Supporting Information for

Copper Catalyzed Direct Trifluoromethylthiolation of Indoles by tert-Butyl 2-((trifluoromethyl)sulfonyl)hydrazine-1-carboxylate

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Contents **Page**

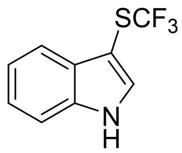
General information	2
Characteristic data for compound **3a-3z**	2-8
Experiments for the mechanistic study	8-22
References	22
^{1}H and ^{13}C NMR Spectra	22-55

1) General information

All solvents were distilled prior to use. For chromatography, 200-300 mesh silica gel (Qingdao, China) was employed. ^{1}H and ^{13}C NMR spectra were recorded at 400 MHz and 100 MHz with Brucker ARX 400 spectrometer. Chemical shifts are reported in ppm using tetramethylsilane as internal standard. Mass spectra were obtained on a Bruker SCION 436-GC SQ mass spectrometer or on a Bruker Apex IV FTMS spectrometer.

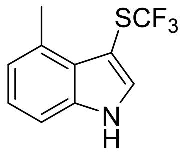
2) Characteristic data for 3a-3z

3-((trifluoromethyl)thio)-1*H*-indole (3a).[1]



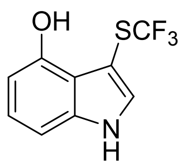
White soild (72 mg, 66%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (s, 1H), 7.84-7.82 (m, 1H), 7.53 (d, *J* = 2.4 Hz, 1H), 7.44-7.42 (m, 1H), 7.33-7.28 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.1, 132.9, 129.6, 129.6 (q, *J* = 307 Hz, 1C), 123.5, 121.7, 119.4, 111.8, 95.6 (q, *J* = 2.0 Hz, 1C) ; ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.46.

4-methyl-3-((trifluoromethyl)thio)-1*H*-indole (3b).[1]



White soild (69 mg, 60%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (s, 1H), 7.52 (d, *J* = 2.0 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 1H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.01 (d, *J* = 6.8 Hz, 1H), 2.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.5, 134.1, 131.8, 129.3 (q, *J* = 307 Hz, 1C), 126.9, 123.6, 123.5, 109.8, 95.2 (q, *J* = 3.0 Hz, 1C), 19.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -45.83.

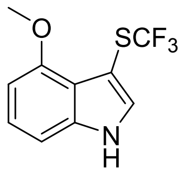
3-((trifluoromethyl)thio)-1*H*-indol-4-ol (3c).[1]



White soild (56 mg, 48%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz,

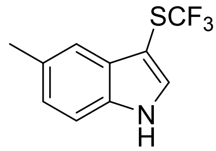
$CDCl_3$) δ 8.62 (s, 1H), 7.44 (s, 1H), 7.18 (t, *J* = 8.0 Hz, 1H), 7.00 (d, *J* = 8.0 Hz, 1H), 6.74 (s, 1H), 6.72 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.6, 137.8, 132.9, 128.4 (q, *J* = 309 Hz, 1C), 125.2, 116.6, 107.2, 104.6, 91.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -45.73.

4-methoxy-3-((trifluoromethyl)thio)-1*H*-indole (3d).[1]



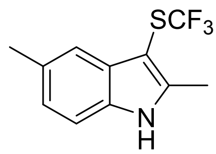
White soild (64 mg, 52%). Eluent: ethyl acetate/petroleum ether = 1/10. ^1H NMR (400 MHz, $CDCl_3$) δ 8.46 (s, 1H), 7.36 (d, *J* = 2.0 Hz, 1H), 7.22 (t, *J* = 8.0 Hz, 1H), 7.00 (d, *J* = 8.0 Hz, 1H), 6.68 (d, *J* = 7.6 Hz, 1H), 3.99 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.6, 138.0, 132.6, 129.6 (q, *J* = 308 Hz, 1C), 124.4, 118.6, 105.0, 102.2, 94.4 (q, *J* = 3.0 Hz, 1C), 55.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -45.39.

5-methyl-3-((trifluoromethyl)thio)-1*H*-indole (3e).[1]



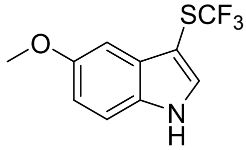
White soild (54 mg, 47%). Eluent: ethyl acetate/petroleum ether = 1/10. ^1H NMR (400 MHz, $CDCl_3$) δ 8.39 (s, 1H), 7.60 (s, 1H), 7.49 (d, *J* = 2.8 Hz, 1H), 7.31(d, *J* = 8.4 Hz, 1H), 7.13 (d, *J* = 8.4 Hz, 1H), 2.51 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.4, 133.0, 131.3, 130.0, 129.6 (q, *J* = 308 Hz, 1C), 125.2, 119.0, 111.5, 95.0 (q, *J* = 2.0 Hz, 1C), 21.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.58.

2,5-Dimethyl-3-((trifluoromethyl)thio)-1*H*-indole (3f).[2]



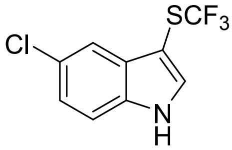
White soild (50 mg, 43%). Eluent: ethyl acetate/petroleum ether = 1/10. ^1H NMR (400 MHz, $CDCl_3$) δ 8.17 (s, 1H), 7.51 (s, 1H), 7.20 (d, *J* = 8.0 Hz, 1H), 7.06 (d, *J* = 8.0 Hz, 1H), 2.55 (s, 1H), 2.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.7, 133.4, 131.0, 130.9, 129.9 (q, *J* = 309 Hz, 1C), 124.2, 118.5, 110.6, 92.0, 21.6, 12.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.45.

5-Methoxy-3-((trifluoromethyl)thio)-1*H*-indole (3g).[3]



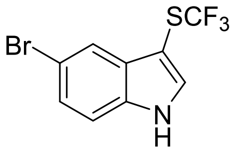
White soild (67 mg, 54%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (s, 1H), 7.45 (d, *J* = 2.8 Hz, 1H), 7.26 (d, *J* = 8.8 Hz, 1H), 7.23 (s, 1H), 6.68 (dd, *J* = 8.8 Hz, 2.0 Hz, 1H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.7, 133.4, 131.1, 130.4, 129.7 (q, *J* = 308 Hz, 1C), 114.1, 112.7, 100.7, 95.1 (q, *J* = 3.0 Hz, 1C), 56.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.61.

5-chloro-3-((trifluoromethyl)thio)-1*H*-indole (3h).[1]



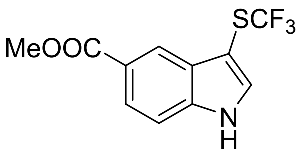
White soild (78 mg, 62%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (s, 1H), 7.75 (s, 1H), 7.50 (d, *J* = 2.4 Hz, 1H), 7.29 (d, *J* = 8.8 Hz, 1H), 6.68 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.5, 134.1, 130.8, 129.4 (q, *J* = 308 Hz, 1C), 127.8, 124.1, 119.0, 112.9, 95.6 (q, *J* = 3.0 Hz, 1C); ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.46.

5-bromo-3-((trifluoromethyl)thio)-1*H*-indole (3i).[1]



White soild (90 mg, 61%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (s, 1H), 7.93 (s, 1H), 7.53 (s, 1H), 7.38 (d, *J* = 8.4 Hz, 1H), 7.28 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.8, 133.9, 131.3, 129.4 (q, *J* = 308 Hz, 1C), 126.7, 122.1, 115.3, 113.3, 95.5 (q, *J* = 2.0 Hz, 1C); ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.45.

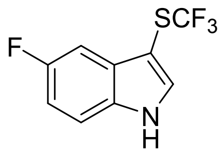
Methyl 3-((trifluoromethyl)thio)-1H-indole-5-carboxylate (3j).[1]



White soild (77 mg, 56%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (s, 1H), 8.55 (s, 1H), 8.02 (d, *J* = 8.4 Hz, 1H), 7.63 (d, *J* = 2.8 Hz, 1H), 7.46 (d,

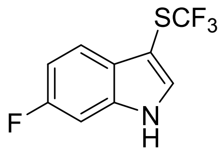
J = 8.4 Hz, 1H), 3.97 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 166.8, 139.1, 137.1, 129.3 (q, J = 308 Hz, 1C), 128.7, 123.4, 122.6, 120.2, 112.8, 92.9 (q, J = 2 Hz, 1C), 51.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.39.

5-fluoro-3-((trifluoromethyl)thio)-1*H*-indole (3k).[1]



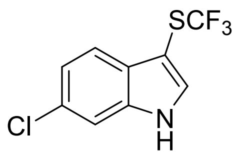
White soild (72 mg, 61%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (s, 1H), 7.57 (d, J = 2.8 Hz, 1H), 7.46 (dd, J = 8.8 Hz, 2.4 Hz, 1H), 7.35 (dd, J = 8.8 Hz, 4.4 Hz, 1H), 7.28 (td, J = 9.0 Hz, 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2(d, J = 236 Hz, 1C), 134.5, 132.6, 130.5(d, J = 11 Hz, 1C), 129.5 (q, J = 308 Hz, 1C), 112.8(d, J = 9 Hz, 1C), 112.3(d, J = 26 Hz, 1C), 104.7(d, J = 25 Hz, 1C), 95.9 (q, J = 2.0 Hz, 1C); ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.58, -121.60.

6-fluoro-3-((trifluoromethyl)thio)-1*H*-indole (3l).[1]



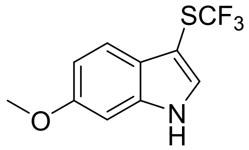
White soild (75 mg, 64%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (s, 1H), 7.72 (dd, J = 8.4 Hz, 5.6 Hz, 1H), 7.52 (s, 1H), 7.11 (d, J = 8.6 Hz, 1H), 7.05 (t, J = 8.6 Hz,, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7(d, J = 239 Hz, 1C), 136.2(d, J = 13 Hz, 1C), 133.3(d, J = 2 Hz, 1C), 129.5 (q, J = 308 Hz, 1C), 126.0, 120.5(d, J = 10 Hz, 1C), 110.7(d, J = 24 Hz, 1C), 98.3(d, J = 27 Hz, 1C), 96.1 (q, J = 2.0 Hz, 1C); ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.49, -119.03.

6-chloro-3-((trifluoromethyl)thio)-1*H*-indole (3m).[1]



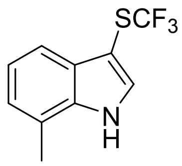
White soild (75 mg, 60%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (s, 1H), 7.71 (d, J = 8.4 Hz, 1H), 7.51 (d, J = 2.8 Hz, 1H), 7.40 (d, J = 1.2 Hz, 1H), 6.68 (dd, J = 8.4 Hz, 1.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.4, 133.5, 129.6, 129.4 (q, J = 308 Hz, 1C), 128.2, 122.6, 120.5, 111.8, 96.2 (q, J = 2 Hz, 1C); ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.43.

6-methoxy-3-((trifluoromethyl)thio)-1*H*-indole (3n).[1]



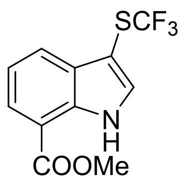
White soild (86 mg, 70%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (s, 1H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.43 (d, *J* = 2.4 Hz, 1H), 6.94 (dd, *J* = 8.8 Hz, 2.0 Hz, 1H), 6.89 (d, *J* = 2.0 Hz, 1H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.5, 137.0, 131.7, 129.5 (q, *J* = 308 Hz, 1C), 123.7, 120.2, 111.8, 95.7, 95.1, 55.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.62.

7-methyl-3-((trifluoromethyl)thio)-1*H*-indole (3o).[1]



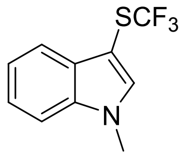
White soild (79 mg, 68%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.42 (d, *J* = 2.8 Hz, 1H), 7.18 (t, *J* = 8.0 Hz, 1H), 7.06 (d, *J* = 2.8 Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.7, 132.6, 129.6 (q, *J* = 308 Hz, 1C), 129.2, 124.1, 121.9, 121.1, 117.1, 95.9 (q, *J* = 2 Hz, 1C), 16.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.45.

Methyl 3-((trifluoromethyl)thio)-1*H*-indole-7-carboxylate (3p).[3]



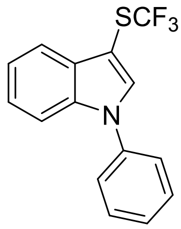
White soild (56 mg, 41%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.25 (s, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.97 (d, *J* = 7.6 Hz, 1H), 7.65 (d, *J* = 2.0 Hz, 1H), 7.32 (t, *J* = 7.6 Hz, 1H), 4.00 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 167.6, 136.2, 134.0, 130.6, 129.4 (q, J = 308 Hz, 1C), 125.7, 125.1, 121.1, 113.6, 95.9 (q, *J* = 3.0 Hz, 1C), 52.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.60.

1-methyl-3-((trifluoromethyl)thio)-1*H*-indole (3q).[1]



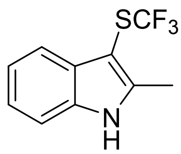
White soild (58 mg, 50%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.6 Hz, 1H), 7.37-7.24 (m, 4H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.3, 137.0, 130.4, 129.6 (q, *J* = 308 Hz, 1C), 123.1, 121.4, 119.5, 110.0, 93.1 (q, *J* = 2 Hz, 1C), 33.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.93.

1-phenyl-3-((trifluoromethyl)thio)-1*H*-indole (3r).[1]



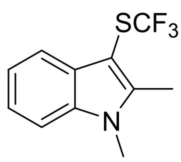
White soild (66 mg, 45%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89-7.87 (m, 1H), 7.67 (s, 1H), 7.59-7.50 (m, 5H), 7.45 (d, *J* = 7.2 Hz, 1H), 7.36-7.30 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.6, 136.7, 136.1, 130.7, 130.0, 129.6 (q, *J* = 308 Hz, 1C), 127.8, 124.8, 123.8, 122.2, 119.8, 111.2, 96.3 (q, *J* = 2 Hz, 1C); ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.33.

2-methyl-3-((trifluoromethyl)thio)-1*H*-indole (3s).[1]



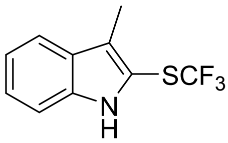
White soild (59 mg, 51%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.69 (d, *J* = 7.2 Hz, 1H), 7.25-7.17 (m, 3H), 2.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.7, 135.1, 130.7, 129.9 (q, *J* = 309 Hz, 1C), 122.7, 121.5, 118.8, 110.9, 92,6 (q, *J* = 3.0 Hz, 1C), 12.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.35.

1,2-Dimethyl-3-((trifluoromethyl)thio)-1*H*-indole (3t).[1]



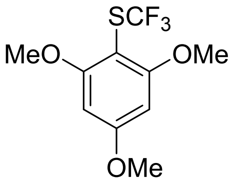
White soild (53 mg, 43%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72-7.70 (m, 1H), 7.27-7.19 (m, 3H), 3.64 (s, 3H), 2.52 (s, 3H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 145.3, 136.9, 130.2, 129.9 (q, J = 309 Hz, 1C), 122.3, 121.2, 118.8, 109.3, 91.1 (q, J = 2.0 Hz, 1C), 30.4, 10.9; ^{19}F NMR (376 MHz, CDCl$_3$) δ -44.86

3-methyl-2-((trifluoromethyl)thio)-1*H*-indole (3u).[1]



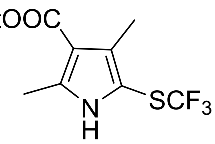
White soild (36 mg, 31%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, CDCl$_3$) δ 8.10 (s, 1H), 7.62 (d, J = 7.6 Hz, 1H), 7.37-7.30 (m, 2H), 7.18 (t, J = 7.2 Hz, 1H), 2.47 (s, 1H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 137.5, 128.9 (q, J = 310 Hz, 1C), 128.1, 124.9, 123.8, 120.2, 120.1, 113.2, 111.2, 9.55; ^{19}F NMR (376 MHz, CDCl$_3$) δ -43.07.

(trifluoromethyl)(2,4,6-trimethoxyphenyl)sulfane (3v).[4]



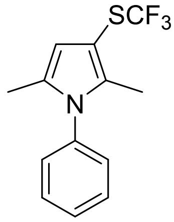
White soild (82 mg, 61%). Eluent: ethyl acetate/petroleum ether = 1/30. ^{1}H NMR (400 MHz, CDCl$_3$) δ 6.15 (s, 2H), 3.86 (s, 6H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 164.5, 163.6, 129.7 (q, J = 309.0 Hz, 1C), 91.9, 91.3, 56.3 (q, J = 4.4 Hz, 1C), 55.5 (q, J = 4.4 Hz, 1C); ^{19}F NMR (376 MHz, CDCl$_3$) δ -43.50.

ethyl 2,4-dimethyl-5-((trifluoromethyl)thio)-1H-pyrrole-3-carboxylate (3w).[4]



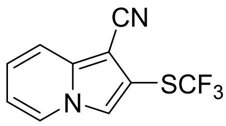
Brown soild (48 mg, 36%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, CDCl$_3$) δ 8.46 (s, 1H), 4.30 (q, J = 7.2 Hz, 2H), 2.53 (s, 3H), 2.36 (s, 3H), 1.36 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 165.3 (q, J = 2.0 Hz, 1C), 140.2, 133.9, 128.6 (q, J = 310.2 Hz, 1C), 113.4, 104.6 (q, J = 2.3 Hz, 1C), 59.7, 14.6, 14.4 (q, J = 3.2 Hz, 1C), 12.2 (q, J = 2.9 Hz, 1C); ^{19}F NMR (376 MHz, CDCl$_3$) δ -44.94.

2,5-dimethyl-1-phenyl-3-((trifluoromethyl)thio)-1H-pyrrole (3x).[4]



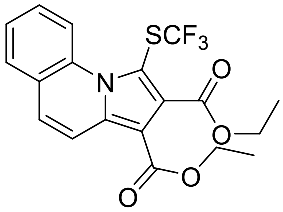
Brown soild (34 mg, 25%). Eluent: petroleum ether. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52-7.43 (m, 3H), 7.22-7.19 (m, 2H), 6.13 (s, 1H), 2.11 (s, 3H), 2.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.4, 136.7, 129.9 (q, J = 307.3 Hz, 1C), 129.6, 129.5, 128.6, 128.2, 112.7, 97.7 (q, J = 2.1 Hz, 1C), 12.9, 11.2 (q, J = 1.8 Hz, 1C); ^{19}F NMR (376 MHz, $CDCl_3$) δ -45.30.

2-((trifluoromethyl)thio)indolizine-1-carbonitrile (3y).[4]



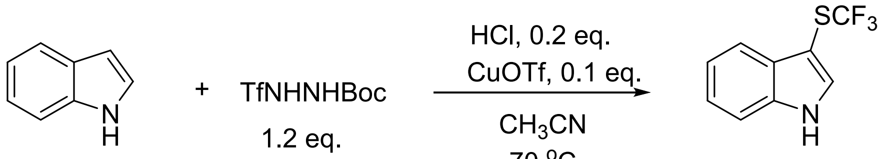
Yellow soild (61 mg, 50%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (d, J = 6.8 Hz, 1H), 7.74 (dt, J = 8.9 Hz, 1.1 Hz, 1H), 7.50 (s, 1H), 7.32 (ddd, J = 8.9 Hz, 6.8 Hz, 1.0 Hz, 1H), 7.02 (td, J = 6.8 Hz, 1.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.3, 129.7, 128.3 (q, J = 311.9 Hz, 1C), 125.5, 125.1, 118.2, 115.2, 114.5, 103.6, 84.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.07.

diethyl 1-((trifluoromethyl)thio)pyrrolo[1,2-a]quinoline-2,3-dicarboxylate (3z).



Yellow soild (58 mg, 28%). Eluent: ethyl acetate/petroleum ether = 1/10. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.88 – 8.59 (m, 1H), 8.37 (d, J = 7.4 Hz, 1H), 7.71-7.68 (m, 1H), 7.62-7.56 (m, 2H), 7.16 (d, J = 7.4 Hz, 1H), 4.47 (q, J = 7.2 Hz, 2H), 4.45 (q, J = 7.2 Hz, 2H), 1.42 (t, J = 7.2 Hz, 3H), 1.41 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 163.8, 133.4, 130.6, 129.4, 129.0, 128.6, 128.3 (q, J = 312.2 Hz, 1C), 127.5, 125.6, 124.9, 121.4, 115.6, 111.1, 105.2 (q, J = 2.5 Hz, 1C), 61.7, 61.6, 14.3, 14.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -42.96. HRMS (ESI) *m/e* calcd for $C_{19}H_{16}NO_4F_3S$ $(M+H)^+$ 412.0825, found 412.0828.

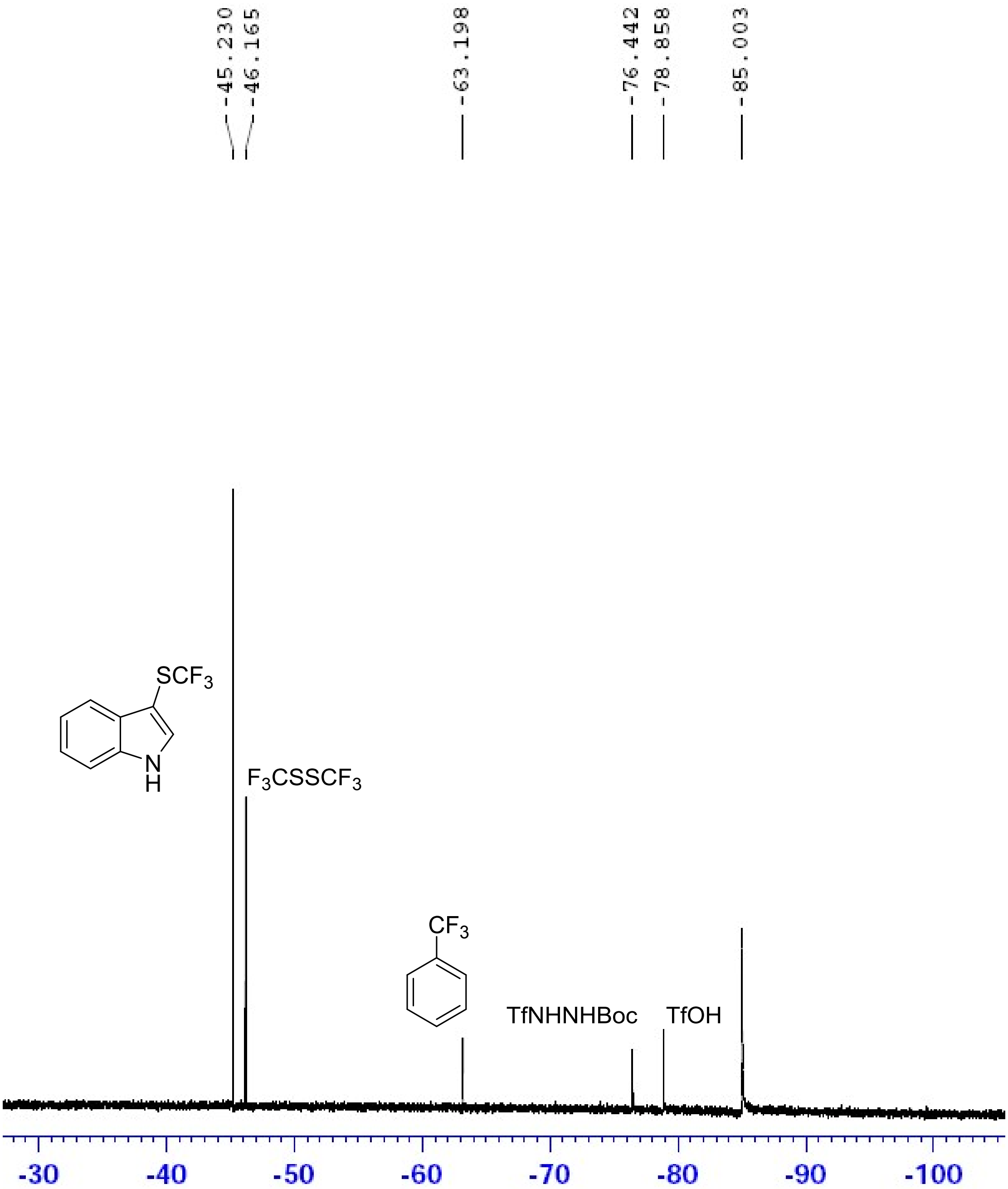
4）Experiments for the mechanistic study



1 2 3a

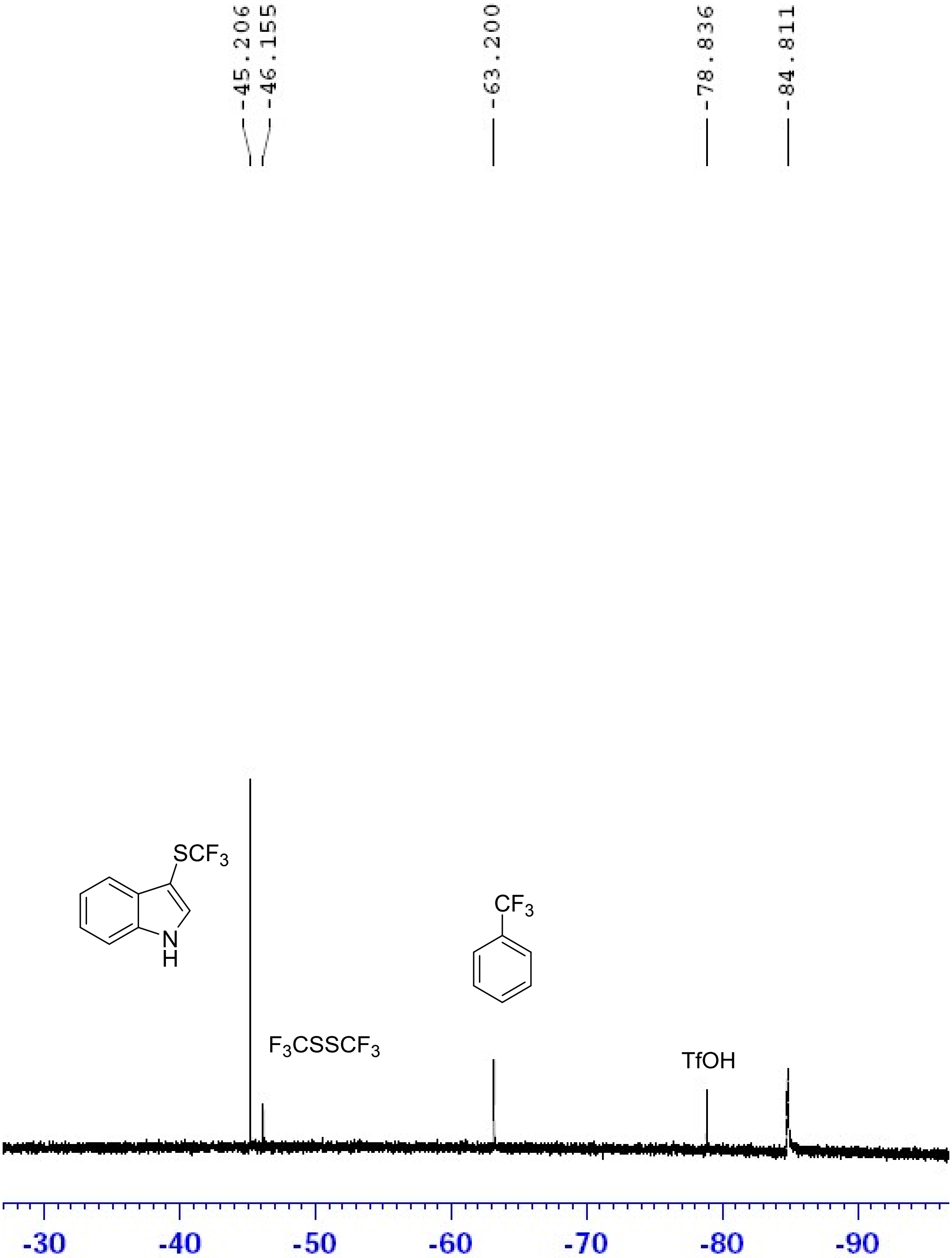
A 15 ml sealing tube with a magnetic stirring bar was charged with indole (59 mg, 0.5 mmol), TfNHNHBoc (158 mg, 0.6 mmol) and CuOTf (11 mg, 0.05 mmol), dry acetonitrile (2 mL) was added via syringe with gentle stirring. Then 12 M HCl (aq) (8 uL, 0.1 mmol) was added to the reaction mixture and the resulting mixture was stirred at 70 ^{o}C and monitored by ^{19}F NMR spectroscopies with $PhCF_3$ (δ = -63.2 ppm) as the internal standard.

15min



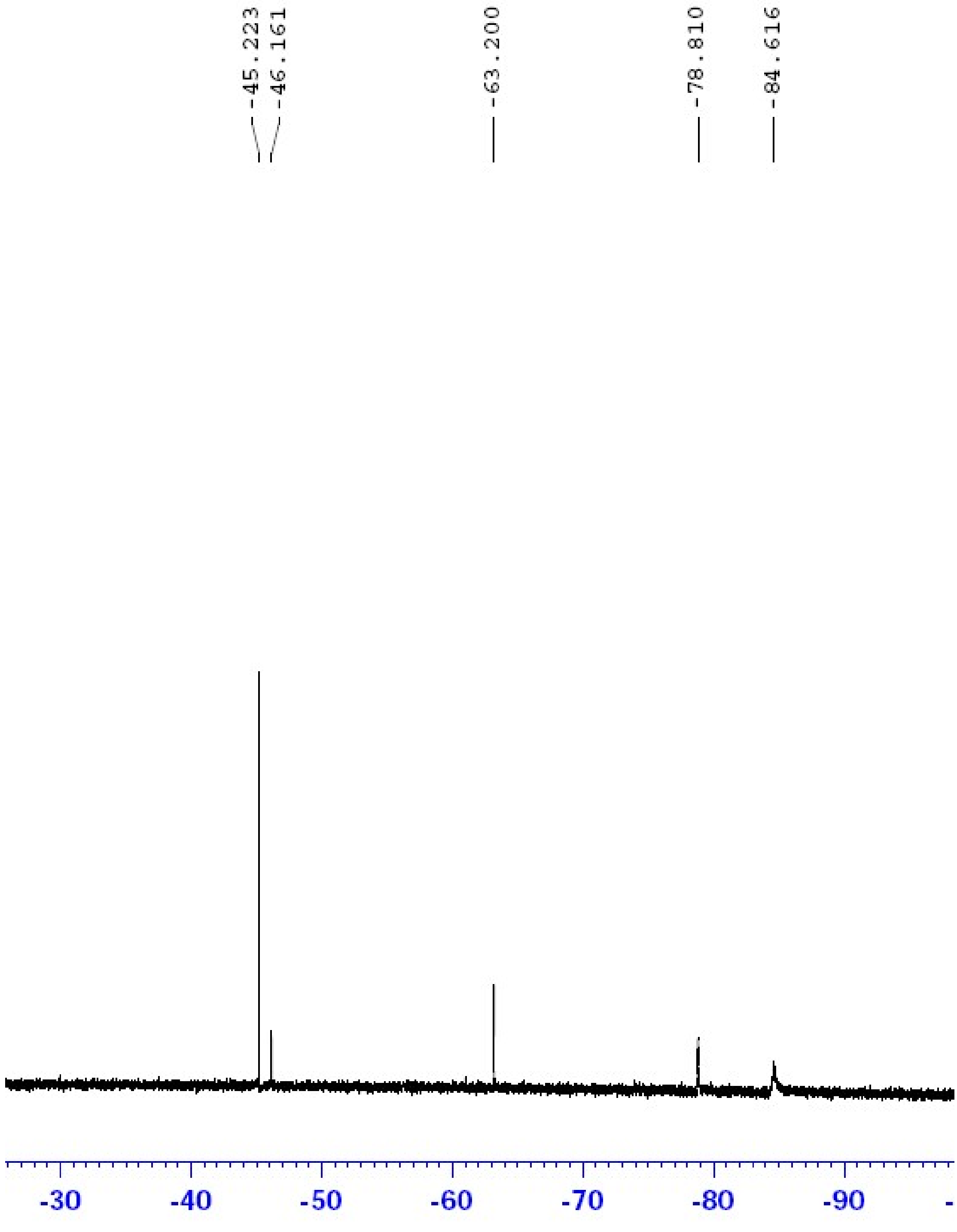
-45.230
-46.165
-63.198
-76.442
-78.858
-85.003
SCF3
N
H
F3CSSCF3
CF3
TfNHNHBoc
TfOH
-30
-40
-50
-60
-70
-80
-90
-100

30min

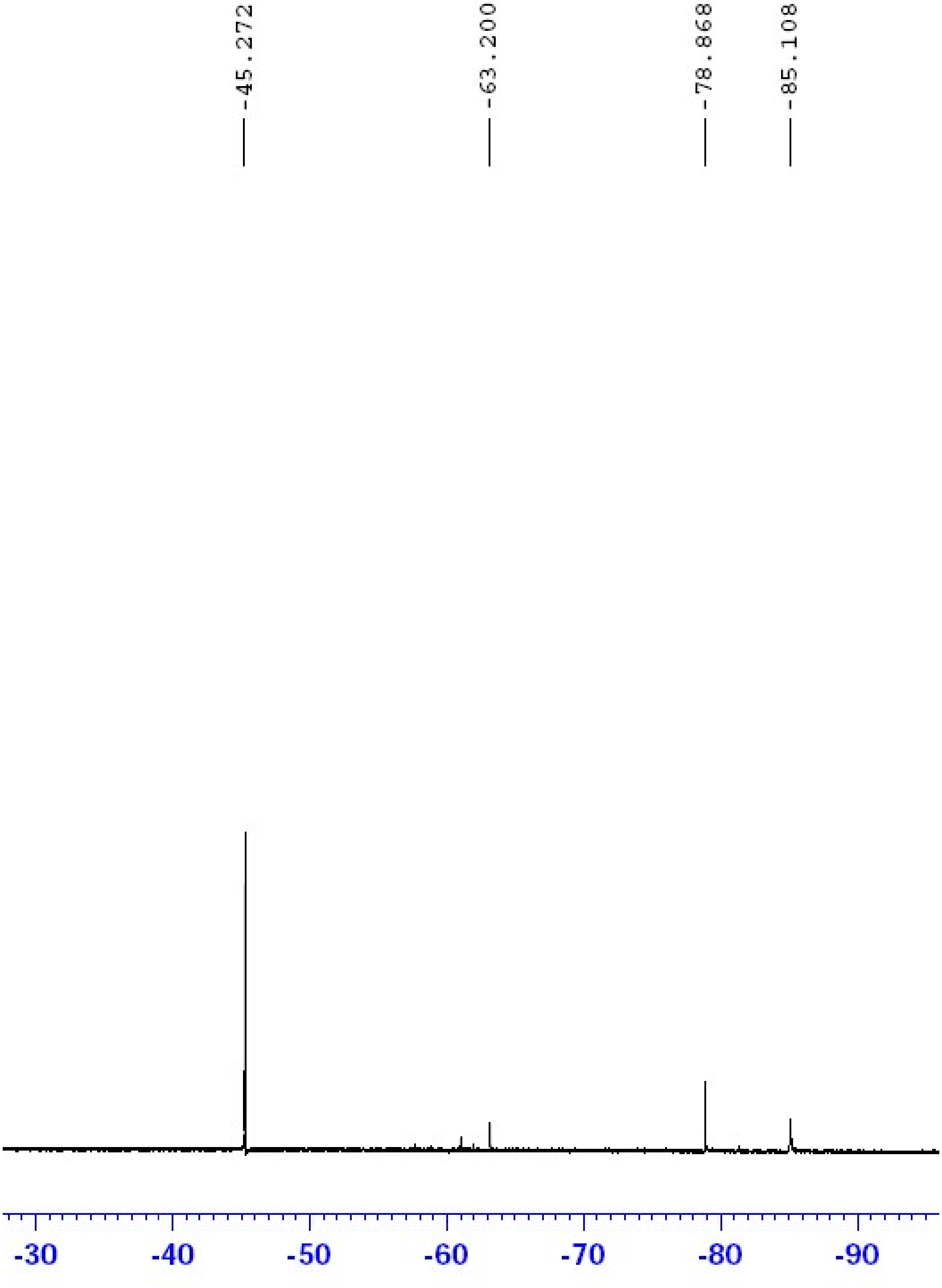


-45.206
-46.155
-63.200
-78.836
-84.811
SCF3
N
H
CF3
F3CSSCF3
TfOH
-30
-40
-50
-60
-70
-80
-90

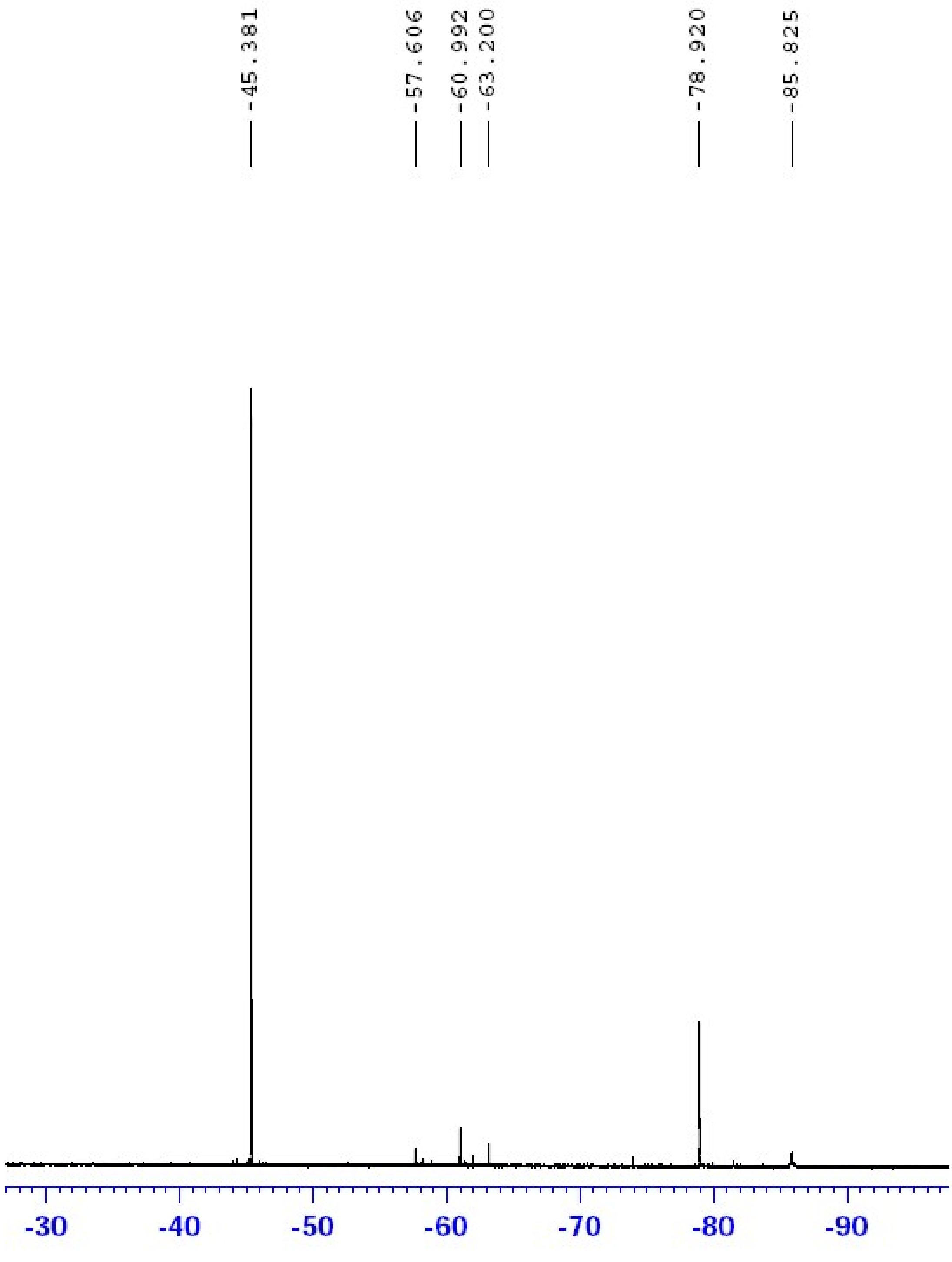
45min



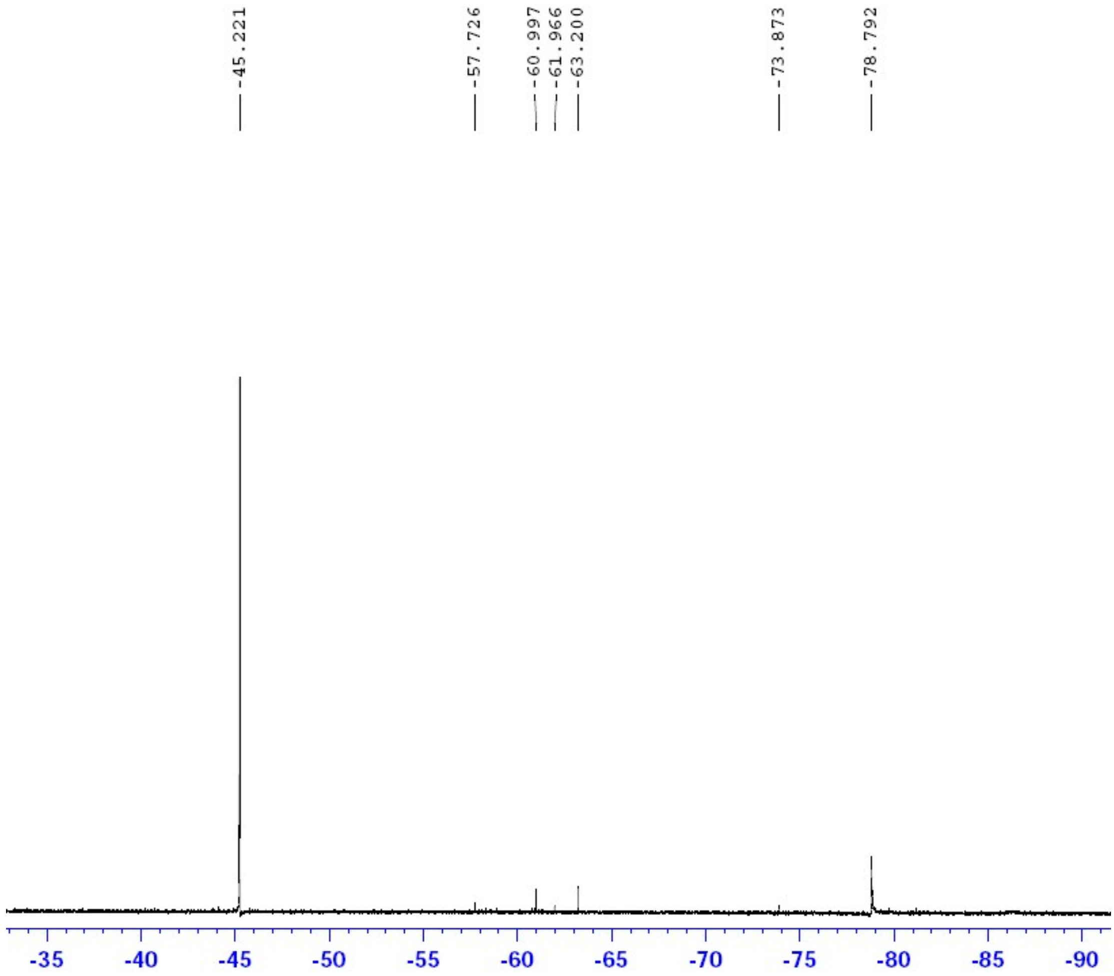
1h



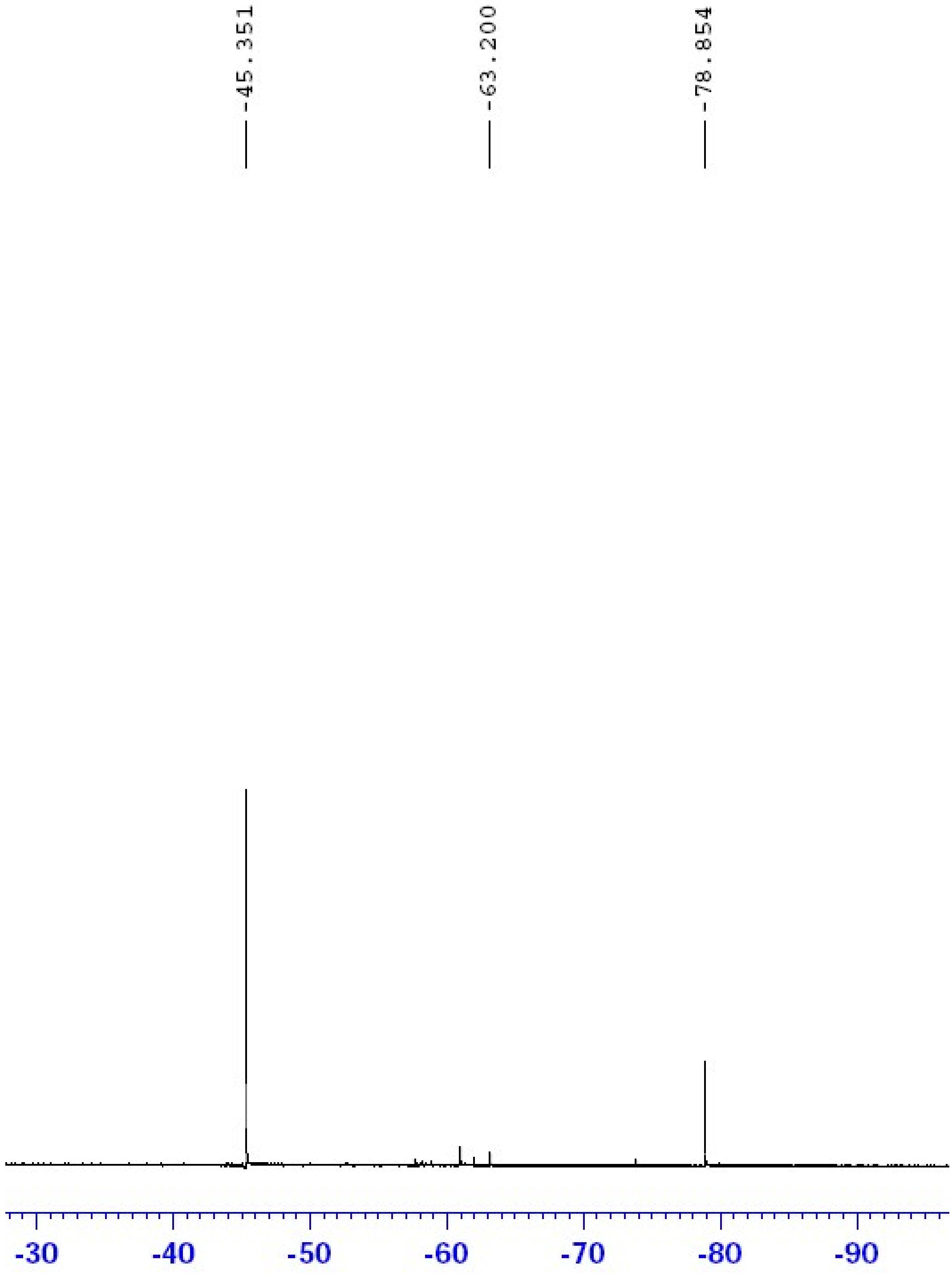
2h

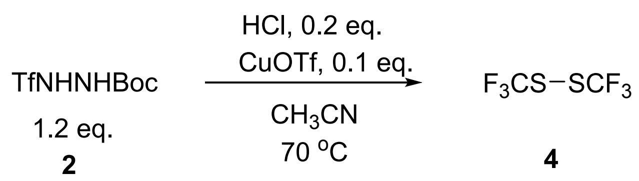


4h


-45.221
-57.726
-60.997
-61.966
-63.200
-73.873
-78.792
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90

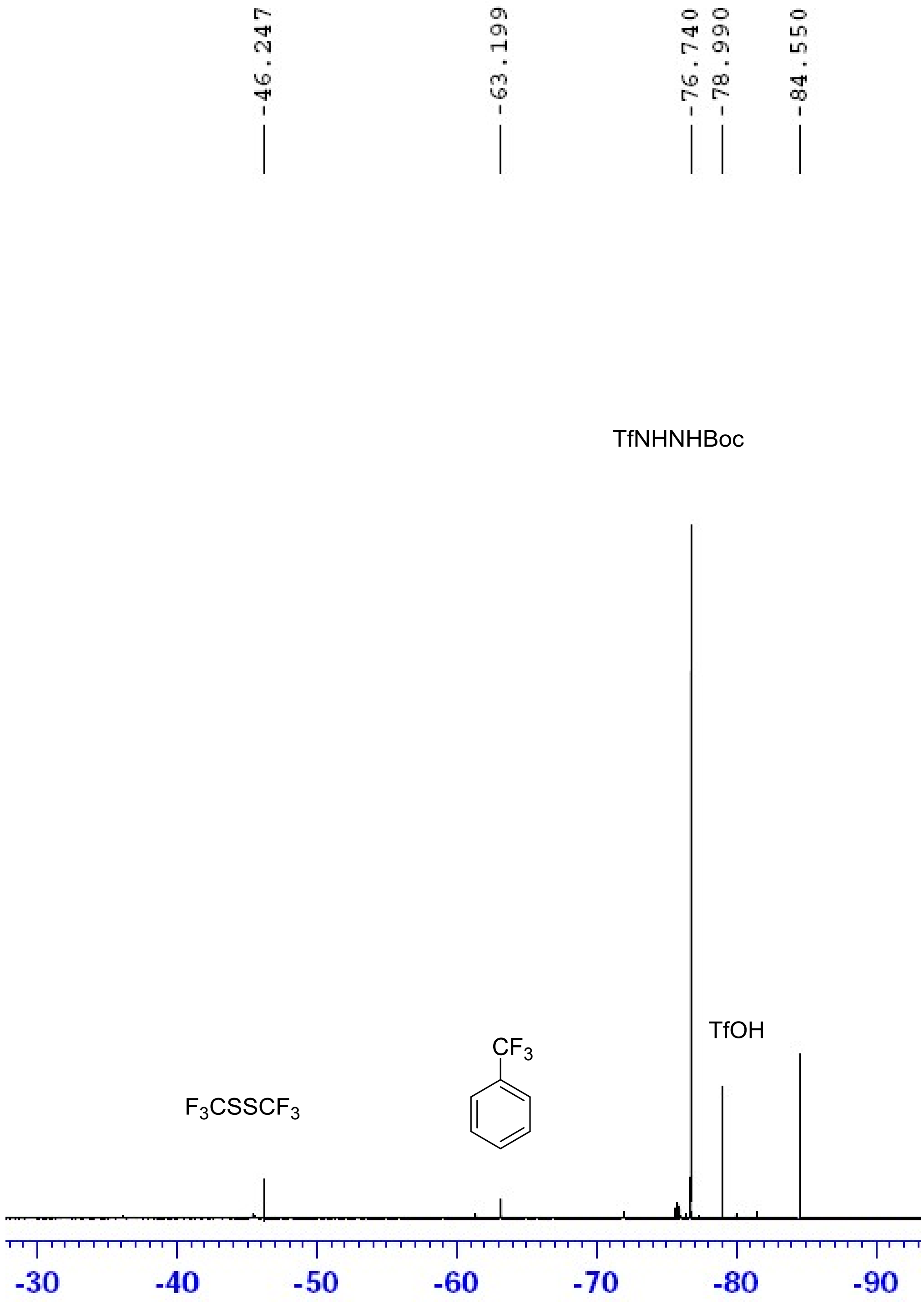
7h



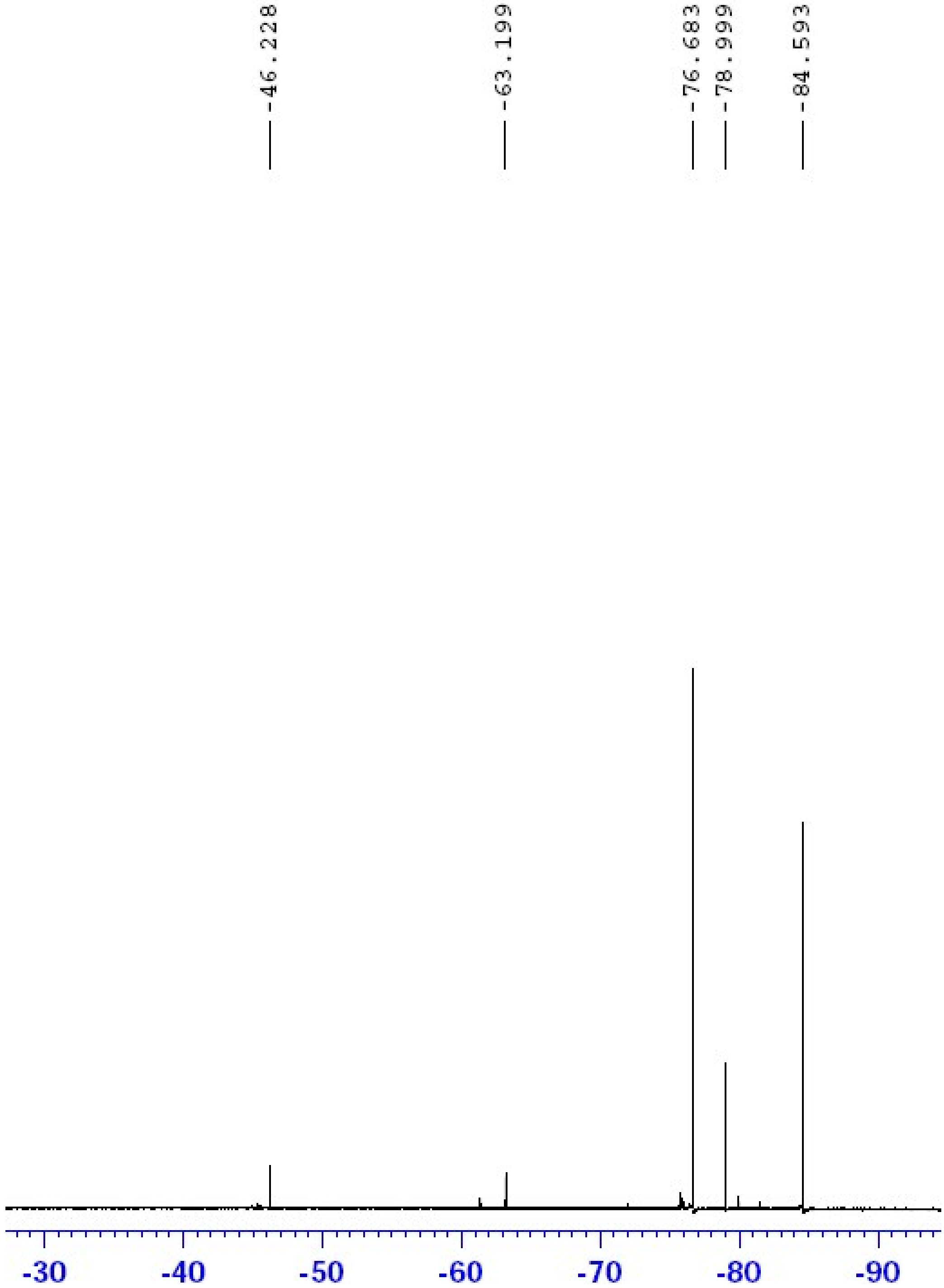


A 15 ml sealing tube with a magnetic stirring bar was charged with TfNHNHBoc (158 mg, 0.6 mmol) and CuOTf (11 mg, 0.05 mmol), dry acetonitrile (2 mL) was added via syringe with gentle stirring. Then 12 M HCl (aq) (8 uL, 0.1 mmol) was added to the reaction mixture and the resulting mixture was stirred at 70 ^{o}C and monitored by ^{19}F NMR spectroscopies with $PhCF_3$ (δ = -63.2 ppm) as the internal standard.

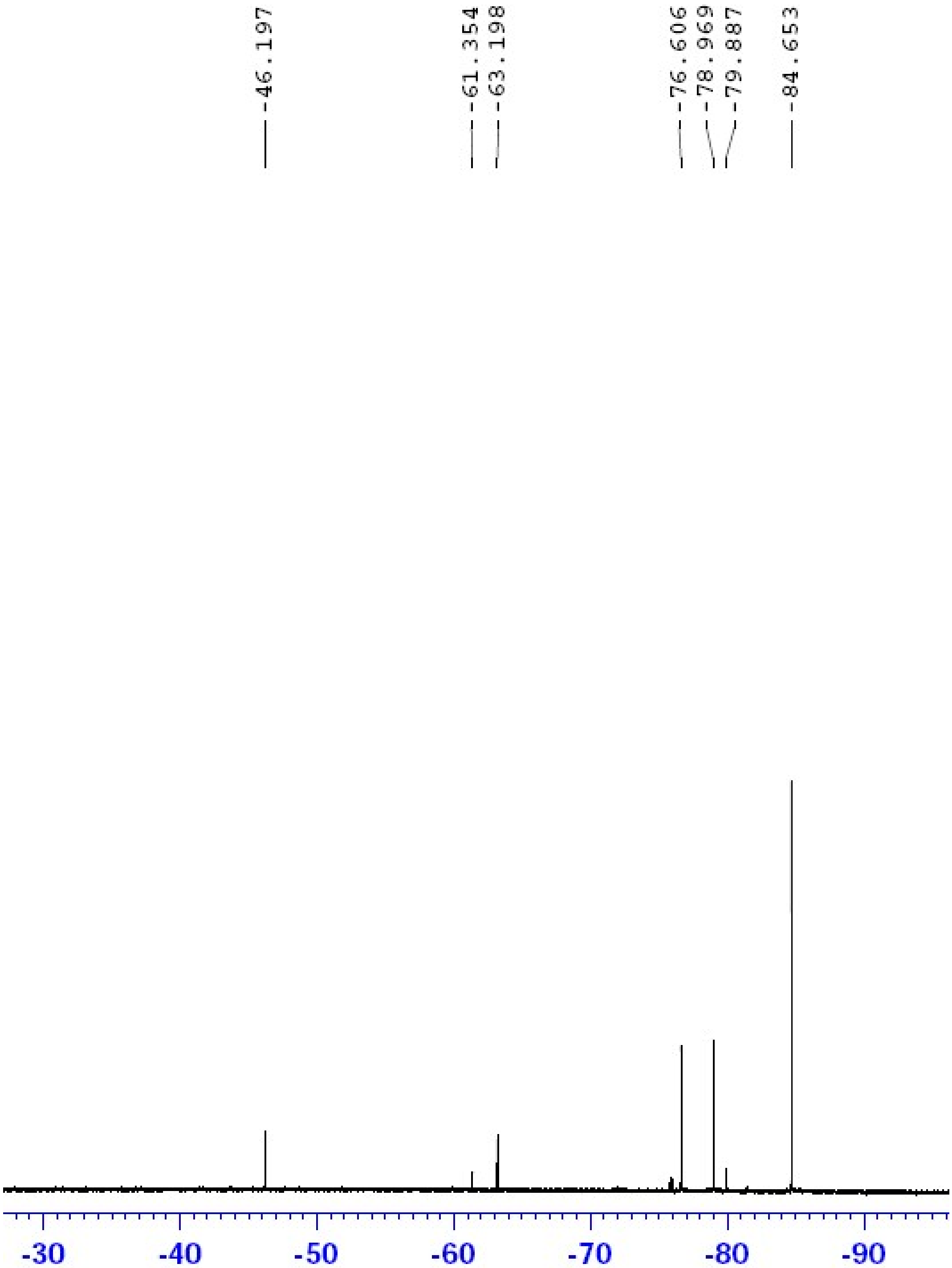
15min


-46.247
-63.199
-76.740
-78.990
-84.550
TfNHNHBoc
TfOH
CF3
F3CSSCF3
-30
-40
-50
-60
-70
-80
-90

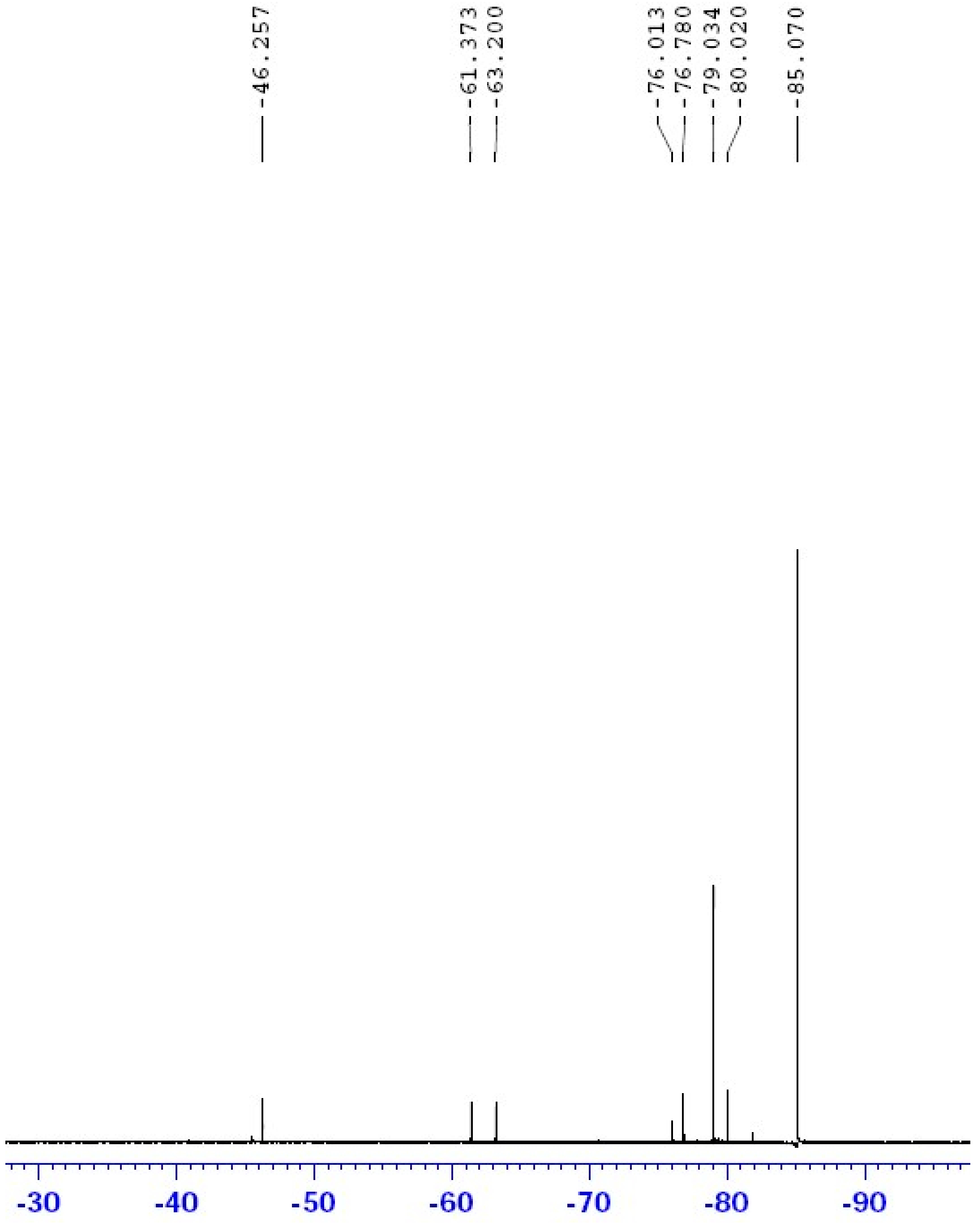
30min

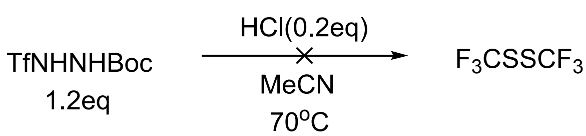


1h

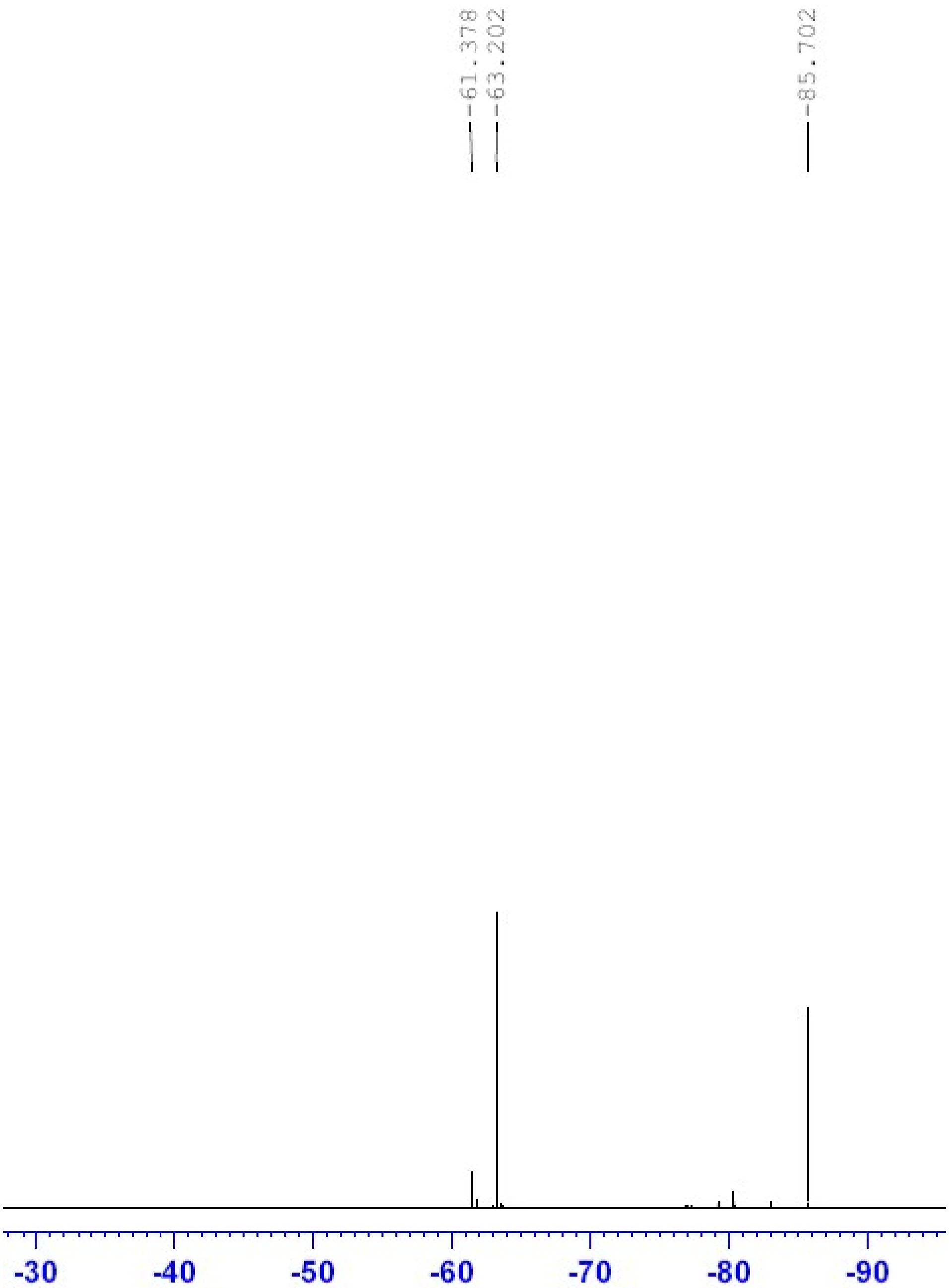


2h





A 15 ml sealing tube with a magnetic stirring bar was charged with TfNHNHBoc (158 mg, 0.6 mmol), dry acetonitrile (2 mL) was added via syringe with gentle stirring. Then 12 M HCl (aq) (8 uL, 0.1 mmol) was added to the reaction mixture and the resulting mixture was stirred at 70 °C and monitored by ^{19}F NMR spectroscopies with $PhCF_3$ (δ = -63.2 ppm) as the internal standard.



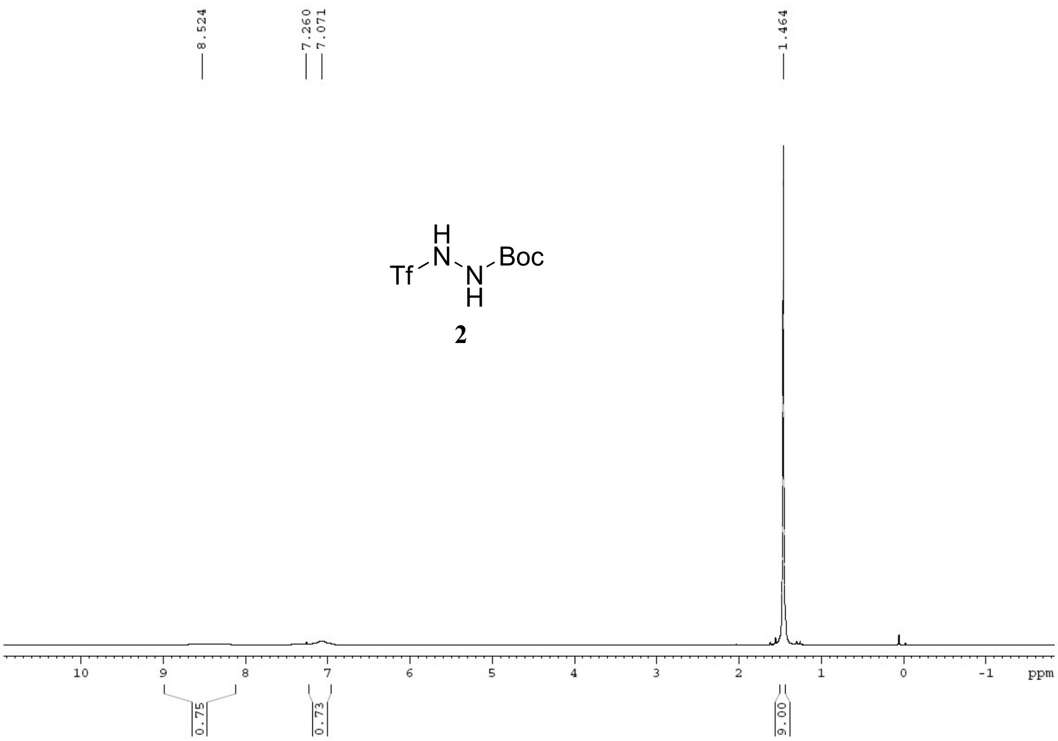
5) References

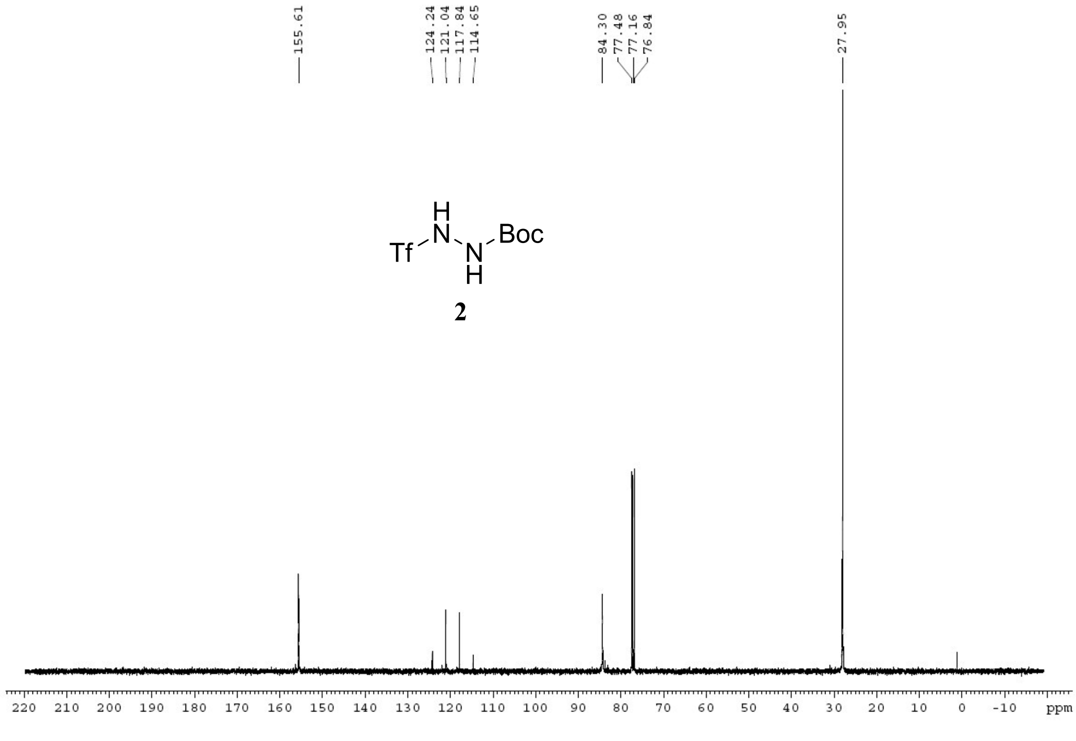
[1] Lu, K.; Deng, Z.; Li, M.; Li, T.; Zhao, X. *Org. Biomol. Chem.* **2017**, *15*, 1254–1260.

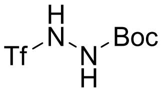
[2] Shao, X.; Xu, C.; Lu, L.; Shen, Q. *J. Org. Chem.* **2015**, *80*, 3012–3021.

[3] Bu, M.; Lu, G.; Cai, C. *Org. Chem. Front.* **2017**, *4*, 266–270.

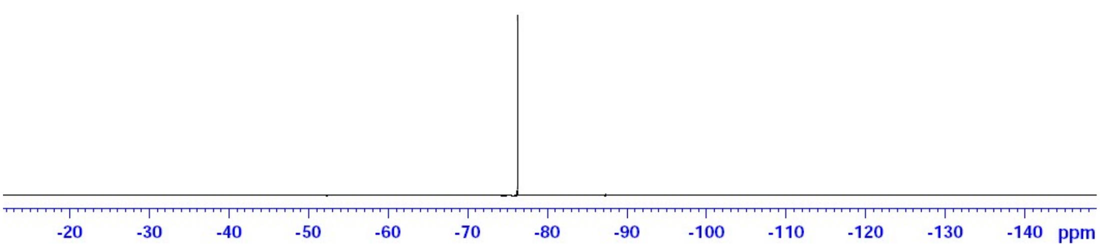
[4] Zhao, X.; Zheng, C.; Tian, M.; Sheng, J.; Tong, Y.; Lu, K. *Tetrahedron* **2017**, *73*, 7233-7238.

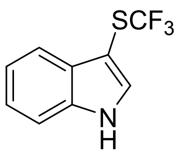

8.524
7.260
7.071
1.464
Tf
N
H
N
H
Boc
2
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
0.75
0.73
9.00


155.61
124.24
121.04
117.84
114.65
84.30
77.48
77.16
76.84
27.95
Tf
N
H
N
H
Boc
2
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

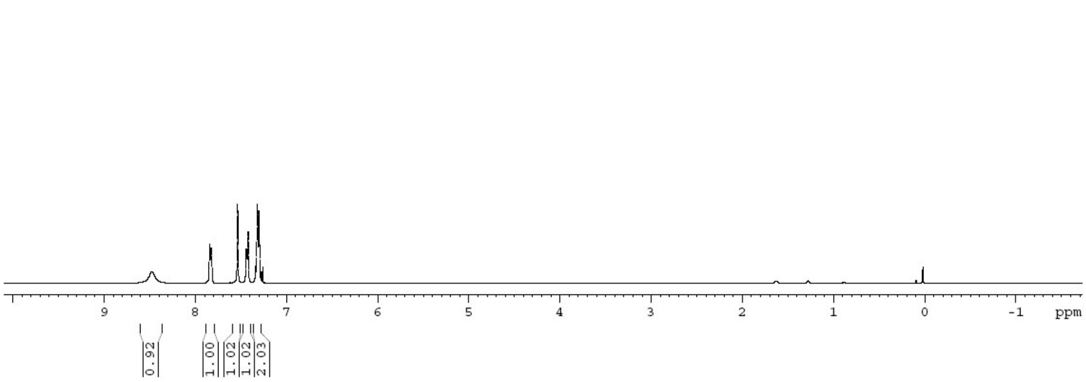


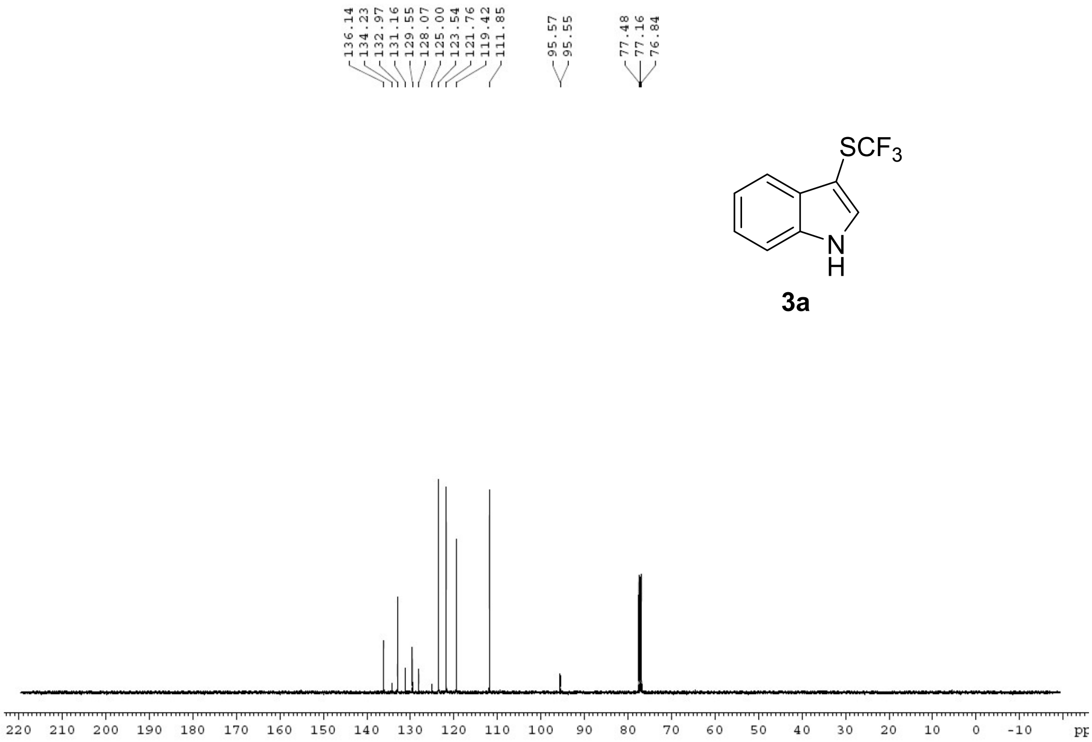
2

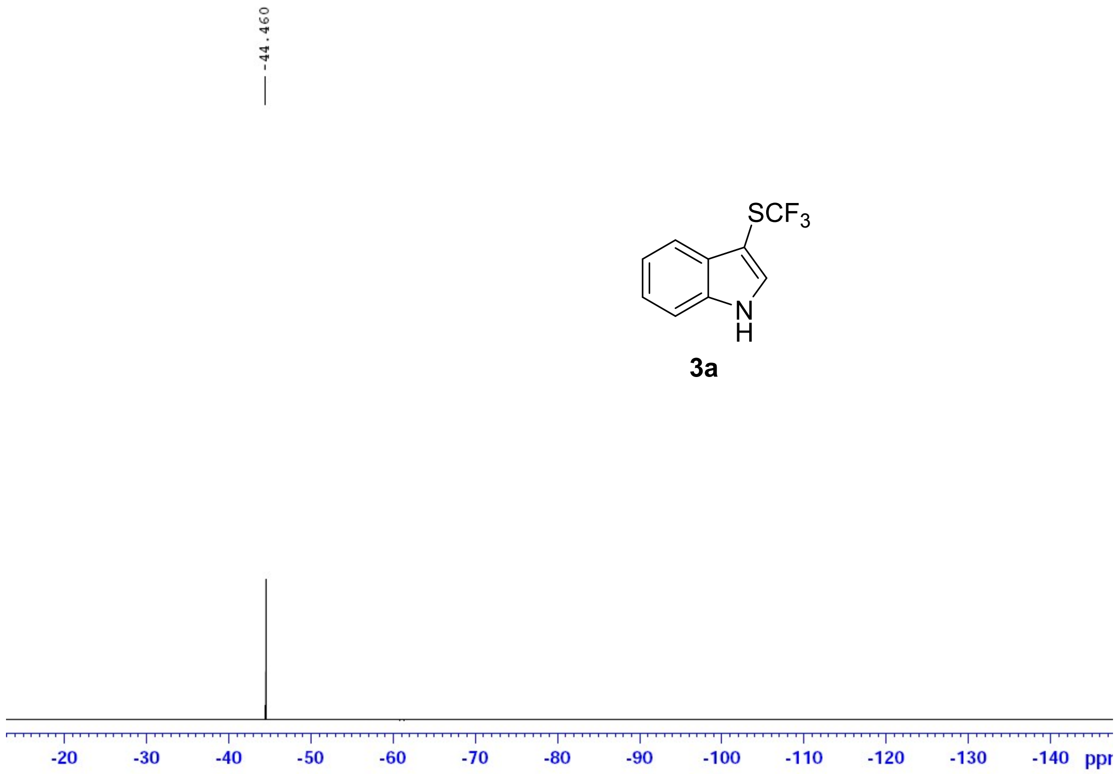


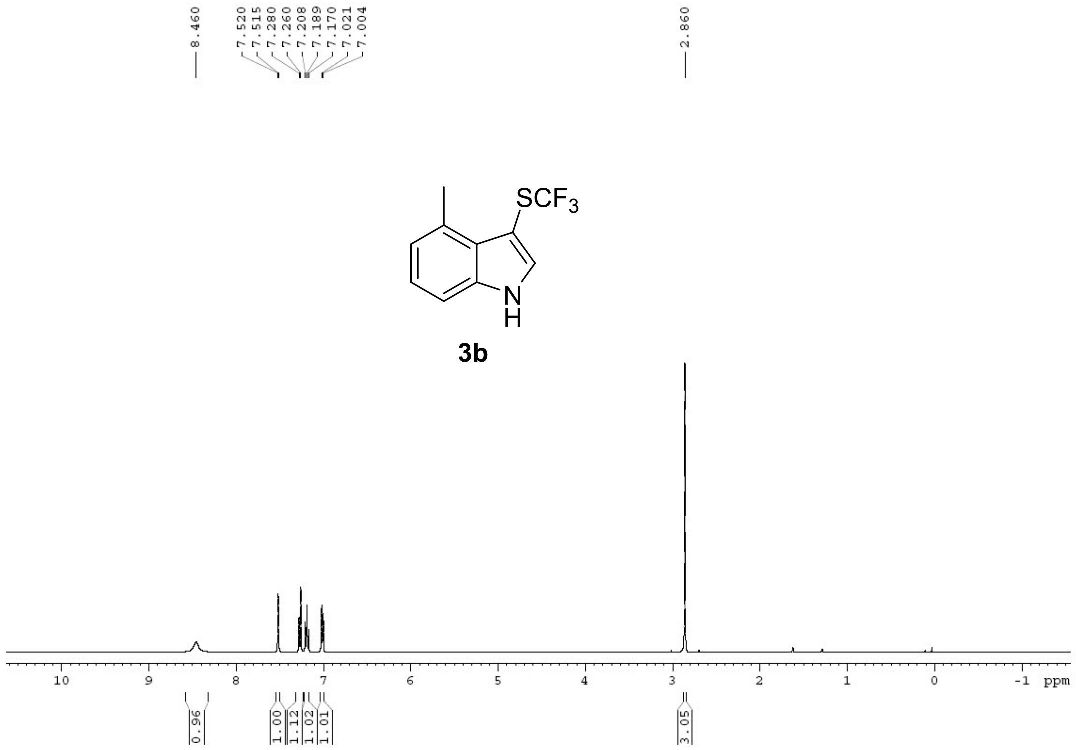


3a

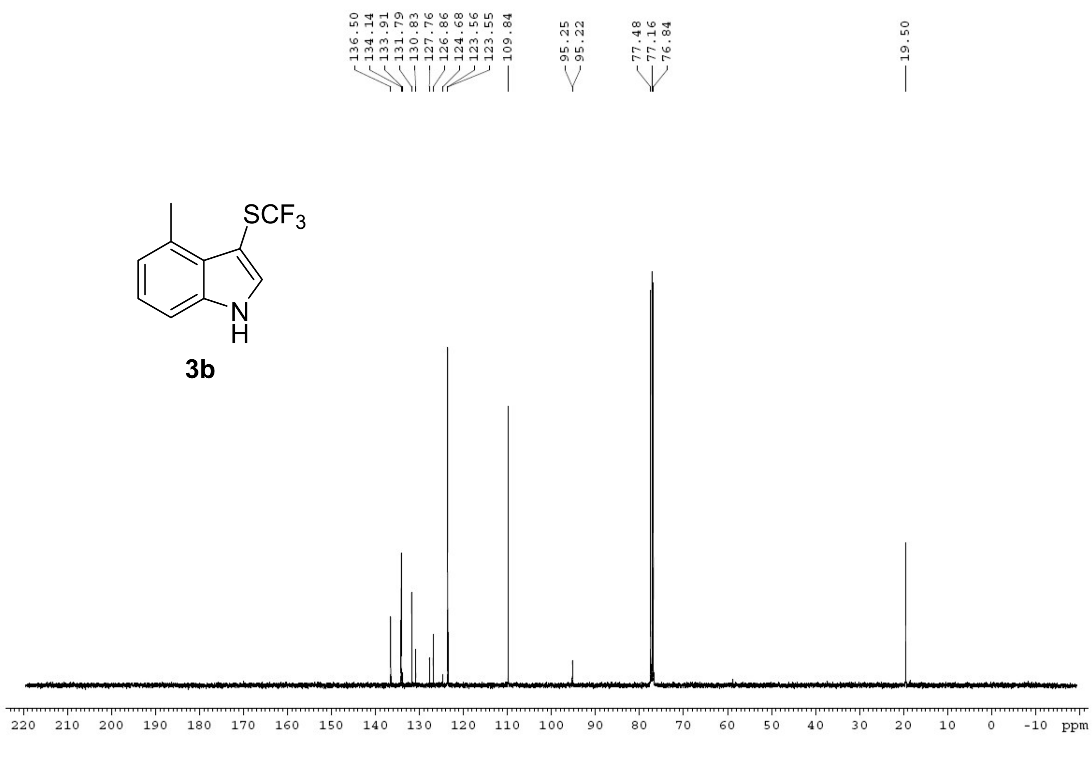



136.14
134.23
132.97
131.16
129.55
128.07
125.00
123.54
121.76
119.42
111.85
95.57
95.55
77.48
77.16
76.84
SCF3
N
H
3a
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 pp

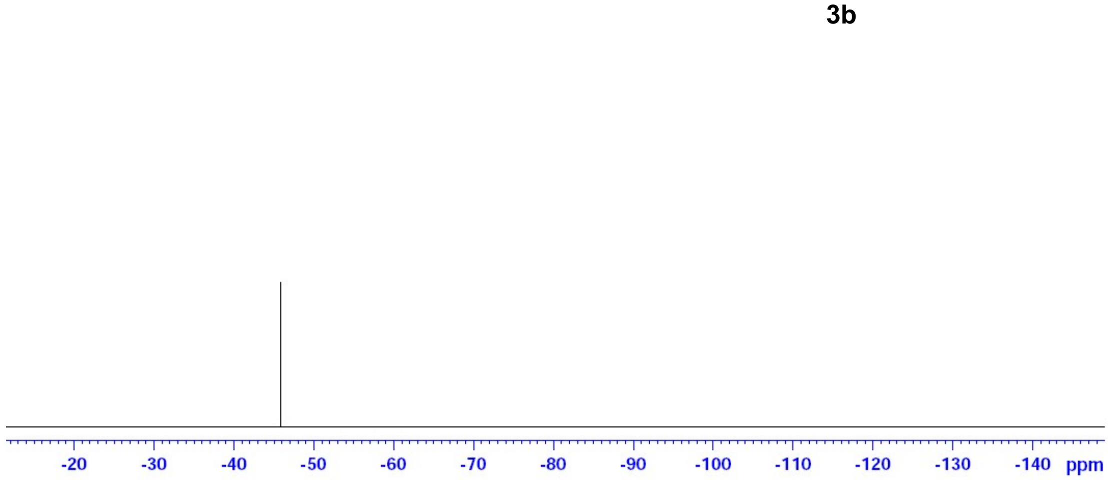

-44.460
SCF3
N
H
3a
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 ppm

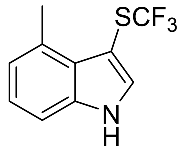


8.460
7.520
7.515
7.280
7.260
7.208
7.189
7.170
7.021
7.004
2.860
SCF3
N
H
3b
10 9 8 7 6 5 4 3 2 1 0 -1 ppm
0.96
1.00
1.12
1.02
1.01
3.05

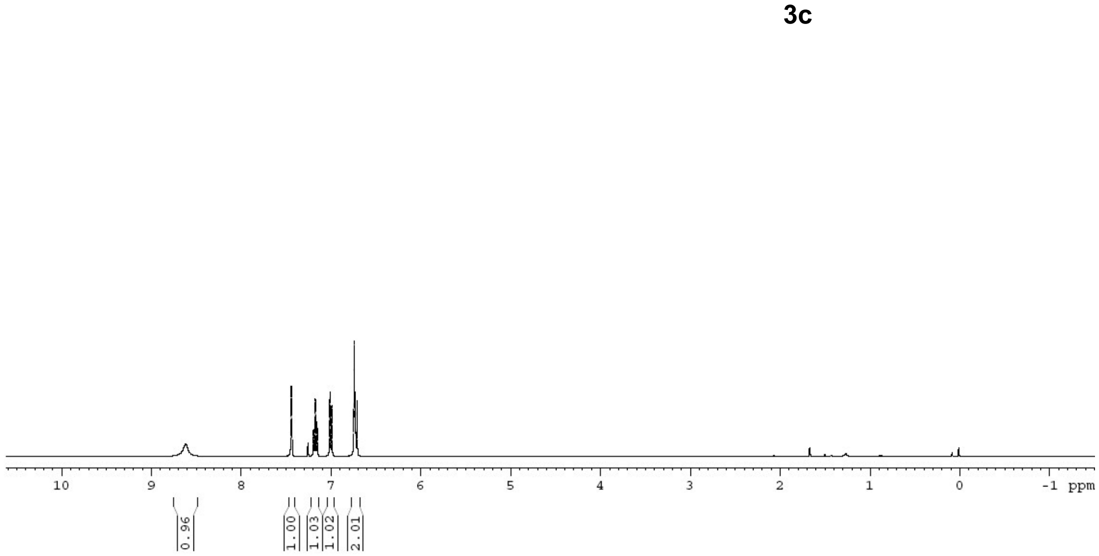


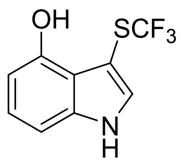
136.50
134.14
133.91
131.79
130.83
127.76
126.86
124.68
123.56
123.55
109.84
95.25
95.22
77.48
77.16
76.84
19.50
SCF3
N
H
3b
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm


-45.825
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 ppm

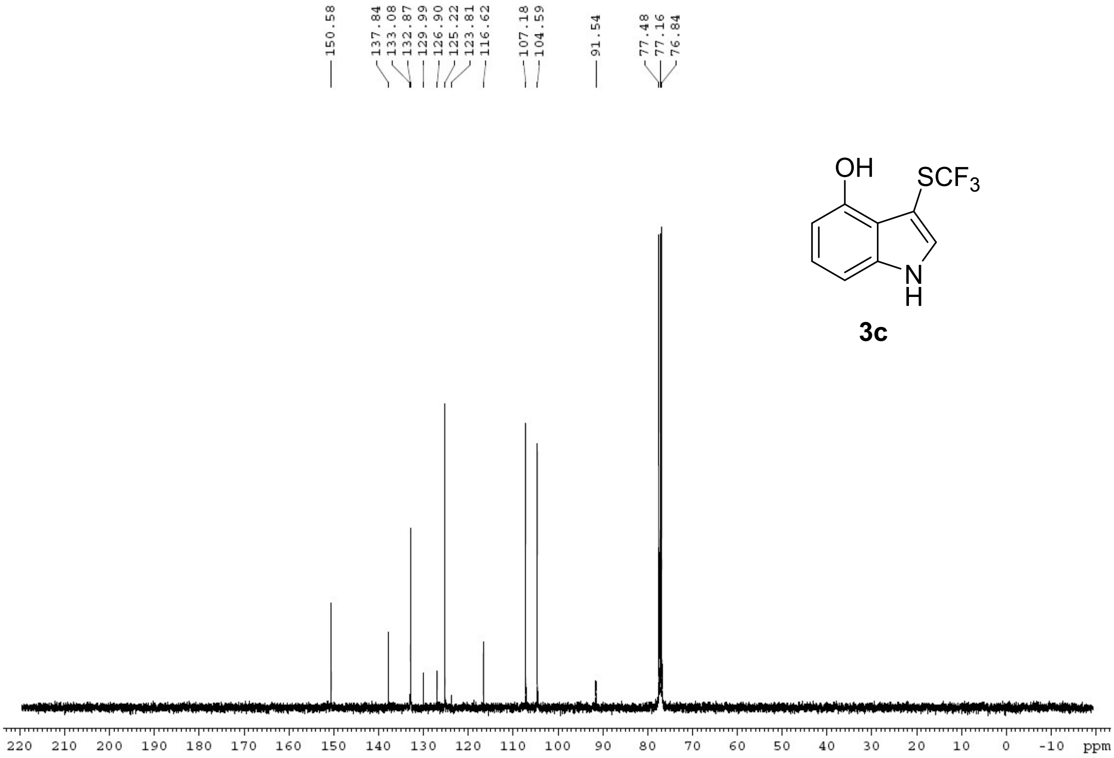

SCF3
N
H

3b


8.620
7.444 7.260 7.197 7.177 7.157 7.015 6.994 6.744 6.733 6.713
10 9 8 7 6 5 4 3 2 1 0 -1 ppm
0.96
1.00 1.03 1.02 2.01


OH
SCF3
N
H

3c


150.58
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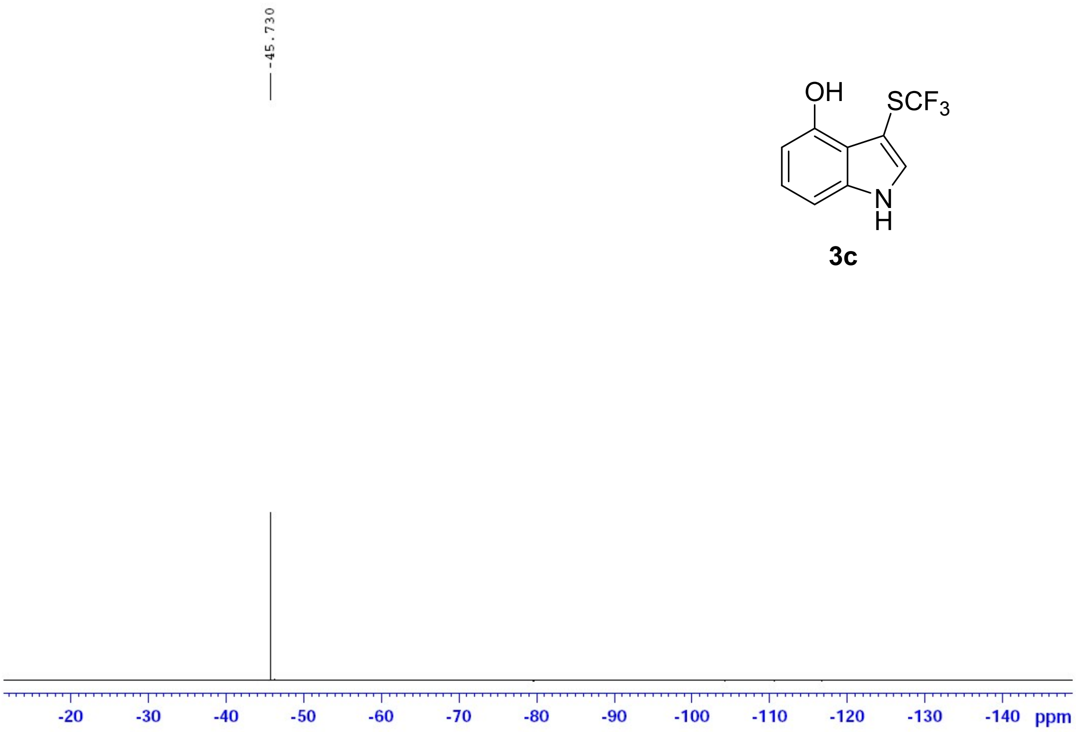
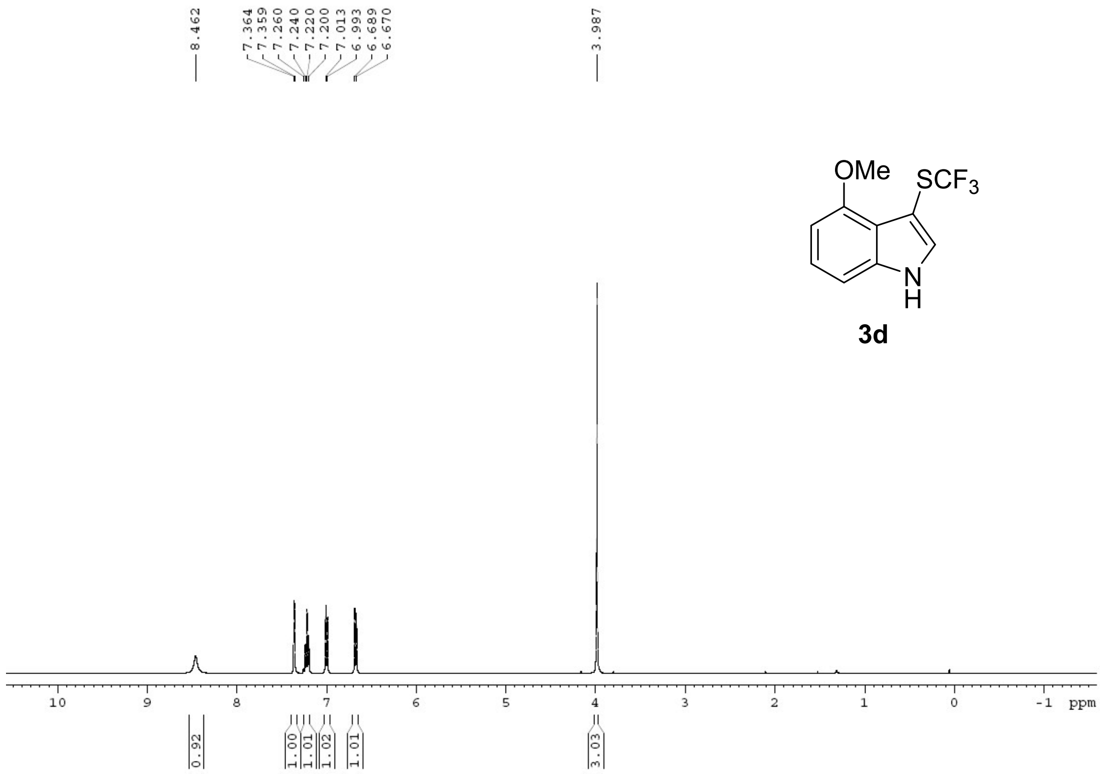
132.87
129.99
126.90
125.22
123.81
116.62
107.18
104.59
91.54
77.48
77.16
76.84
OH
SCF3
N
H
ppm

3c


-45.730
OH
SCF3
N
H
ppm

3c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7.359
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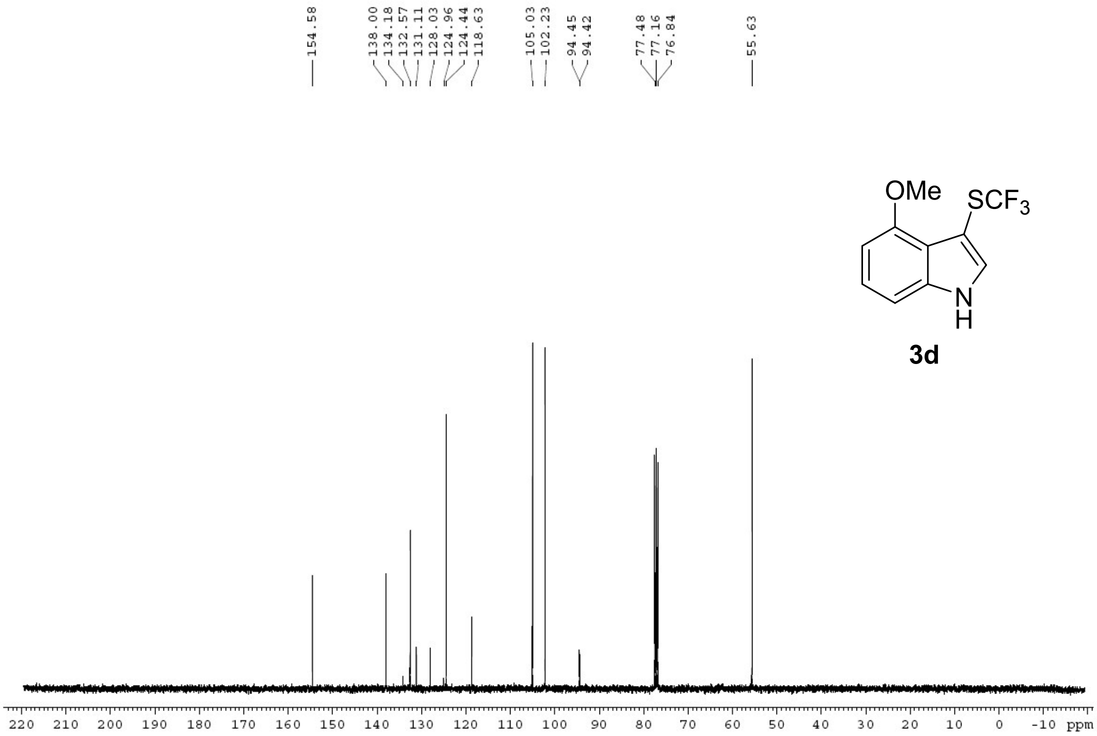
7.240
7.220
7.200
7.013
6.993
6.689
6.670
3.987
OMe
SCF3
N
H
3d
10 9 8 7 6 5 4 3 2 1 0 -1 ppm
0.92
1.00
1.01
1.01
1.02
1.01
3.03


154.58
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131.11
128.03
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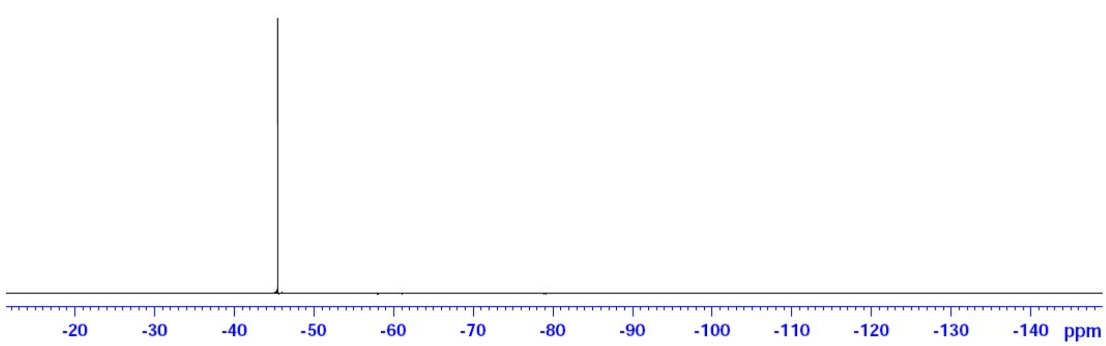
124.44
118.63
105.03
102.23
94.45
94.42
77.48
77.16
76.84
55.63
OMe
SCF3
N
H
3d
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm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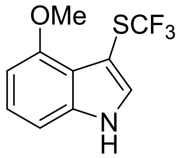
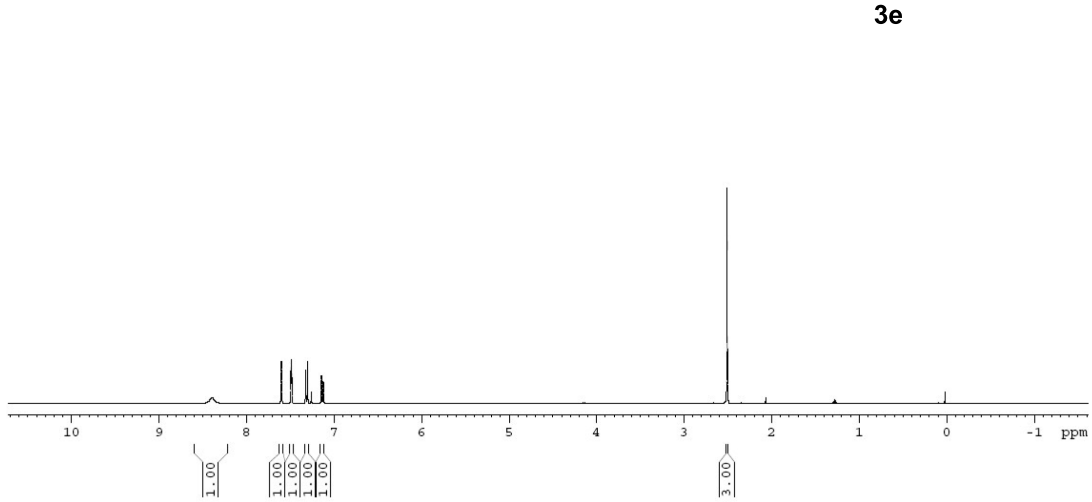
-120
-130
-140
ppm


OMe
SCF3
N
H

3d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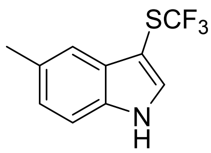
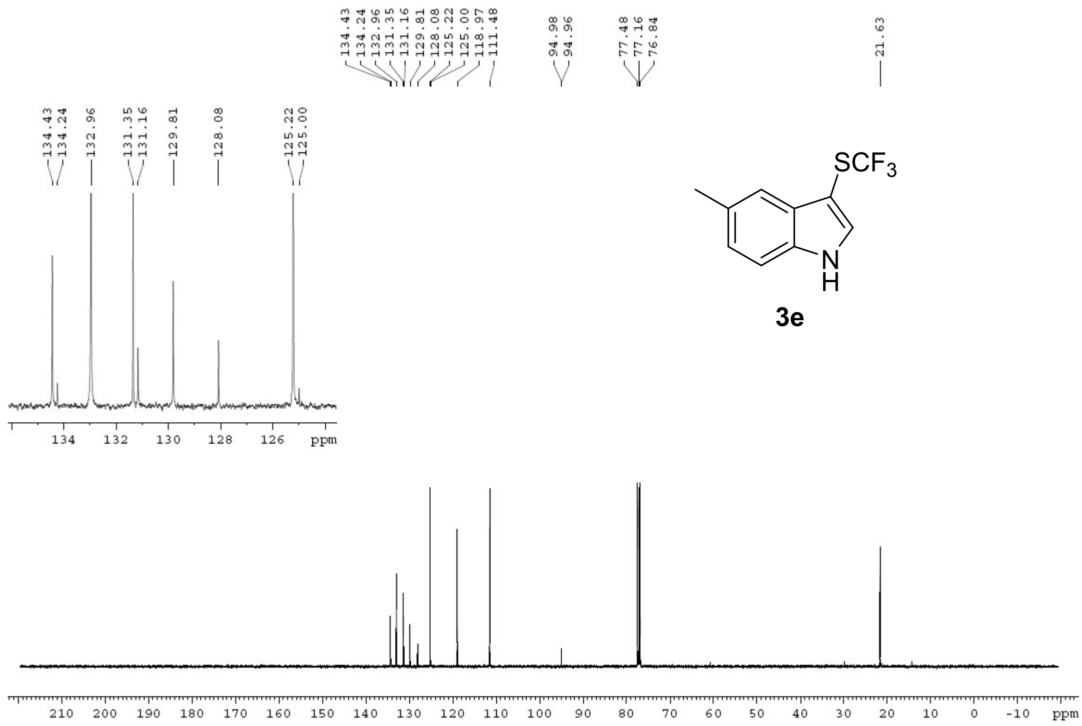
7.324
7.303
7.260
7.145
7.124
2.511
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
1.00
1.00
1.00
1.00
1.00
3.00


SCF3
N
H

3e


134.43
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125.00
118.97
111.48
94.98
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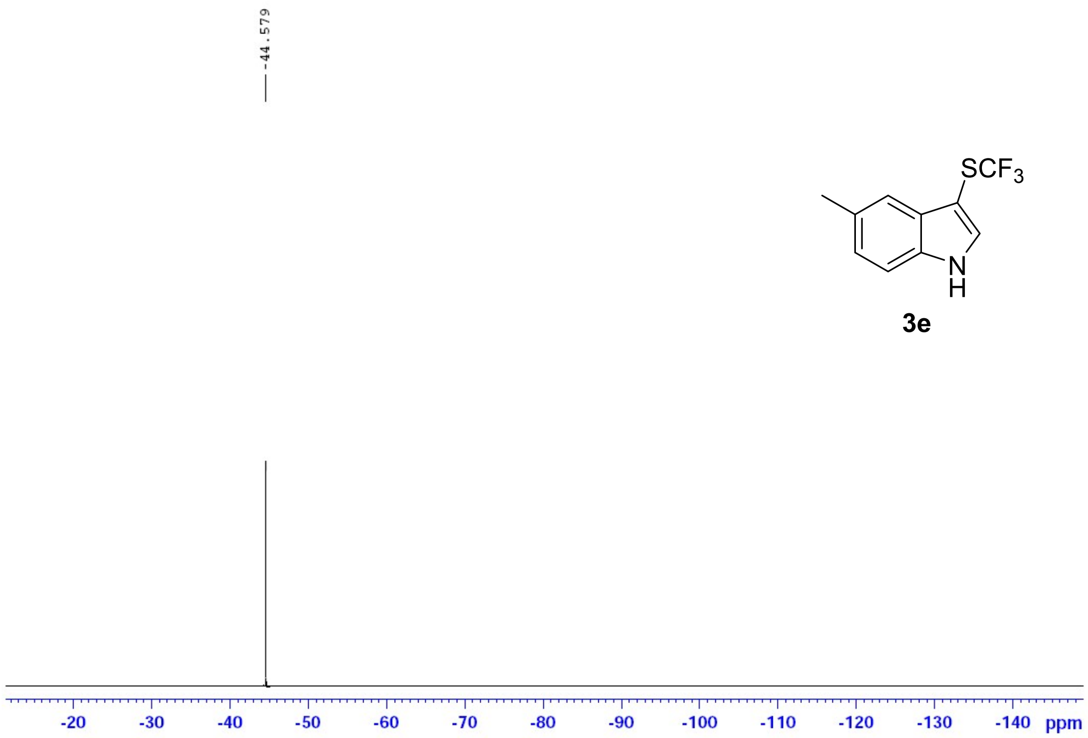
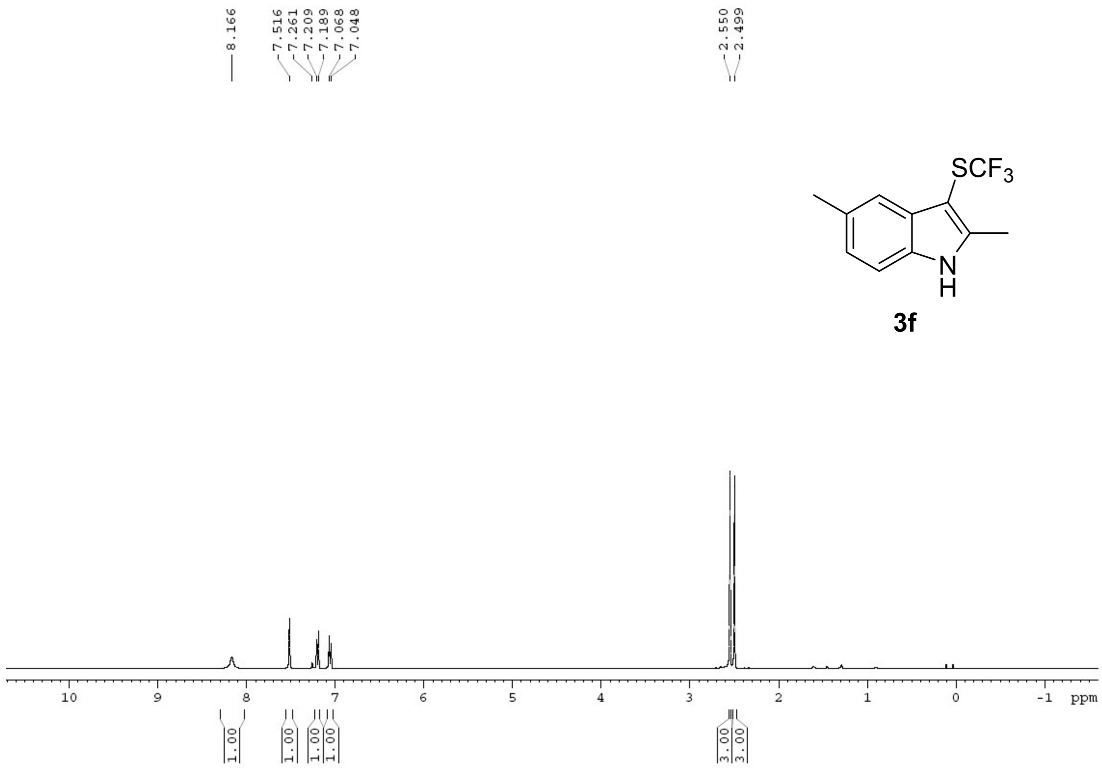
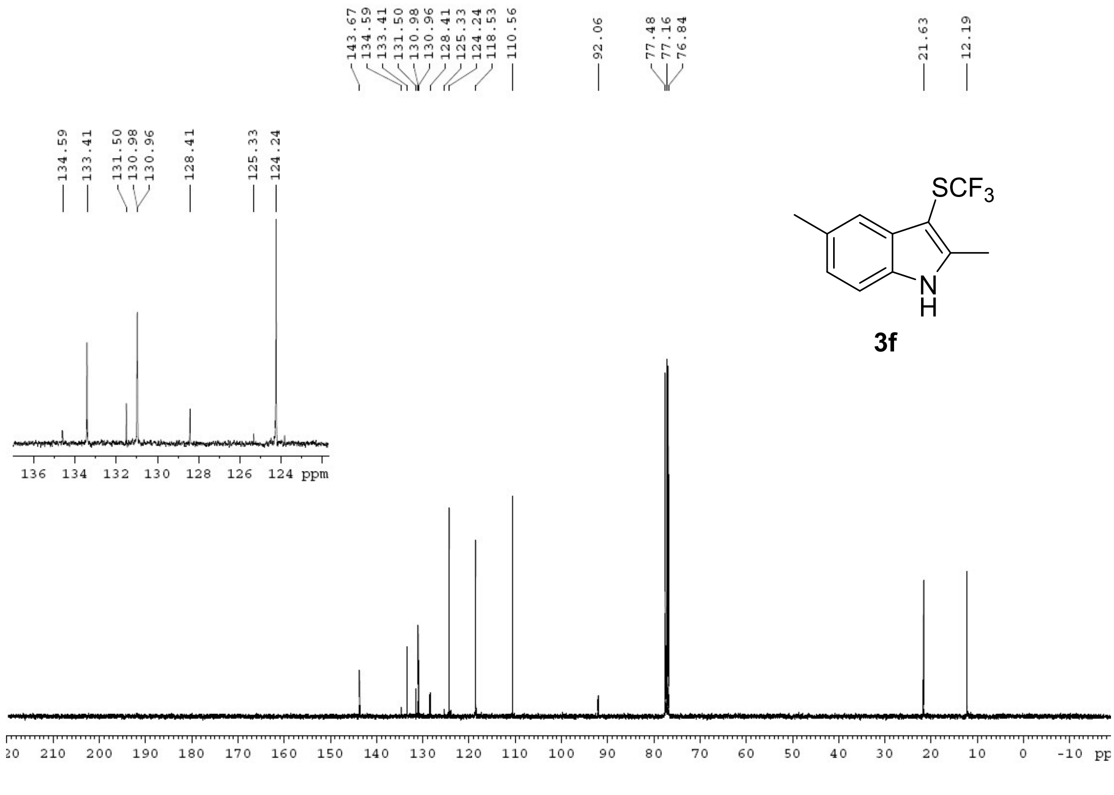
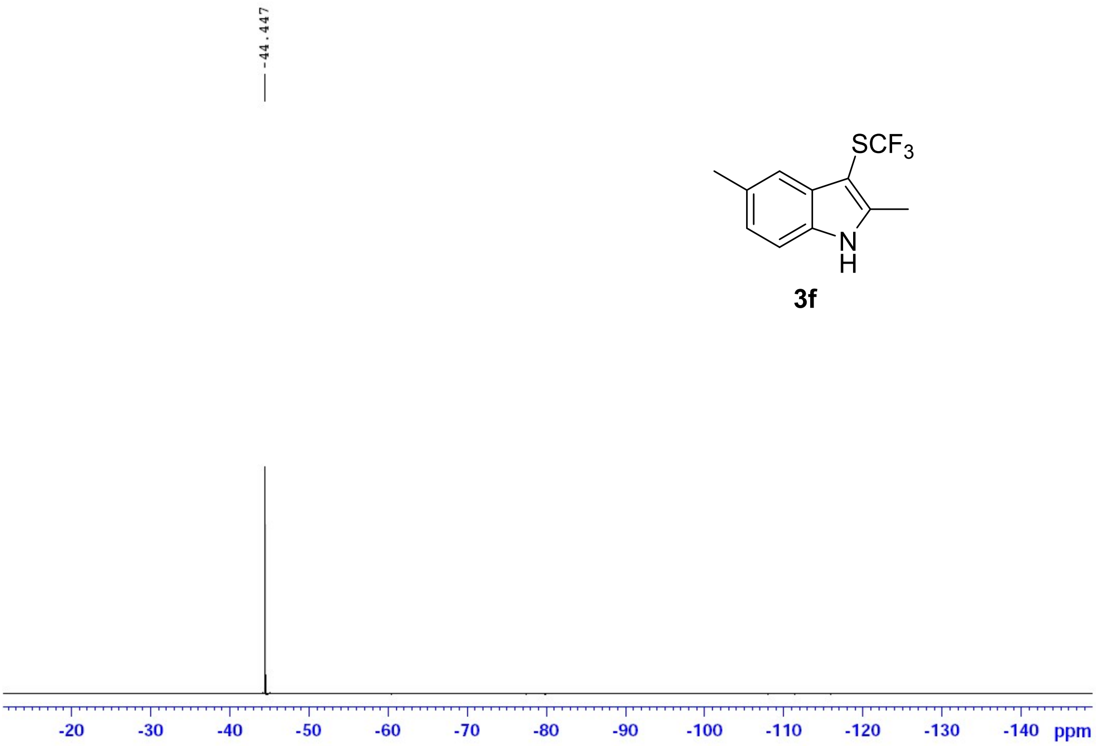
77.48
77.16
76.84
21.63
SCF_3
N
H
3e
134 132 130 128 126 ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm


-44.579
SCF_3
N
H
3e
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 ppm


8.166
7.516
7.261
7.209
7.189
7.068
7.048
2.550
2.499
SCF3
N
H
3f
ppm
1.00
1.00
1.00
1.00
3.00
3.00


143.67
134.59
133.41
131.50
130.98
130.96
128.41
125.33
124.24
118.53
110.56
92.06
77.48
77.16
76.84
21.63
12.19
SCF3
N
H
3f
ppm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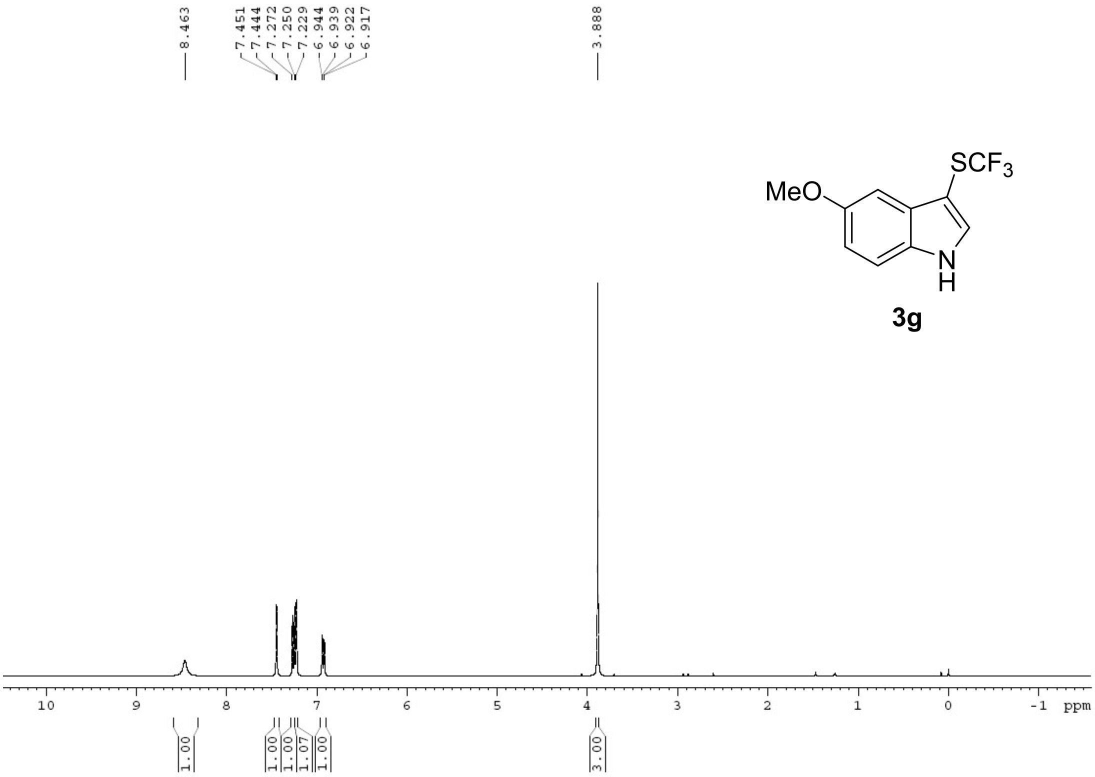
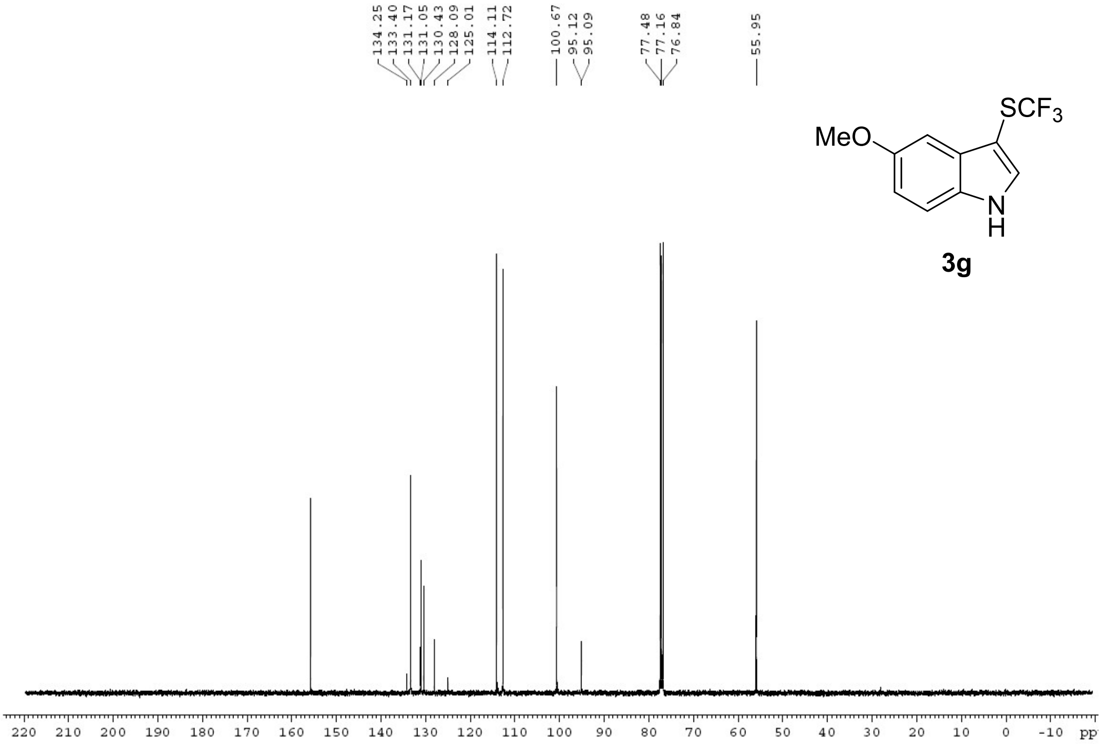
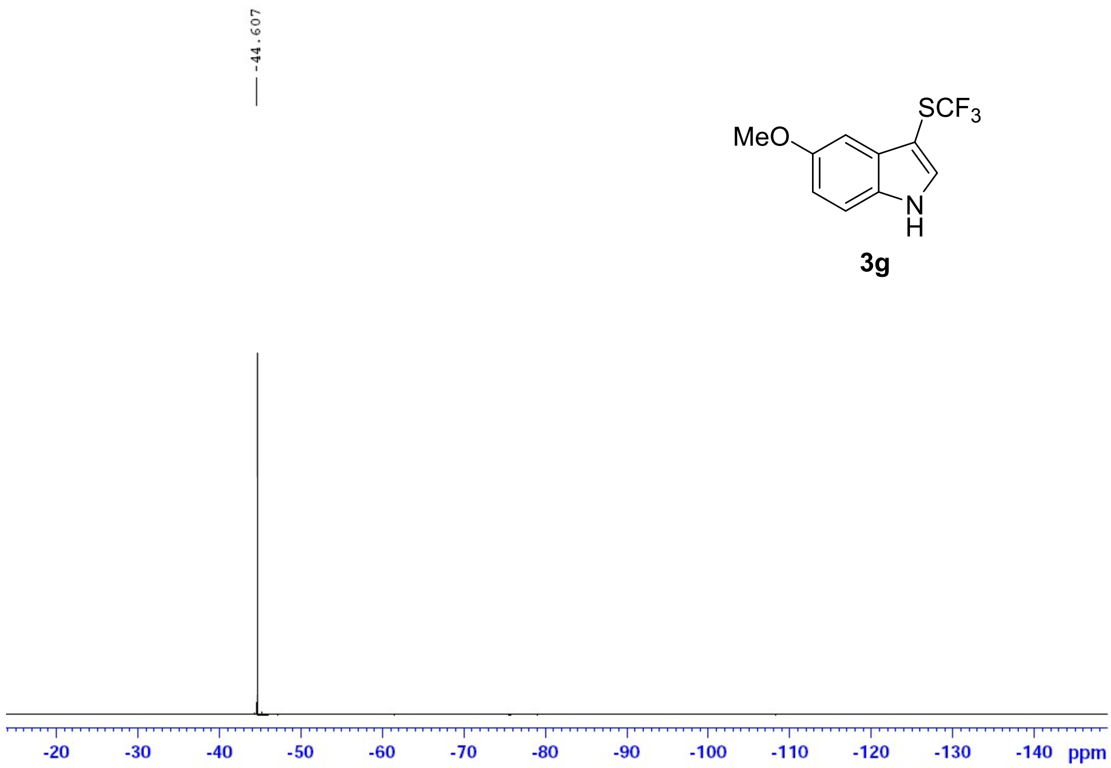
SCF3
N
H
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 ppm

3f


8.463
7.451
7.444
7.272
7.250
7.229
6.944
6.939
6.922
6.917
3.888
SCF3
MeO
N
H
10 9 8 7 6 5 4 3 2 1 0 -1 ppm
1.00
1.00
1.00
1.07
1.00
3.00

3g


134.25
133.40
131.17
131.05
130.43
128.09
125.01
114.11
112.72
100.67
95.12
95.09
77.48
77.16
76.84
55.95
SCF$_3$
MeO
N
H
3g
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 pp


-44.607
SCF$_3$
MeO
N
H
3g
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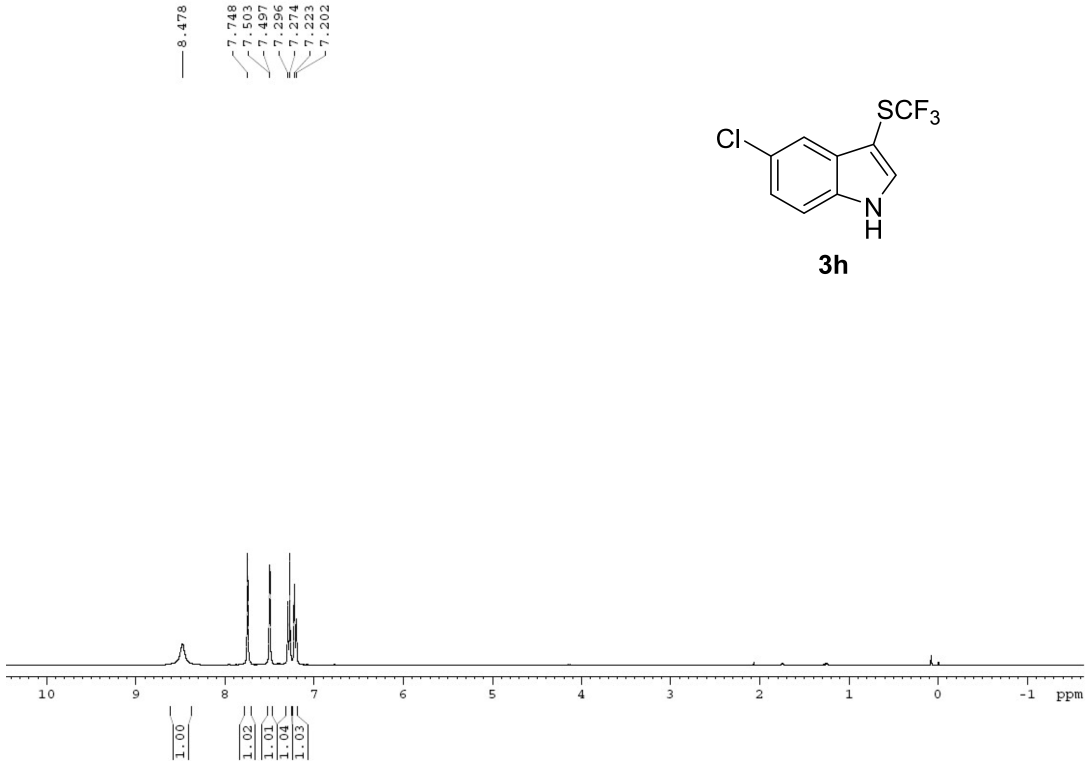
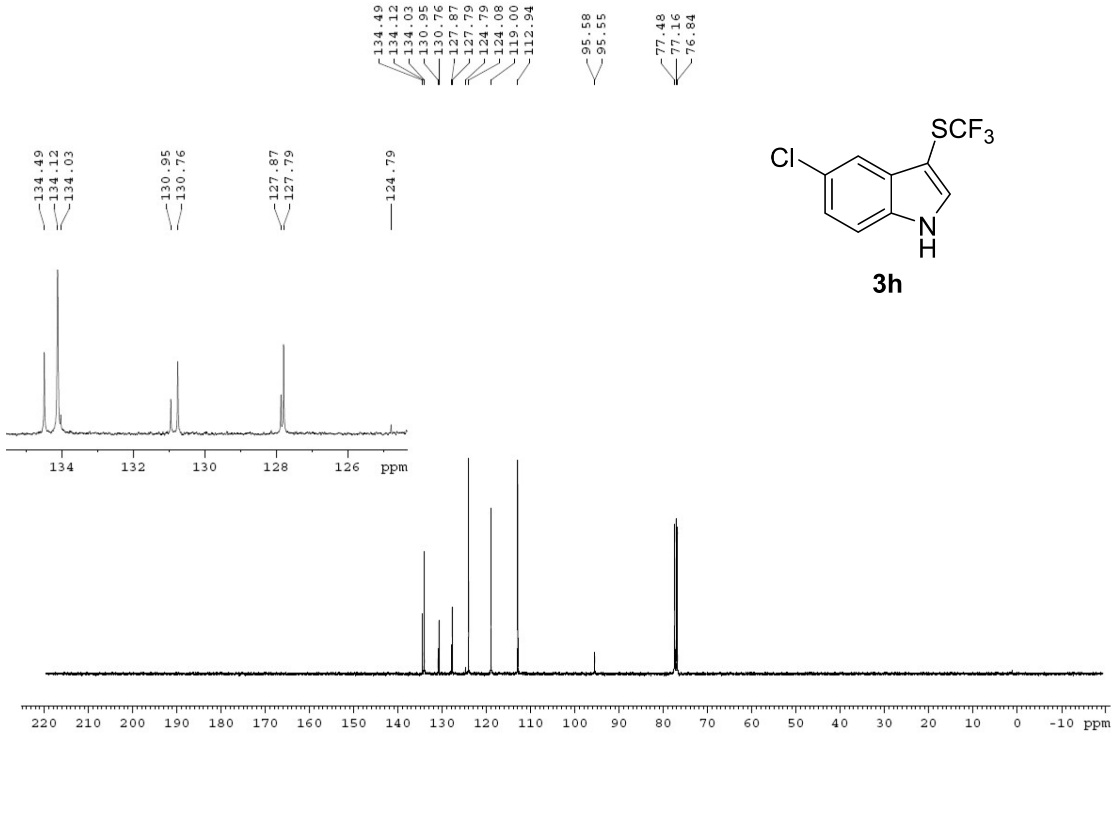
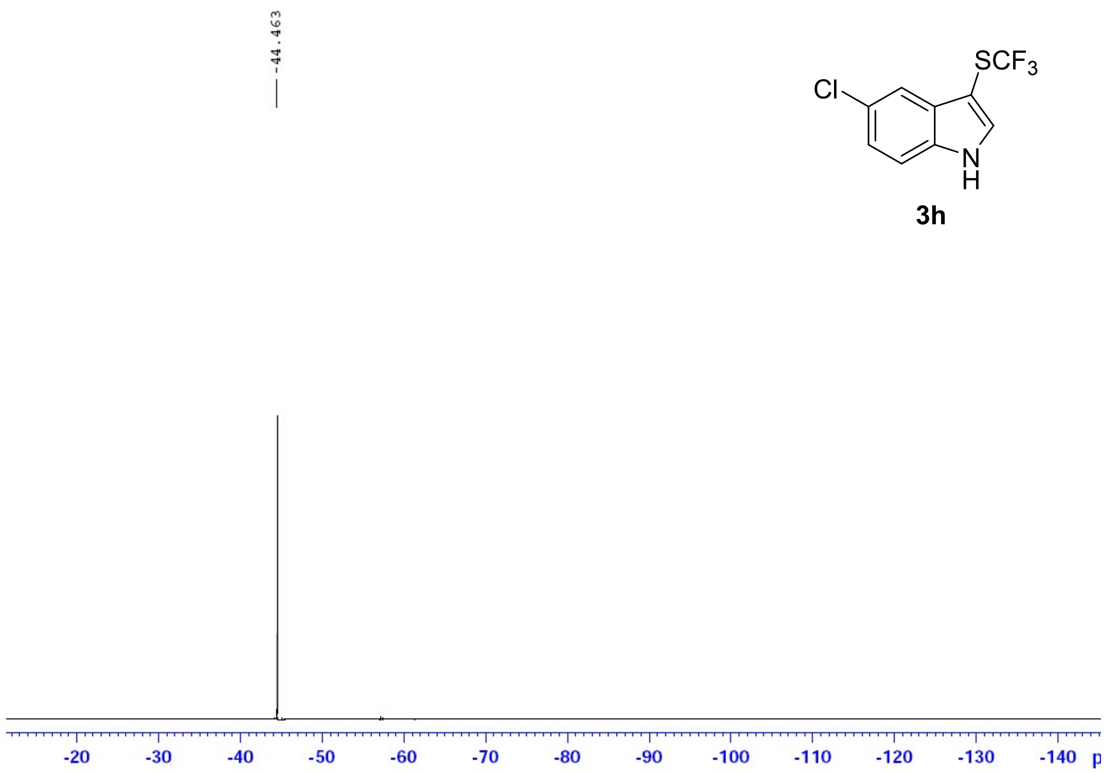
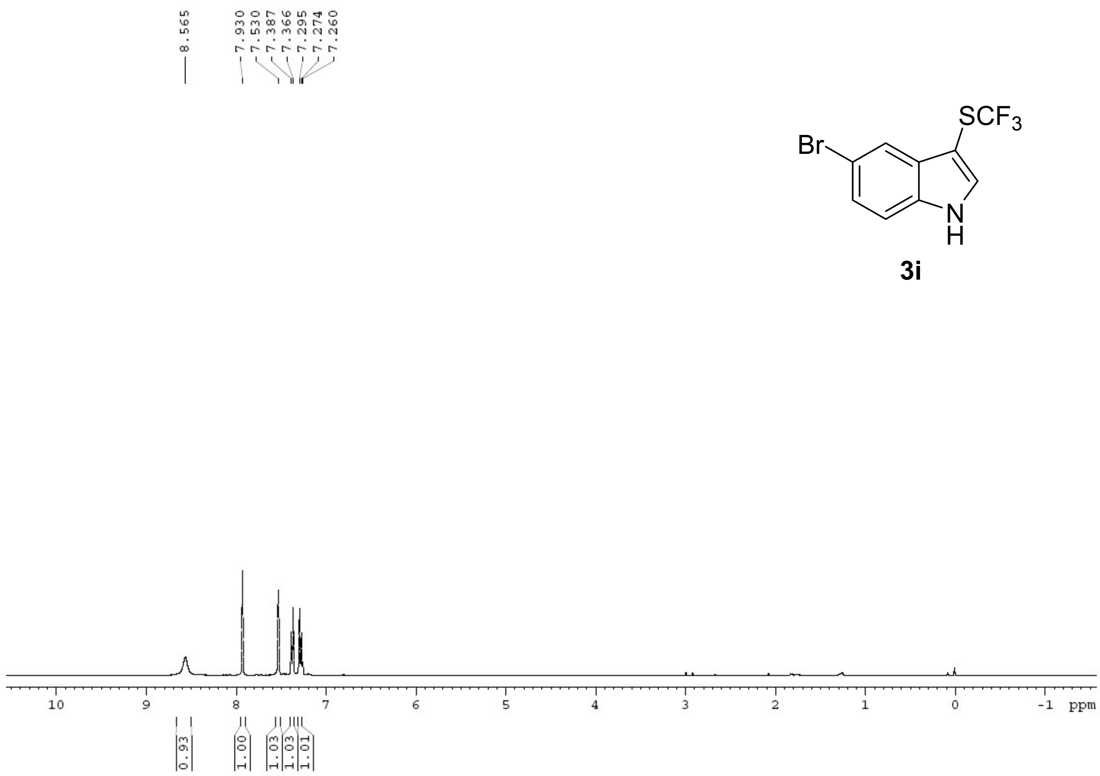
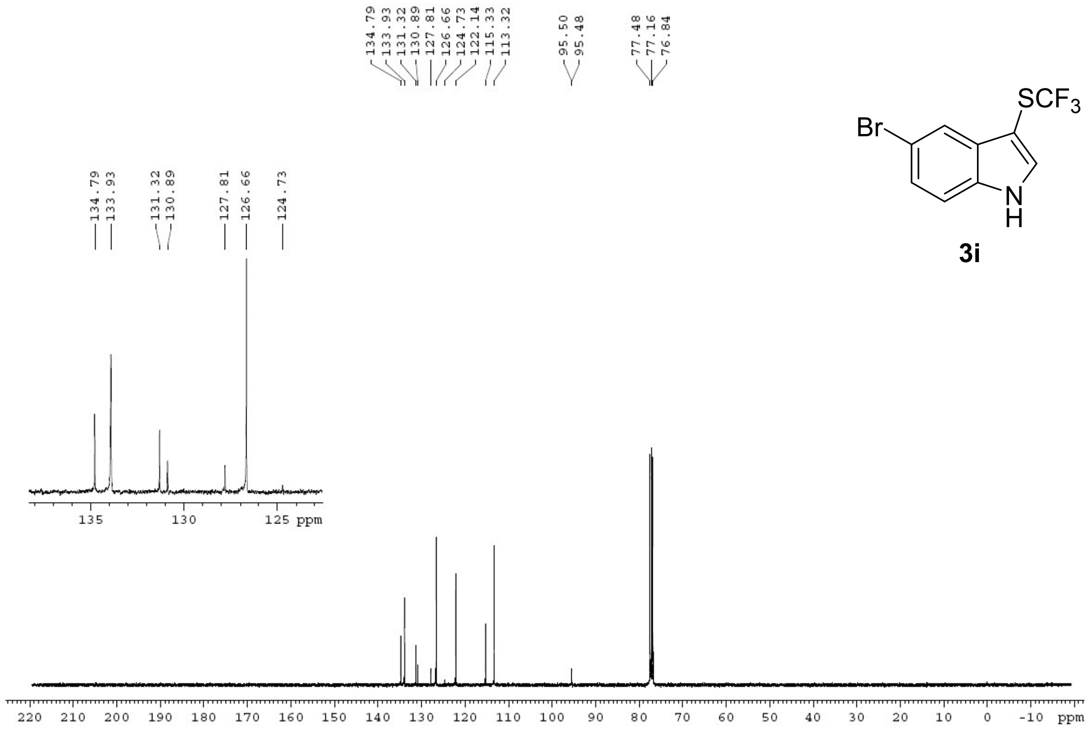

8.478
7.748
7.503
7.497
7.296
7.274
7.223
7.202
Cl
SCF3
N
H
3h
10 9 8 7 6 5 4 3 2 1 0 -1 ppm
1.00
1.02
1.01
1.04
1.03

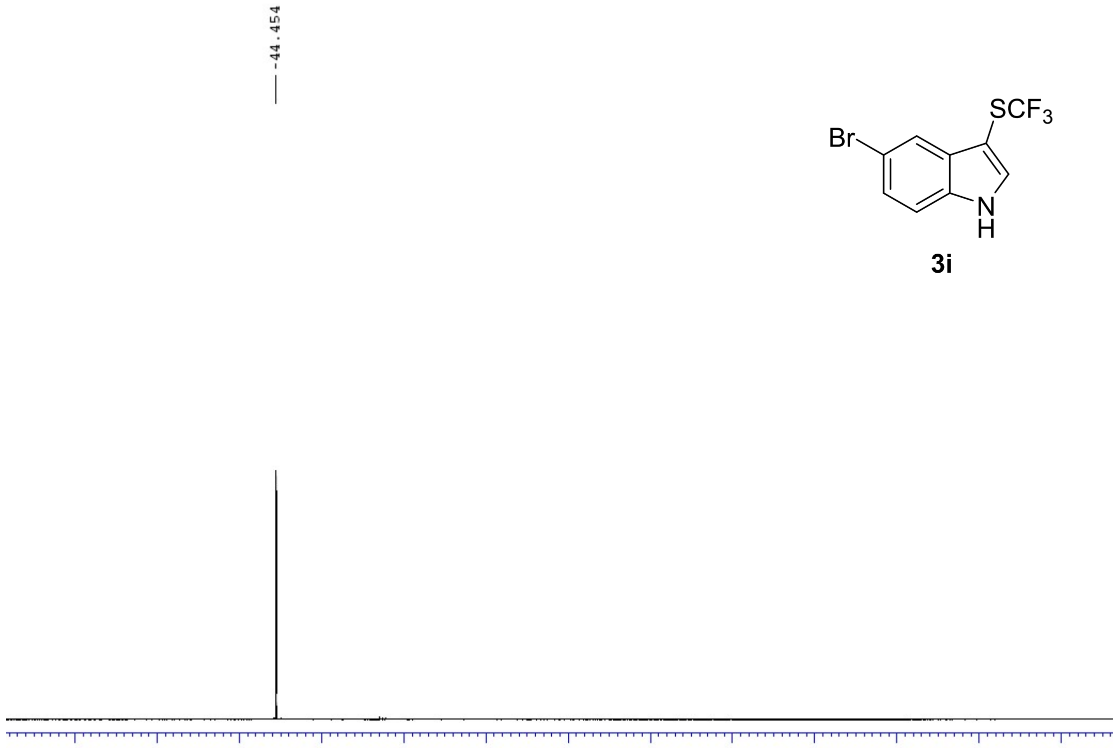

134.49
134.12
134.03
130.95
130.76
127.87
127.79
124.79
124.08
119.00
112.94
95.58
95.55
77.48
77.16
76.84
Cl
SCF3
N
H
3h
134 132 130 128 126 ppm
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm


-44.463
SCF3
Cl
N
H
3h
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140

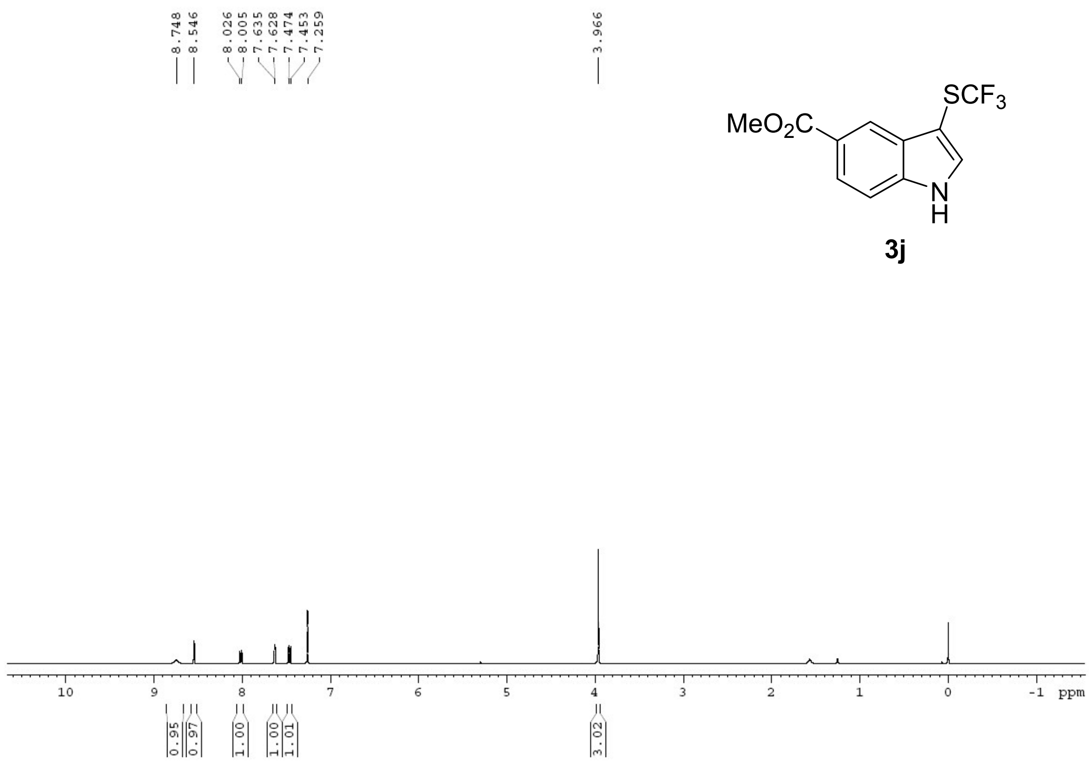

8.565
7.930
7.530
7.387
7.366
7.295
7.274
7.260
SCF3
Br
N
H
3i
10 9 8 7 6 5 4 3 2 1 0 -1 ppm
0.93
1.00
1.03
1.03
1.01


134.79
133.93
131.32
130.89
127.81
126.66
124.73
122.14
115.33
113.32
95.50
95.48
77.48
77.16
76.84
SCF3
Br
N
H
135
130
125 ppm
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

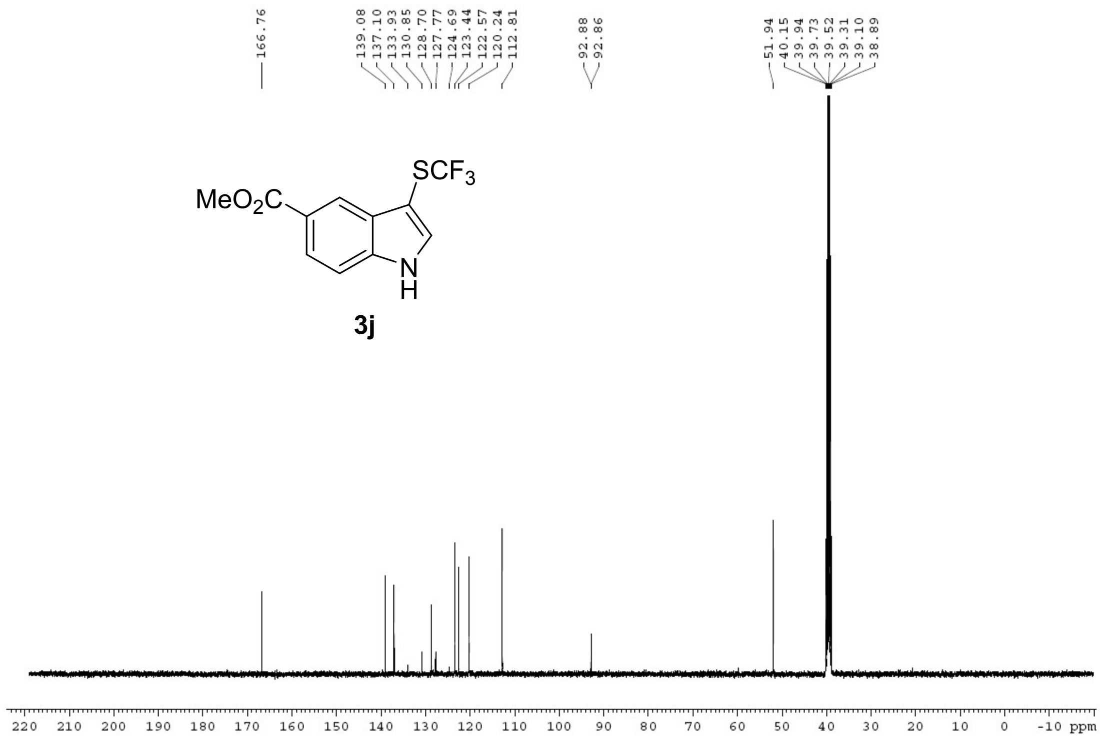
3i


-44.454
SCF3
Br
N
H
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140

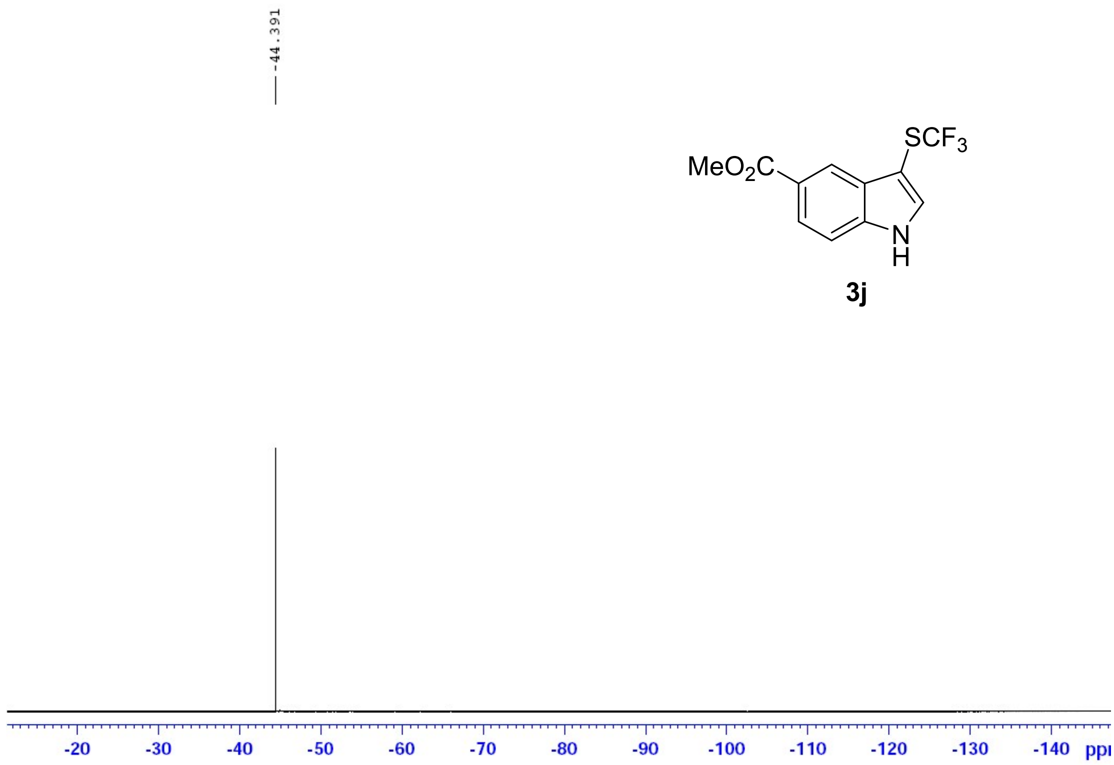
3i



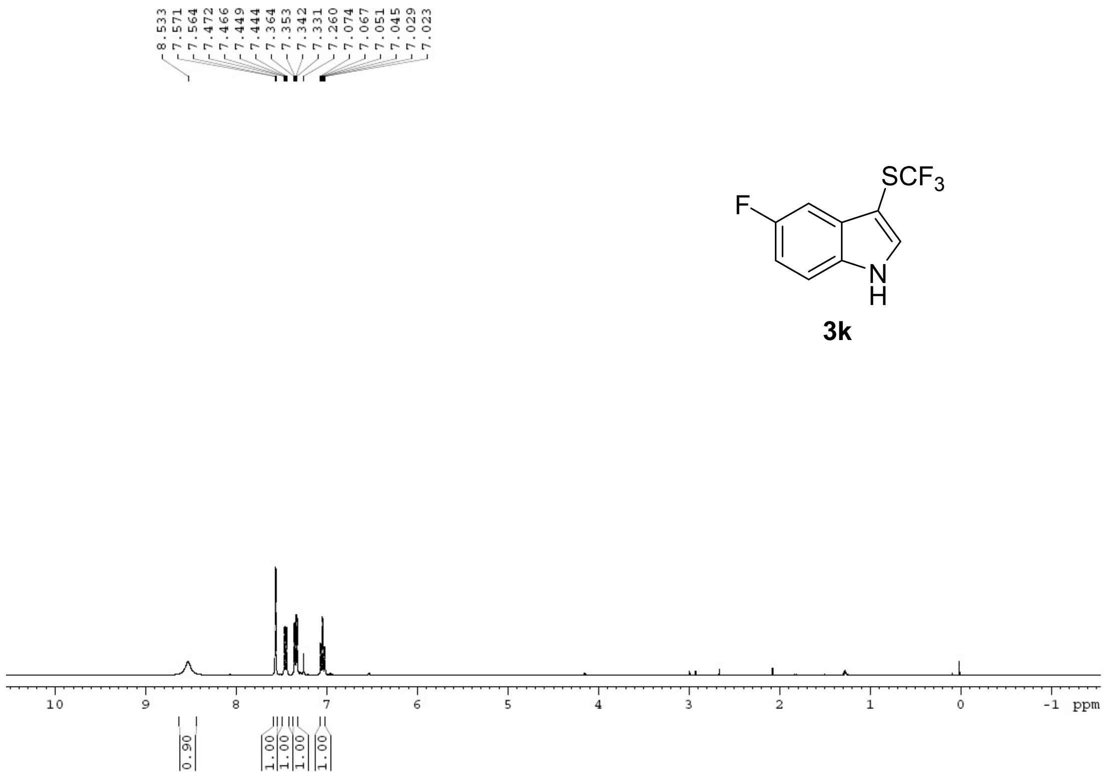
8.748
8.546
8.026
8.005
7.635
7.628
7.474
7.453
7.259
3.966
SCF3
MeO2C
N
H
3j
10 9 8 7 6 5 4 3 2 1 0 -1 ppm
0.95
0.97
1.00
1.00
1.01
3.02



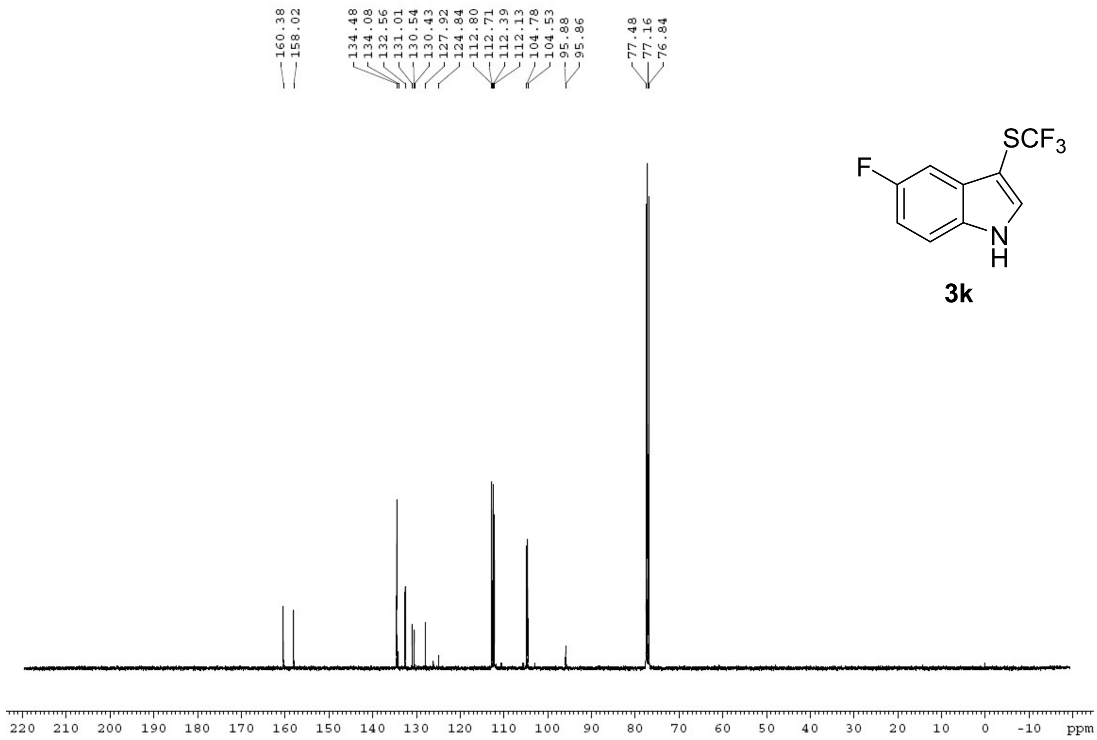
166.76
139.08
137.10
133.93
130.85
128.70
127.77
124.69
123.44
122.57
120.24
112.81
92.88
92.86
51.94
40.15
39.94
39.73
39.52
39.31
39.10
38.89
SCF3
MeO2C
N
H
3j
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm


-44.391
MeO2C
SCF3
N
H
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 ppm

3j


8.533
7.571
7.564
7.472
7.466
7.449
7.444
7.364
7.353
7.342
7.331
7.260
7.074
7.067
7.051
7.045
7.029
7.023
F
SCF3
N
H
10 9 8 7 6 5 4 3 2 1 0 -1 ppm
0.90
1.00
1.00
1.00
1.00

3k


160.38
158.02
134.48
134.08
132.56
131.01
130.54
130.43
127.92
124.84
112.80
112.71
112.39
112.13
104.78
104.53
95.88
95.86
77.48
77.16
76.84
F
SCF3
N
H
3k
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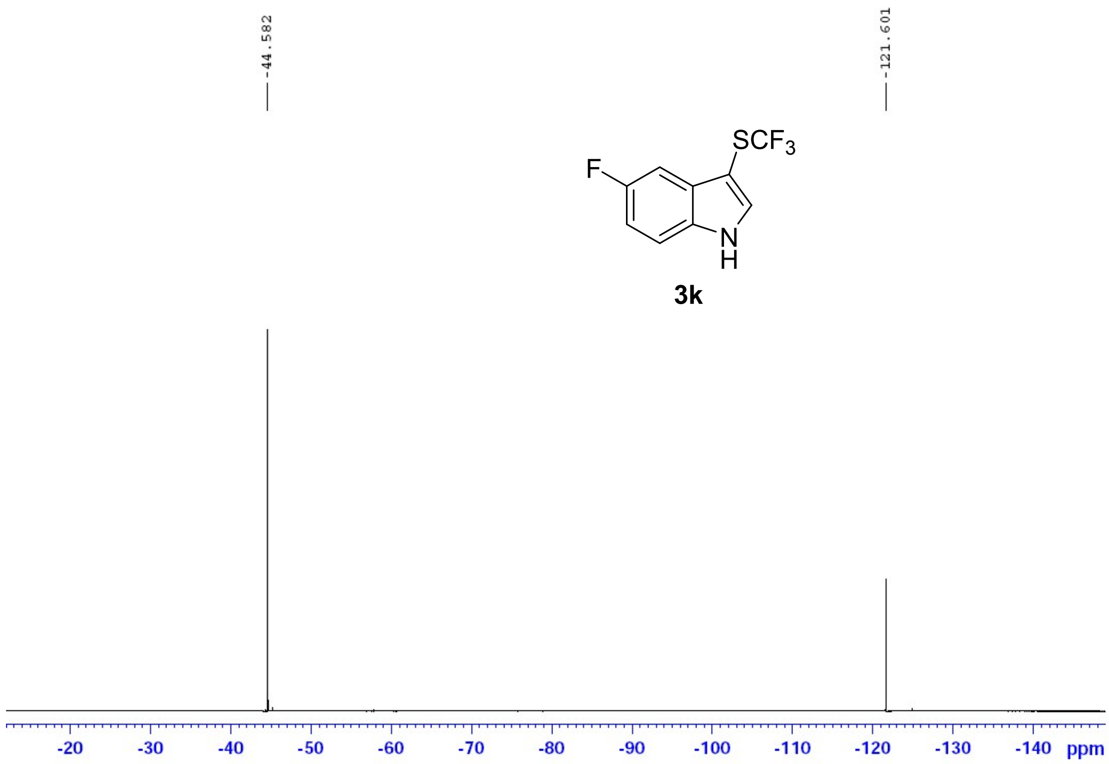
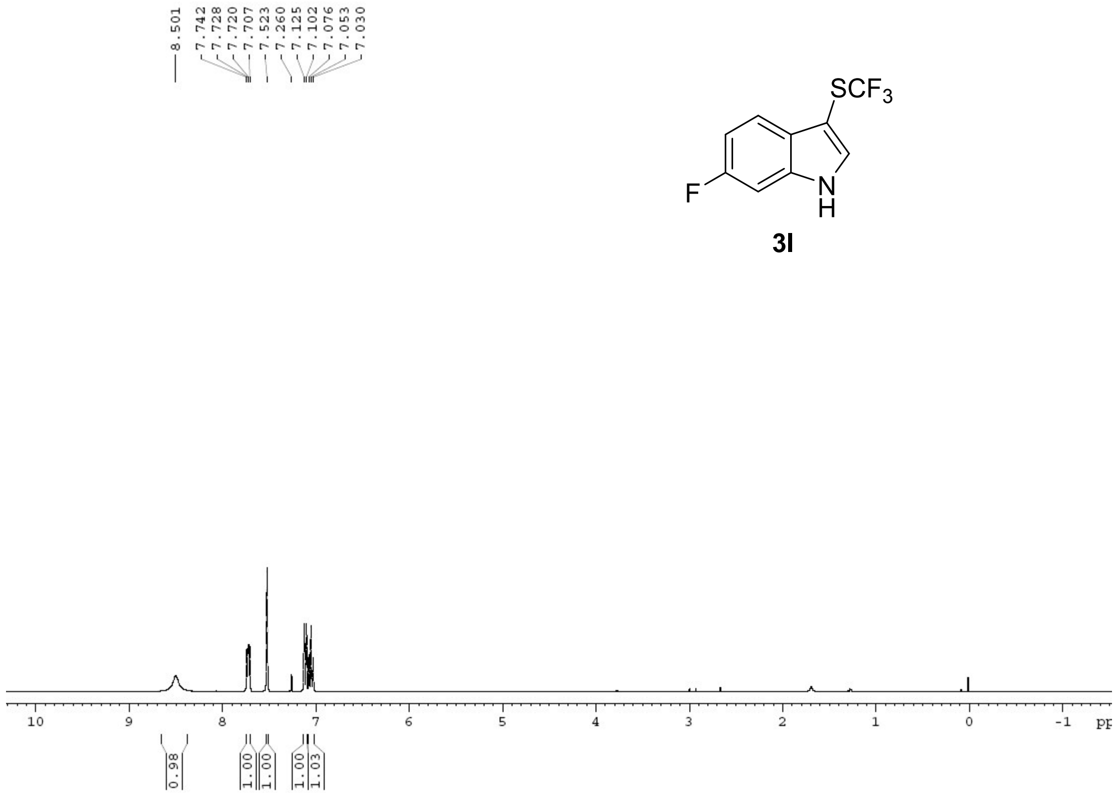
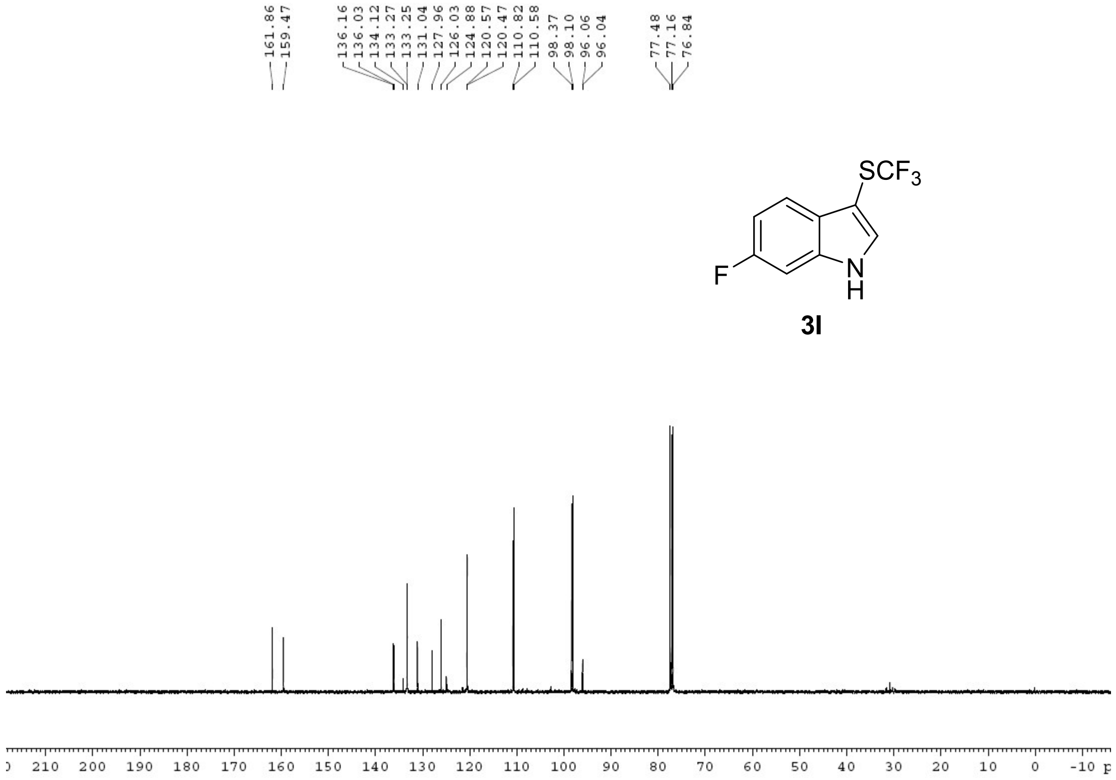
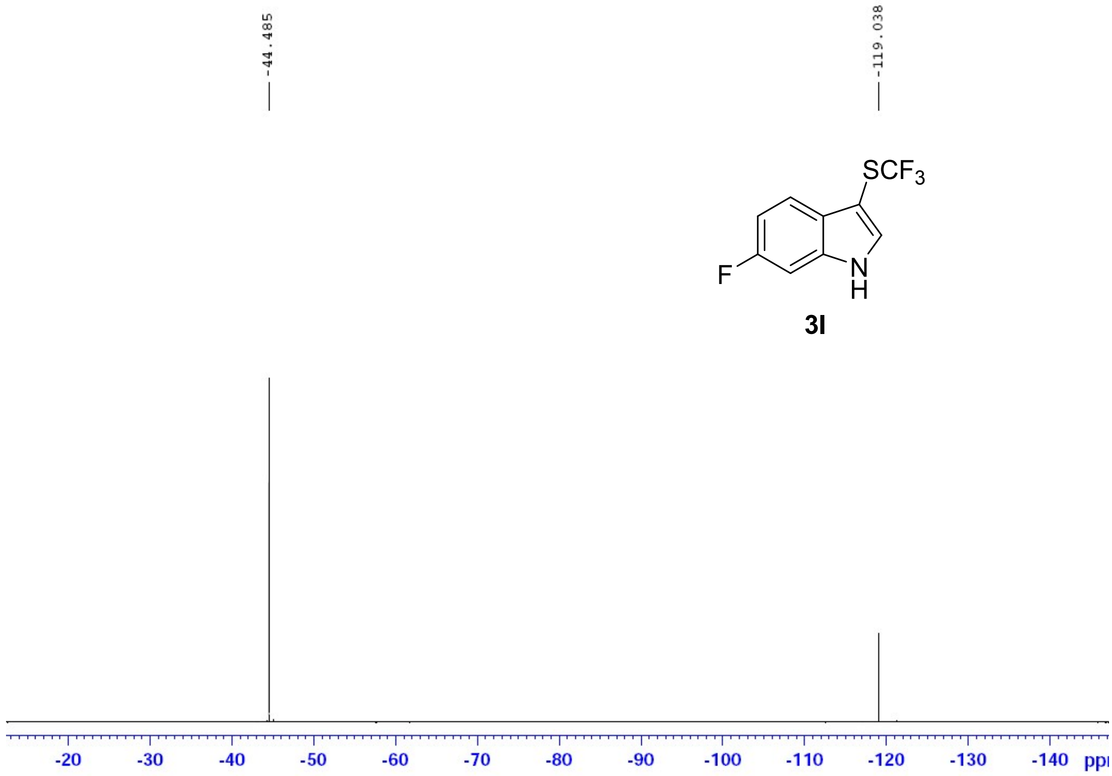
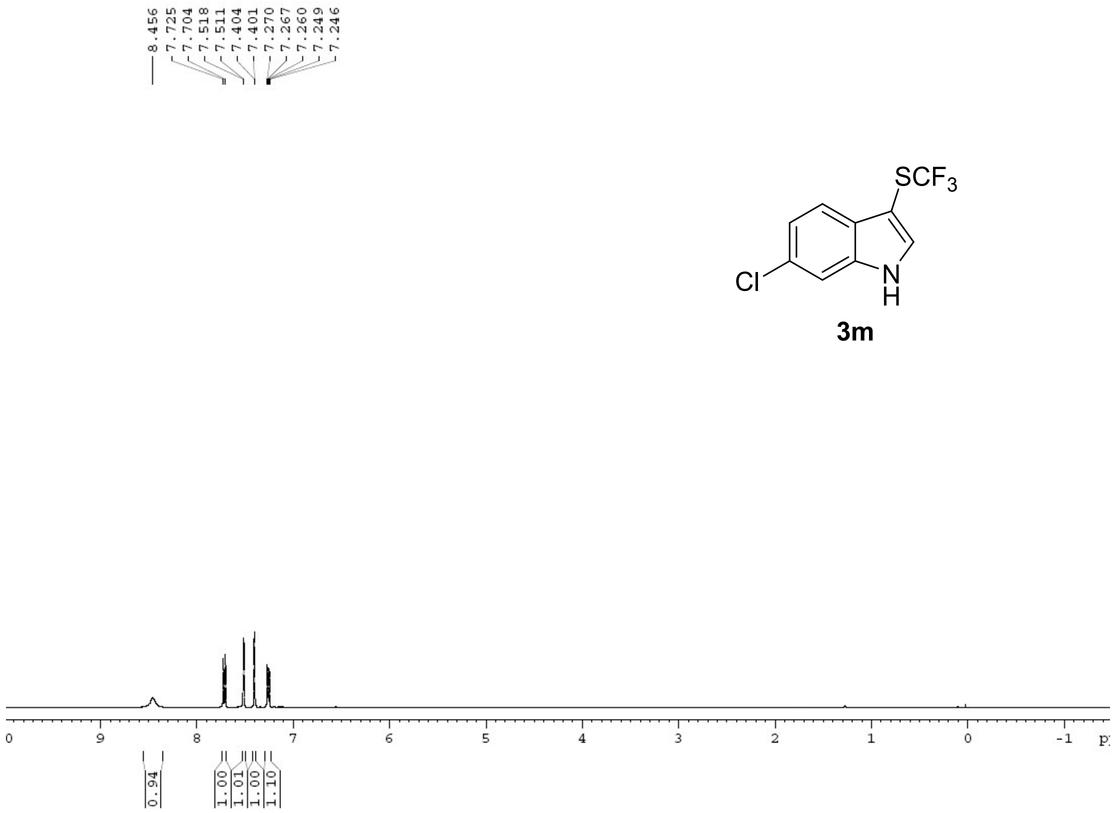

-44.582
-121.601
F
SCF3
N
H
3k
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 ppm


8.501
7.742
7.728
7.720
7.707
7.523
7.260
7.125
7.102
7.076
7.053
7.030
SCF3
F
N
H
3l
10 9 8 7 6 5 4 3 2 1 0 -1 pp
0.98
1.00
1.00
1.00
1.03

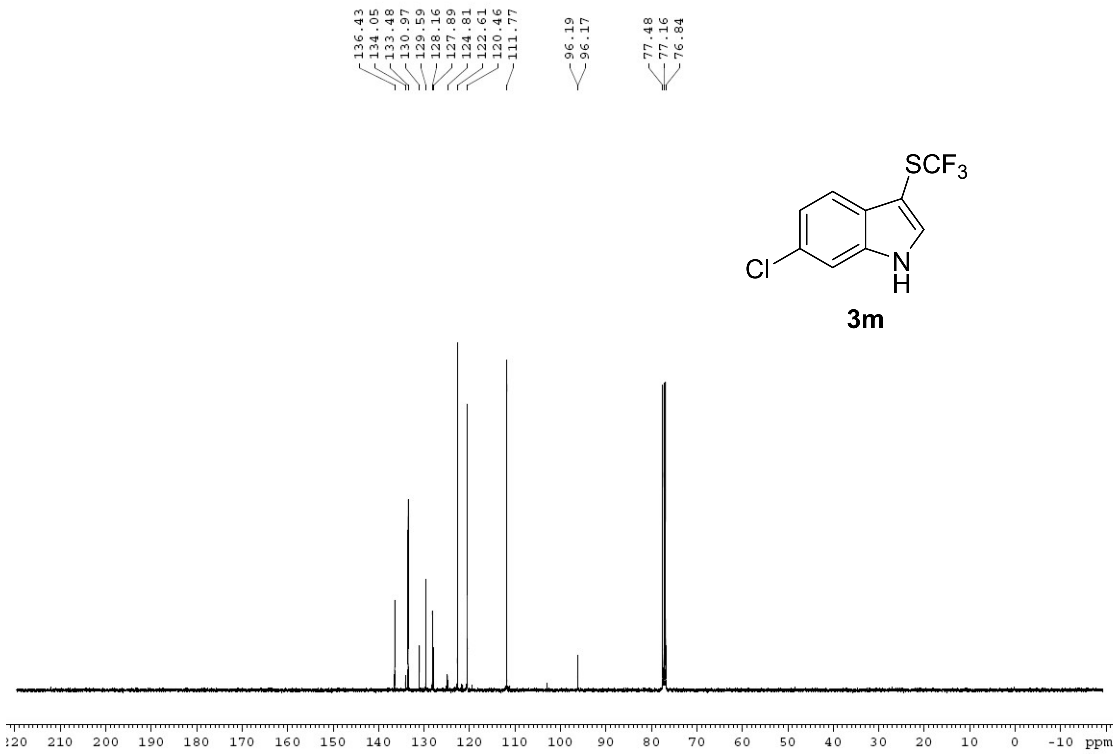

161.86
159.47
136.16
136.03
134.12
133.27
133.25
131.04
127.96
126.03
124.88
120.57
120.47
110.82
110.58
98.37
98.10
96.06
96.04
77.48
77.16
76.84
SCF3
F
N
H
3l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

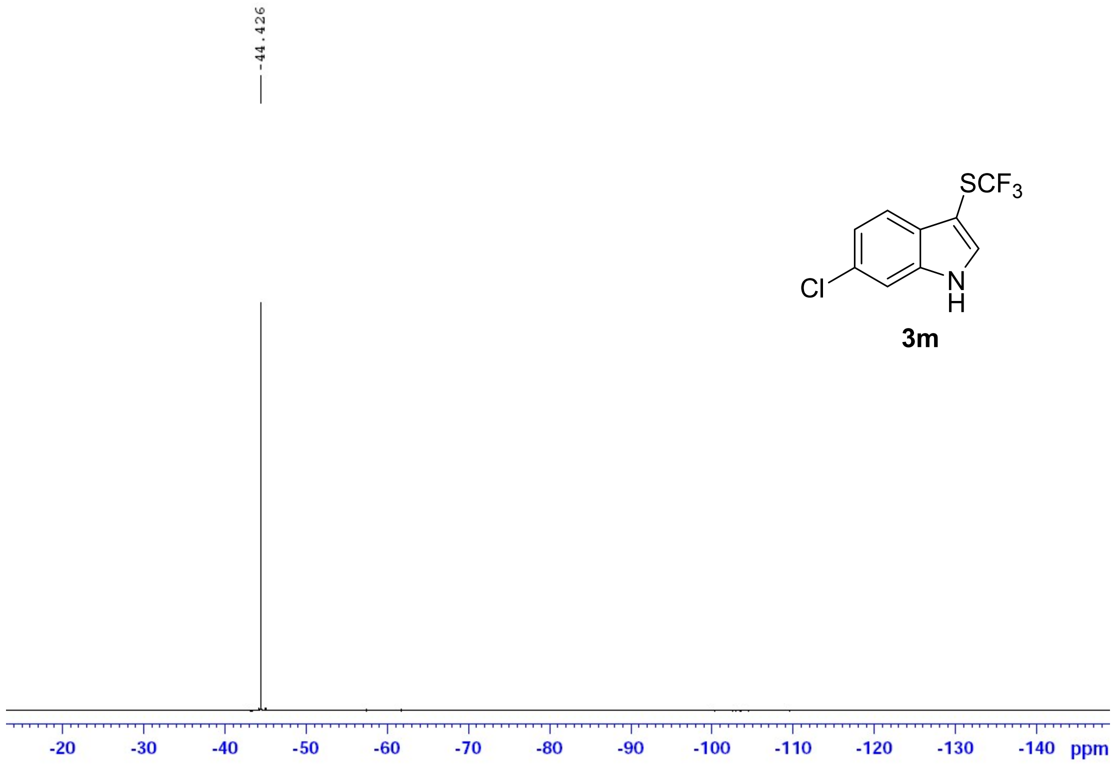

-44.485
-119.038
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
ppm

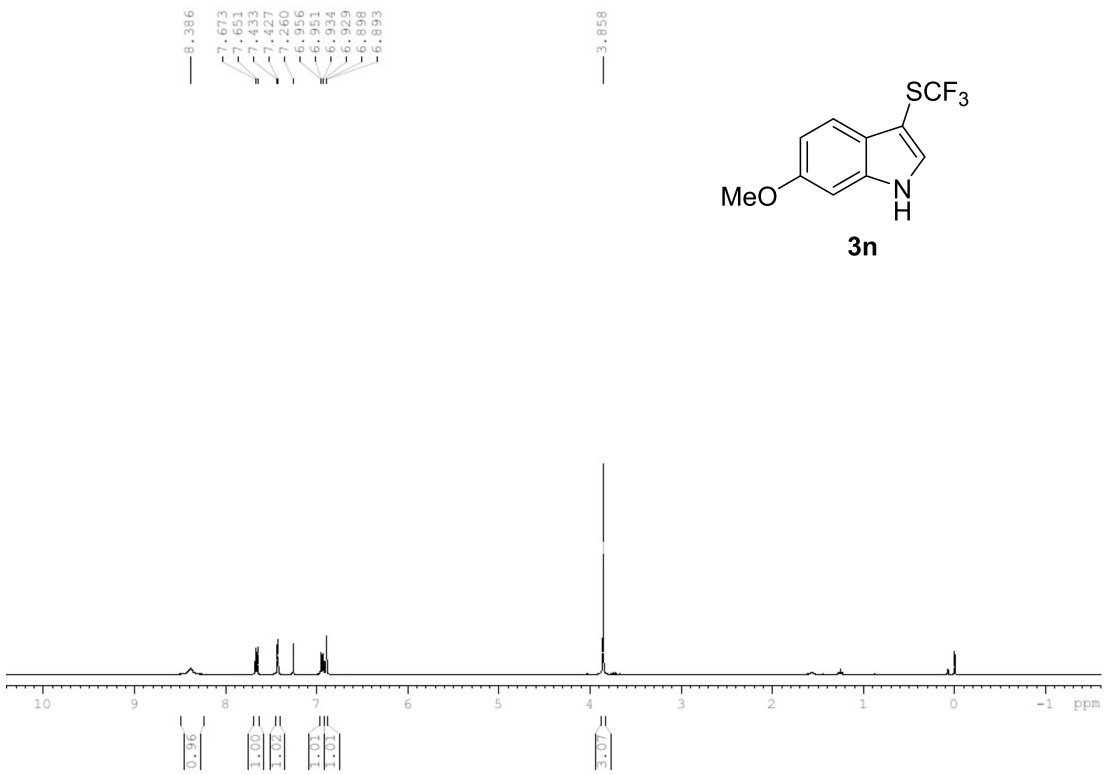
3l

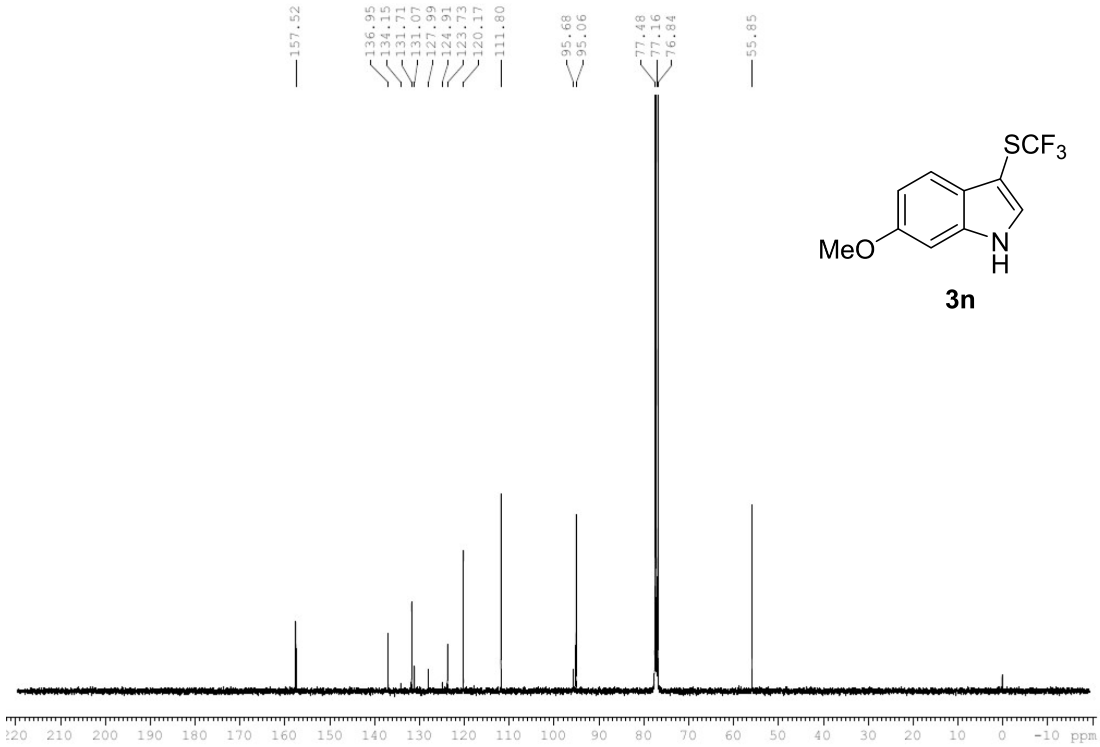

8.456
7.725
7.704
7.518
7.511
7.404
7.401
7.270
7.267
7.260
7.249
7.246
0.94
1.00
1.01
1.00
1.10

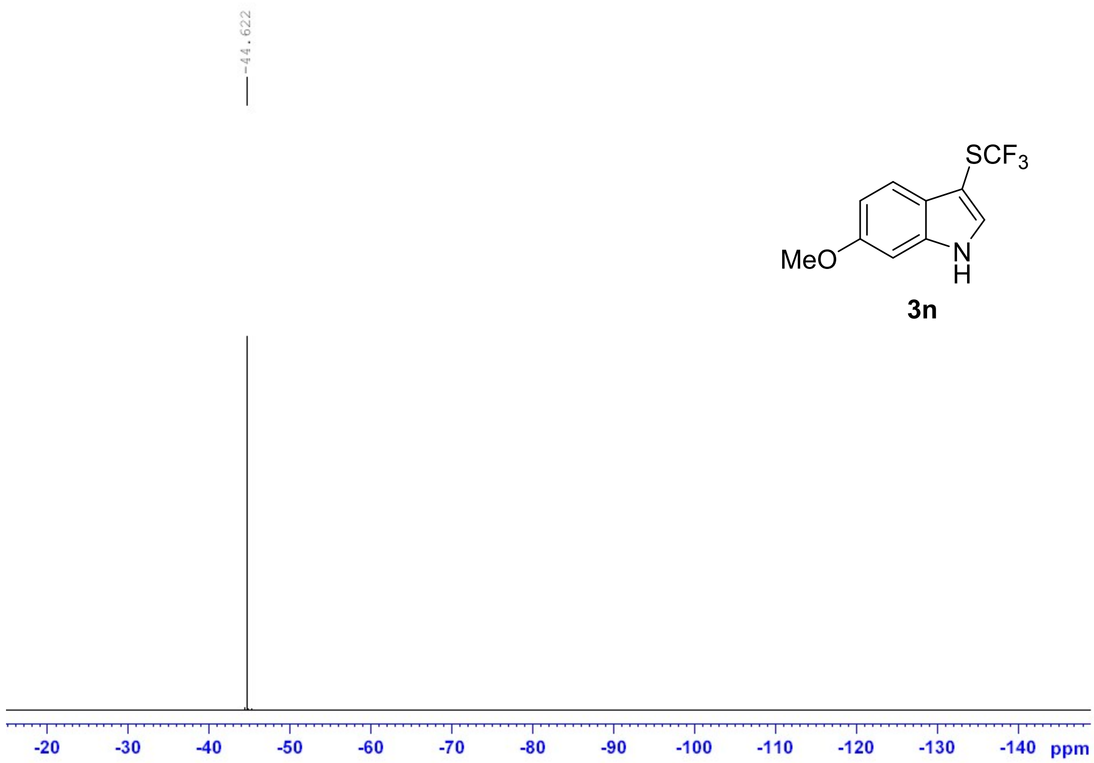
3m


136.43
134.05
133.48
130.97
129.59
128.16
127.89
124.81
122.61
120.46
111.77
96.19
96.17
77.48
77.16
76.84
SCF3
Cl
N
H
3m
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

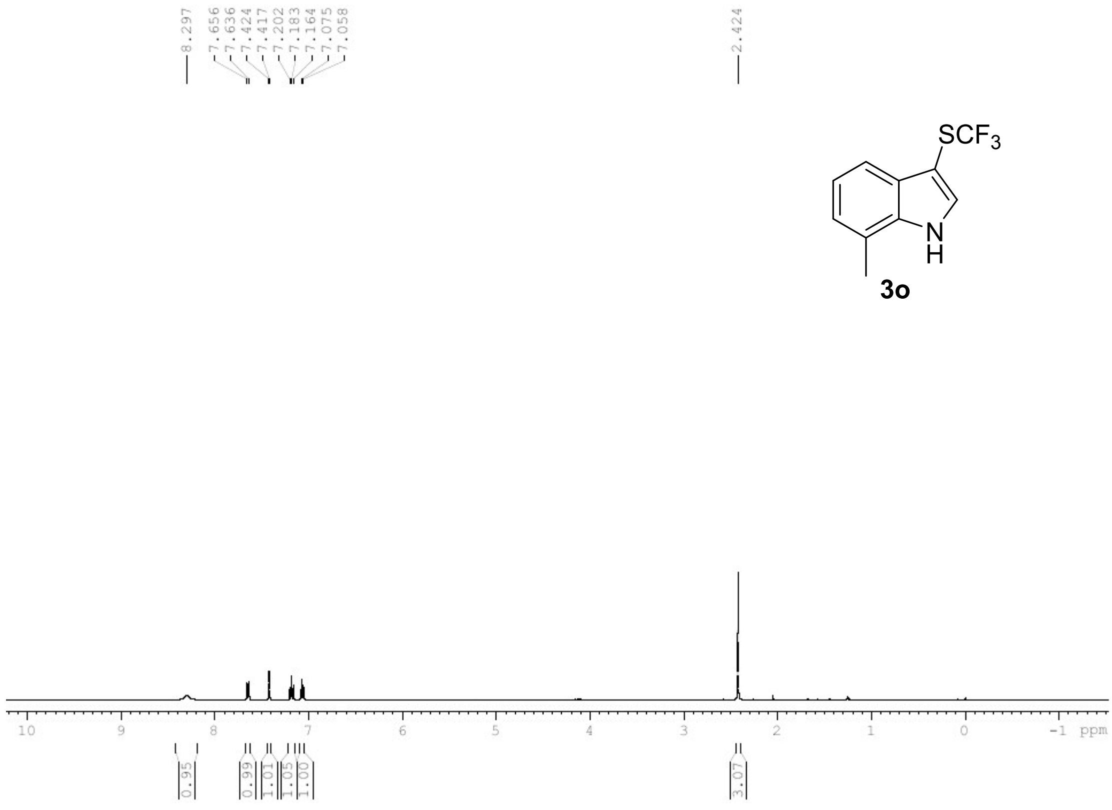

-44.426
SCF3
Cl
N
H
3m
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 ppm


8.386
7.673
7.651
7.433
7.427
7.260
6.956
6.951
6.934
6.929
6.898
6.893
3.858
SCF3
MeO
N
H
3n
10 9 8 7 6 5 4 3 2 1 0 -1 ppm
0.96
1.00
1.02
1.01
1.01
3.07

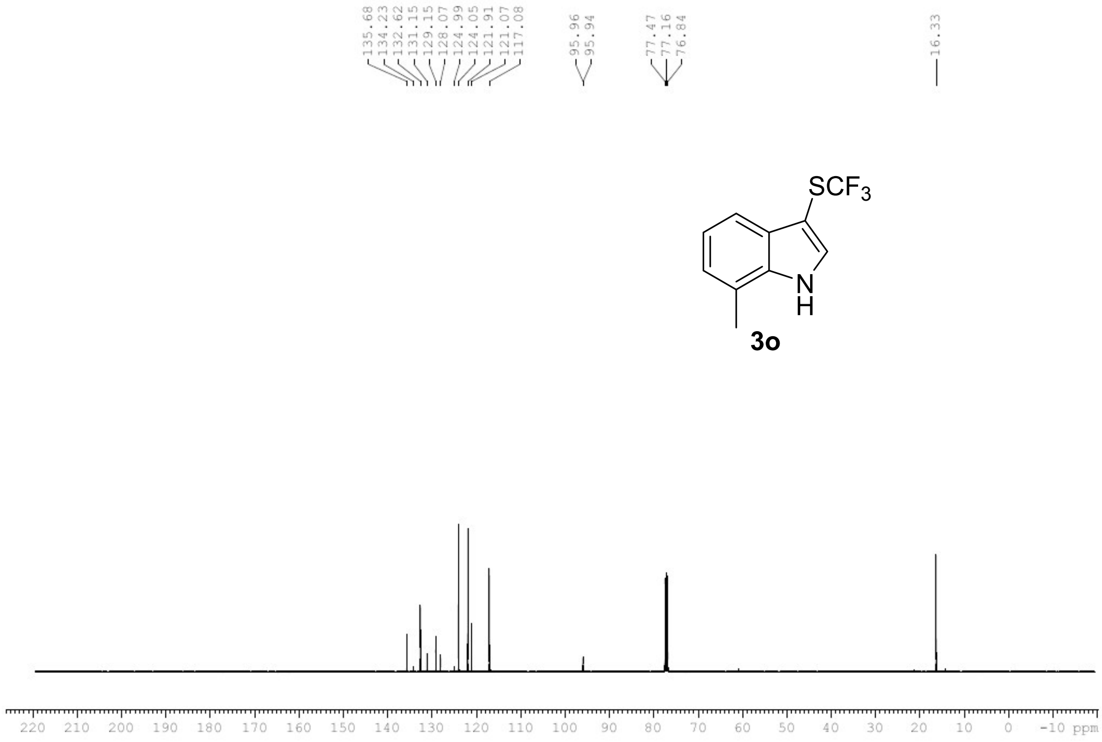

157.52
136.95
134.15
131.71
131.07
127.99
124.91
123.73
120.17
111.80
95.68
95.06
77.48
77.16
76.84
55.85
SCF3
MeO
N
H
3n
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

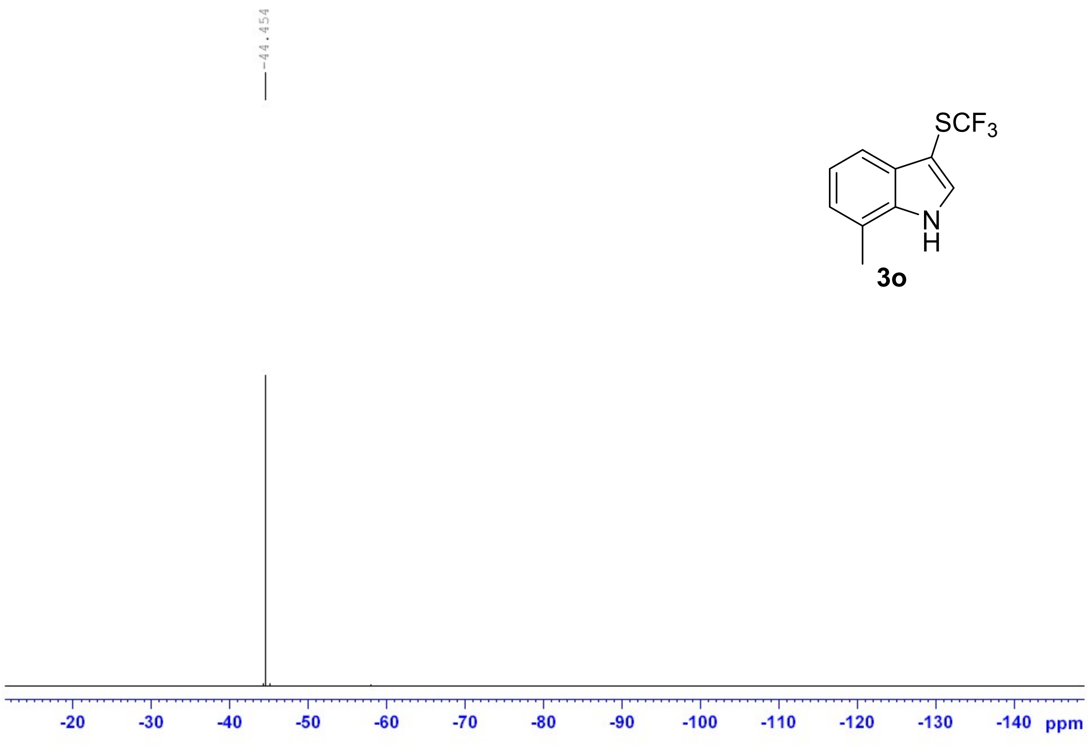


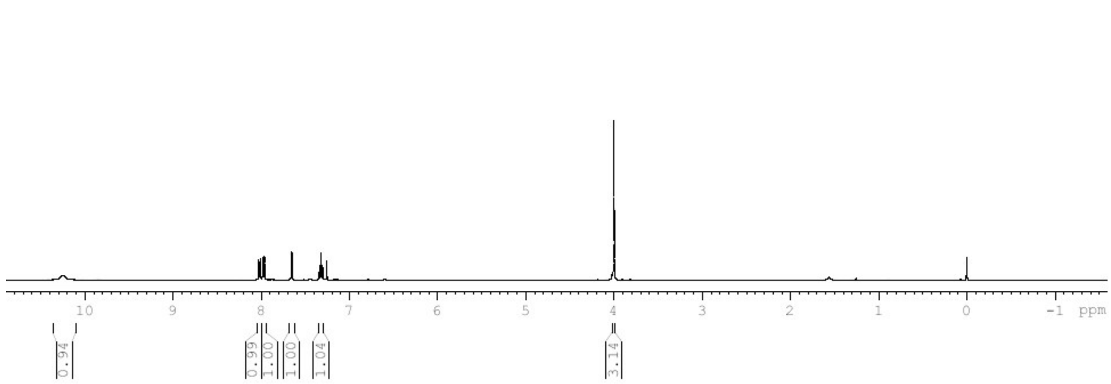
-44.622
SCF3
MeO
N
H
3n
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 ppm

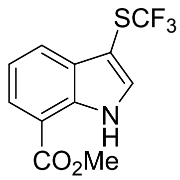


8.297
7.656
7.636
7.424
7.417
7.202
7.183
7.164
7.075
7.058
2.424
SCF3
N
H
3o
10 9 8 7 6 5 4 3 2 1 0 -1 ppm
0.95
0.99
1.01
1.05
1.00
3.07

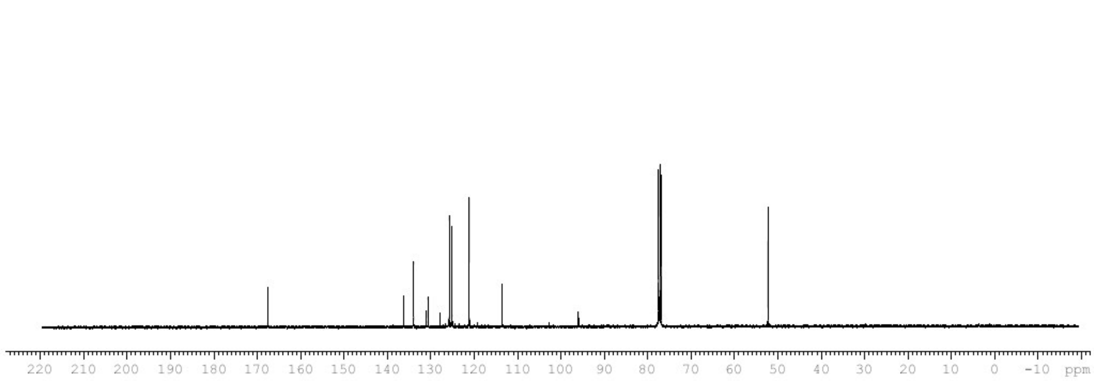

135.68
134.23
132.62
131.15
129.15
128.07
124.99
124.05
121.91
121.07
117.08
95.96
95.94
77.47
77.16
76.84
16.33
SCF3
N
H
3o
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

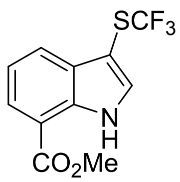

-44.454
SCF3
N
H
3o
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 ppm


10.249
8.032
8.012
7.983
7.964
7.659
7.654
7.342
7.322
7.303
7.260
4.004
0.94
0.99
1.00
1.00
1.04
3.14
ppm

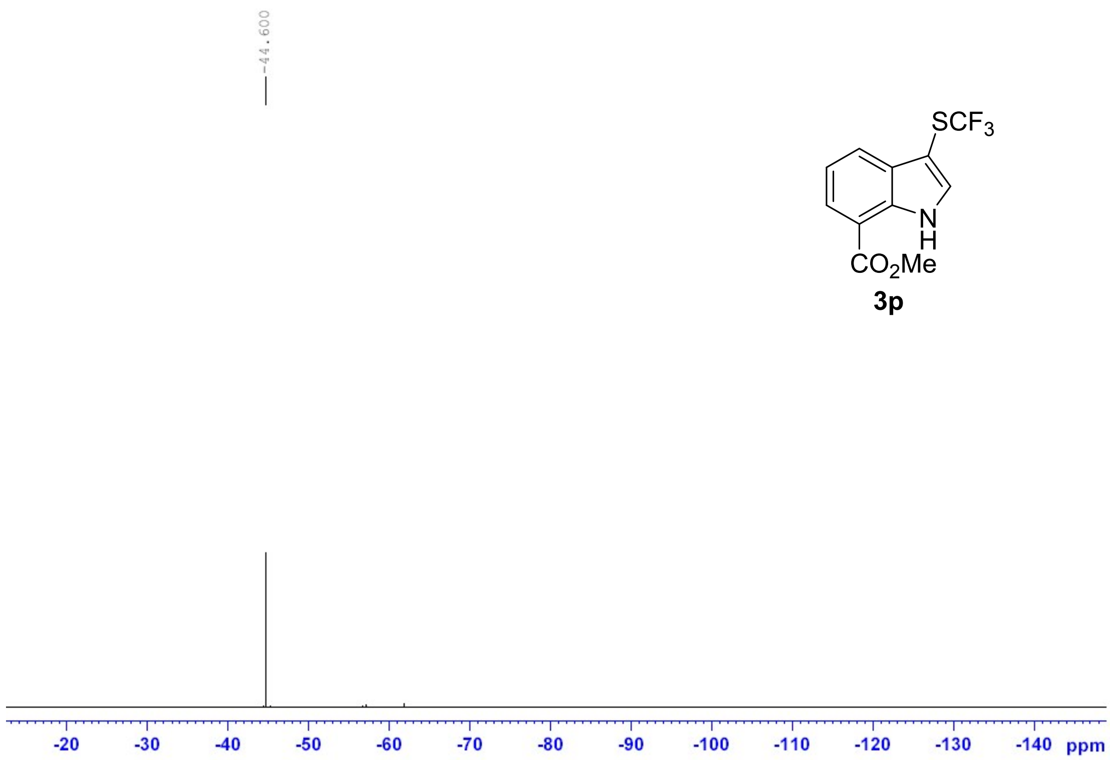

SCF3
N
H
CO2Me

3p


167.58
136.20
133.96
130.97
130.62
127.89
125.72
125.12
124.81
121.10
113.56
95.98
95.95
77.48
77.16
76.84
52.24
ppm

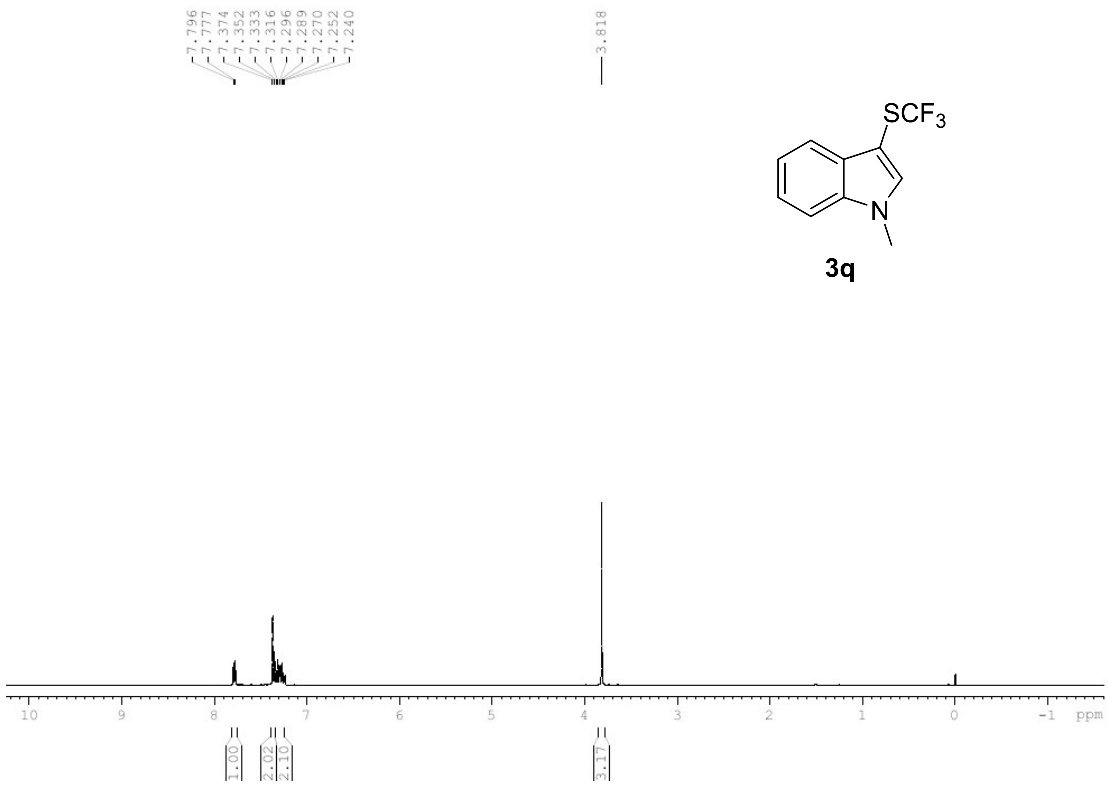

SCF3
N
H
CO2Me

3p



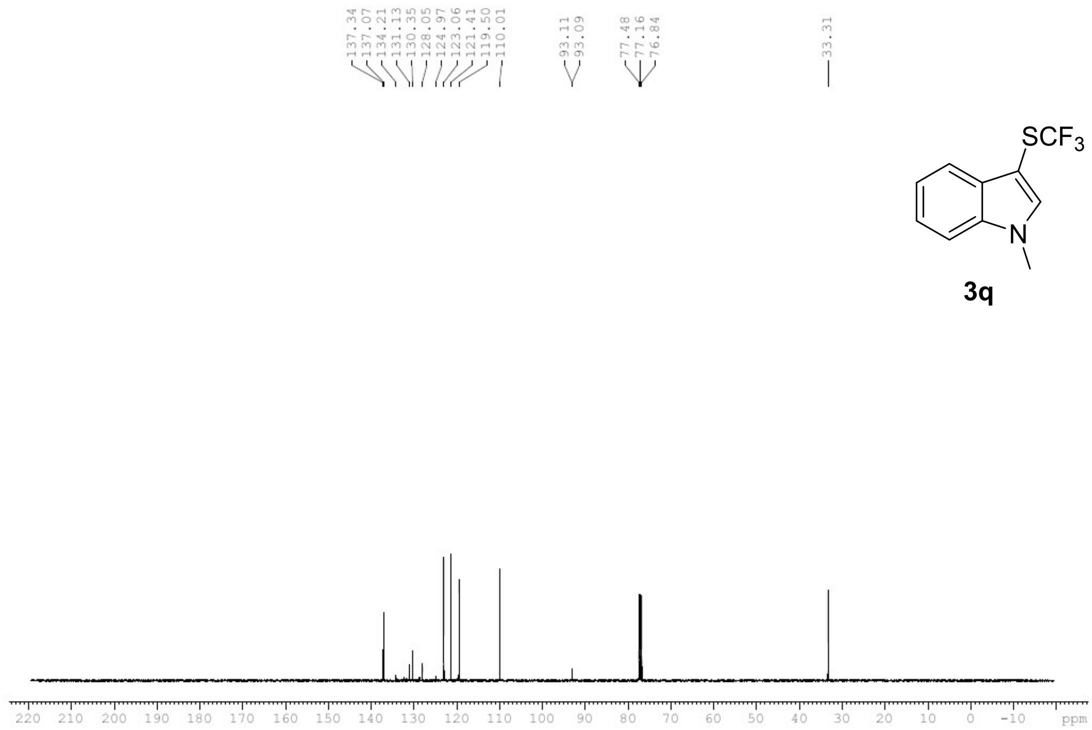
-44.600
SCF3
N
H
CO2Me
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
ppm

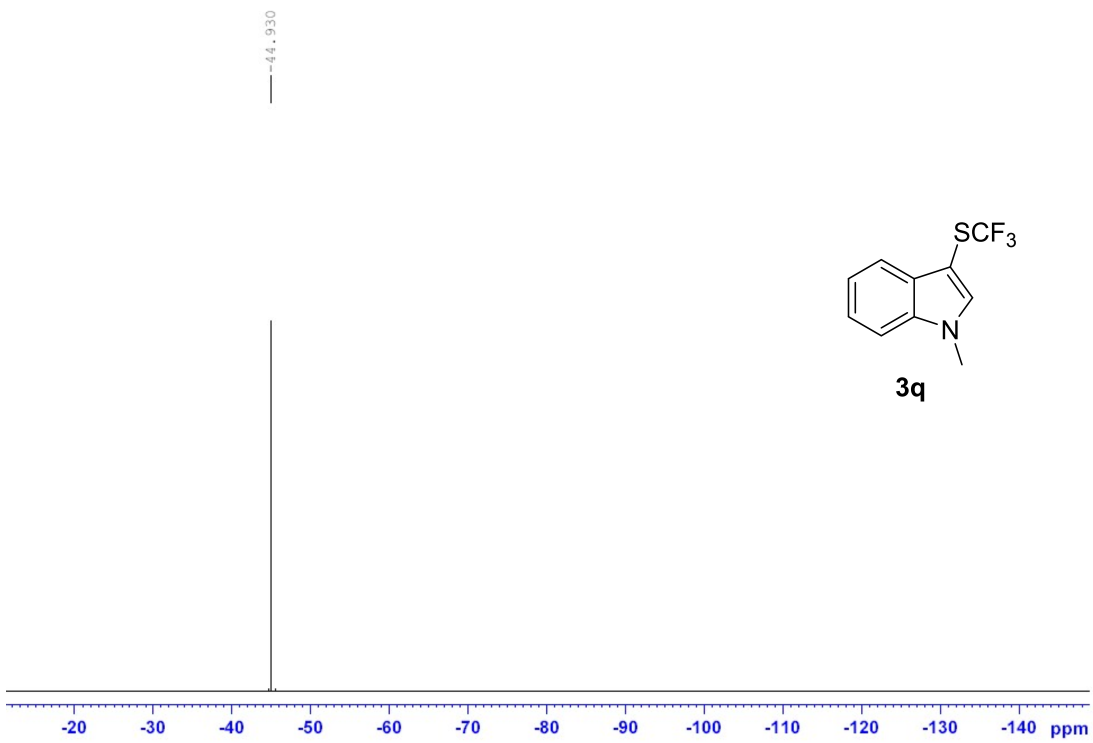
3p

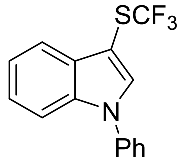


7.796
7.777
7.374
7.352
7.333
7.316
7.296
7.289
7.270
7.252
7.240
3.818
SCF3
N
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
1.00
2.02
2.10
3.17

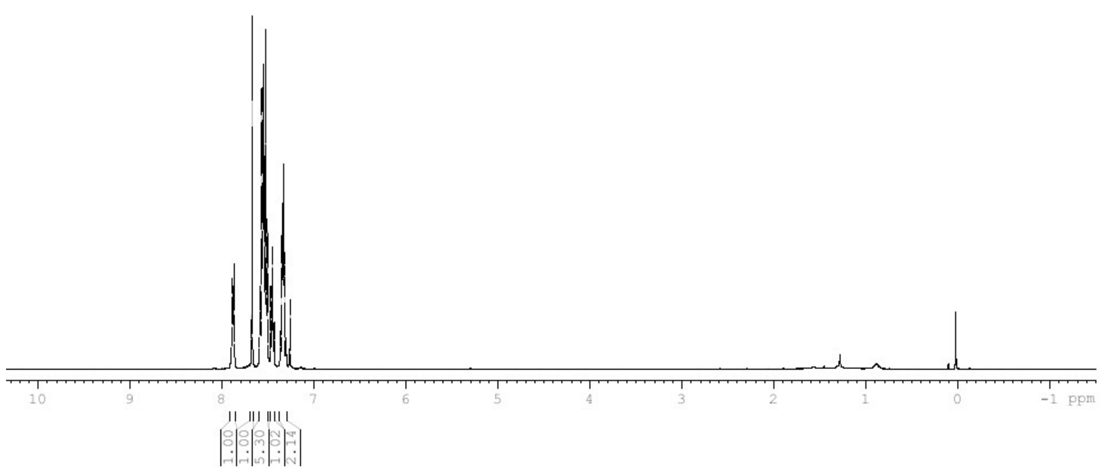
3q

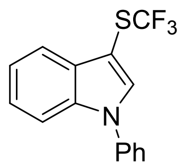

137.34
137.07
134.21
131.13
130.35
128.05
124.97
123.06
121.41
119.50
110.01
93.11
93.09
77.48
77.16
76.84
33.31
SCF3
N
3q
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm


-44.930
SCF3
N
3q
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 ppm

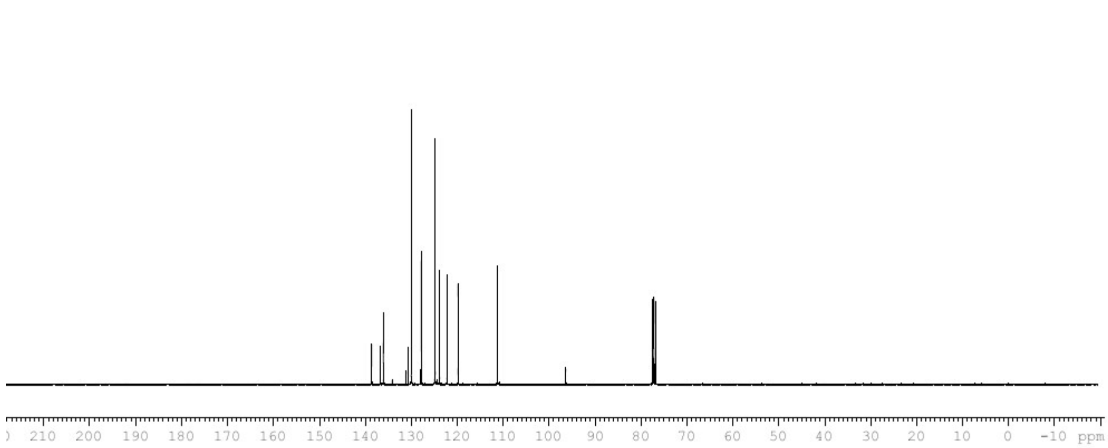

SCF3
N
Ph

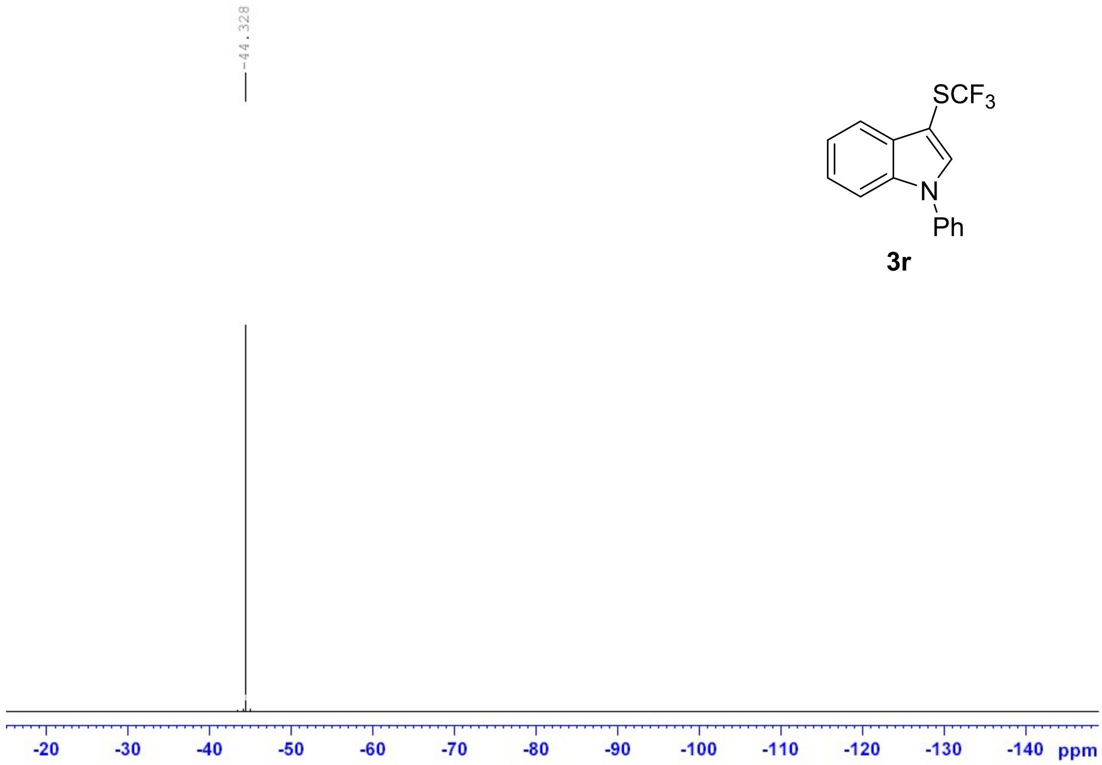
3r


7.892
7.888
7.871
7.673
7.589
7.568
7.550
7.529
7.509
7.471
7.453
7.435
7.364
7.346
7.335
7.327
7.306
7.260
10
9
8
7
6
5
4
3
2
1
0
-1 ppm
1.00
1.00
5.30
1.02
2.14


SCF3
N
Ph

3r


138.59
136.74
136.05
134.19
131.10
130.69
129.97
128.02
127.82
124.94
124.80
123.83
122.21
119.81
111.24
96.39
96.37
77.48
77.16
76.84
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10 ppm


-44.328
SCF_3
N
Ph
3r
-20
-30
-40
-50
-60
-70
-80
-90
-100
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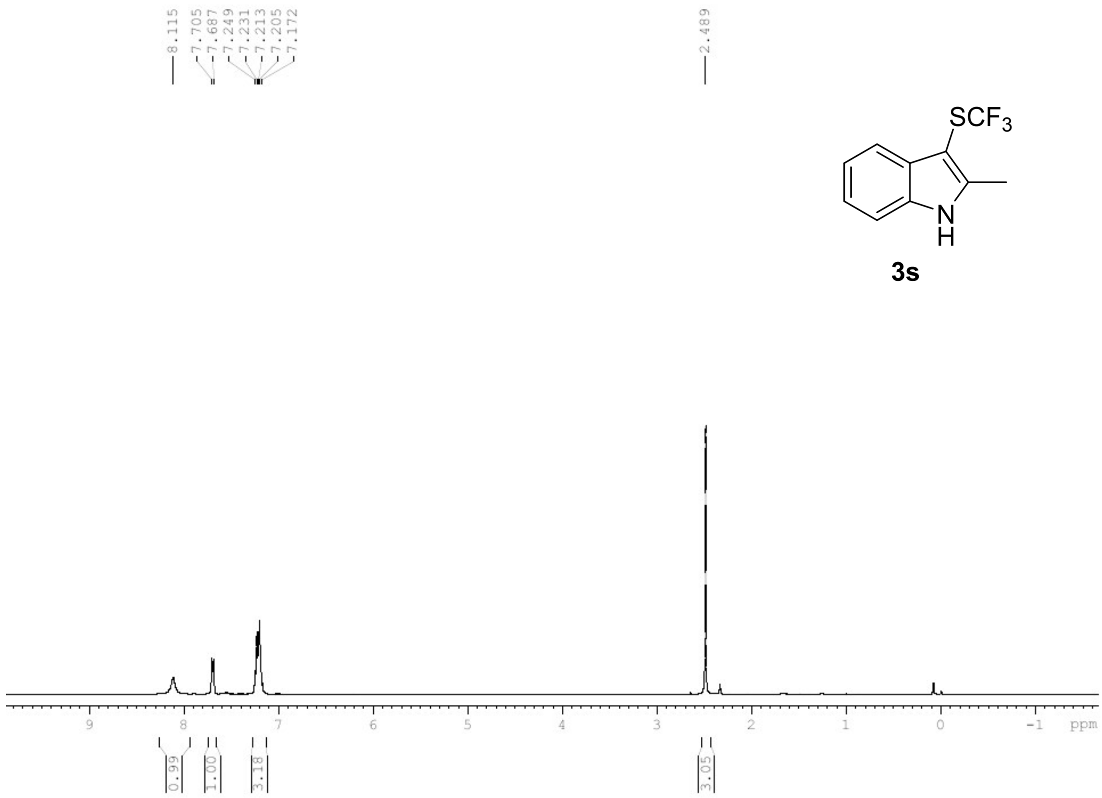
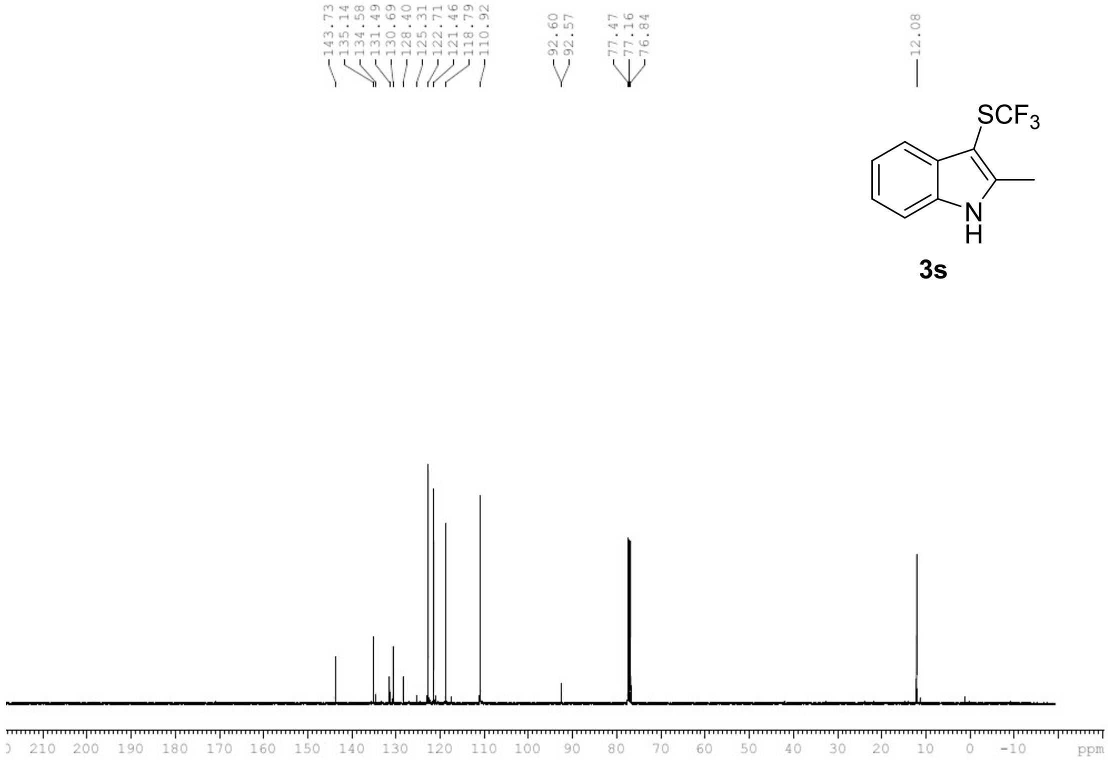
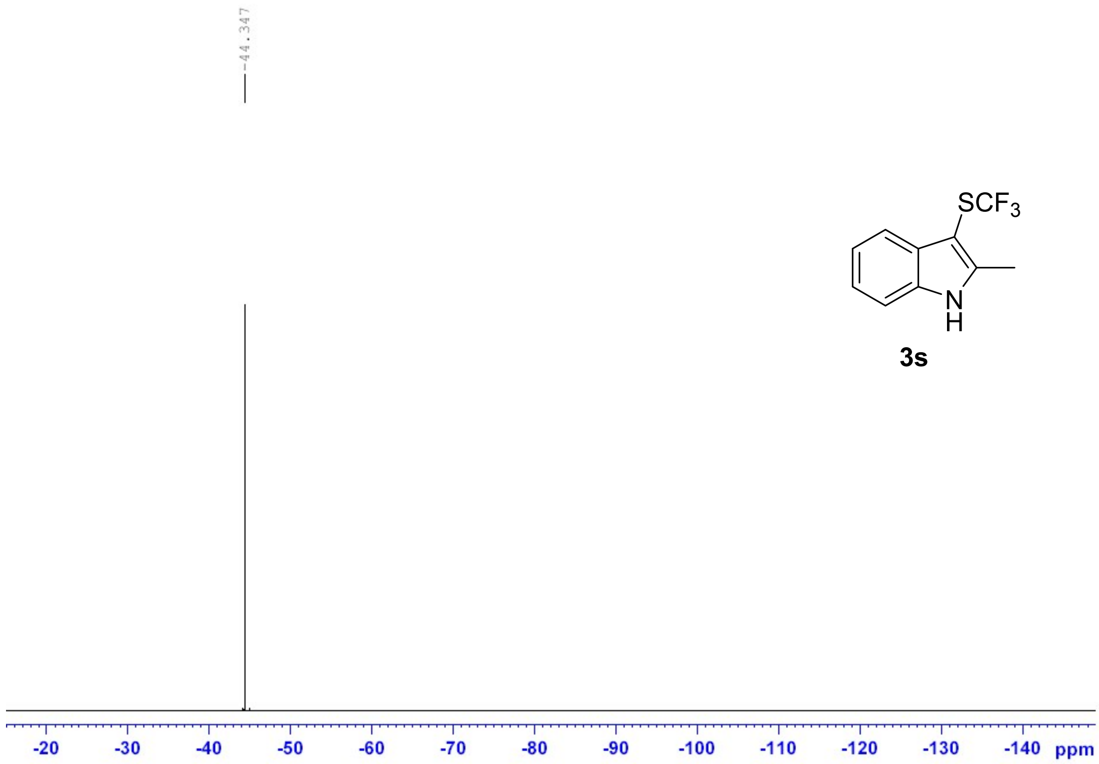
-120
-130
-140
ppm

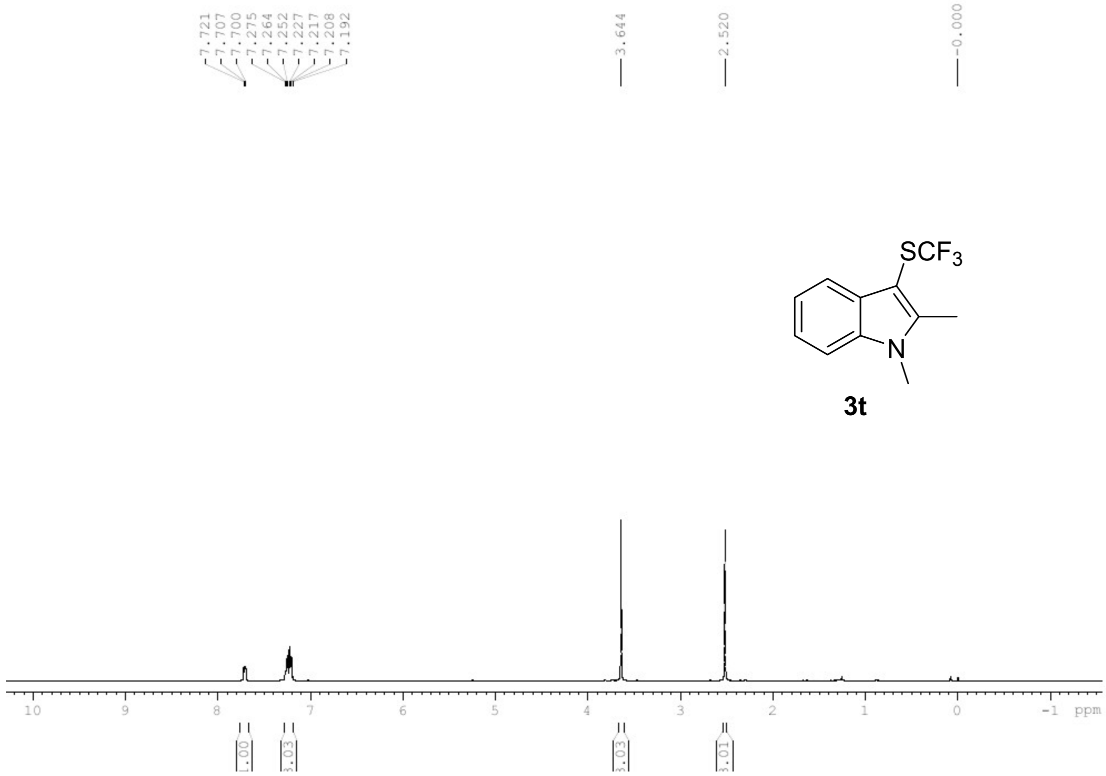

8.115
7.705
7.687
7.249
7.231
7.213
7.205
7.172
2.489
SCF_3
N
H
3s
9
8
7
6
5
4
3
2
1
0
-1
ppm
0.99
1.00
3.18
3.05

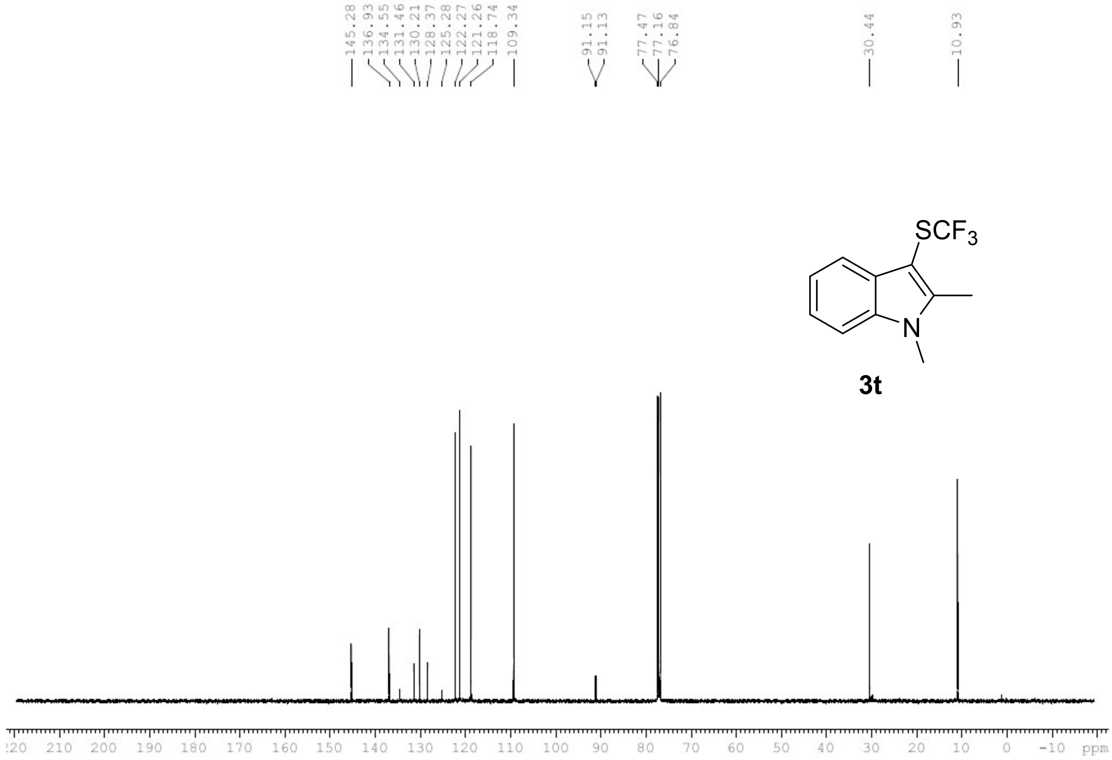


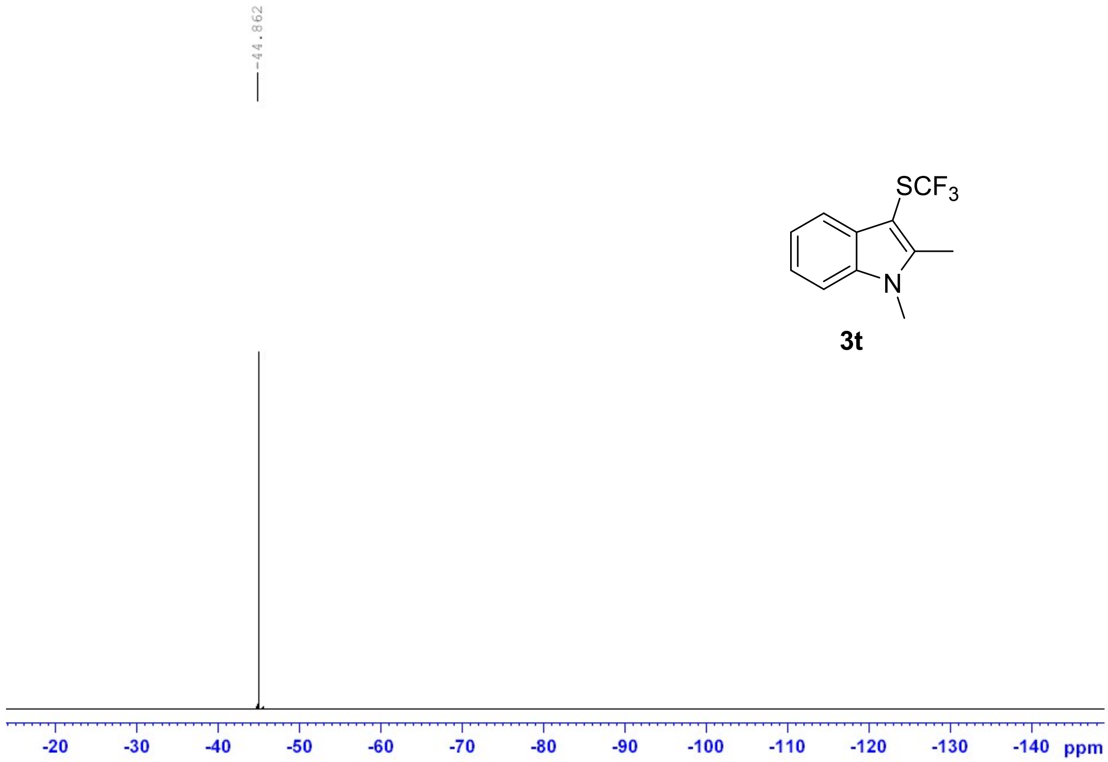
143.73
135.14
134.58
131.49
130.69
128.40
125.31
122.71
121.46
118.79
110.92
92.60
92.57
77.47
77.16
76.84
12.08
SCF_3
N
H
3s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm



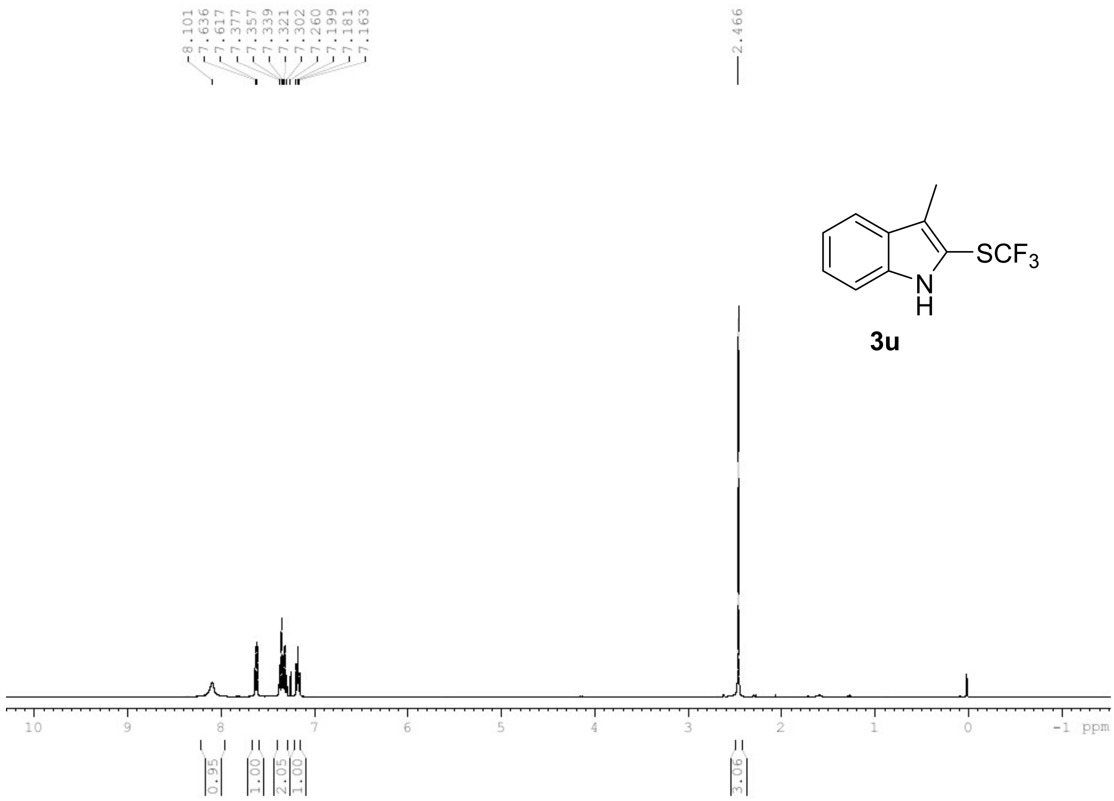
-44.347
SCF_3
N
H
3s
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 ppm


7.721
7.707
7.700
7.275
7.264
7.252
7.227
7.217
7.208
7.192
3.644
2.520
0.000
SCF3
N
3t
10 9 8 7 6 5 4 3 2 1 0 -1 ppm
.00
3.03
3.03
3.01

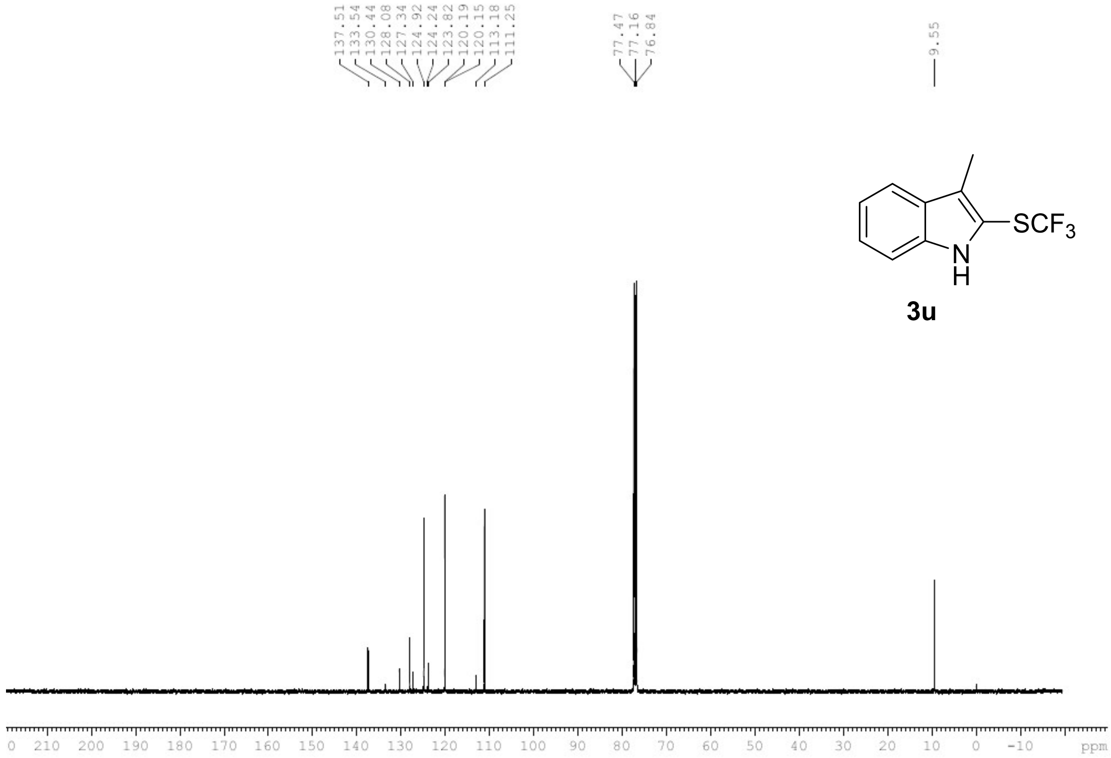

145.28
136.93
134.55
131.46
130.21
128.37
125.28
122.27
121.26
118.74
109.34
91.15
91.13
77.47
77.16
76.84
30.44
10.93
SCF3
N
3t
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

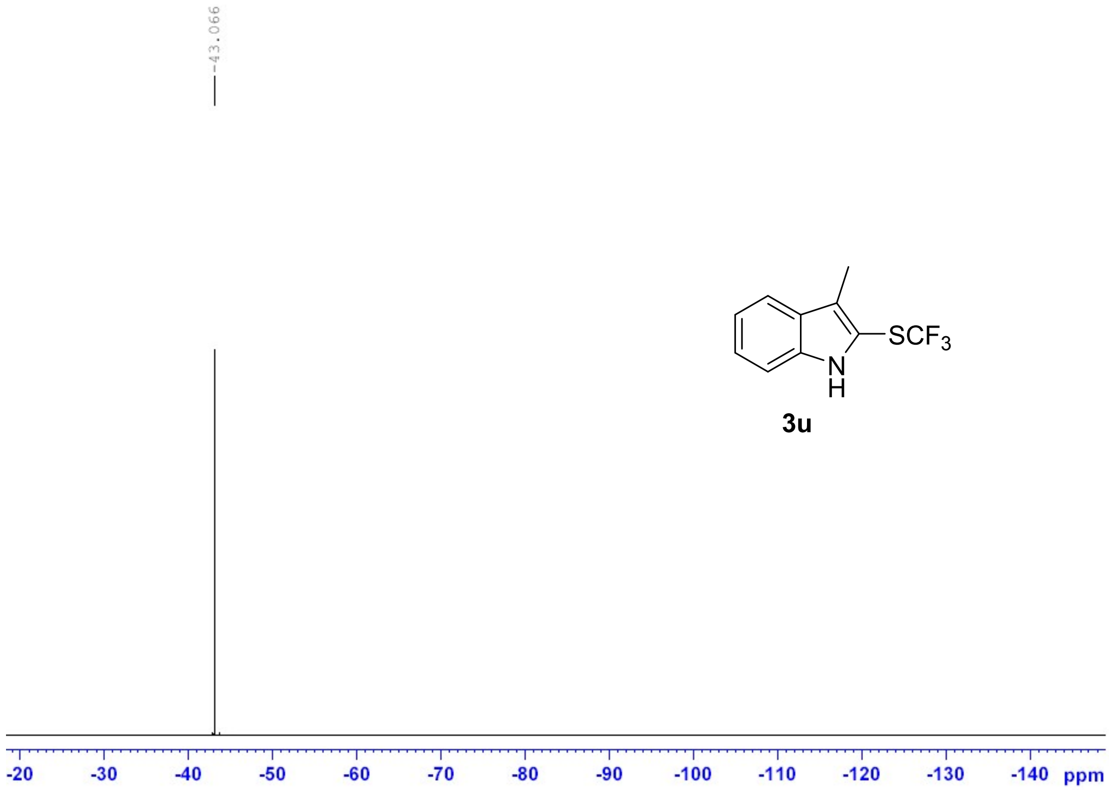


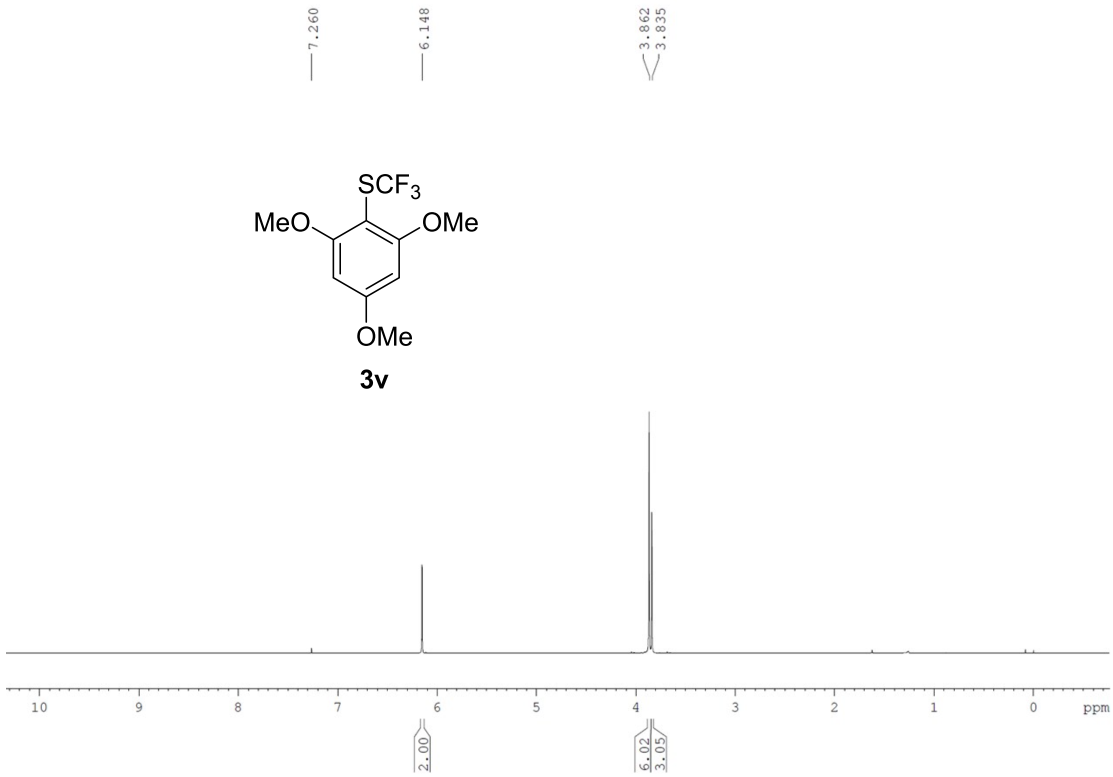
-44.862
SCF3
N
3t
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
ppm



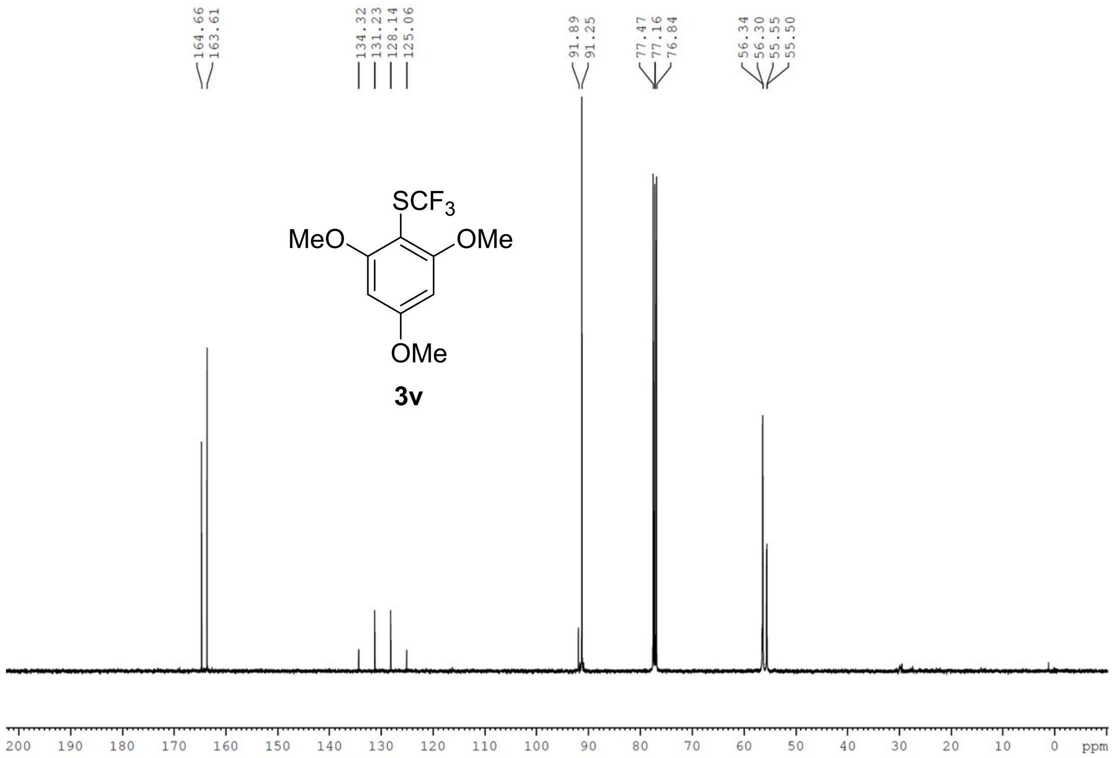
8.101
7.636
7.617
7.377
7.357
7.339
7.321
7.302
7.260
7.199
7.181
7.163
2.466
SCF3
N
H
3u
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
0.95
1.00
2.05
1.00
3.06


137.51
133.54
130.44
128.08
127.34
124.92
124.24
123.82
120.19
120.15
113.18
111.25
77.47
77.16
76.84
9.55
SCF3
N
H
3u
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

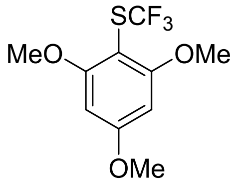

-43.066
SCF3
N
H
3u
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 ppm


7.260
6.148
3.862
3.835
SCF3
MeO
OMe
OMe
10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
6.02
3.05

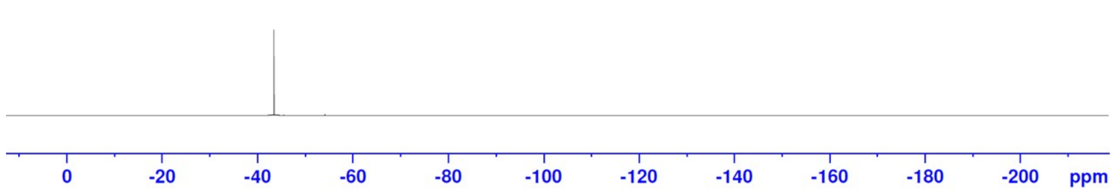
3v


164.66
163.61
134.32
131.23
128.14
125.06
91.89
91.25
77.47
77.16
76.84
56.34
56.30
55.55
55.50
SCF3
MeO
OMe
OMe
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

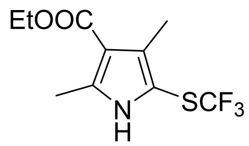
3v



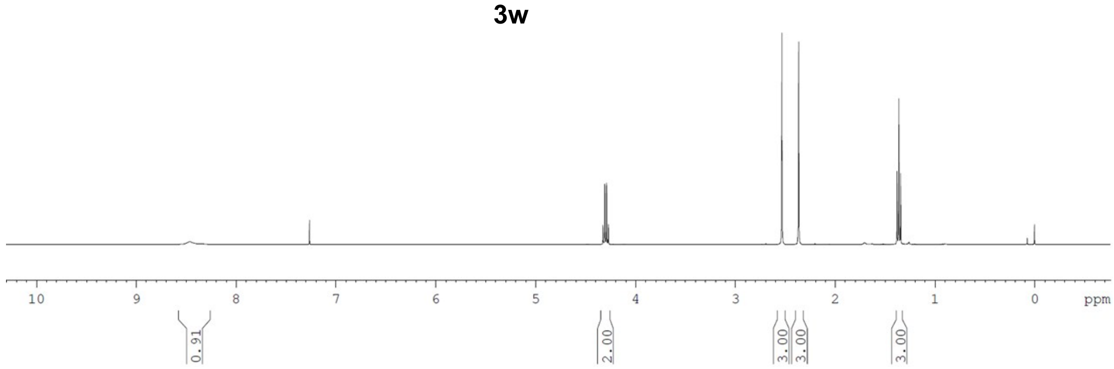
3v



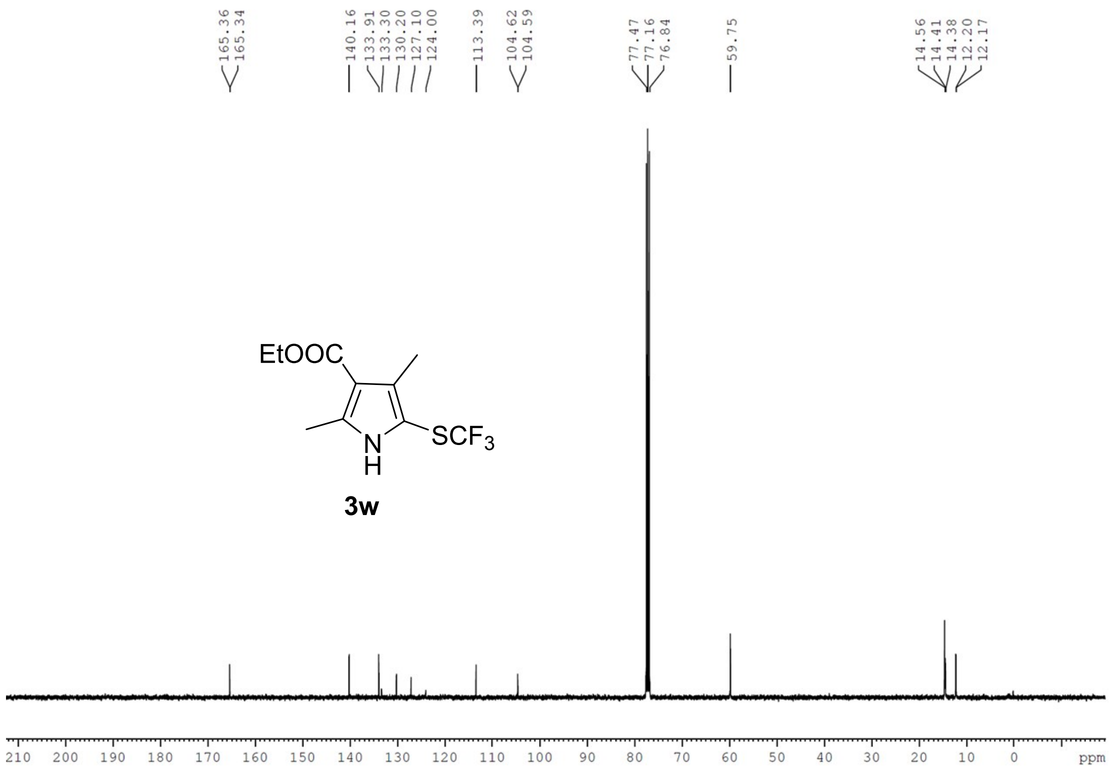
-43.500
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

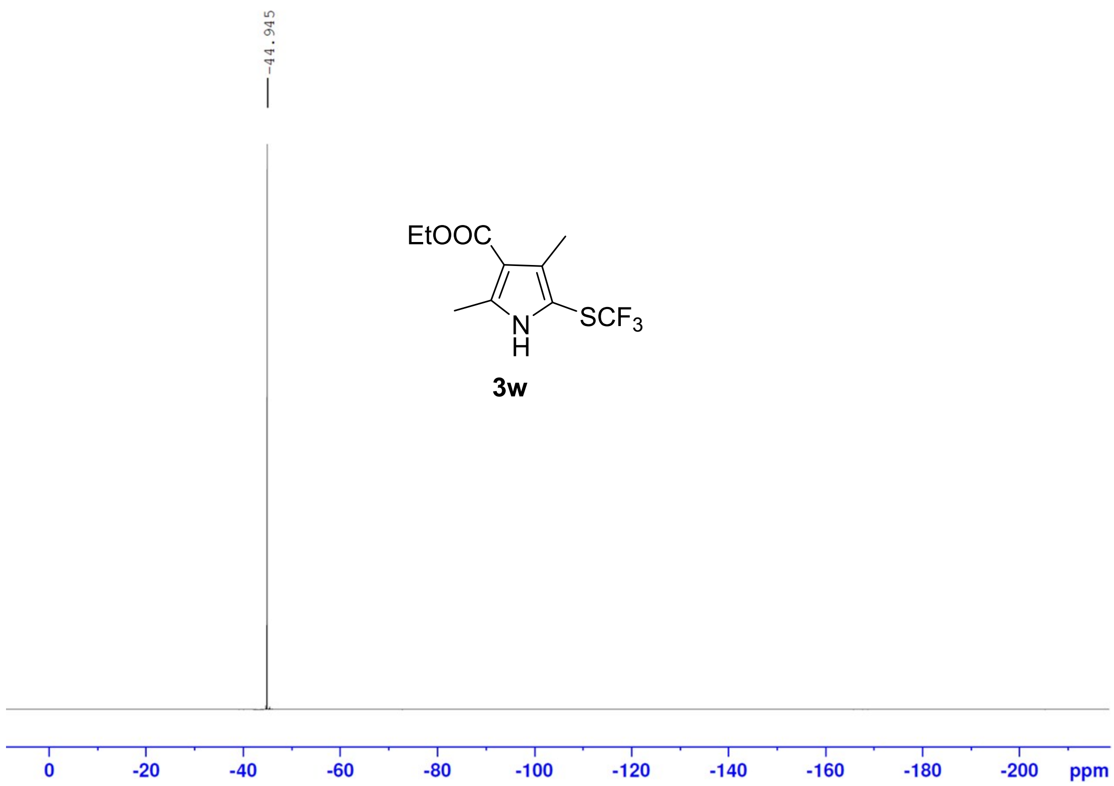


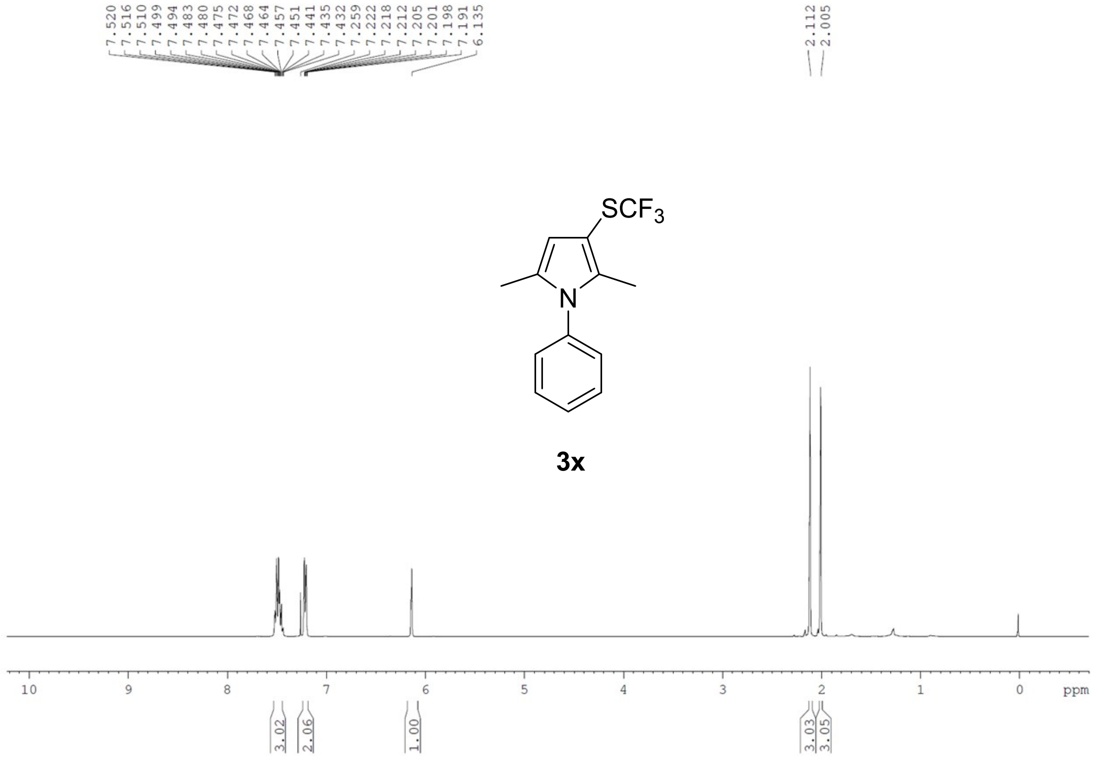
3w

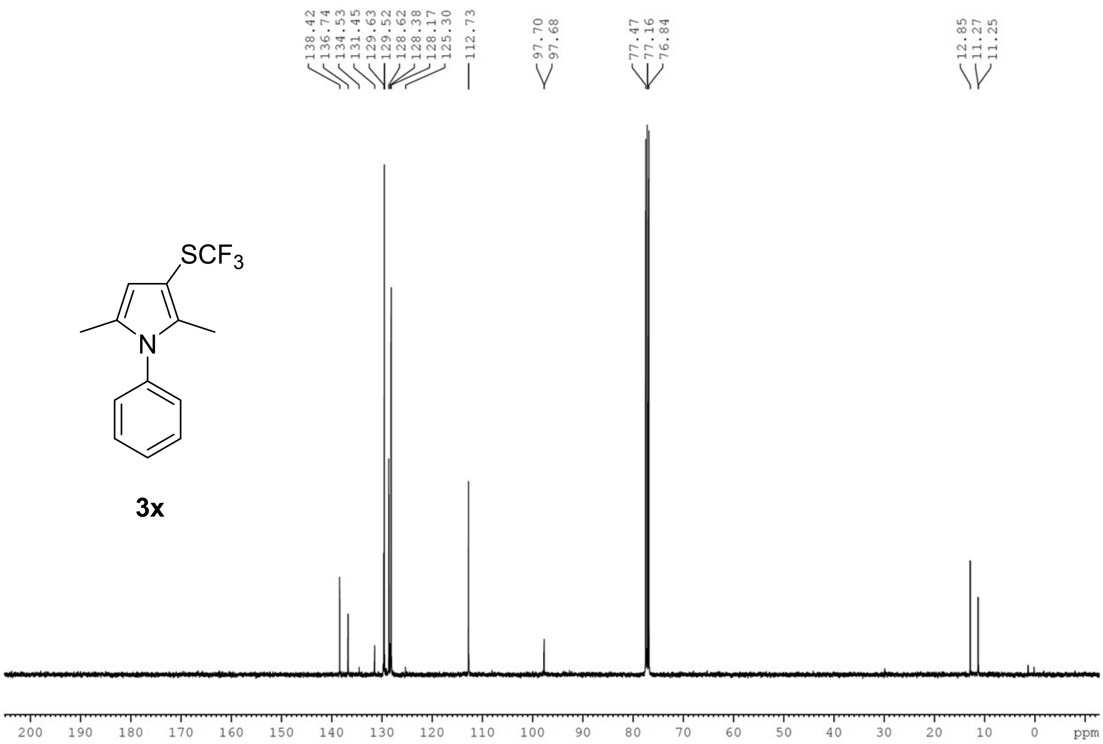


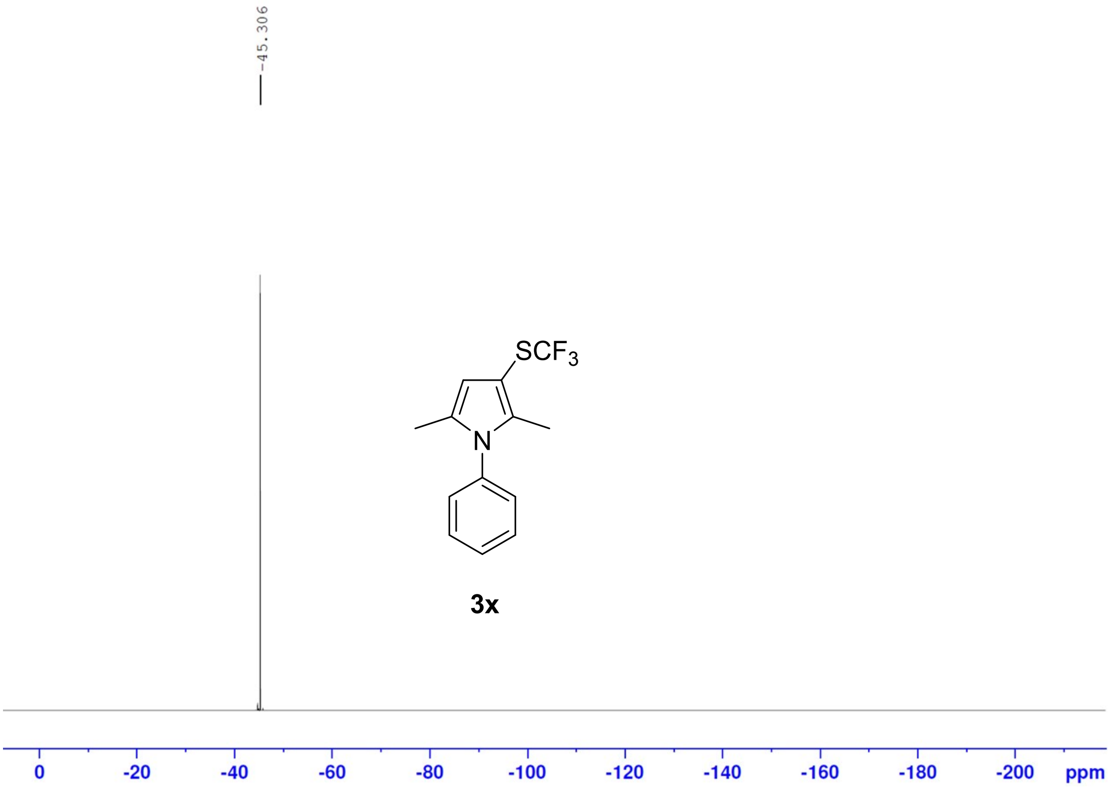
8.461
7.263
4.323
4.305
4.287
4.269
2.530
2.362
1.377
1.359
1.341
10
9
8
7
6
5
4
3
2
1
0
ppm
0.91
2.00
3.00
3.00
3.00

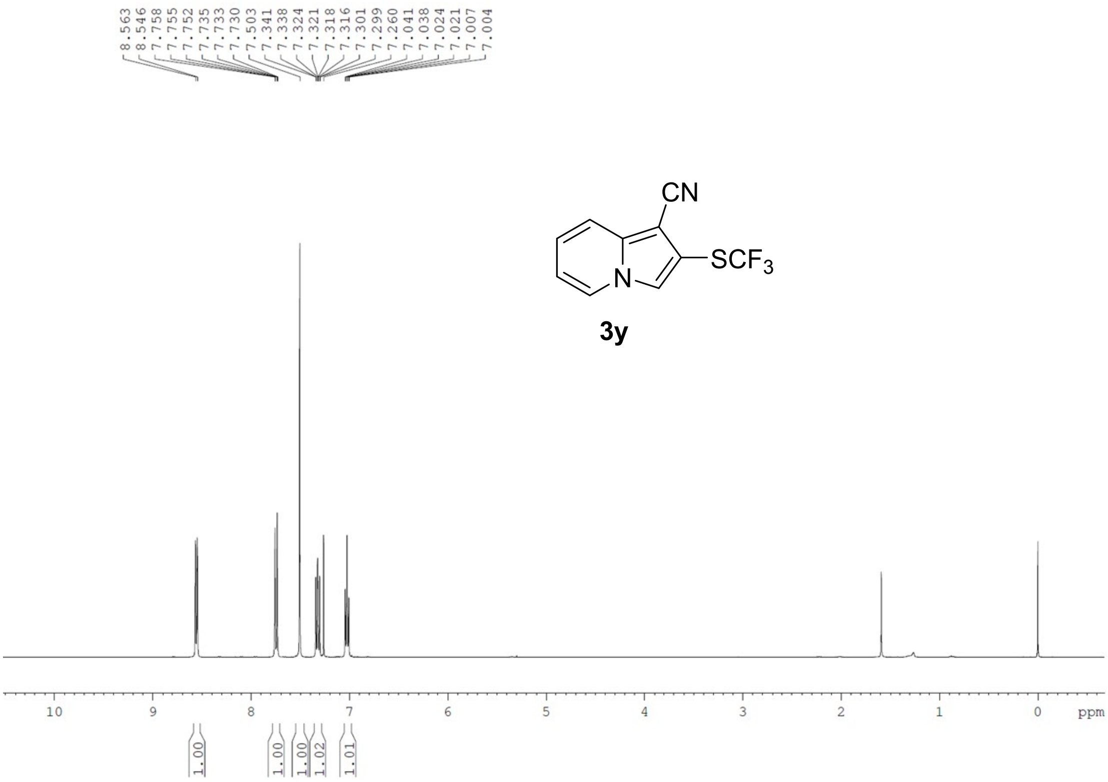

165.36
165.34
140.16
133.91
133.30
130.20
127.10
124.00
113.39
104.62
104.59
77.47
77.16
76.84
59.75
14.56
14.41
14.38
12.20
12.17
EtOOC
SCF3
N
H
3w
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

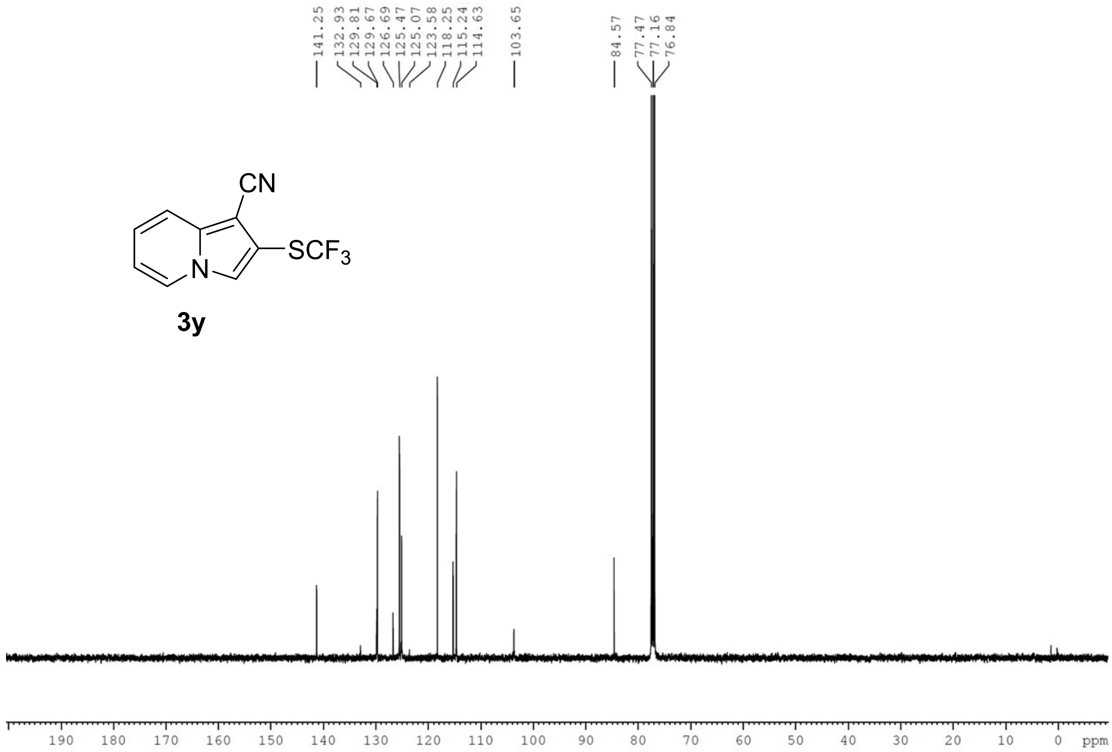

-44.945
EtOOC
SCF3
N
H
3w
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm

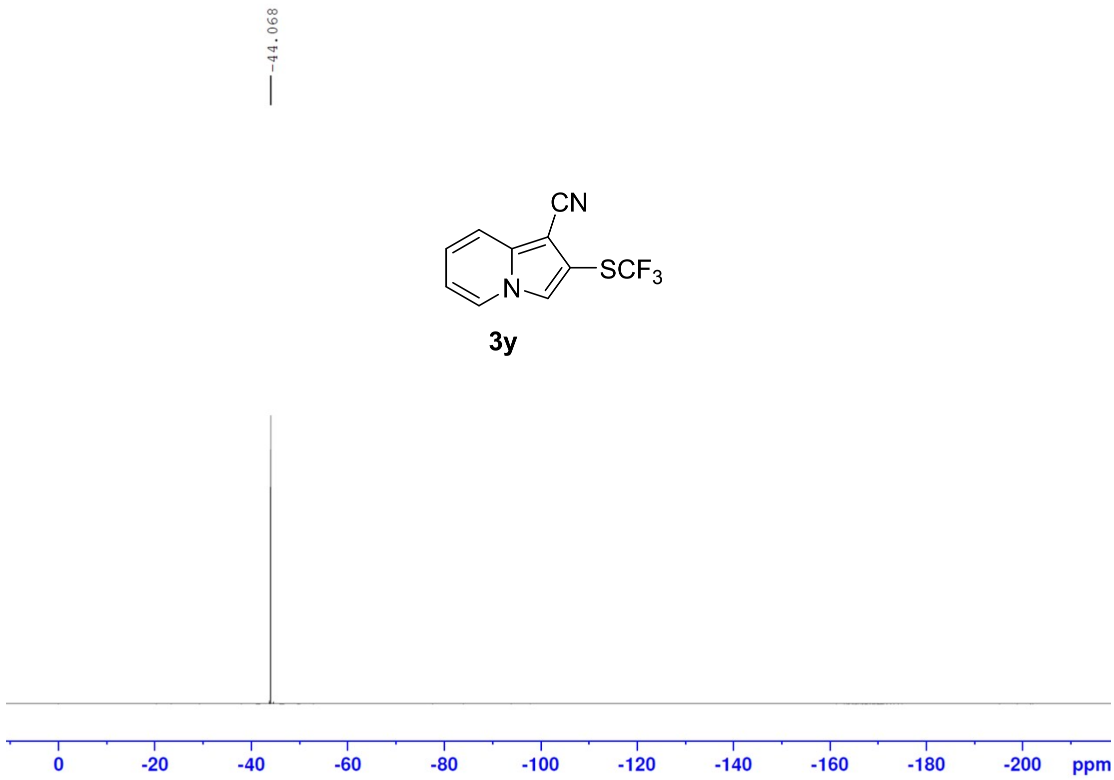

7.520
7.516
7.510
7.499
7.494
7.483
7.480
7.475
7.472
7.468
7.464
7.457
7.451
7.441
7.435
7.432
7.259
7.222
7.218
7.212
7.205
7.201
7.198
7.191
6.135
2.112
2.005
SCF3
N
3x
10 9 8 7 6 5 4 3 2 1 0 ppm
3.02
2.06
1.00
3.03
3.05

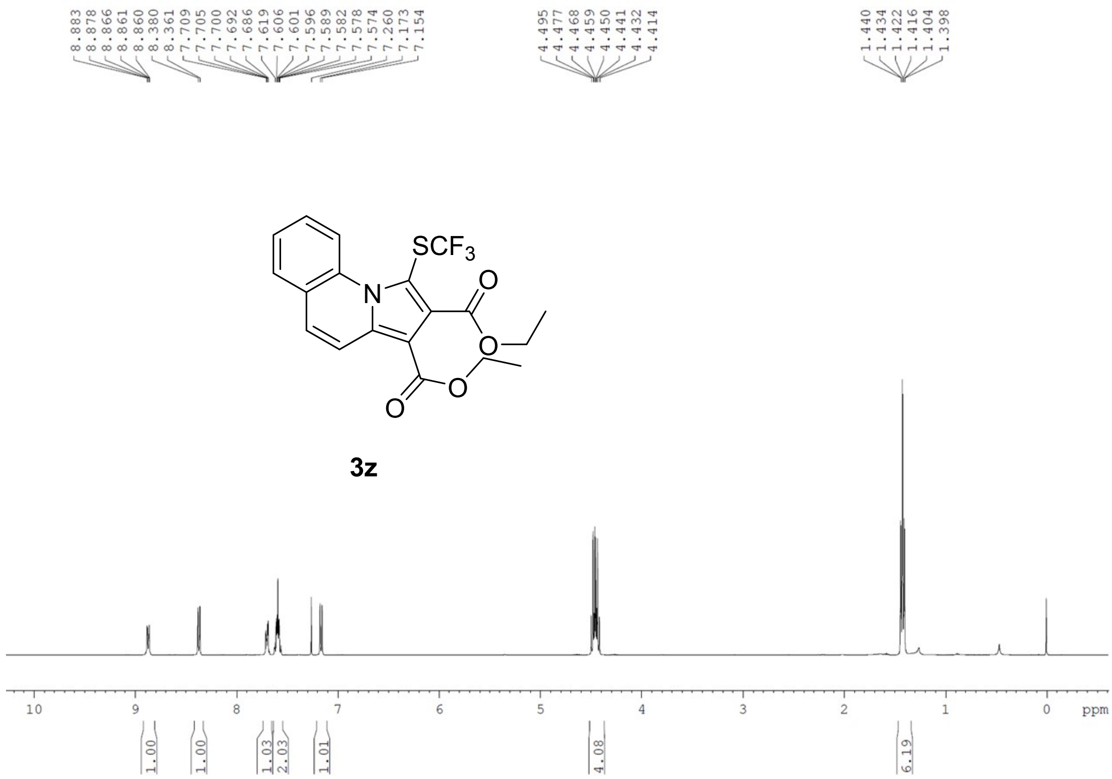

138.42
136.74
134.53
131.45
129.63
129.52
128.62
128.38
128.17
125.30
112.73
97.70
97.68
77.47
77.16
76.84
12.85
11.27
11.25
SCF3
N
3x
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

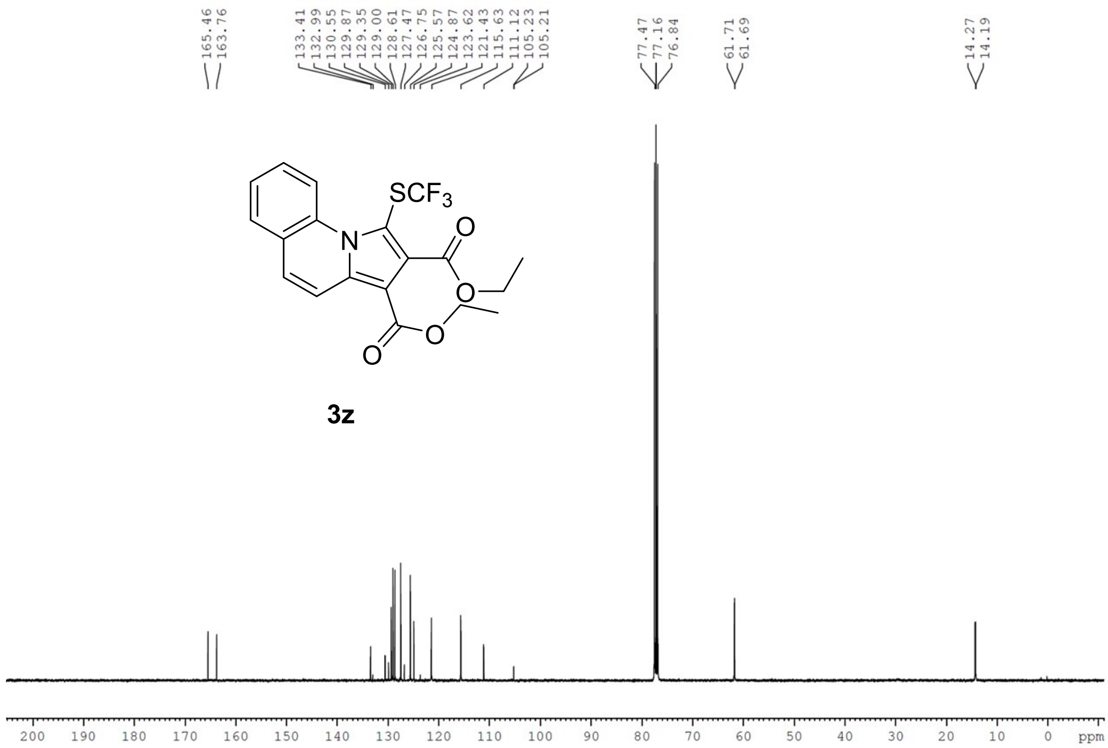

-45.306
SCF3
N
3x
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

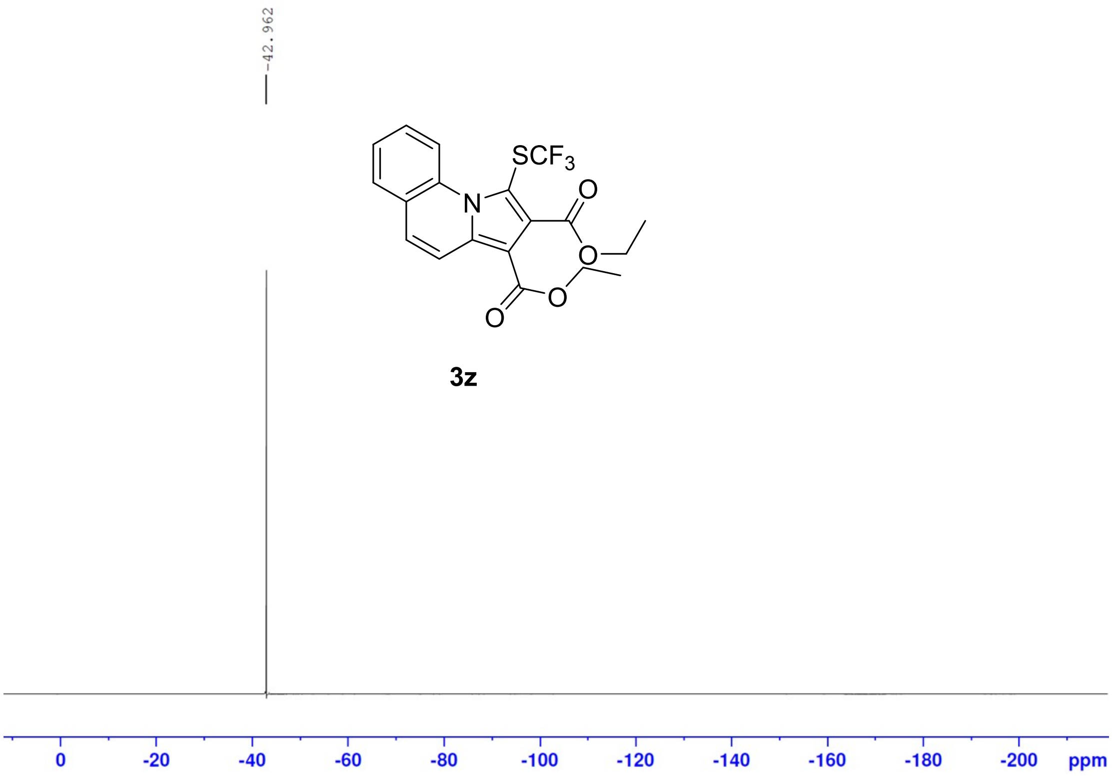

8.563
8.546
7.758
7.755
7.752
7.735
7.733
7.730
7.503
7.341
7.338
7.324
7.321
7.318
7.316
7.301
7.299
7.260
7.041
7.038
7.024
7.021
7.007
7.004
CN
SCF3
N
3y
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
1.00
1.02
1.01


141.25
132.93
129.81
129.67
126.69
125.47
125.07
123.58
118.25
115.24
114.63
103.65
84.57
77.47
77.16
76.84
CN
SCF3
N
3y
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


-44.068
CN
SCF3
N
3y
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm


8.883 8.878 8.866 8.861 8.860 8.380 8.361 7.709 7.705 7.700 7.692 7.686 7.619 7.606 7.601 7.596 7.589 7.582 7.578 7.574 7.260 7.173 7.154
4.495 4.477 4.468 4.459 4.450 4.441 4.432 4.414
1.440 1.434 1.422 1.416 1.404 1.398
SCF3
N
O
O
O
O
3z
10 9 8 7 6 5 4 3 2 1 0 ppm
1.00 1.00 1.03 2.03 1.01 4.08 6.19


165.46 163.76
133.41 132.99 130.55 129.87 129.35 129.00 128.61 127.47 126.75 125.57 124.87 123.62 121.43 115.63 111.12 105.23 105.21
77.47 77.16 76.84
61.71 61.69
14.27 14.19
SCF3
N
O
O
O
O
3z
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



-42.962
SCF3
N
O
O
O
O
3z
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm