Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supplementary Information for

Reactions of Triflate Esters and Triflamides with an Organic Neutral Super-Electron-Donor

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- Experimental Procedures and Spartan computational files: pages 2-8

- NMR spectra + Mass Spectrum of ^{18}O-DMF and **24** (in expt where ^{18}O-DMF was used)

Supplementary Information

Experimental Details.

All Gas Chromatography Mass Spectrometry (GC-MS) was performed on an Ion Trap Mass Spectrometer/Trace GC instrument with ZB-5 column (30 metres), at 1ml/min He gas flow rate and temperature range of 50 to 320 ^{o}C with an increment of 10 to 20 ^{o}C/min.
Flash chromatography was performed using silica gel 60 (200-400 mesh). Thin layer chromatography (TLC) was performed using aluminium sheets of silica gel 60 F_{254} and was visualised under UV lamp (254 nm). The plates were developed with acidic methanolic vanillin solutions.
All reagents were obtained from commercial suppliers and used without further purification unless otherwise stated. As required, organic solvents were dried and / or distilled prior to use. Tetrahydrofuran, dichloromethane, hexane, diethyl ether and toluene were dried and deoxygenated with a column-based solvent purification system by and the moisture content of the solvents was analysed using a Karl Fischer coulometer. A 500 ml bottle of anhydrous DMF was sealed with a septum and degassed with argon bubbled through a needle, with stirring over 2h. The sealed bottle was transferred to a glovebox and stored under oxygen-free, moisture-free conditions.
All reactions requiring anhydrous conditions were performed in flame-dried apparatus under a nitrogen or argon atmosphere. Organic extracts were, in general, dried over anhydrous sodium sulfate (Na_2SO_4).
The IUPAC names of some compounds were obtained using ChemDraw Ultra version 11.0.

***N,N,N',N'*-Tetramethyl-7,8-dihydro-6H-dipyrido[1,2-a;2',1'-c][1,4]diazepine-2,12-diamine (13)**[1]
A mixture of 1,3-*bis*(*N,N*-dimethyl-4-aminopyridinium)propane diiodide (8.10 g, 15 mmol, 1 eq.) and NaH (60% dispersed in mineral oil, 6 g, 150 mmol, 10 eq.) was placed under argon in a Schlenk flask equipped with a dry-ice cooler. The mixture was washed with hexane and the hexane removed. While stirring, ammonia gas was condensed into the flask (70 ml), the mixture was kept under reflux for 4 h and then the ammonia was allowed to evaporate over 3 h, followed by putting under vacuum. The solid was then extracted with diethyl ether, the solvent was removed and the residue dried under vacuum to give *N,N,N',N'*-tetramethyl-7,8-dihydro-6H-dipyrido[1,2-a;2',1'c][1,4]di-azepine-2,12-diamine **13** (3.56 g, 83.4%) as a purple-black, moisture-sensitive and oxygen-sensitive powder, M.pt. = 131-133 ^{o}C; ^{1}H NMR (400 MHz, C_6D_6) :δ 1.00 (2H, quintet, J = 6.3 Hz), 2.46 (12H, s), 3.03 (4H, t, J = 6.3 Hz), 4.91 (2H, dd, J = 7.5, 2.2 Hz), 5.14 (2H, d, J = 2.2 Hz), 5.64 ppm, (2H, d, J = 7.5 Hz); ^{13}C NMR (100 MHz, C_6D_6) *:* δ_C 24.5, 40.8, 52.6, 95.8, 96.2, 116.0, 138.7, 143.7 ppm. λ_{max} (MeCN) = 260 (ε = 30000 M^{-1} cm^{-1}), 345 (ε = 15000 M^{-1} cm^{-1}), 520 (ε = 2500 M^{-1} cm^{-1}) nm.

General procedure A - preparation of triflates: Alcohol or phenol starting material (1.0 eq.) was dissolved in dry dichloromethane (2 ml), pyridine (1.0 eq.) was added and the flask cooled to -78^{o}C. A solution of trifluoromethanesulfonic anhydride (1.5 eq.) in DCM (2 ml) at -78^{o}C was added dropwise to the stirred alcohol or phenol solution. The dry-ice bath was removed from and the reaction mixture allowed to warm to room temperature. Water (10ml) was then added, followed by dichloromethane (10ml). The reaction solution was then washed with further portions of water (3 x 10 ml) and brine (1 x 10ml), dried over Na_2SO_4 and the solvent was evaporated. The crude organic residue was then eluted (dichloromethane on silica gel), to afford the pure corresponding trifluoromethanesulfonate ester.

3-Phenylpropyl-1-trifluoromethanesulfonate (21):[2a]
Phenylpropan-1-ol **24** (0.08 ml, 0.6 mmol, 1.0 eq.) was reacted according to procedure A to afford 3-phenylpropyl-1-trifluoromethanesulfonate **21** as a colourless oil (0.153g, 0.57 mmol, 95%); IR (thin film) ν = 3066, 3030, 2935, 2865,1498, 1455, 1412, 1246, 1207, 1145, 984, 930, 831, 800, 747, 700, 615, 576 and 519 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.14-2.20 (2H, m), 2.78 (2H, t, J = 7.3 Hz), 4.54 (2H, t, J = 6.3 Hz), 7.20 (2H, d, J = 7.4 Hz), 7.25 (1H, t, J = 7.4 Hz) and 7.33 ppm (2H, t, J = 7.4 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 31.1, 31.5, 76.9, 119.0 (q, J = 318 Hz, CF_3) 126.9, 128.7, 129.1, 139.8 ppm. *m/z* (EI) 268.0 ([M]$^{+}$, 18%), 118.0 (35), 117.0 (71), 91.0 (100).

Figure below: Phenylpropyl triflate **21** (Spartan'04 using DFT 6-31G*)

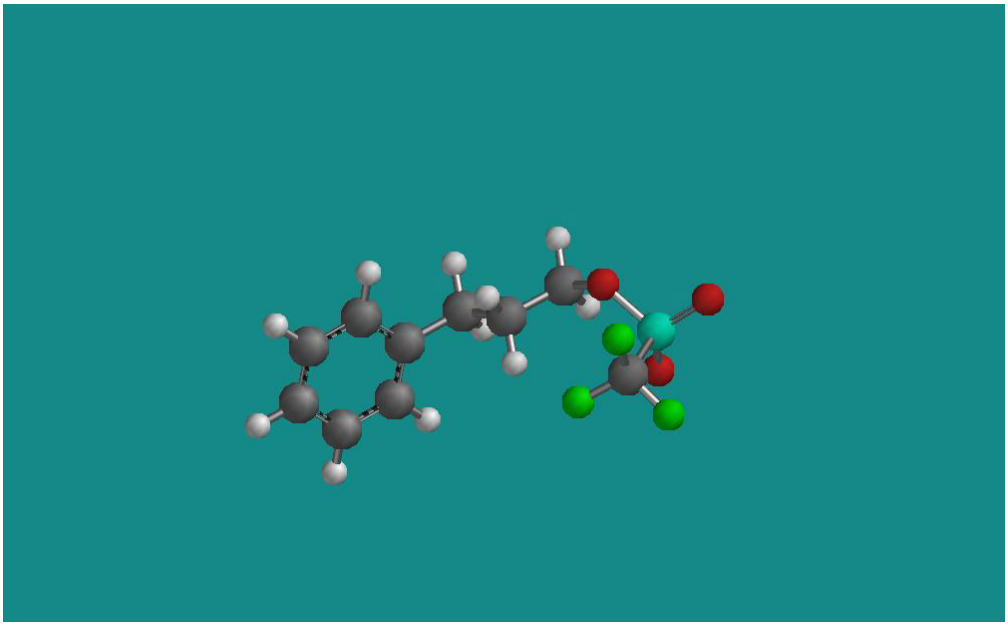
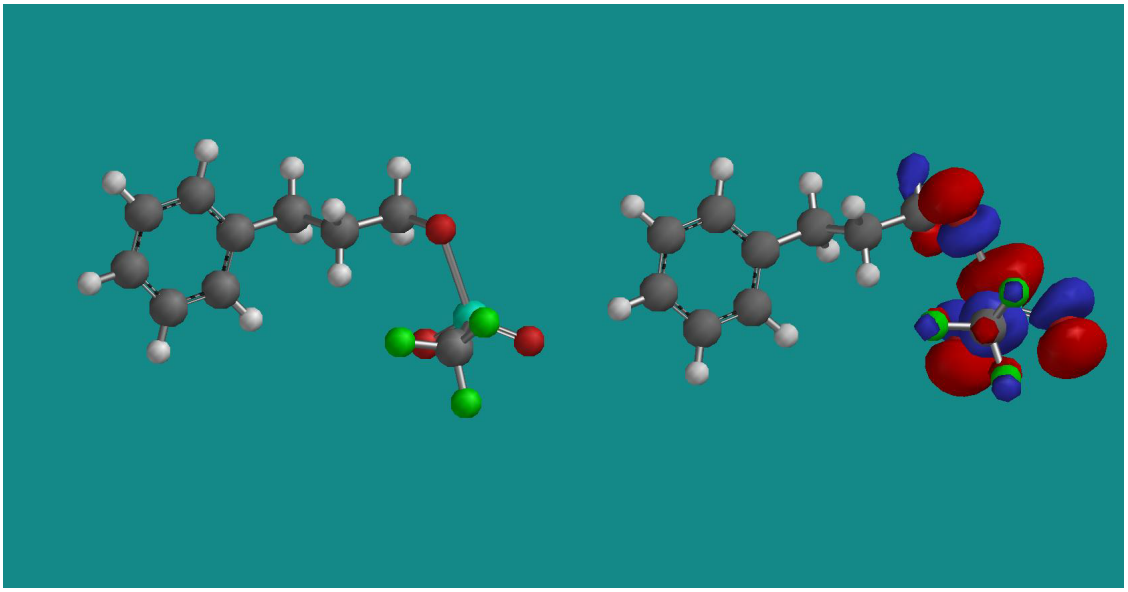


Figure below: Phenylpropyl triflate **21** radical-anion (Spartan'04 using DFT 6-31G*) (SOMO is depicted bottom right)



4-Phenylbutyl-1-trifluoromethanesulfonate (22):[2b]
4-Phenylbutan-1-ol **25** (150 mg, 1.0 mmol, 1.0 eq.) was reacted according to procedure A to afford 4-phenylbutyl-1-trifluoromethanesulfonate **22** as a colourless oil (263 mg, 0.93 mmol, 93%); IR (thin film) ν = 3064, 3029, 2944, 2864, 1497, 1454, 1412, 1246, 1206, 1146, 991, 932, 838, 748, 700, 615, 578 and 526 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ = 1.75-1.81 (2H, m), 1.84-1.90 (2H, m), 2.69 (2H, t, J = 7.4 Hz), 4.58 (2H, t, J = 6.3 Hz), 7.18-7.32 ppm (5H, m); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 27.0, 28.9, 35.2, 77.8, 119.0 (q, J = 318 Hz, CF_3),126.4, 128.6, 128.8, 141.5 ppm. *m/z* (ESI) 281.9 ($[M]^+$, 23%), 132.0 (34), 104.1 (83), 91.1 (100), 65.1 (27).

5-Phenylpentyl-1-trifluoromethanesulfonate (23)[3]
5-Phenylpentan-1-ol **26** (164 mg, 1.0 mmol, 1.0 eq.) was reacted according to procedure A to afford 5-phenylpentyl-1-trifluoromethanesulfonate **23** as a colourless oil (279 mg, 0.94 mmol, 94%); IR (thin film) ν = 3030, 3934, 2865, 1412, 1247, 1207, 1145, 930, 799, 746 and 616 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ = 1.55-1.61 (2H, m), 1.66-172 (2H, m), 1.84-1.90 (2H, m), 2.69 (2H, t, J = 7.4 Hz), 4.58 (2H, t, J = 6.3 Hz), 7.17-7.22 (3H, m) and 7.26-7.31 ppm (2H, m); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 25.0, 29.5, 31.0, 35.9, 77.8, 119.0 (q, J = 317 Hz, CF_3), 126.2, 128.7, 128.7 and 142.2 ppm. *m/z* (EI) 295.9 ($[M]^+$, 22%), 146.1 (32), 104.1 (38). 91.2 (100), 65.1 (22).

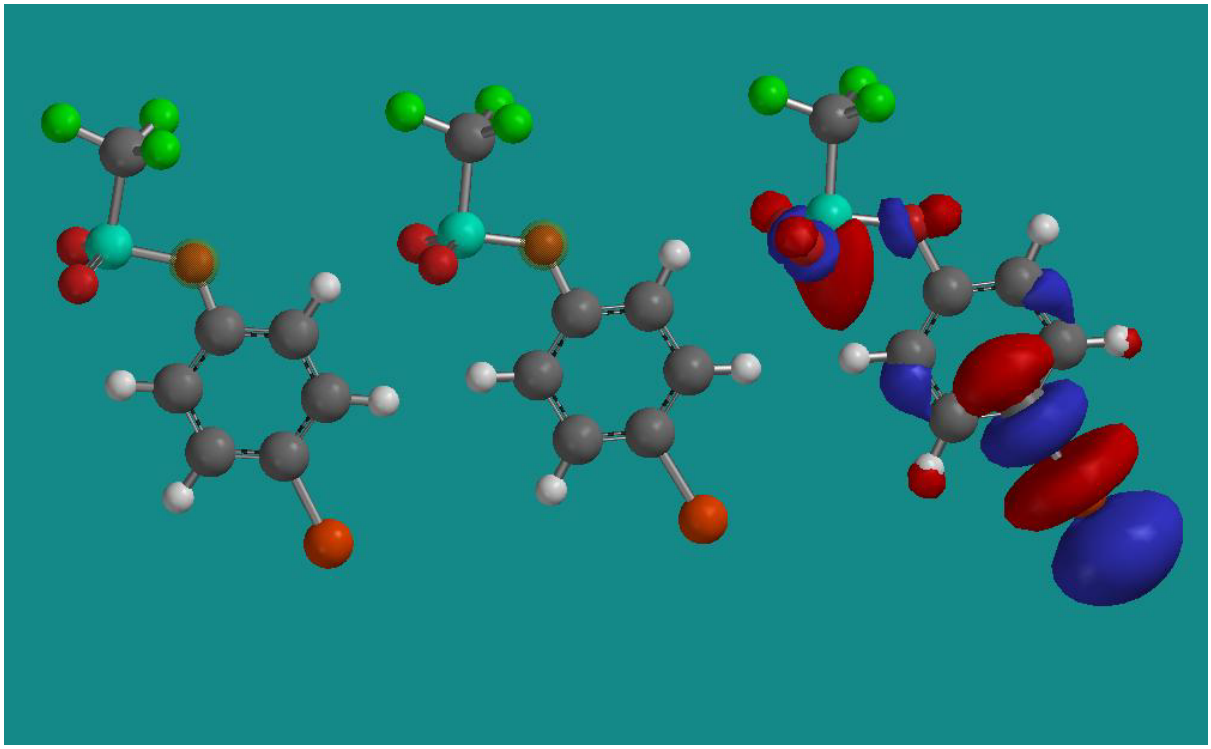
2,3-Dihydro-1H-inden-5-yl trifluoromethanesulfonate (40)[4]
2,3-Dihydro-1H-inden-5-ol **41** (201 mg, 1.5 mmol, 1.0 eq.) was reacted according to procedure A to afford 2,3-dihydro-1H-inden-5-yl trifluoromethanesulfonate **40** as a colourless oil (359 mg, 1.35 mmol, 90%); [Found: $(M)^+$, 266.0220. $C_{10}H_9F_3O_3S$ requires $(M)^+$, 266.0219]; IR (thin film) ν = 2957, 2850, 1611, 1593, 1480, 1423, 1250, 1212, 1142, 1100, 933, 870, 852, 608, and 502 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 2.45 (2H, quintet, J = 7.4 Hz), 2.93 (2H, t, J = 7.4 Hz), 2.96 (2H, t, J = 7.4 Hz), 7.02 (1H, m), 7.12 (1H, d, J = 1.8 Hz) and 7.25 ppm (1H, d, J = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 26.1, 32.7, 33.3, 117.7, 119.1 (q, J = 319 Hz, CF_3), 119.2, 125.8, 145.0, 147.2, 148.6 ppm.

2-Allylphenyl trifluoromethanesulfonate (45)[5]
2-Allylphenol (268 mg, 2.0 mmol, 1.0 eq.) was reacted according to procedure A to afford 2-allylphenyl trifluoromethanesulfonate **45** as a colourless oil (493 mg, 1.85 mmol, 93%); [Found: $(M)^+$ 266.0219. $C_{10}H_9F_3O_3S$ requires $(M)^+$, 266.0219]; IR (thin film) ν = 3085, 2985, 2923, 1642, 1488, 1454, 1422, 1250, 1214, 1140, 1105, 1073, 891, 181, 767 and 606 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ = 3.49 (2H, dt, J = 6.6, 1.3 Hz), 5.11-5.18 (2H, m), 5.89-5.97 (1H, m) and 7.28-7.36 ppm (4H, m); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 34.3, 117.8, 119.0 (q, J = 318 Hz, CF_3), 121.7, 128.5, 128.7, 131.8, 133.2, 134.9, 148.3 ppm.

4-Bromophenyl trifluoromethanesulfonate (47)[6]
4-Bromophenol **48** (346 mg, 2.0 mmol, 1.0 eq.) was reacted according to procedure A to afford 4-bromophenyl-1-trifluoromethanesulfonate **47** as a colourless oil (591 mg, 1.94 mmol, 97%); [Found: $(M)^+$ 303.9011 $C_7H_4BrF_3O_3S$ requires $(M)^+$, 303.9011]; IR (thin film) ν = 3103, 1481, 1428, 1401, 1251, 1216, 1174, 1141, 1071, 1013, 886, 832, 779, 750, 628, 607 and 525 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ = 7.18 (2H, d, J = 9.0 Hz) and 7.60 ppm (2H, d, J = 9.0 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 119.0 (q, J = 319 Hz, CF_3), 122.4, 123.4, 133.8, 148.8 ppm.

Compound **47**: calculations below with Spartan'04 (Wavefunction Inc) using DFT 6-31G*

Below left: *p*-bromophenyl triflate Spartan'04 using DFT 6-31G*
Below Centre: *p*-bromophenyl triflate radical-anion Spartan'04 using DFT 6-31G*
Below right: *p*-bromophenyl triflate radical-anion Spartan'04 using DFT 6-31G* showing SOMO



General procedure B - reductions of triflates: Donor **13** (128 mg, 0.45 mmol, 1.5 eq.) was dissolved in degassed DMF (2 ml) in a glove-box. This solution was directly pipetted onto the dry and degassed selected substrate (0.3 mmol, 1.0 eq.). The mixture was left to stir for 2 h at ambient temperature, then added to water (75 ml), before extracting with diethyl ether (4 x 50 ml). The combined organic layers were then washed with water (2 x 50 ml), brine (50 ml) and dried over Na_2SO_4. The crude organic residue, obtained after evaporation under reduced pressure, was eluted with ethyl acetate on silica gel, to afford the pure corresponding products as reported.

3-Phenylpropan-1-ol (24)[7]
3-Phenylpropyl-1-trifluoromethanesulfonate **21** (81 mg, 0.3 mmol, 1.0 eq.), was reacted according to procedure B to afford 3-phenylpropan-1-ol **24** as a colourless oil, (37 mg, 0.27 mmol, 90%); IR (Thin film) ν = 3335, 3033, 2932, 2941, 1605, 1495, 1450, 1055, 1032, 749 and 701 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ = 1.62 (s, OH), 1.89-1.95 (2H, m), 2.72 (2H, t, J = 7.7 Hz), 3.70 (2H, t, J = 6.5 Hz), 7.20-7.23 (3H, m), 7.31 ppm (2H, t, J = 7.4); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 32.4, 34.5, 62.6, 126.2, 128.7, 128.8, 142.1. *m/z* (EI) 135.93 ($[M]^+$).

4-Phenylbutan-1-ol (25)[7]
4-Phenylbutyl-1-trifluoromethanesulfonate **22** (85 mg, 0.3 mmol, 1.0 eq.), was reacted according to procedure B to afford 4-phenylbutan-1-ol **25** as a colourless oil, (41 mg, 0.28 mmol, 91%); IR (Thin film) ν = 3294, 3028, 1497, 1429, 1249, 1217, 1078, 1029, 746 and 698 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ = 1.38 (1H, s), 1.60-1.65 (2H, m), 1.69-1.75 (2H, m), 2.66 (2H, t, J = 7.6 Hz), 3.68 (2H, t, J = 7.6 Hz), 7.18-7.20 (3H, m) and 7.27-7.31 ppm (2H, m); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 27.8, 32.6, 36.0, 63.2, 126.1, 128.6, 128.7, 142.6 ppm. *m/z* (ESI) 150.0 ($[M]^+$, 30%), 132.2 (64), 104.3 (100), 91.1 (42), 65.2 (12).

5-Phenylpentan-1-ol (26)[7]
5-Phenylpentyl-1-trifluoromethanesulfonate **23** (89 mg, 0.3 mmol, 1.0 eq.), was reacted according to procedure B to afford 5-phenylpentan-1-ol **26** as a colourless oil, (42 mg, 0.26 mmol, 85%); IR (thin film) ν = 2957, 2850, 1611, 1593, 1480, 1423, 1250, 1212, 1142, 1100, 933, 870, 852, 608, and 502 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ = 1.39-1.45 (2H, m), 1.59-1.64 (2H, m), 1.65-1.70 (2H, m), 2.64 (2H, t, J = 7.7 Hz), 3.65 (2H, t, J = 6.6 Hz), 7.18-7.12 (3H, m), 7.27-7.30 (2H, m); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 25.7, 31.6, 33.0, 36.2, 63.3, 126.0, 128.6, 128.7, 142.9 ppm. *m/z* (ESI) 186.93 ($[M+Na]^+$).

2,3-Dihydro-1H-inden-5-ol (41)[7]
2,3-Dihydro-1H-inden-5-yl trifluoromethanesulfonate **40** (80 mg, 0.3 mmol, 1.0 eq.), was reacted according to procedure B to afford 2,3-dihydro-1H-inden-5-ol **41** as a white solid (36 mg, 0.27 mmol, 89%); M.pt. = 56-57 °C (Lit.[8] = 56 °C), ^1H NMR (400 MHz, $CDCl_3$): δ = 2.08 (2H, quintet, J = 7.4 Hz), 2.84 (2H, t, J = 7.2 Hz), 2.87 (2H, t, J = 7.2 Hz), 4.51 (1H, br. s) 6.61 (1H, dd, J = 8.0, 2.5 Hz), 6.72 (1H, d, J = 2.0 Hz) and 7.08 ppm (1H, d, J = 8.1 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 26.2, 32.3, 33.4, 111.7, 113.3, 123.3, 136.7, 146.4, 154.5 ppm. *m/z* (ESI) 133.07 ($[M-H]^-$, 100%).

(Trifluoromethylsulfonyl)methylbenzene (44)[9]
Donor **13** (128 mg, 0.45 mmol, 1.5 eq.) was dissolved in degassed DMF (2 ml) in a glovebox. This solution was directly pipetted onto the dry and degassed 2,3-dihydro-1H-inden-5-yl trifluoromethanesulfonate **40** (80 mg, 0.3 mmol, 1.0 eq.). The mixture was left to stir for 2h at ambient temperature, before benzyl bromide (308 mg, 1.8 mmol, 4.0 eq.) was added to the reaction mixture and stirred overnight. The reaction vessel was sealed and removed to a fumehood and water (75 ml) added, before extraction with diethyl ether (5 x 50 ml). The combined organic layers were then washed with water (2 x 50 ml), brine (50 ml) and dried over Na_2SO_4. The crude organic obtained after evaporation under reduced pressure was purified by column chromatography to give (trifluoromethylsulfonyl)-methylbenzene **44** as a white crystalline solid (61 mg, 274 mmol, 91%); M.pt. 100-101°C (Lit.[9] = 104 °C); Found $(M)^+$, 224.0114. $C_8H_7F_3O_2S$ requires $(M)^+$, 224.0113. IR (KBr) ν = 3007, 2953, 1625, 1494, 1459, 1361, 1202, 1120, 774, 720, 697, 634, 525 and 507 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ = 4.49 (2H, s) and 7.43-7.48 ppm (5H, m); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 56.5, 120.1 (q, J = 326 Hz, CF_3), 123.5, 129.6, 130.4, 131.6 ppm.

2-(Prop-1-enyl)phenol (46)[7]
2-Allylphenyl trifluoromethanesulfonate **45** (80 mg, 0.3 mmol, 1.0 eq.), was reacted according to procedure B to afford 2-(prop-1-enyl)phenol **46** as a colourless oil, (38mg, 0.286 mmol, 95%); IR (Thin Film) ν = 3410, 3034, 2912, 2852, 1654, 1581, 1446, 1284, 1172, 964 and 746 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 1.93 (3H, dd, J = 6.6, 1.7 Hz), 4.96 (s, OH), 6.23 (1H, dq, J = 15.9, 6.6 Hz), 6.59-6.63 (1H, m), 6.81 (1H, dd, J = 8.0, 1.0 Hz), 6.91 (1H, td, J = 7.7, 7.4, 1.0 Hz), 7.12 (1H, td, J = 8.0, 7.4, 1.6 Hz) and 7.32 ppm (1H, dd, J = 7.7, 1.6 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 19.3, 116.0, 121.2, 125.4, 125.7, 127.7, 128.3, 128.7, 152.7. *m/z* (ESI) 133.10 ($[M-H]^-$).

4-Bromophenol (48)[7]
4-Bromophenyl-1-trifluoromethanesulfonate **47** (92 mg, 0.3 mmol, 1.0 eq.), was reacted according to procedure B to afford 4-bromophenol **48** as a colourless crystalline solid, (44mg, 0.252 mmol, 84%); M.pt. = 66-68 °C (Lit.[10] = 66-68 °C); IR (thin film) ν = 3342, 3062, 2943, 2665, 1588, 1487, 1437, 1331, 1211, 1116, 1070, 999, 936, 827, 695 and 632 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 4.69 (1H, s, OH), 6.73 (2H, d, J = 8.9 Hz) and 7.35 ppm (2H, d, J = 8.9 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 113.3, 117.5, 132.8, 155.0 ppm. *m/z* (ESI) 170.9 ($[M-H]^-$, 100%).

1-(Benzyloxy)-4-bromobenzene (49) and (Trifluoromethylsulfonyl)methylbenzene (44)
Donor **13** (427 mg, 1.5 mmol, 1.5 eq.) was dissolved in degassed DMF (5 ml). This solution was directly pipetted onto the dry 4-bromophenyl trifluoromethanesulfonate **47** (305 mg, 1.0 mmol, 1.0 eq.). The mixture was left to stir for 16h at ambient

temperature, before benzyl bromide (1.03 g, 6.0 mmol, 6.0 eq.) was added to the reaction mixture and stirred overnight. The reaction vessel was sealed and removed to a fumehood and water (75 ml) added, before extraction with ethyl acetate (5 x 50 ml). The combined organic layers were then washed with water (2 x 50 ml), brine (50 ml) and dried over Na_2SO_4. The crude organic obtained after evaporation under reduced pressure was purified by column chromatography in diethyl ether and petroleum ether (40 - 60 ^oC) to give 1-(benzyloxy)-4-bromobenzene **49** as a white crystalline solid (231 mg, 0.88 mmol, 88%) and trifluoromethylsulfonyl)methylbenzene **44** as a white crystalline solid (132 mg, 0.59 mmol, 59%);
1-(Benzyloxy)-4-bromobenzene: M.pt. 58-60 ^oC [Lit.[11] 59-60 ^oC]. IR (thin film) ν = 3338, 3034, 2891, 2080, 1893, 1573, 1491, 1453, 1379, 1285, 1233, 1112, 1073, 1047, 993, 909, 823 and 739 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 5.06 ppm (2H, s), 6.87 (2H, d, J = 9.0 Hz) and 7.33-7.45 ppm (7H, m). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 69.7, 112.6, 116.2, 126.9, 127.6, 128.1, 131.8, 136.1, 157.4 ppm.

Data for (Trifluoromethylsulfonyl)methylbenzene **44** were consistent with those reported above.

Reaction of substrate 21 in ^{18}O labelled dimethylformamide:

(i) Preparation of ^{18}O- dimethylformamide.[12]
Dry dimethylformamide (7.7 ml, 0.1 mol) and dry benzoyl chloride (11.6 mL, 0.1 mol) were taken in a three necked flask equipped with a calcium chloride drying tube. The flask was then cooled to 0 ^oC and ^{18}O labelled water (20% mole of ^{18}O isotope, 1.83g, 0.1 mol) was introduced slowly into the reaction flask. The contents solidified instantaneously due to the formation of benzoic acid Mass spectrometry of the crude reaction mixture indicated the presence of ^{18}O labelled dimethylformamide. Petroleum ether (40 - 60 ^oC, 10 ml) was added to the reaction flask and stirred for 10 min and sodium bicarbonate (8.4 g, 0.1 mol) was added to the reaction flask. When the evolution of carbon dioxide ceased, the contents were extracted with acetone (3 x 20 ml). The combined acetone layers were dried over anhydrous potassium carbonate and filtered, and the resulting solution was concentrated under vacuum. The crude product was purified by distillation (90 ^oC @ 30 mm Hg) and provided ^{18}O-labelled dimethylformamide (13% mole of ^{18}O isotope, 5.6 g, 78 %).
^{18}O-DMF IR (Thin film) ν = 3480, 2939, 1660, 1388, 1257, 1092 and 1060 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$) δ = 2.80 (3H, s), 2.89 (3H, s) and 7.94 ppm (1H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 31.3, 36.4 and 162.4 ppm; m/z (ESI) 76.2 ($[M+H]^+$, 13%), 74.2, ($[M+H]^+$, 100).

(ii) Reaction with substrate **21**
Dry ^{18}O-enriched DMF (2 mL) was added to 3-phenylpropyl-1-trifluoromethanesulfonate (80 mg, 0.3 mmol), followed by 4-DMAP donor (128 mg, 0.45 mmol, 1.5 equiv) in a glove box and the reaction flask was sealed. After stirring at room temperature for 2 h, the reaction was then quenched with water (10 mL) and extracted with diethyl ether (3 x 10 mL). The combined ether phases were washed again with water (10 mL), brine (10 mL) and dried over anhydrous sodium sulfate. The resulting solution was concentrated and purified by column chromatography (20% diethyl ether in petroleum ether) to provide 3-phenylpropan-1-ol (18 mg, 44%). The spectral data were consistent with the previous data of the same compound. Mass spectroscopy showed that there was no enrichment of ^{18}O in the alcohol product and the data were given in the supporting information.

Preparation of triflamides:
9-(Trifluoromethylsulfonyl)-2,3,4,9-tetrahydro-1H-carbazole (51)
2,3,4,9-Tetrahydro-1H-carbazole **52** (685 mg, 4.0 mmol, 1.0 eq.) was dissolved in dry THF (10 ml). The reaction vessel was cooled to -78^oC before *n*-butyllithium was added dropwise (4.4 mmol, 1.1 eq.) and stirred for 30 min. Trifluoromethanesulfonic anhydride (1.24 g, 4.4 mmol, 1.1 eq.) in dichloromethane (10 ml) at -78^oC, under argon was added dropwise to the stirred solution of 2,3,4,9-tetrahydro-1H-carbazole. On complete addition, the reaction vessel was warmed to room temperature and stirred overnight. The reaction mixture was quenched with water (25 ml) and washed with further portions of water (3 x 25 ml) and brine (1 x 20 ml) before being dried over Na_2SO_4 and evaporated. The crude organic residue was purified on silica gel, (10% ethyl acetate in hexane), to afford 9-(trifluoromethylsulfonyl)-2,3,4,9-tetrahydro-1H-carbazole **51** as colourless crystals (413 mg, 1.36 mmole 34%); M.pt. = 60-61^oC; [Found: $(M)^+$, 303.0533. $C_{13}H_{12}F_3NO_2S$ requires $(M)^+$, 303.0535]; IR (KBr) ν = 3437, 2944, 1441, 1412, 1224, 1196, 1151, 1116, and 609 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ = 1.86-1.95 (4H, m), 2.66-2.69 (2H, m), 2.86-2.96 (2H, m), 7.30-7.35 (2H, m), 7.43-7.45 (1H, m) and 7.93-7.94 ppm (1H,m); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 21.5, 22.2, 23.4, 24.3, 114.6, 118.8, 119.3 (q, J = 322.7 Hz, CF_3), 121.1, 125.1, 125.2, 130.9, 136.1, 136.5 ppm.

***N*-Benzyl-*N*-phenyl-1,1,1-trifluoromethanesulfonamide (53)** [13,14]
N-Benzylaniline **54** (277 mg, 1.51 mmol) in dry dichloromethane (5 ml) was cooled to -78^oC under an inert atmosphere and triethylamine (202 mg, 2.0 mmol, 1.0 eq.) was added. Trifluoromethanesulfonic anhydride (846 mg, 3.0 mmol, 1.5 eq.) in dry dichloromethane (5 ml) was added, cooled to -78^oC, to the stirred *N*-benzyl aniline solution. The cooling was then removed and the reaction mixture was stirred for a further 2h. It was then quenched with water (15 ml) and washed with further portions of water (4 x 15 ml) before drying and evaporation. The crude organic residue was purified on silica gel,

[10% ethyl acetate in hexane], to afford *N*-benzyl-1,1,1-trifluoro-*N*-phenylmethanesulfonamide **53** as pale yellow crystals, (318 mg, 1.00 mmol, 66%); M.pt. = 76-77°C (Lit.[12] 78-79°C); [Found $(M)^+$, 315.0535. $C_{14}H_{12}F_3NO_2S$ requires $(M)^+$, 315.0531]. IR (KBr) ν = 3064, 3032, 2925, 2854, 1595, 1493, 1456, 1391, 1229, 1207, 1141, 1086, 1060, 882, 714, 695, 601, 575 and 524 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ = 4.92 (2H, s), 7.13-7.19 (4H, m), and 7.30-7.34 ppm (6H, m); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 57.7, 120.9 (q, J = 321 Hz, CF_3), 128.8, 129.0, 129.3, 129.5, 129.7, 129.7, 134.6, 136.9 ppm.

General procedure C - reductions of triflamides: Donor **13** (256 mg, 0.90 mmol, 3.0 eq.) was dissolved in degassed DMF (2 ml) in a glovebox. This solution was directly pipetted onto the dry and degassed selected substrate (0.3 mmol, 1 eq.). The mixture was left to stir overnight at 100 °C, then added to water (75 ml), and extracted with diethyl ether (50 ml and 4 x 50 ml). The combined organic layers were then washed with water (2 x 50 ml), brine (50 ml) and dried over Na_2SO_4. The crude organic residue obtained after evaporation under reduced pressure was purified by column chromatography to give the corresponding products as reported.

2,3,4,9-Tetrahydro-1H-carbazole (52)[7]

9-(Trifluoromethylsulfonyl)-2,3,4,9-tetrahydro-1H-carbazole **51** (91 mg, 0.3 mmol, 1.0 eq.) was reacted according to procedure C, to afford 2,3,4,9-tetrahydro-1H-carbazole **52** as a white solid, (27 mg, 0.16 mmol, 53%); M.pt. = 113-115 °C (Lit.[15] 114-115 °C); IR ν (powder) = 3397, 2926, 2846, 1467, 1363, 1284, 1144, 1008, 972, 918 and 719 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ = 1.87-1.97 (4H, m), 2.72-2.76 (4H, m), 7.09 (1H, td, 7.4, 1.2 Hz), 7.13 (1H, td, 7.4, 1.4 Hz), 7.28-7.30 (1H, m), 7.47-7.49 (1H, m), and 7.65 ppm (1H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 21.2, 23.6, 23.6, 23.6, 110.5, 110.7, 118.1, 119.4, 121.3, 128.2, 134.4, 136.0 ppm. *m*/*z* (ESI) 172.07 ($[M+H]^+$).

***N*-benzylaniline (54)**[7]

N-Benzyl-1,1,1-trifluoro-*N*-phenylmethanesulfonamide **53** (95 mg, 0.3 mmol, 1.0 eq.), was reacted according to procedure C, [but reacting for 2 days] to afford *N*-benzyl aniline **54** as a white/yellow crystalline solid (22 mg, 0.12 mmol, 40%); M.pt. = 32-34 °C (Lit.[16] 33-34 °C); IR (powder) ν = 3417, 3051, 3022, 2926, 1601, 1508, 1447, 1360, 1301, 1105, 956, 827 and 688 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 4.35 (2H, s), 6.67 (2H, d, J = 7.8 Hz), 6.74 (1H, t, J = 7.3 Hz), 7.17-7.22 (2H, m), 7.28-7.31 (1H, m) and 7.40-7.41 ppm (4H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 48.7, 113.2, 117.9, 127.6, 127.9, 129.0, 129.6, 139.8, 148.5 ppm; *m*/*z* (ESI) 183.98 ($[M+H]^+$).

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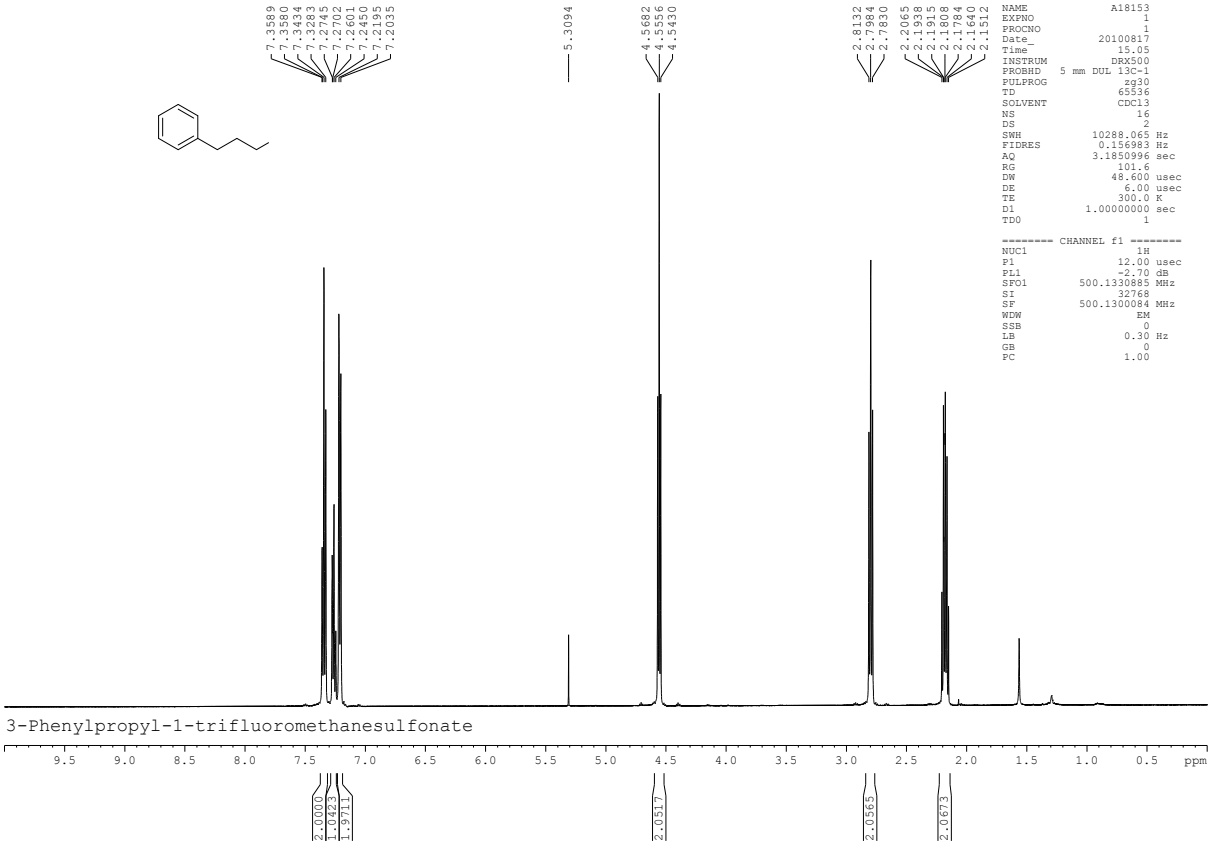

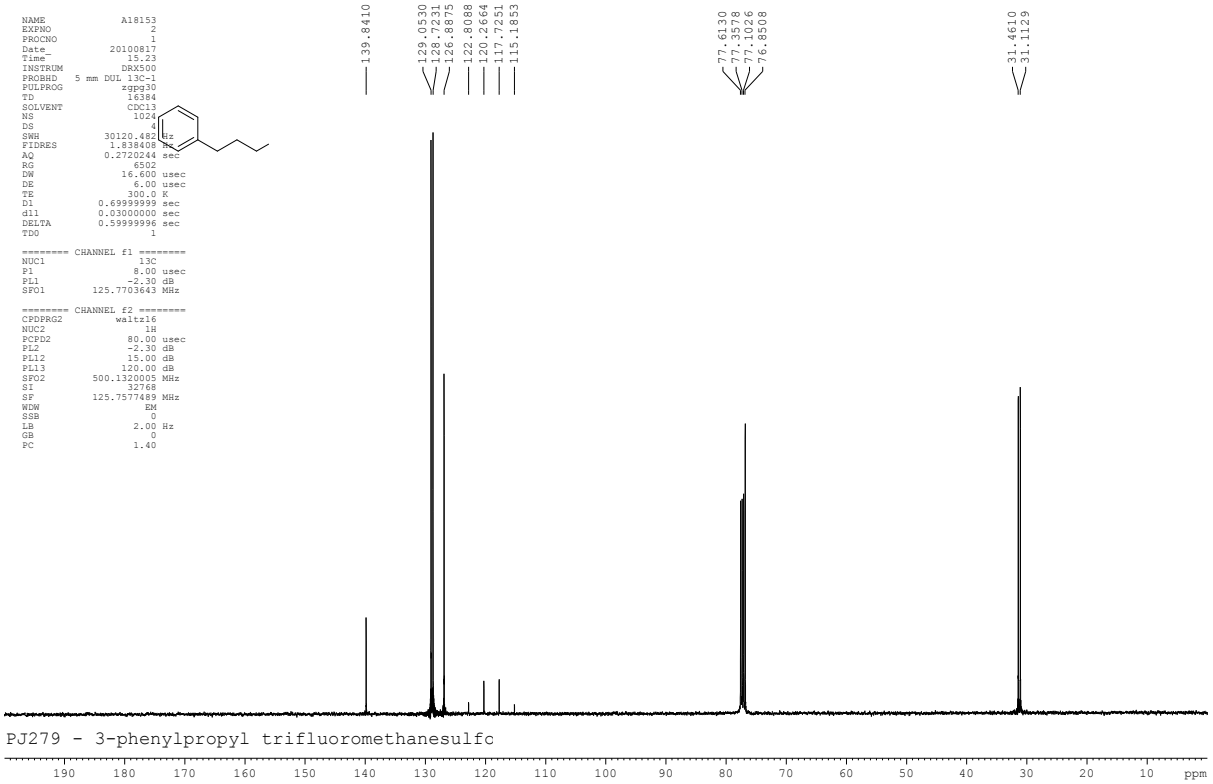

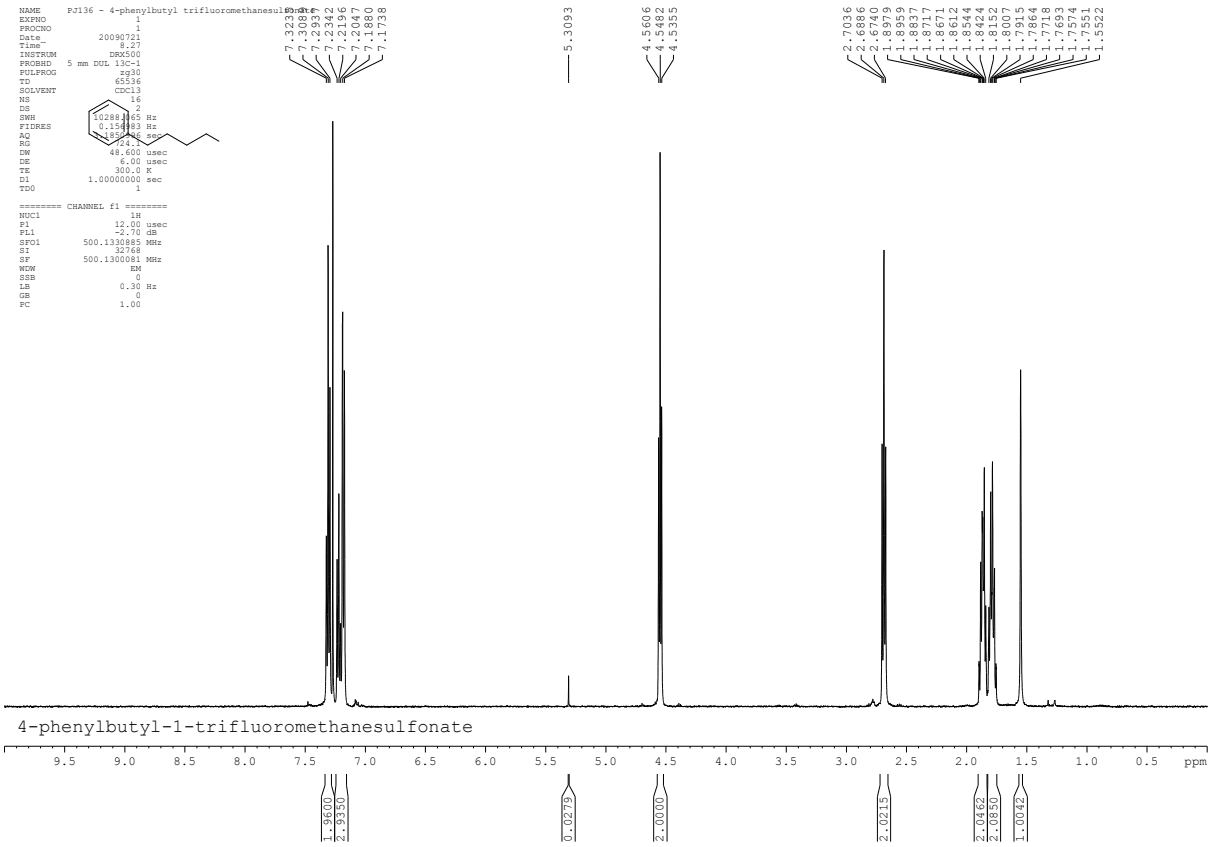

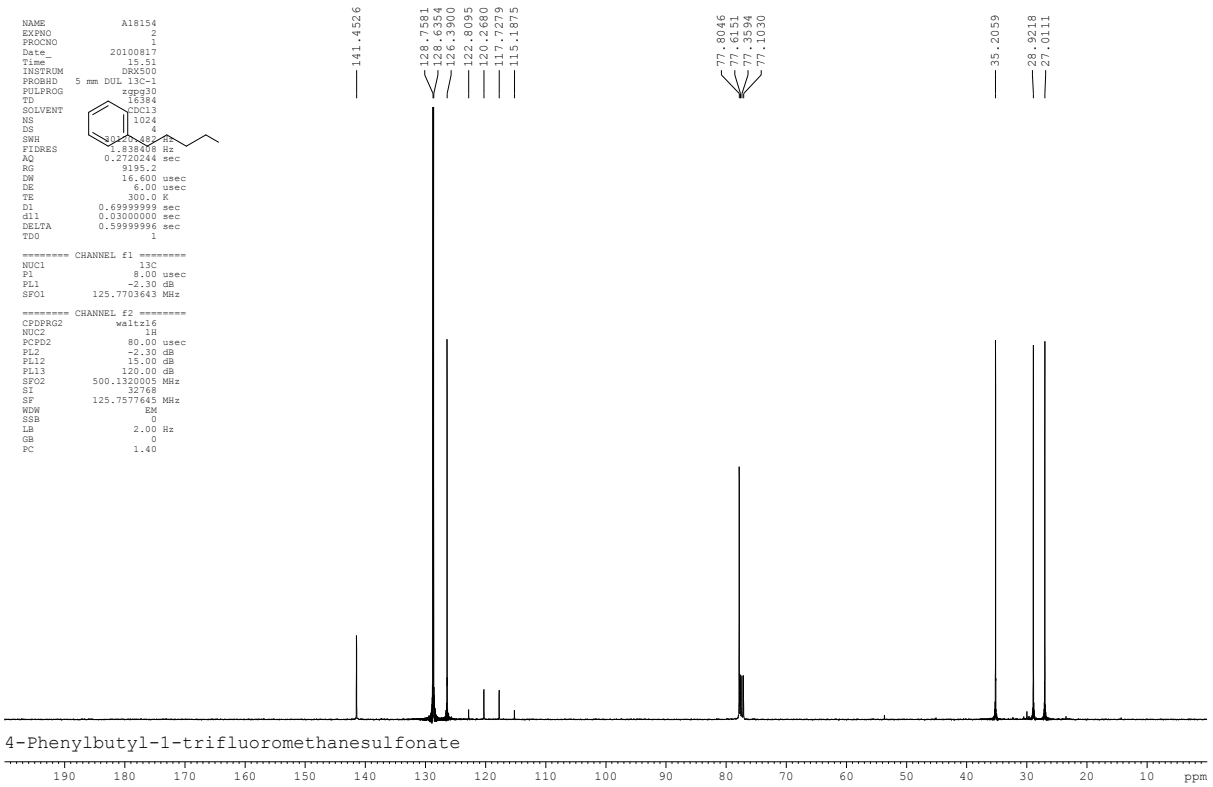

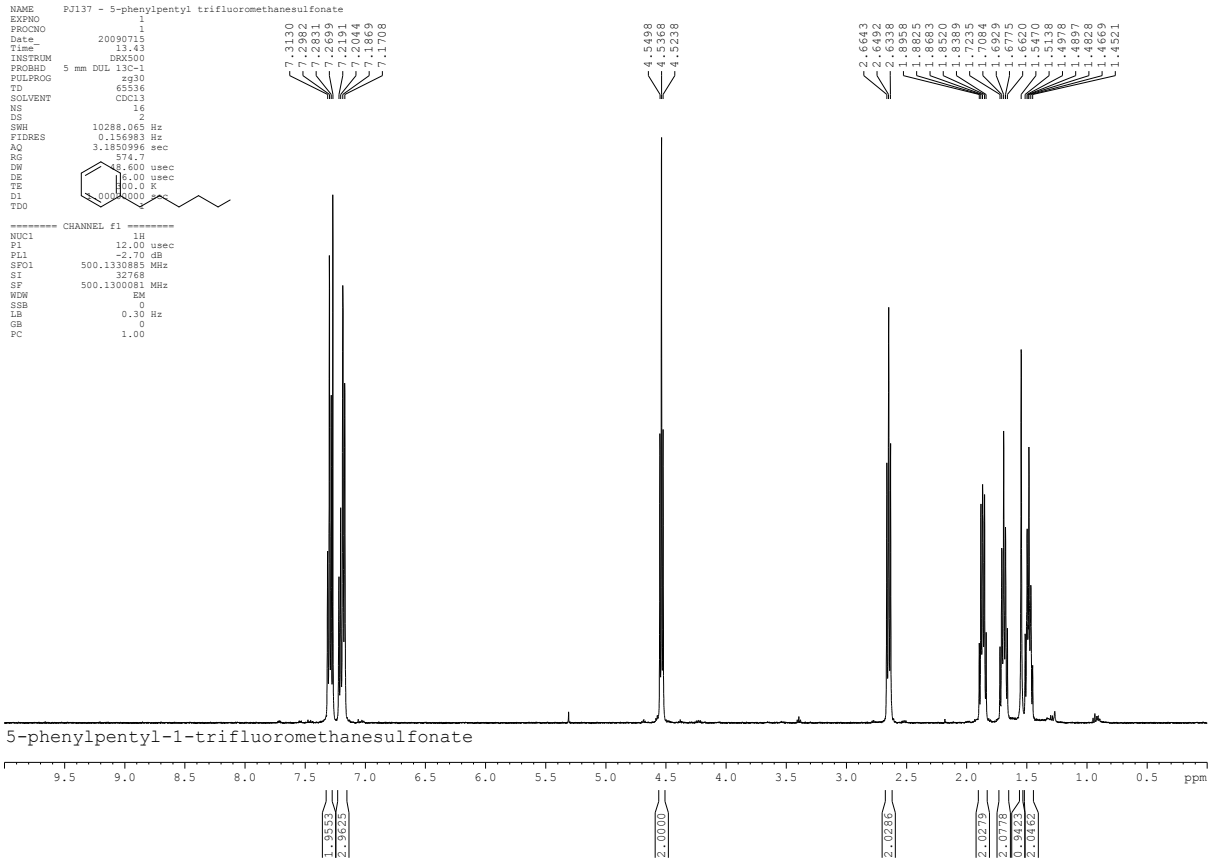

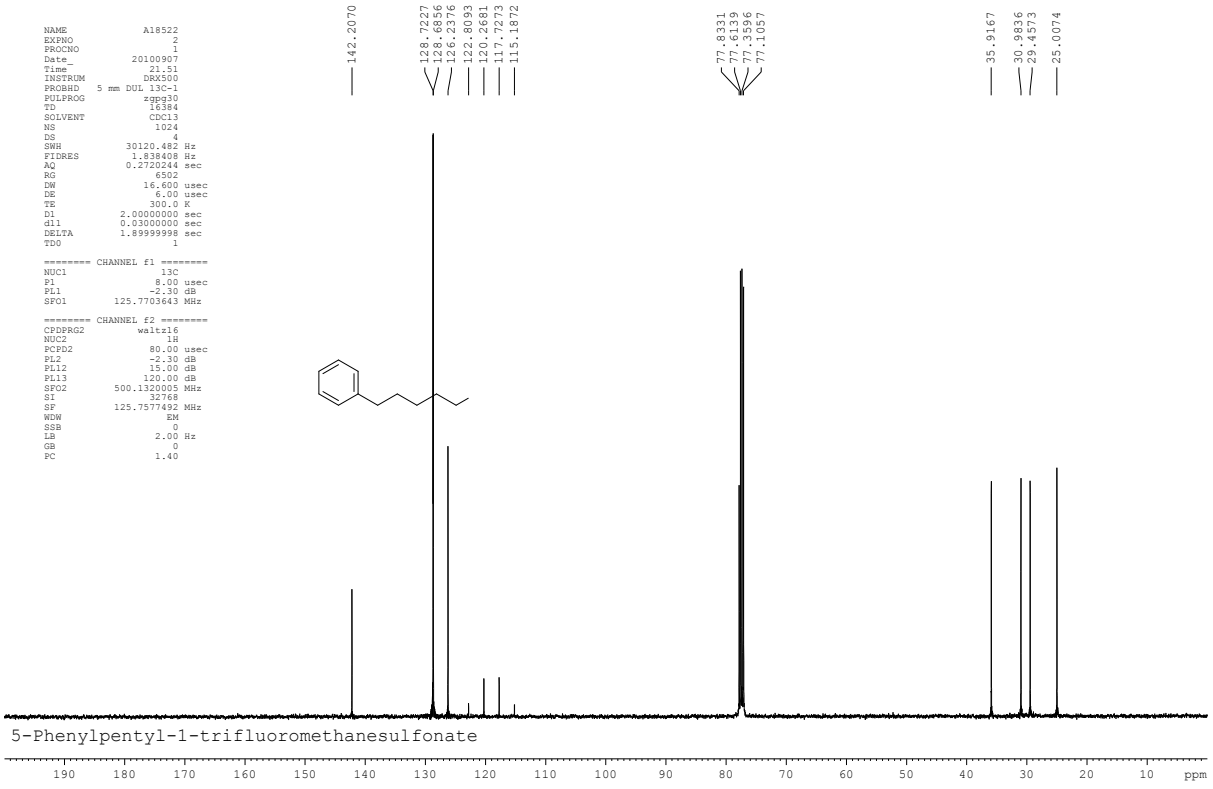

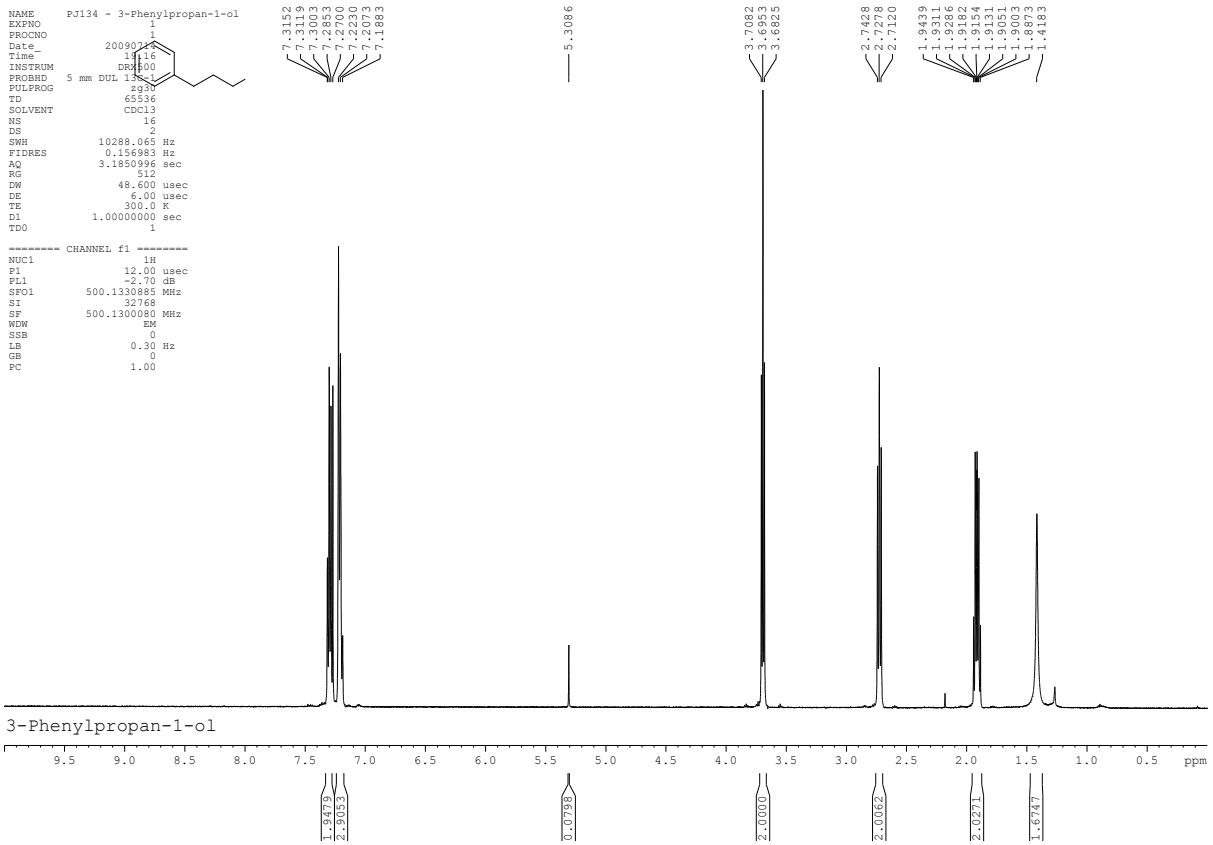

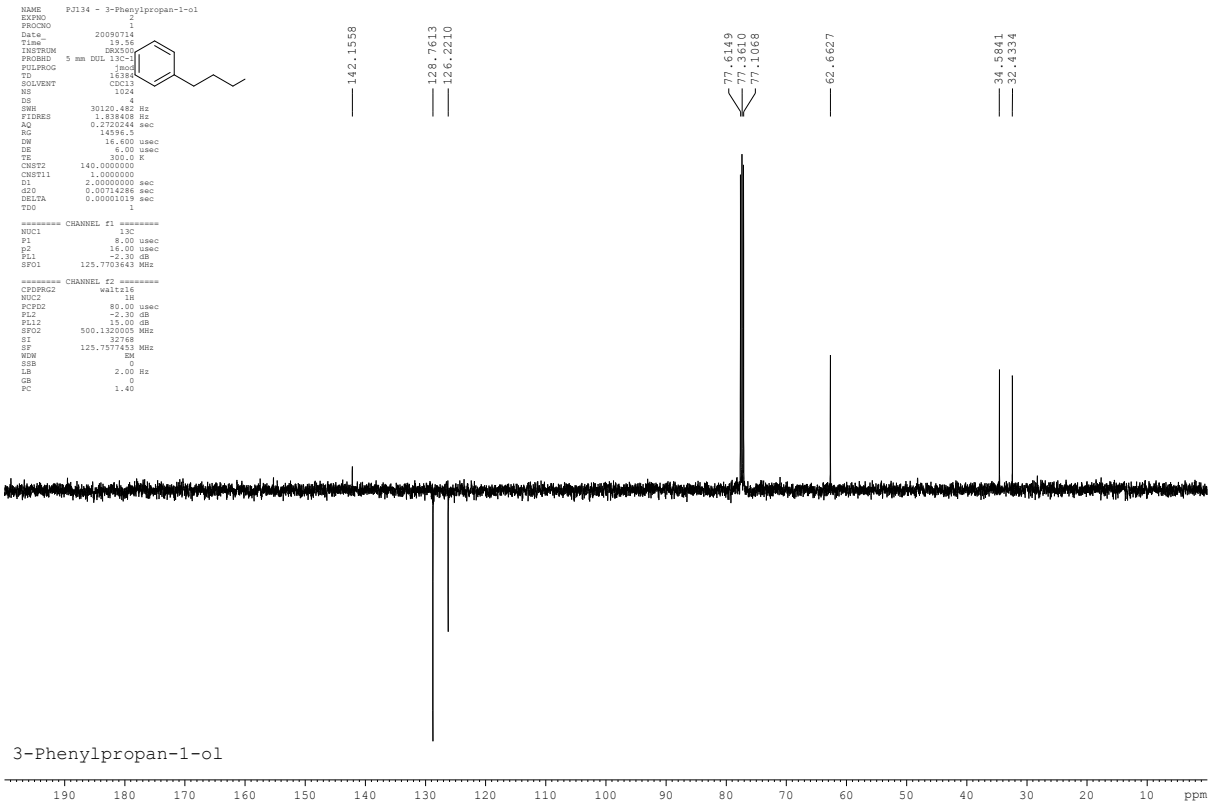

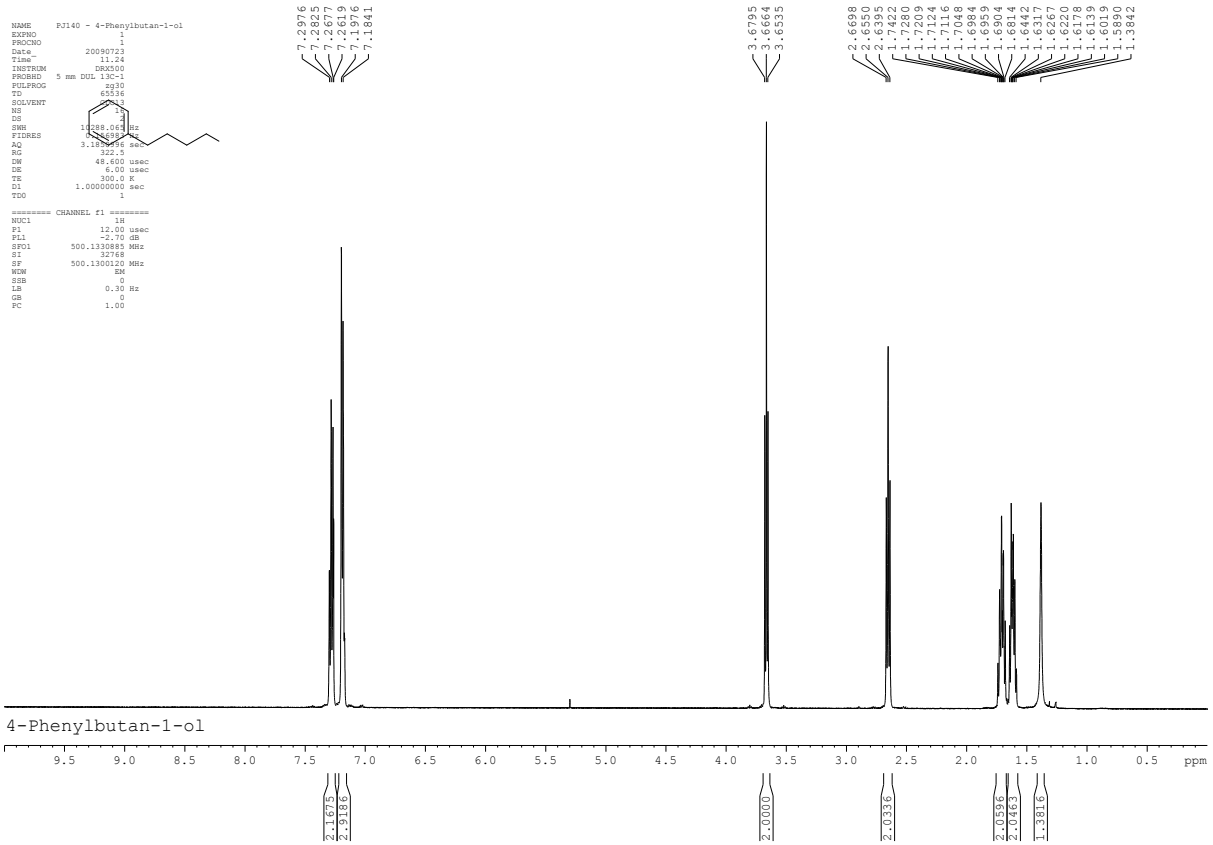

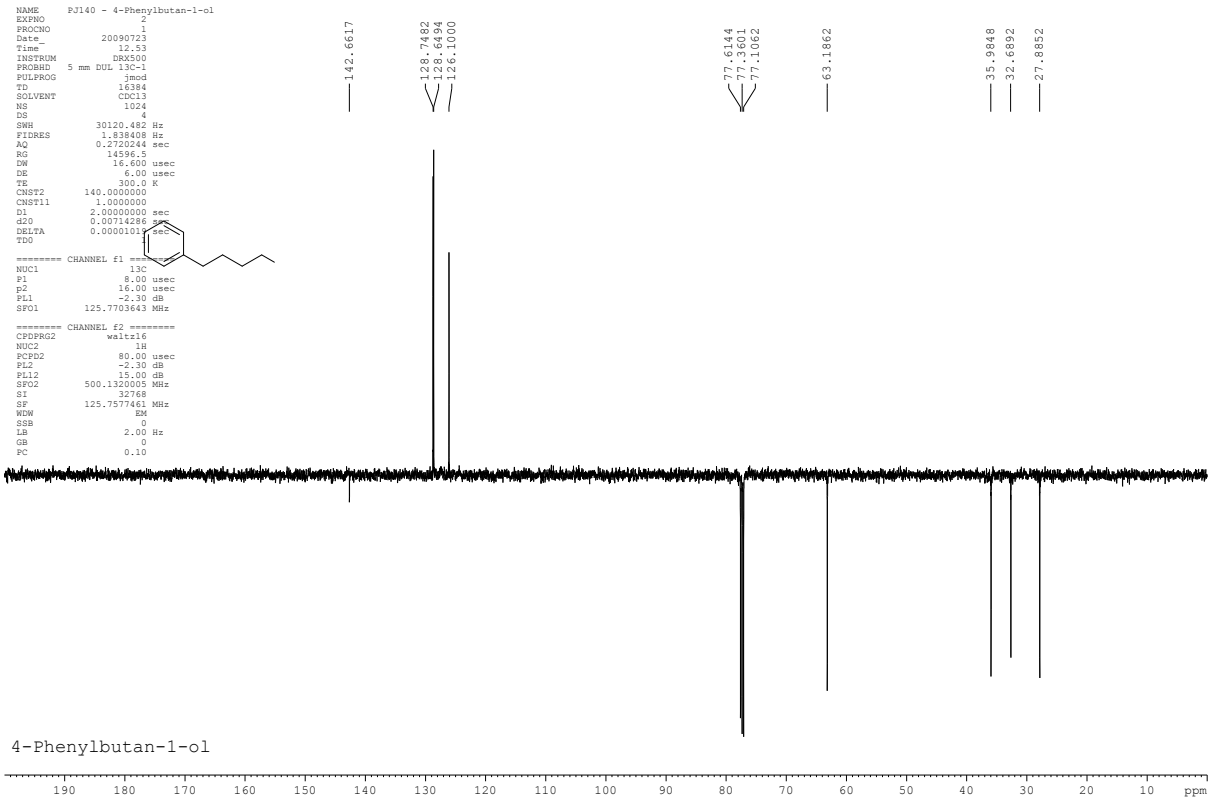

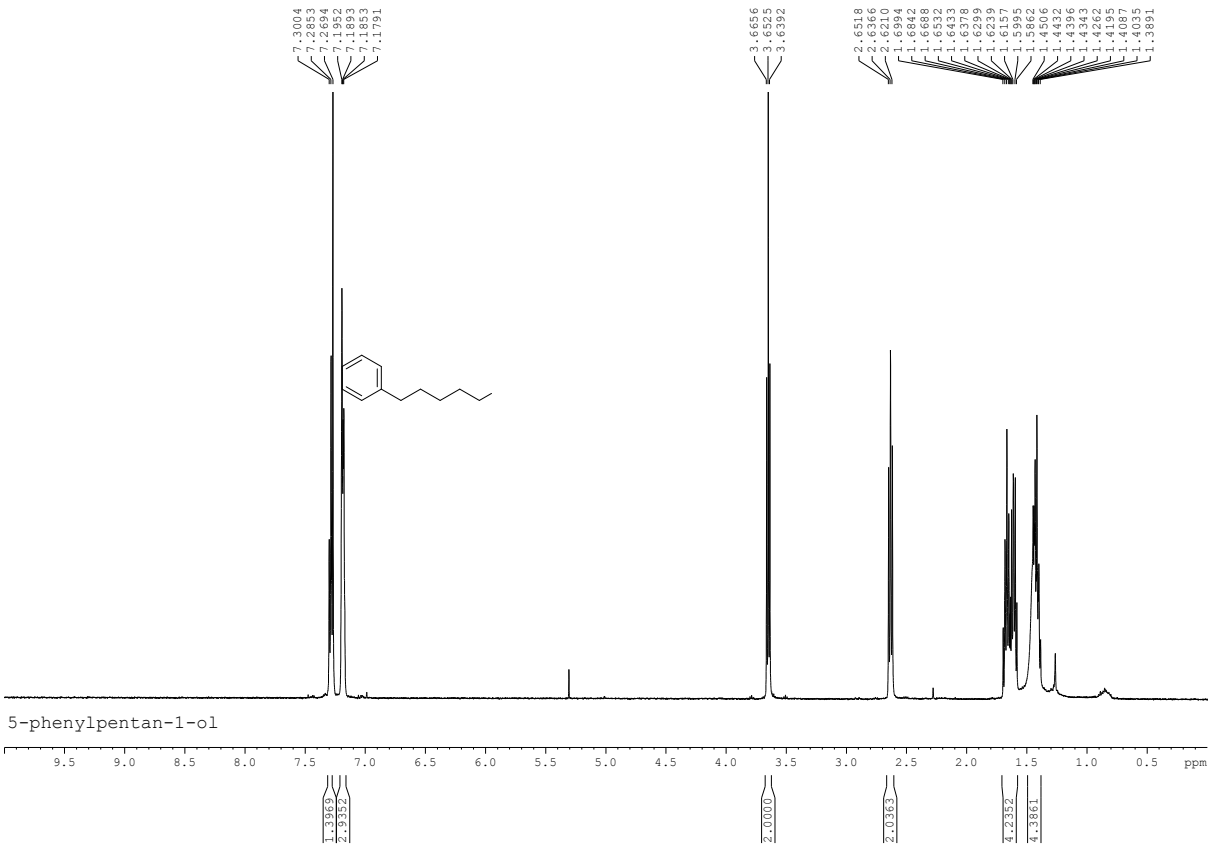
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1.4343
1.4262
1.4195
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5-phenylpentan-1-ol
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
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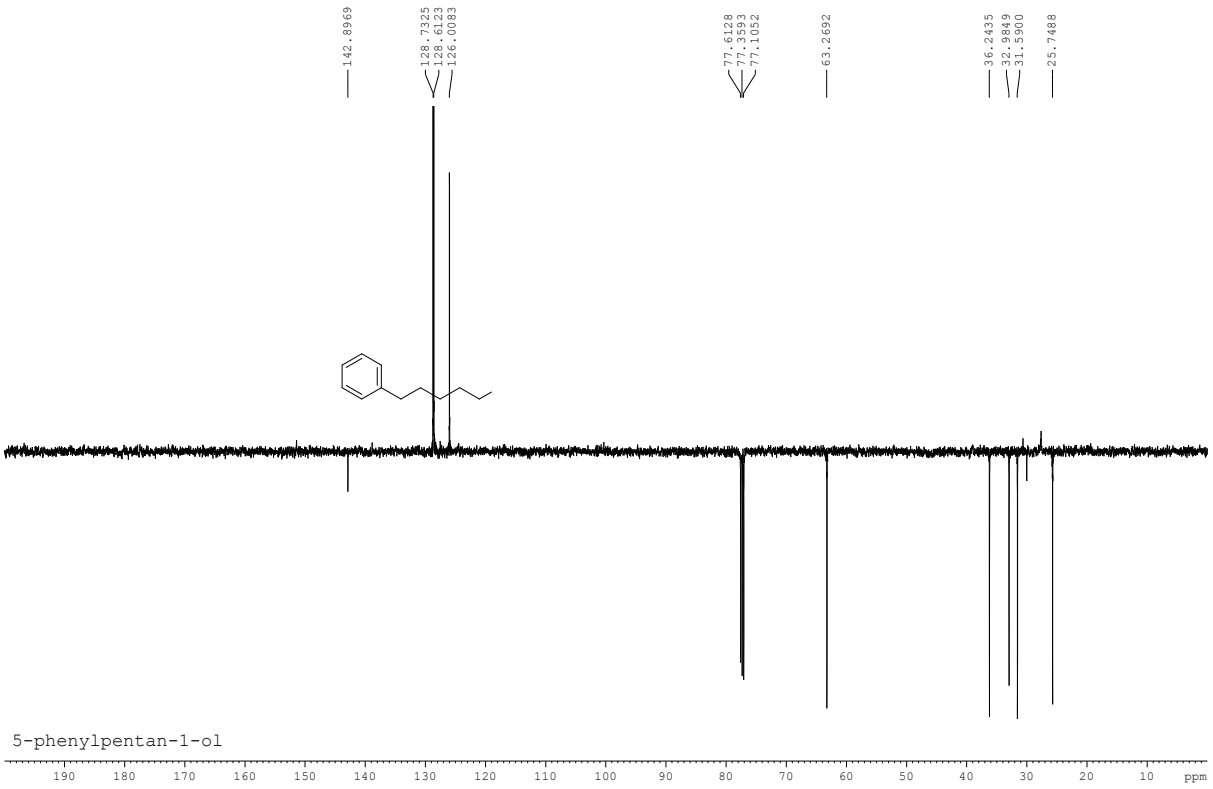
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5-phenylpentan-1-ol
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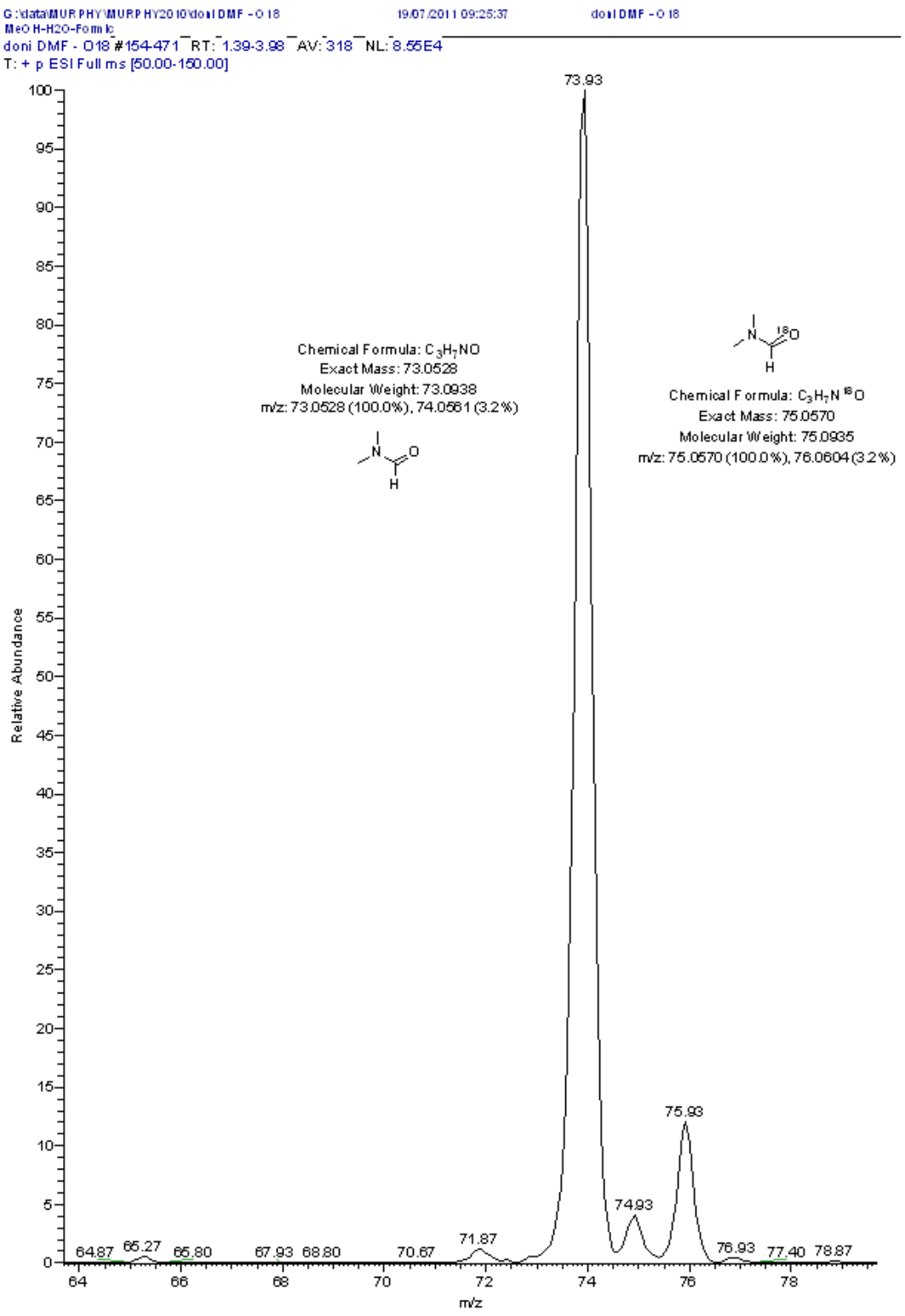
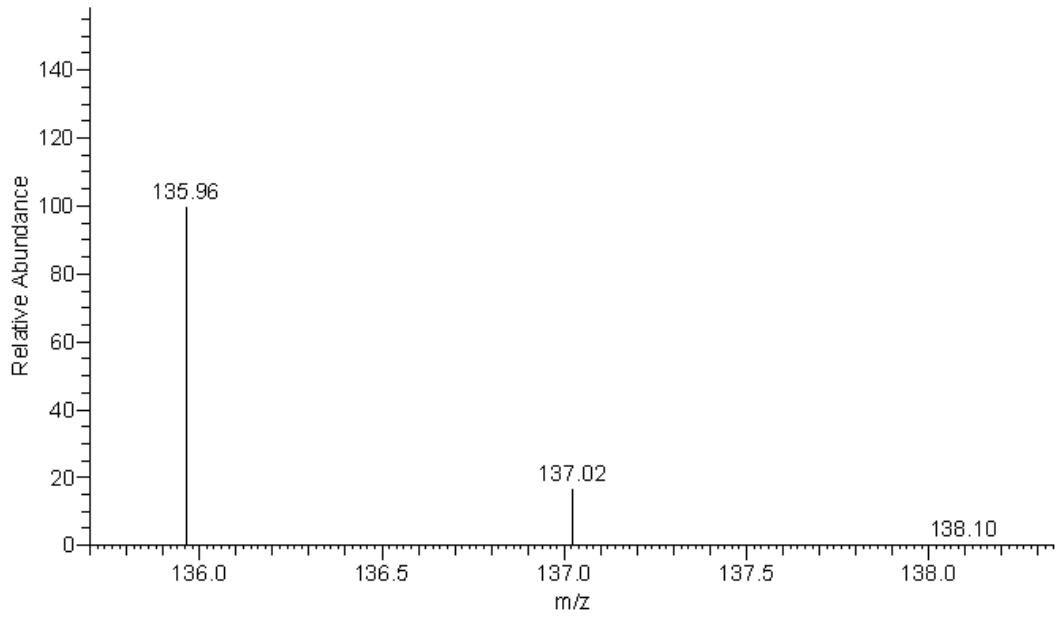
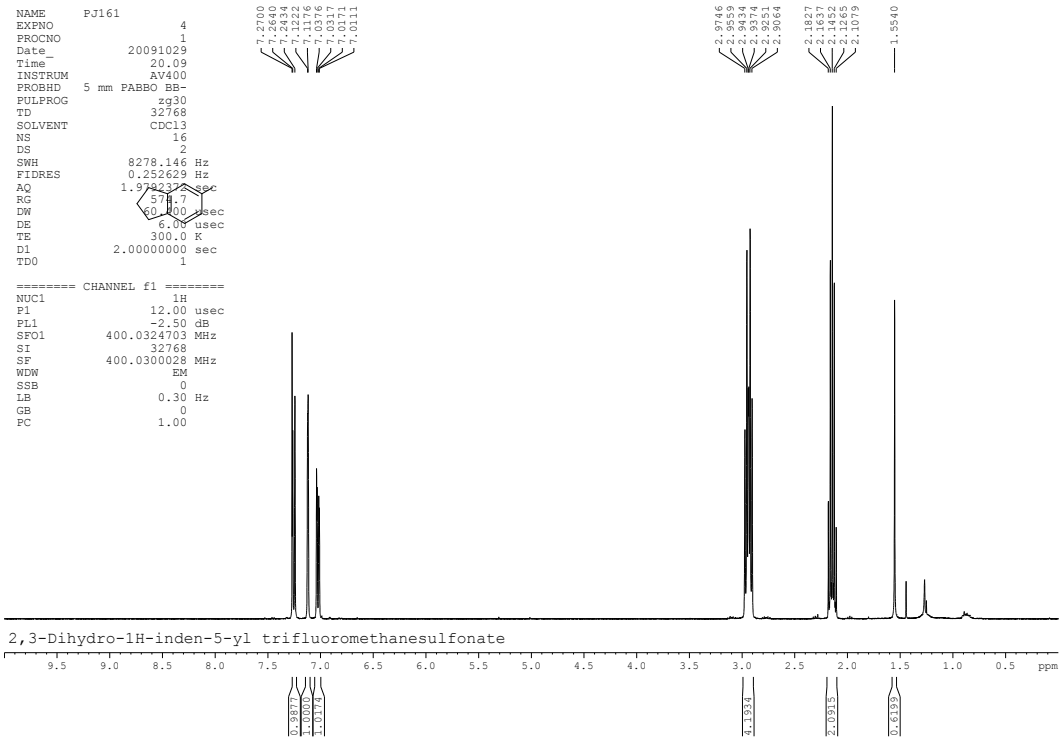


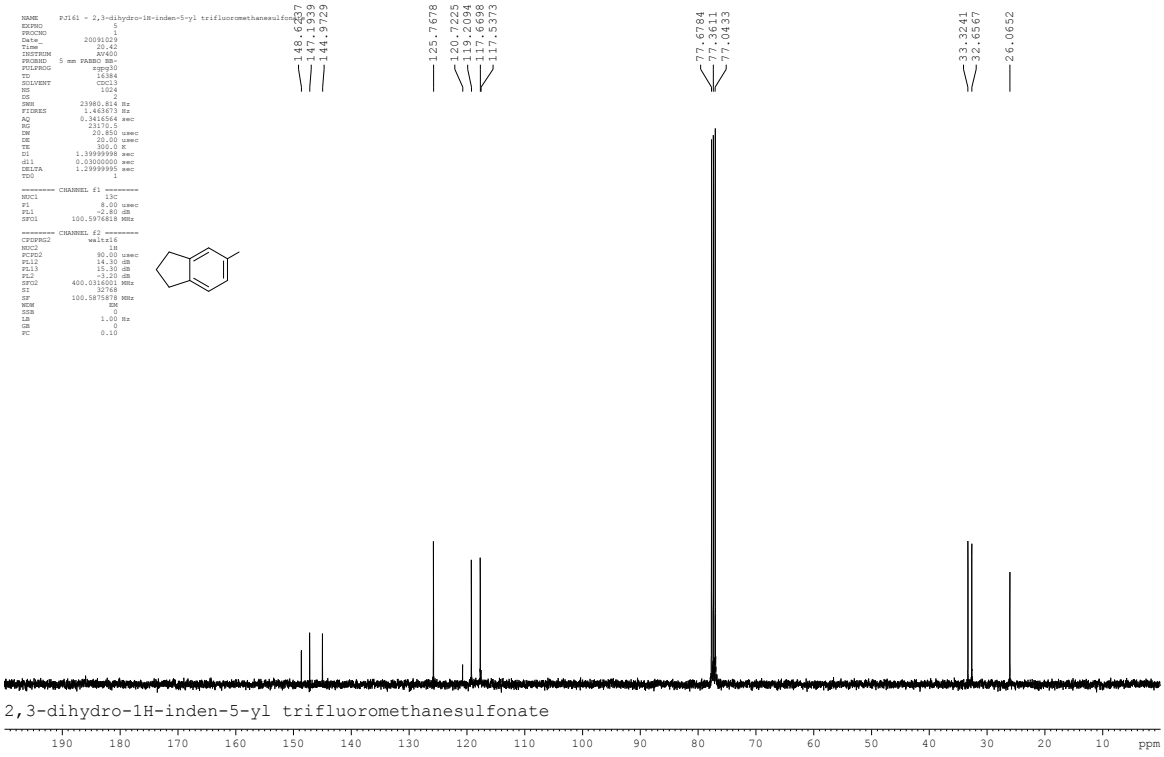
Mass spectrum of labelled DMF, showing incorporation of ^{18}O (75.93)

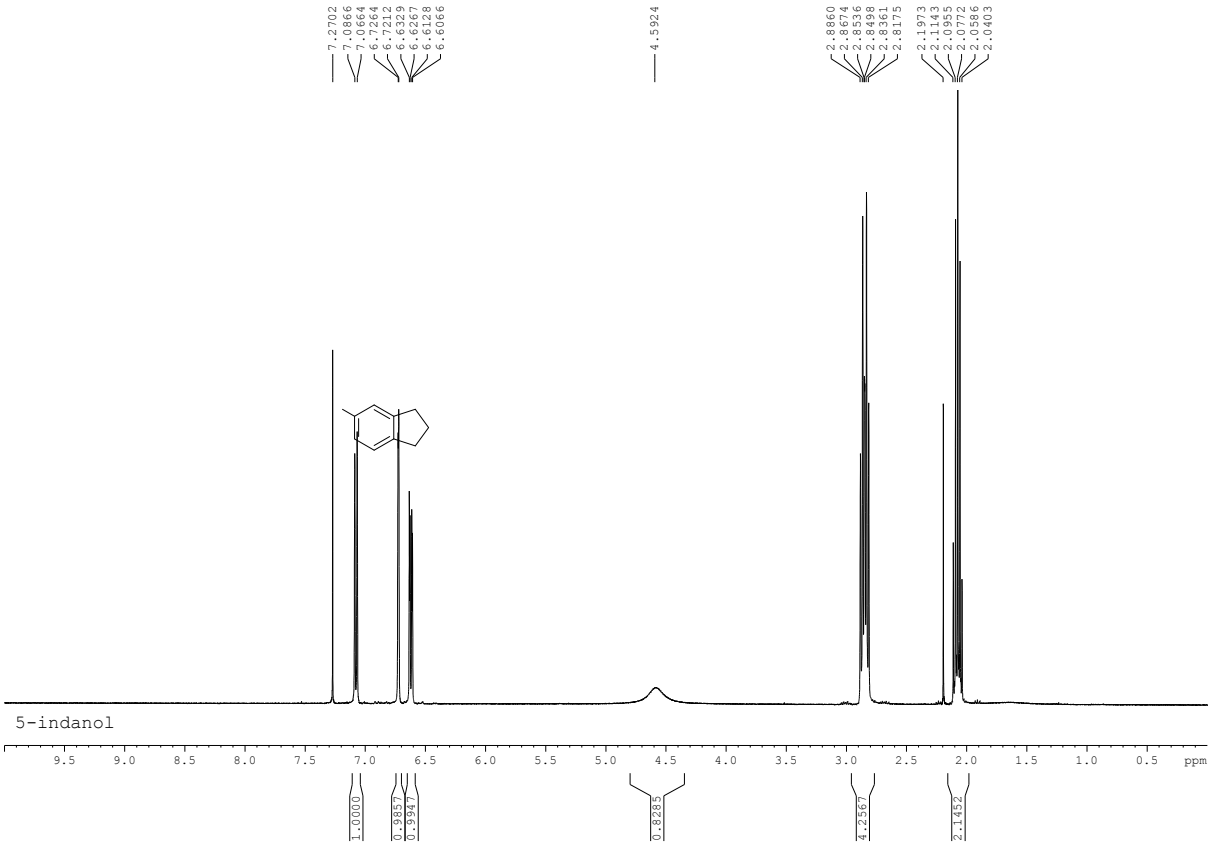


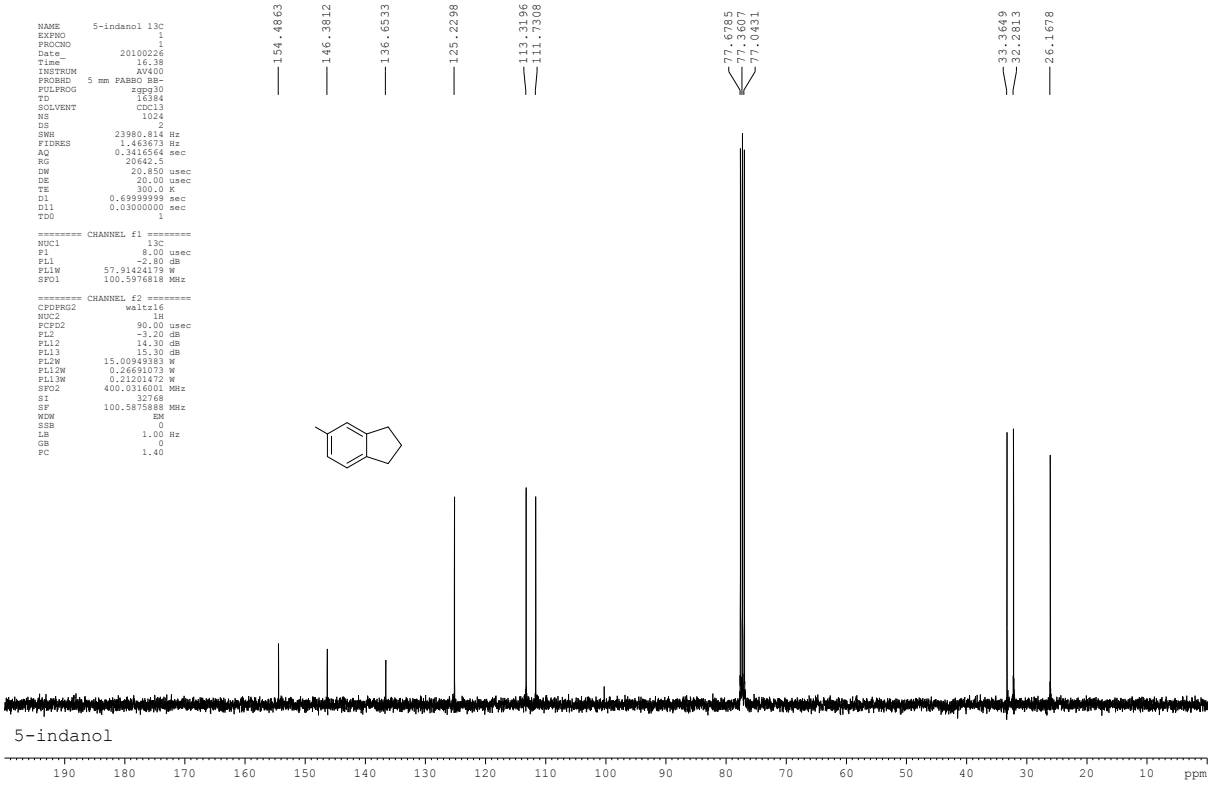
m/z	Intensity	Relative
135.96	14595.4	100.00
137.02	2439.1	16.71
138.10	106.1	0.73

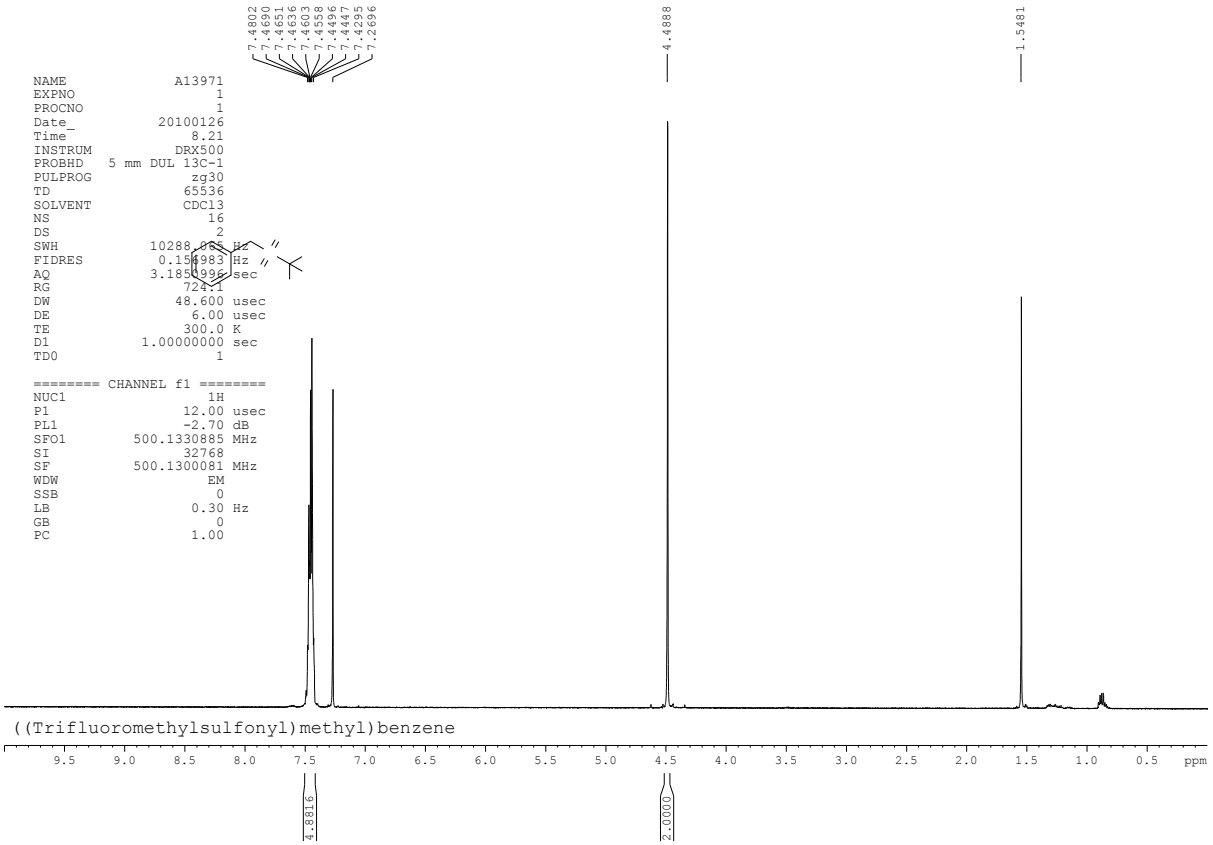
Expansion of the mass spectrum of $Ph(CH_2)_3OH$ **24** formed from the experiment conducted in ^{18}O-enriched DMF. Mass spectrum shows no enrichment of the peak at 138.10 (M+2) compared to the unlabelled peak at 135.96 (M with ^{16}O present).

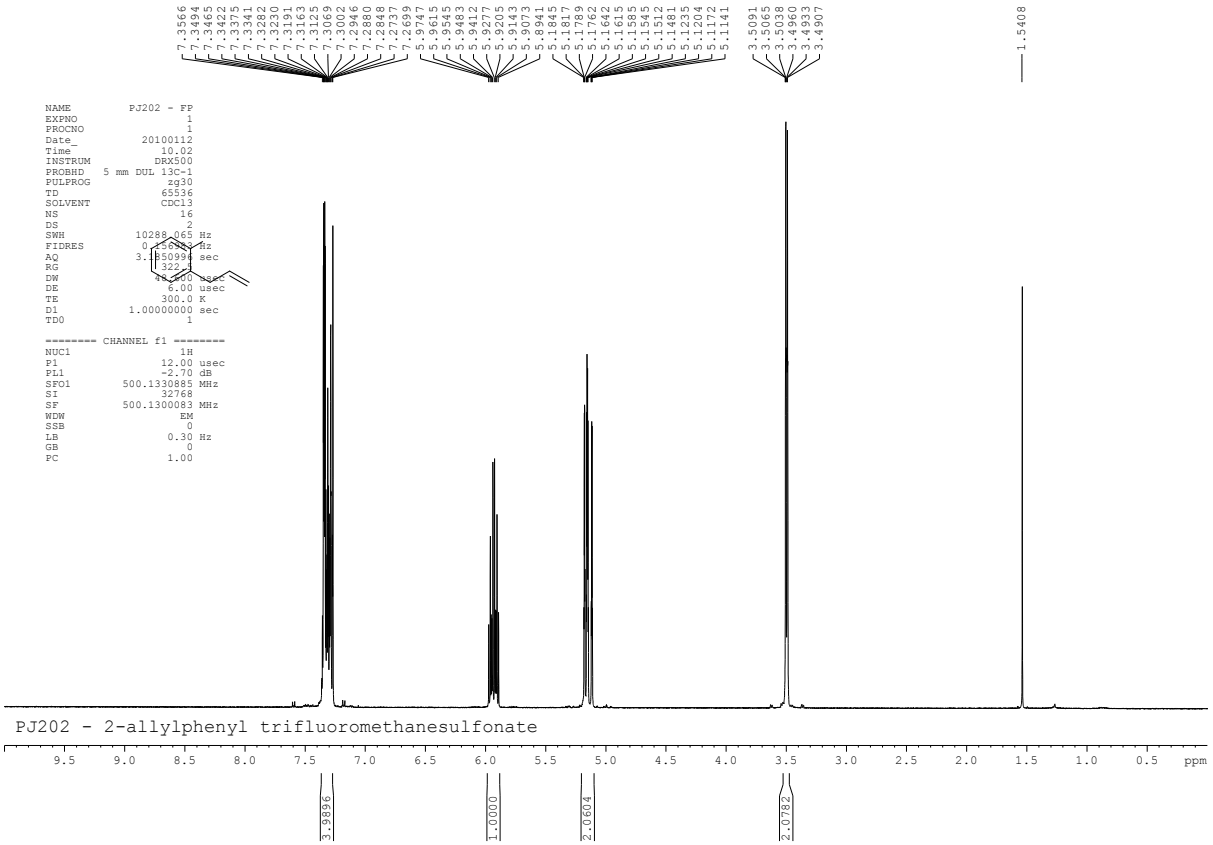


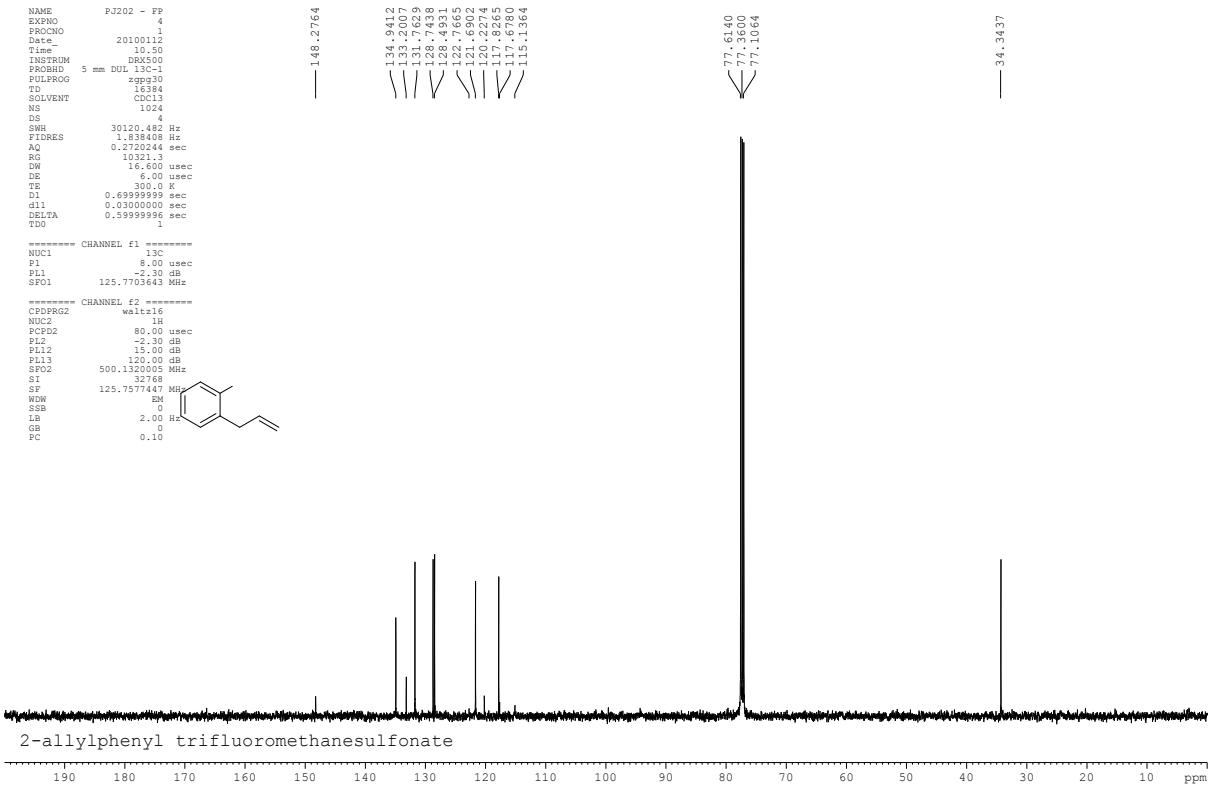


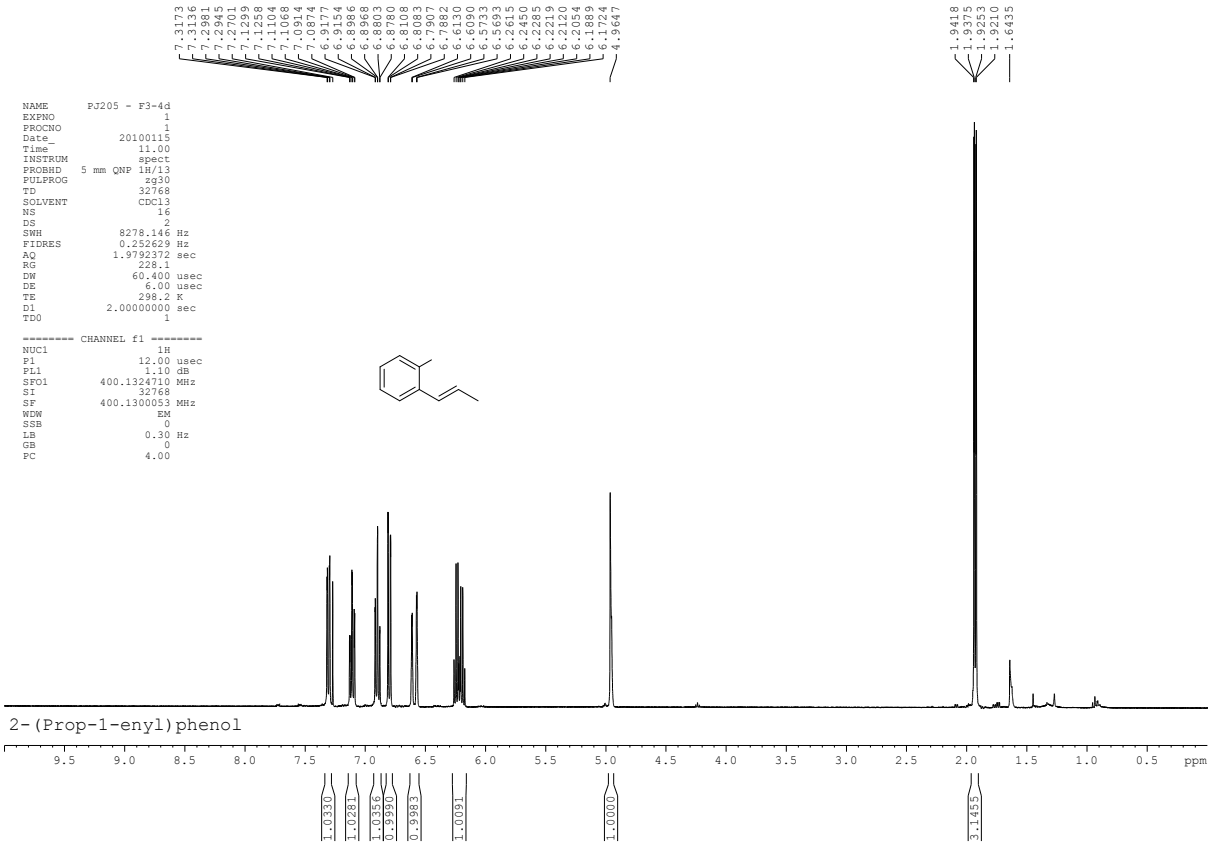








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SOLVENT CDCl3
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FIDRES 0.252629 Hz
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RG 228.1
DW 60.400 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
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P1 12.00 usec
PL1 1.10 dB
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2-(Prop-1-enyl)phenol
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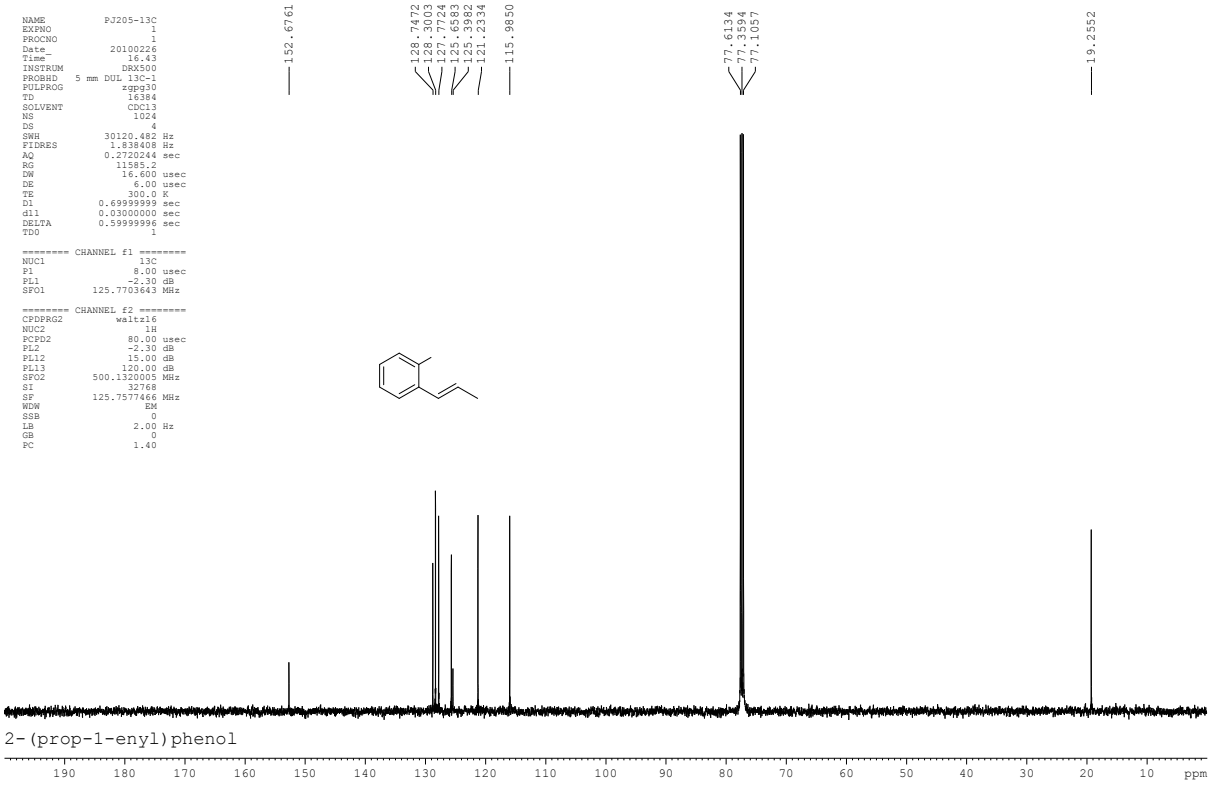
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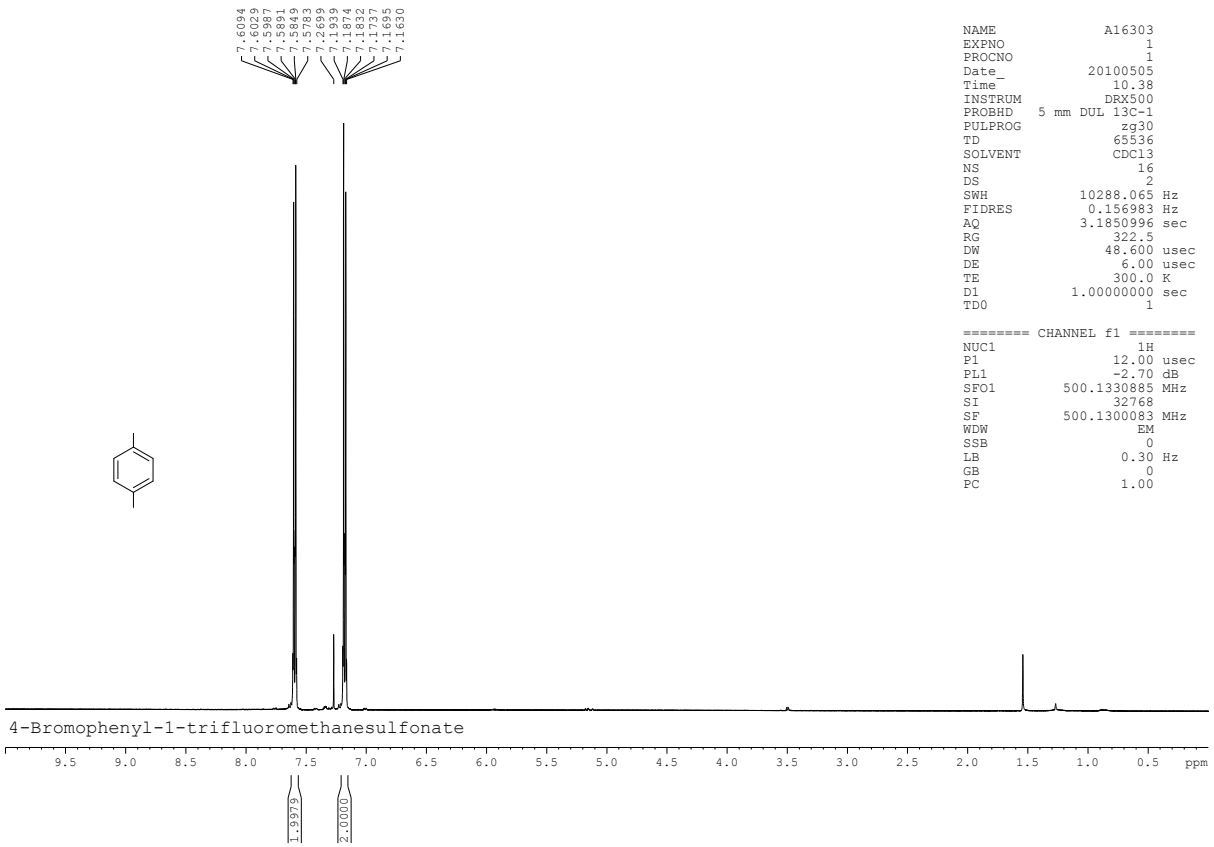
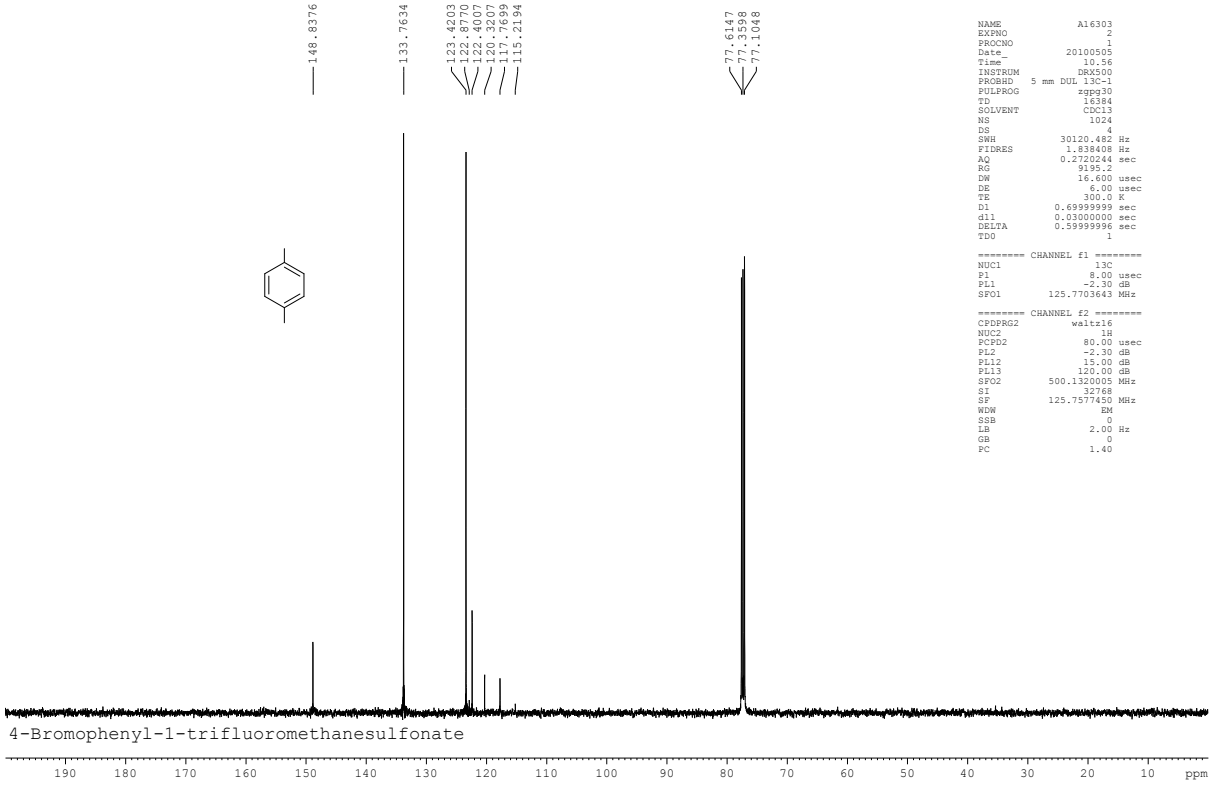
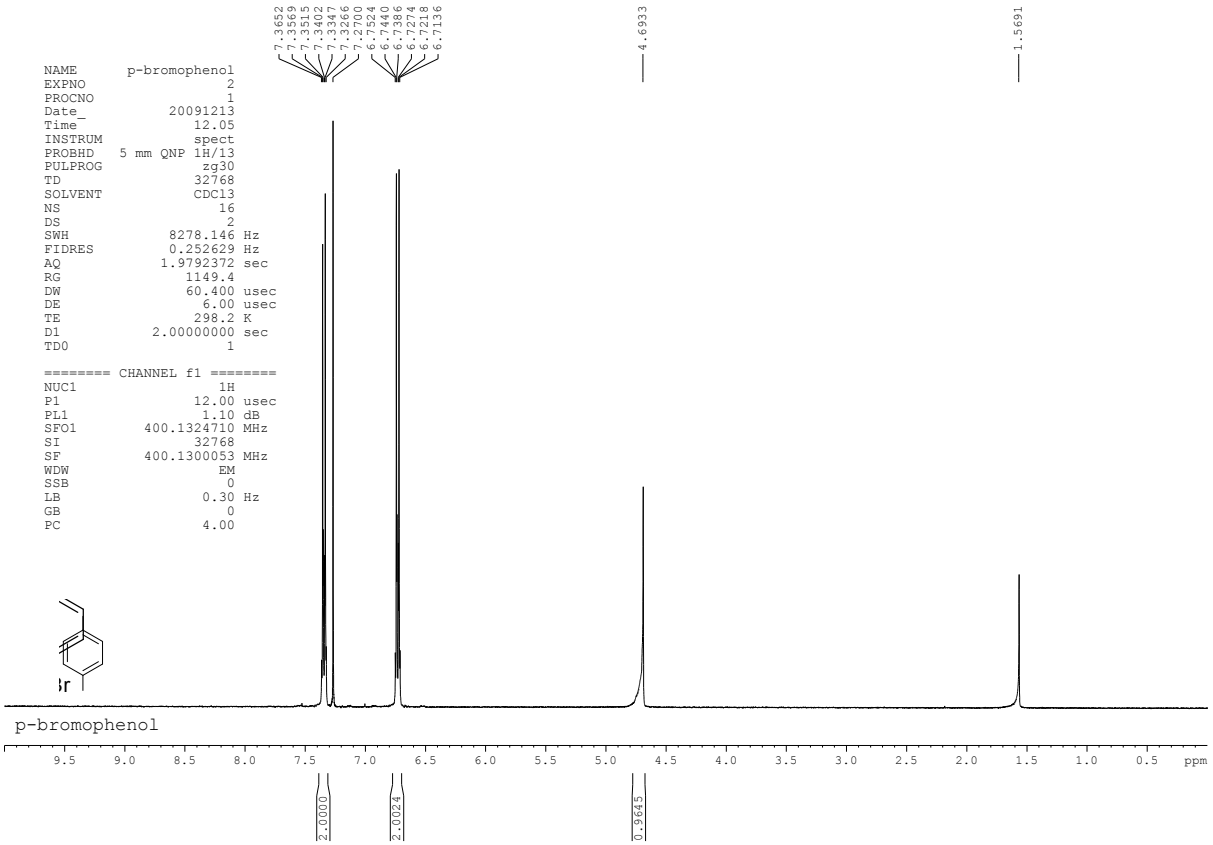
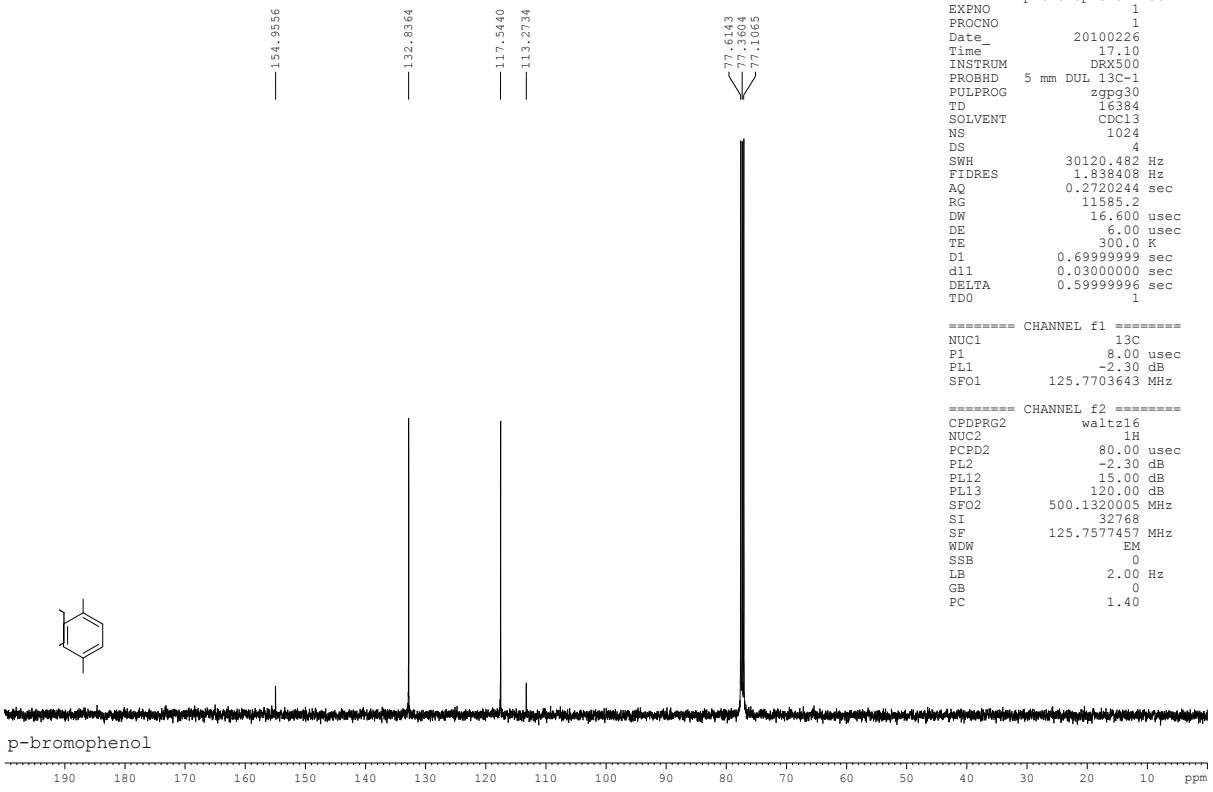
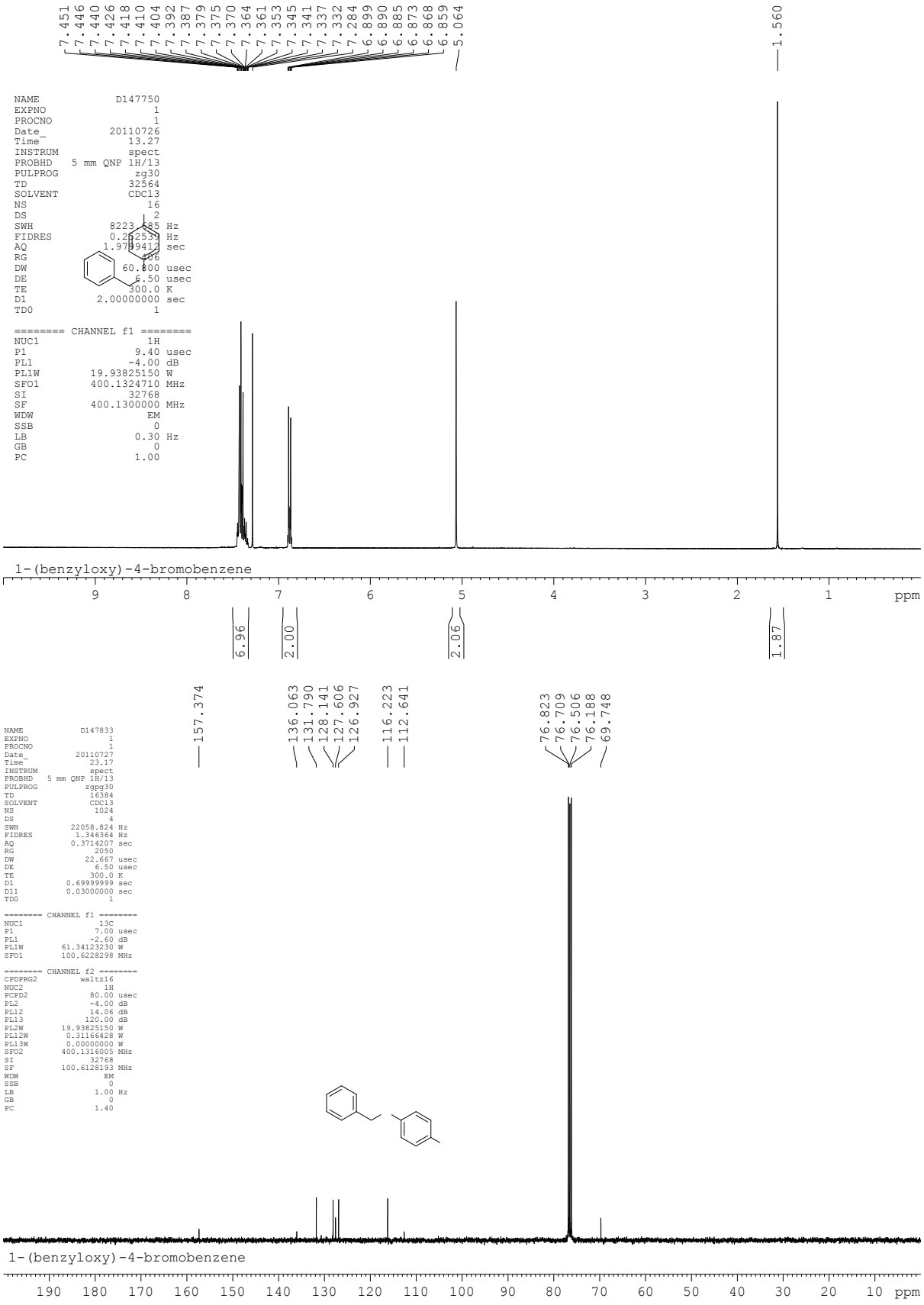
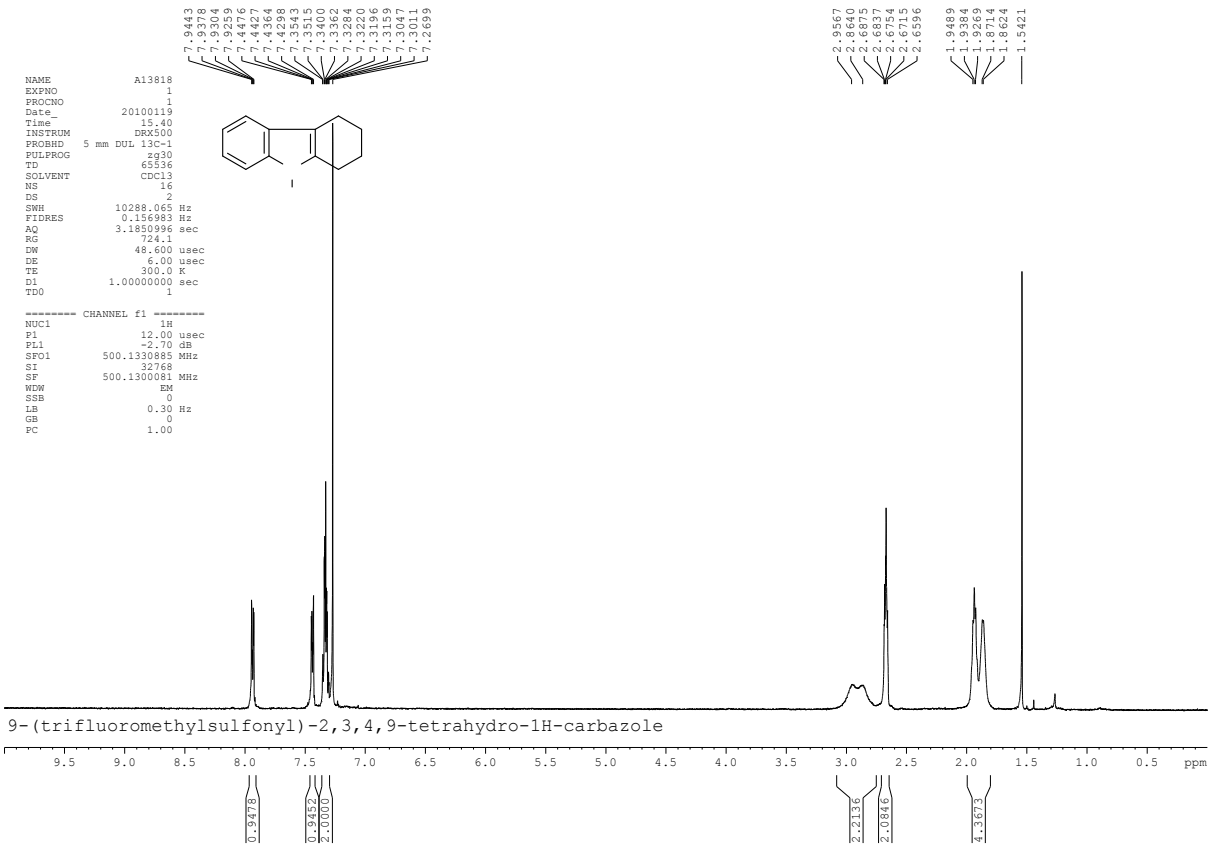


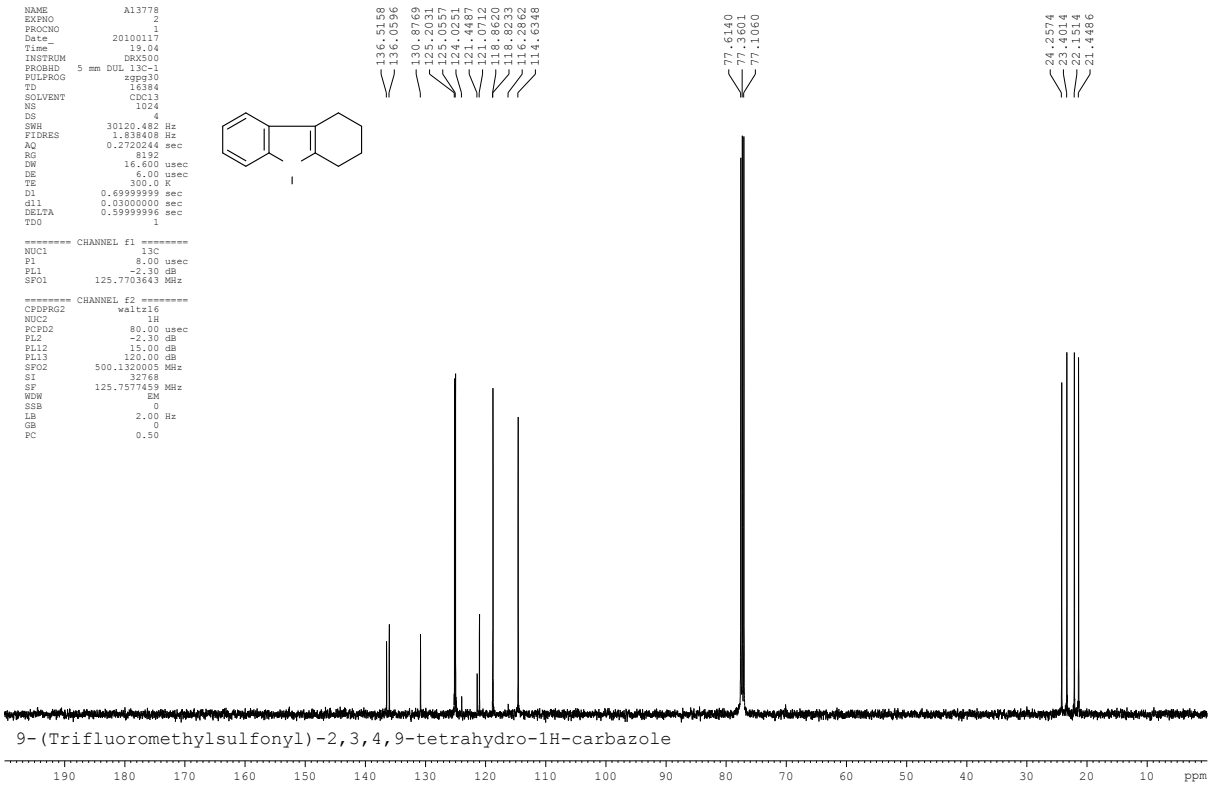


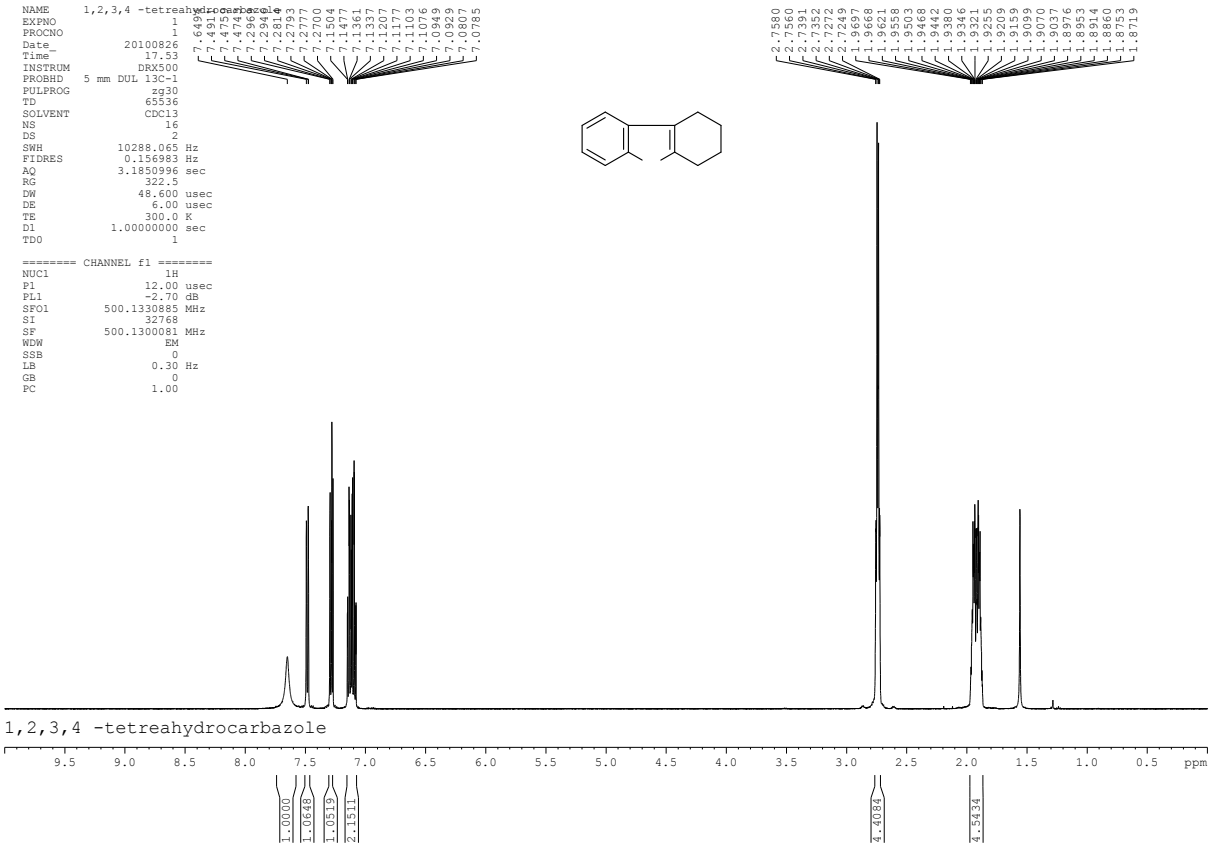


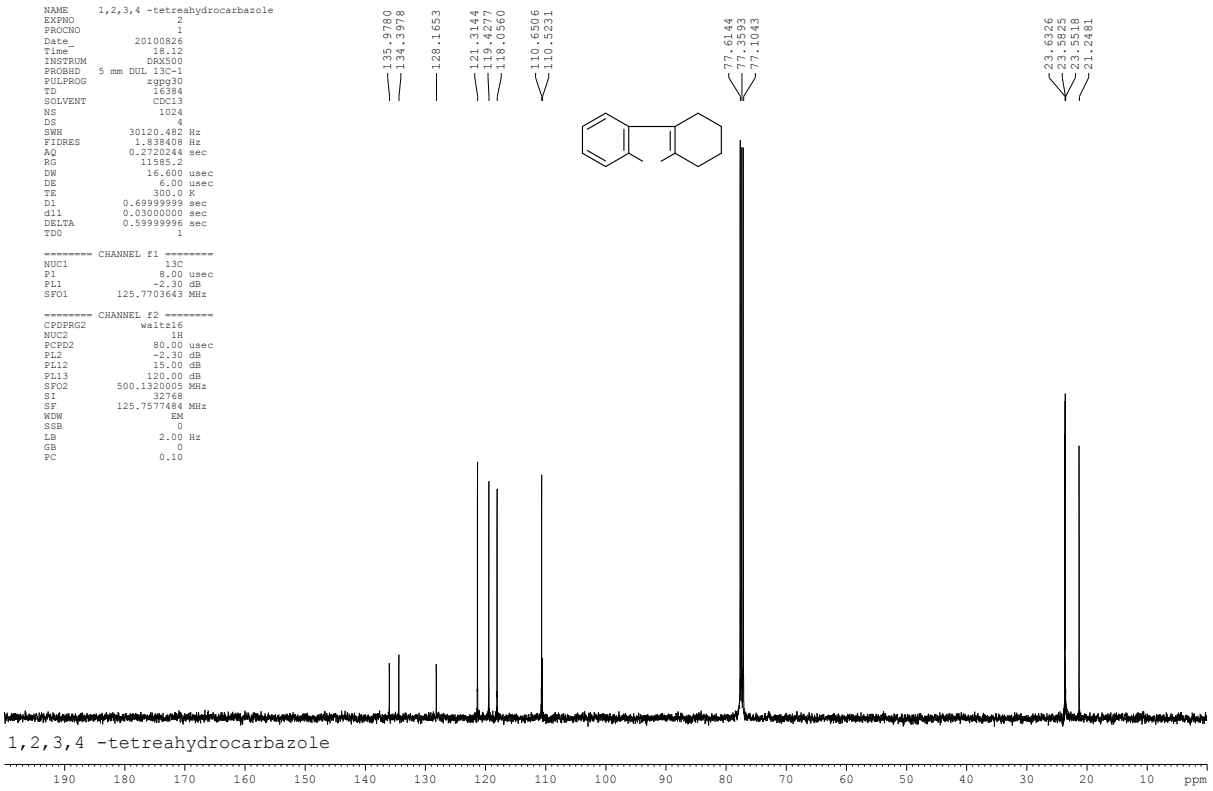


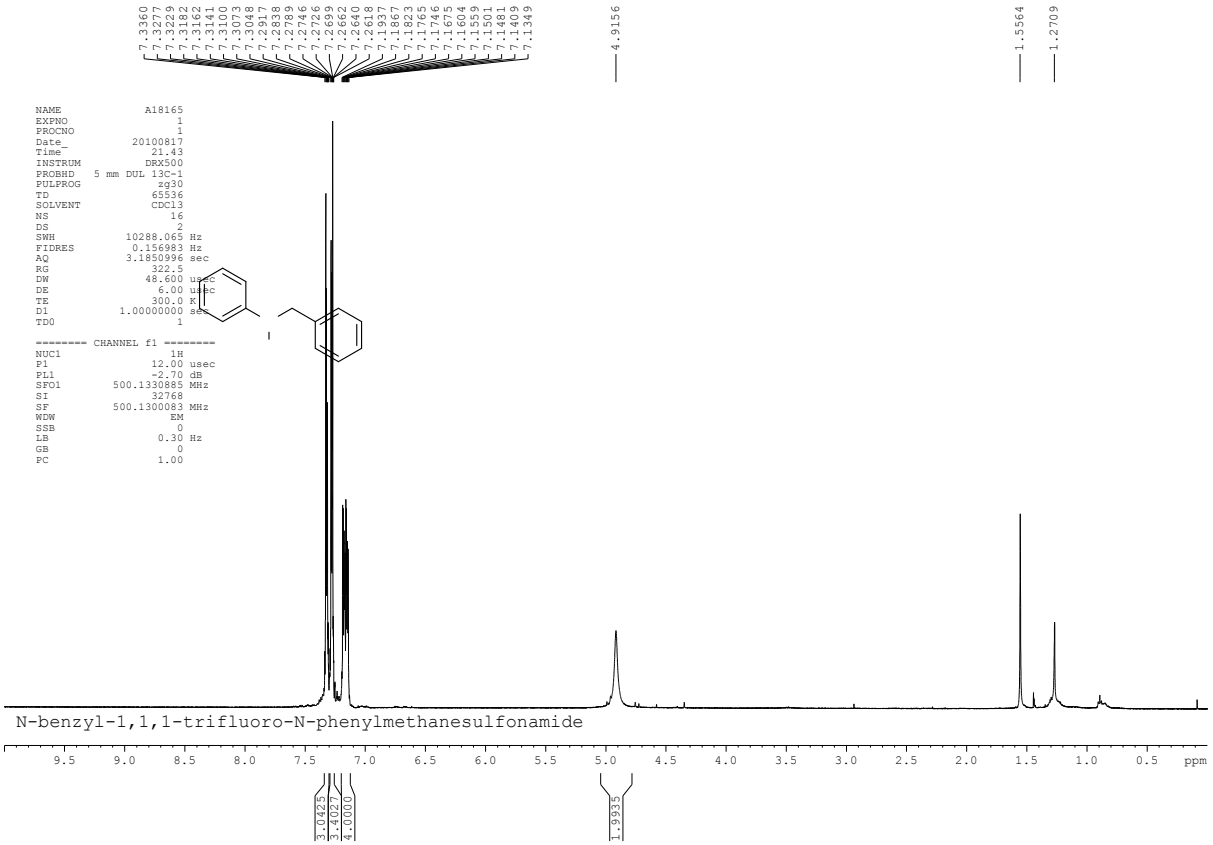


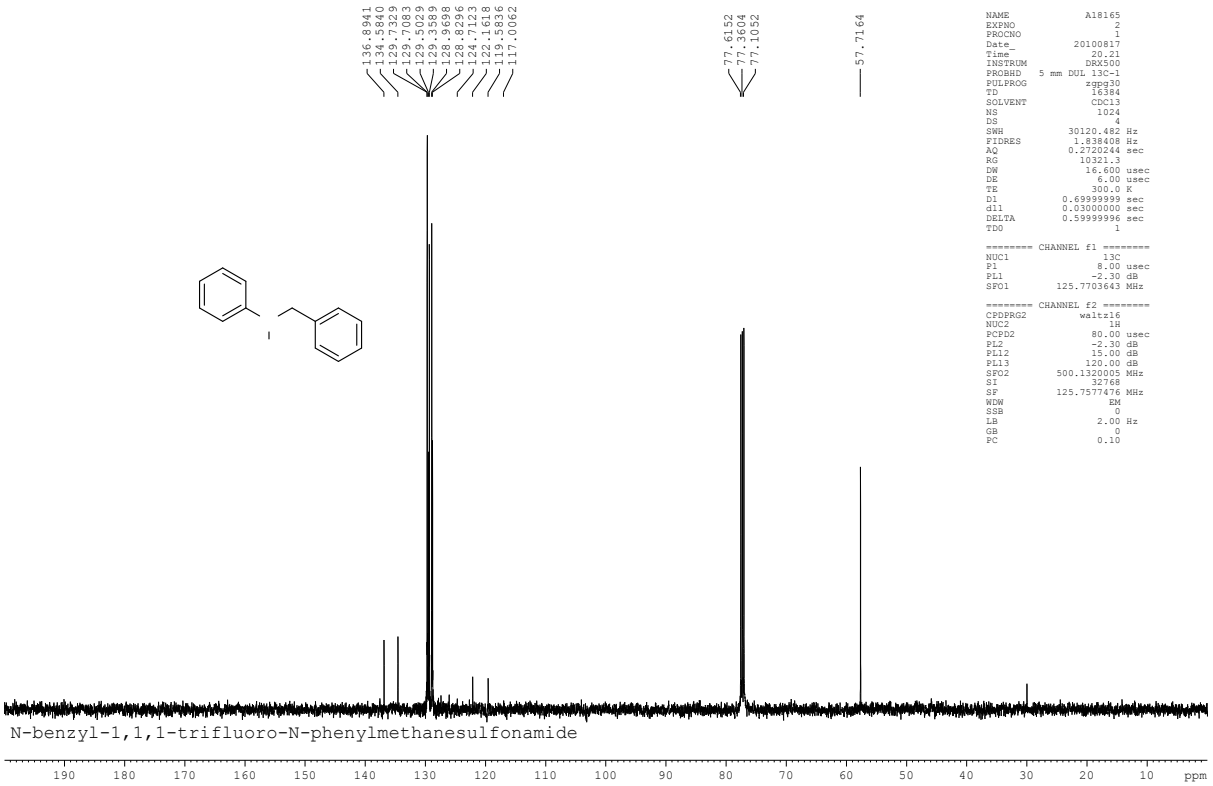


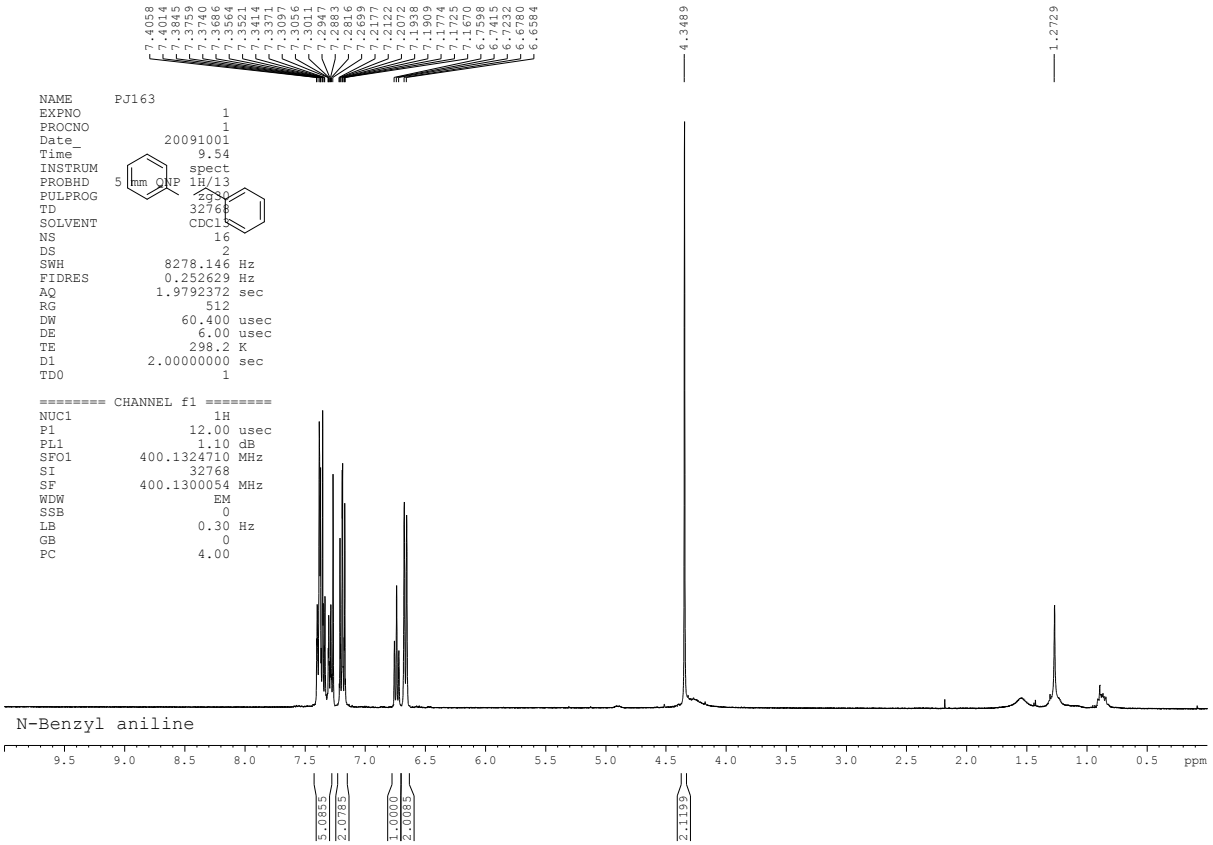


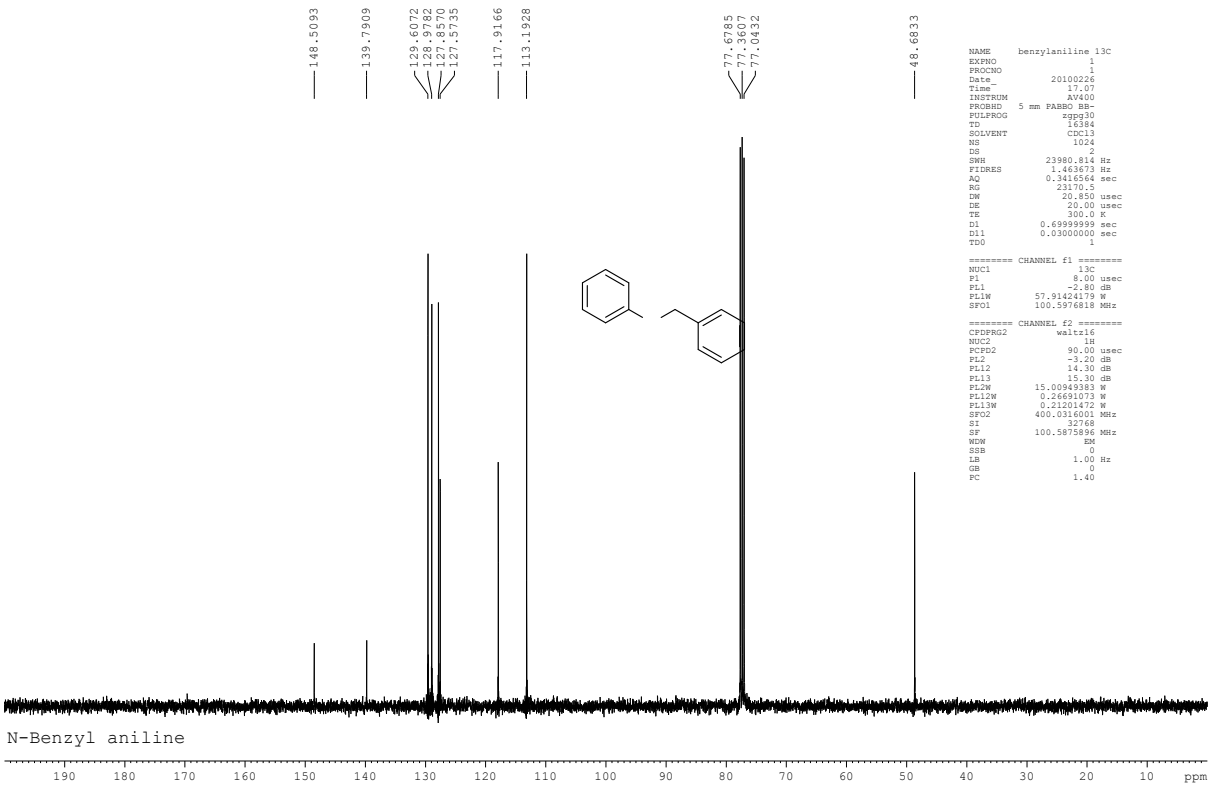

NAME 1,2,3,4 -tetreahydrocarbazole
EXPNO 1
PROCNO 1
Date_ 20100826
Time_ 17.53
INSTRUM DRX500
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10288.065 Hz
FIDRES 0.156983 Hz
AQ 3.1850996 sec
RG 322.5
DW 48.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -2.70 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.649 7.495 7.475 7.474 7.296 7.294 7.281 7.279 7.277 7.270 7.197 7.194 7.137 7.135 7.207 7.177 7.103 7.076 7.049 7.029 7.007 7.005
2.580 2.560 2.391 2.352 2.272 2.249 1.968 1.962 1.958 1.950 1.946 1.942 1.938 1.934 1.921 1.915 1.909 1.903 1.901 1.897 1.895 1.893 1.891 1.886 1.875 1.871
1,2,3,4 -tetreahydrocarbazole
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.0000 1.0648 1.0519 2.1511 4.4084 4.5434


NAME 1,2,3,4 -tetreahydrocarbazole
EXPNO 2
PROCNO 1
Date_ 20100826
Time_ 18.12
INSTRUM DRX500
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 16384
SOLVENT CDCl3
NS 1024
DS 4
SWH 30120.482 Hz
FIDRES 1.838408 Hz
AQ 0.2720244 sec
RG 11585.2
DW 16.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.69999999 sec
d11 0.03000000 sec
DELTA 0.59999996 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 -2.30 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.30 dB
PL12 15.00 dB
PL13 120.00 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577484 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 0.10
135.9780 134.3978 128.1653 121.3144 119.4277 118.0560 110.6506 110.5231 77.6144 77.3593 77.1043 23.6326 23.5825 23.5518 21.2481
1,2,3,4 -tetreahydrocarbazole
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.3360
7.3277
7.3229
7.3182
7.3162
7.3141
7.3100
7.3073
7.3048
7.2917
7.2838
7.2789
7.2746
7.2676
7.2662
7.2640
7.2618
7.1937
7.1867
7.1823
7.1765
7.1746
7.1675
7.1604
7.1559
7.1501
7.1481
7.1409
7.1349
4.9156
1.5564
1.2709
NAME A18165
EXPNO 1
PROCNO 1
Date_ 20100817
Time_ 21.43
INSTRUM DRX500
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10288.065 Hz
FIDRES 0.156983 Hz
AQ 3.1850996 sec
RG 322.5
DW 48.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -2.70 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300083 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
N-benzyl-1,1,1-trifluoro-N-phenylmethanesulfonamide
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
3.0425
3.4027
4.0000
1.9935


136.8941
134.5840
129.7329
129.7083
129.5029
129.3589
128.9698
128.8296
124.7123
122.1618
119.5836
117.0062
77.6152
77.3604
77.1052
57.7164
NAME A18165
EXPNO 2
PROCNO 1
Date_ 20100817
Time_ 20.21
INSTRUM DRX500
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 16384
SOLVENT CDCl3
NS 1024
DS 4
SWH 30120.482 Hz
FIDRES 1.838408 Hz
AQ 0.2720244 sec
RG 10321.3
DW 16.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.69999999 sec
d11 0.03000000 sec
DELTA 0.59999996 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 -2.30 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.30 dB
PL12 15.00 dB
PL13 120.00 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577476 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 0.10
N-benzyl-1,1,1-trifluoro-N-phenylmethanesulfonamide
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.4058
7.4014
7.3945
7.3758
7.3740
7.3686
7.3564
7.3521
7.3414
7.3371
7.3097
7.3056
7.3011
7.2947
7.2883
7.2816
7.2699
7.2177
7.2122
7.2072
7.1938
7.1908
7.1774
7.1725
7.1670
6.7598
6.7415
6.7232
6.6780
6.6584
4.3489
1.2729
NAME PJ163
EXPNO 1
PROCNO 1
Date_ 20091001
Time 9.54
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 512
DW 60.400 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 1.10 dB
SFO1 400.1324710 MHz
SI 32768
SF 400.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
N-Benzyl aniline
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
5.0855
2.0785
1.0000
2.0085
2.1199


148.5093
139.7909
129.6072
128.9782
127.8570
127.5735
117.9166
113.1928
77.6785
77.3607
77.0432
48.6833
NAME benzylaniline 13C
EXPNO 1
PROCNO 1
Date_ 20100226
Time 17.07
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16384
SOLVENT CDCl3
NS 1024
DS 2
SWH 23980.814 Hz
FIDRES 1.463673 Hz
AQ 0.3416564 sec
RG 23170.5
DW 20.850 usec
DE 20.00 usec
TE 300.0 K
D1 0.69999999 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 -2.80 dB
PL1W 57.91424179 W
SFO1 100.5976818 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.20 dB
PL12 14.30 dB
PL13 15.30 dB
PL2W 15.00949383 W
PL12W 0.26691073 W
PL13W 0.21201472 W
SFO2 400.0316001 MHz
SI 32768
SF 100.5875896 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N-Benzyl aniline
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm