 (q, 2H, *J* = 6.8 Hz), 2.08 (s, 3H), 0.98 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 201.8, 167.7, 141.4, 128.7, 127.7, 126.9, 65.2, 61.5, 50.9, 30.0, 13.8; IR: ν_{max} (ATR, cm^{-1}) 2159, 2028, 1736, 1361, 1144, 700, 495, 445; EIMS (*m/z*): 278 (85%), 253 (25%), 207 (100%), 205 (55%), 178 (50%), 167 (60%), 165 (65%), 152 (35%); ESI-HRMS: Calculated for $[M]^+$ $C_{19}H_{20}O_3$, 296.1412; found, 296.1395.

Benzhydryl(phenyl)sulphane (4f)[6]

295 mg, 1.07 mmol, 98%, white solid; Mp: 76–80 °C; TLC: 0.55 (50:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.59–7.55 (m, 4H), 7.20–7.44 (m, 11H), 5.71 (s, 1H); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 140.9, 136.1, 130.4, 128.6, 128.4, 128.3, 127.1, 126.5, 57.3; IR: ν_{max} (ATR, cm^{-1}) 2159, 2028, 1479, 1024, 732, 694, 411; EIMS (*m/z*): 276 ($[M]^+$, 10%), 168 (20%), 167 (80%), 165 (60%), 152 (30%); ESI-HRMS: Calculated for $[M]^+$ $C_{19}H_{16}S$, 276.0973; found, 276.1003.

(*O*-*l*-Menthyl)methylenedibenzene (4g)[7]

299 mg, 0.927 mmol, 85%, white solid; Mp: 68–70 °C; TLC: 0.74 (50:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.36–7.16 (m, 10H), 5.54 (s, 1H), 3.12 (td, 1H, *J* = 10.5, 4.3 Hz), 2.35 (t, 1H, *J* = 6.9 Hz), 2.16–2.12 (m, 1H), 1.60–1.53 (m, 2H), 1.32–1.23 (m, 2H), 0.97–0.80 (m, 9H), 0.42 (d, 3H, *J* = 6.6 Hz); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 143.8, 142.5, 128.2, 128.0, 127.9, 127.4, 126.8, 126.6, 79.8, 75.7, 48.7, 40.3, 34.5, 31.4, 25.0, 22.8, 22.4, 21.3, 15.6; IR: ν_{max} (ATR, cm^{-1}) 2941, 2159, 2031, 1453, 1044, 764, 737, 699, 613, 452; EIMS (*m/z*): 304 (20%), 180 (20%), 168 (80%), 167 (100%), 165 (80%), 152 (80%), 137 (70%); ESI-HRMS: Calculated for $[M]^+$ $C_{23}H_{30}O$, 322.2297; found, 322.2299.

4-Benzhydrylphenol (4h)[8]

238 mg, 0.914 mmol, 84%, light yellow solid; Mp: 110–113 °C (Lit. 112–115 °C); TLC: 0.23 (8:1 hexane/EtOAc); ^{1}H NMR: (400 MHz, $CDCl_3$) δ_H: 7.33 (t, 4H, *J* = 7.4 Hz), 7.26 (t, 2H, *J* = 7.2 Hz), 7.17 (d, 4H, *J* = 7.2 Hz), 7.02 (d, 2H, *J* = 8.4 Hz), 6.77 (d, 2H, *J* = 8.8 Hz), 5.54 (s, 1H); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 153.7, 144.1, 136.2, 130.5, 129.3, 128.2, 126.2, 115.1, 55.9; IR: ν_{max} (ATR, cm^{-1}) 3022, 2160, 2031, 1510, 1450, 1237, 698, 565, 446; EIMS (*m/z*): 260 ($[M]^+$, 100%), 259 (35%), 229 (25%), 183 (80%), 181 (35%), 165 (60%), 152 (30%); ESI-HRMS: Calculated for $[M]^+$ $C_{19}H_{16}O$, 260.1201; found, 260.1193.

1-Benzhydrylnaphthalen-2-ol (4i)[9]

332 mg, 1.07 mmol, 98%, white foam; TLC: 0.44 (8:1 hexane/EtOAc); ^{1}H NMR: (400 MHz, $CDCl_3$) δ_H: 8.20 (d, 1H, *J* = 8.8 Hz), 7.94 (d, 1H, *J* = 8.0 Hz), 7.89 (d, 1H, *J* = 8.8 Hz), 7.56

(t, 1H, *J* = 7.4 Hz), 7.35–7.49 (m, 11 H), 7.25 (d, 1H, *J* = 9.2 Hz), 6.63 (s, 1H), 5.44 (s, 1H); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 152.7, 141.6, 133.3, 129.6, 129.0, 128.9, 128.7, 128.2, 127.1, 126.7, 125.2, 123.1, 122.8, 120.2, 119.7, 48.4; IR: ν_{max} (ATR, cm^{-1}) 3498, 2160, 2031, 1598, 1465, 1202, 815, 745, 700, 508; EIMS (*m/z*): 310 ($[M]^+$, 100%), 307 (70%), 233 (20%), 231 (90%), 215 (30%), 202 (35%), 167 (60%), 165 (45%); ESI-HRMS: Calculated for $[M]^+$ $C_{23}H_{18}O$, 310.1358; found, 310.1348.

3-Benzhydryl-1*H*-indole (4j)[10]

247 mg, 0.872 mmol, 80%, white solid; Mp: 113–115 °C; TLC: 0.39 (8:1 hexane/EtOAc); ^{1}H NMR: (400 MHz, $CDCl_3$) δ_H: 7.79 (s, 1H), 7.25–7.36 (m, 12H), 7.22 (t, 1H, *J* = 7.6 Hz), 7.05 (t, 1H, *J* = 7.4 Hz), 6.55 (d, 1H, *J* = 1.6 Hz), 5.73 (s, 1H); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 143.9, 136.6, 129.0, 128.2, 126.9, 126.2, 124.0, 122.0, 119.8, 119.8, 119.3, 111.0, 48.7; IR: ν_{max} (ATR, cm^{-1}) 3379, 2160, 2029, 1450, 746, 696, 504; EIMS (*m/z*): 283 ($[M]^+$, 90%), 282 (25%), 206 (100%), 204 (30%); ESI-HRMS: Calculated for $[M]^+$ $C_{21}H_{17}N$, 283.1361; found, 283.1356.

Methyl 5-*O*-benzhydryl-2,3-isopropylidene-β-D-riboside (4k)

291 mg, 0.786 mmol, 72%, white solid; Mp: 75–79 °C; TLC: 0.43 (8:1 Hexane:EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H 7.41 (d, 4H, *J* = 7.5 Hz), 7.34 (t, 4H, *J* = 5.9 Hz), 7.27 (d, 2H, *J* = 6.9 Hz), 5.41 (s, 1H), 5.01 (s, 1H), 4.76 (d, 1H, *J* = 5.9 Hz), 4.61 (d, 1H, *J* = 5.9 Hz), 4.51 (t, 1H, *J* = 6.9 Hz), 3.47–3.60 (m, 2H), 3.27 (s, 3H), 1.54 (s, 3H), 1.35 (s, 3H); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C : 141.9, 141.8, 128.2, 127.3, 127.3, 126.8, 126.8, 112.1, 109.2, 85.2, 85.1, 82.1, 82.1, 69.8, 54.6, 26.4, 24.9; IR: ν_{max} (ATR, cm^{-1}) 2941, 2509, 2159, 2029, 1976, 1453,

1092, 1059, 1047, 873, 696, 449; EIMS (*m/z*): 323 (30%), 207 (20%), 183 (20%), 167 (100%); ESI-HRMS: Calculated for $[M]^+$ $C_{22}H_{26}O_5$, 370.1780; found, 370.1776.

Benzylation of phenols

To a solution of benzyl chloride (0.245 mL, 2.10 mmol) and *n*-TBAB (69 mg, 10 mol %) in toluene (2 mL) was added 1.5 equivalents of the phenol. KOH (0.238 g, 2.1 mmol) dissolved in water (2 mL) was added to the reaction mixture. This mixture was heated to 80 °C for 12 hours. The reaction mixture was diluted with Et_2O (10 mL), washed with water (2 × 5 mL) and dried over magnesium sulphate. The organic solvent was removed under reduced pressure and the resulting residue purified by flash silica column chromatography using the eluents as detailed below (for TLC analysis)

Benzylphenyl ether (5a)[11]

379 mg, 2.06 mmol, 98%, white solid; Mp: 30–33 °C; TLC: 0.64 (20:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.37–7.55 (m, 8H), 7.09 (d, 2H, J = 8.7 Hz), 5.14 (s, 2H); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 158.7, 137.0, 129.4, 128.5, 127.8, 127.4, 120.9, 114.8, 69.8; IR: ν_{max} (ATR, cm^{-1}) 3036, 2907, 2159, 32031, 1584, 1490, 1455, 1376, 1237, 1169, 1011, 742, 689, 506; EIMS (*m/z*): 184 ($[M]^+$, 10%), 91 (100%); ESI-HRMS: Calculated for $[M]^+$ $C_{13}H_{12}O$, 184.0888; found, 184.0882.

***p*-Cresyl benzyl ether (5b)[11,12]**

412 mg, 2.08 mmol, >98%, white solid; Mp: 100–102 °C; TLC: 0.68 (10:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.45–7.32 (m, 5H), 7.10 (d, 2H, J = 8.1 Hz), 6.89 (d, 2H, J

= 8.1 Hz), 5.05 (s, 2H), 2.30 (s, 3H); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 156.7, 137.3, 130.1, 129.9, 128.5, 127.8, 127.4, 114.7, 70.0, 20.5; IR: ν_{max} (ATR, cm^{-1}) 2159, 1610, 1508, 1381, 1236, 1009, 807, 732, 694, 409; EIMS (*m/z*): 198 ($[M]^+$, 10%), 91 (100%); ESI-HRMS: Calculated for $[M]^+$ $C_{14}H_{14}O$, 198.1045; found, 198.1046.

Al(OTf)$_3$ catalysed rearrangement of phenol derived benzylic ethers

To a solution of Al(OTf)$_3$ (5 mg, 1 mol %) in nitroethane (2 mL) was added benzyl ether **5a** or **5b** (1.0 mmol) and the mixture was heated at 80 °C for 5 hours. The reaction was quenched by the addition of saturated aqueous sodium bicarbonate (5 mL). The reaction mixture was extracted with Et_2O (3 × 5 mL), and the combined organic layers washed with water (2 × 5 mL) and dried over magnesium sulphate. The solvent was removed under reduced pressure and the residue purified by flash silica column chromatography (10:1 hexane/EtOAc).

2-Benzylphenol (6a)[13]

181 mg, 0.98 mmol, 98%, yellow oil; TLC: 0.52 (10:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.22–7.32 (m, 5H), 7.15–7.11 (m, 2H), 6.89 (t, 1H, *J* = 7.4 Hz), 6.78 (d, 1H, *J* = 7.5 Hz), 4.71 (br s, 1H), 4.00 (s, 2H); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 153.7, 139.8, 131.0, 128.7, 128.6, 127.8, 126.9, 126.3, 120.9, 115.7, 36.3; IR: ν_{max} (ATR, cm^{-1}) 3531, 3026, 1921, 2442, 2159, 2029, 1976, 1493, 1452, 1167, 1093, 752, 728, 696, 492; EIMS (*m/z*): 184 ($[M]^+$, 100%), 183 (50%), 165 (50%), 106 (50%); ESI-HRMS: Calculated for $[M]^+$ $C_{13}H_{12}O$, 184.0888; found, 184.0779.

2-Benzyl-4-methylphenol (6b)[14]

196 mg, 0.99 mmol, >98%, clear oil; TLC: 0.53 (10:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.32–7.24 (m, 5H), 6.93–6.91 (m, 2H), 6.67 (d, 1H, J = 8.7 Hz), 4.59 (s, 1H), 3.96 (s, 2H), 2.26 (s, 3H); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 151.4, 140.0, 131.5, 130.1, 128.6, 128.1, 126.7, 126.3, 115.6, 36.3, 20.5; IR: ν_{max} (ATR, cm^{-1}) 3529, 3026, 2921, 2521, 2159, 2030, 1494, 1452, 1185, 1101, 810, 696, 435; EIMS (*m/z*): 198 ($[M]^+$, 100%), 183 (30%), 165 (20%), 120 (50%); ESI-HRMS: Calculated for $[M]^+$ $C_{14}H_{14}O$, 198.1045; found, 198.1051.

General procedure for the $Al(OTf)_3$ catalysed nucleophilic substitution of *trans*-1,3-diphenylprop-2-en-1-ol (**7**)

To a mixture of *trans*-1,3-diphenylprop-2-en-1-ol (0.231 g, 1.1 mmol) and $Al(OTf)_3$ (5 mg, 1 mol %) in nitroethane (2 mL) was added 1 equivalent of the appropriate nucleophile. The mixture was allowed to stir for 1 hour at room temperature and the reaction was quenched by the addition of saturated aqueous sodium bicarbonate (5 mL). The reaction mixture was extracted with Et_2O (3 × 5 mL), the combined organic layers washed with water (2 × 5 mL) and dried with magnesium sulphate. The solvent was removed under reduced pressure and the residue purified by flash silica column chromatography using the eluents given below.

1-Ethoxy-1,3-diphenylpropene (8a)[15]

223 mg, 0.936 mmol, 85%, clear oil; TLC: 0.51 (50:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.43–7.18 (m, 10H), 6.61 (d, 1H, J = 15.9 Hz), 6.31 (dd, 1H, J = 16.1, 7.0 Hz), 4.92 (d, 1H, J = 7.2 Hz), 3.59 (dq, 1H, J = 9.1, 7.0 Hz), 3.49 (dq, 1H, J = 9.3, 7.2 Hz), 1.27 (t,

3H, *J* = 7.0 Hz); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 141.5, 136.6, 131.1, 130.6, 128.5, 127.6, 126.8, 126.6, 82.5, 64.0, 15.3; IR: ν_{max} (ATR, cm^{-1}) 2159, 2030, 1720, 2602, 1450, 1214, 1097, 1017, 747, 696, 499; EIMS (*m/z*): 238 ($[M]^+$, 100%); ESI-HRMS: Calculated for $[M]^+$ $C_{17}H_{18}O$, 238.1358; found, 238.1343.

1-Allyloxy-1,3-diphenylpropene (8b)[16]

231 mg, 0.923 mmol, 84%, clear oil; TLC: 0.52 (50:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.49–7.24 (m, 10H), 6.68 (d, 1H, *J* = 16.2 Hz), 6.36 (dd, 1H, *J* = 15.8, 7.1 Hz), 6.03 (ddt, 1H, *J* = 17.2, 9.9 Hz), 5.38 (dq, 1H, *J* = 17.2, 1.7 Hz), 5.26 (dq, 1H, *J* = 9.9, 5.2 Hz), 5.04 (d, 1H, *J* = 7.2 Hz), 4.10 (dt, 2H, *J* = 9.9, 1.5 Hz); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 141.1, 136.5, 134.8, 131.3, 130.2, 128.5, 127.7, 127.6, 126.8, 126.5, 116.9, 81.7, 69.2; IR: ν_{max} (ATR, cm^{-1}) 3030, 2159, 2029, 1719, 1450, 1269, 1025, 748, 696, 483; EIMS (*m/z*):192 (100%), 191 (60%), 189 (30%), 165 (50%), 115 (40%), 105 (30%), 77 (40%); ESI-HRMS: M^+ Calcd for $C_{18}H_{18}O$, 250.1358; found, 250.1352.

2-Propynyloxy-1,3-diphenylpropene (8c)[17]

262 mg, 1.06 mmol, 96%, clear oil; TLC: 0.33 (50:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.44–7.20 (m, 10H), 6.66 (d, 1H, *J* = 15.9 Hz), 6.29 (d, 1H, *J* = 16.1, 7.7 Hz), 5.20 (d, 1H, *J* = 7.2 Hz), 4.24 (dd, 1H, *J* = 15.5, 2.5 Hz), 4.14 (dd, 1H, *J* = 15.6, 2.4 Hz), 2.45 (t, 1H, *J* = 1.9 Hz); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 140.2, 136.4, 132.4, 129.1, 128.6, 127.9, 127.1, 126.6, 80.9, 79.8, 74.4, 55.3; IR: ν_{max} (ATR, cm^{-1}) 3288, 3029, 2511, 2159, 2030, 1494, 1450, 1068, 1026, 967, 746, 695, 458; ESI-HRMS: Calculated for $[M]^+$ $C_{18}H_{16}O$, 248.1201; found, 248.1218.

3-(1,3-Diphenylprop-2-en-1-yl)pentane-2,4-dione (8d)[15]

315 mg, 1.08 mmol, 98%, white solid; Mp: 78–80 °C; TLC: 0.54 (4:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.31–7.18 (m, 10H), 6.45 (d, 1H, *J* = 15.9 Hz), 6.23 (dd, 1H, *J* = 15.4, 7.1 Hz), 4.38–4.36 (m, 2H), 2.24 (s, 3H), 1.92 (s, 3H); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 202.4, 202.3, 139.9, 136.6, 131.3, 129.1, 128.7, 128.3, 127.7, 127.4, 127.0, 126.1, 74.1, 48.9, 29.8, 29.5; IR: ν_{max} (ATR, cm^{-1}) 3026, 2918, 2439, 2160, 1976, 2721, 1359, 1138, 974, 693, 420; EIMS (*m/z*): 274 (40%), 249 (80%), 232 (35%), 193 (65%), 191 (50%), 178 (45%), 115 (95%), 91 (100%); ESI-HRMS: Calculated for $[M]^+$ $C_{20}H_{20}O_2$, 292.1463; found, 292.1461.

Ethyl 2-(1,3-diphenylprop-2-en-1-yl)acetylacetonate (8e)[15]

348 mg, 1.08 mmol, 98%, clear oil, diastereomeric mixture – the two sets of data below represent each set of enantiomers; TLC: 0.5 (8:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.48–7.33 (m, 10H), 6.61 (d, 1H, *J* = 11.1 Hz), **6.56 (d, 1H, *J* = 11.4 Hz)**, 6.44 (dd, 1H, *J* = 15.9, 8.1 Hz), **6.38 (dd, 1H, *J* = 15.1, 8.2 Hz)**, 4.43 (t, 1H, *J* = 9.8 Hz), 4.36–4.20 (m, 3H), **4.08 (q, 2H, *J* = 6.9 Hz)**, 2.44 (s, 3H), **2.18 (s, 3H)**, 1.35 (t, 3H, *J* = 8.1 Hz), **1.12 (t, 3H, *J* = 7.0 Hz)**; ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 201.6, **201.4**, 167.8, **167.5**, 140.3, **140.1**, 136.7, **136.6**, 131.7, **131.4**, 129.4, **129.2**, 128.8, **128.6**, 128.4, 127.9, **127.9**, 127.5, **127.5**, 127.1, **127.0**, 126.3, **126.2**, 65.4, **65.1**, 61.5 (OCH_2CH_3), **61.3**, **48.7**, 30.0, **29.8**, 14.1; IR: ν_{max} (ATR, cm^{-1}) 3028, 2512, 2159, 2028, 1452, 1153, 965, 745, 685, 486; EIMS (*m/z*): 304 (95%), 279 15%), 233 (50%), 193 (80%), 115 (95%), 91 (45%); EI-HRMS: Calculated for $[M]^+$ $C_{21}H_{22}O_3$, 322.1569; found, 322.1556.

(1,3-Diphenylprop-2-en-1-yl)(phenyl)sulphane (8f)[18]

304 mg, 0.943 mmol, 86%, white solid; Mp: 69–72 °C; TLC: 0.49 (50:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.56–7.27 (m, 10H), 6.60 (dd, 1H, *J* = 15.5, 8.2 Hz), 6.42 (d, 1H, *J* = 15.3 Hz), 5.06 (d, 1H, *J* = 8.1 Hz); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 140.1, 136.6, 134.8, 133.0, 131.4, 129.0, 128.6, 128.4, 127.9, 127.5, 127.4, 126.4; IR: ν_{max} (ATR, cm^{-1}) 3060, 3027, 2509, 2160, 2030, 1478, 1438, 1025, 968, 739, 687, 487; ESI-HRMS: Calculated for $[M]^+$ $C_{21}H_{17}S$, 301.1051; found, 301.1059.

4-(1,3-Diphenylprop-2-en-1-yl)phenol (8g)[15]

273 mg, 0.903 mmol, 82%, yellow oil; TLC: 0.44 (10:1 toluene/EtOAC); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.37–7.16 (m, 10H), 7.08 (d, 2H, *J* = 8.1 Hz), 6.77 (d, 2H, *J* = 7.8 Hz), 6.63 (dd, 1H, *J* = 15.9, 7.5 Hz), 6.31 (d, 1H, *J* = 16.1 Hz), 4.82 (d, 1H, *J* = 7.5 Hz), 4.74 (s, 1H); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 153.9, 143.7, 137.3, 135.8, 132.8, 131.1, 129.8, 128.6, 128.5, 128.4, 127.3, 126.4, 126.4, 115.3, 53.3; IR: ν_{max} (ATR, cm^{-1}) 3317, 3025, 2494, 2159, 2030, 1510, 1171, 744, 695, 475; EIMS (*m/z*): 286 ($[M]^+$, 50%), 209 (35%), 208 (100%), 207 (70%), 192 (70%), 165 (35%), 121 (90%), 105 (50%); ESI-HRMS: Calculated for $[M]^+$ $C_{21}H_{18}O$, 286.1358; found, 286.1351.

1-(1,3-Diphenylprop-2-en-1-yl)naphthalen-2-ol (8h)[19]

300 mg, 0.892 mmol, 81%, yellow oil; TLC: 0.44 (8:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.98 (d, 1H, *J* = 8.7 Hz), 7.79 (d, 1H, *J* = 7.8 Hz), 7.73 (d, 1H, *J* = 8.7 Hz), 7.43 (t, 1H, *J* = 7.0 Hz), 7.20–7.38 (m, 11H), 7.10 (d, 1H, *J* = 8.7 Hz), 6.97 (dd, 1H, *J* = 6.6, 1.2 Hz), **6.91 (dd, 1H, *J* = 7.1, 1.0 Hz)**, 6.49 (d, 1H, *J* = 15.6 Hz), 5.87 (d, 1H, *J* = 6.6 Hz), 5.52

(s, 1H); ^{13}CNMR: (75 MHz, $CDCl_3$) δ_C: 152.2, 141.6, 136.7, 133.1, **133.0**, 130.0, **129.7**, 129.3, 128.9, 128.8, 128.5, 128.0, 127.6, 126.8, 126.7, 126.4, 123.2, 123.0, 119.7, 119.1, 45.2; IR: ν_{max} (ATR, cm^{-1}) 2361, 2159, 2031, 1260, 813, 692, 48; EIMS (*m/z*): 336 ($[M]^+$, 50%), 334 (90%), 260 (35%), 257 (90%), 245 (95%), 231 (95%), 215 (80%), 202 (60%), 115 (40%), 105 (40%); ESI-HRMS: Calculated for $[M]^+$ $C_{25}H_{20}O$, 336.1514; found, 336.1499.

3-(1,3-Diphenylprop-2-en-1-yl)-1*H*-indole (8i)[15]

296 mg, 0.957 mmol, 87%, yellow oil; TLC: 0.36 (8:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.87 (s, 1H), 7.53 (d, 1H, *J* = 8.1 Hz), 7.45–7.22 (m, 12H), 7.12 (t, 1H, *J* = 7.5 Hz), 6.88 (d, 1H, *J* = 2.3 Hz), 6.82 (dd, 1H, *J* = 15.7, 7.4 Hz), 6.53 (d, 1H, *J* = 15.9 Hz), 5.20 (d, 1H, *J* = 7.2 Hz); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 143.3, 137.4, 136.6, 132.5, 130.5, 128.4, 128.4, 127.1, 126.7, 126.3, 126.3, 122.6, 122.0, 119.8, 119.4, 118.5, 111.1, 46.1; IR: ν_{max} (ATR, cm^{-1}) 3057, 2923, 2509, 2160, 1977, 1695, 1450, 742, 695, 511; EIMS (*m/z*): 309 ($[M]^+$, 5%), 208 (25%), 207 (35%), 149 (30%), 105 (35%), 77 (50%); ESI-HRMS: Calculated for $[M]^+$ $C_{23}H_{19}N$, 309.1517; found, 309.1506.

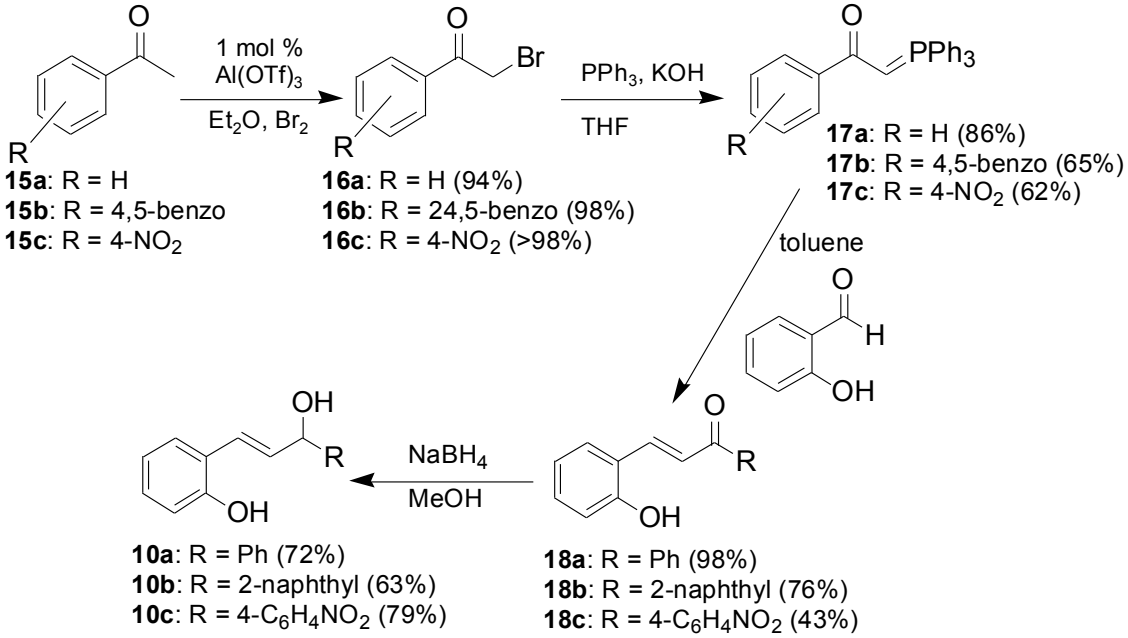
***N*-Benzhydryl-4-methylbenzenesulphonamide (9a)[20]**

364 mg, 1.08 mmol, 98%, white solid; Mp: 150–152 °C; TLC: 0.46 (4:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.55 (d, 2H, *J* = 7.8 Hz), 7.16–7.07 (m, 12 H), 5.67 (d, 1H, *J* = 7.7 Hz), 5.57 (d, 1H, *J* = 7.7 Hz), 2.34 (s, 3H); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 143.0, 140.5, 137.3, 129.2, 128.4, 127.4, 127.3, 127.1, 61.2, 21.4; IR: ν_{max} (ATR, cm^{-1}) 3246, 2159, 2030, 1450, 1313, 1157, 1058, 698, 672, 406; EIMS (*m/z*): 218 (10%), 207 (30%), 182 (70%), 91 (100%); ESI-HRMS: Calculated for $[M]^+$ $C_{20}H_{19}NO_2S$, 337.1136; found, 337.1125.

(*E*)-*N*-(1,3-Diphenyl-prop-2-en-1-yl)-4-methylbenzenesulphonamide (9b)[15]

396 mg, 1.09 mmol, >98%, white solid; Mp: 130–132 °C; TLC: 0.43 (4:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.67 (d, 2H, *J* = 8.1 Hz), 7.21–7.11 (m, 10H), 7.10 (d, 2H, *J* = 8.1 Hz), 6.33 (1H, *J* = 15.9 Hz), 6.07 (d, 1H, *J* = 15.9, 6.6 Hz), 5.58 (d, 1H, *J* = 7.5 Hz), 5.11 (t, 1H, *J* = 7.0 Hz), 2.28 (s, 3H); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 143.1, 139.6, 137.7, 136.0, 131.9, 129.3, 128.6, 128.3, 128.1, 127.7, 127.6, 127.2, 127.0, 126.4, 59.7, 21.3; IR: ν_{max} (ATR, cm^{-1}) 3290, 3028, 2480, 2160, 1977, 1425, 1324, 1292, 1151, 966, 751, 667, 447; EIMS (*m/z*): 192 (70%), 191 (40%), 165 (20%), 91 (100%); ESI-HRMS: Calculated for $[M]^+$ $C_{22}H_{21}NO_2S$, 363.1293; found, 363.1297.

General procedure for the α-bromination of acetophenones



Scheme S1. Synthesis of phenylpropenols **10**.

Acetophenones **15** (Scheme S1, 8.32 mmol), respectively, and $Al(OTf)_3$ (39 mg, 82 μmol) were dissolved in Et_2O (5 mL) in a two necked flask equipped with a reflux condenser. To this solution was added bromine (0.42 mL, 8.32 mmol) by means of a dropping funnel so as to maintain a gentle reflux. Upon completion of the addition of bromine the solvent was removed under reduced pressure, under a constant stream of nitrogen using an aqueous sodium bicarbonate trap to scrub the HBr. The residue was washed with *n*-hexane (5 mL) and then water (5 × 10 mL). The white solid product was collected and dried under reduced pressure and required no further purification.

2-Bromo-1-phenylethanone (16a)[21]

1.557 g, 7.82 mmol, 94%, white solid; Mp: 42–45 °C; ^{1}H NMR: (400 MHz, $CDCl_3$) δ_H: 7.97 (d, 2H, *J* = 8.0 Hz), 7.59 (t, 1H, *J* = 7.4 Hz), 7.48 (t, 2H, *J* = 7.4 Hz), 4.44 (s, 2H); ^{13}C NMR: (100 MHz, $CDCl_3$) δ_C: 191.3, 133.9, 129.7, 128.9, 128.8, 30.9; IR: ν_{max} (ATR, cm^{-1}) 3065, 3002, 1953, 1476, 2160, 2028, 1690, 1580, 1447, 1389, 1281, 1196, 991, 745, 685, 620, 504.

2-Bromo-1-(naphthalen-2-yl)ethanone (16b)[22]

2.031 g, 8.15 mmol, 98%, white solid; Mp: 79–81 °C; ^{1}H NMR: (400 MHz, $CDCl_3$) δ_H: 8.49 (s, 1H), 8.00 (d, 1H, *J* = 8.4 Hz), 7.96 (d, 1H, *J* = 8.0 Hz), 7.91–7.86 (m, 2H), 7.61 (t, 1H, *J* = 7.6 Hz), 7.56 (t, 1H, *J* = 7.6 Hz), 4.56 (s, 2H); ^{13}C NMR: (100 MHz, $CDCl_3$) δ_C: 1919.2, 135.8, 132.2, 131.2, 130.9, 129.7, 129.0, 128.8, 127.8, 127.0, 124.1, 30.9; IR: ν_{max} (ATR, cm^{-1}) 2442, 2159, 2026, 1976, 1689, 1384, 1158, 1029, 853, 810, 678, 514.

2-Bromo-1-(4-nitrophenyl)ethanone (16c)[22]

2.018 g, 8.24 mmol, >98%, white solid; Mp: 91–93 °C; ^{1}H NMR: (400 MHz, $CDCl_3$) δ_H: 8.31 (d, 2H, *J* = 8.4 Hz), 8.13 (d, 2H, *J* = 8.4 Hz), 4.45 (s, 2H); ^{13}C NMR: (100 MHz, $CDCl_3$) δ_C: 189.9, 150.6, 138.3, 130.0, 124.0, 30.2; IR: ν_{max} (ATR, cm^{-1}) 3109, 2446, 2160, 2031, 1977, 1699, 1515, 1341, 1191, 998, 841, 744, 480.

Wittig ylide formation from the corresponding bromides

Triphenyl phosphine (1.00 g, 3.81 mmol) was dissolved in THF (5 mL). To this mixture was added α-bromoacetophenones **16** (3.81 mmol), respectively, in five portions. The mixture was stirred at room temperature overnight. The resulting white precipitate was collected by filtration, washed with *n*-hexane (5 × 5 mL) and dried under reduced pressure. The dried white solid was dissolved in MeOH (20 mL). To this solution was added KOH (2.14 g, 38.1 mmol) dissolved in H_2O (20 mL) in a dropwise fashion. The mixture was allowed to stir at room temperature for 2 hours. The MeOH was removed under reduced pressure and the crude reaction mixture extracted with Et_2O (3 × 10 mL). The combined organic layers were washed with water (3 × 10 mL) and dried over magnesium sulphate. The solvent was removed under reduced pressure to afford the ylide, which was purified by re-crystallisation from hot ethanol.

1-Phenyl-2-(triphenylphosphoranylidene)ethanone (17a)[23]

1.248 g, 3.28 mmol, 86%, white solid; Mp: 175–178 °C; ^{1}H NMR: (400 MHz, $CDCl_3$) δ_H: 7.99–7.94 (m, 2H), 7.70 (dd, 6H, *J* = 12.2, 7.8 Hz), 7.55–7.52 (m, 3H), 7.46–7.45 (m, 6H), 7.40–7.30 (m, 3H), 4.41 (d, 1H, *J* = 24.4 Hz); ^{13}C NMR: (100 MHz, $CDCl_3$) δ_C: 184.7, 141.1 (d, *J* = 13.0 Hz), 133.0 (d, *J* = 10.1 Hz), 132.0, 129.3, 128.8 (d, *J* = 12.2 Hz), 127.6, 127.4, 126.8, 126.4, 50.6 (d, *J* = 111.0 Hz); ^{31}P NMR: (160 MHz, $CDCl_3$) δ_P: 16.96; IR: ν_{max} (ATR,

cm^{-1}) 3049, 2505, 2160, 2028, 1976, 1587, 1513, 1436, 1385, 1104, 873, 747, 710, 689, 461; EIMS (*m/z*): 380 ($[M]^+$, 85%), 379 (100%), 303 (100%), 277 (60%), 202 (40%), 183 (70%); ESI-HRMS: Calculated for $[M]^+$ $C_{26}H_{21}OP$, 380.1330; found 380.1314.

1-(2-Naphthalenyl)-2-(triphenylphosphoranylidene)ethanone (17b)[24]

1.068 g, 2.48 mmol, 65%, yellow solid; Mp: 186–189 °C; ^{1}H NMR: (400 MHz, $CDCl_3$) δ_H: 8.50 (s, 1H), 8.06 (d, 1H, *J* = 8.4 Hz), 7.88–7.72 (m, 9H), 7.69–7.45 (m,11H), 4.57 (d, 1H, *J* = 24.4 Hz); ^{13}C NMR: (100 MHz, $CDCl_3$) δ_C: 184.6, 138.5 (d, *J* = 14.5 Hz) 134.1, 133.2 (d, *J* = 10.1 Hz), 133.0, 132.1, 128.9 (d, *J* = 12.3 Hz), 127.4, 127.1, 126.5, 126.2, 125.7, 124.9, 51.6, (d, *J* = 111.0 Hz); P^{31} NMR: (160 MHz, $CDCl_3$) δ_P: 17.02; IR: ν_{max} (ATR, cm^{-1}) 3050, 2504, 2159, 2028, 2977, 1520, 2435, 1395, 1105, 873, 757, 691, 435; EIMS (*m/z*): 430 ($[M]^+$, 95%), 429 (100%), 401 (25%), 303 (90%), 277 (65%), 183 (55%); ESI-HRMS: Calculated for $[M]^+$ $C_{30}H_{23}OP$, 430.1487; found, 430.1484.

1-(4-Nitrophenyl)-2-(triphenylphosphoranylidene)ethanone (17c)[24]

1.004 g, 2.36 mmol, 62%, yellow solid; Mp: 161–162 °C; ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 8.16 (d, 2H, *J* = 11.6 Hz), 8.05 (d, 2H, *J* = 12.0 Hz), 7.72–7.65 (m, 6H), 7.60–7.55 (m, 3H), 7.51–7.45 (m, 6H), 4.49 (d, 1H, *J* = 30.4 Hz); ^{13}C NMR: (100 MHz, $CDCl_3$) δ_C: 181.8, 148.2, 147.1 (d, *J* = 15.0 Hz), 133.1 (d, *J* = 10.2 Hz), 132.0, 129.0 (d, *J* = 12.2 Hz), 127.7, 126.6, 125.6, 123.1, 53.7 (d, *J* = 109.0 Hz); ^{31}P NMR: (160 MHz, $CDCl_3$) δ_P: 17.02; IR: ν_{max} (ATR, cm^{-1}) 3065, 2442, 2159, 2031, 1976, 1525, 1436, 1407, 1339, 1103, 863, 715, 692, 512; EIMS (*m/z*): 425 ($[M]^+$, 60%), 424 (100%), 303 (75%), 277 (65%), 183 (65%); ESI-HRMS: Calculated for $[M]^+$ $C_{26}H_{20}NO_3P$, 425.1181; found, 425.1174.

General procedure for the synthesis of 2-hydroxychalcones via the Wittig reaction

The Wittig reagents **17** (2.62 mmol) were respectively dissolved in toluene (10 mL) in a two necked flask equipped with a reflux condenser. To this solution was added salicylaldehyde (0.321 g, 2.63 mmol) dissolved in toluene (5 mL) and the reaction mixture was stirred under reflux for 1 hour. The toluene was removed under reduced pressure and the residue purified by flash silica column chromatography (4:1 hexane/EtOAc).

(*E*)-3-(2-Hydroxyphenyl)-1-phenylprop-2-en-1-one (18a)[25]

577 mg, 2.57 mmol, 98%, yellow solid; Mp: 152–154 °C; TLC: 0.24 (4:1 hexane/EtOAc); ^{1}H NMR: (400 MHz, $CDCl_3$) δ_H: 8.13 (d, 1H, *J* = 16.0 Hz), 8.02 (d, 2H, *J* = 7.6 Hz), 7.69 (d, 1H, *J* = 16.0 Hz), 7.59–7.47 (m, 4H), 7.26 (t, 1H, *J* = 8.0 Hz), 6.95 (t, 1H, *J* = 7.4 Hz), 6.90 (d, 1H, *J* = 8.4 Hz), 6.35 (br s, 1H); ^{13}C NMR: (100 MHz, $CDCl_3$) δ_C: 191.8, 155.7, 140.8, 138.3, 132.7, 131.8, 129.6, 128.6, 122.9, 122.2, 121.0, 116.6; IR: ν_{max} (ATR, cm^{-1}) 3185, 2504, 2159, 2028, 1976, 1638, 1560, 1455, 1344, 1229, 1022, 731, 513, 471; EIMS (*m/z*): 224 ($[M]^+$, 15%), 208 (35%), 207 100%), 178 (55%), 147 (20%), 105 (25%), 77 (25%); ESI-HRMS: Calculated for $[M]^+$ $C_{15}H_{12}O_2$, 224.0837; found, 224.0832.

(*E*)-3-(2-Hydroxyphenyl)-1-(naphthalen-2-yl)prop-2-en-1-one (18b)[26]

546 mg, 1.99 mmol, 76%, yellow solid; Mp: 156–159 °C; TLC: 0.48 (2:1 hexane/EtOAc); ^{1}H NMR: (400 MHz, DMSO) δ_H: 10.17 (s, 1H), 8.85 (s, 1H), 8.11–7.92 (m, 5H), 7.65 (t, 2H, *J* = 8.4 Hz), 7.28 (t, 1H, *J* = 7.6 Hz), 6.95 (d, 1H, *J* = 8.0 Hz), 6.80 (t, 1H, *J* = 7.6 Hz); ^{13}C NMR: (100 MHz, DMSO) δ_C: 189.15, 157.2, 139.3, 135.2, 134.9, 132.3, 132.1, 130.1, 129.6, 128.6,

128.5, 128.4, 127.7, 126.9, 124.2, 121.4, 120.8, 119.4, 116.2; IR: ν_{max} (ATR, cm^{-1}) 3184, 2522, 2159, 2030, 1976, 1645, 1585, 1458, 1333, 1187, 986, 826, 746, 586, 431; EIMS (*m/z*): 274 ($[M]^+$, 10%), 258 (30%), 257 (100%), 228 (20%), 155 (15%), 127 (20%); ESI-HRMS: Calculated for $[M]^+$ $C_{19}H_{14}O_2$, 274.0994; found, 274.0988.

(*E*)-3-(2-Hydroxyphenyl)-1-(4-nitrophenyl)-2-propen-1-one (18c)[27]

303 mg, 1.13 mmol, 43%, yellow solid; Mp: 195–200 °C; TLC: 0.61 (2:1 hexane/EtOAc); ^1H NMR: (400 MHz, DMSO) δ_H: 10.40 (s, 1H), 8.34 (d, 2H, *J* = 8.4 Hz), 8.27 (d, 2H, *J* = 8.4 Hz), 8.07 (d, 1H, *J* = 15.6 Hz), 7.85 (d, 1H, *J* = 5.2 Hz), 7.83 (d, 1H, *J* = 15.6 Hz), 7.28 (t, 1H, *J* = 7.4 Hz), 6.96 (d, 1H, *J* = 8.0 Hz), 6.87 (t, 1H, *J* = 7.2 Hz); ^{13}C NMR: (100 MHz, DMSO) δ_C: 188.6, 157.6, 149.6, 142.7, 141.1, 132.5, 129.6, 128.9, 128.8, 123.8, 121.0, 120.6, 119.4, 116.3; IR: ν_{max} (ATR, cm^{-1}) 3462, 3333, 2447, 2160, 2029, 1976, 1673, 1651, 1572, 1518, 1339, 1214, 1033, 848, 755, 426; EIMS (*m/z*): 269 ($[M]^+$, 25%), 252 (95%), 206 (50%), 150 (40%), 147 (50%), 119 (45%); ESI-HRMS: Calculated for $[M]^+$ $C_{15}H_{11}O_4N$, 269.0688; found, 269.0681.

General procedure for the sodium borohydride reduction of 2-hydroxychalcones

Compounds **18** (4.46 mmol) were respectively dissolved in MeOH (10 mL) and the mixture cooled to 0 °C. To this solution was added $NaBH_4$ (0.675 g, 17.8 mmol) in six portions. The resultant mixture was allowed to warm to room temperature and stirred for 1 hour. The reaction was quenched by the addition of 1 M HCl (10 mL), the mixture extracted with Et_2O (3 × 5 mL) and the combined organic layers washed with water (2 × 5 mL) and dried with magnesium sulphate. The solvent was removed under reduced pressure and the residue purified by flash silica column chromatography (2:1 hexane/EtOAc).

(*E*)-2-(1-Hydroxy-1-phenylprop-2-en-3-yl)phenol (10a)[28]

727 mg, 3.21 mmol, 72%, white solid; Mp: 102–105 °C; TLC: 0.31 (2:1 hexane/EtOAc); ^{1}H NMR: (400 MHz, DMSO) δ_H: 9.58 (s, 1H), 7.39 (d, 2H, *J* = 7.2 Hz), 7.35–7.30 (m, 3H), 7.22 (t, 1H, *J* = 7.2 Hz), 7.25 (t, 1H, *J* = 8.4 Hz), 6.83 (d, 1H, *J* = 16.0 Hz), 6.86–6.81 (m, 1H), 6.73 (t, 1H, *J* = 7.4 Hz), 6.53 (dd, 1H, *J* = 16.0, 6.4 Hz,), 5.55 (d, 1H, *J* = 4.4 Hz), 5.22 (t, 1H, *J* = 5.6 Hz); ^{13}C NMR: (100 MHz, DMSO) δ_C: 154.7, 144.8, 133.0, 128.2, 128.1, 126.7, 126.6, 126.2, 123.6, 123.3, 119.1, 115.7, 73.8; IR: ν_{max} (ATR, cm^{-1}) 2922, 2441, 2159, 2030, 1976, 1731, 1599, 1487, 1450, 1022, 751, 697, 414; EIMS (*m/z*): 223 ([M-3H]$^+$, 20%), 222 (45%), 221 (30%), 208 (70%), 207 (100%), 105 (95%), 77 (60%); ESI-HRMS: Calculated for [M]$^+$ $C_{15}H_{14}O_2$, 226.0994; found, 226.0981.

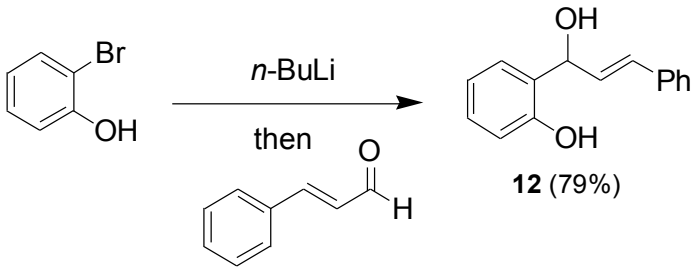
(*E*)-2-(1-Hydroxy-1-(naphthalen-2-yl)prop-2-en-3-yl)phenol (10b)[29]

776 mg, 2.81 mmol, 63%, off white solid; Mp: 103–105 °C; TLC: 0.43 (3:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, DMSO) δ_H: 9.61 (s, 1H), 7.91–7.87 (m, 4H), 7.56 (dd, 1H, *J* = 11.2, 2.0 Hz), 7.52–7.44 (m2H), 7.37 (dd, 1H, 10.4, 2.0 Hz), 7.04 (dt, 1H, *J* = 14.1, 4.8 Hz), 6.93 (d, 1H, *J* = 21.2 Hz), 6.84 (d, 1H, *J* = 11.2 Hz), 6.74 (t, 1H, *J* = 10.2 Hz), 6.44 (dd, 1H, *J* = 21.2, 8.8 Hz), 5.72 (d, 1H, *J* = 5.6 Hz), 5.41 (t, 1H, *J* = 6.8 Hz); ^{13}C NMR: (75 MHz, DMSO) δ_C: 154.7, 142.3, 132.9, 132.8, 132.2, 128.3, 127.8, 127.6, 127.5, 126.7, 126.0, 125.6, 125.1, 124.2, 123.9, 123.4, 119.1, 115.7, 73.9; IR: ν_{max} (ATR, cm^{-1}) 3343, 3051, 2556, 2159, 2030, 1976, 1453, 1246, 1089, 818, 753, 455; EIMS (*m/z*): 276 ([M]$^+$, 5%), 260 (100%), 258 (50%), 257 (40%), 154 (30%); ESI-HRMS: Calculated for [M]$^+$ $C_{19}H_{16}O_2$, 276.1150; found, 276.1142.

(*E*)-2-(1-Hydroxy-1-(4-nitrophenyl)prop-2-en-3-yl)phenol (10c)

956 mg, 3.52 mmol, 79%, red solid; Mp: 139–142 °C; TLC: 0.44 (2:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, DMSO) δ_H: 9.65 (s, 1H), 8.21 (d, 2H, *J* = 11.6 Hz), 7.67 (d, 2H, *J* = 11.2 Hz), 7.35 (dd, 1H, *J* = 10.2, 2.2 Hz), 7.05 (t, 1H, *J* = 9.2 Hz), 6.90 (d, 1H, *J* = 21.1 Hz), 6.82 (dd, 1H, *J* = 10.8, 1.6 Hz), 6.73 (t, 1H, *J* = 10.6 Hz), 6.33 (dd, 1H, *J* = 21.1, 9.0 Hz), 5.92 (d, 1H, *J* = 4.8 Hz), 5.39 (d, 1H, *J* = 6.0 Hz); ^{13}C NMR: (75 MHz, DMSO) δ_C: 154.8, 152.6, 146.4, 131.7, 128.6, 127.2, 126.9, 124.9, 123.5, 123.0, 119.2, 115.7, 73.1; IR: ν_{max} (ATR, cm^{-1}) 2159, 2031, 1516, 1454, 1343, 855, 752, 699, 474; EI-HRMS: Calculated for $[M]^+$ $C_{15}H_{13}NO_4$, 271.0845; found, 271.0832.

(*E*)-2-(1-Hydroxy-3-phenylprop-2-en-1-yl)phenol (12)[29]



Scheme S2. Synthesis of **12**, an isomer of **10a**.

To an oven-dried two necked reaction flask were added anhydrous THF (5 mL) and *n*-BuLi (2.31 mmol, 0.9 M) at 0 °C, after which 2-bromophenol (0.200 g, 1.16 mmol) dissolved in THF (2 mL) was added. The mixture was allowed to warm to room temperature and stirred for 2 hours after which it was cooled to –78 °C. To the solution was added *trans*-cinnamaldehyde (0.146 mL, 1.16 mmol) dissolved in THF (5 mL) and the mixture was allowed to warm to 0 °C and stirred for 1 hour. The reaction was quenched by the addition of

saturated aqueous NH_4Cl (10 mL). The reaction mixture was diluted with Et_2O (10 mL) and the organic layer washed with water (2 × 5 mL) and dried with magnesium sulphate. The organic solvent was removed under reduced pressure and the resulting residue purified by flash silica column chromatography (4:1 hexane/EtOAc).

207 mg, 0.916 mmol, 79%, yellow oil; TLC: 0.37 (4:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, DMSO) δ_H: 9.43 (br s, 1H), 7.38 (d, 2H, *J* = 7.2 Hz), 7.29 (t, 2H, *J* = 7.2 Hz), 7.20 (d, 1H, *J* = 7.2 Hz), 7.22–7.17 (m, 1H), 7.06 (t, 1H, *J* = 7.5 Hz), 6.82–6.80 (m, 2H), 6,59 (d, 1H, *J* = 16.1 Hz), 6.40 (dd, 1H, *J* = 16.1, 5.0 Hz), 5.57 (d, 1H, *J* = 5.0 Hz); ^{13}C NMR: (75 MHz, DMSO) δ_C: 153.9, 136.9, 133.0, 130.3, 128.6, 127.6, 127.2, 126.8, 126.2, 119.0, 115.0, 67.5; IR: ν_{max} (ATR, cm^{-1}) 3028, 1732, 1603, 1485, 1452, 1226, 1202, 750, 696, 409; EI-HRMS: Calculated for $[M]^+$ $C_{15}H_{14}O_2$, 226.0994; found, 226.0986.

General procedure for the cyclisation of "activated" diols

$Al(OTf)_3$ (4 mg, 8.8 μmol) was dissolved in DCM (10 mL) and **10a** (0.200 g, 0.884 mmol) was added. The reaction mixture was allowed to stir at room temperature for 1 hour. The reaction was quenched with 5% aqueous sodium bicarbonate (5 mL). The aqueous portion was extracted with Et_2O (3 × 5 mL) and the combined organic layers washed with water (2 × 5 mL) and dried with magnesium sulphate. The volatile component was removed under reduced pressure and the residue purified by column chromatography (20:1 hexane/EtOAc).

2-Phenyl-2*H*-chromene (11a)[28,30]

155 mg, 0.743 mmol, 84%, yellow oil; TLC: 0.55 (20:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.46 (dd, 2H, *J* = 7.9, 1.7 Hz), 7.40–7.32 (m, 3H), 7.11 (td, 1H, *J* = 10.6,

1.8 Hz), 7.02 (dd, 1H, *J* = 10.7, 1.8 Hz), 6.86 (td, 1H, *J* = 10.3, 1.8 Hz), 6.79 (dd, 1H, *J* = 8.1, 1.7 Hz), 6.53 (dd, 1H, *J* = 9.9, 2.0 Hz), 5.92 (dd, 1H, *J* = 3.4, 2.0 Hz), 5.80 (dd, 1H, *J* = 9.9, 3.4 Hz); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 153.1, 140.8, 129.4, 128.6, 128.3, 127.0, 126.6, 124.8, 124.0, 121.3, 121.1, 116.0, 77.1; IR: ν_{max} (ATR, cm^{-1}) 2921, 2442, 2159, 2029, 1976, 1449, 1259, 1014, 752, 697, 509; EIMS (*m/z*): 208 ($[M]^+$, 65%), 207 (100%), 178 (30%), 131 (40%); ESI-HRMS: Calculated for $[M]^+$ $C_{15}H_{12}O$, 208.0888; found, 208.0882.

2-(Naphthalen-2-yl)-2*H*-chromene (11b)[29,30]

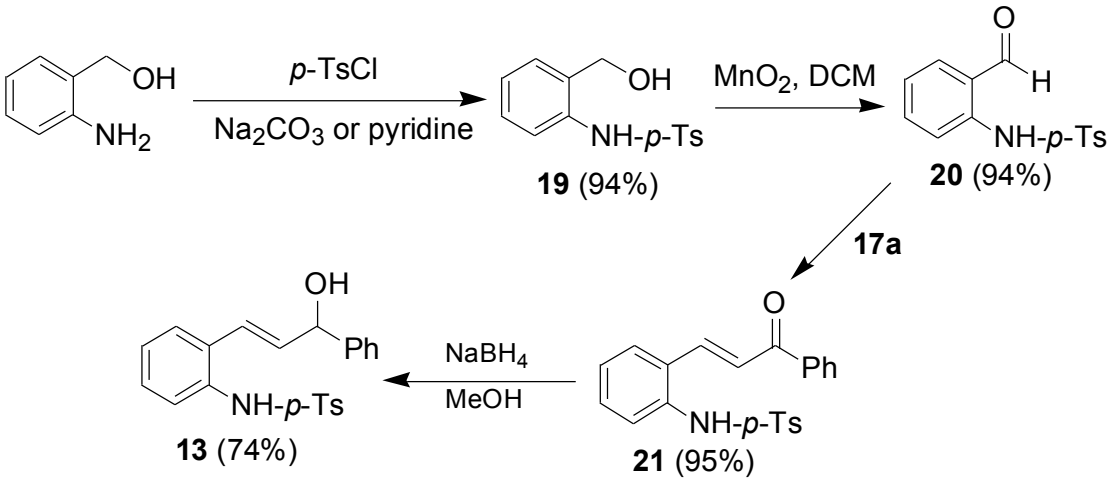
146 mg, 0.566 mmol, 64%, white solid; Mp: 88–90 °C; TLC: 0.62 (20:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.89–7.82 (m, 4H), 7.63 (dd, 1H, *J* = 8.2, 2.0 Hz), 7.53–7.47 (m, 2H), 7.15 (td, 1H, *J* = 7.9, 1.7 Hz), 7.06 (dd, 1H, *J* = 7.5, 1.6 Hz), 6.90 (td, 1H, *J* = 7.5, 1.3 Hz), 6.85 (dd, 1H, *J* = 8.1, 1.4 Hz), 6.60 (dd, 1H, *J* = 9.9, 1.6 Hz), 6.11 (dd, 1H, *J* = 3.2, 1.6 Hz), 5.89 (dd, 1H, *J* = 9.9, 3.2 Hz); ^{13}C NMR: (75 MHz, $CDCL_3$) δ_C: 153.2, 138.0, 133.3, 133.2, 129.5, 128.6, 128.2, 127.7, 126.6, 126.2, 126.0, 124.9, 124.7, 124.2, 121.3, 121.2, 116.0, 77.2; IR: ν_{max} (ATR, cm^{-1}) 3054, 2159, 2031, 1601, 1483, 1230, 1108, 798, 740, 410; EIMS (*m/z*): 258 ($[M]^+$, 100%), 257 (95%), 131 (25%); ESI-HRMS: Calculated for $[M]^+$ $C_{19}H_{14}O$, 258.1045; found, 258.1040.

2-(4-Nitrophenyl)-2*H*-chromene (11c)

128 mg, 0.504 mmol, 57%, yellow oil; TLC: 0.60 (20:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 8.20 (d, 2H, *J* = 10.2 Hz), 7.60 (d, 2H, *J* = 10.1 Hz), 7.13 (td, 1H, *J* = 10.3, 2.2 Hz), 7.01 (dd, 1H, *J* = 9.8, 2.2 Hz), 6.88 (td, 1H, *J* = 10.2, 2.0 Hz), 6.81 (dd, 1H, *J* = 10.3, 1.8 Hz), 6.56 (dd, 1H, *J* = 10.0, 2.0 Hz), 5.99 (dd, 1H, *J* = 4.8, 2.0 Hz), 5.78 (dd, 1H, *J* = 10.0, 4.8 Hz); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 152.6, 147.9, 129.9, 127.5, 126.9, 125.0,

123.9, 123.3, 121.8, 121.0, 116.0, 75.7; IR: ν_{max} (ATR, cm^{-1}) 2923, 2156, 2030, 1605, 1518, 1344, 1012, 853, 753, 509; EIMS (*m/z*): 253 ($[M]^+$, 10%), 252 (10%), 218 (20%), 207 (10%), 178 (10%), 130 (30%), 68 (100%); ESI-HRMS: Calculated for $[M]^+$ $C_{15}H_{11}NO_3$, 253.0739; found, 253.0708.

***N*-(2-(Hydroxyphenyl)-4-methylbenzenesulphonamide (19)[31]**



Scheme S3. Synthesis of benzenesulphonamide **13**.

2-Aminobenzylalcohol (0.200 g, 1.62 mmol) was dissolved in Et_2O (5 mL) and Na_2CO_3 (0.190 g, 1.78 mmol) was added. To the mixture was added *p*-tosylchloride (0.340 g, 1.78 mmol) and the reaction mixture was then heated to reflux temperature for 12 hours.

Alternatively, 2-aminobenzylalcohol (0.200 g, 1.62 mmol) was dissolved in Et_2O (10 mL) and pyridine (0.78 mL, 9.72 mmol) was added, after which *p*-tosylchloride (0.340 g, 1.78 mmol) was added. The reaction mixture was then heated under reflux for 3 hours.

After the elapsed time the reaction mixture was diluted with Et_2O (10 mL) and washed with H_2O (10 mL) then with 1 M HCl (10 mL). The organic layer was extracted with 1 M NaOH

(4 × 10 mL). The basic aqueous extractions were combined, cooled to 0 °C and neutralised with concentrated HCl. The white precipitate was filtered off and dried under reduced pressure, and required no further purification.

578 mg, 1.52 mmol, 94%, white solid; Mp: 144–146 °C; ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.88 (br s, 1H), 7.62 (d, 2H, *J* = 8.4 Hz), 7.40 (d, 1H, *J* = 8.1 Hz), 7.24 (t, 1H, *J* = 4.3 Hz), 7.19 (d, 2H, *J* = 8.1 Hz), 7.07–7.05 (m, 2H), 4.37 (s, 2H), 2.36 (s, 3H); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 143.8, 136.9, 136.4, 131.6, 129.6, 129.2, 129.0, 127.0, 125.3, 123.4, 63.9, 21.5; IR: ν_{max} (ATR, cm^{-1}) 3430, 2506, 2027, 1977, 1412, 1315, 1150, 1031, 928, 761, 547, 470; ESI-HRMS: Calculated for $[M]^+$ $C_{14}H_{16}O_3S$, 278.0851; found, 278.0850.

_N_-(2-(Formylphenyl)-4-methylbenzenesulphonamide (20)[32]

Benzylalcohol **19** (1.20 g, 4.35 mmol) was dissolved in DCM (10 mL) and MnO_2 (1.51 g, 17.4 mmol) was added. The reaction mixture was stirred under reflux for 12 hours. After the elapsed reaction time the solids were filtered off and the volatile component removed under reduced pressure. The residue was purified by flash silica column chromatography.

861 mg, 3.13 mmol, 72%, yellow solid; Mp: 131–133 °C; TLC: 0.51 (2:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H : 10.8 (br s, 1H, N<u>H</u>Ts), 9.79 (s, 1H), 7.74 (d, 2H, *J* = 8.4 Hz), 7.64 (d, 1H, *J* = 8.1 Hz), 7.56 (dd, 1H, *J* = 7.7, 1.4 Hz), 7.47 (dt, 1H, *J* = 8.1, 1.0 Hz), 7.20 (d, 2H, *J* = 8.4 Hz), 7.13 (dt, 1H, *J* = 7.6, 1.1 Hz), 2.33 (s, 3H); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C : 195.0, 144.2, 139.8, 136.2, 136.1, 135.7, 129.7, 127.2, 122.9, 121.7, 117.6, 21.4; IR: ν_{max} (ATR, cm^{-1}) 3115, 2513, 2160, 2030, 1976, 1662, 1581, 1493, 1455, 1337, 1154, 929, 812, 758, 659, 543, 452; EIMS (*m/z*): 275 ($[M]^+$, 50%), 218 (20%), 120 (100%), 119 (40%); ESI-HRMS: Calculated for $[M]^+$ $C_{14}H_{13}NO_3S$, 275.0616; found, 275.0568.

(*E*)-4-Methyl-*N*-(2-(3-oxo-3-phenylprop-1-enyl)phenyl)benzenesulphonamide (21)[33]

20 (0.501 g, 1.82 mmol) was dissolved in toluene (10 mL) in a two necked flask equipped with a reflux condenser. To this was added **17a** (0.692 g, 1.82 mmol) dissolved in toluene (5 mL). The reaction mixture was stirred under reflux for 1 hour. The toluene was removed under reduced pressure and the residue purified by flash silica column chromatography.

652 mg, 1.73 mmol, 95%, yellow solid; Mp: 175–177 °C; TLC: 0.46 (2:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H : 7.84 (d, 2H, *J* = 7.2 Hz), 7.59 (d, 1H, *J* = 15.6 Hz), 7.50–7.40 (m, 3H), 7.44 (d, 2H, *J* = 8.4 Hz), 7.37 (d, 2H, *J* = 7.6 Hz), 7.28 (dt, 1H, *J* = 10.7, 3.9 Hz), 7.14–7.19 (m, 2H), 7.09 (d, 1H, *J* = 15.6 Hz), 7.00 (d, 2H), 2.03 (s, 3H); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C : 190.0, 143.9, 139.0, 137.6, 135.8, 135.3, 133.1, 131.1, 130.9, 129.7, 129.7, 128.7, 128.6, 127.7, 127.2, 127.2, 124.3; IR: ν_{max} (ATR, cm^{-1}) 3181, 2501, 2159, 2030, 1976, 1592, 1456, 1341, 1156, 1019, 755, 682, 450; ESI-HRMS: Calculated for $[M]^+$ $C_{22}H_{20}NO_3S$, 378.1164; found, 378.1156.

(*E*)-*N*-(2-(3-Hydroxy-3-phenylprop-1-enyl)phenyl)-4-methylbenzenesulphonamide (13)[34]

Reduction of **21** (650 mg, 1.33 mmol) was carried out in a fashion similar to the reduction of compounds **18** to form compounds **10**.

373 mg, 0.984 mmol, 74%, white solid; Mp: 146–148 °C; TLC: 0.34 (2:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, DMSO) δ_H : 9.69 (br s, 1H), 7.54 (d, 2H, *J* = 8.1 Hz), 7.49 (d, 1H, *J* = 4.8 Hz), 7.35–7.25 (m, 5H), 7.30 (d, 2H, *J* = 7.8Hz), 7.13–7.11 (m, 2H), 6.93–6.92 (m, 1H), 6.82 (d, 1H, *J* = 15.9 Hz), 6.19 (dd, 1H, *J* = 15.9, 6.6 Hz), 5.56 (d, 1H, *J* = 4.2 Hz), 5.11 (dd, 1H, *J* = 6.6, 4.2 Hz), 2.33 (s, 3H); ^{13}C NMR: (75 MHz, DMSO) δ_C : 144.4, 143.0, 137.4, 134.6, 133.7, 133.4, 129.6, 128.1, 127.7, 127.0, 126.9, 126.7, 126.3. 125.9, 123.8, 73.6, 21.0; IR: ν_{max} (ATR, cm^{-1}) 3266, 2488, 2159, 2028, 1976, 1486, 1394, 1326, 1155, 1090, 765, 671,

514; EIMS (*m/z*): 361 (10%), 284 (20%), 206 (90%), 205 (80%), 204 (60%), 155 (30%), 128 (60%), 101 (20%), 91 (100%), 77 (50%); ESI-HRMS: Calculated for $[M]^+$ $C_{22}H_{21}NO_3S$, 379.1242; found, 379.1236.

2-Phenyl-1-*p*-tosyl-1,2-dihydroquinoline (14)[34]

To $Al(OTf)_3$ (8 mg, 15.8 µmol) dissolved in DCM (10 mL) was added **13** (0.6 g, 1.58 mmol). The reaction mixture was allowed to stir at reflux temperature for 1 hour after which the reaction was quenched by the addition of aqueous sodium bicarbonate (5 mL). The aqueous portion was extracted with Et_2O (3 x 5 mL) and the combined organic layers washed with water (2 × 5 mL) and dried with magnesium sulphate. The solvent was removed under reduced pressure and the resulting residue purified by flash silica column chromatography (2:1 hexane/EtOAc).

491 mg, 1.36 mmol, 86%, white solid; Mp: 123–126 °C; TLC: 0.69 (2:1 hexane/EtOAc); ^{1}H NMR: (300 MHz, $CDCl_3$) δ_H: 7.65 (d, 1H, *J* = 7.8 Hz), 7.35–7.32 (m, 4H), 7.23–7.06 (m, 5H), 7.08 (t, 2H, *J* = 8.4 Hz), 6.96 (d, 1H, *J* = 7.9 Hz), 6.27 (d, 1H, *J* = 9.5 Hz), 6.03 (d, 1H, *J* = 5.9 Hz), 5.88 (dd, 1H, *J* = 9.5, 5.9 Hz), 2.33 (s, 3H); ^{13}C NMR: (75 MHz, $CDCl_3$) δ_C: 143.4, 138.3, 136.0, 132.8, 129.0, 128.6, 128.3, 128.1, 127.8, 127.5, 127.3, 127.1, 126.4, 126.2, 125.4, 56.8, 21.4; IR: ν_{max} (ATR, cm^{-1}) 2160, 2031, 1451, 1334, 1154, 811, 775, 690, 655, 575, 471; EIMS (*m/z*): 361 (M, 20%), 206 (100%), 205 (40%), 155 (30%), 128 (30%); ESI-HRMS: Calculated for $[M]^+$ $C_{22}H_{19}NO_2S$, 361.1136; found, 361.1154.

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28. Compound **10a** has been previously synthesised but has not been fully characterised (SciFinder Scholar search). Kouhkan, M.; Zeynizadeh, B.; *Bull. Kor. Chem. Soc.* **2010**, *31*, 2961–2966.

29. For compound **11b**, see the following reference. Compounds **10b** and **12** have been previously synthesised but have not been fully characterised (SciFinder Scholar search). Compounds **11b** and **12** are both reported in Zeng, B.-S.; Yu, X.; Siu, P. W.; Scheidt K. A.; *Chem. Sci.* **2014***, 5*, 2277–2281.

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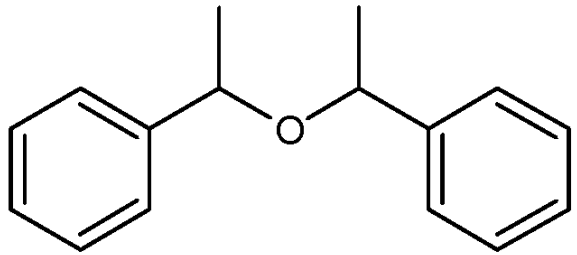
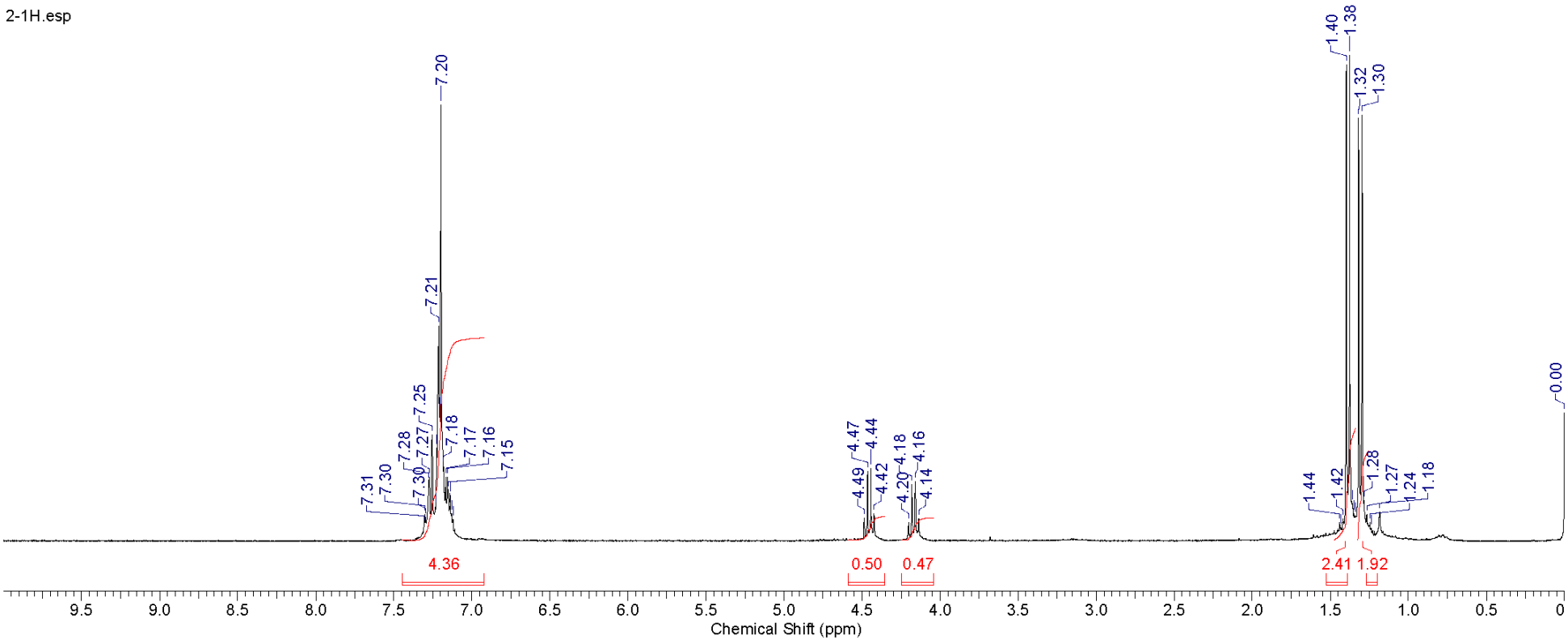
2

Formula $C_{16}H_{18}O$	***FW***	226.3135	

Acquisition Time (sec)	2.0000	***Comment***	CC2-1H	***Date***	Aug 8 2008	***Date Stamp***	Aug 8 2008		
File Name	C:\Users\User\Desktop\adam\CCclean\CC2-1H.fid\fid			***Frequency (MHz)***	300.06	***Nucleus***	1H	***Number of Transients***	1
Original Points Count	9600	***Points Count***	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	8.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	1467.7166	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4800.00	***Temperature (degree C)***	AMBIENT TEMPERATURE		

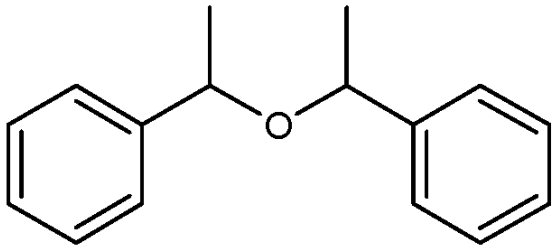


2-1H.esp



2

Formula $C_{16}H_{18}O$	***FW***	226.3135							
Acquisition Time (sec)	1.8150	***Comment***	CC2-13C	***Date***	Aug 8 2008	***Date Stamp***	Aug 8 2008		
File Name	C:\Users\User\Desktop\adam\CCclean\CC2-13C.fid\fid			***Frequency (MHz)***	75.46	***Nucleus***	13C	***Number of Transients***	136
Original Points Count	34053	***Points Count***	65536	***Pulse Sequence***	s2pul	***Receiver Gain***	37.00		
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	7541.7852	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	18761.73
Temperature (degree C)	AMBIENT TEMPERATURE								



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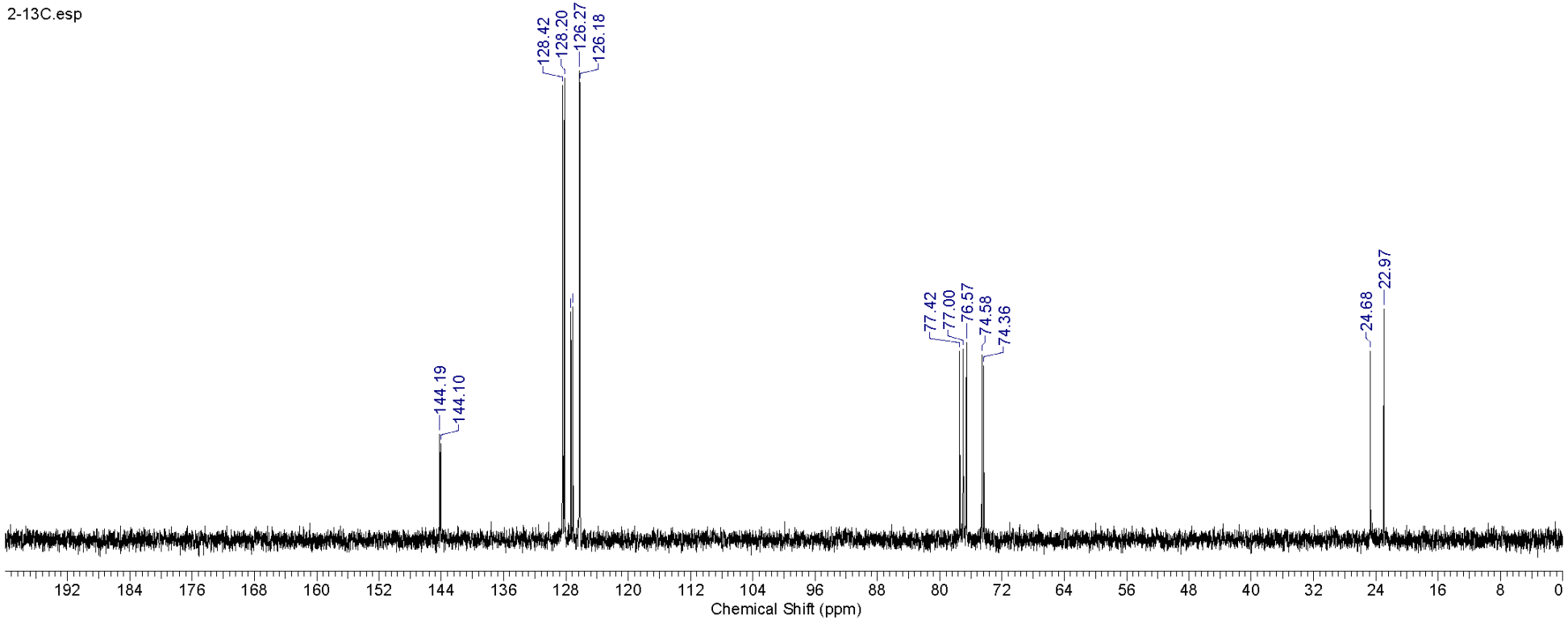
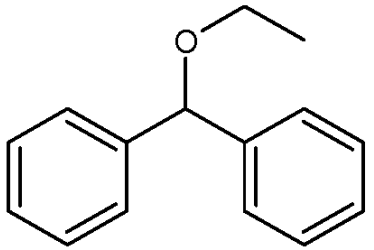


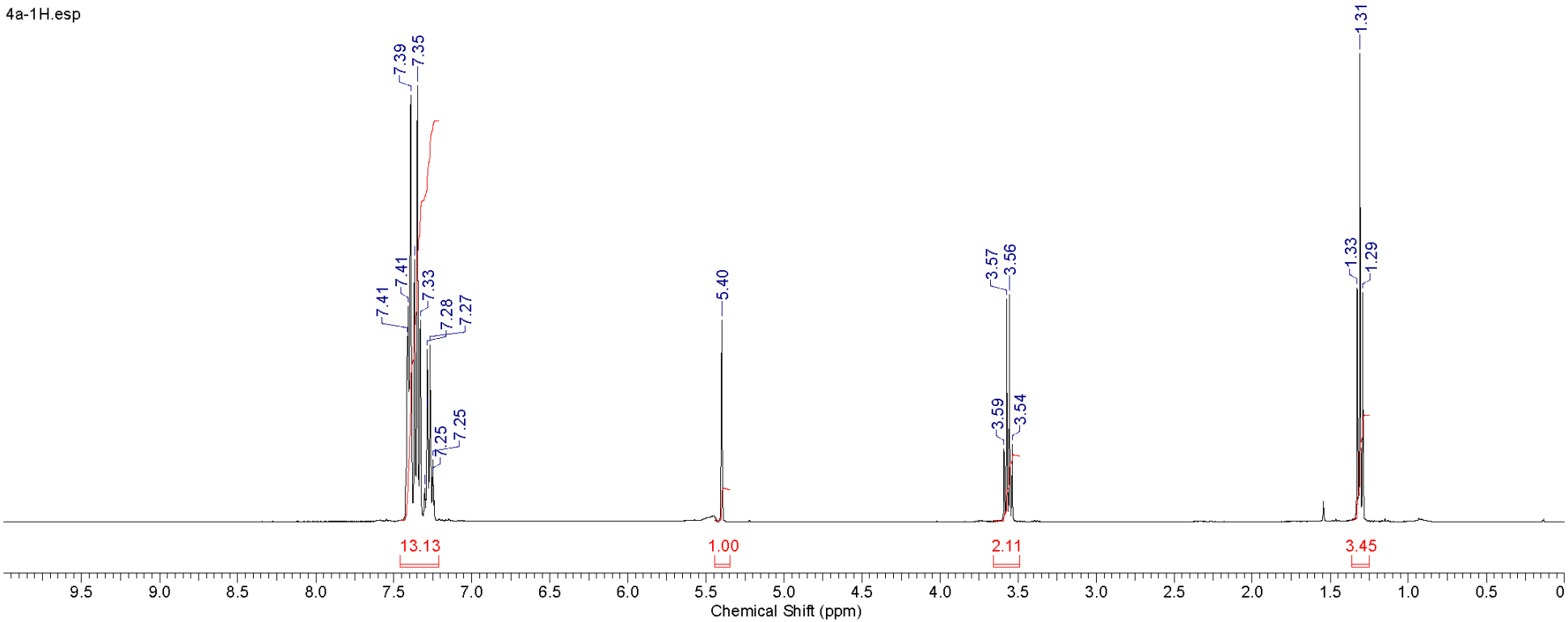
2

Formula $C_{15}H_{16}O$	***FW***	212.2869	

Acquisition Time (sec)	3.9846	***Comment***	CC1-1H	***Date***	26 Oct 2010 14:03:12			***Date Stamp***	26 Oct 2010 14:03:12
File Name	C:\Users\User\Desktop\adam\nmr\CC1\1\fid			***Frequency (MHz)***	400.17	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	40.30	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2455.1277
Spectrum Type	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	23.600				



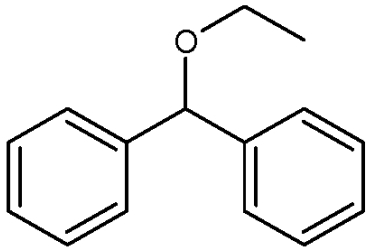
4a-1H.esp

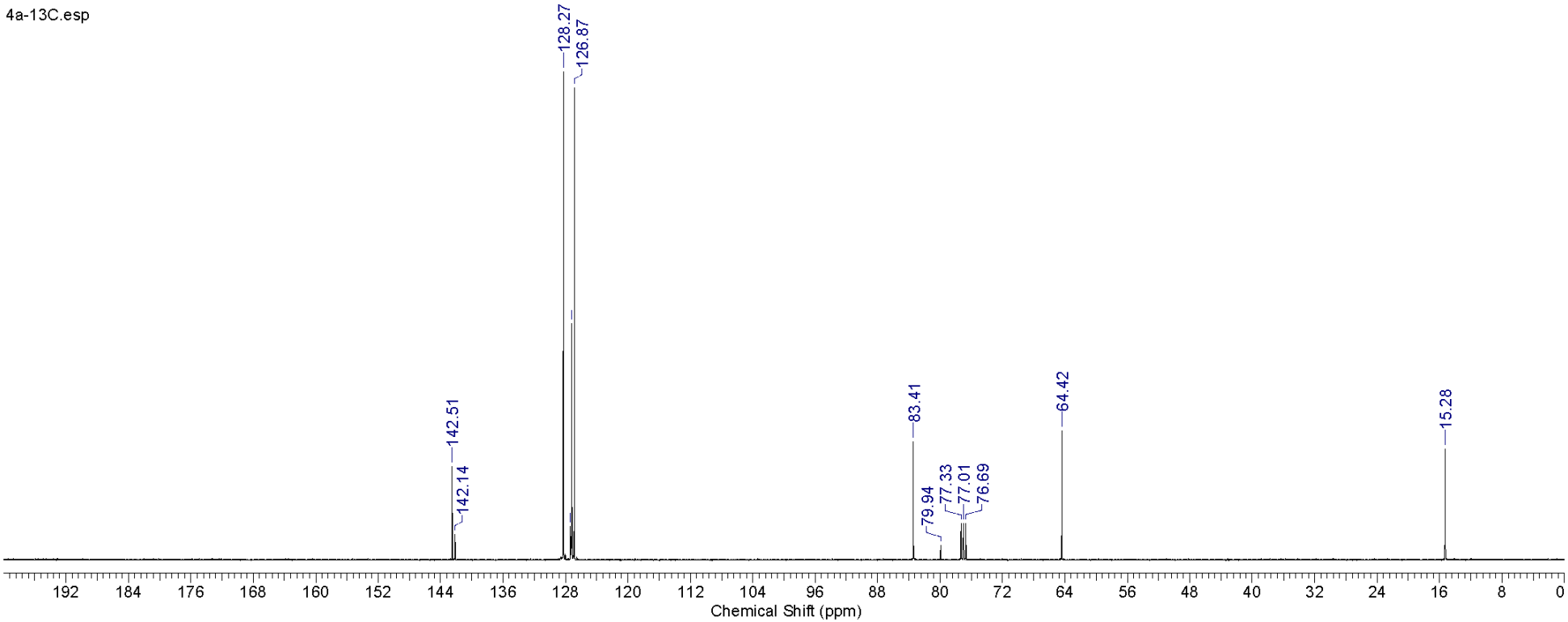


2

Formula $C_{15}H_{16}O$	***FW***	212.2869	

Acquisition Time (sec)	1.3631	***Comment***	CC1-13C	***Date***	27 Oct 2010 15:11:28			***Date Stamp***	27 Oct 2010 15:11:28
File Name	C:\Users\User\Desktop\adam\nmr\CC1\2\fid			***Frequency (MHz)***	100.62	***Nucleus***	13C	***Number of Transients***	450
Origin	spect	***Original Points Count***	32768	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgig30
Receiver Gain	114.00	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10035.5586
Spectrum Type	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	25.000				

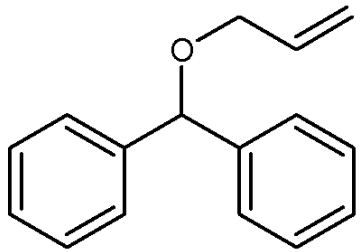


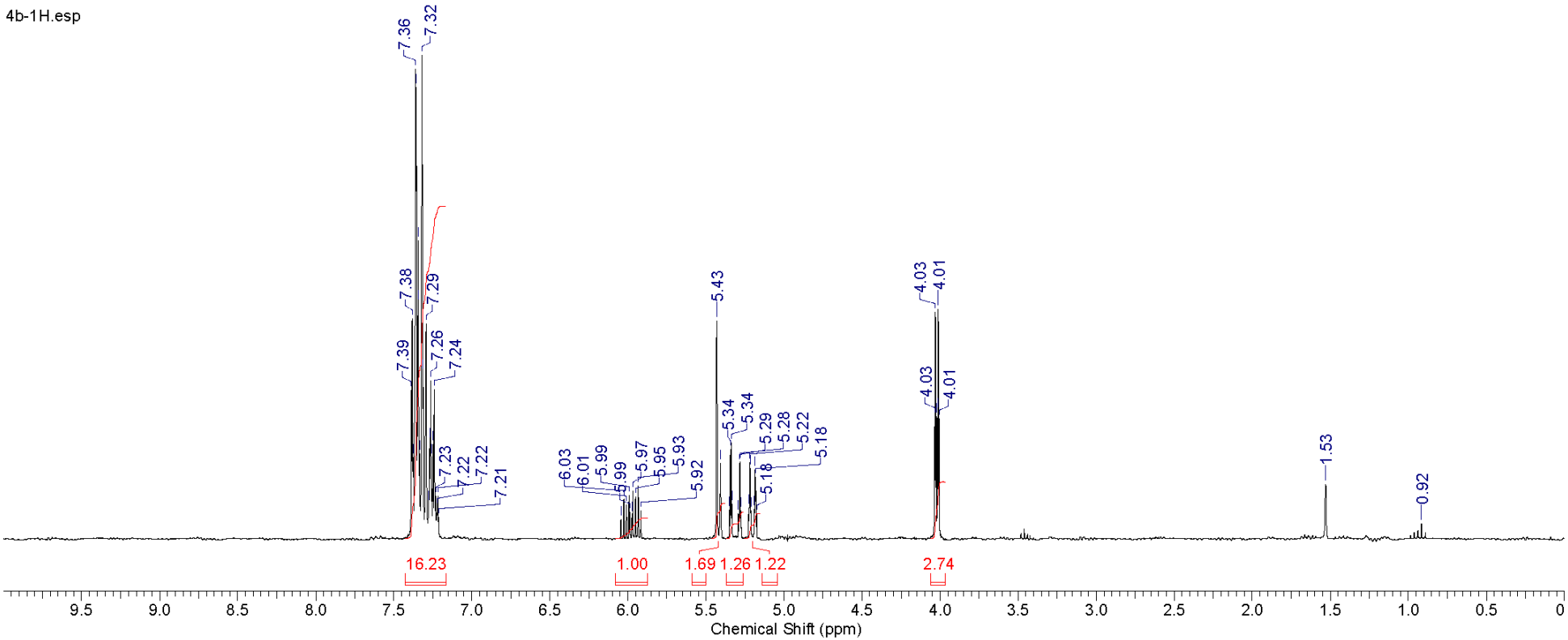


2

Formula $C_{16}H_{16}O$	FW	224.2976

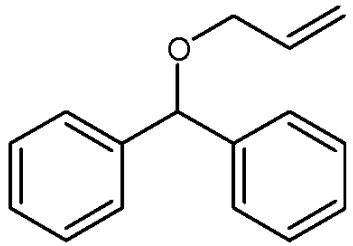
Acquisition Time (sec)	2.0000	**Comment**	CC3-1H	**Date**	Feb 21 2011	**Date Stamp**	Feb 21 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC3-1H.fid\fid			**Frequency (MHz)**	300.08	**Nucleus**	1H	**Number of Transients**	4
Original Points Count	9600	**Points Count**	16384	**Pulse Sequence**	s2pul	**Receiver Gain**	3.00	**Solvent**	CHLOROFORM-d
Spectrum Offset (Hz)	1493.5874	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	4800.00	**Temperature (degree C)**	AMBIENT TEMPERATURE		

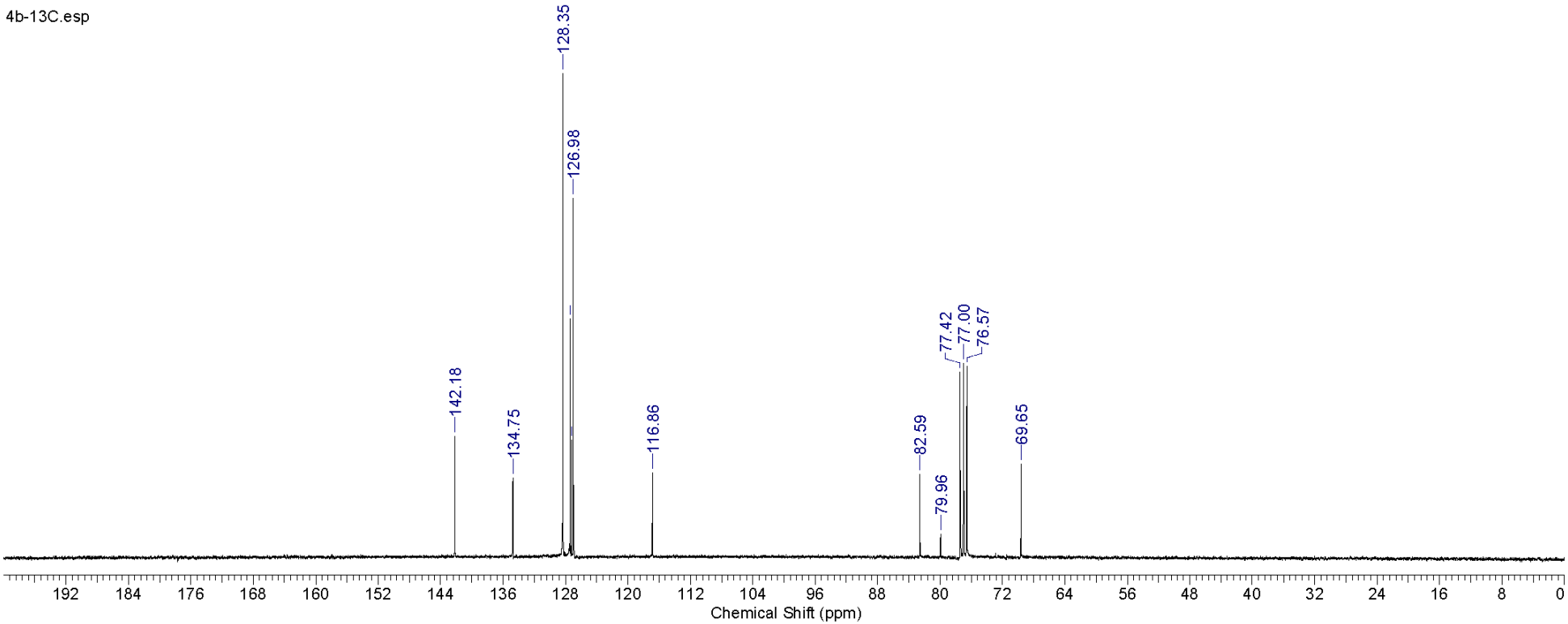




2

Formula $C_{16}H_{16}O$	***FW***	224.2976							
Acquisition Time (sec)	1.8150	***Comment***	CC3-13C	***Date***	Feb 21 2011	***Date Stamp***	Feb 21 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC3-13C.fid\fid			***Frequency (MHz)***	75.46	***Nucleus***	13C	***Number of Transients***	5000
Original Points Count	34053	***Points Count***	65536	***Pulse Sequence***	s2pul	***Receiver Gain***	30.00		
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	7541.6602	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	18761.73
Temperature (degree C)	AMBIENT TEMPERATURE								

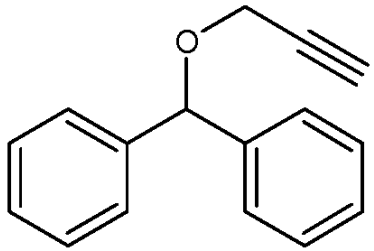


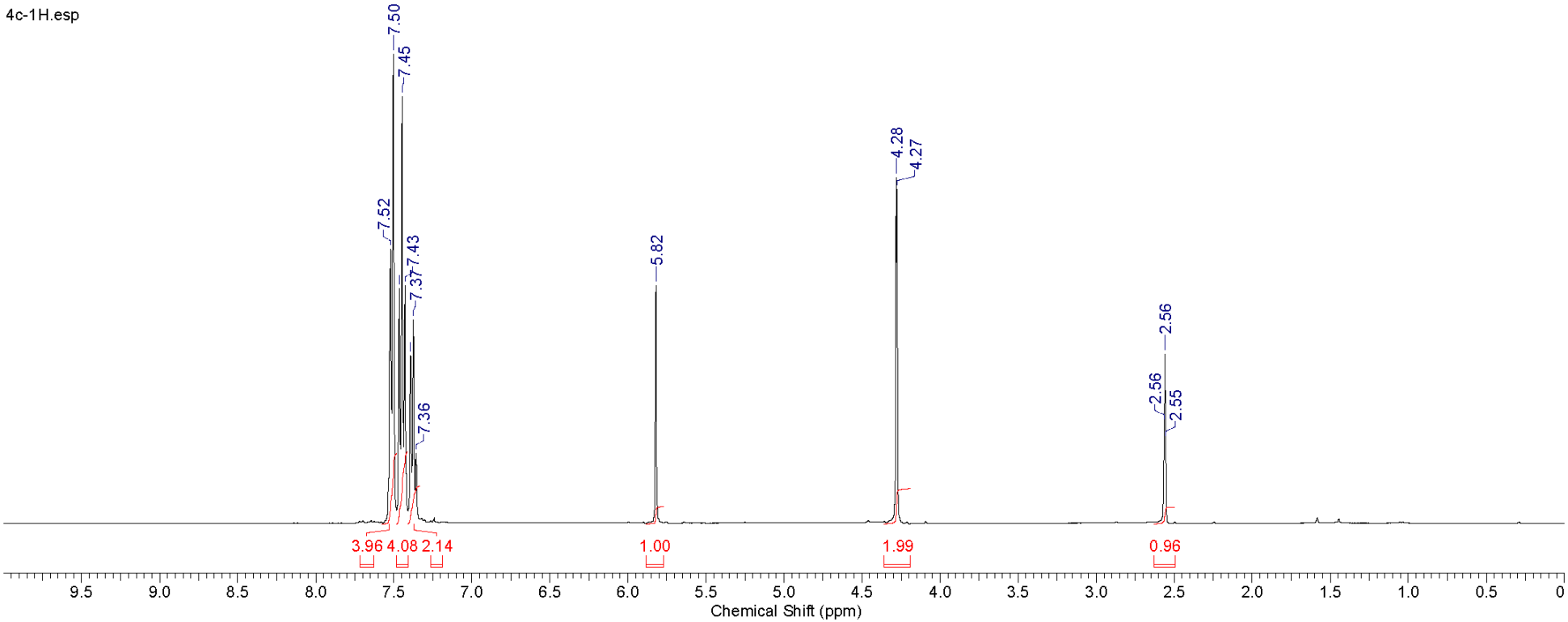


2

Formula $C_{16}H_{14}O$	***FW***	222.2818	

Acquisition Time (sec)	3.9846	***Comment***	CC4-1H	***Date***	28 Oct 2010 11:44:32			***Date Stamp***	28 Oct 2010 11:44:32
File Name	C:\Users\User\Desktop\adam\nmr\CC4\1\fid			***Frequency (MHz)***	400.17	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	16.00	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2455.4199
Spectrum Type	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	22.600				

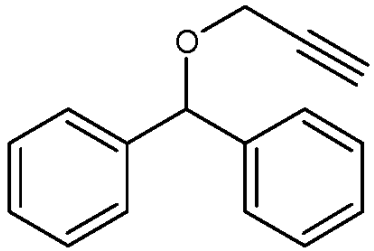


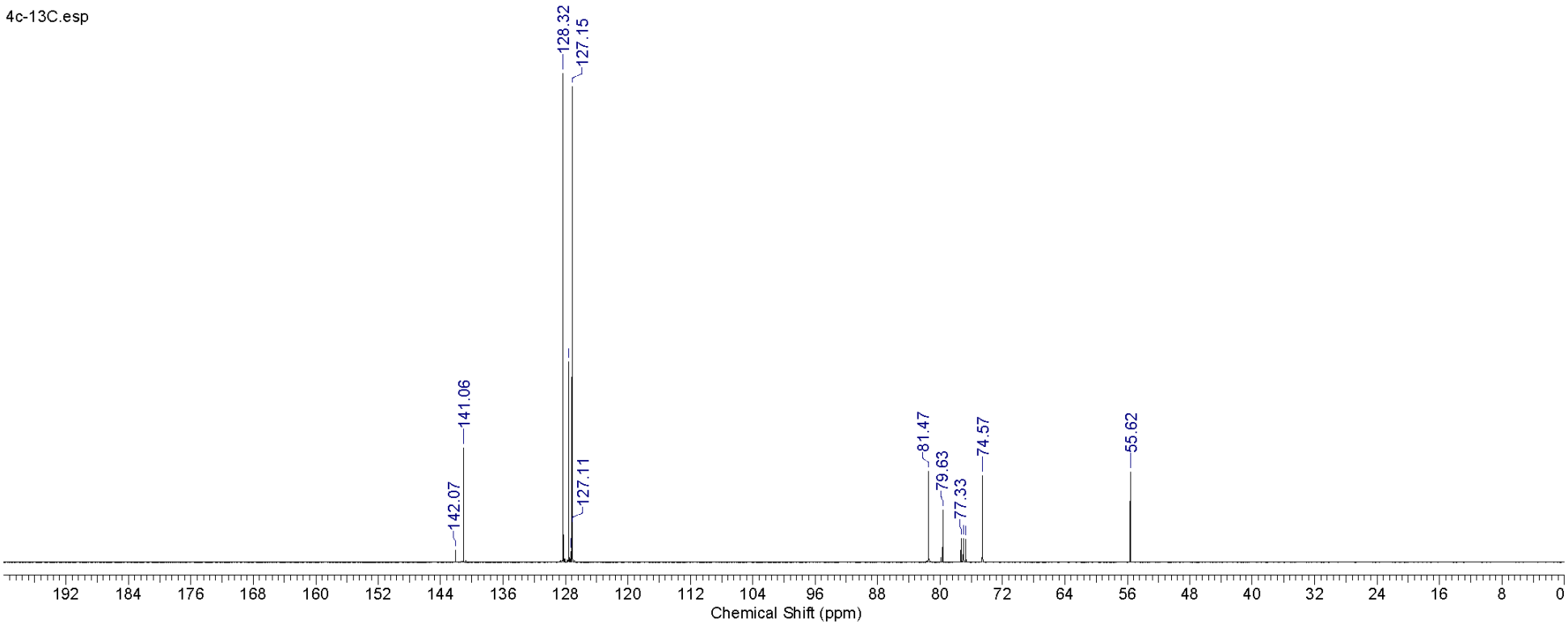


2

Formula $C_{16}H_{14}O$	***FW***	222.2818	

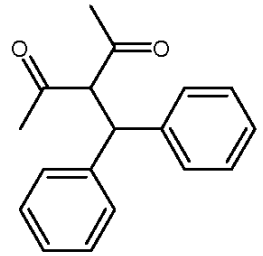
Acquisition Time (sec)	1.3631	***Comment***	CC4-13C	***Date***	28 Oct 2010 12:10:08			***Date Stamp***	28 Oct 2010 12:10:08
File Name	C:\Users\User\Desktop\adam\nmr\CC4\2\fid			***Frequency (MHz)***	100.62	***Nucleus***	13C	***Number of Transients***	450
Origin	spect	***Original Points Count***	32768	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgig30
Receiver Gain	114.00	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10028.1855
Spectrum Type	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	23.100				



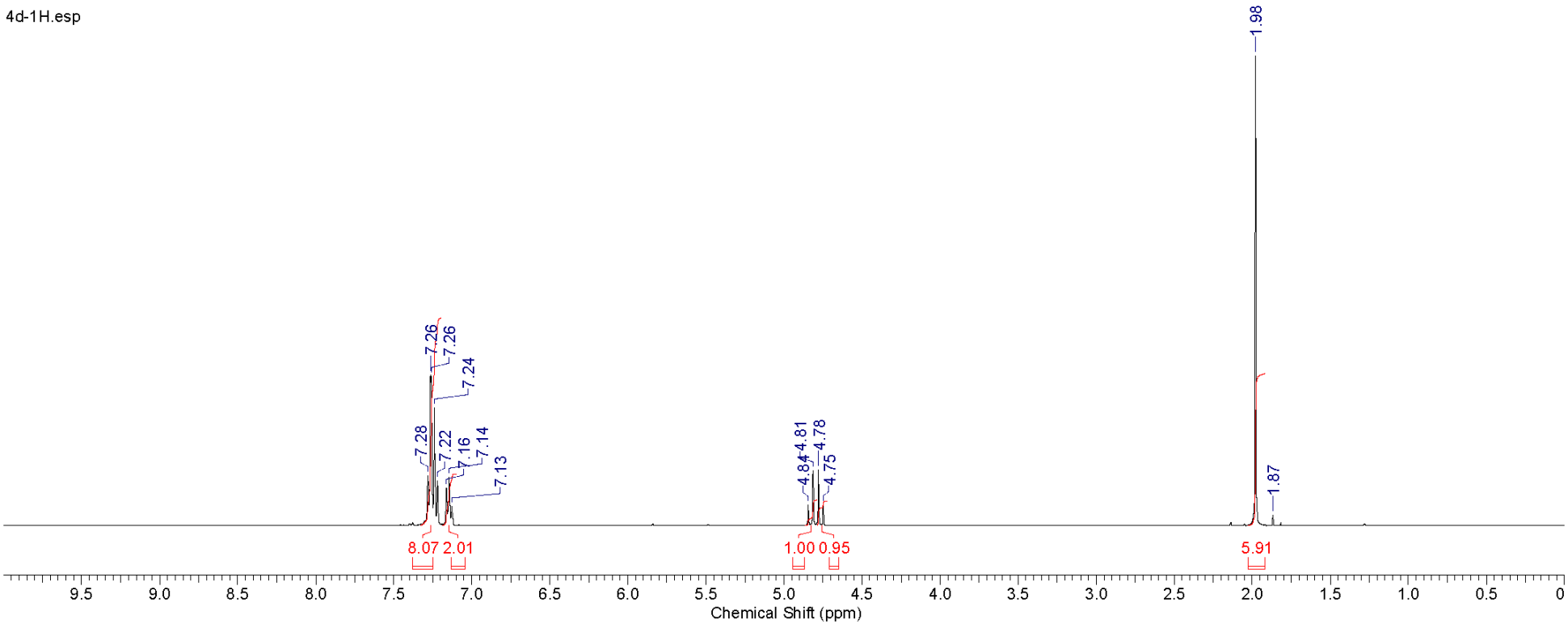


Formula $C_{18}H_{18}O_2$	FW	266.3343

Acquisition Time (sec)	3.9846	**Comment**	CC40-1H	**Date**	28 Oct 2010 14:26:40			**Date Stamp**	28 Oct 2010 14:26:40
File Name	C:\Users\User\Desktop\adam\nmr\CC40\1\fid			**Frequency (MHz)**	400.17	**Nucleus**	1H	**Number of Transients**	16
Origin	spect	**Original Points Count**	32768	**Owner**	nmrsu	**Points Count**	32768	**Pulse Sequence**	zg30
Receiver Gain	20.20	**SW(cyclical) (Hz)**	8223.68	**Solvent**	CHLOROFORM-d			**Spectrum Offset (Hz)**	2458.0571
Spectrum Type	STANDARD	**Sweep Width (Hz)**	8223.43	**Temperature (degree C)**	23.700				

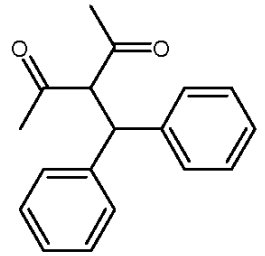


4d-1H.esp

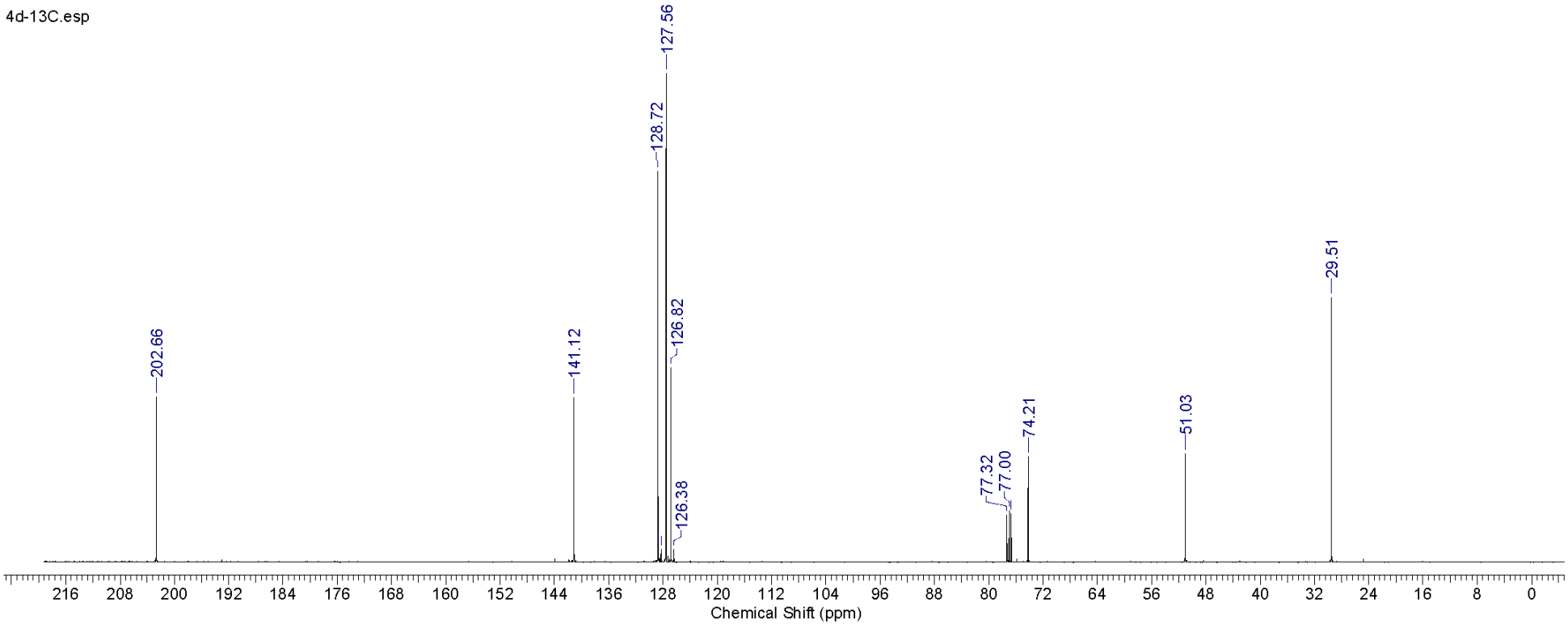


Formula $C_{18}H_{18}O_2$	FW	266.3343

Acquisition Time (sec)	1.3631	**Comment**	CC40-13C	**Date**	28 Oct 2010 14:54:24			**Date Stamp**	28 Oct 2010 14:54:24
File Name	C:\Users\User\Desktop\adam\nmr\CC40\2\fid			**Frequency (MHz)**	100.62	**Nucleus**	13C	**Number of Transients**	450
Origin	spect	**Original Points Count**	32768	**Owner**	nmrsu	**Points Count**	32768	**Pulse Sequence**	zgig30
Receiver Gain	114.00	**SW(cyclical) (Hz)**	24038.46	**Solvent**	CHLOROFORM-d			**Spectrum Offset (Hz)**	10037.5996
Spectrum Type	STANDARD	**Sweep Width (Hz)**	24037.73	**Temperature (degree C)**	24.300				

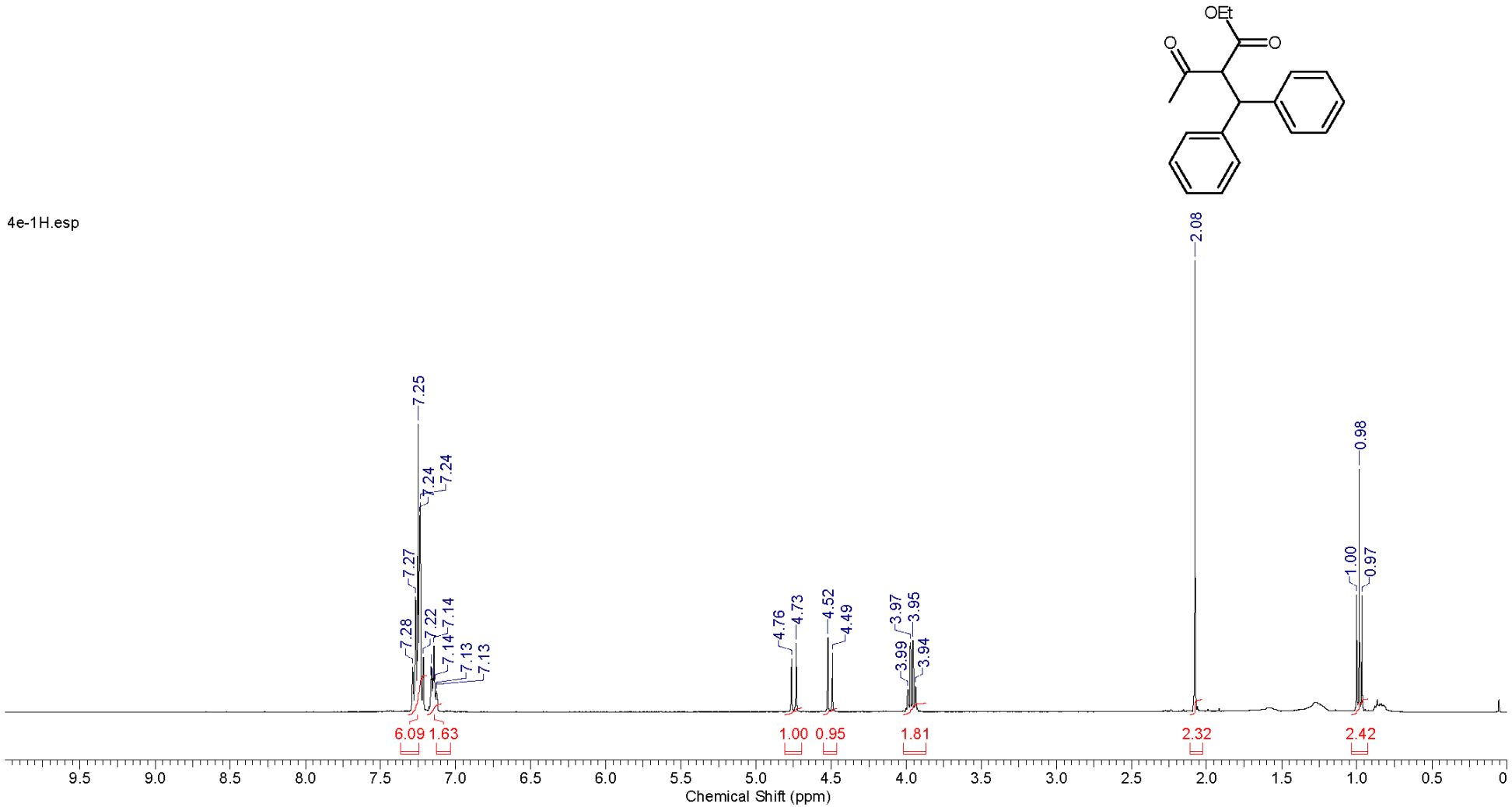


4d-13C.esp



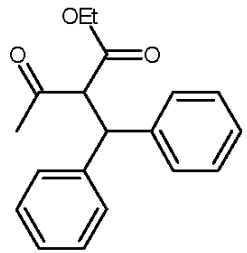
Formula $C_{17}H_{15}O_2$?	FW	251.2998+?

Acquisition Time (sec)	3.9846	**Comment**	CC41-1H-1	**Date**	02 Nov 2010 13:58:56			**Date Stamp**	02 Nov 2010 13:58:56
File Name	C:\Users\User\Desktop\adam\nmr\CC41\3\fid			**Frequency (MHz)**	400.17	**Nucleus**	1H	**Number of Transients**	16
Origin	spect	**Original Points Count**	32768	**Owner**	nmrsu	**Points Count**	32768	**Pulse Sequence**	zg30
Receiver Gain	128.00	**SW(cyclical) (Hz)**	8223.68	**Solvent**	CHLOROFORM-d			**Spectrum Offset (Hz)**	2455.4636
Spectrum Type	STANDARD	**Sweep Width (Hz)**	8223.43	**Temperature (degree C)**	24.400				



Formula $C_{17}H_{15}O_2$?	FW 251.2998+?

Acquisition Time (sec)	1.3631	**Comment**	CC41-13C	**Date**	02 Nov 2010 15:49:52			**Date Stamp**	02 Nov 2010 15:49:52
File Name	C:\Users\User\Desktop\adam\nmr\CC41\4\fid			**Frequency (MHz)**	100.62	**Nucleus**	13C	**Number of Transients**	450
Origin	spect	**Original Points Count**	32768	**Owner**	nmrsu	**Points Count**	32768	**Pulse Sequence**	zgig30
Receiver Gain	114.00	**SW(cyclical) (Hz)**	24038.46	**Solvent**	CHLOROFORM-d			**Spectrum Offset (Hz)**	10060.0840
Spectrum Type	STANDARD	**Sweep Width (Hz)**	24037.73	**Temperature (degree C)**	24.100				



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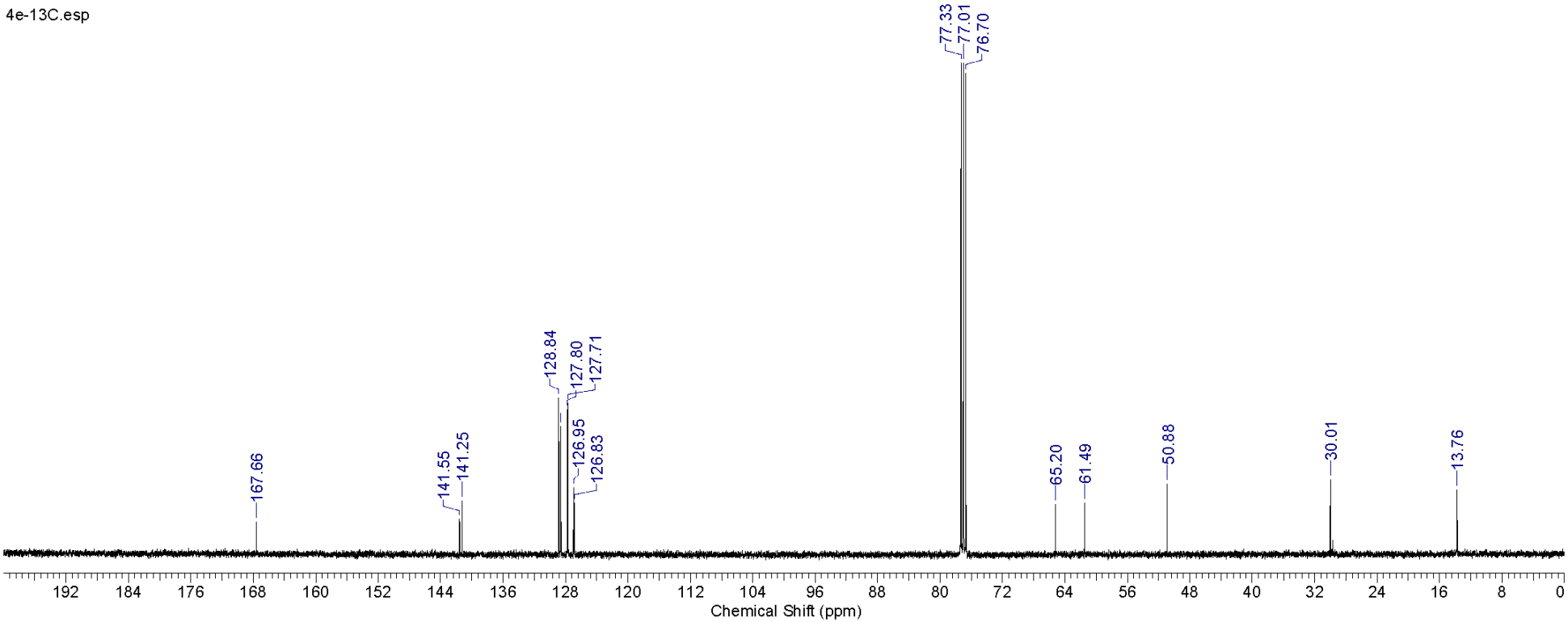
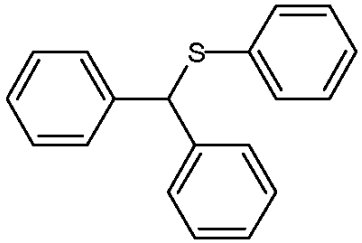
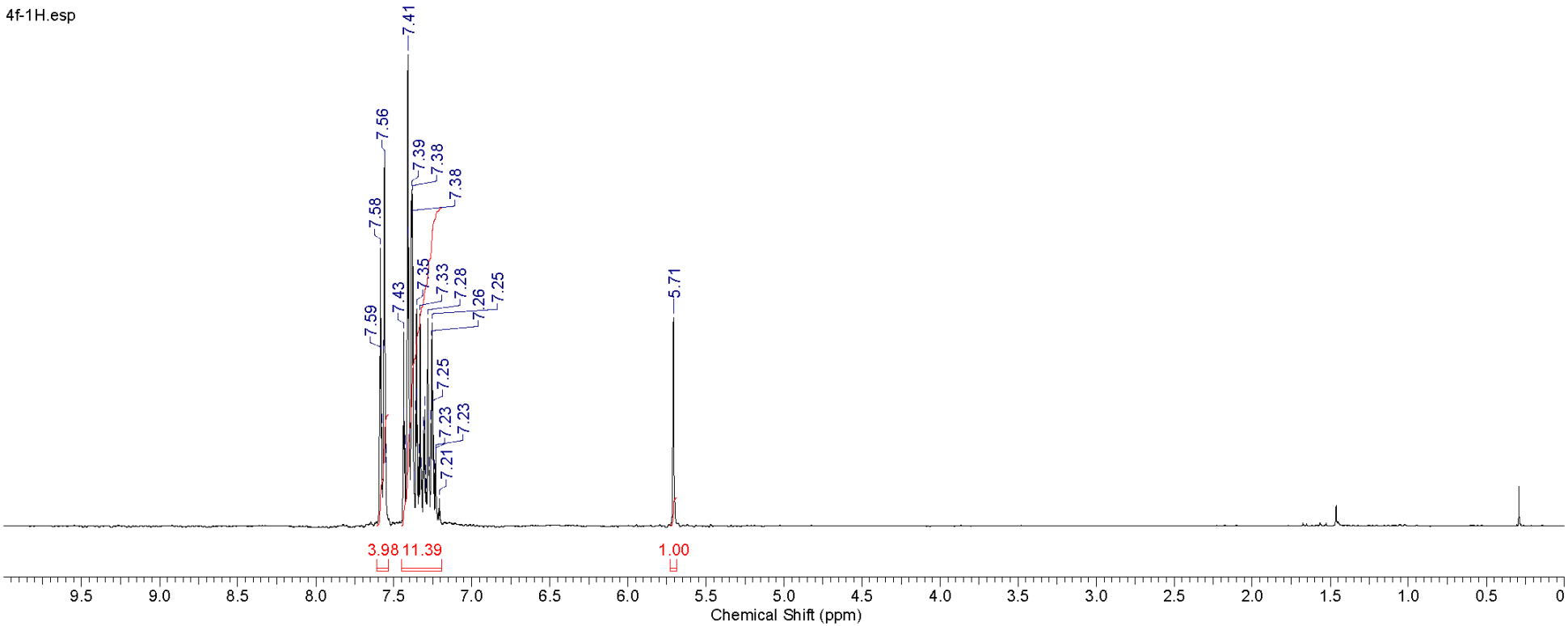


Formula $C_{19}H_{16}S$	FW	276.3953

Acquisition Time (sec)	2.0000	**Comment**	CC119-1H	**Date**	Feb 16 2011	**Date Stamp**	Feb 16 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC119-1H.fid\fid			**Frequency (MHz)**	300.08	**Nucleus**	1H	**Number of Transients**	8
Original Points Count	9600	**Points Count**	16384	**Pulse Sequence**	s2pul	**Receiver Gain**	8.00	**Solvent**	CHLOROFORM-d
Spectrum Offset (Hz)	1497.9822	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	4800.00	**Temperature (degree C)**	AMBIENT TEMPERATURE		

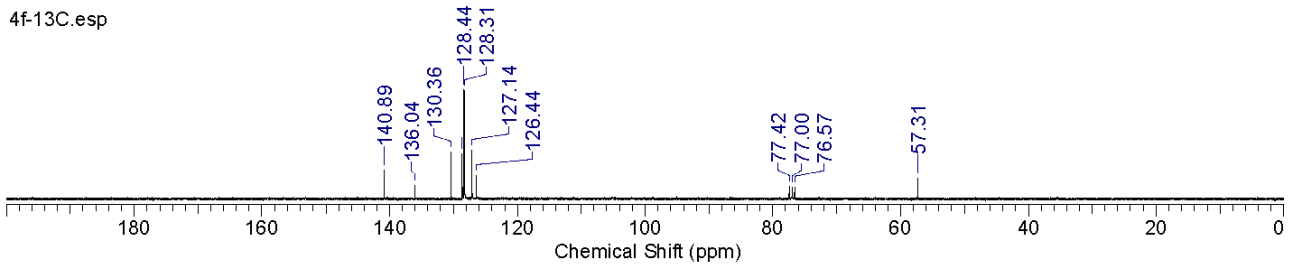


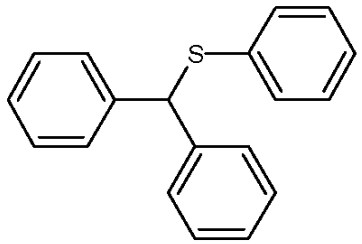


Formula $C_{19}H_{16}S$	FW	276.3953

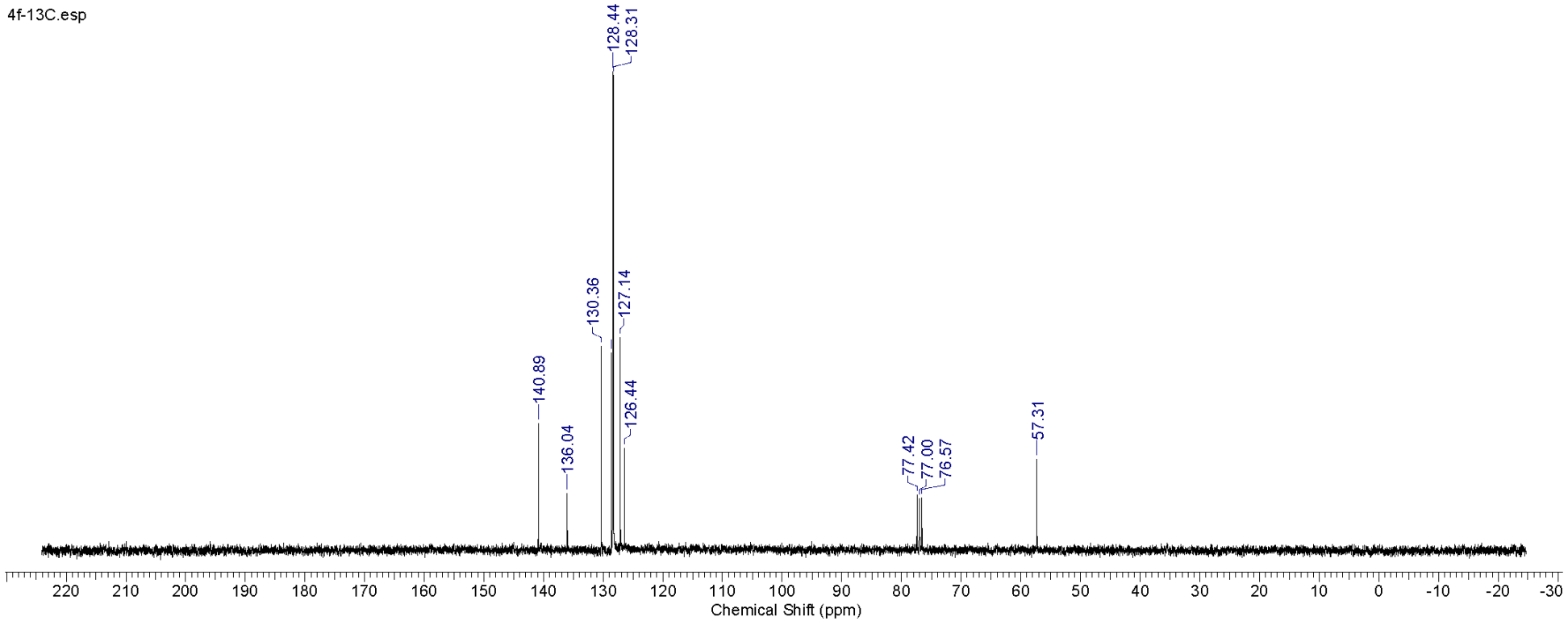
Acquisition Time (sec)	1.8150	**Comment**	CC119-13C	**Date**	Feb 16 2011	**Date Stamp**	Feb 16 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC119-13C.fid\fid			**Frequency (MHz)**	75.46	**Nucleus**	13C	**Number of Transients**	32
Original Points Count	34053	**Points Count**	65536	**Pulse Sequence**	s2pul	**Receiver Gain**	30.00		
Solvent	CHLOROFORM-d			**Spectrum Offset (Hz)**	7523.9121	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	18761.73
Temperature (degree C)	AMBIENT TEMPERATURE								

4f-13C.esp



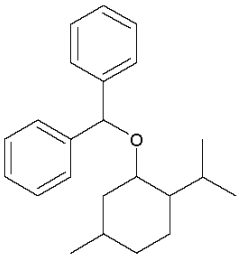


4f-13C.esp

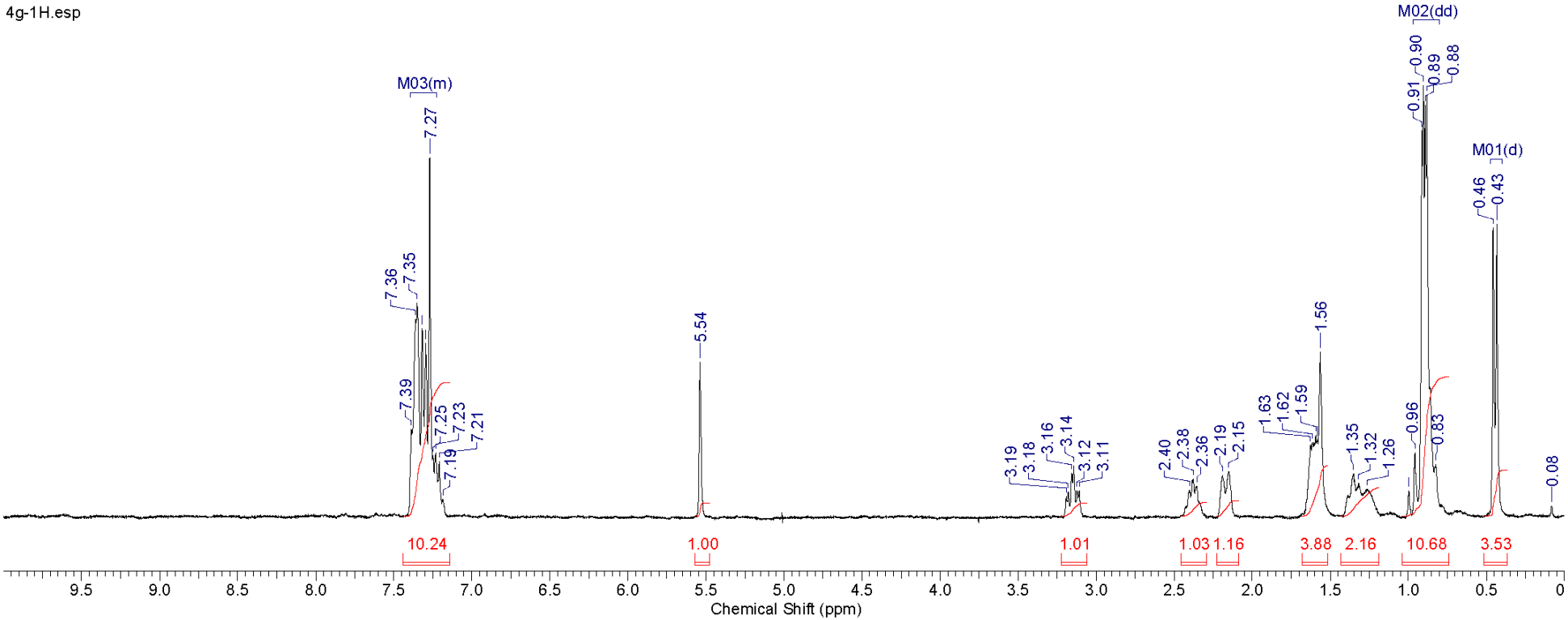


Formula $C_{29}H_{30}O$	FW	322.4837

Acquisition Time (sec)	2.0000	**Comment**	CC29-1H	**Date**	Oct 6 2011	**Date Stamp**	Oct 6 2011
File Name	C:\Users\User\Documents\PhD\PhD NMR data\CCclean\CC29-1H.fid\fid					**Frequency (MHz)**	300.08
Nucleus	1H	**Number of Transients**	4	**Original Points Count**	9600	**Points Count**	16384
Pulse Sequence	s2pul	**Receiver Gain**	14.00	**Solvent**	CHLOROFORM-d		
Spectrum Offset (Hz)	1503.7727	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	4800.00	**Temperature (degree C)**	AMBIENT TEMPERATURE

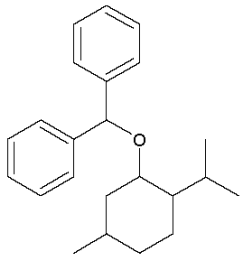


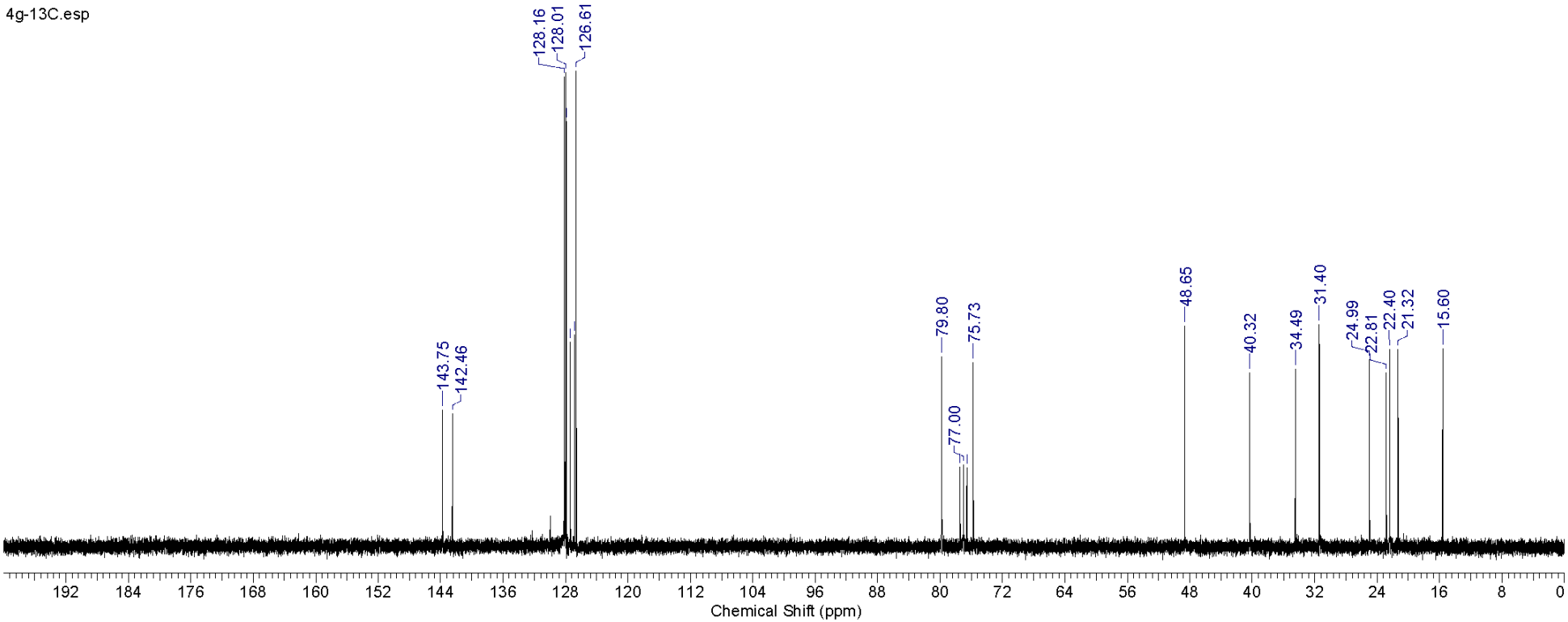
4g-1H.esp



Formula $C_{29}H_{30}O$	FW	322.4837

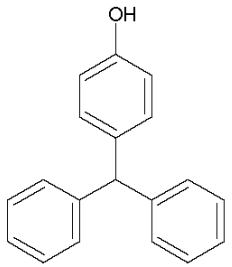
Acquisition Time (sec)	1.8150	**Comment**	CC29-13C	**Date**	Oct 6 2011	**Date Stamp**	Oct 6 2011
File Name	C:\Users\User\Documents\PhD\PhD NMR data\CCclean\CC29-13C.fid\fid					**Frequency (MHz)**	75.46
Nucleus	13C	**Number of Transients**	276	**Original Points Count**	34053	**Points Count**	65536
Pulse Sequence	s2pul	**Receiver Gain**	30.00	**Solvent**	CHLOROFORM-d		
Spectrum Offset (Hz)	7526.7744	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	18761.73	**Temperature (degree C)**	AMBIENT TEMPERATURE

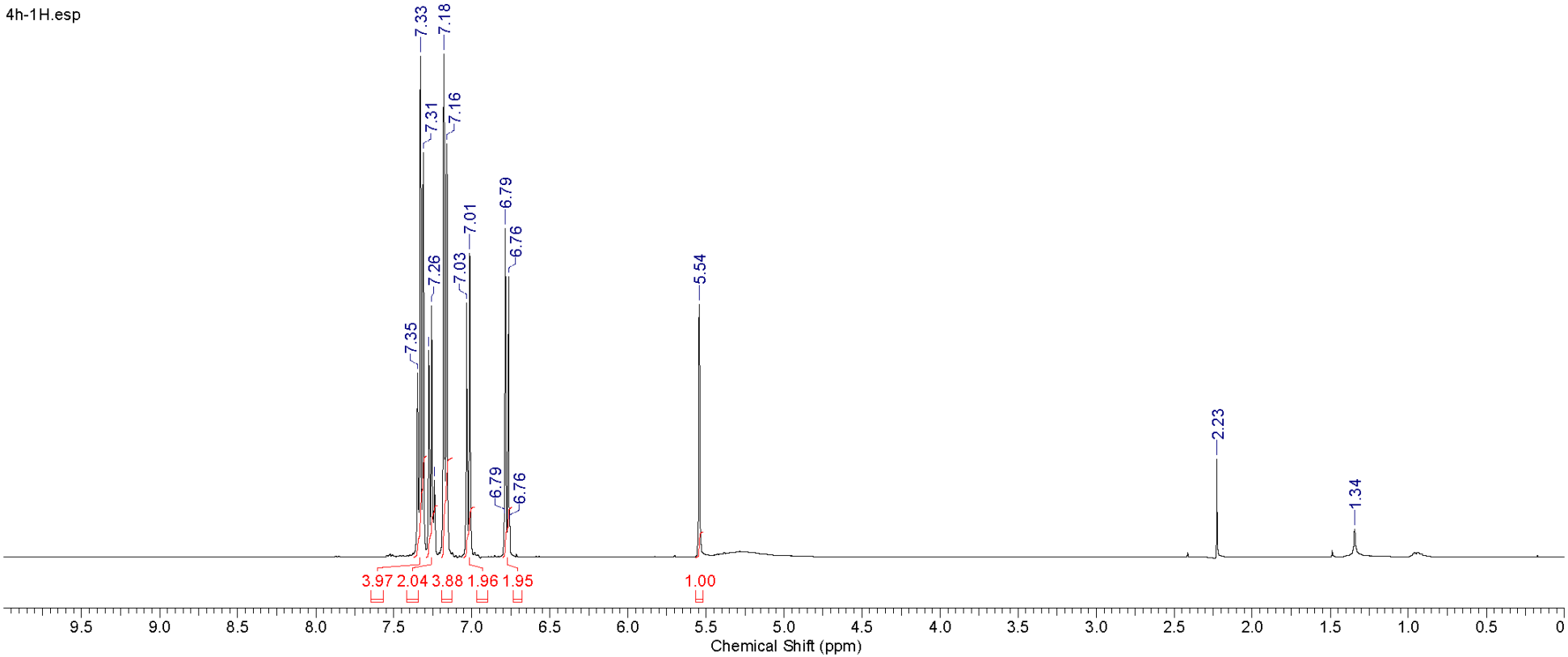




Formula $C_{19}H_{16}O$	***FW***	260.3297	

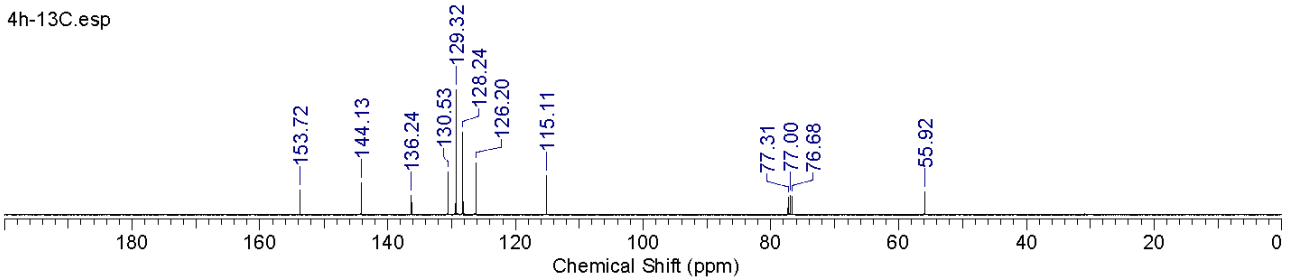
Acquisition Time (sec)	3.9846	***Comment***	CC45-1H	***Date***	28 Oct 2010 13:31:12			***Date Stamp***	28 Oct 2010 13:31:12
File Name	C:\Users\User\Desktop\adam\nmr\CC45\1\fid			***Frequency (MHz)***	400.17	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	36.00	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2457.4846
Spectrum Type	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	23.300				

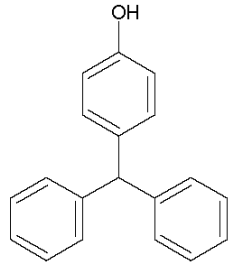


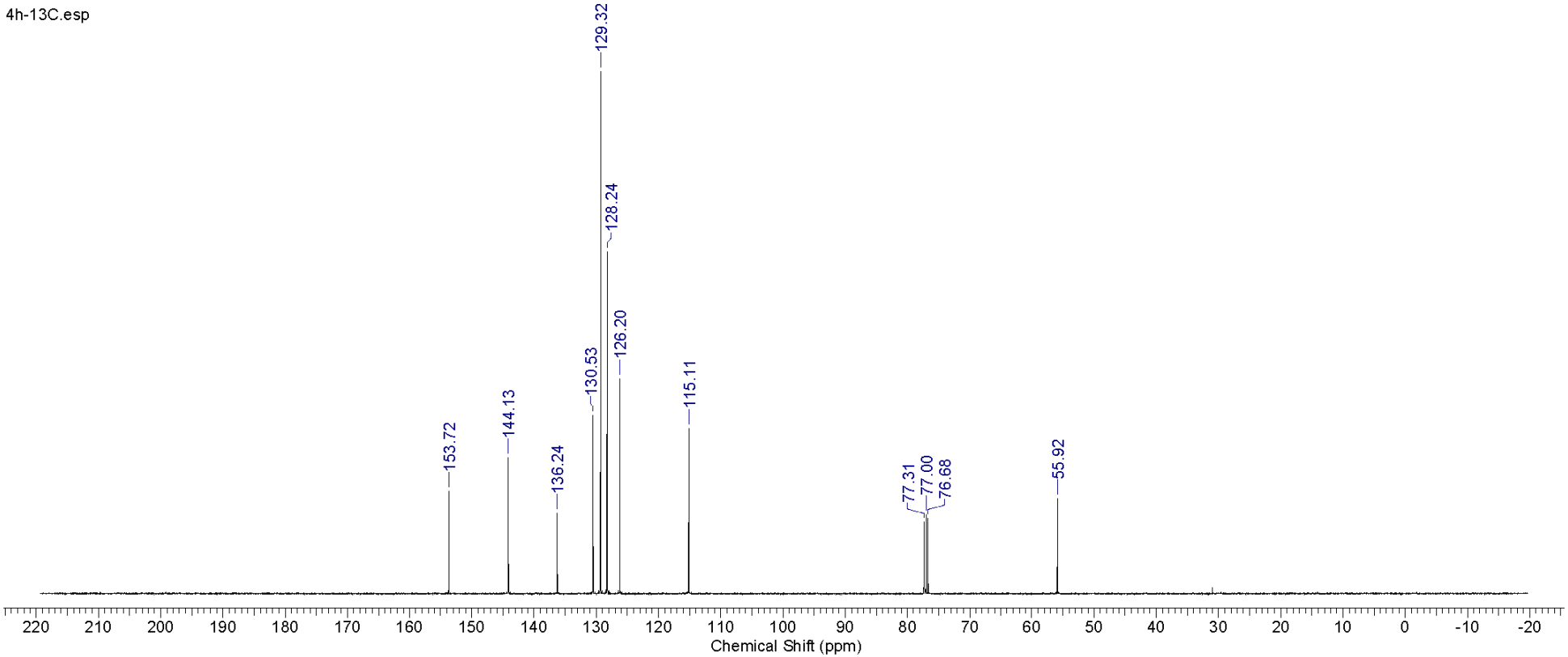


Formula $C_{19}H_{16}O$	FW	260.3297

Acquisition Time (sec)	1.3631	**Comment**	CC45-13C	**Date**	28 Oct 2010 13:58:56			**Date Stamp**	28 Oct 2010 13:58:56
File Name	C:\Users\User\Desktop\adam\nmr\CC45\2\fid			**Frequency (MHz)**	100.62	**Nucleus**	13C	**Number of Transients**	450
Origin	spect	**Original Points Count**	32768	**Owner**	nmrsu	**Points Count**	32768	**Pulse Sequence**	zgig30
Receiver Gain	128.00	**SW(cyclical) (Hz)**	24038.46	**Solvent**	CHLOROFORM-d			**Spectrum Offset (Hz)**	10045.2051
Spectrum Type	STANDARD	**Sweep Width (Hz)**	24037.73	**Temperature (degree C)**	23.800				

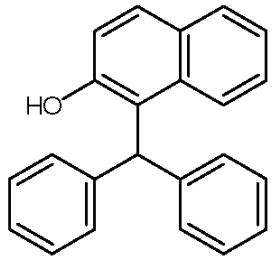


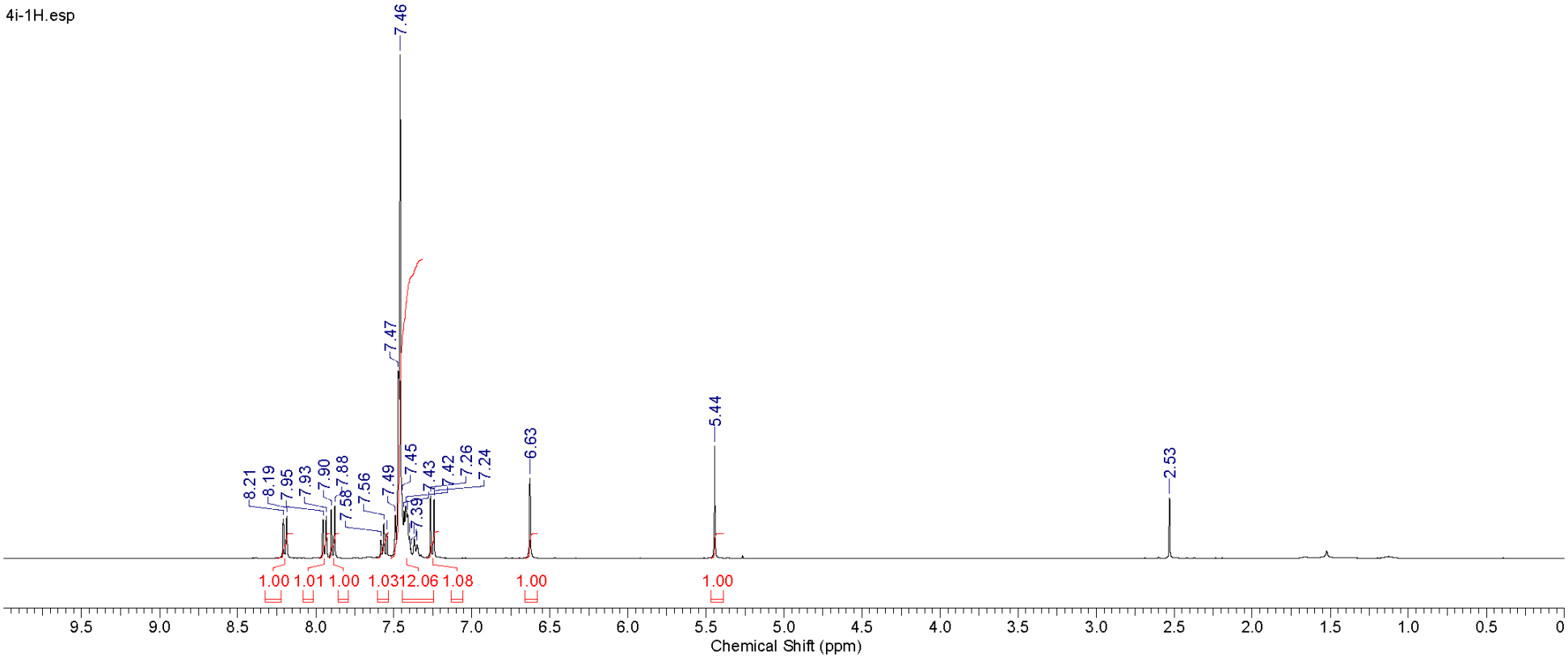




Formula $C_{23}H_{18}O$	FW	310.3884

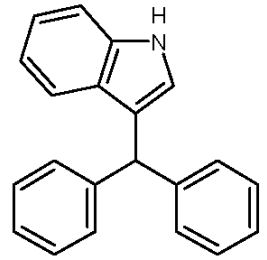
Acquisition Time (sec)	3.9846	**Comment**	CC44-1H	**Date**	28 Oct 2010 15:56:16			**Date Stamp**	28 Oct 2010 15:56:16
File Name	C:\Users\User\Desktop\adam\nmr\CC44\1\fid			**Frequency (MHz)**	400.17	**Nucleus**	1H	**Number of Transients**	16
Origin	spect	**Original Points Count**	32768	**Owner**	nmrsu	**Points Count**	32768	**Pulse Sequence**	zg30
Receiver Gain	18.00	**SW(cyclical) (Hz)**	8223.68	**Solvent**	CHLOROFORM-d			**Spectrum Offset (Hz)**	2455.6116
Spectrum Type	STANDARD	**Sweep Width (Hz)**	8223.43	**Temperature (degree C)**	24.500				

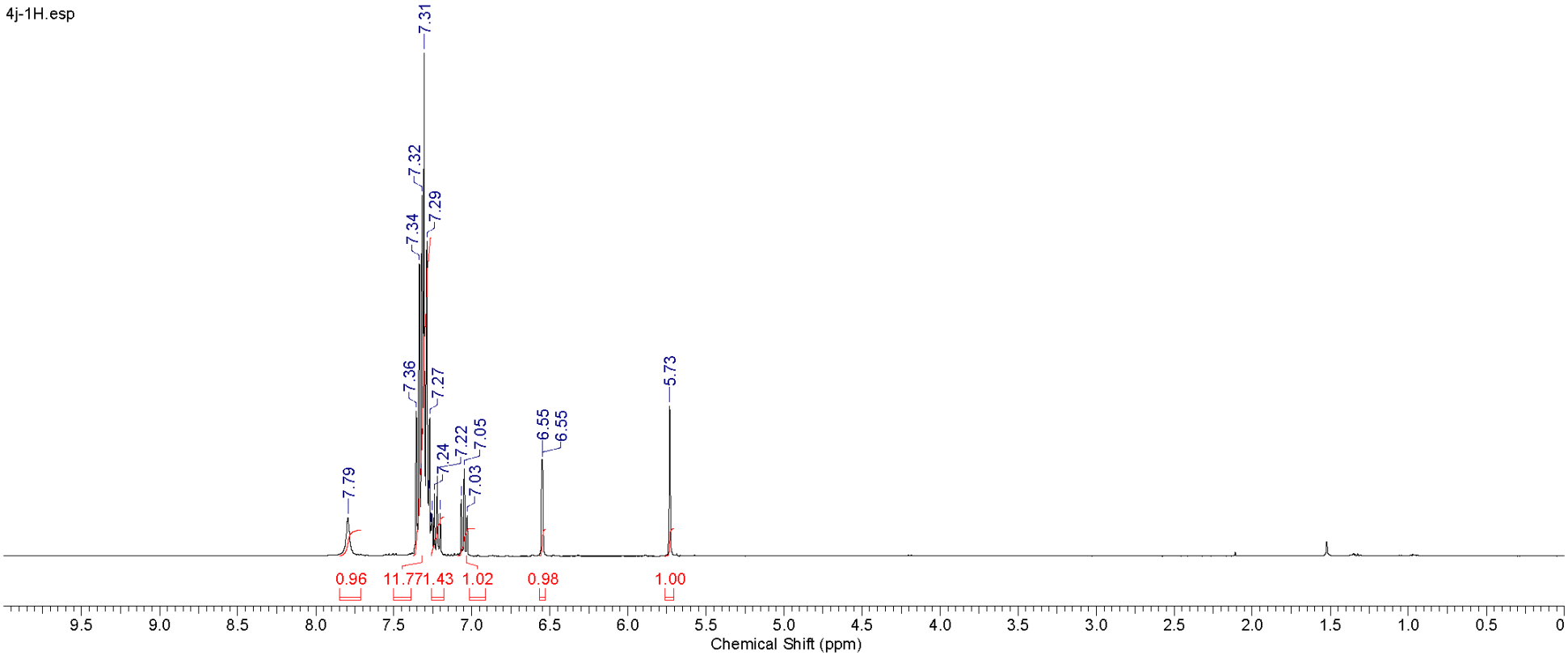




Formula $C_{21}H_{17}N$	FW	283.3664

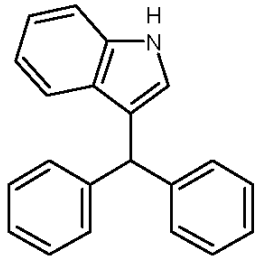
Acquisition Time (sec)	3.9846	**Comment**	CC46-1H	**Date**	01 Nov 2010 15:00:48			**Date Stamp**	01 Nov 2010 15:00:48
File Name	C:\Users\User\Desktop\adam\nmr\CC46\1\fid			**Frequency (MHz)**	400.17	**Nucleus**	1H	**Number of Transients**	16
Origin	spect	**Original Points Count**	32768	**Owner**	nmrsu	**Points Count**	32768	**Pulse Sequence**	zg30
Receiver Gain	50.80	**SW(cyclical) (Hz)**	8223.68	**Solvent**	CHLOROFORM-d			**Spectrum Offset (Hz)**	2455.3635
Spectrum Type	STANDARD	**Sweep Width (Hz)**	8223.43	**Temperature (degree C)**	23.500				

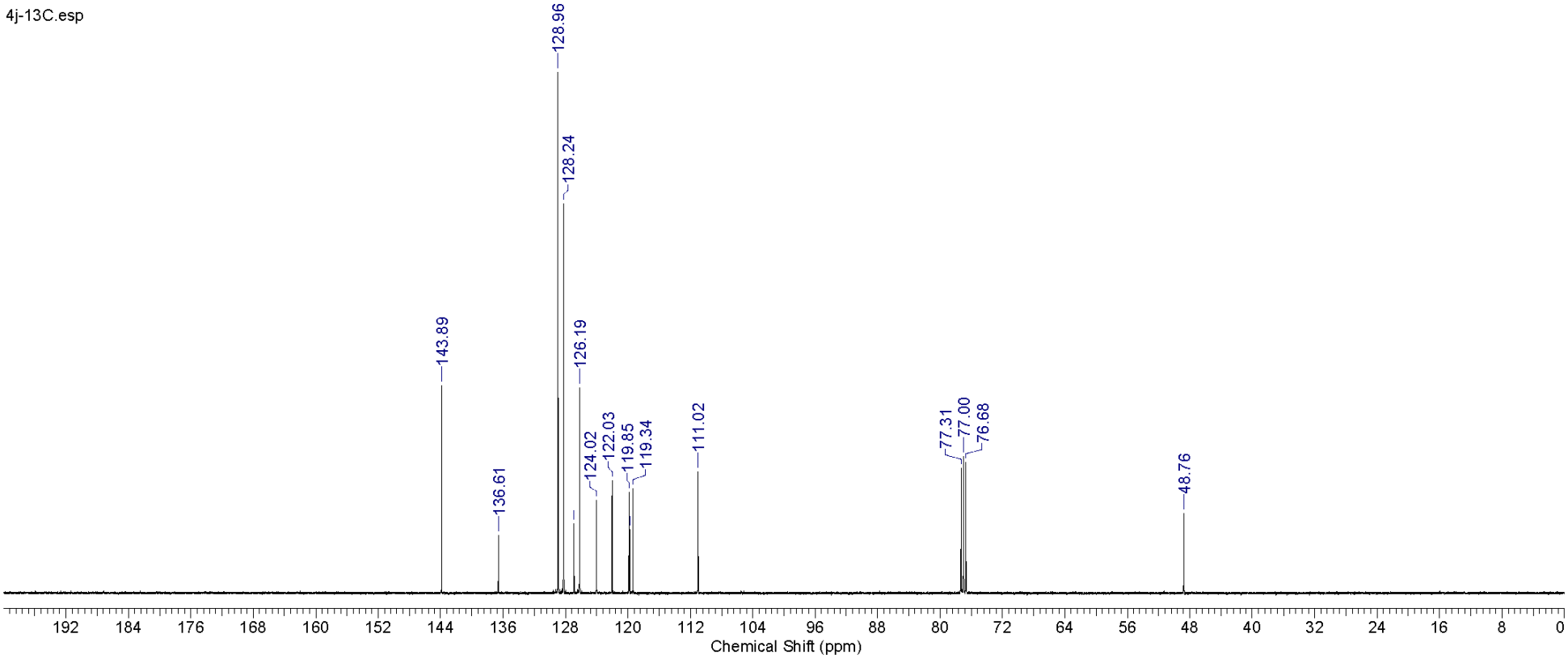




Formula $C_{21}H_{17}N$	FW	283.3664

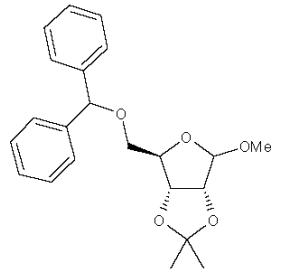
Acquisition Time (sec)	1.3631	**Comment**	CC46-13C	**Date**	01 Nov 2010 15:24:16			**Date Stamp**	01 Nov 2010 15:24:16
File Name	C:\Users\User\Desktop\adam\nmr\CC46\2\fid			**Frequency (MHz)**	100.62	**Nucleus**	13C	**Number of Transients**	400
Origin	spect	**Original Points Count**	32768	**Owner**	nmrsu	**Points Count**	32768	**Pulse Sequence**	zgig30
Receiver Gain	114.00	**SW(cyclical) (Hz)**	24038.46	**Solvent**	CHLOROFORM-d			**Spectrum Offset (Hz)**	10045.9463
Spectrum Type	STANDARD	**Sweep Width (Hz)**	24037.73	**Temperature (degree C)**	24.000				

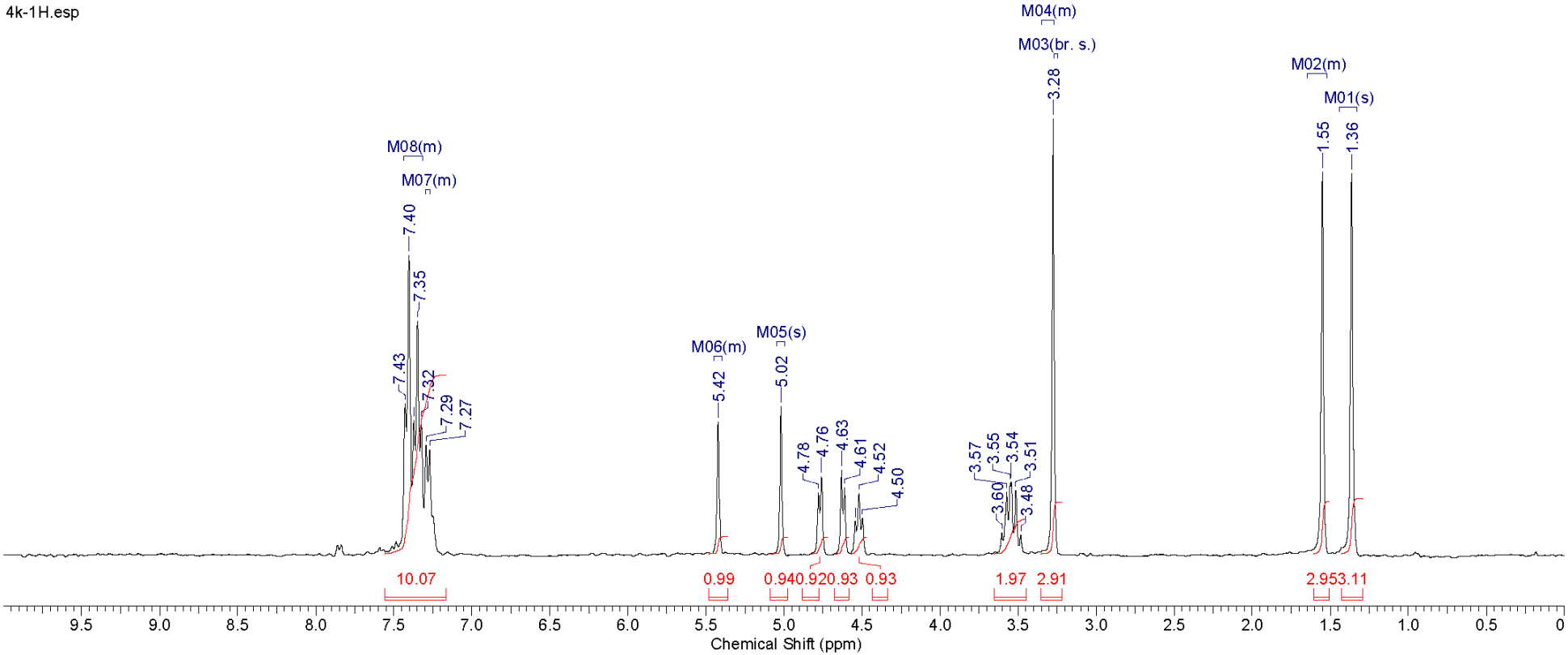




Formula $C_{22}H_{26}O_5$	FW	370.4388

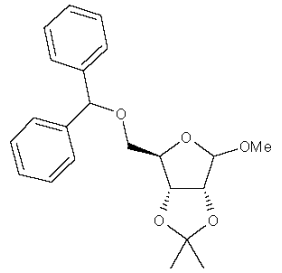
Acquisition Time (sec)	2.0000	**Comment**	CC23-1H	**Date**	Oct 8 2011	**Date Stamp**	Oct 8 2011
File Name	C:\Users\User\Documents\PhD\Green chem article\NMR data\4k\CC23-1H.fid\fid					**Frequency (MHz)**	300.08
Nucleus	1H	**Number of Transients**	4	**Original Points Count**	9600	**Points Count**	131072
Pulse Sequence	s2pul	**Receiver Gain**	3.00	**Solvent**	CHLOROFORM-d		
Spectrum Offset (Hz)	1493.8297	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	4800.00	**Temperature (degree C)**	AMBIENT TEMPERATURE

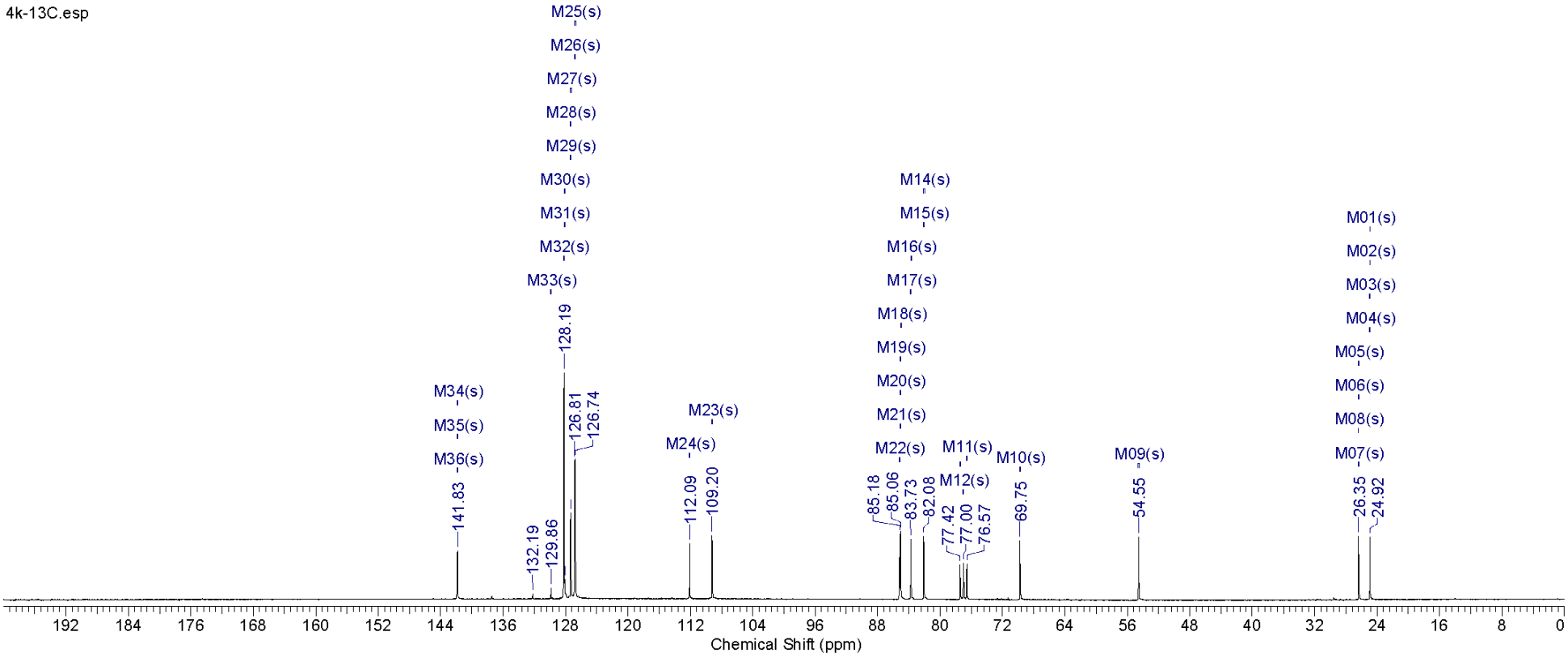




Formula $C_{22}H_{26}O_5$	FW	370.4388

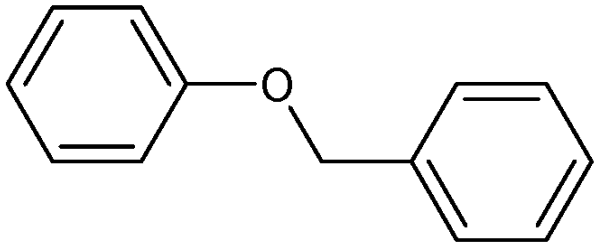
Acquisition Time (sec)	1.8150	**Comment**	CC23-13C	**Date**	Oct 8 2011	**Date Stamp**	Oct 8 2011
File Name	C:\Users\User\Documents\PhD\Green chem article\NMR data\4k\CC23-13C.fid\fid					**Frequency (MHz)**	75.46
Nucleus	13C	**Number of Transients**	5080	**Original Points Count**	34053	**Points Count**	65536
Pulse Sequence	s2pul	**Receiver Gain**	29.00	**Solvent**	CHLOROFORM-d		
Spectrum Offset (Hz)	7525.9155	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	18761.73	**Temperature (degree C)**	AMBIENT TEMPERATURE

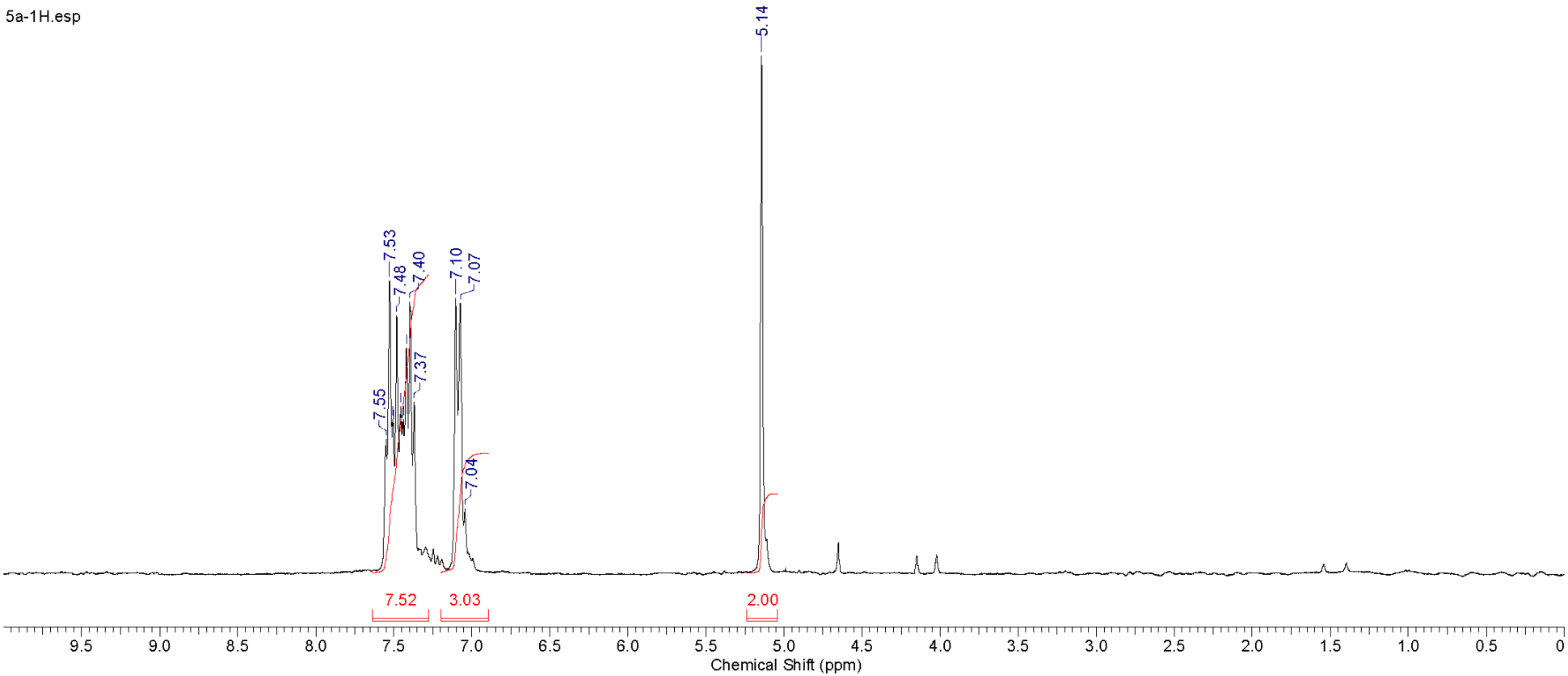




Formula $C_{13}H_{12}O$	FW	184.2338

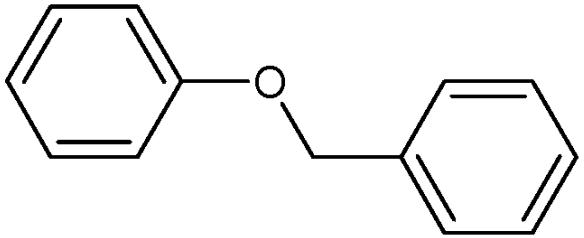
Acquisition Time (sec)	2.0000	*Comment*	CC148-1H	*Date*	Jul 28 2011	*Date Stamp*	Jul 28 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC148-1H.fid\fid			*Frequency (MHz)*	300.08	*Nucleus*	1H	*Number of Transients*	4
Original Points Count	9600	*Points Count*	16384	*Pulse Sequence*	s2pul	*Receiver Gain*	9.00	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	1497.0046	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	4800.00	*Temperature (degree C)*	AMBIENT TEMPERATURE		

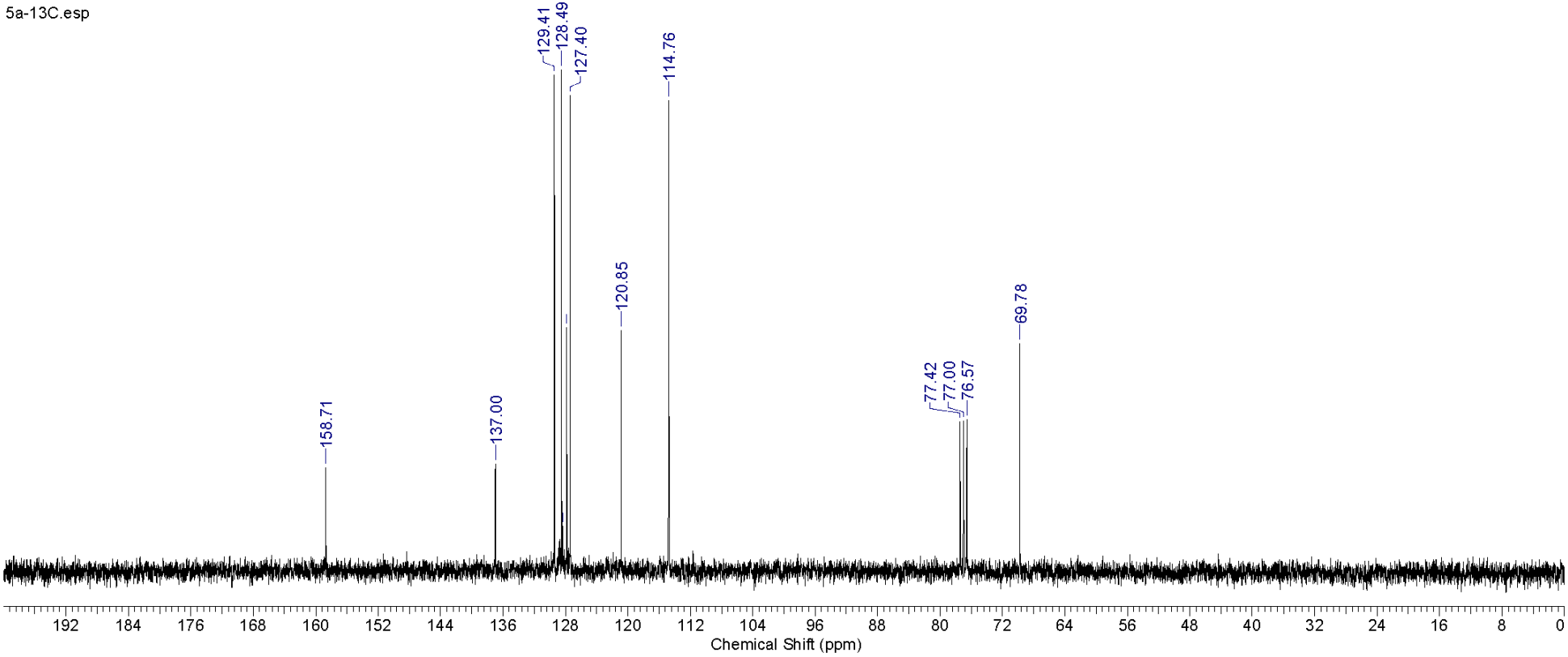




Formula $C_{13}H_{12}O$	FW	184.2338

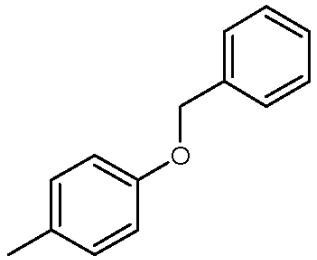
Acquisition Time (sec)	1.8150	**Comment**	CC148-13C	**Date**	Jul 28 2011	**Date Stamp**	Jul 28 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC148-13C.fid\fid			**Frequency (MHz)**	75.46	**Nucleus**	13C	**Number of Transients**	60
Original Points Count	34053	**Points Count**	65536	**Pulse Sequence**	s2pul	**Receiver Gain**	29.00		
Solvent	CHLOROFORM-d			**Spectrum Offset (Hz)**	7529.9233	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	18761.73
Temperature (degree C)	AMBIENT TEMPERATURE								



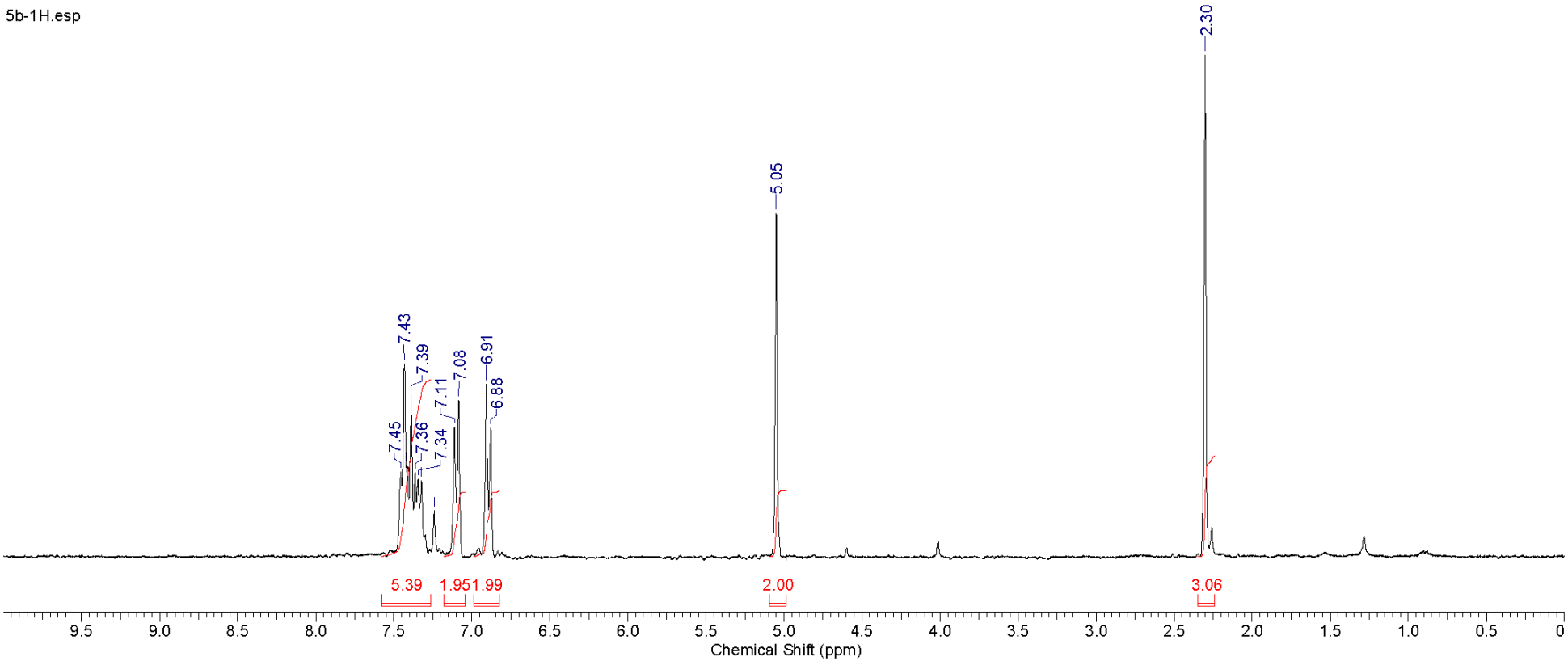


Formula $C_{14}H_{14}O$	FW	198.2604

Acquisition Time (sec)	2.0000	***Comment***	CC173-1H	***Date***	Sep 8 2011	***Date Stamp***	Sep 8 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC173-1H.fid\fid			***Frequency (MHz)***	300.08	***Nucleus***	1H	***Number of Transients***	4
Original Points Count	9600	***Points Count***	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	1495.6379	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4800.00	***Temperature (degree C)***	AMBIENT TEMPERATURE		

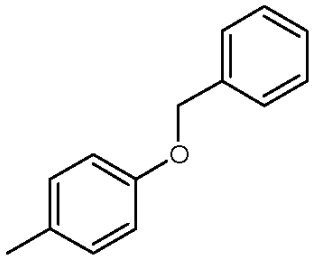


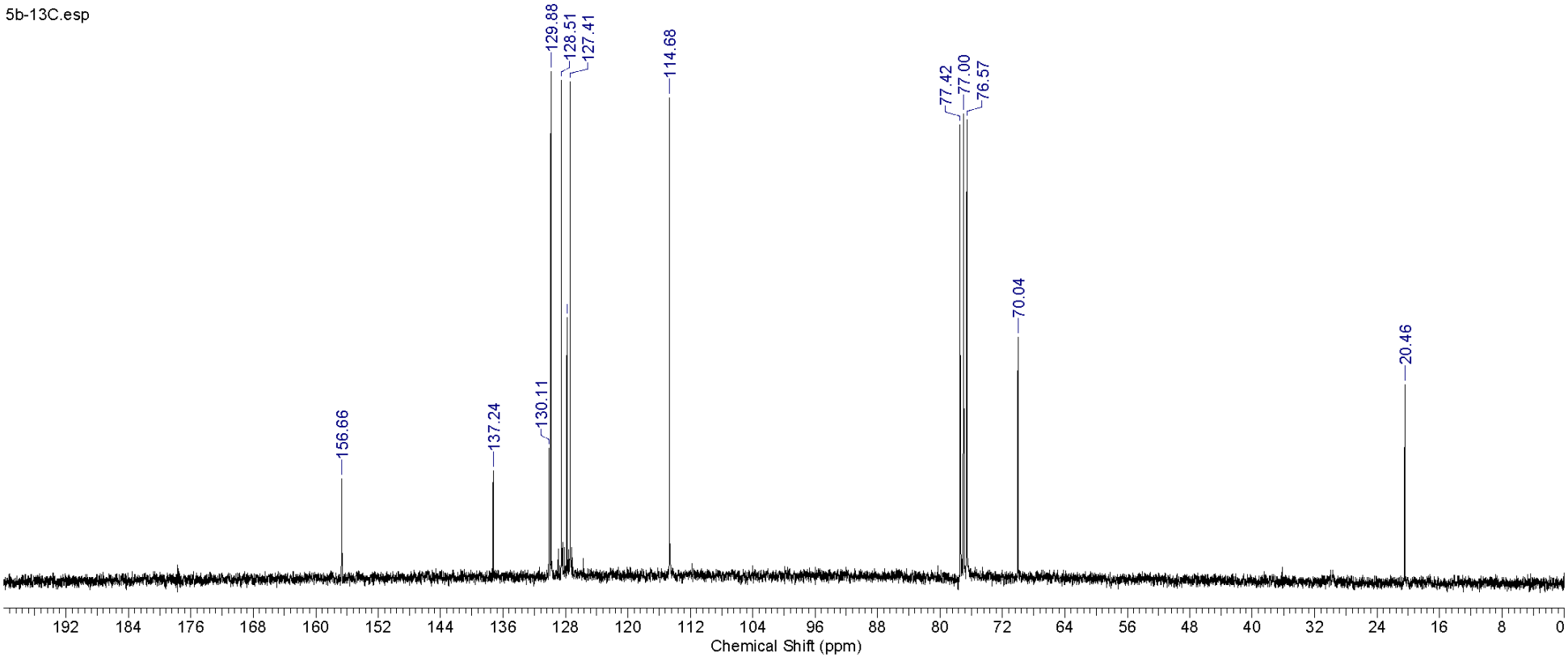
5b-1H.esp



Formula $C_{14}H_{14}O$	FW	198.2604

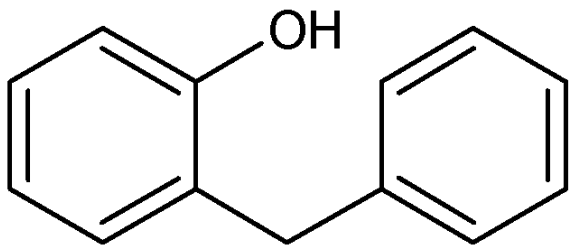
Acquisition Time (sec)	1.8150	**Comment**	CC173-13C	**Date**	Sep 8 2011	**Date Stamp**	Sep 8 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC173-13C.fid\fid			**Frequency (MHz)**	75.46	**Nucleus**	13C	**Number of Transients**	2700
Original Points Count	34053	**Points Count**	65536	**Pulse Sequence**	s2pul	**Receiver Gain**	30.00		
Solvent	CHLOROFORM-d			**Spectrum Offset (Hz)**	7541.6602	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	18761.73
Temperature (degree C)	AMBIENT TEMPERATURE								

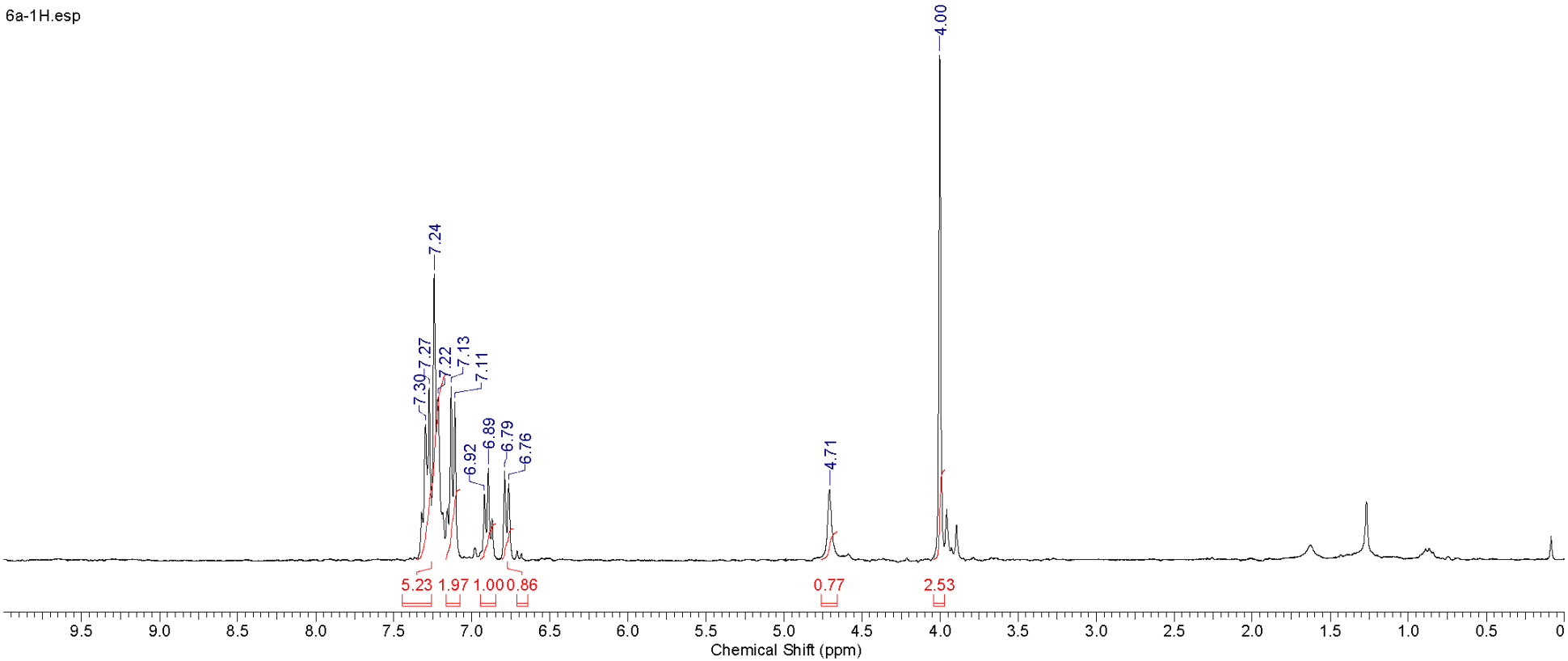




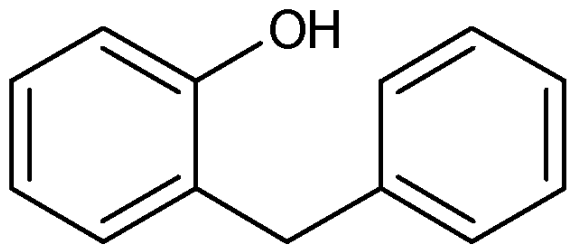
Formula $C_{13}H_{12}O$	FW	184.2338

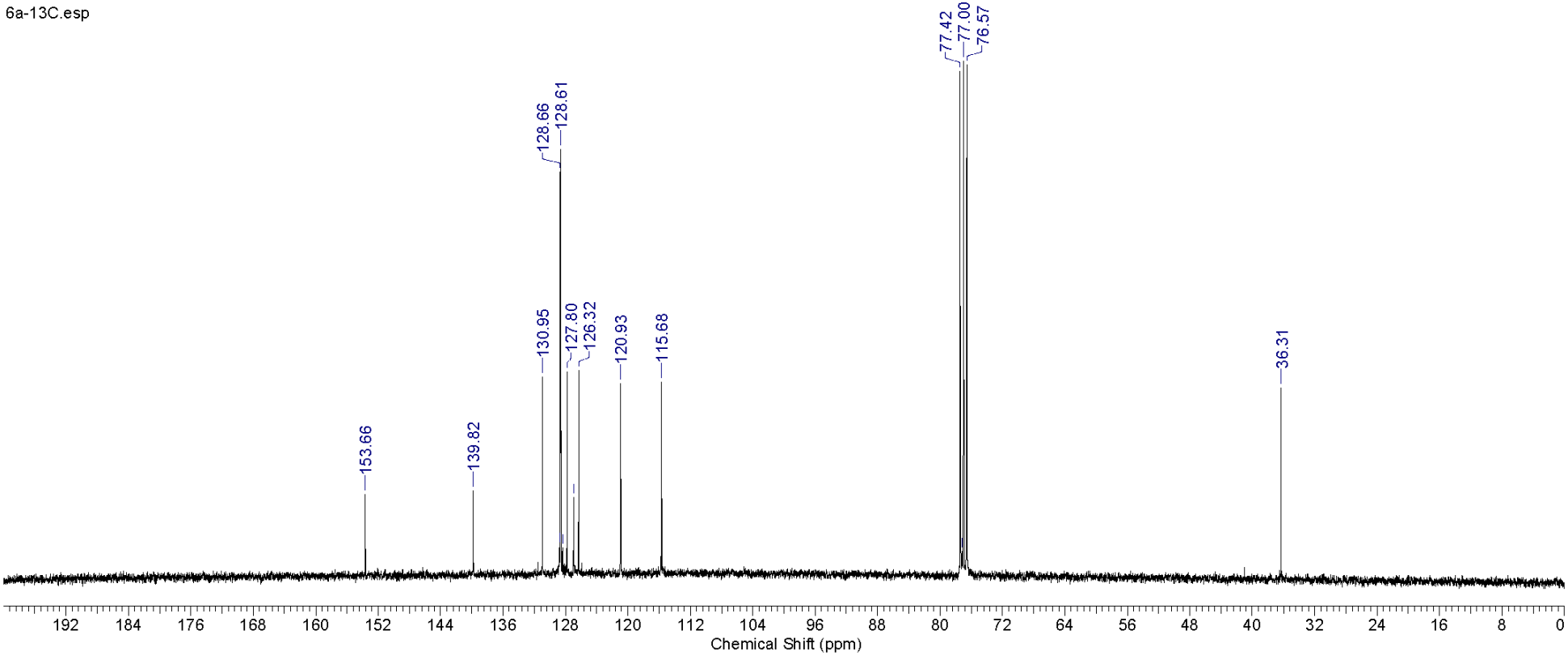
Acquisition Time (sec)	2.0000	***Comment***	CC152-1H	***Date***	Sep 28 2011	***Date Stamp***	Sep 28 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC152-1H.fid\fid			***Frequency (MHz)***	300.08	***Nucleus***	1H	***Number of Transients***	4
Original Points Count	9600	***Points Count***	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	7.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	1496.5173	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4800.00	***Temperature (degree C)***	AMBIENT TEMPERATURE		





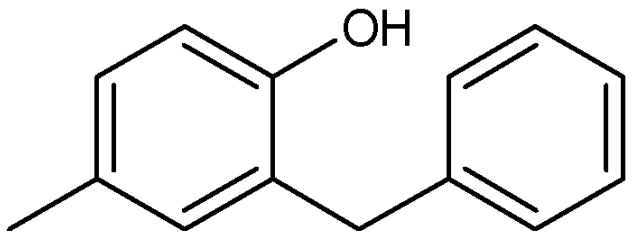
Formula $C_{13}H_{12}O$	***FW***	184.2338							
Acquisition Time (sec)	1.8150	***Comment***	CC152-13C	***Date***	Oct 1 2011	***Date Stamp***	Oct 1 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC152-13C.fid\fid			***Frequency (MHz)***	75.46	***Nucleus***	13C	***Number of Transients***	5564
Original Points Count	34053	***Points Count***	65536	***Pulse Sequence***	s2pul	***Receiver Gain***	30.00		
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	7542.5186	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	18761.73
Temperature (degree C)	AMBIENT TEMPERATURE								



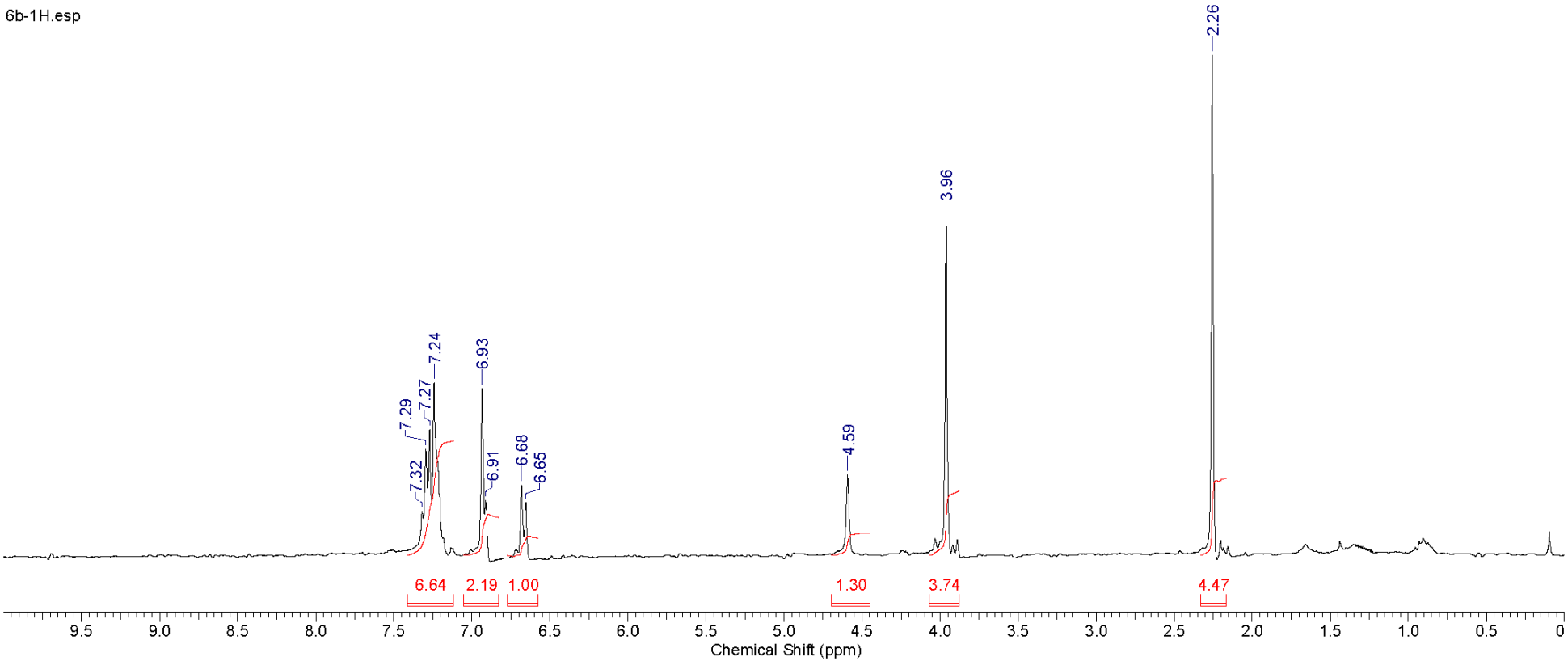


Formula $C_{14}H_{14}O$	FW	198.2604

Acquisition Time (sec)	2.0000	***Comment***	CC174-1H	***Date***	Sep 28 2011	***Date Stamp***	Sep 28 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC174-1H.fid\fid			***Frequency (MHz)***	300.08	***Nucleus***	1H	***Number of Transients***	4
Original Points Count	9600	***Points Count***	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	2.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	1491.2437	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4800.00	***Temperature (degree C)***	AMBIENT TEMPERATURE		

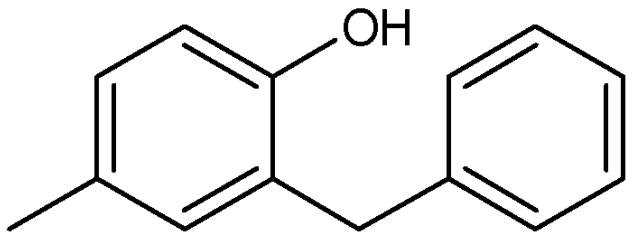


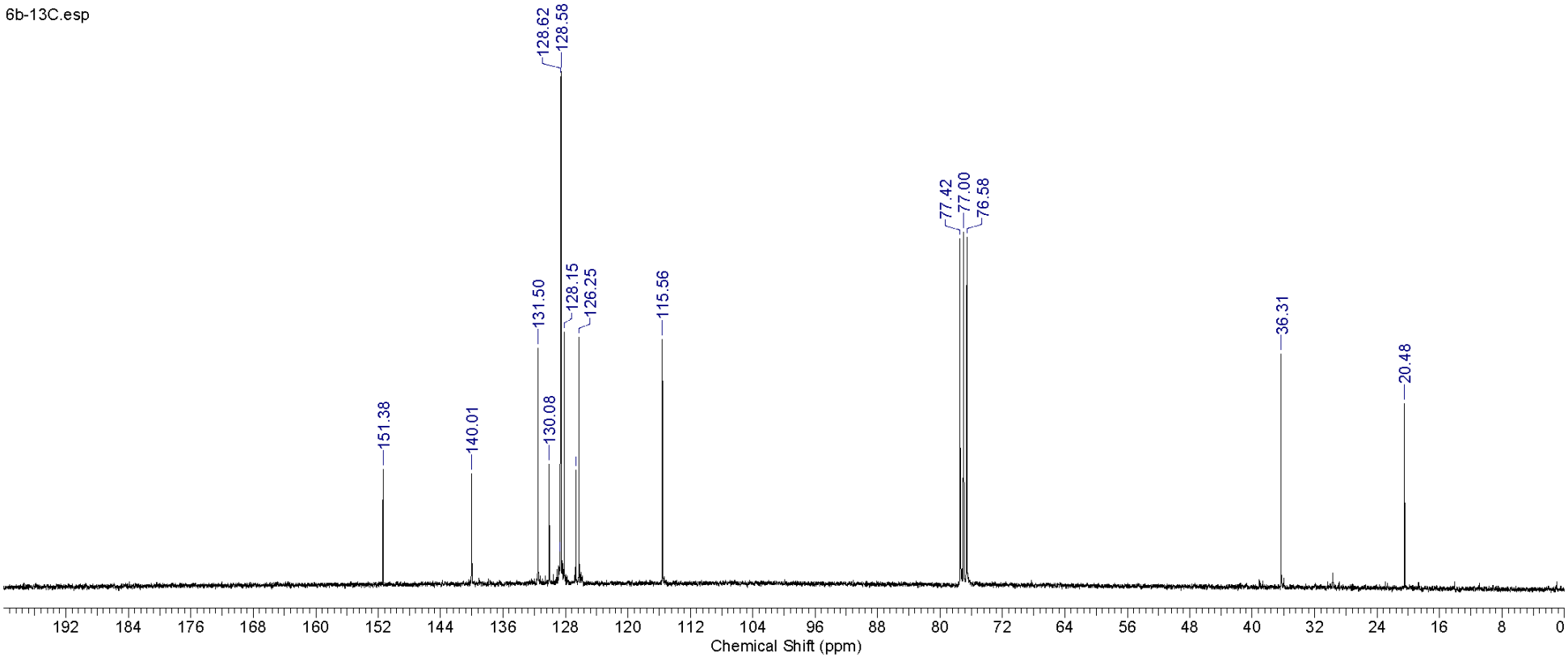
6b-1H.esp



Formula $C_{14}H_{14}O$	FW	198.2604

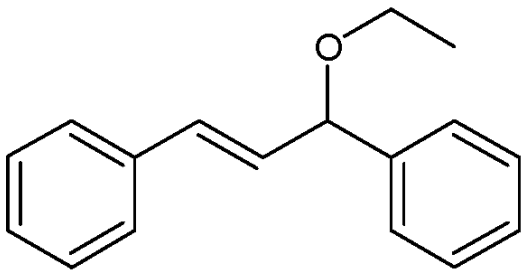
Acquisition Time (sec)	1.8150	**Comment**	CC174-13C	**Date**	Oct 2 2011	**Date Stamp**	Oct 2 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC174-13C.fid\fid			**Frequency (MHz)**	75.46	**Nucleus**	13C	**Number of Transients**	9148
Original Points Count	34053	**Points Count**	65536	**Pulse Sequence**	s2pul	**Receiver Gain**	30.00		
Solvent	CHLOROFORM-d			**Spectrum Offset (Hz)**	7540.2358	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	18761.73
Temperature (degree C)	AMBIENT TEMPERATURE								



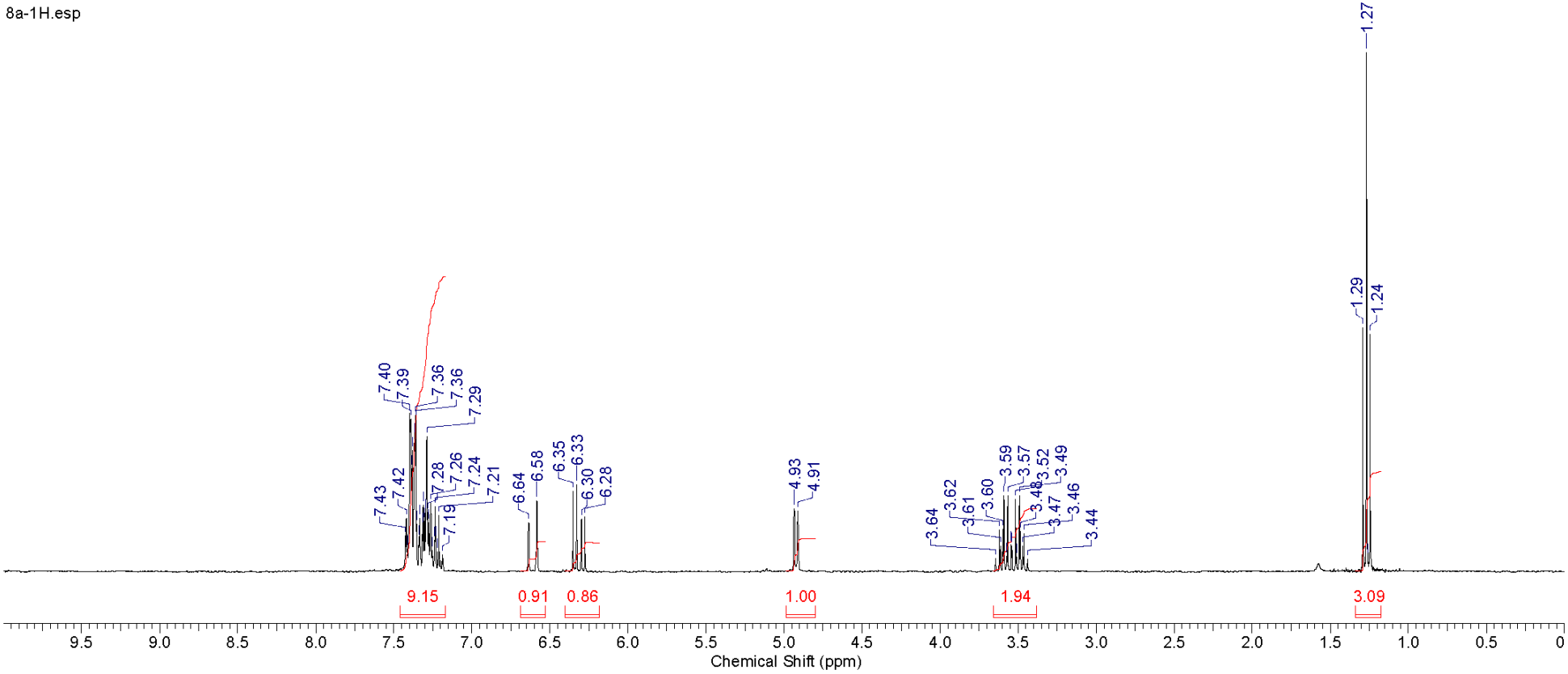


Formula $C_{17}H_{18}O$	FW	238.3242

Acquisition Time (sec)	2.0000	*Comment*	CC81-1H	*Date*	Feb 23 2011	*Date Stamp*	Feb 23 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC81-1H.fid\fid			*Frequency (MHz)*	300.08	*Nucleus*	1H	*Number of Transients*	4
Original Points Count	9600	*Points Count*	16384	*Pulse Sequence*	s2pul	*Receiver Gain*	2.00	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	1493.0132	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	4800.00	*Temperature (degree C)*	AMBIENT TEMPERATURE		

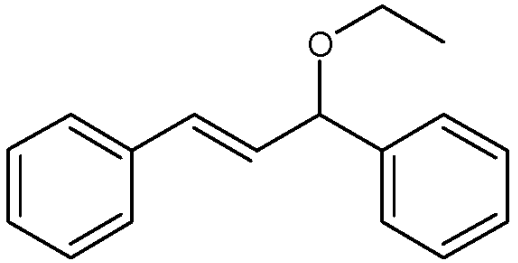


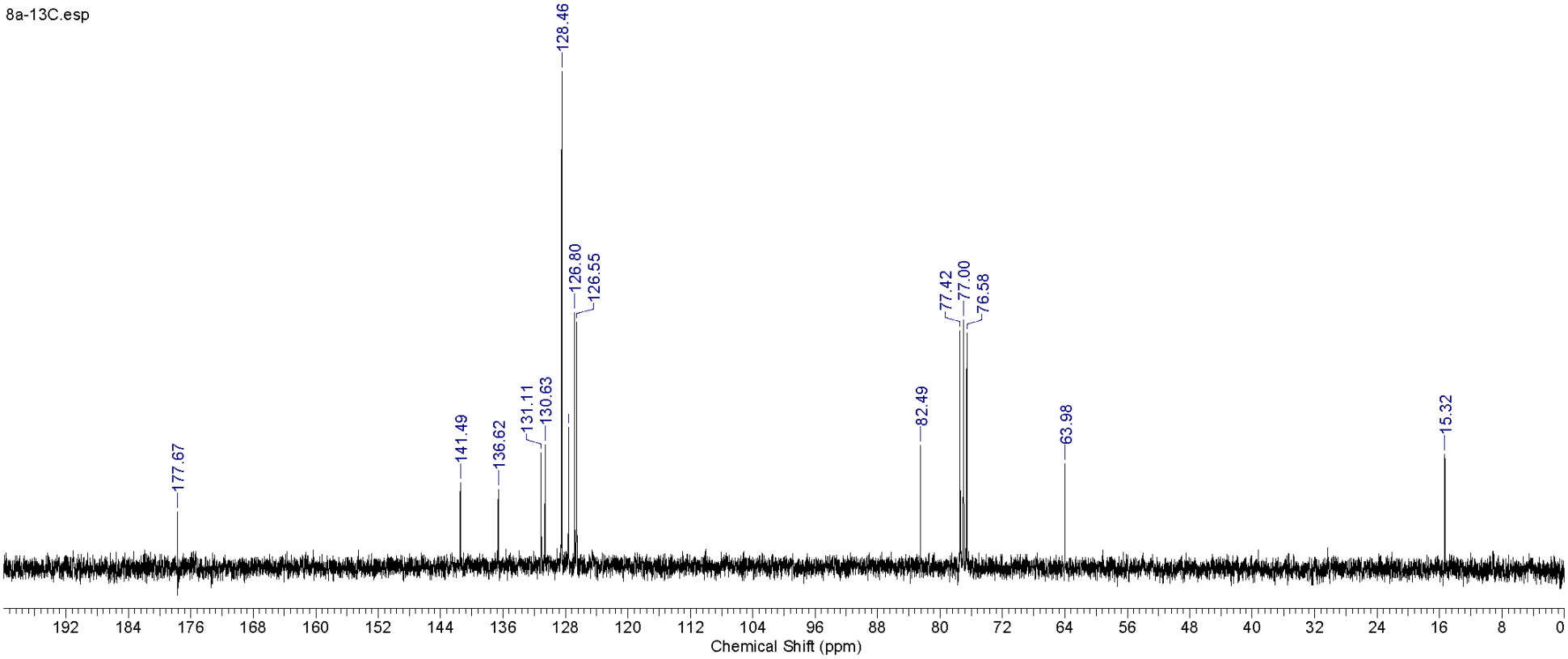
8a-1H.esp



Formula $C_{17}H_{18}O$	FW	238.3242

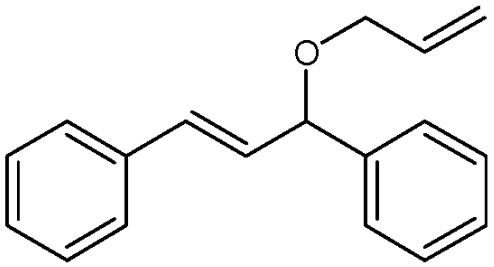
Acquisition Time (sec)	1.8150	*Comment*	CC81-13C	*Date*	Feb 23 2011	*Date Stamp*	Feb 23 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC81-13C.fid\fid			*Frequency (MHz)*	75.46	*Nucleus*	13C	*Number of Transients*	152
Original Points Count	34053	*Points Count*	65536	*Pulse Sequence*	s2pul	*Receiver Gain*	33.00		
Solvent	CHLOROFORM-d			*Spectrum Offset (Hz)*	7541.6680	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	18761.73
Temperature (degree C)	AMBIENT TEMPERATURE								

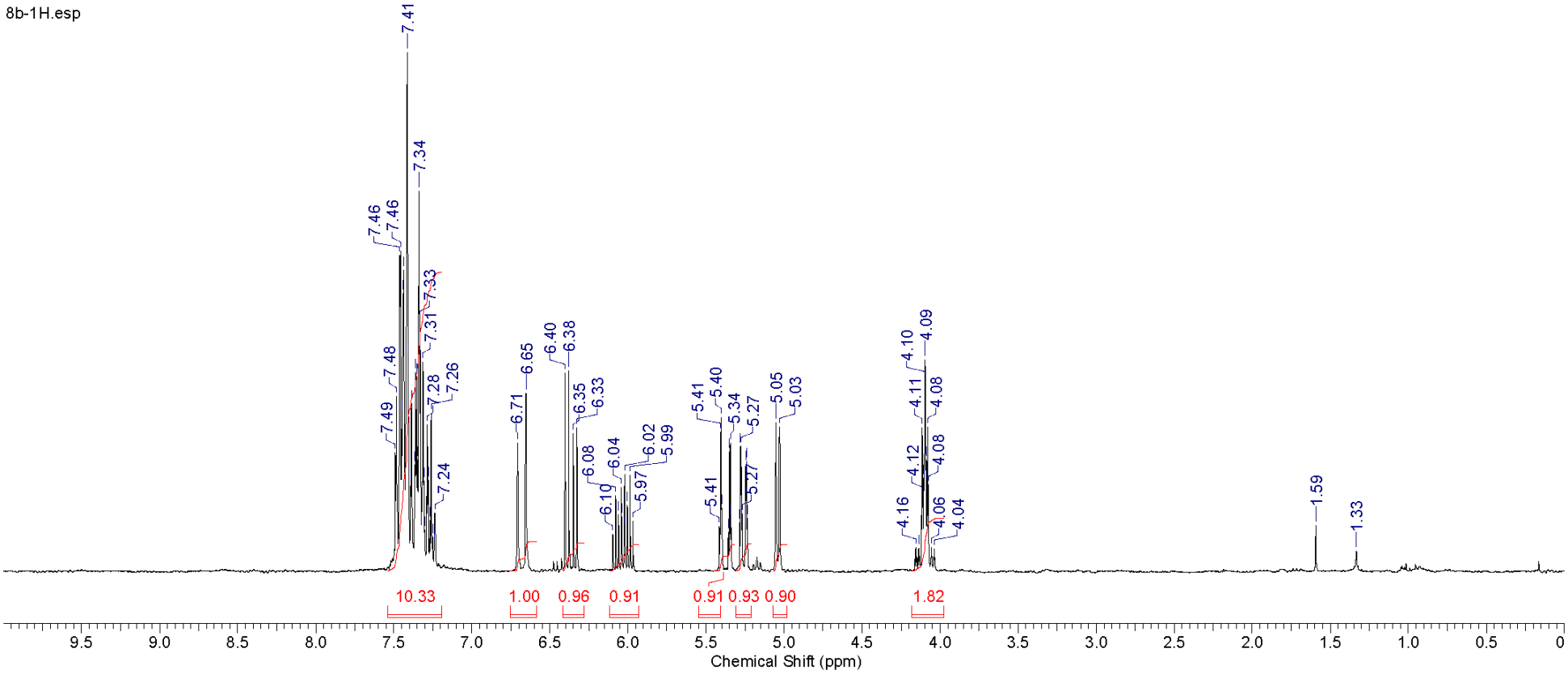




Formula $C_{18}H_{18}O$	FW	250.3349

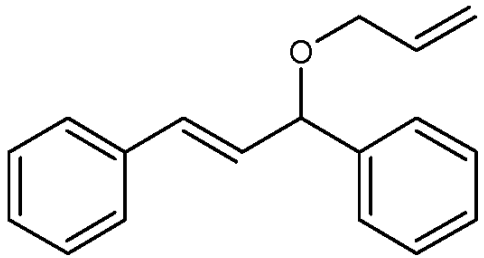
Acquisition Time (sec)	2.0000	**Comment**	CC79-1H	**Date**	Feb 14 2011	**Date Stamp**	Feb 14 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC79-1H.fid\fid			**Frequency (MHz)**	300.08	**Nucleus**	1H	**Number of Transients**	8
Original Points Count	9600	**Points Count**	16384	**Pulse Sequence**	s2pul	**Receiver Gain**	10.00	**Solvent**	CHLOROFORM-d
Spectrum Offset (Hz)	1493.4601	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	4800.00	**Temperature (degree C)**	AMBIENT TEMPERATURE		

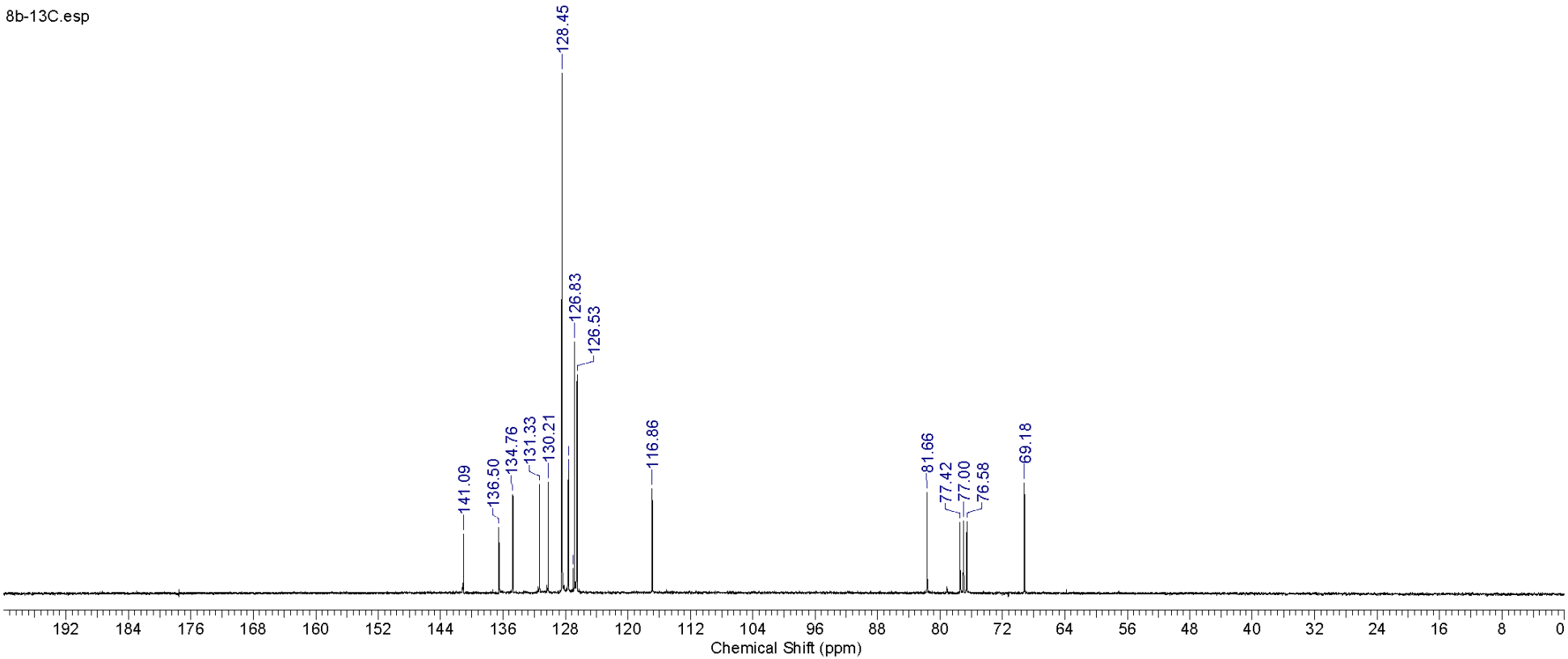




Formula $C_{18}H_{18}O$	FW	250.3349

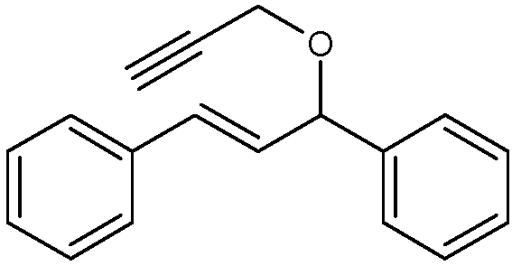
Acquisition Time (sec)	1.8150	**Comment**	CC79-13C	**Date**	Feb 14 2011	**Date Stamp**	Feb 14 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\Cc79-13C.fid\fid			**Frequency (MHz)**	75.46	**Nucleus**	13C	**Number of Transients**	2316
Original Points Count	34053	**Points Count**	65536	**Pulse Sequence**	s2pul	**Receiver Gain**	33.00		
Solvent	CHLOROFORM-d			**Spectrum Offset (Hz)**	7533.9307	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	18761.73
Temperature (degree C)	AMBIENT TEMPERATURE								

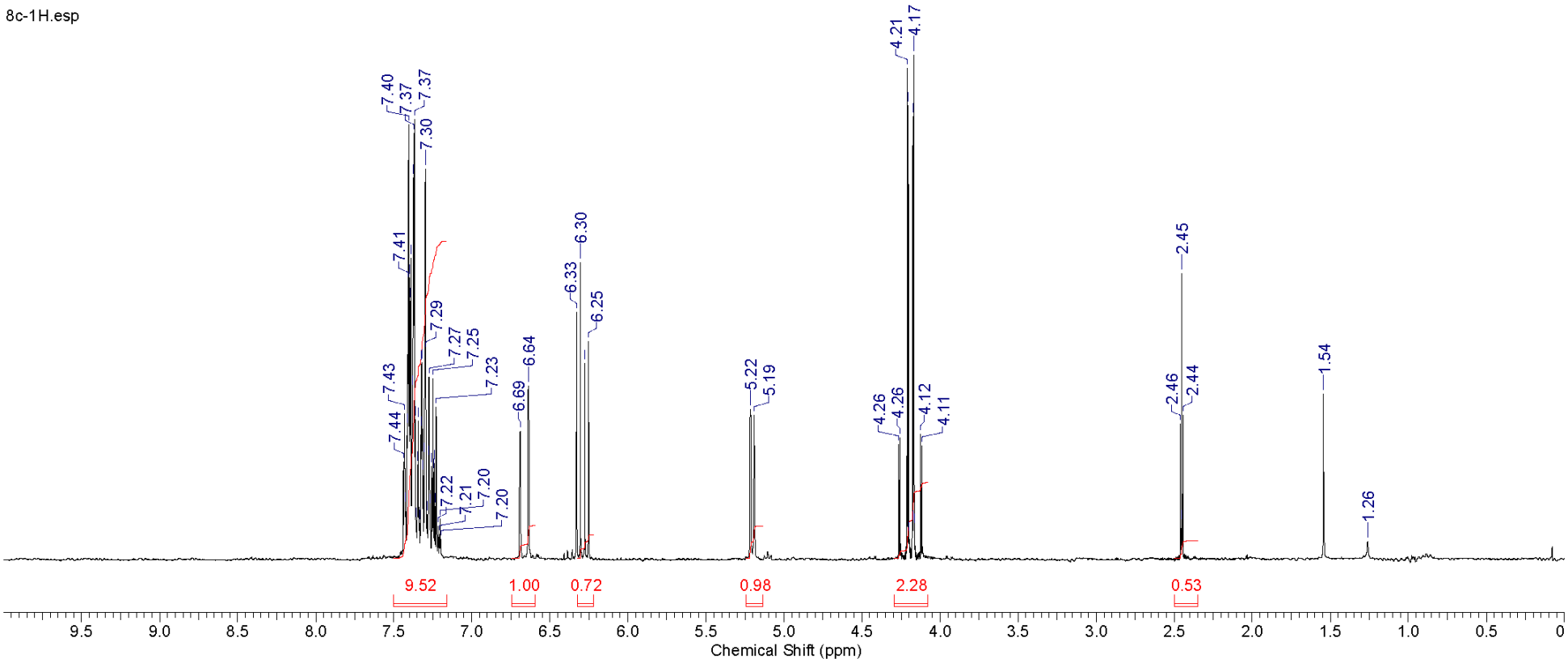




Formula $C_{18}H_{16}O$	FW	248.3190

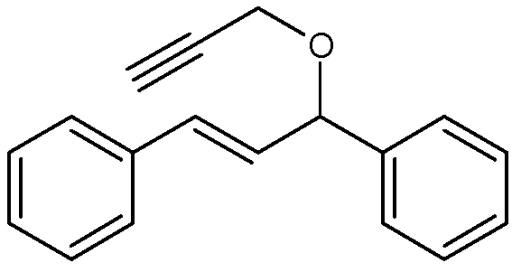
Acquisition Time (sec)	2.0000	***Comment***	CC118-1H	***Date***	Feb 15 2011	***Date Stamp***	Feb 15 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC118-1H.fid\fid			***Frequency (MHz)***	300.08	***Nucleus***	1H	***Number of Transients***	8
Original Points Count	9600	***Points Count***	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	8.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	1495.0859	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4800.00	***Temperature (degree C)***	AMBIENT TEMPERATURE		

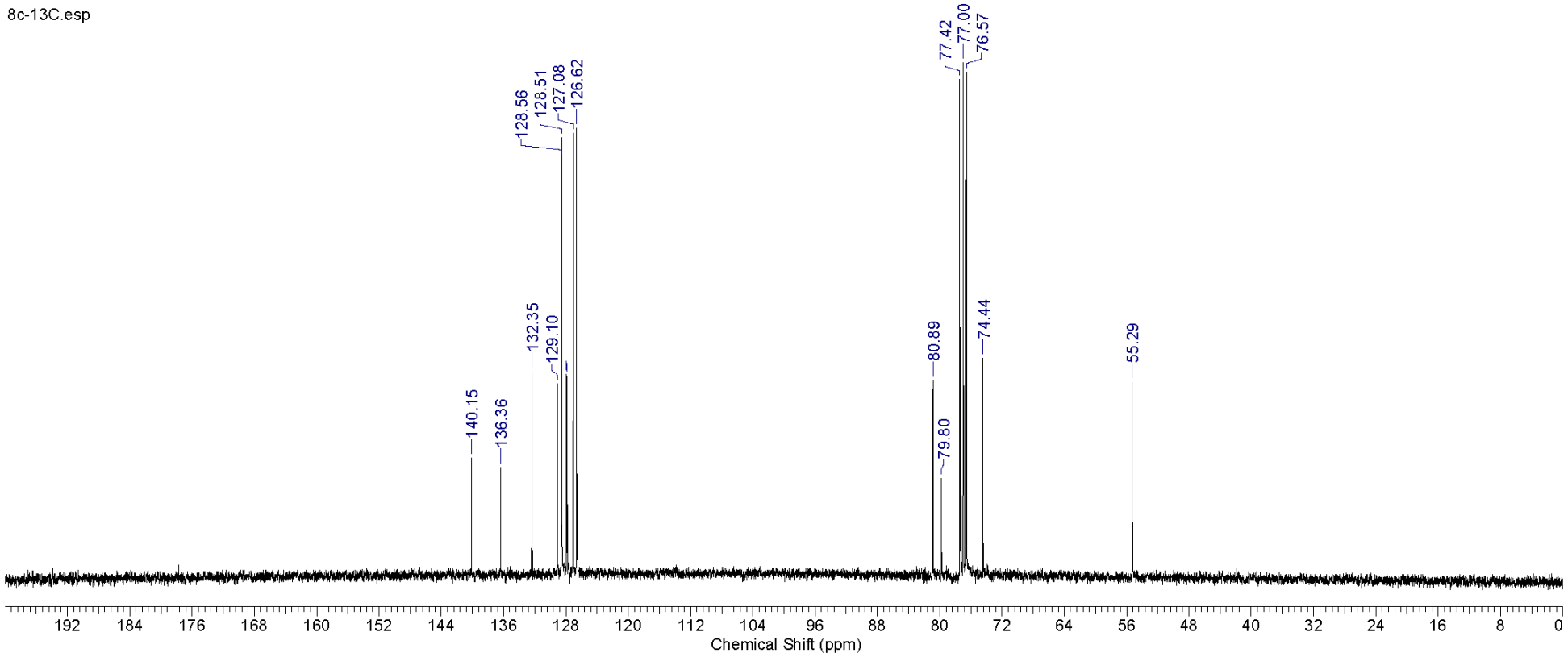




Formula $C_{18}H_{16}O$	FW	248.3190

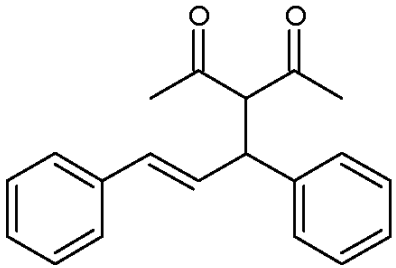
Acquisition Time (sec)	1.8150	**Comment**	CC118-13C	**Date**	Feb 15 2011	**Date Stamp**	Feb 15 2011
File Name	C:\Users\User\Desktop\adam\CCclean\CC118-13C.fid\fid			**Frequency (MHz)**	75.46	**Nucleus**	13C
Number of Transients	3172	**Original Points Count**	34053	**Points Count**	65536	**Pulse Sequence**	s2pul
Receiver Gain	33.00	**Solvent**	CHLOROFORM-d			**Spectrum Offset (Hz)**	7542.2329
Spectrum Type	STANDARD	**Sweep Width (Hz)**	18761.73	**Temperature (degree C)**	AMBIENT TEMPERATURE		



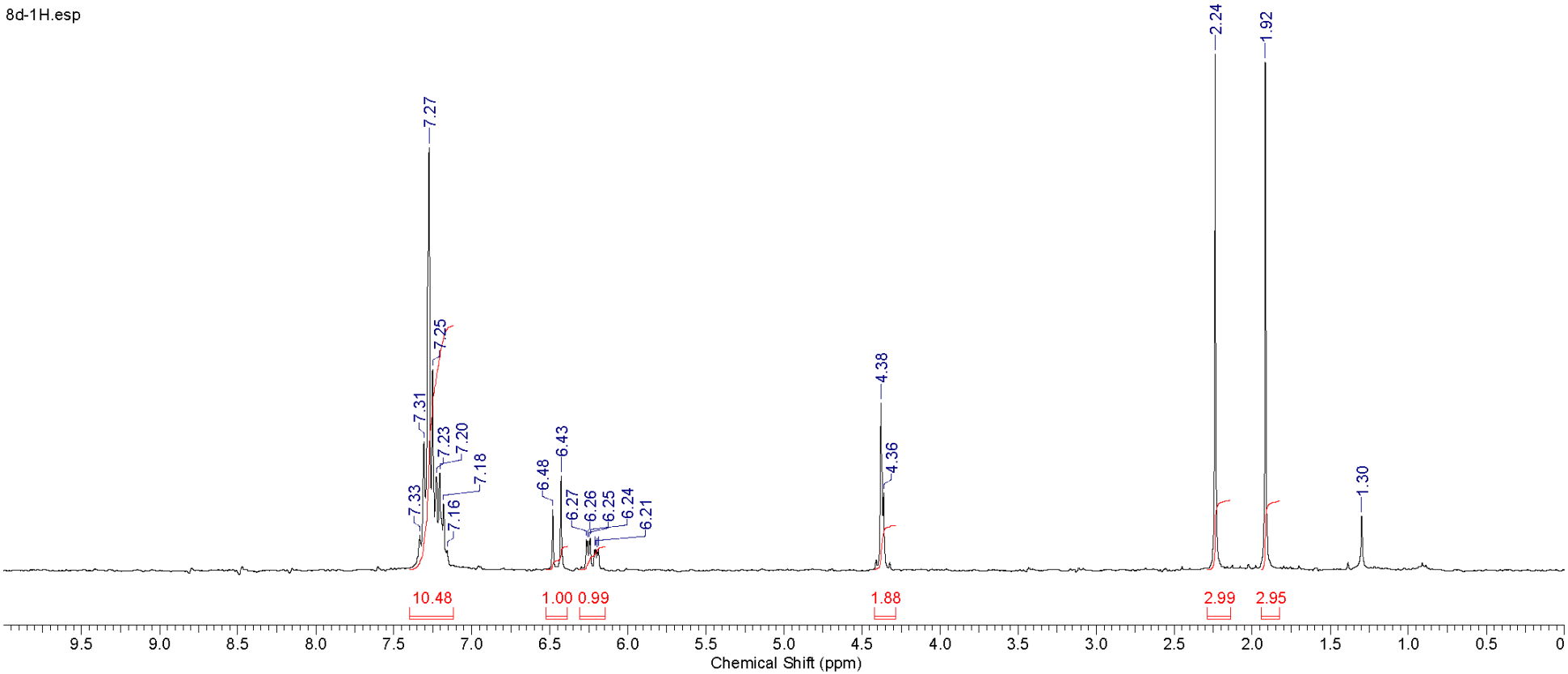


Formula $C_{20}H_{20}O_2$	FW	292.3716

Acquisition Time (sec)	2.0000	*Comment*	CC61-1H	*Date*	Feb 1 2011	*Date Stamp*	Feb 1 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC61-1H.fid\fid			*Frequency (MHz)*	300.08	*Nucleus*	1H	*Number of Transients*	8
Original Points Count	9600	*Points Count*	16384	*Pulse Sequence*	s2pul	*Receiver Gain*	3.00	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	1493.7749	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	4800.00	*Temperature (degree C)*	AMBIENT TEMPERATURE		

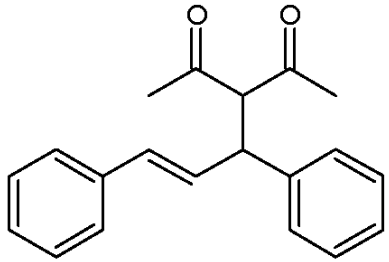


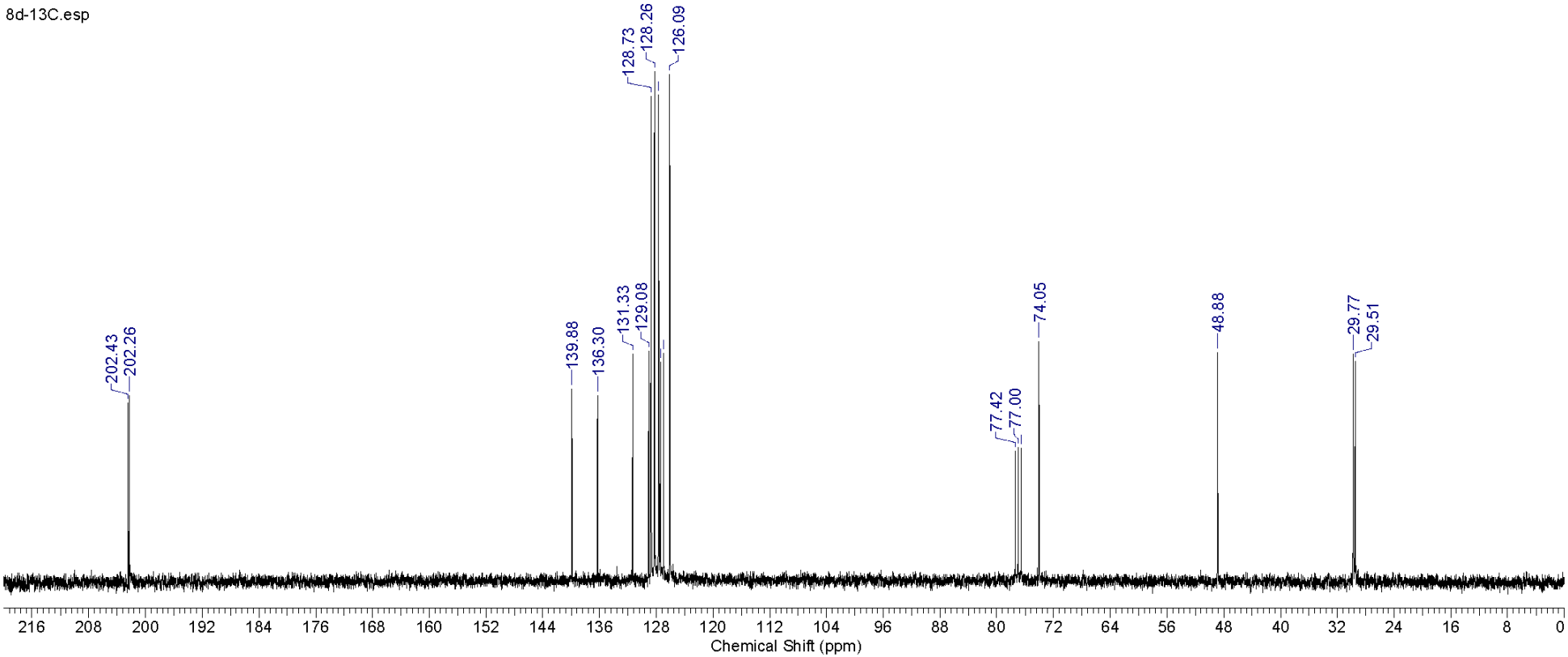
8d-1H.esp



Formula $C_{20}H_{20}O_2$	FW	292.3716

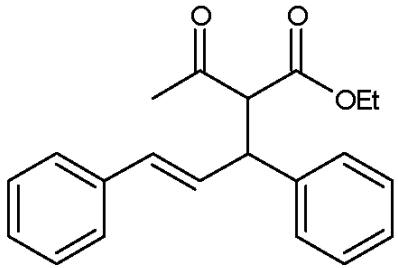
Acquisition Time (sec)	1.8150	**Comment**	CC61-13C	**Date**	Feb 1 2011	**Date Stamp**	Feb 1 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC61-13C.fid\fid			**Frequency (MHz)**	75.46	**Nucleus**	13C	**Number of Transients**	100
Original Points Count	34053	**Points Count**	65536	**Pulse Sequence**	s2pul	**Receiver Gain**	29.00		
Solvent	CHLOROFORM-d			**Spectrum Offset (Hz)**	7521.0488	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	18761.73
Temperature (degree C)	AMBIENT TEMPERATURE								



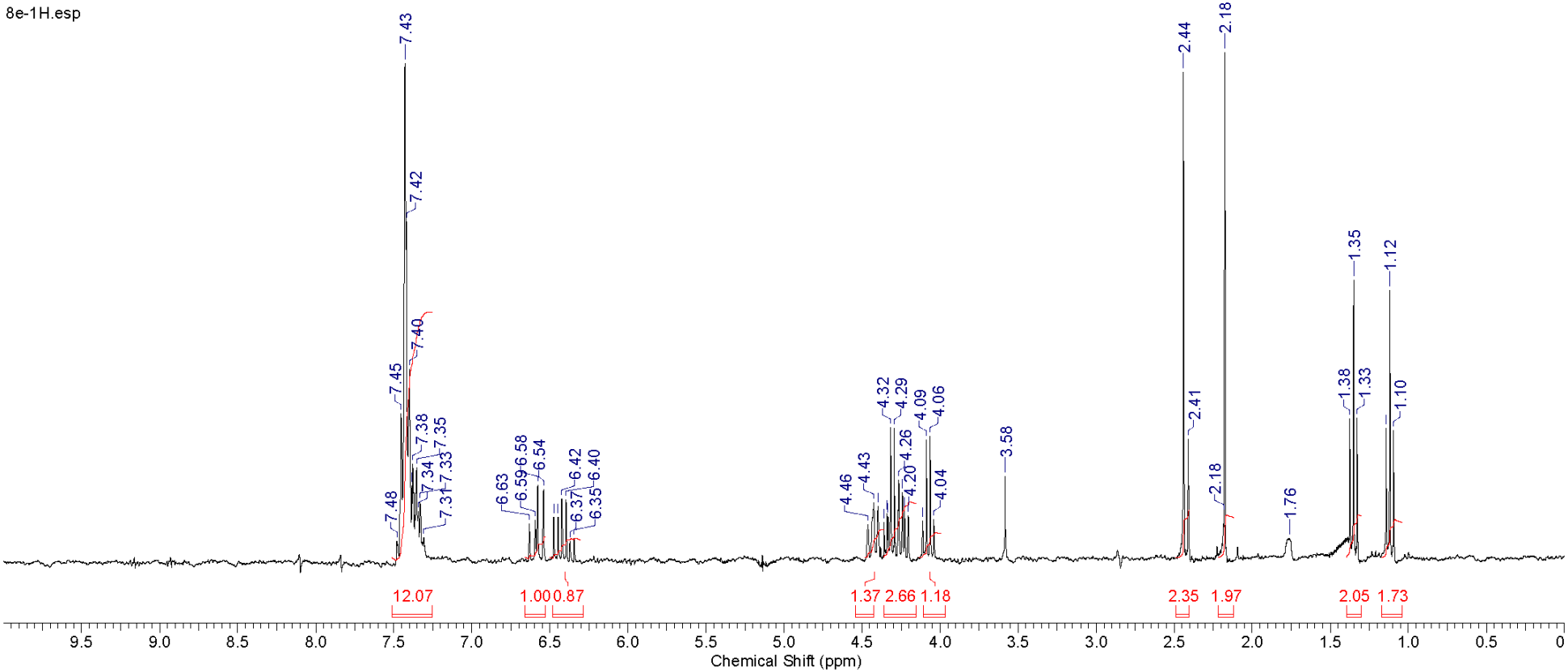


Formula $C_{21}H_{22}O_3$	FW	322.3976

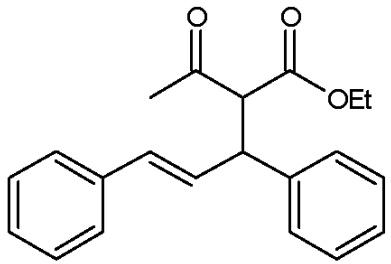
Acquisition Time (sec)	2.0000	***Comment***	CC63-1H	***Date***	Feb 4 2011	***Date Stamp***	Feb 4 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC63-1H.fid\fid			***Frequency (MHz)***	300.08	***Nucleus***	1H	***Number of Transients***	1
Original Points Count	9600	***Points Count***	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	4.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	1541.7954	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4800.00	***Temperature (degree C)***	AMBIENT TEMPERATURE		

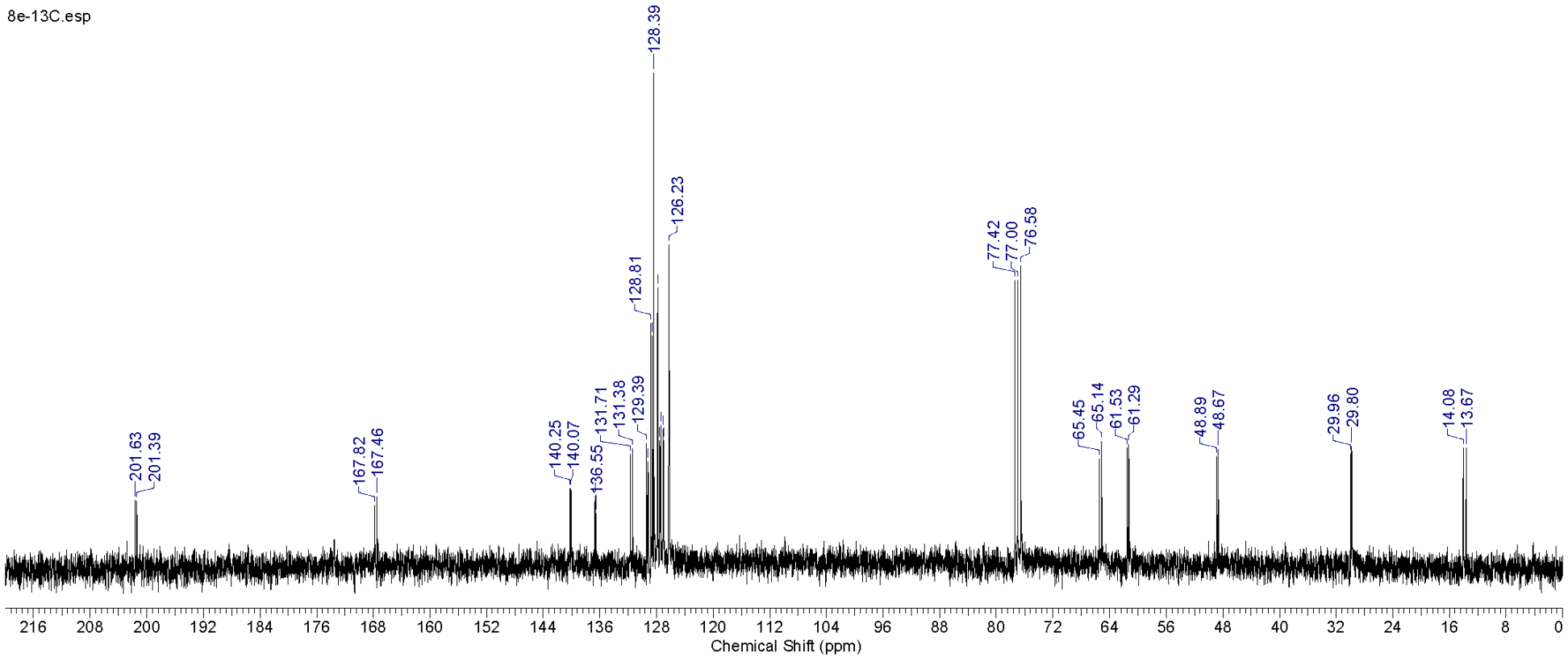


8e-1H.esp



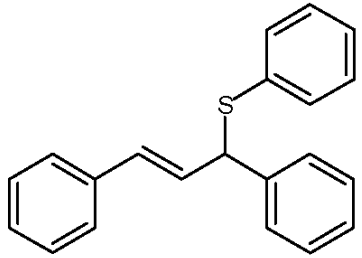
Formula $C_{21}H_{22}O_3$	***FW***	322.3976							
Acquisition Time (sec)	1.8150	***Comment***	CC63-13C	***Date***	May 17 2010	***Date Stamp***	May 17 2010		
File Name	C:\Users\User\Desktop\adam\CCclean\CC63-13C.fid\fid			***Frequency (MHz)***	75.46	***Nucleus***	13C	***Number of Transients***	156
Original Points Count	34053	***Points Count***	65536	***Pulse Sequence***	s2pul	***Receiver Gain***	35.00		
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	7536.9263	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	18761.73
Temperature (degree C)	AMBIENT TEMPERATURE								

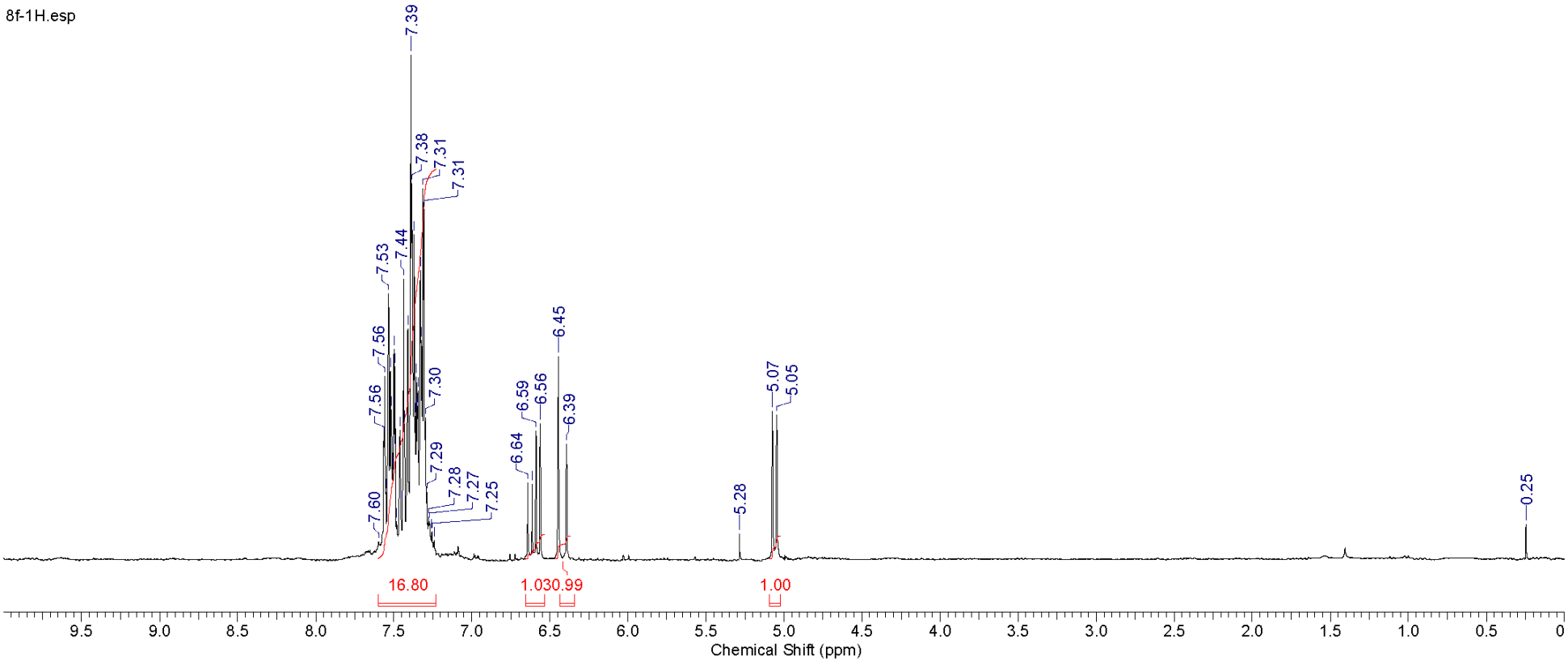




Formula $C_{21}H_{18}S$	FW	302.4326

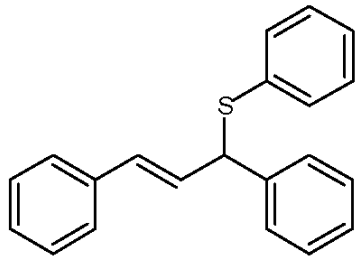
Acquisition Time (sec)	2.0000	***Comment***	CC120-1H	***Date***	Feb 25 2011	***Date Stamp***	Feb 25 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC120-1H.fid\fid			***Frequency (MHz)***	300.08	***Nucleus***	1H	***Number of Transients***	6
Original Points Count	9600	***Points Count***	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	8.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	1498.8611	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4800.00	***Temperature (degree C)***	AMBIENT TEMPERATURE		

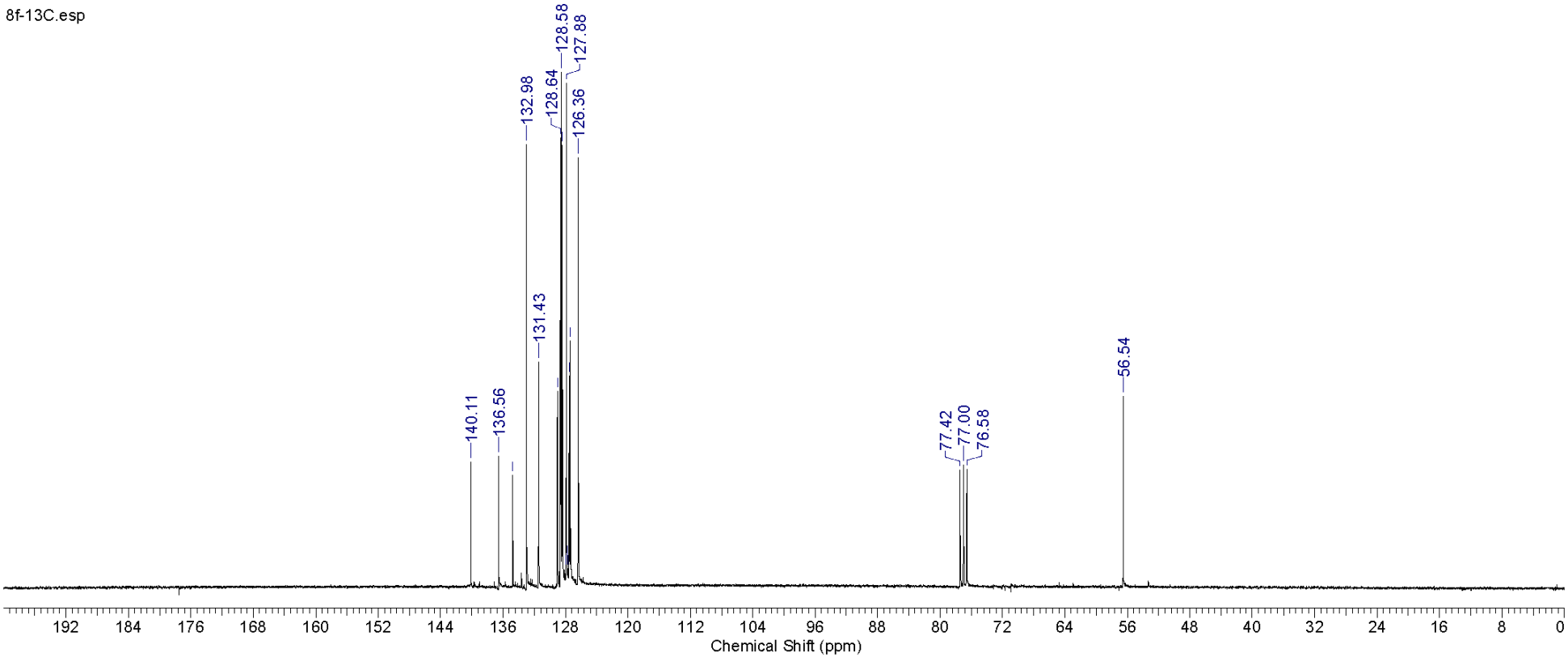




Formula $C_{21}H_{18}S$	FW	302.4326

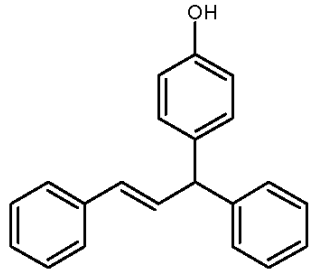
Acquisition Time (sec)	1.8150	**Comment**	CC120-13C	**Date**	Feb 25 2011	**Date Stamp**	Feb 25 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\Cc120-13C.fid\fid			**Frequency (MHz)**	75.46	**Nucleus**	13C	**Number of Transients**	5000
Original Points Count	34053	**Points Count**	65536	**Pulse Sequence**	s2pul	**Receiver Gain**	33.00		
Solvent	CHLOROFORM-d			**Spectrum Offset (Hz)**	7527.6333	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	18761.73
Temperature (degree C)	AMBIENT TEMPERATURE								

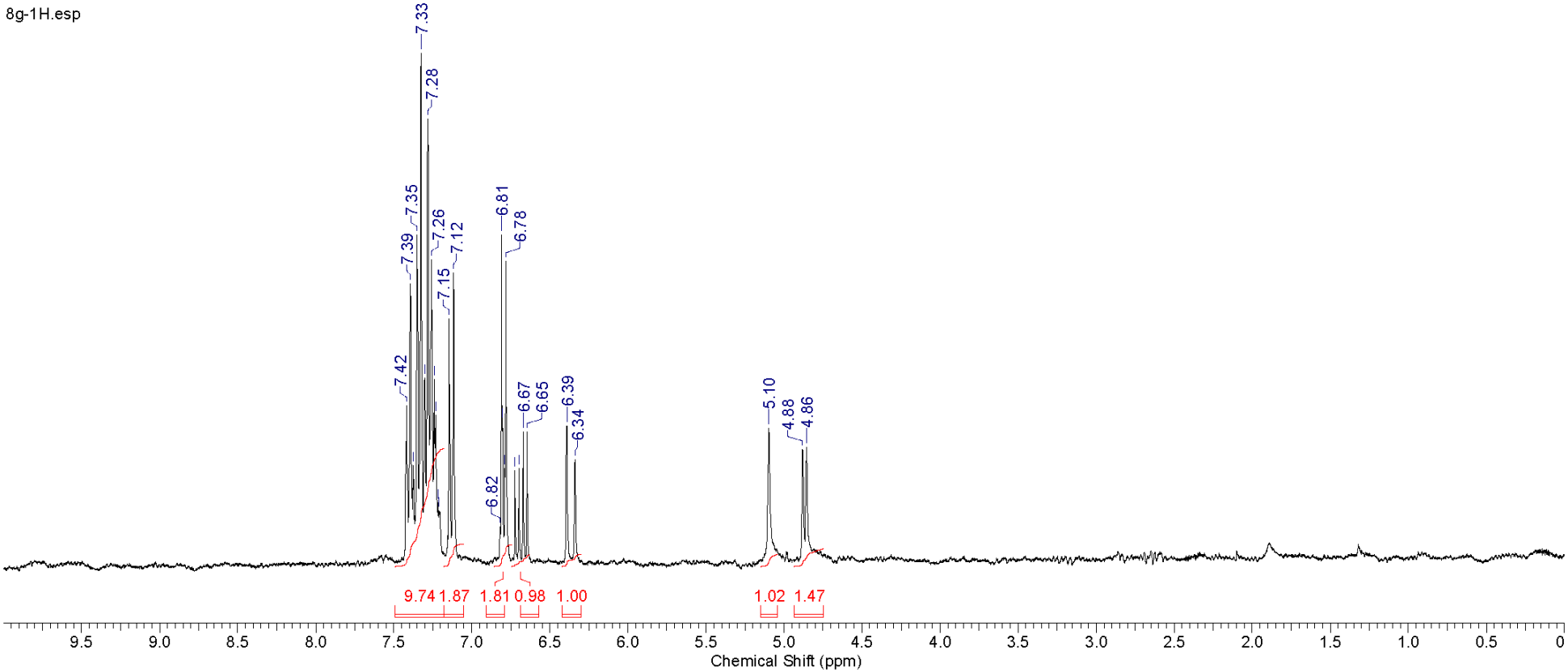




Formula $C_{21}H_{18}O$	FW	286.3670

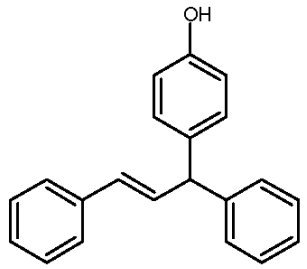
Acquisition Time (sec)	2.0000	**Comment**	cc65-1H	**Date**	Feb 8 2011	**Date Stamp**	Feb 8 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC65-1H-2.fid\fid			**Frequency (MHz)**	300.08	**Nucleus**	1H	**Number of Transients**	1
Original Points Count	9600	**Points Count**	16384	**Pulse Sequence**	s2pul	**Receiver Gain**	14.00	**Solvent**	CHLOROFORM-d
Spectrum Offset (Hz)	1495.3453	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	4800.00	**Temperature (degree C)**	AMBIENT TEMPERATURE		



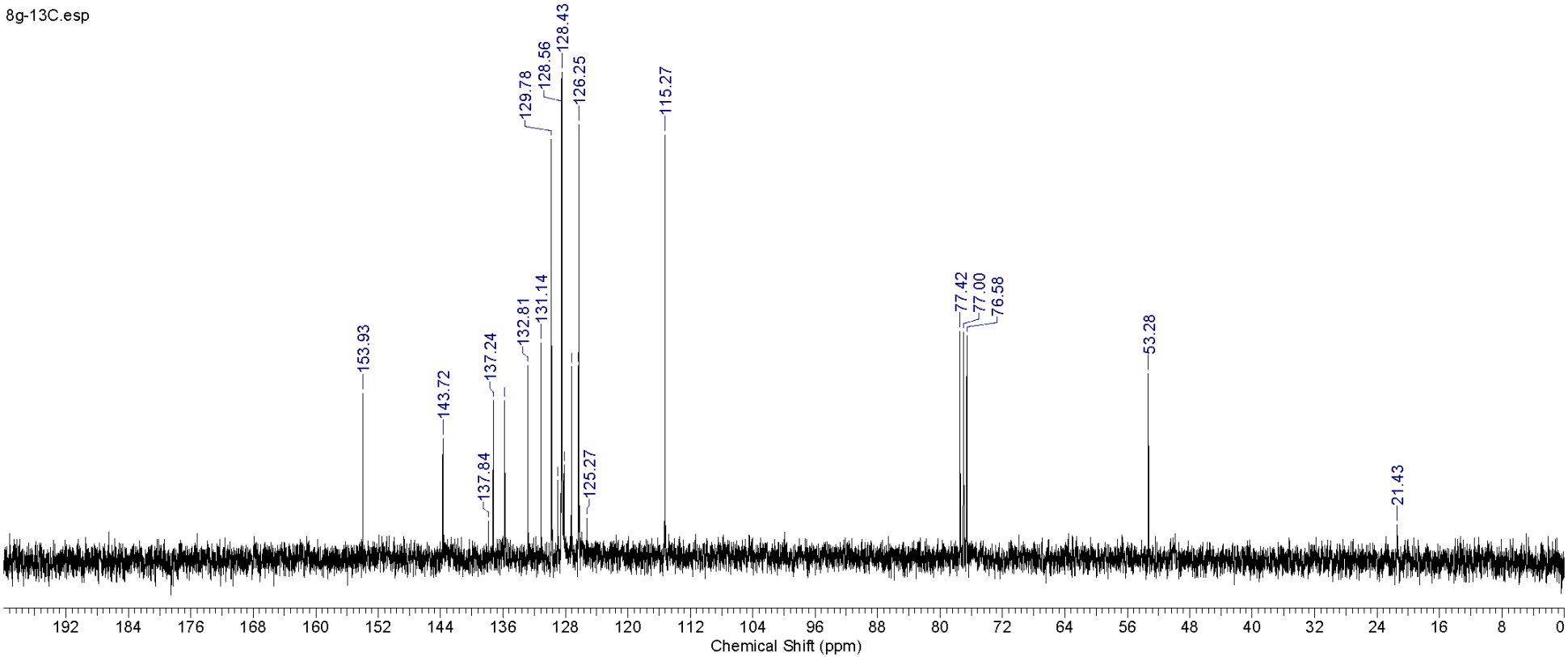


Formula $C_{21}H_{18}O$	FW	286.3670

Acquisition Time (sec)	1.8150	**Comment**	CC65-13C	**Date**	Feb 9 2011	**Date Stamp**	Feb 9 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC65-13C.fid\fid			**Frequency (MHz)**	75.46	**Nucleus**	13C	**Number of Transients**	108
Original Points Count	34053	**Points Count**	65536	**Pulse Sequence**	s2pul	**Receiver Gain**	30.00		
Solvent	CHLOROFORM-d			**Spectrum Offset (Hz)**	7537.3662	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	18761.73
Temperature (degree C)	AMBIENT TEMPERATURE								

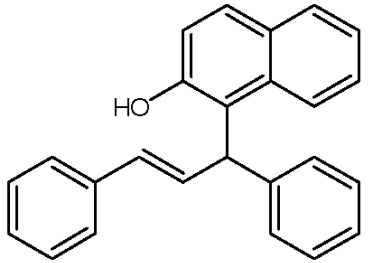


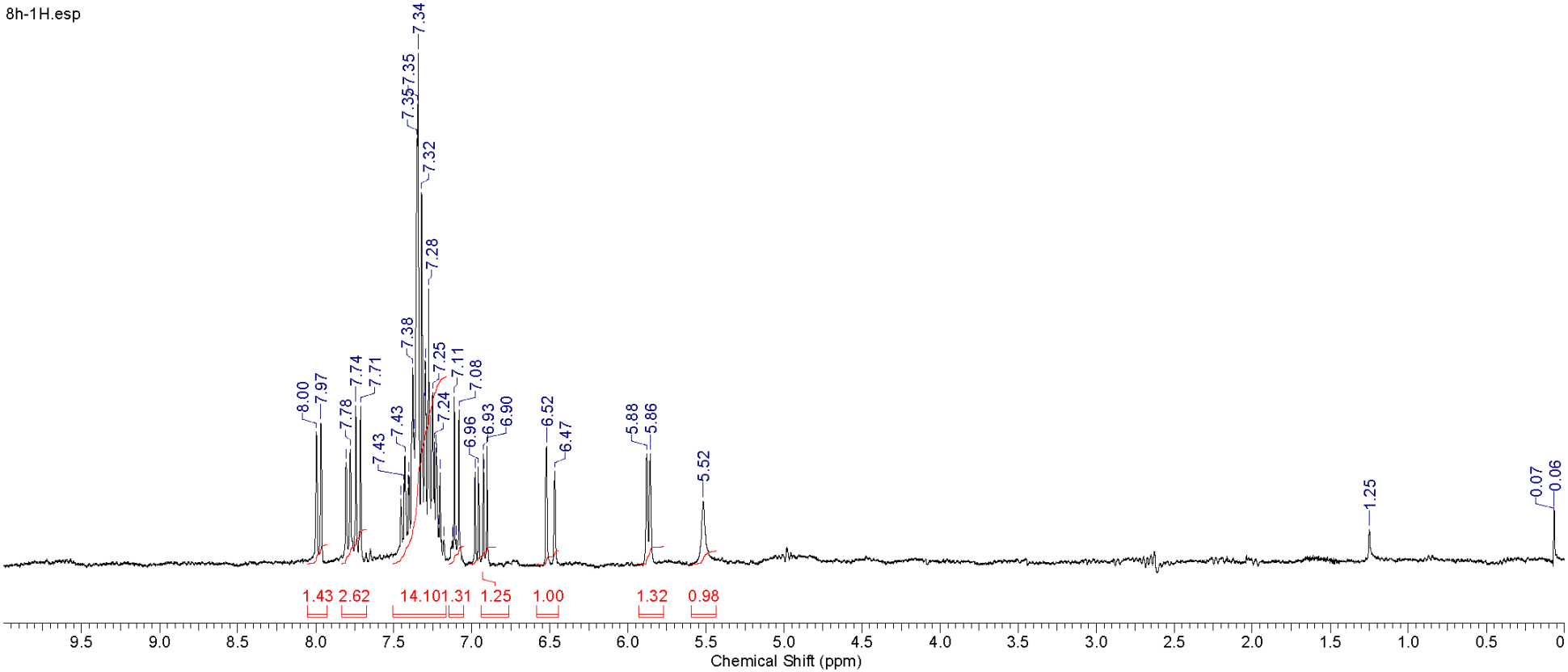
8g-13C.esp



Formula $C_{25}H_{20}O$	FW	336.4257

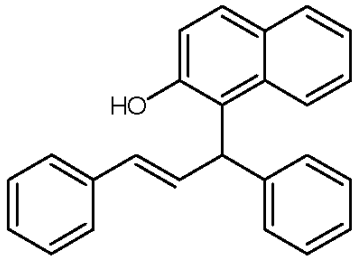
Acquisition Time (sec)	2.0000	*Comment*	CC64-1H	*Date*	Feb 7 2011	*Date Stamp*	Feb 7 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC64-1H.fid\fid			*Frequency (MHz)*	300.08	*Nucleus*	1H	*Number of Transients*	1
Original Points Count	9600	*Points Count*	16384	*Pulse Sequence*	s2pul	*Receiver Gain*	14.00	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	1494.7594	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	4800.00	*Temperature (degree C)*	AMBIENT TEMPERATURE		

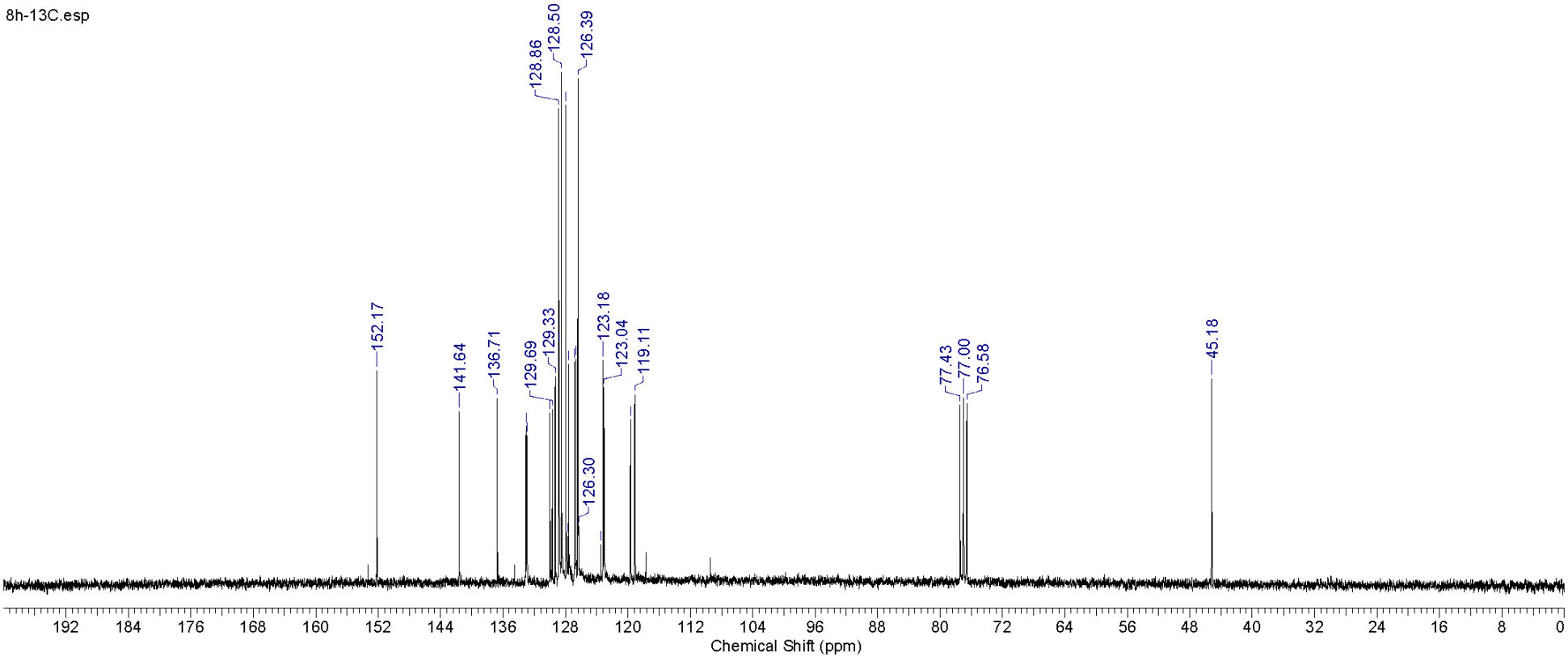




Formula $C_{25}H_{20}O$	FW	336.4257

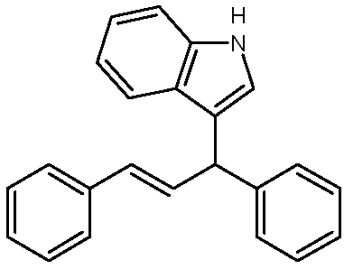
Acquisition Time (sec)	1.8150	**Comment**	CC64-13C	**Date**	Feb 7 2011	**Date Stamp**	Feb 7 2011
File Name	C:\Users\User\Desktop\adam\CCclean\CC64-13C.fid\fid			**Frequency (MHz)**	75.46	**Nucleus**	13C
Original Points Count	34053	**Points Count**	65536	**Pulse Sequence**	s2pul	**Receiver Gain**	28.00
Solvent	CHLOROFORM-d			**Spectrum Offset (Hz)**	7531.0684	**Spectrum Type**	STANDARD
Sweep Width (Hz)	18761.73	**Temperature (degree C)**	AMBIENT TEMPERATURE				

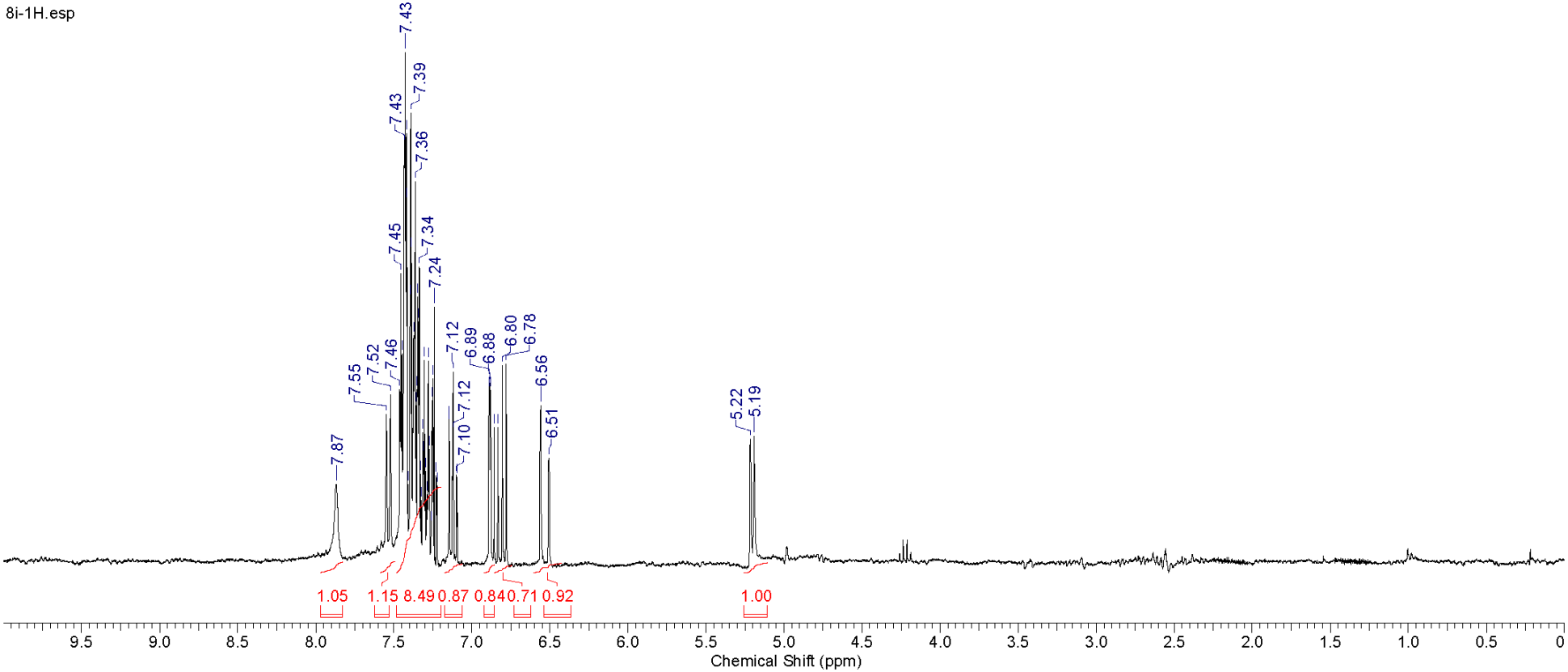




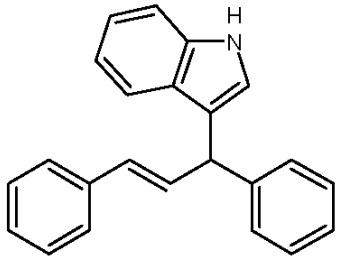
Formula $C_{23}H_{19}N$	FW	309.4037

Acquisition Time (sec)	2.0000	*Comment*	CC66-1H	*Date*	Feb 9 2011	*Date Stamp*	Feb 9 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC66-1H.fid\fid			*Frequency (MHz)*	300.08	*Nucleus*	1H	*Number of Transients*	1
Original Points Count	9600	*Points Count*	16384	*Pulse Sequence*	s2pul	*Receiver Gain*	13.00	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	1495.6384	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	4800.00	*Temperature (degree C)*	AMBIENT TEMPERATURE		

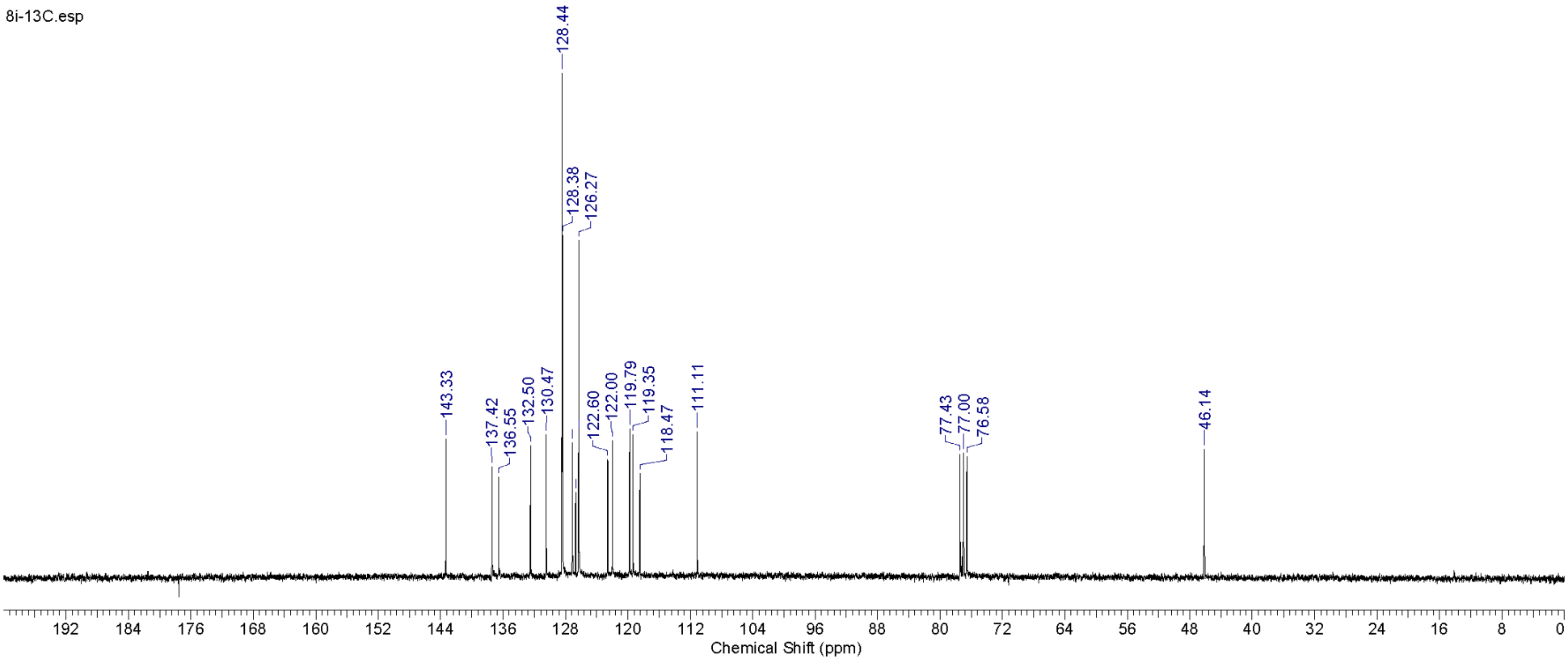




Formula $C_{23}H_{19}N$	***FW***	309.4037							
Acquisition Time (sec)	1.8150	***Comment***	CC66-13C	***Date***	Feb 9 2011	***Date Stamp***	Feb 9 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC66-13C.fid\fid			***Frequency (MHz)***	75.46	***Nucleus***	13C	***Number of Transients***	816
Original Points Count	34053	***Points Count***	65536	***Pulse Sequence***	s2pul	***Receiver Gain***	30.00		
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	7532.2134	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	18761.73
Temperature (degree C)	AMBIENT TEMPERATURE								

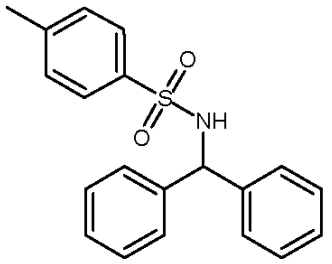


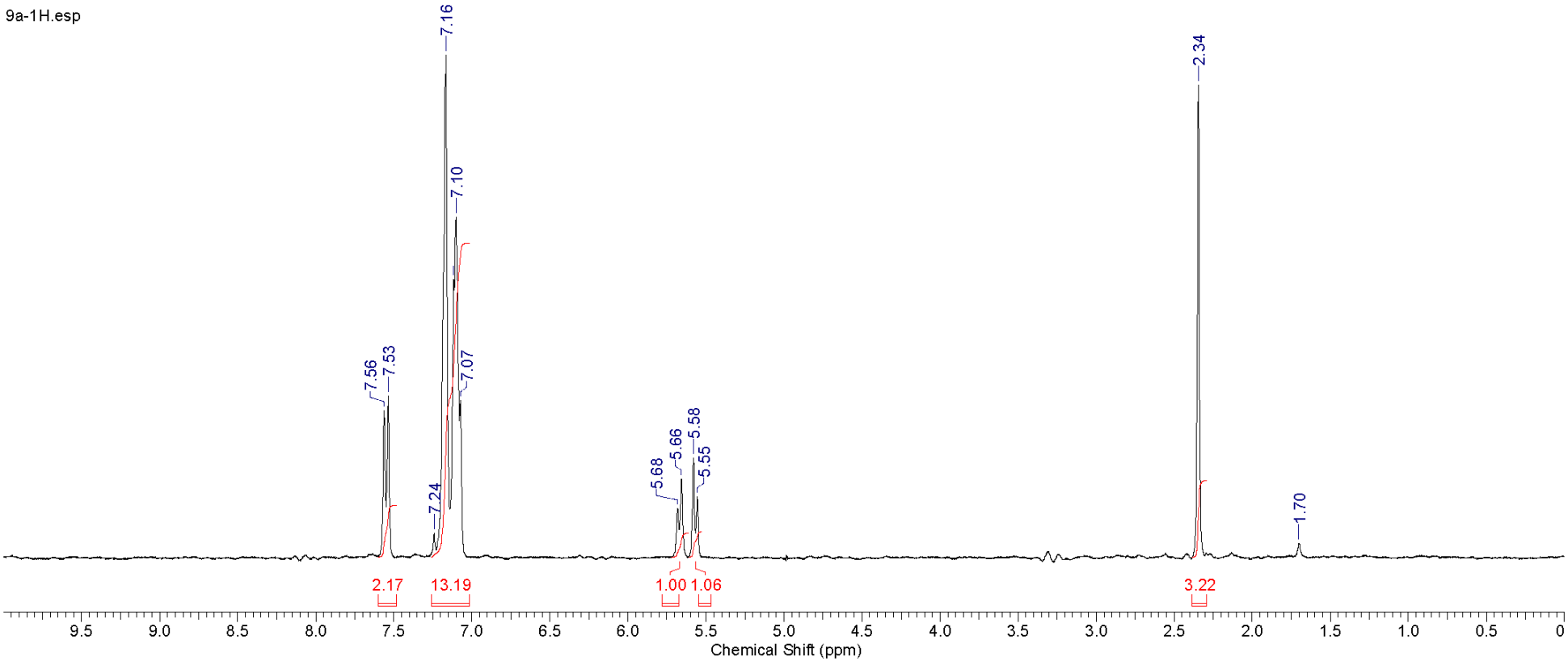
8i-13C.esp



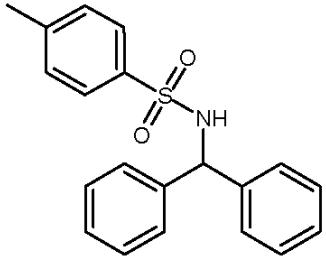
Formula $C_{20}H_{19}NO_2S$	FW	337.4354

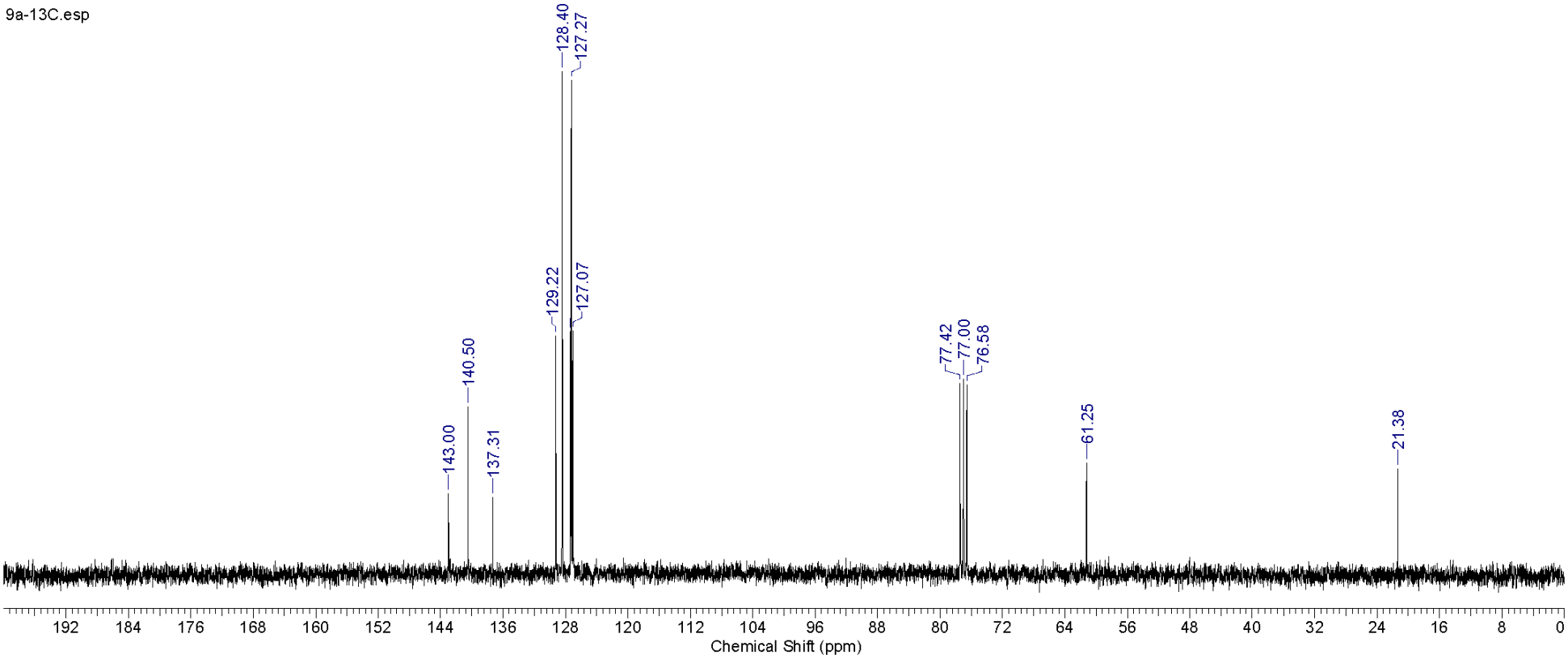
Acquisition Time (sec)	2.0000	**Comment**	CC180-1H	**Date**	Nov 8 2011	**Date Stamp**	Nov 8 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC180-1H.fid\fid			**Frequency (MHz)**	300.08	**Nucleus**	1H	**Number of Transients**	4
Original Points Count	9600	**Points Count**	16384	**Pulse Sequence**	s2pul	**Receiver Gain**	11.00	**Solvent**	CHLOROFORM-d
Spectrum Offset (Hz)	1495.6384	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	4800.00	**Temperature (degree C)**	AMBIENT TEMPERATURE		





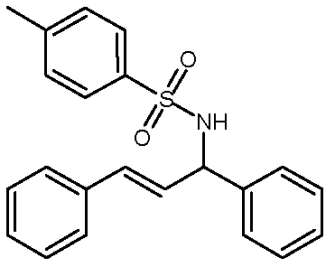
Formula $C_{20}H_{19}NO_2S$	***FW***	337.4354							
Acquisition Time (sec)	1.8150	***Comment***	CC18-13C	***Date***	Nov 8 2011	***Date Stamp***	Nov 8 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC180-13C.fid\fid			***Frequency (MHz)***	75.46	***Nucleus***	13C	***Number of Transients***	108
Original Points Count	34053	***Points Count***	65536	***Pulse Sequence***	s2pul	***Receiver Gain***	30.00		
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	7537.6597	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	18761.73
Temperature (degree C)	AMBIENT TEMPERATURE								



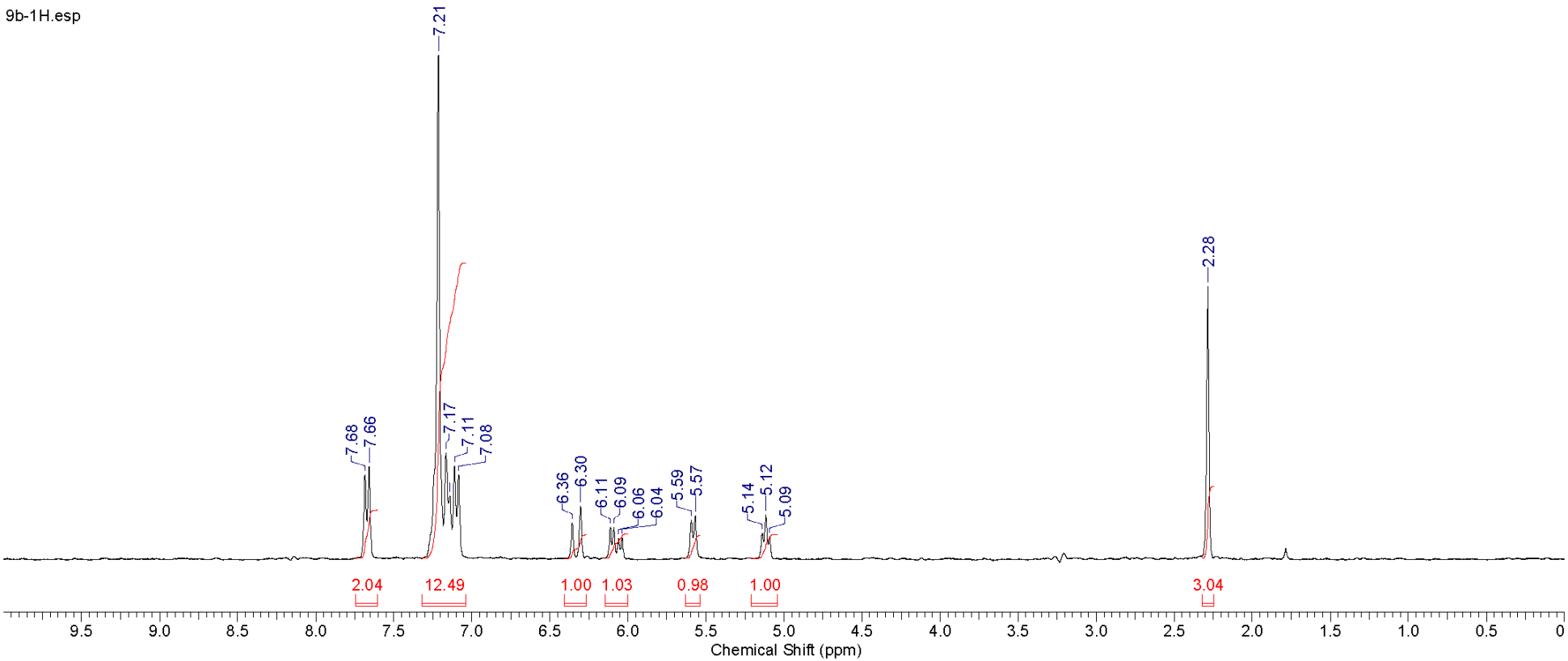


Formula $C_{22}H_{21}NO_2S$	FW	363.4726

Acquisition Time (sec)	2.0000	**Comment**	CC181-1H	**Date**	Nov 8 2011	**Date Stamp**	Nov 8 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC181-1H.fid\fid			**Frequency (MHz)**	300.08	**Nucleus**	1H	**Number of Transients**	4
Original Points Count	9600	**Points Count**	16384	**Pulse Sequence**	s2pul	**Receiver Gain**	10.00	**Solvent**	CHLOROFORM-d
Spectrum Offset (Hz)	1494.8887	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	4800.00	**Temperature (degree C)**	AMBIENT TEMPERATURE		

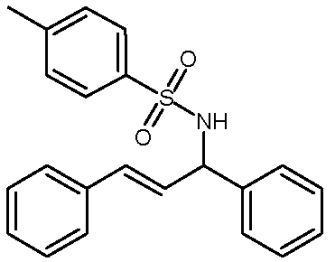


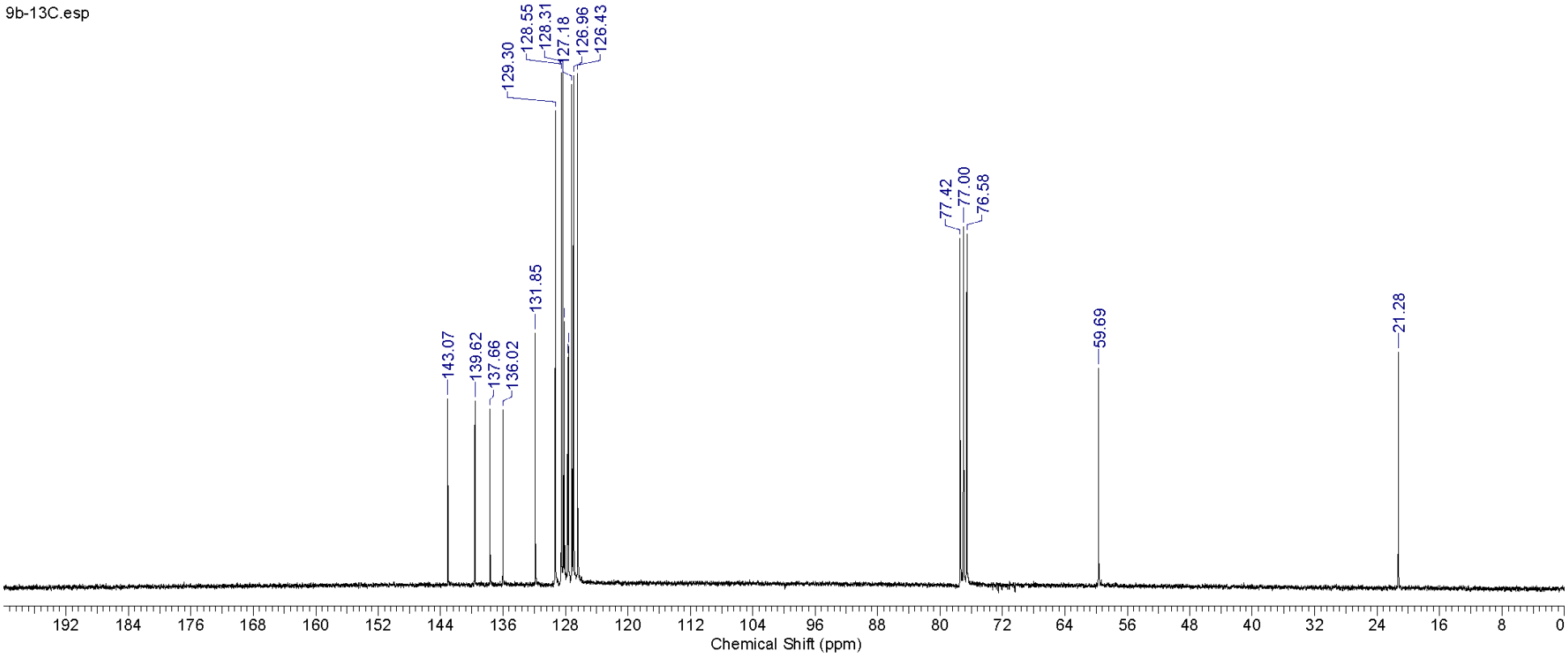
9b-1H.esp



Formula $C_{22}H_{21}NO_2S$	FW	363.4726

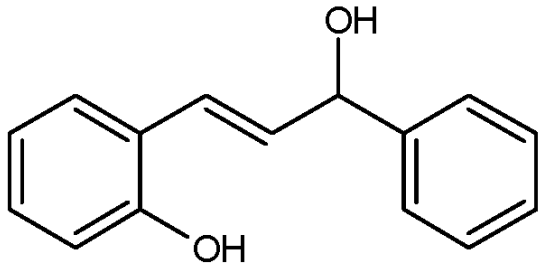
Acquisition Time (sec)	1.8150	**Comment**	CC181-13C	**Date**	Nov 8 2011	**Date Stamp**	Nov 8 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC181-13C.fid\fid			**Frequency (MHz)**	75.46	**Nucleus**	13C	**Number of Transients**	6964
Original Points Count	34053	**Points Count**	65536	**Pulse Sequence**	s2pul	**Receiver Gain**	30.00		
Solvent	CHLOROFORM-d			**Spectrum Offset (Hz)**	7535.0762	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	18761.73
Temperature (degree C)	AMBIENT TEMPERATURE								

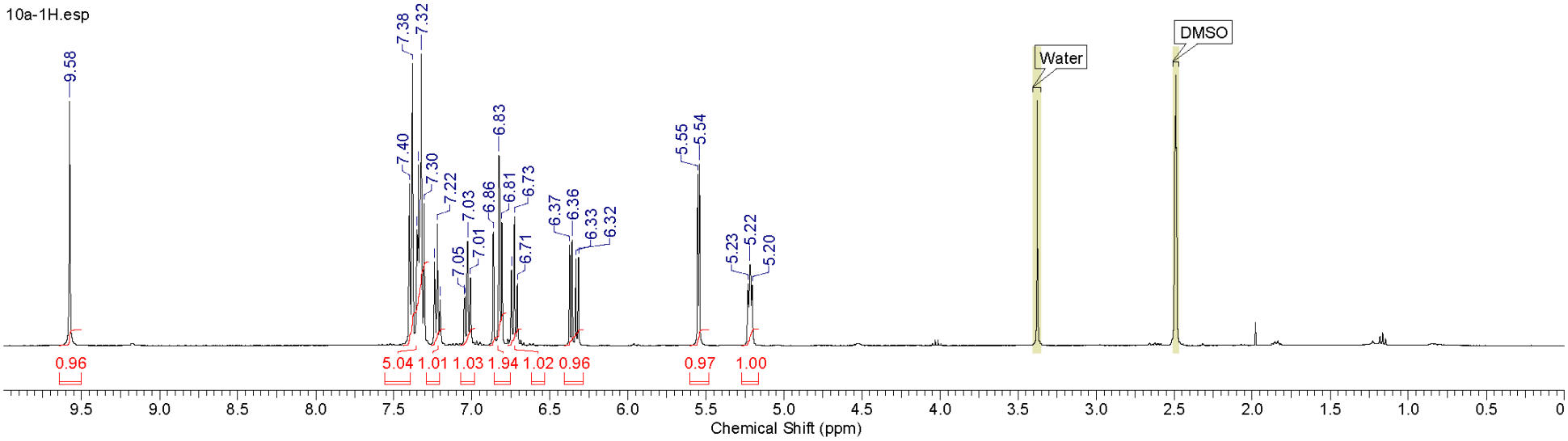




Formula $C_{15}H_{14}O_2$	FW	226.2705

Acquisition Time (sec)	3.9846	**Comment**	CC92-1H-DMSO			**Date**	20 Oct 2010 16:53:52
Date Stamp	20 Oct 2010 16:53:52			**File Name**	C:\Users\User\Desktop\adam\nmr\CC92\7\fid	**Frequency (MHz)**	400.17
Nucleus	1H	**Number of Transients**	16	**Origin**	spect	**Original Points Count**	32768	**Owner**	nmrsu
Points Count	32768	**Pulse Sequence**	zg30	**Receiver Gain**	64.00	**SW(cyclical) (Hz)**	8223.68	**Solvent**	DMSO-d6
Spectrum Offset (Hz)	2465.7646	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	8223.43	**Temperature (degree C)**	24.500		

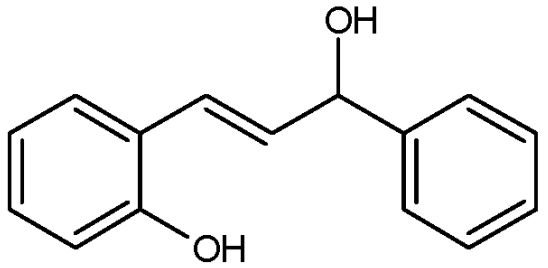




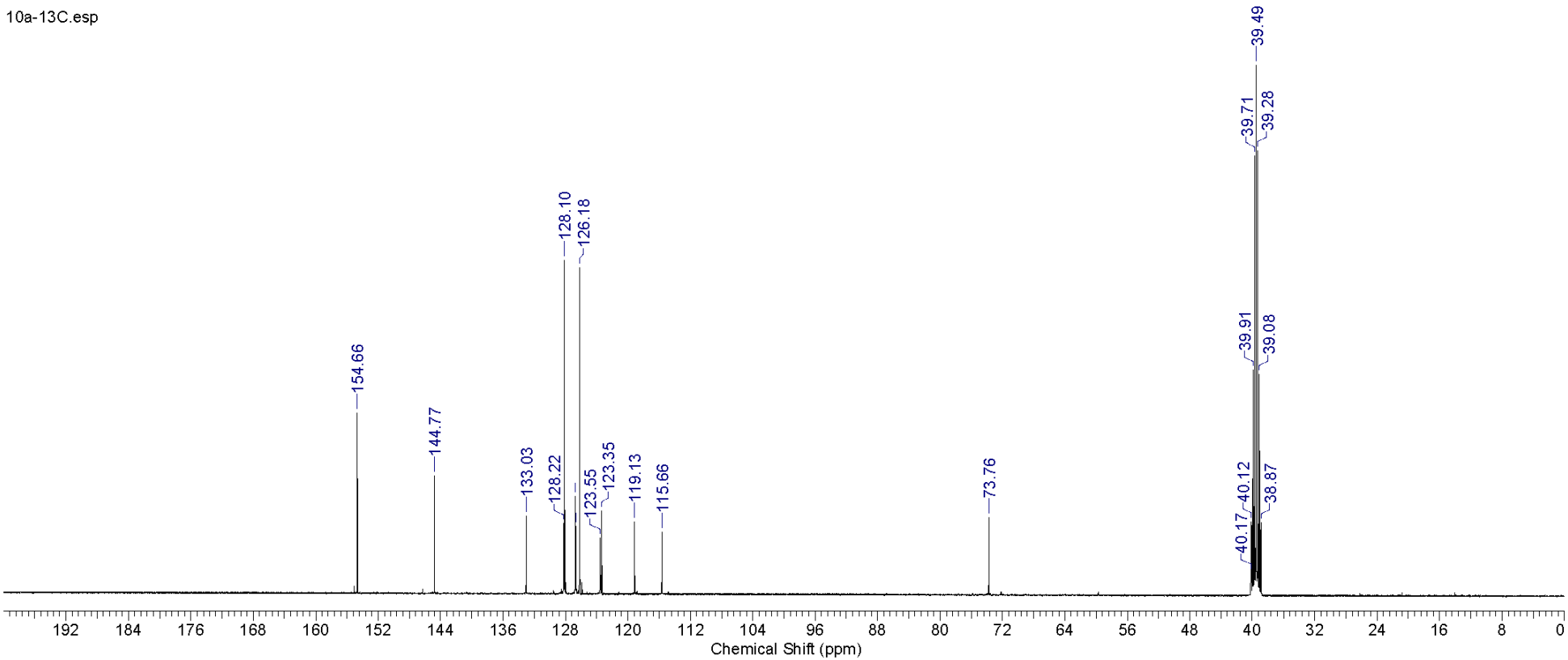
No.	(ppm)	Annotation	Layer No.	Created By	Created At	Modified By	Modified At
1	[2.47 .. 2.51]	DMSO	1	User	Fri 2012/03/23 03:13:33 PM		
2	[3.36 .. 3.40]	Water	1	User	Fri 2012/03/23 03:13:33 PM		

Formula $C_{15}H_{14}O_2$	FW	226.2705

Acquisition Time (sec)	1.3631	**Comment**	5 mm PABBO BB-1H/D Z-GRD Z108618/0217			**Date**	20 Oct 2010 23:00:48
Date Stamp	20 Oct 2010 23:00:48			**File Name**	C:\Users\User\Desktop\adam\nmr\CC92\8\fid	**Frequency (MHz)**	100.62
Nucleus	13C	**Number of Transients**	5500	**Origin**	spect	**Original Points Count**	32768	**Owner**	nmrsu
Points Count	32768	**Pulse Sequence**	zgig30	**Receiver Gain**	101.00	**SW(cyclical) (Hz)**	24038.46	**Solvent**	DMSO-d6
Spectrum Offset (Hz)	10013.3662	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	24037.73	**Temperature (degree C)**	23.400		

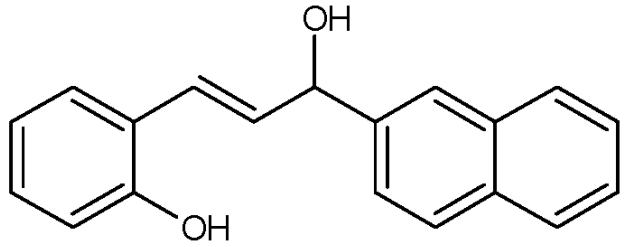


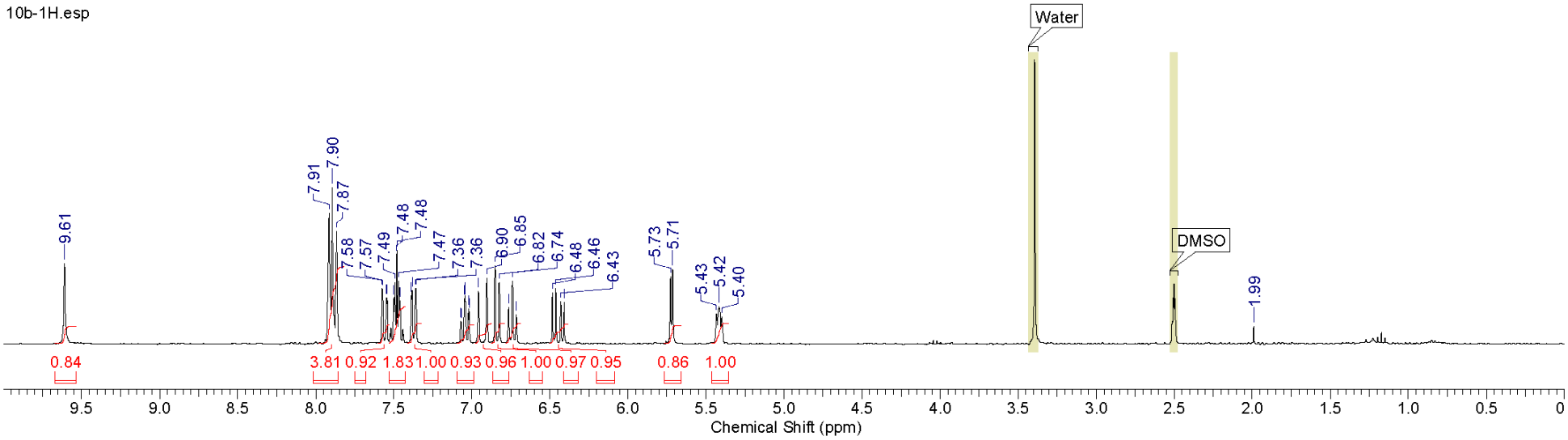
10a-13C.esp



Formula $C_{19}H_{16}O_2$	FW	276.3291

Acquisition Time (sec)	2.0000	**Comment**	CC109-1H-DMSO			**Date**	Feb 28 2011	**Date Stamp**	Feb 28 2011
File Name	C:\Users\User\Desktop\adam\CCclean\CC109-1H-DMSO.fid\fid					**Frequency (MHz)**	300.08	**Nucleus**	1H
Number of Transients	8	**Original Points Count**	9600	**Points Count**	16384	**Pulse Sequence**	s2pul	**Receiver Gain**	2.00
Solvent	DMSO-d6	**Spectrum Offset (Hz)**	1505.6711	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	4800.00		
Temperature (degree C)	AMBIENT TEMPERATURE								

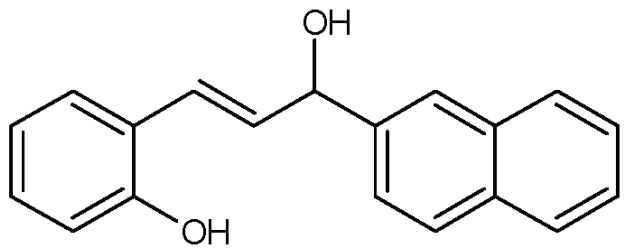




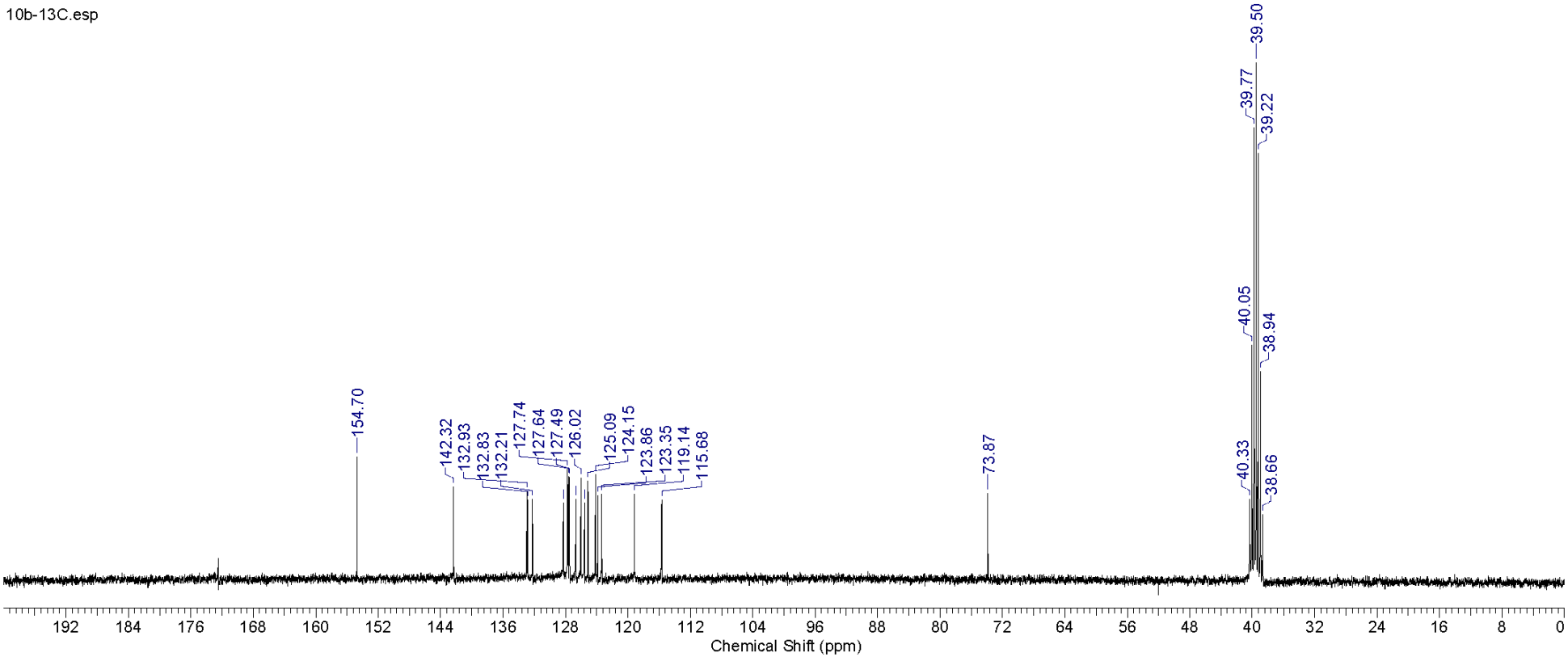
No.	(ppm)	Annotation	Layer No.	Created By	Created At	Modified By	Modified At
1	[2.48 .. 2.53]	DMSO	1	User	Sun 2012/03/11 11:49:29 AM		
2	[3.37 .. 3.43]	Water	1	User	Sun 2012/03/11 11:49:29 AM		

Formula $C_{19}H_{16}O_2$	FW	276.3291

Acquisition Time (sec)	1.8150	**Comment**	CC109-13C-DMSO			**Date**	Feb 28 2011
Date Stamp	Feb 28 2011	**File Name**	C:\Users\User\Desktop\adam\CCclean\CC109-13C-DMSO.fid\fid				
Frequency (MHz)	75.46	**Nucleus**	13C	**Number of Transients**	1464	**Original Points Count**	34053
Points Count	65536	**Pulse Sequence**	s2pul	**Receiver Gain**	29.00	**Solvent**	DMSO-d6
Spectrum Offset (Hz)	7510.5420	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	18761.73	**Temperature (degree C)**	AMBIENT TEMPERATURE

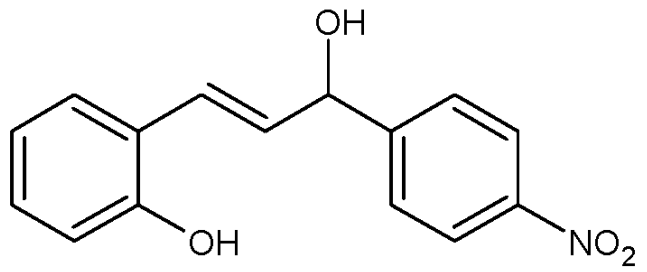


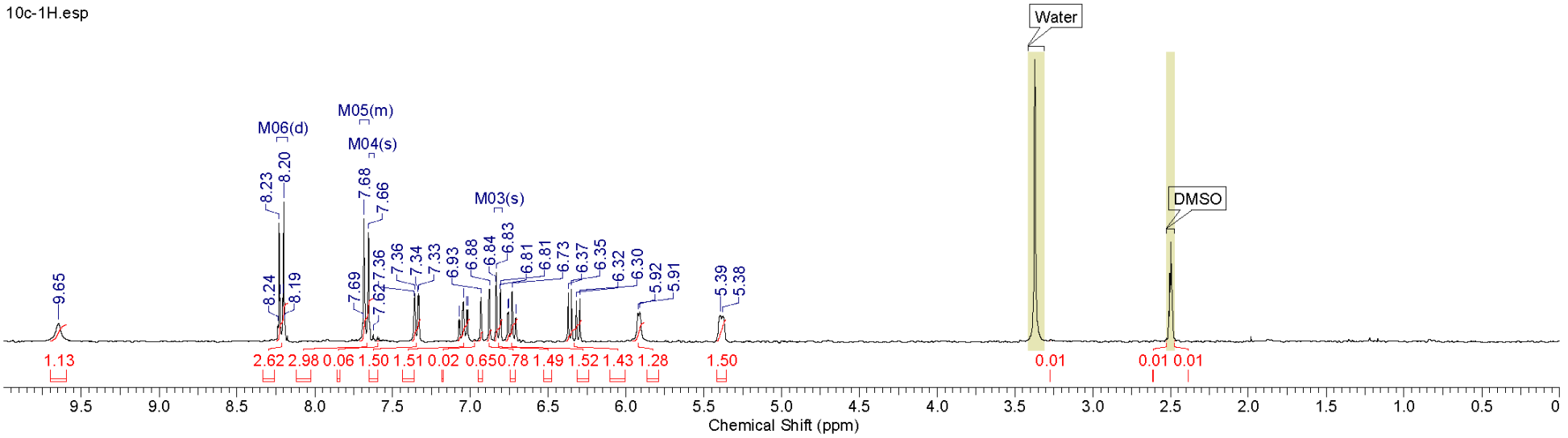
10b-13C.esp



Formula $C_{15}H_{13}NO_4$	FW	271.2680

Acquisition Time (sec)	2.0000	**Comment**	CC107-1H	**Date**	Mar 8 2011	**Date Stamp**	Mar 8 2011		
File Name	C:\Users\User\Documents\PhD\PhD NMR data\CCclean\CC107-1H.fid\fid					**Frequency (MHz)**	300.08	**Nucleus**	1H
Number of Transients	4	**Original Points Count**	9600	**Points Count**	131072	**Pulse Sequence**	s2pul	**Receiver Gain**	4.00
Solvent	DMSO-d6	**Spectrum Offset (Hz)**	1505.0852	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	4800.00		
Temperature (degree C)	AMBIENT TEMPERATURE								

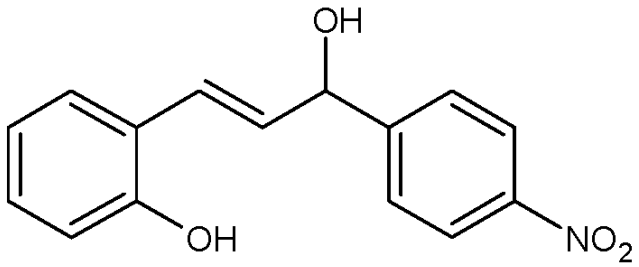




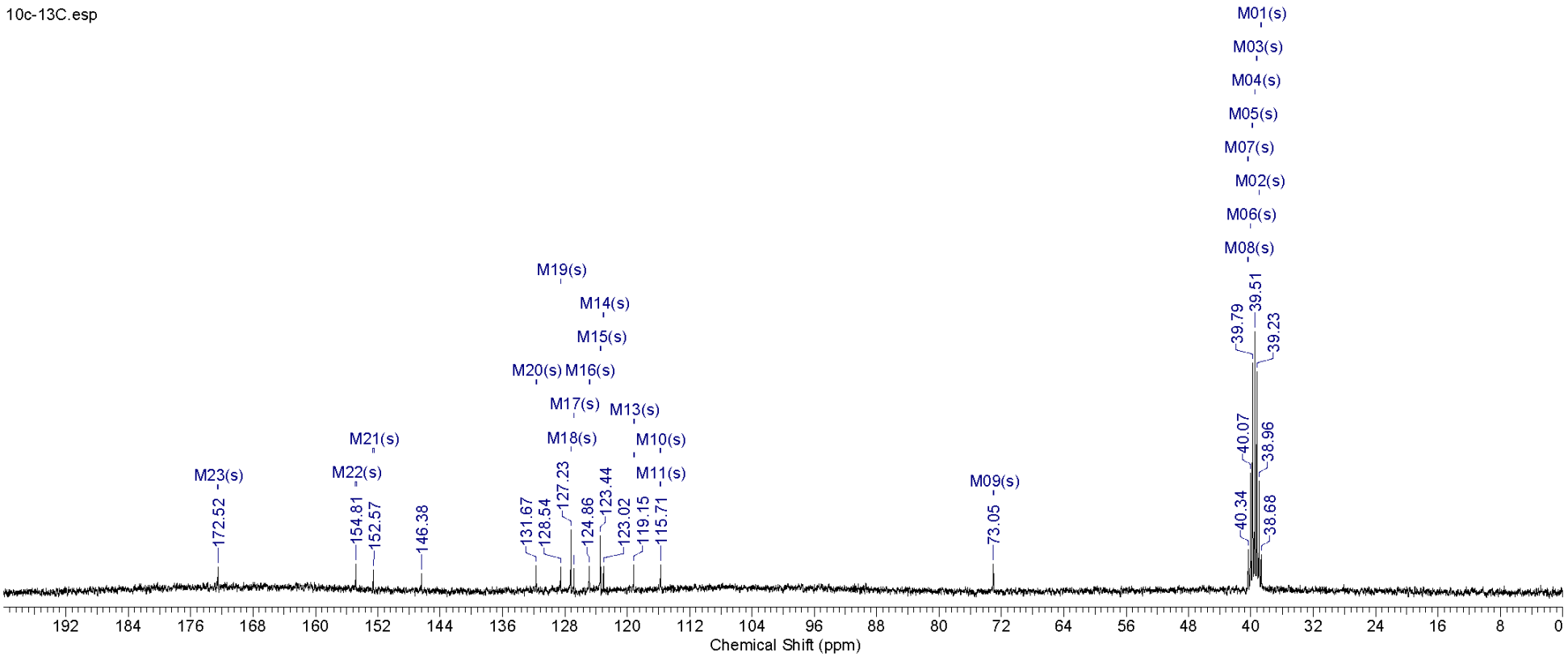
No.	(ppm)	Annotation	Layer No.	Created By	Created At	Modified By	Modified At
1	[2.48 .. 2.52]	DMSO	1	User	Thu 2017/02/09 08:37:14 PM		
2	[3.31 .. 3.42]	Water	1	User	Thu 2017/02/09 08:37:14 PM		

Formula $C_{15}H_{13}NO_4$	FW	271.2680

Acquisition Time (sec)	1.8150	**Comment**	CC107-13C	**Date**	Mar 8 2011	**Date Stamp**	Mar 8 2011
File Name	C:\Users\User\Documents\PhD\PhD NMR data\CCclean\CC107-13C.fid\fid					**Frequency (MHz)**	75.46
Nucleus	13C	**Number of Transients**	356	**Original Points Count**	34053	**Points Count**	65536
Pulse Sequence	s2pul	**Receiver Gain**	33.00	**Solvent**	DMSO-d6	**Spectrum Offset (Hz)**	7511.8789
Spectrum Type	STANDARD	**Sweep Width (Hz)**	18761.73	**Temperature (degree C)**	AMBIENT TEMPERATURE		

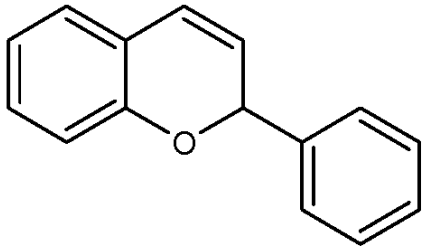


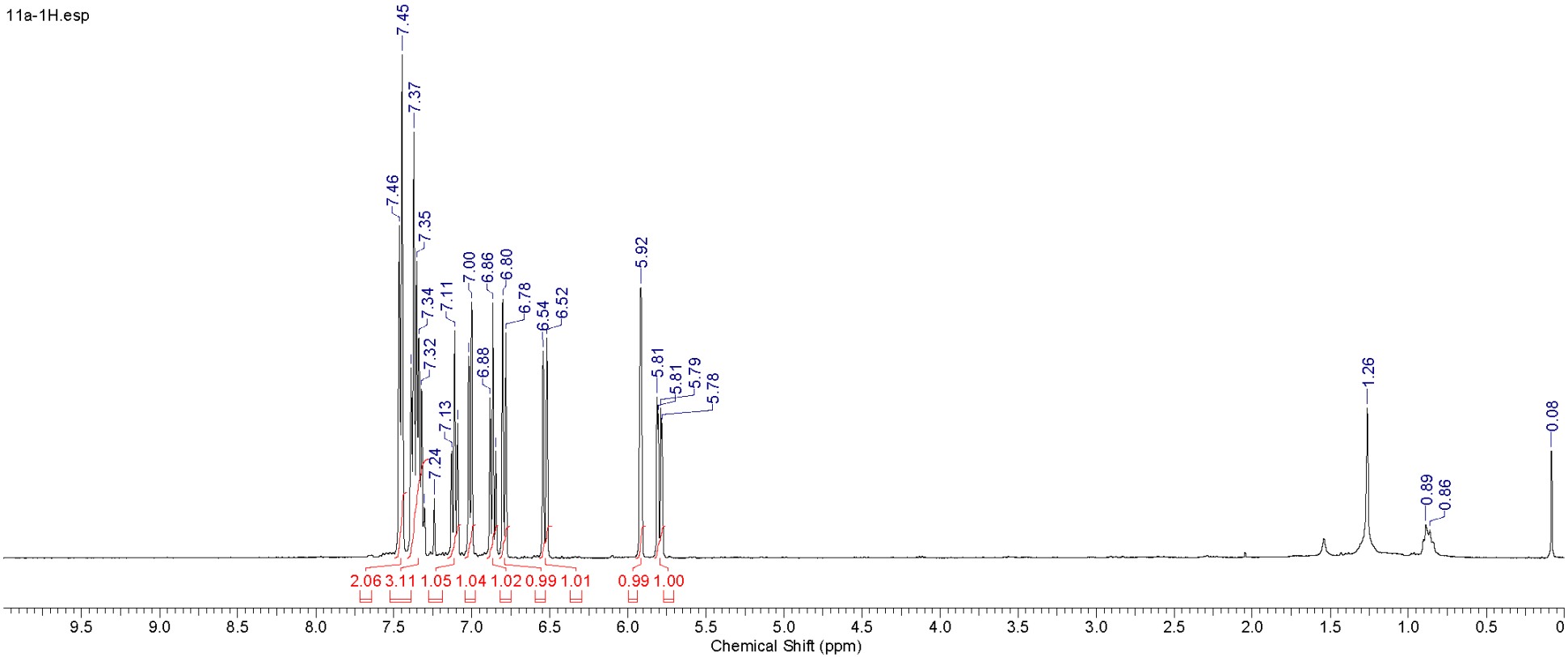
10c-13C.esp



Formula $C_{15}H_{12}O$	FW	208.2552

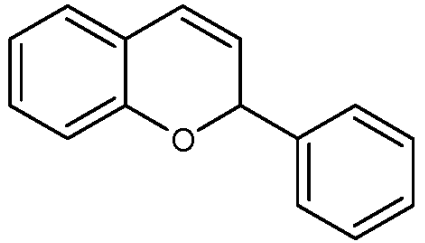
Acquisition Time (sec)	3.9846	**Comment**	CC97d-1H	**Date**	14 Sep 2010 08:49:36			**Date Stamp**	14 Sep 2010 08:49:36
File Name	C:\Users\User\Desktop\adam\nmr\CC97d\1\fid			**Frequency (MHz)**	400.17	**Nucleus**	1H	**Number of Transients**	16
Origin	spect	**Original Points Count**	32768	**Owner**	nmrsu	**Points Count**	32768	**Pulse Sequence**	zg30
Receiver Gain	80.60	**SW(cyclical) (Hz)**	8223.68	**Solvent**	CHLOROFORM-d			**Spectrum Offset (Hz)**	2454.8315
Spectrum Type	STANDARD	**Sweep Width (Hz)**	8223.43	**Temperature (degree C)**	20.500				

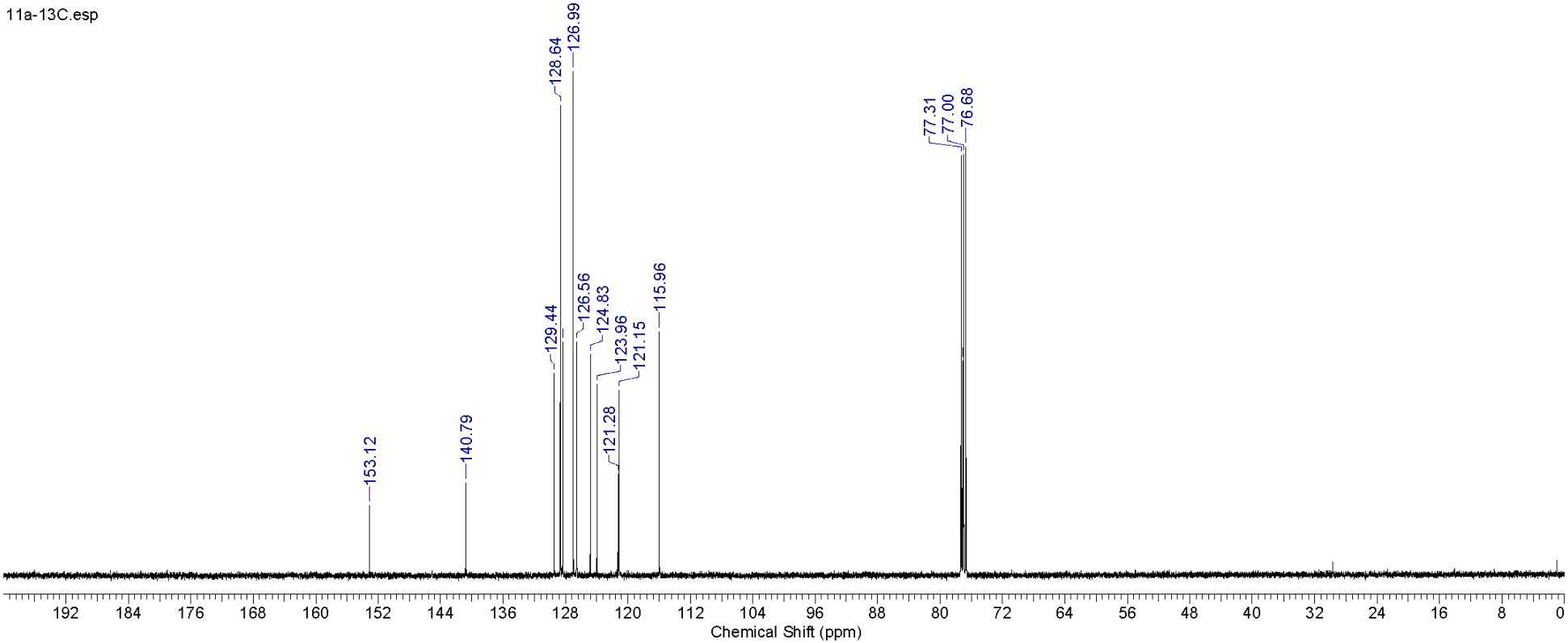




Formula $C_{15}H_{12}O$	FW	208.2552

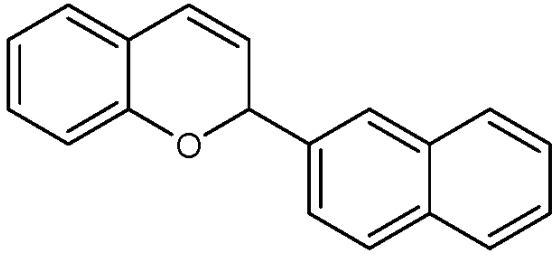
Acquisition Time (sec)	1.3631	**Comment**	CC97d-13C	**Date**	14 Sep 2010 09:13:04			**Date Stamp**	14 Sep 2010 09:13:04
File Name	C:\Users\User\Desktop\adam\nmr\CC97d\2\fid			**Frequency (MHz)**	100.62	**Nucleus**	13C	**Number of Transients**	384
Origin	spect	**Original Points Count**	32768	**Owner**	nmrsu	**Points Count**	32768	**Pulse Sequence**	zgig30
Receiver Gain	114.00	**SW(cyclical) (Hz)**	24038.46	**Solvent**	CHLOROFORM-d			**Spectrum Offset (Hz)**	10054.7500
Spectrum Type	STANDARD	**Sweep Width (Hz)**	24037.73	**Temperature (degree C)**	21.000				

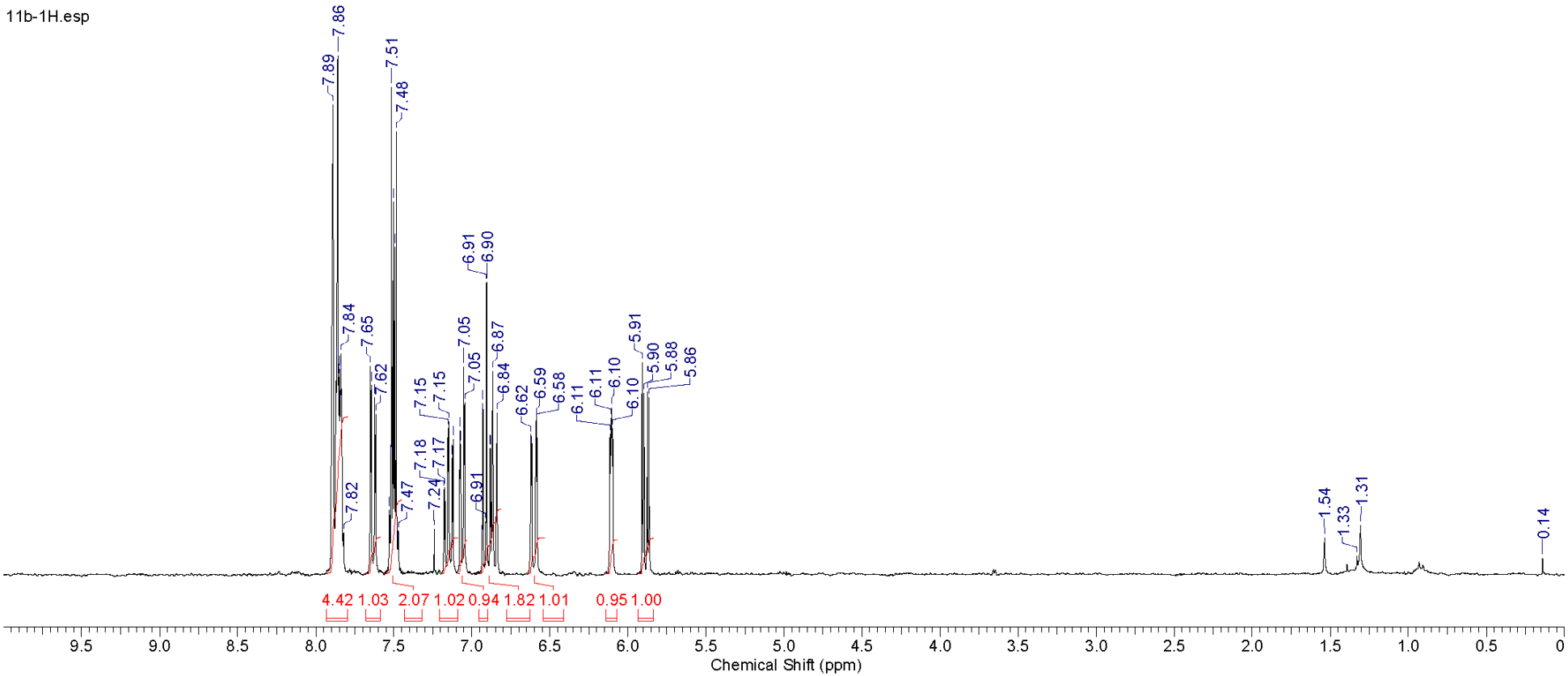




Formula $C_{19}H_{14}O$	FW	258.3139

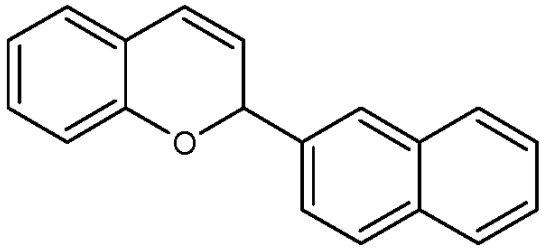
Acquisition Time (sec)	2.0000	**Comment**	CC110-1H	**Date**	Mar 2 2011	**Date Stamp**	Mar 2 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC110-1H.fid\fid			**Frequency (MHz)**	300.08	**Nucleus**	1H	**Number of Transients**	6
Original Points Count	9600	**Points Count**	16384	**Pulse Sequence**	s2pul	**Receiver Gain**	2.00	**Solvent**	CHLOROFORM-d
Spectrum Offset (Hz)	1495.0524	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	4800.00	**Temperature (degree C)**	AMBIENT TEMPERATURE		

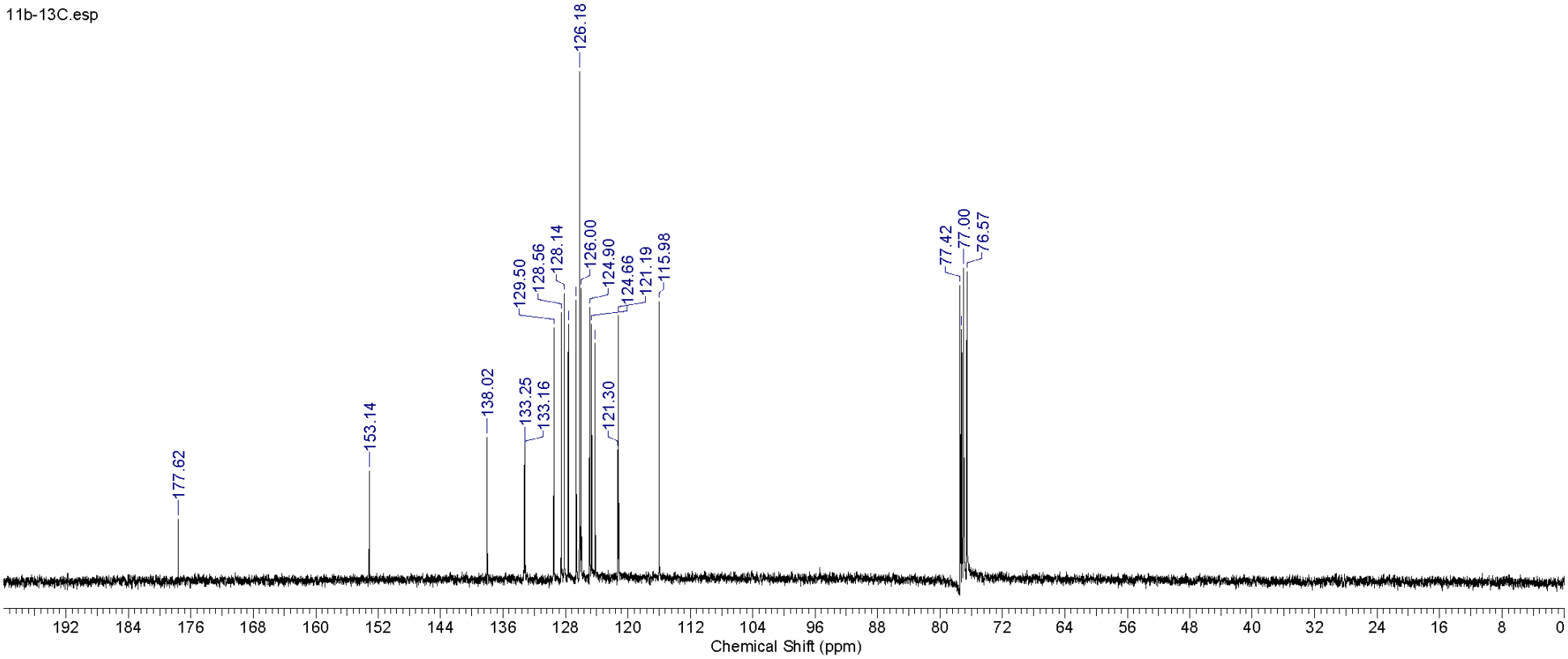




Formula $C_{19}H_{14}O$	FW	258.3139

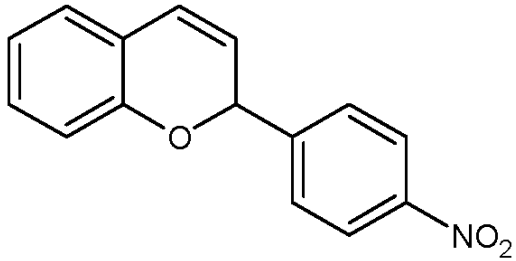
Acquisition Time (sec)	1.8150	*Comment*	CC110-13C	*Date*	Mar 2 2011	*Date Stamp*	Mar 2 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC110-13C.fid\fid			*Frequency (MHz)*	75.46	*Nucleus*	13C	*Number of Transients*	1344
Original Points Count	34053	*Points Count*	65536	*Pulse Sequence*	s2pul	*Receiver Gain*	30.00		
Solvent	CHLOROFORM-d			*Spectrum Offset (Hz)*	7538.5112	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	18761.73
Temperature (degree C)	AMBIENT TEMPERATURE								



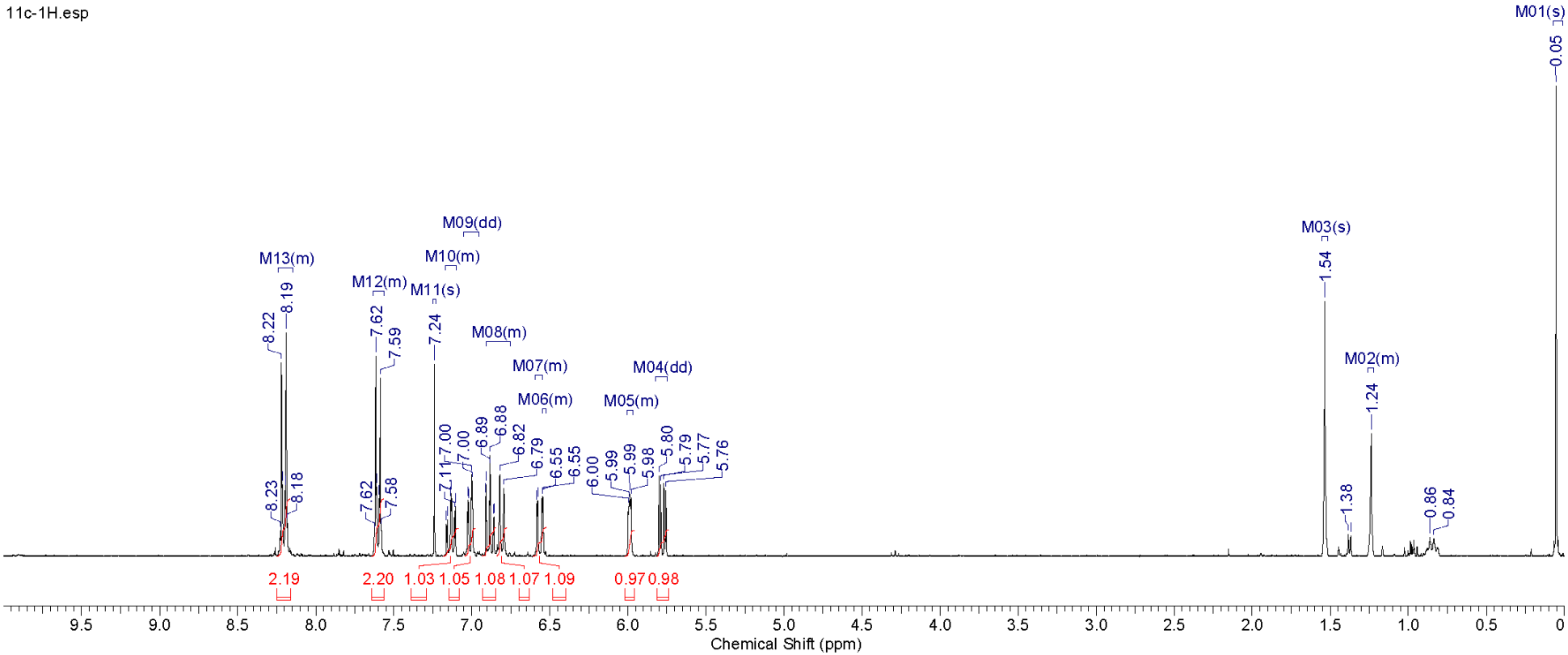


Formula $C_{15}H_{11}NO_3$	***FW***	253.2527	

Acquisition Time (sec)	2.0000	***Comment***	CC108-1H	***Date***	Mar 9 2011	***Date Stamp***	Mar 9 2011
File Name	C:\Users\User\Documents\PhD\PhD NMR data\CCclean\CC108-1H.fid\fid					***Frequency (MHz)***	300.08
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	9600	***Points Count***	131072
Pulse Sequence	s2pul	***Receiver Gain***	20.00	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	1495.0524	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4800.00	***Temperature (degree C)***	AMBIENT TEMPERATURE

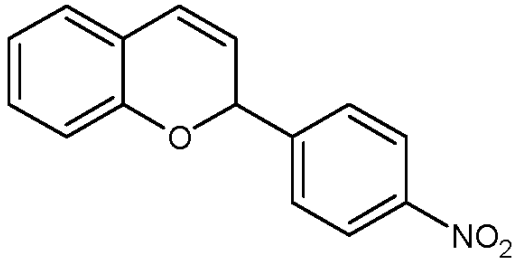


11c-1H.esp

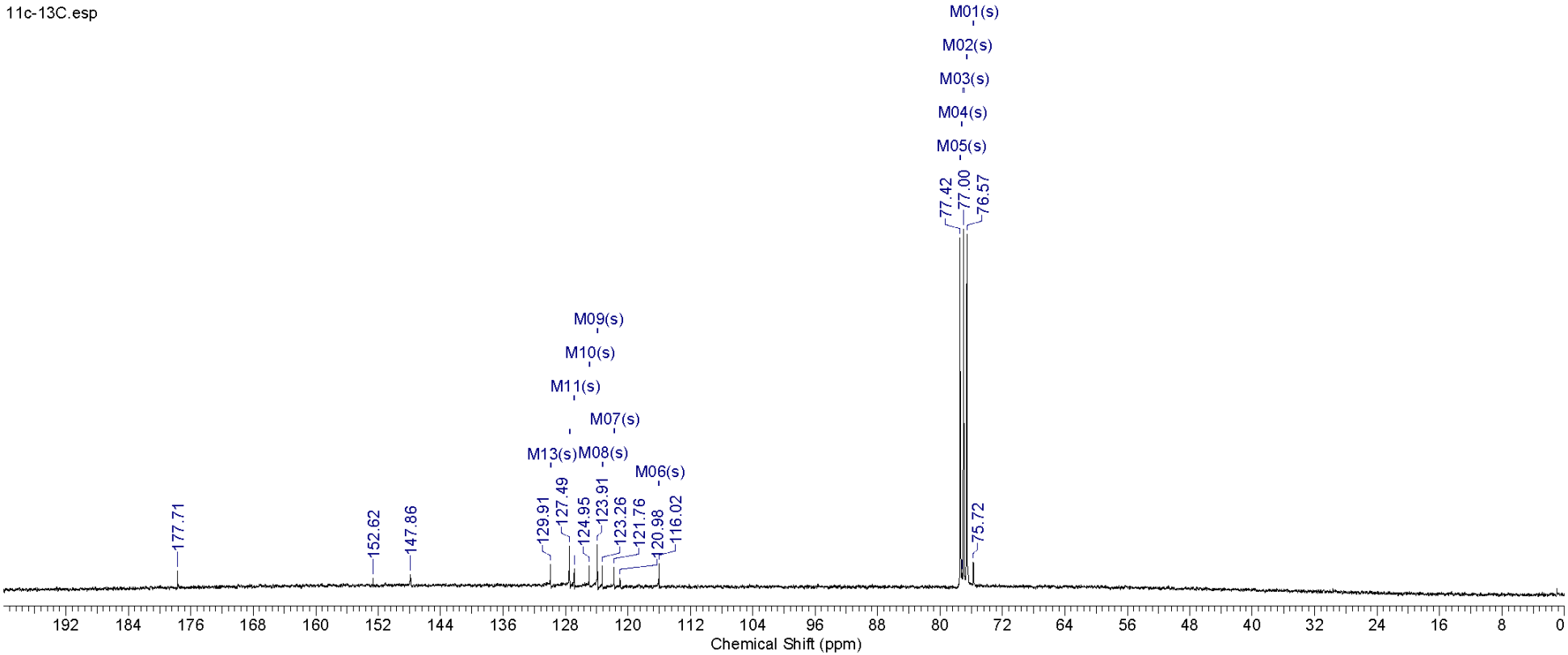


Formula $C_{15}H_{11}NO_3$	FW	253.2527

Acquisition Time (sec)	1.8150	**Comment**	CC108-13C	**Date**	Mar 9 2011	**Date Stamp**	Mar 9 2011
File Name	C:\Users\User\Documents\PhD\PhD NMR data\CCclean\CC108-13C.fid\fid					**Frequency (MHz)**	75.46
Nucleus	13C	**Number of Transients**	20688	**Original Points Count**	34053	**Points Count**	65536
Pulse Sequence	s2pul	**Receiver Gain**	30.00	**Solvent**	CHLOROFORM-d		
Spectrum Offset (Hz)	7545.6675	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	18761.73	**Temperature (degree C)**	AMBIENT TEMPERATURE

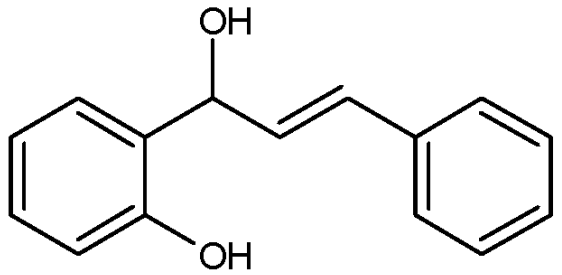


11c-13C.esp

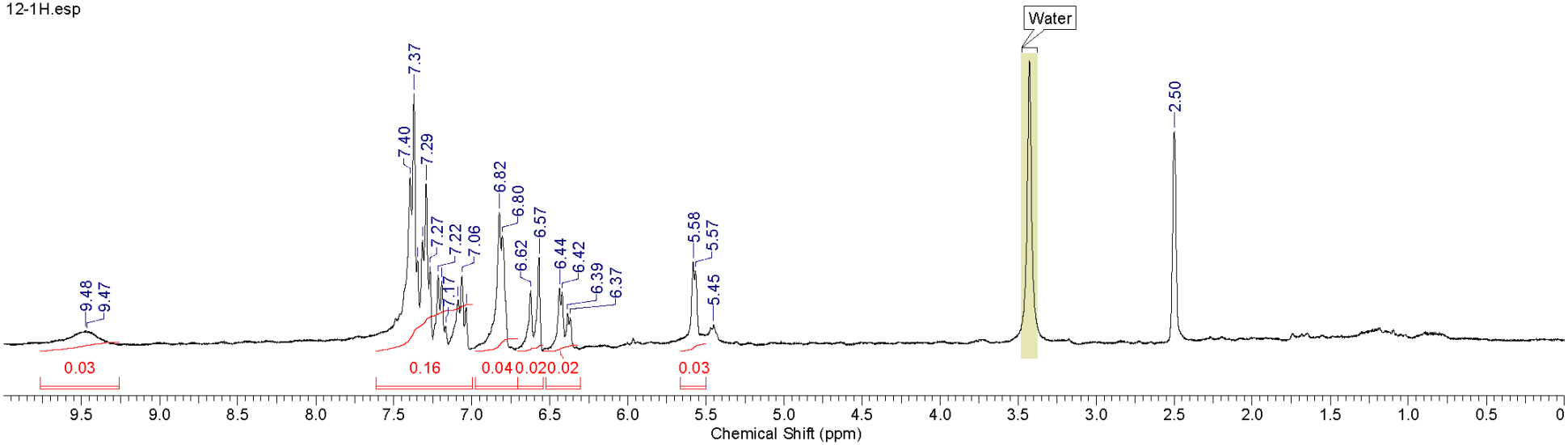


Formula $C_{15}H_{14}O_2$	FW	226.2705

Acquisition Time (sec)	2.0000	**Comment**	CC178-1H	**Date**	Sep 20 2011	**Date Stamp**	Sep 20 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC178-1H.fid\fid			**Frequency (MHz)**	300.08	**Nucleus**	1H	**Number of Transients**	4
Original Points Count	9600	**Points Count**	16384	**Pulse Sequence**	s2pul	**Receiver Gain**	13.00	**Solvent**	DMSO-d6
Spectrum Offset (Hz)	1505.9641	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	4800.00	**Temperature (degree C)**	AMBIENT TEMPERATURE		



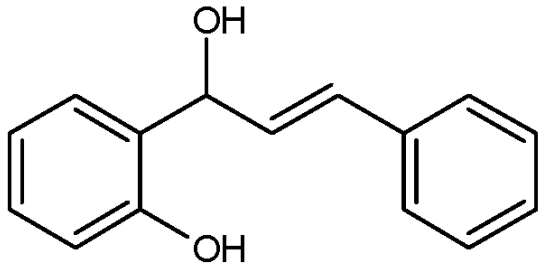
12-1H.esp



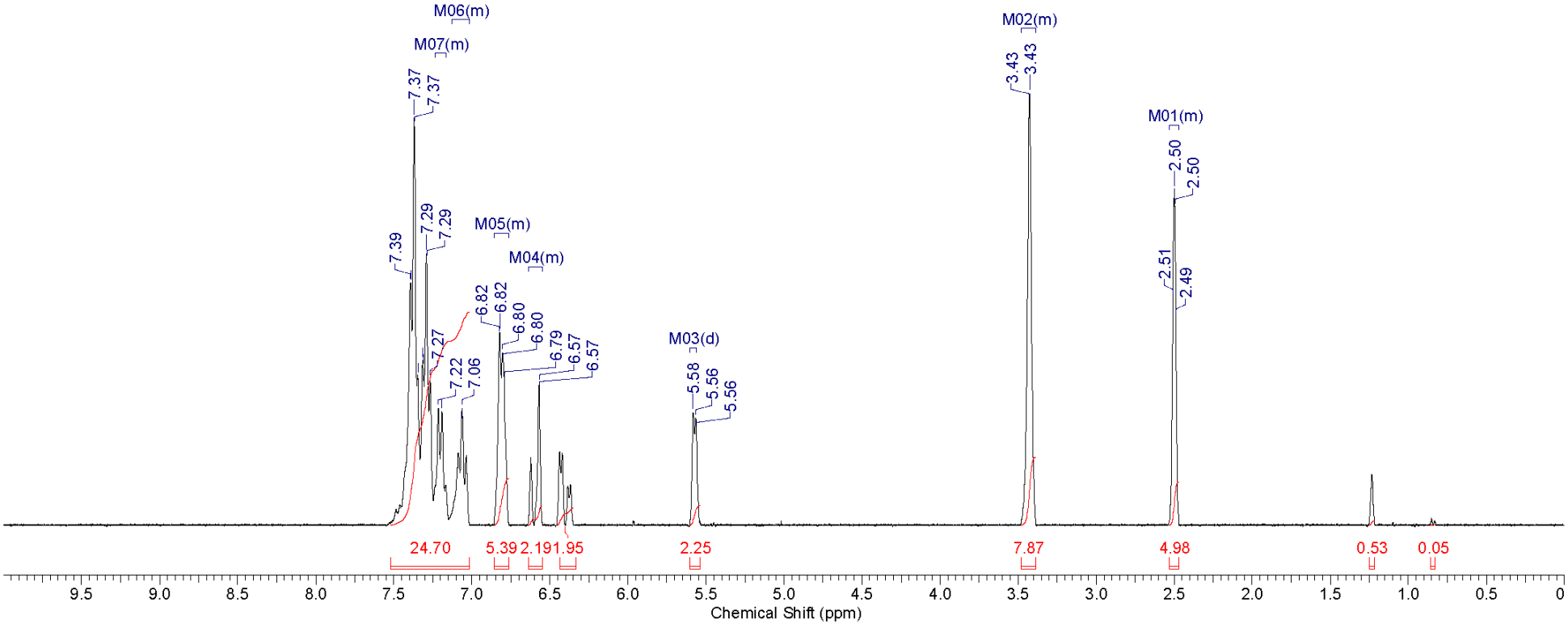
No.	(ppm)	Annotation	Layer No.	Created By	Created At	Modified By	Modified At
1	[3.38 .. 3.48]	Water	1	User	Sun 2012/03/11 12:17:09 PM		

Formula $C_{15}H_{14}O_2$	FW	226.2705

Acquisition Time (sec)	2.0000	**Comment**	CC178-1H	**Date**	Sep 20 2011	**Date Stamp**	Sep 20 2011
File Name	C:\Users\User\Documents\PhD\PhD NMR data\CCclean\CC178-1H.fid\fid					**Frequency (MHz)**	300.08
Nucleus	1H	**Number of Transients**	4	**Original Points Count**	9600	**Points Count**	131072
Pulse Sequence	s2pul	**Receiver Gain**	13.00	**Solvent**	DMSO-d6	**Spectrum Offset (Hz)**	1505.9641
Spectrum Type	STANDARD	**Sweep Width (Hz)**	4800.00	**Temperature (degree C)**	AMBIENT TEMPERATURE		

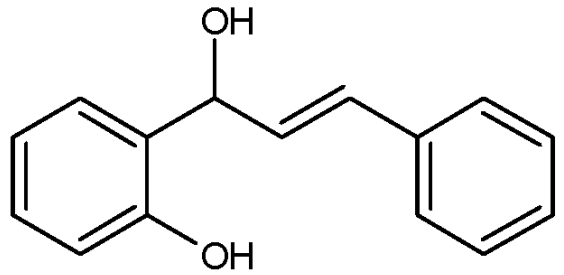


12-1H-2nd spectra.esp

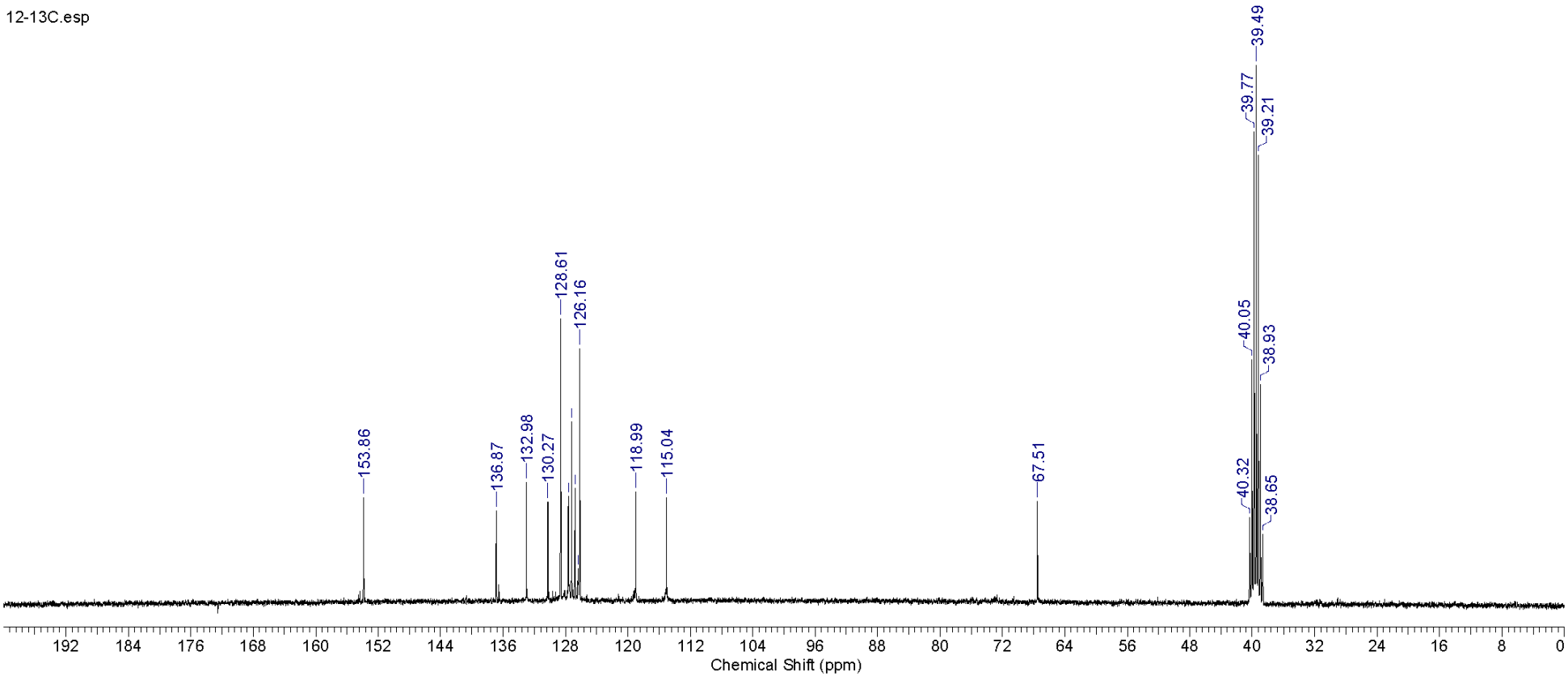


Formula $C_{15}H_{14}O_2$	FW	226.2705

Acquisition Time (sec)	1.8150	***Comment***	CC178-13C	***Date***	Sep 20 2011	***Date Stamp***	Sep 20 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC178-13C.fid\fid			***Frequency (MHz)***	75.46	***Nucleus***	13C	***Number of Transients***	4268
Original Points Count	34053	***Points Count***	65536	***Pulse Sequence***	s2pul	***Receiver Gain***	30.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	7513.4043	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	18761.73	***Temperature (degree C)***	AMBIENT TEMPERATURE		

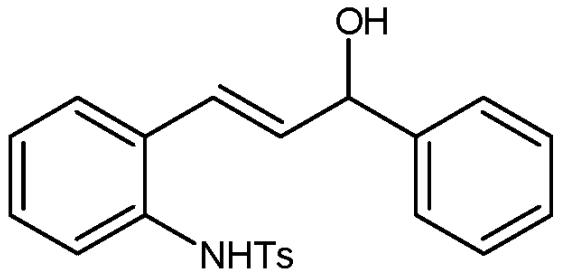


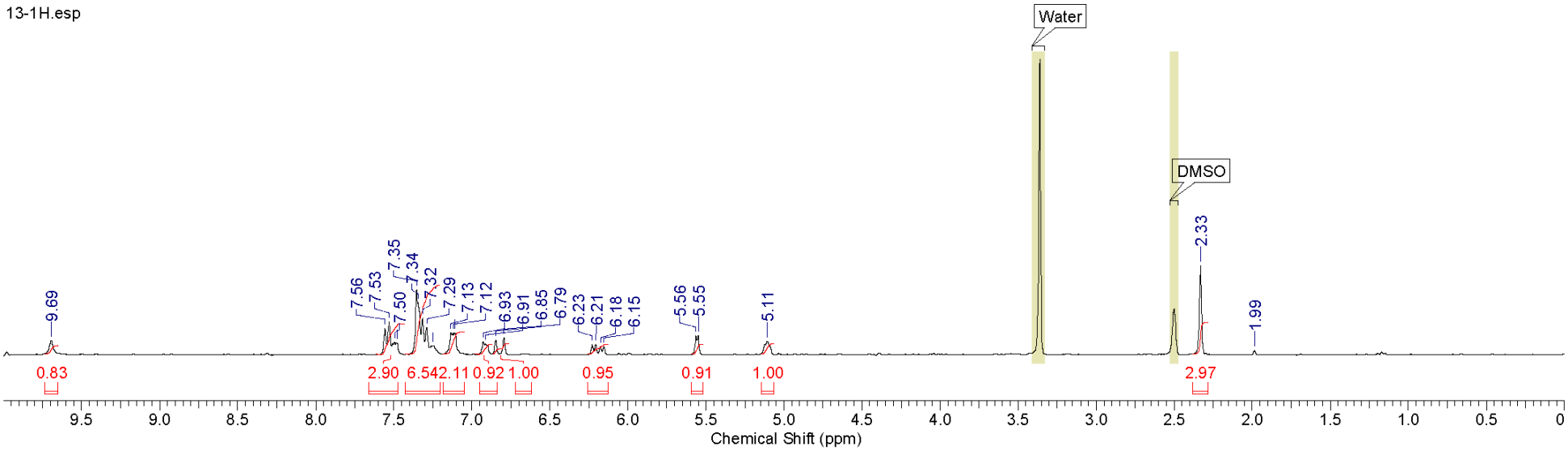
12-13C.esp



Formula $C_{22}H_{21}NO_3S$	FW	379.4720

Acquisition Time (sec)	2.0000	**Comment**	CC133-1H	**Date**	May 18 2011	**Date Stamp**	May 18 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC133-1H.fid\fid			**Frequency (MHz)**	300.08	**Nucleus**	1H	**Number of Transients**	6
Original Points Count	9600	**Points Count**	16384	**Pulse Sequence**	s2pul	**Receiver Gain**	4.00	**Solvent**	DMSO-d6
Spectrum Offset (Hz)	1505.3820	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	4800.00	**Temperature (degree C)**	AMBIENT TEMPERATURE		

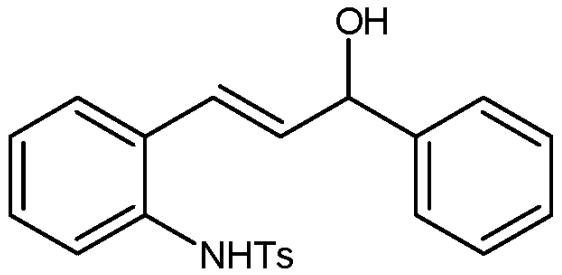




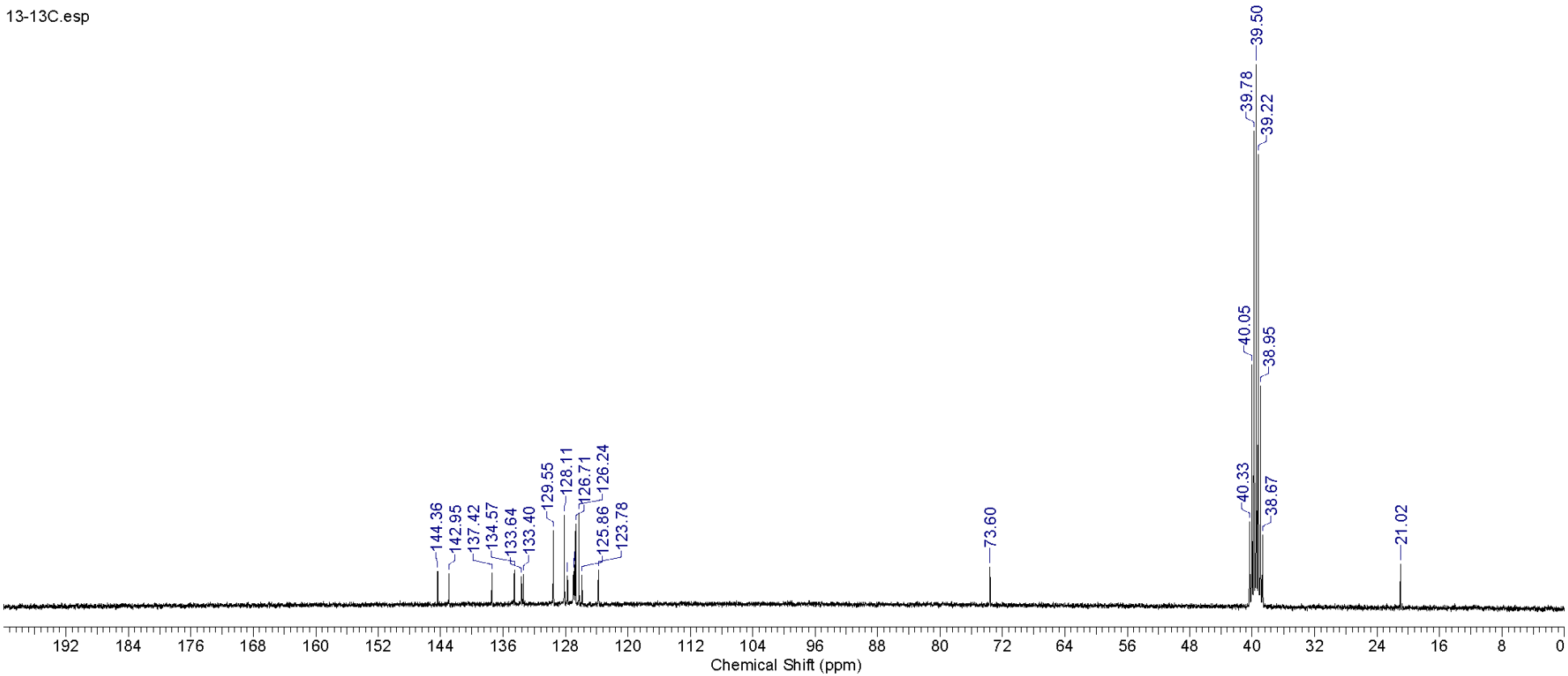
No.	(ppm)	Annotation	Layer No.	Created By	Created At	Modified By	Modified At
1	[2.48 .. 2.52]	DMSO	1	User	Sun 2012/03/11 12:58:59 PM		
2	[3.33 .. 3.41]	Water	1	User	Sun 2012/03/11 12:58:59 PM		

Formula $C_{22}H_{21}NO_3S$	FW	379.4720

Acquisition Time (sec)	1.8150	**Comment**	CC133-13C	**Date**	May 18 2011	**Date Stamp**	May 18 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC133-13C.fid\fid			**Frequency (MHz)**	75.46	**Nucleus**	13C	**Number of Transients**	5000
Original Points Count	34053	**Points Count**	65536	**Pulse Sequence**	s2pul	**Receiver Gain**	29.00	**Solvent**	DMSO-d6
Spectrum Offset (Hz)	7512.2593	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	18761.73	**Temperature (degree C)**	AMBIENT TEMPERATURE		

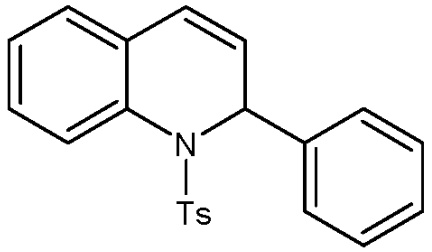


13-13C.esp

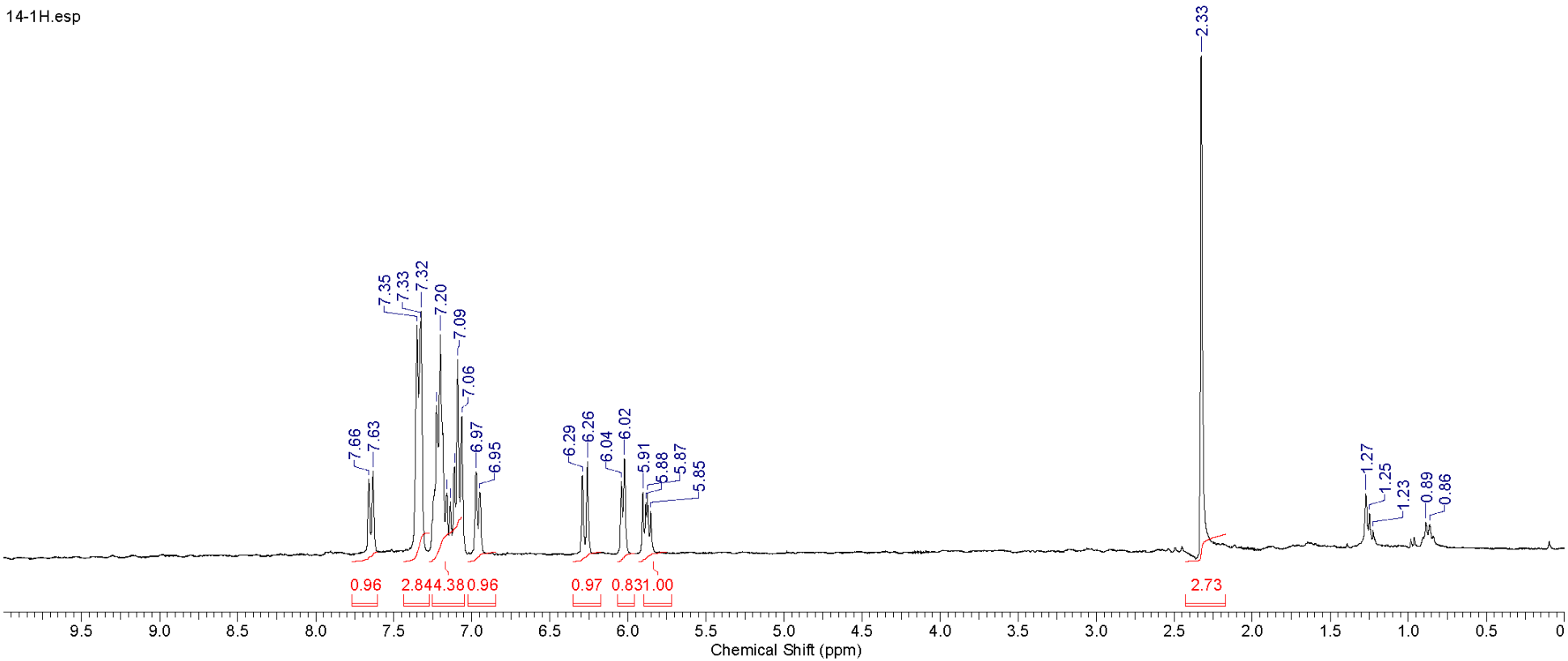


Formula $C_{22}H_{19}NO_2S$	FW	361.4568

Acquisition Time (sec)	2.0000	**Comment**	CC138-1H	**Date**	May 26 2011	**Date Stamp**	May 26 2011		
File Name	C:\Users\User\Desktop\adam\CCclean\CC138-1H.fid\fid			**Frequency (MHz)**	300.08	**Nucleus**	1H	**Number of Transients**	4
Original Points Count	9600	**Points Count**	16384	**Pulse Sequence**	s2pul	**Receiver Gain**	11.00	**Solvent**	CHLOROFORM-d
Spectrum Offset (Hz)	1494.8170	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	4800.00	**Temperature (degree C)**	AMBIENT TEMPERATURE		

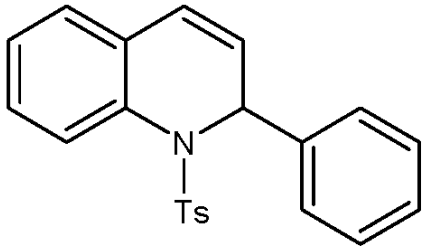


14-1H.esp



Formula $C_{22}H_{19}NO_2S$	FW	361.4568

Acquisition Time (sec)	1.8150	***Comment***	CC138-13C	***Date***	May 26 2011	***Date Stamp***	May 26 2011
File Name	C:\Users\User\Desktop\adam\CCclean\CC138-13C.fid\fid			***Frequency (MHz)***	75.46	***Nucleus***	13C
Number of Transients	6028	***Original Points Count***	34053	***Points Count***	65536	***Pulse Sequence***	s2pul
Receiver Gain	28.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	7535.3623
Spectrum Type	STANDARD	***Sweep Width (Hz)***	18761.73	***Temperature (degree C)***	AMBIENT TEMPERATURE		



14-13C.esp