Copper-Catalyzed Ring-Opening Trifluoromethylthiolation/ Trifluoromethylselenolation of Cyclopropanols with $TsSCF_3$ or *Se*-(trifluoromethyl) 4-methoxybenzenesulfonoselenoate

Ankun Li,[a,c] Xiaoxing Wang,[a,c] Yuqing Liu,[a] Delong Hao,[a] Xia Zhao,[a,*] and Kui Lu[b,*]

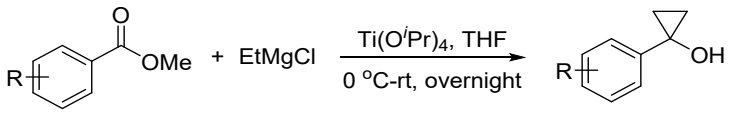
[a] *College of Chemistry, Tianjin Key Laboratory of Structure and Performance for Functional Molecules, Key laboratory of Inorganic-organic Hybrid Functional Material Chemistry, Ministry of Education, Tianjin Normal University, Tianjin, China, 300387, hxxyzhx@mail.tjnu.edu.cn*

[b] *China International Science and Technology Cooperation Base of Food Nutrition/Safety and Medicinal Chemistry, College of Biotechnology, Tianjin University of Science & Technology, Tianjin, China, 300457, lukui@tust.edu.cn*

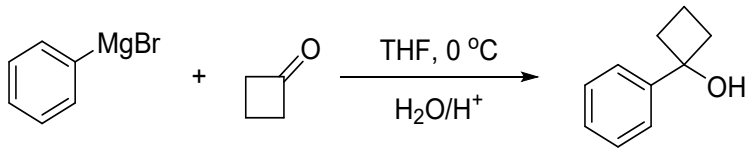
[c] These authors contributed equally to this work.

Contents Page

1) General Procedure for Preparation of cyclopropanols and cyclobutanol (1) [1-5.]

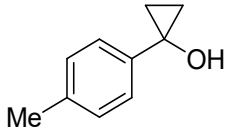


To a 200 mL round-bottomed flask was sequentially added ester (10 mmol, 1.0 eq.), titanium tetraisopropoxide (14 mmol, 1.4 eq.) and THF (40 mL). Then the solution was stirred at 0 °C followed by adding ethylmagnesium chloride (14 mL, 28 mmol, 2.8 eq., 2 M in THF) over 10 minutes. The suspension was warmed to room temperature and stirred overnight before quenching by slow addition of cold H_2SO_4 solution (0.1 M, 40 mL). The mixture was extracted with ethyl acetate (40 mL×3). The combined organic layers were washed with brine (40 mL), dried over anhydrous Na_2SO_4, filtered and concentrated in vacuo to give a residue which was purified by silica gel column chromatography (ethyl acetate/petroleum ether) to afford the desired cyclopropanols (**1**).

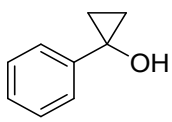


To a 100 mL flame-dried round-bottomed flask tube equipped with a magnetic stir bar was added cyclobutanone (10 mmol, 700 mg, 1.0 equiv.) and dry THF (10 mL), the reaction mixture was cooled to 0 °C, then phenylmagnesium bromide (20 mmol, 2.0 eq., 1.0 M in Et_2O) was added drop wise over 30 min at 0 °C. The mixture was warmed to room temperature and was stirred overnight. Then the mixture was quenched with NH_4Cl (aq). (10 mL) and extracted with ethyl acetate (30.0 mL×3). The combined organic phase was washed with brine (20 mL) and dried over anhydrous Na_2SO_4, filtered and concentrated in vacuo to give a residue which purified by column chromatography (eluent: petroleum ether: ethyl acetate = 10:1) to afford **1-phenylcyclobutan-1-ol.**

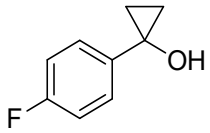
2) Characterization data for compound 1



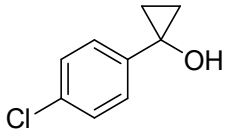
1-(*p*-tolyl)cyclopropan-1-ol (1a): 755.8 mg, 51% yield ; a pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.18 (d, J = 8.0 Hz, 2H), 7.12 (d, J = 8.0 Hz, 2H), 2.32 (s, 3H), 1.19 (dd, J_1 = 7.5 Hz, J_2 = 5.2 Hz, 2H), 0.97 (dd, J_1 = 7.2 Hz, J_2 = 5.0 Hz, 2H).



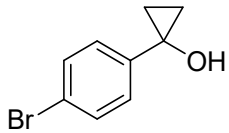
1-phenylcyclopropan-1-ol (1b): 506.6 mg, 74% yield; a colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.32 (s, 2H), 7.30 (d, J = 3.0 Hz, 2H), 7.24-7.20 (m, 1H), 2.37 (s, 1H), 1.24 (q, J = 5.4 Hz, 2H), 1.02 (q, J = 5.0 Hz, 2H).



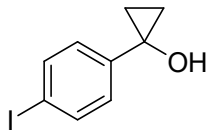
1-(4-fluorophenyl)cyclopropan-1-ol (1c): 1.2 g, 79% yield; a pale yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.27-7.24 (m, 2H), 7.00 (d, J = 8.6 Hz, 2H), 2.56 (s, 1H), 1.21 (dd, J_1 = 7.3 Hz, J_2 = 5.2 Hz, 2H), 0.97 (dd, J_1 = 7.4 Hz, J_2 = 5.3 Hz, 2H).



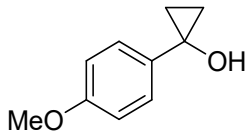
1-(4-chlorophenyl)cyclopropan-1-ol (1d): 450.0 mg, 27% yield; a light yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.28 (d, J = 8.7 Hz, 2H), 7.21 (d, J = 8.6 Hz, 2H), 2.21 (s, 1H), 1.27 (dd, J_1 = 7.5 Hz, J_2 = 5.5 Hz, 2H), 1.01 (dd, J_1 = 7.2 Hz, J_2 = 5.1 Hz, 2H).



1-(4-bromophenyl)cyclopropan-1-ol (1e): 469.5mg, 43% yield; a white solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44 (d, J = 8.5 Hz, 2H), 7.16 (d, J = 8.5 Hz, 2H), 1.99 (s, 1H), 1.28 (dd, J_1 = 7.5 Hz, J_2 = 5.4 Hz, 2H), 1.02 (dd, J_1 = 7.2 Hz, J_2 = 5.1 Hz, 2H).

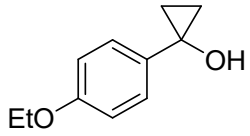


1-(4-iodophenyl)cyclopropan-1-ol (1f): 660.0 mg, 25% yield; a white solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.17 (d, J = 5.0 Hz,1H), 6.97-6.89 (m, 2H), 6.86 (d, J = 3.3 Hz,1H), 2.81 (s, 1H), 1.28 (dd, J_1 = 7.4 Hz, J_2 = 5.5 Hz, 2H), 1.05 (dd, J_1 = 7.0 Hz, J_2 = 5.1 Hz, 2H).

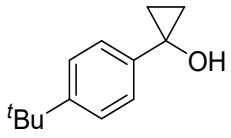


1-(4-methoxyphenyl)cyclopropan-1-ol (1g): 476.2 mg, 29% yield; a pale yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.28-7.26 (m,2H), 6.88-6.86 (m, 2H), 3.80 (s, 3H), 1.83 (s, 1H), 1.20 (dd, J_1

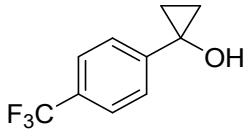
= 7.3 Hz, J_2 = 5.1 Hz, 2H), 0.98 (dd, J_1 = 7.2 Hz, J_2 = 5.1 Hz, 2H).



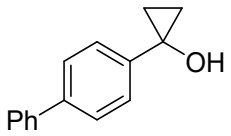
1-(4-ethoxyphenyl)cyclopropan-1-ol (1h): 1.0 g, 58% yield; a pale yellow solid;^{1}H NMR (400 MHz, $CDCl_3$): δ 7.27 (d, J = 2.4 Hz, 1H), 7.24 (t, J = 2.0 Hz, 1H), 6.87-6.85 (m, 2H), 4.02 (q,J = 7.0 Hz,2H), 1.41 (t, J = 7.0 Hz,3H), 1.19 (dd, J_1 = 8.1 Hz, J_2 = 6.2 Hz, 2H), 0.97 (dd, J_1 = 7.0 Hz, J_2 = 5.0 Hz, 2H).



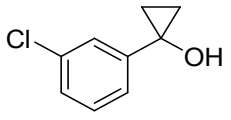
1-(4-(tert-butyl)phenyl)cyclopropan-1-ol (1i): 583.9 mg, 61% yield; a colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 (d, J = 2.8 Hz, 1H), 7.36 (d, J = 3.0 Hz, 1H), 7.27 (d, J = 2.2 Hz, 1H), 7.24 (t, J = 2.0 Hz, 1H), 1.32 (s, 9H), 1.24 (dd, J_1 = 7.3 Hz, J_2 = 5.0 Hz, 2H), 1.03 (dd, J_1 = 7.5 Hz, J_2 = 5.2 Hz, 2H).



1-(4-(trifluoromethyl)phenyl)cyclopropan-1-ol (1j): 652.3 mg, 32% yield; a light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 (d, J = 8.3 Hz, 2H), 7.37 (d, J = 8.2 Hz, 2H), 2.18 (s, 1H), 1.36 (dd, J_1 = 7.7, J_2 = 5.5 Hz, 2H), 1.10 (dd, J_1 = 7.3 Hz, J_2 = 5.2 Hz, 2H).

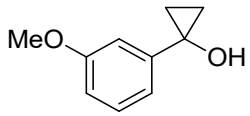


1-([1,1'-biphenyl]-4-yl)cyclopropan-1-ol (1k): 329.3 mg, 16% yield; a light yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (t, J = 8.1 Hz, 4H), 7.44 (t, J = 7.8 Hz, 2H),7.38 (d, J = 8.3 Hz, 2H),7.34 (t, J = 7.4 Hz, 1H), 2.34 (s, 1H), 1.31 (dd, J_1 = 7.6, J_2 = 5.4 Hz, 2H), 1.10 (dd, J_1 = 7.2 Hz, J_2 = 5.0 Hz, 2H).

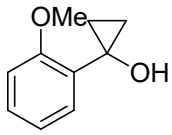


1-(3-chlorophenyl)cyclopropan-1-ol (1l): 930.0 mg, 58% yield; a light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.27 (t, J = 1.8 Hz, 1H), 7.23 (d, J = 3.2 Hz, 1H), 7.18 (t, J = 1.4 Hz, 1H), 7.10 (dt,

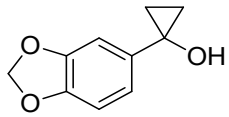
J_1 = 7.6, J_2 = 1.4 Hz, 1H), 2.57 (s, 1H), 1.25 (dd, J_1 = 7.4, J_2 = 5.3 Hz, 2H), 1.01 (dd, J_1 = 7.2 Hz, J_2 = 5.1 Hz, 2H).



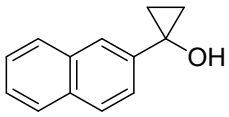
1-(3-methoxyphenyl)cyclopropan-1-ol (1m): 656.8 mg, 40% yield; a light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.13 (t, J = 8.0 Hz, 1H), 6.81 (d, J = 2.3 Hz, 1H), 6.72 (d, J = 6.8 Hz, 1H), 6.66 (dd, J_1 = 8.2, J_2 = 2.1 Hz, 1H), 3.70 (s, 3H), 2.78 (s, 1H), 1.14 (dd, J_1 = 7.5, J_2 = 5.3 Hz, 2H), 0.93 (dd, J_1 = 7.1 Hz, J_2 = 4.9 Hz, 2H).



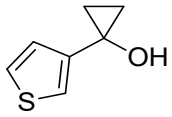
1-(2-methoxyphenyl)cyclopropan-1-ol (1n): 657.0 mg, 40% yield; a light yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.26 (t, J = 8.1 Hz, 1H), 7.20 (d, J = 7.8 Hz, 1H), 6.90 (t, J = 7.1 Hz, 2H), 3.92 (s, 3H), 1.10 (dd, J_1 = 7.2, J_2 = 5.8 Hz, 2H), 0.91 (dd, J_1 = 6.4 Hz, J_2 = 5.4 Hz, 2H).



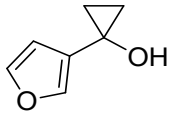
1-(benzo[*d*][1,3]dioxol-5-yl)cyclopropan-1-ol (1o): 803.5 mg, 45% yield; a white solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.84-6.82 (m, 2H),6.78 (s, 1H), 5.94 (s, 2H), 2.24 (s, 1H),1.20 (dd, J_1 = 7.4 Hz, J_2 = 5.3 Hz, 2H), 0.96 (dd, J_1 = 7.1, J_2 = 5.0 Hz, 2H).



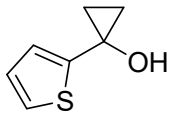
1-(naphthalen-2-yl)cyclopropan-1-ol (1p): 773.8 mg, 42% yield; a white solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (s, 1H), 7.84-7.82 (m, 2H), 7.80 (d, J = 3.7 Hz, 1H), 7.50-7.48 (m, 1H), 7.47-7.44 (m, 1H), 7.31 (dd, J_1 = 8.6 Hz, J_2 = 1.8 Hz, 1H), 2.50 (s, 1H), 1.35 (dd, J_1 = 7.6, J_2 = 5.4 Hz, 2H), 1.17 (dd, J_1 = 7.2 Hz, J_2 = 5.1 Hz, 2H).



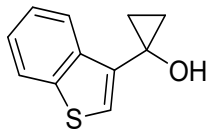
1-(thiophen-3-yl)cyclopropan-1-ol (1q): 630.0 mg, 45% yield; a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.26 (dd, J_1 = 5.0, J_2 = 3.2 Hz, 1H), 7.17-7.12 (m, 1H), 6.82 (d, J = 5.0 Hz, 1H), 2.55 (s, 1H), 1.21 (dd, J_1 = 7.6, J_2 = 5.6 Hz, 2H), 0.98 (dd, J_1 = 7.1 Hz, J_2 = 5.2 Hz, 2H).



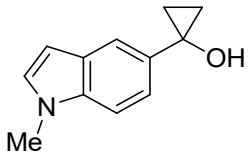
1-(furan-3-yl)cyclopropan-1-ol (1r): 260.7 mg, 21% yield; a light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 (d, J = 7.3, 1H), 7.82-7.81 (m, 1H), 7.33-7.31 (m,1H), 2.60 (s, 1H), 1.15 (dd, J_1 = 7.3, J_2 = 5.2 Hz, 2H), 0.96 (dd, J_1 = 7.0 Hz, J_2 = 5.0 Hz, 2H).



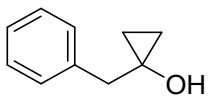
1-(thiophen-2-yl)cyclopropan-1-ol (1s): 525.0 mg, 37% yield; a light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.16 (d, J = 5.0 Hz, 1H), 6.93 (t, J = 3.6 Hz, 1H), 6.86 (d, J = 3.3 Hz, 1H), 2.81 (s, 1H), 1.28 (dd, J_1 = 7.4, J_2 = 5.5 Hz, 2H), 1.05 (dd, J_1 = 7.0 Hz, J_2 = 5.1 Hz, 2H).



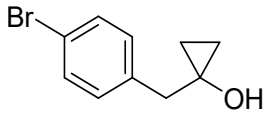
1-(benzo[*b*]thiophen-3-yl)cyclopropan-1-ol (1t): 994.6mg, 52% yield; a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14 (d, J = 7.7 Hz, 1H), 7.84 (d, J = 7.8 Hz, 1H), 7.41 (t, J = 6.6 Hz, 1H), 7.38-7.34 (m, 1H),7.29 (s, 1H), 2.45 (s, 1H), 1.21 (dd, J_1 = 7.4 Hz, J_2 = 5.3 Hz, 2H), 1.00 (dd, J_1 = 6.8, J_2 = 4.9 Hz, 2H).



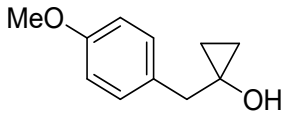
1-(1-methyl-1*H*-indol-5-yl)cyclopropan-1-ol(1u): 356 mg, 19 %; a light yellow solid; R_f (PE : EA = 10 : 1) = 0.35; m.p. = 43-44°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.64 (d, J = 0.8 Hz, 1H), 7.29-7.23 (m, 2H), 7.04 (d, J = 3.0 Hz, 1H), 6.45 (dd, J_1 = 3.0 Hz, J_2 = 0.3 Hz,1H), 3.77 (s, 3H), 1.21 (dd, J_1 = 7.3 Hz, J_2 = 5.0 Hz,2H), 1.04 (dd, J_1 = 7.0 Hz, J_2 = 4.7 Hz,2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 135.9, 134.9, 129.4, 128.4, 120.1, 117.9, 109.3, 101.0, 57.6, 32.9, 16.5; IR (KBr, υ cm^{-1}): 3671, 3365, 3085, 2932, 2877, 2820, 1569, 1492, 1447, 1423, 1338, 1241, 887, 863, 805, 723; HRMS (ESI) m/z calcd for $C_{12}H_{13}NONa^+$ $(M+Na)^+$210.0889, found 210.0889.



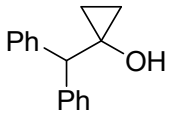
1-benzylcyclopropan-1-ol (1v): 965.8 mg, 65% yield; a colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36-7.25 (m, 5H), 2.89 (s, 2H), 1.94 (s, 1H), 0.82 (dd, J_1 = 6.7, J_2 = 5.7 Hz, 2H), 0.65 (dd, J_1 = 6.7 Hz, J_2 = 5.0 Hz, 2H).



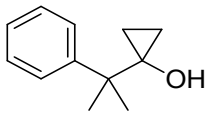
1-(4-methoxybenzyl)cyclopropan-1-ol (1w): 1.55 g, 87% yield; a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.21 (d, J = 8.3 Hz, 2H), 6.87 (d, J = 8.3 Hz, 2H), 3.80 (s, 3H), 2.82 (s, 2H), 2.11 (s, 1H), 0.81-0.79 (m, 2H), 0.63-0.60 (m, 2H).



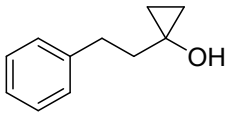
1-(4-bromobenzyl)cyclopropan-1-ol (1x): 2.24 g, 98% yield; a white solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51 (d, J = 8.3 Hz, 2H), 7.18 (d, J = 8.3 Hz, 2H), 2.83 (s, 2H), 1.77 (s, 1H), 0.82 (dd, J_1 = 6.7, J_2 = 5.6 Hz, 2H), 0.63 (dd, J_1 = 6.7 Hz, J_2 = 5.1 Hz, 2H).



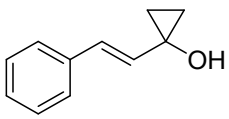
1-benzhydrylcyclopropan-1-ol (1y): 964.5 mg, 43% yield; a light yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38-7.36 (m, 4H), 7.34-7.30 (m, 4H), 7.25-7.23 (m, 2H), 3.89 (s, 1H), 0.94 (dd, J_1 = 6.9, J_2 = 5.4 Hz, 2H), 0.69 (dd, J_1 = 6.8 Hz, J_2 = 5.2 Hz, 2H).



1-(2-phenylpropan-2-yl)cyclopropan-1-ol (1z): 761.0 mg, 43% yield; a colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51 (dd, J_1 = 8.6 Hz, J_2 = 1.3 Hz, 2H), 7.33 (t, J = 7.4 Hz, 2H), 7.21 (t, J = 6.6 Hz, 1H), 1.67 (s, 1H), 1.28 (s, 6H), 0.84 (dd, J_1 = 7.2, J_2 = 5.2 Hz, 2H), 0.71 (dd, J_1 = 7.0 Hz, J_2 = 5.0 Hz, 2H).

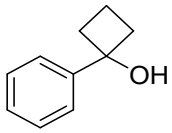


1-phenethylcyclopropan-1-ol (1aa): 1.47 g, 91% yield; a colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31-7.27 (m, 2H), 7.23-7.18 (m, 3H), 2.88-2.84 (m, 2H), 1.90-1.86 (m, 2H), 1.78 (s, 1H), 0.77 (dd, J_1 = 6.5, J_2 = 5.4 Hz, 2H), 0.47 (dd, J_1 = 6.5 Hz, J_2 = 5.0 Hz, 2H).



(*E*)-1-styrylcyclopropan-1-ol (1ab): 170.0 mg, 11% yield; a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36-7.29 (m, 4H), 7.21 (t, J = 7.2 Hz, 1H), 6.66 (d, J = 15.8 Hz, 1H), 5.98 (d, J = 15.8

Hz, 1H), 2.24 (s, 1H), 1.17 (dd, J_1 = 7.4, J_2 = 5.3 Hz, 2H), 0.87 (dd, J_1 = 7.1 Hz, J_2 = 4.9 Hz, 2H).



1-phenylcyclobutan-1-ol (**1ac**) 960.8 mg, 65% yield; a pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46-7.44 (m, 2H), 7.33 (t, J = 7.4 Hz, 2H), 7.26-7.22 (m, 1H), 2.62 (s, 1H), 2.54-2.47 (m, 2H), 2.35-2.78 (m, 2H), 2.02-1.91 (m, 2H), 1.70-1.59 (m, 1H).

3) References

1. X. P. He, Y. J. Shu, J. J. Dai, W. M. Zhang and H. J. Xu, Copper-Catalysed Ring-Opening Trifluoromethylation of Cyclopropanols. *Org. Biomol. Chem.* 2015, **13**, 7159.

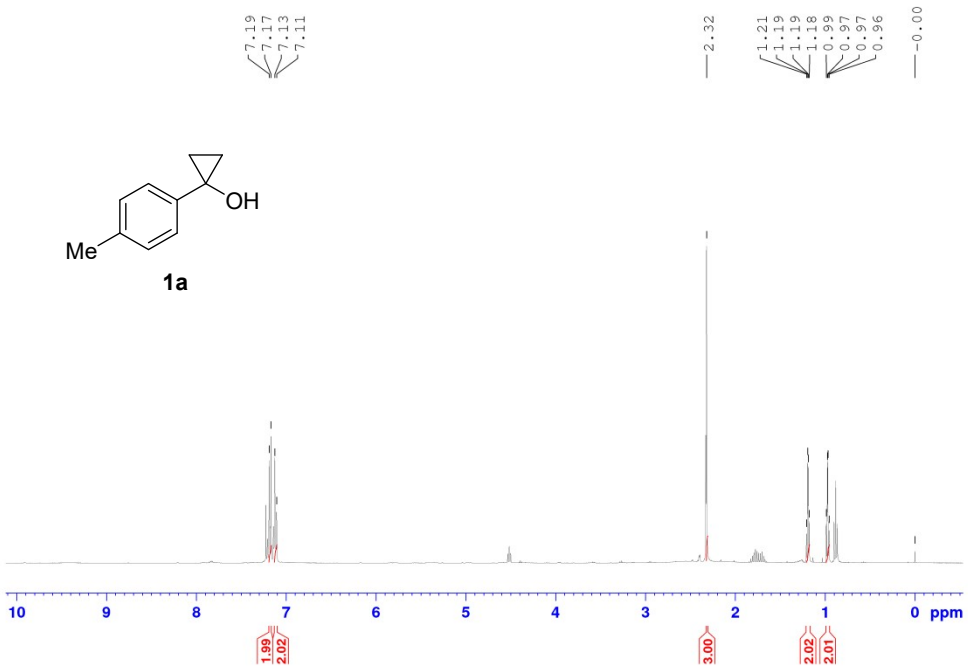
2. W.Huang and F. Meng, Cobalt-Catalyzed Diastereo-and Enantioselective Hydroalkylation of Cyclopropenes with Cobalt-Homoenolates. *Angew. Chem. Int. Ed.* 2021, **60**, 2694.

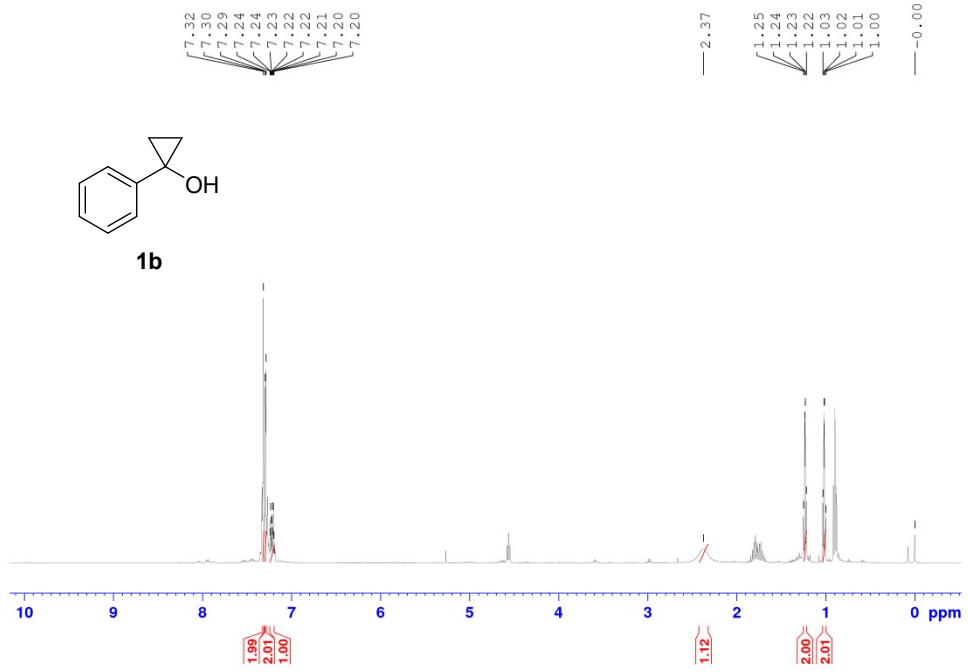
3. B. Q. Cheng, S. X. Zhang, Y. Y. Cui and Z. L. Shen, Copper(II)-Mediated Ring Opening/Alkynylation of Tertiary Cyclopropanols by Using Nonmodified Terminal Alkynes. *Org. Lett.* 2020, **22**, 5456.

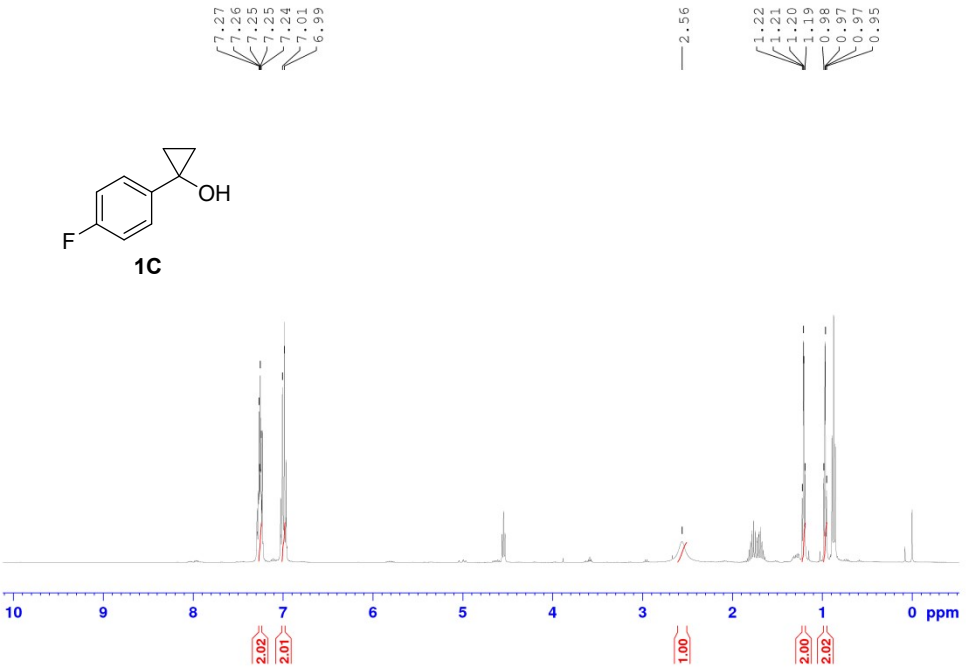
4. L. Cardinale, M. Neumeier, M. Majek and A. Wangelina, Aryl Pyrazoles from Photocatalytic Cycloadditions of Arenediazonium. *Org. Lett.* 2020, **22**, 7219.

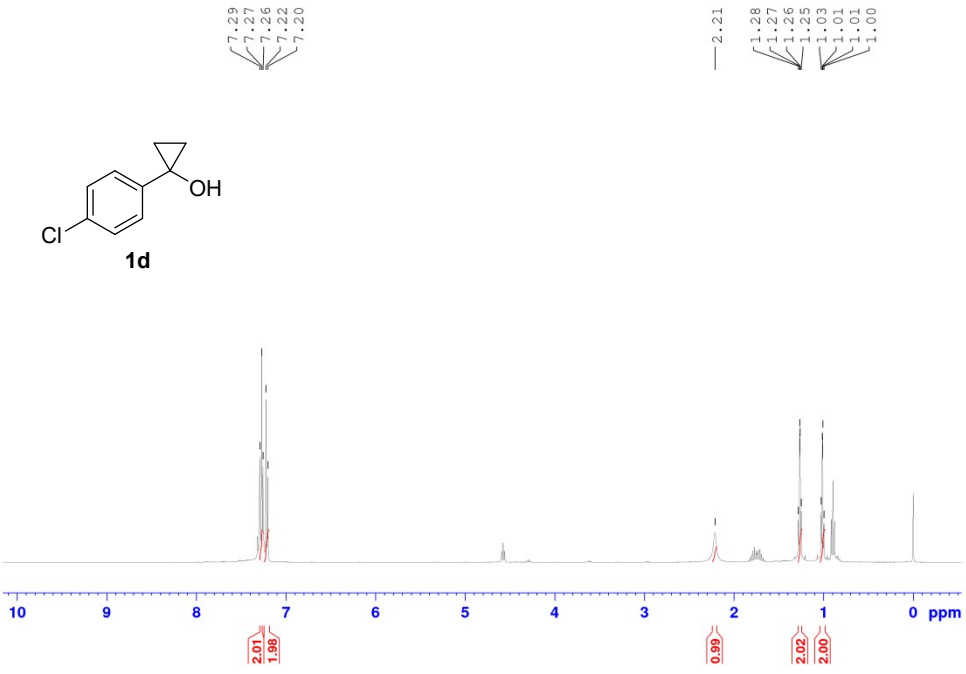
5. Xu, B.; Wang, D.; Hu, Y.; Shen, Q. Silver-Catalyzed Ring-Opening Difluoromethylthiolation/Trifluoromethylthiolation of Cycloalkanols with $PhSO_2SCF_2H$ or $PhSO_2SCF_3$. *Org. Chem. Front*., **2018**, *5*, 1462-1465.

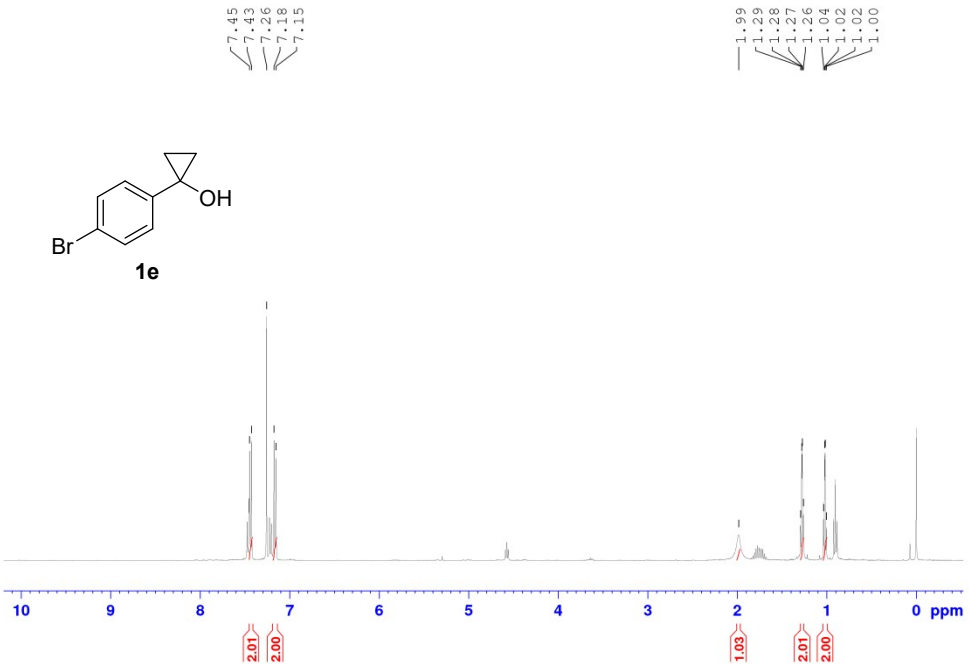
4) Spectra for 1



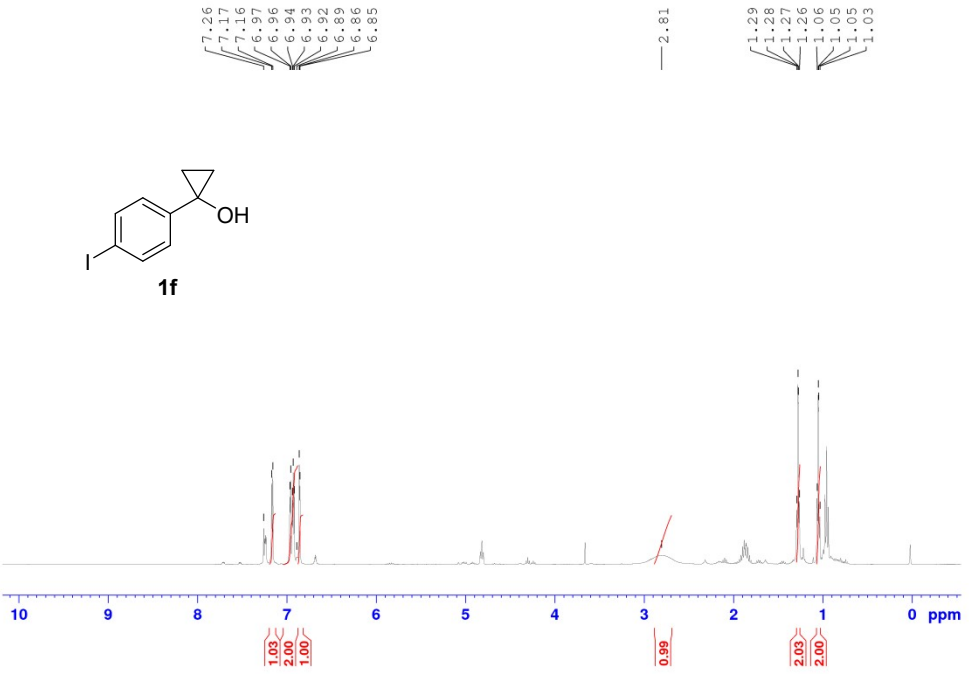



7.27
7.26
7.25
7.25
7.24
7.01
6.99
2.56
1.22
1.21
1.20
1.19
0.98
0.97
0.97
0.95
OH
F
1C
10
9
8
7
6
5
4
3
2
1
0 ppm
2.02
2.01
1.00
2.00
2.02

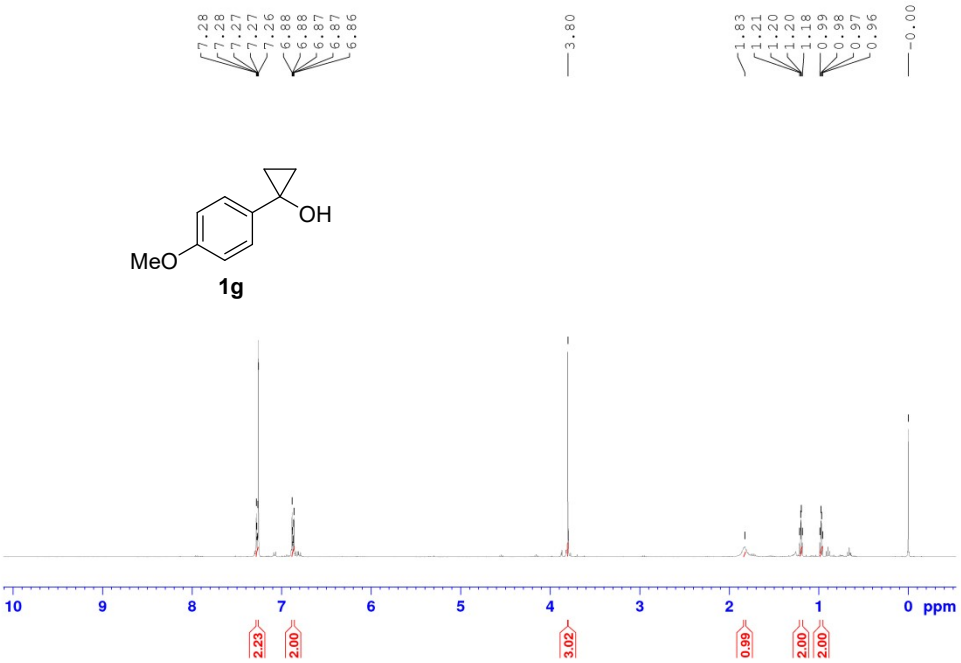

7.29
7.27
7.26
7.22
7.20
2.21
1.28
1.27
1.26
1.25
1.03
1.01
1.01
1.00
OH
Cl
1d
10
9
8
7
6
5
4
3
2
1
0 ppm
2.01
1.98
0.99
2.02
2.00


7.45
7.43
7.26
7.18
7.15
1.99
1.29
1.28
1.27
1.26
1.04
1.02
1.02
1.00
OH
Br
10
9
8
7
6
5
4
3
2
1
0 ppm
2.01
2.00
1.03
2.01
2.00

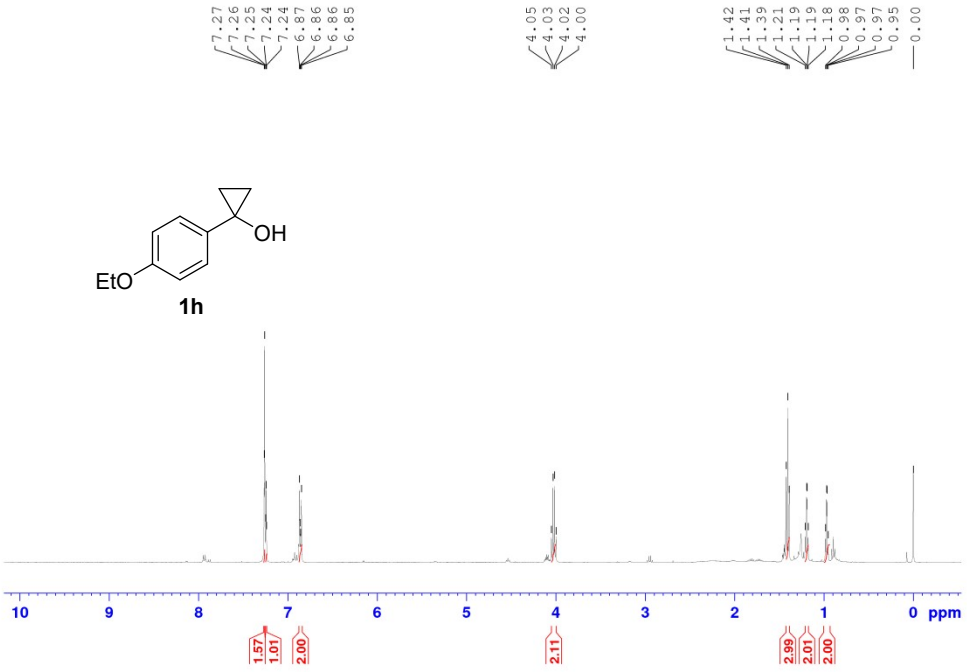
1e


7.26
7.17
7.16
6.97
6.96
6.94
6.93
6.92
6.89
6.86
6.85
2.81
1.29
1.28
1.27
1.26
1.06
1.05
1.05
1.03
OH
I
10
9
8
7
6
5
4
3
2
1
0 ppm
1.03
2.00
1.00
0.99
2.03
2.00

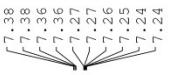
1f

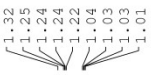

7.28
7.28
7.27
7.27
7.26
6.88
6.88
6.87
6.87
6.86
3.80
1.83
1.21
1.20
1.20
1.18
0.99
0.98
0.97
0.96
0.00
OH
MeO
10
9
8
7
6
5
4
3
2
1
0 ppm
2.23
2.00
3.02
0.99
2.00
2.00

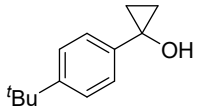
1g


7.27
7.26
7.25
7.24
7.24
6.87
6.86
6.86
6.85
4.05
4.03
4.02
4.00
1.42
1.41
1.39
1.21
1.19
1.19
1.18
0.98
0.97
0.97
0.95
0.00
OH
EtO
10
9
8
7
6
5
4
3
2
1
0 ppm
1.57
1.01
2.00
2.11
2.59
2.01
2.00

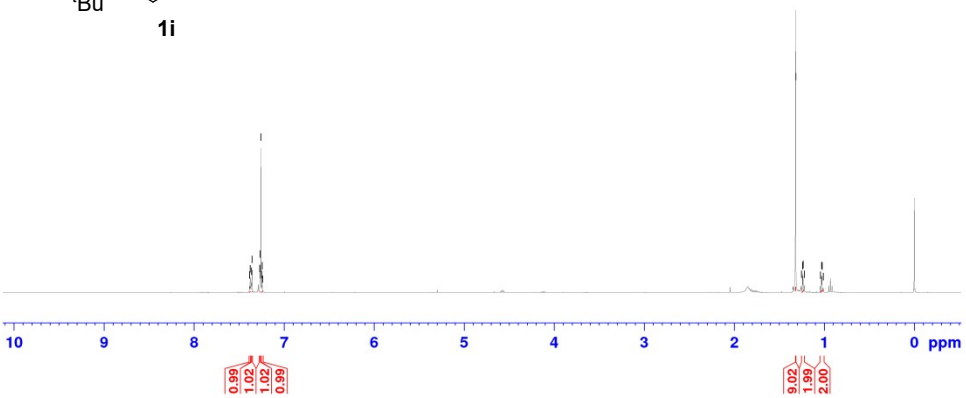
1h


7.38
7.38
7.36
7.27
7.27
7.26
7.25
7.24
7.24

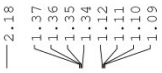

1.32
1.25
1.24
1.24
1.22
1.04
1.03
1.03
1.01

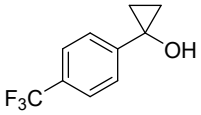

OH
tBu

1i

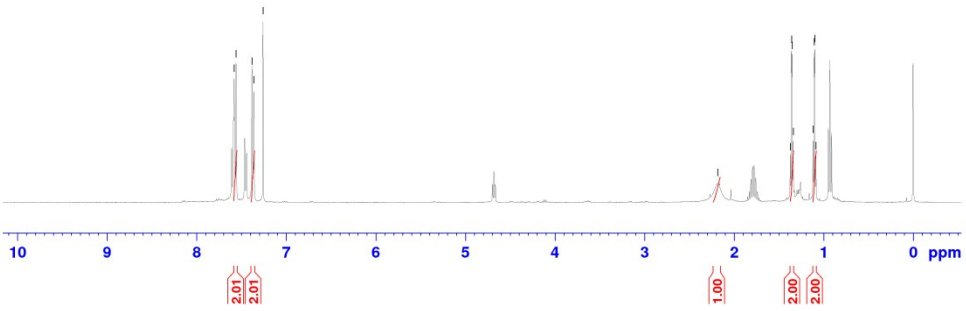

10
9
8
7
6
5
4
3
2
1
0 ppm
0.99
1.02
1.02
0.99
9.02
1.99
2.00

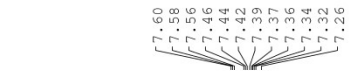

7.58
7.56
7.38
7.36
7.26

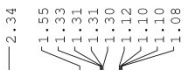

2.18
1.37
1.36
1.35
1.34
1.12
1.11
1.10
1.09

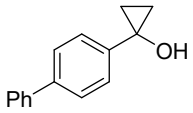

OH
F3C

1j

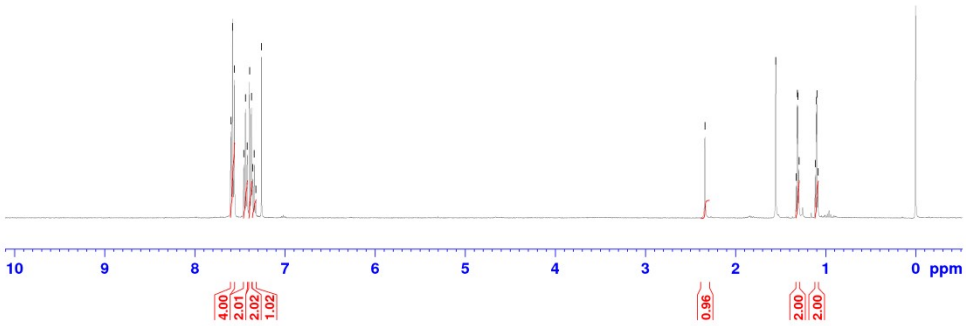

10
9
8
7
6
5
4
3
2
1
0 ppm
2.01
2.01
1.00
2.00
2.00

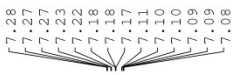

7.60
7.58
7.56
7.46
7.44
7.42
7.39
7.37
7.36
7.34
7.32
7.26

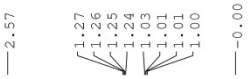

2.34
1.55
1.33
1.31
1.31
1.30
1.12
1.10
1.10
1.08

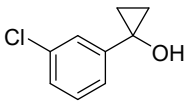

OH
Ph

1k

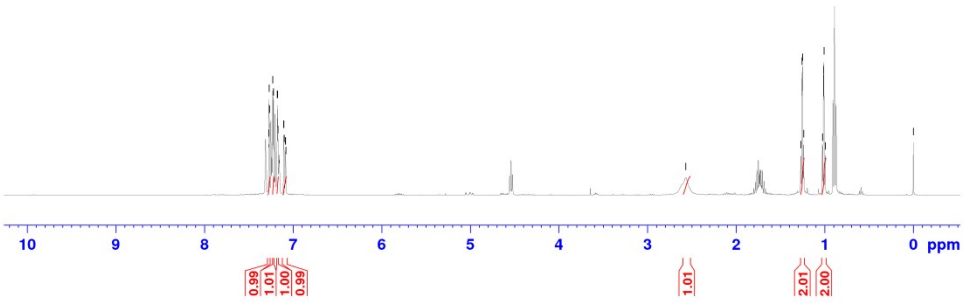

10
9
8
7
6
5
4
3
2
1
0 ppm
4.00
2.01
2.02
1.02
0.96
2.00
2.00

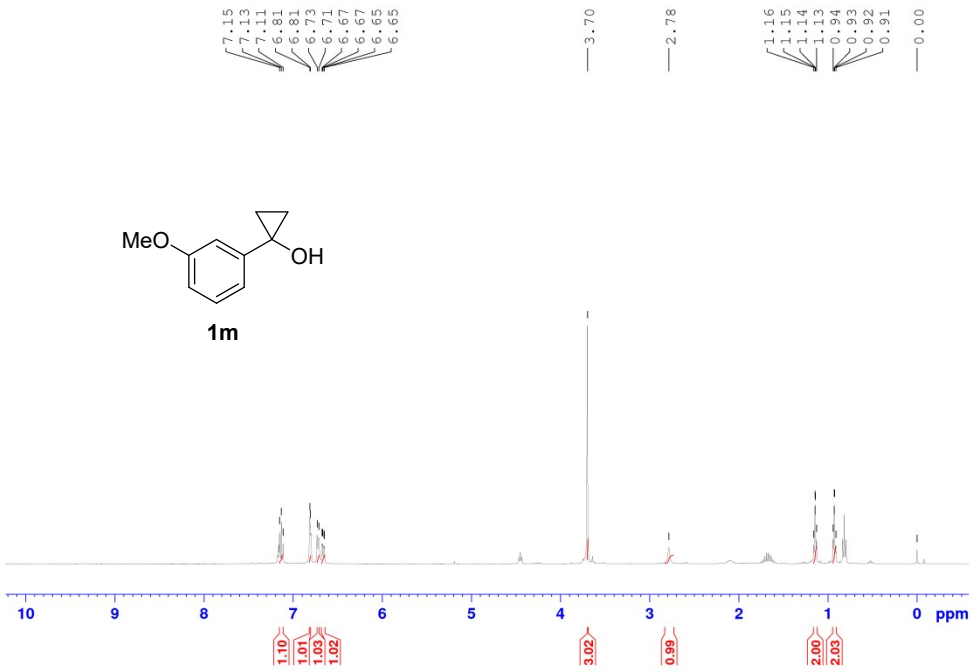

7.28
7.27
7.27
7.23
7.22
7.18
7.18
7.17
7.11
7.10
7.10
7.09
7.09
7.08


2.57
1.27
1.26
1.25
1.24
1.03
1.01
1.01
1.00
0.00

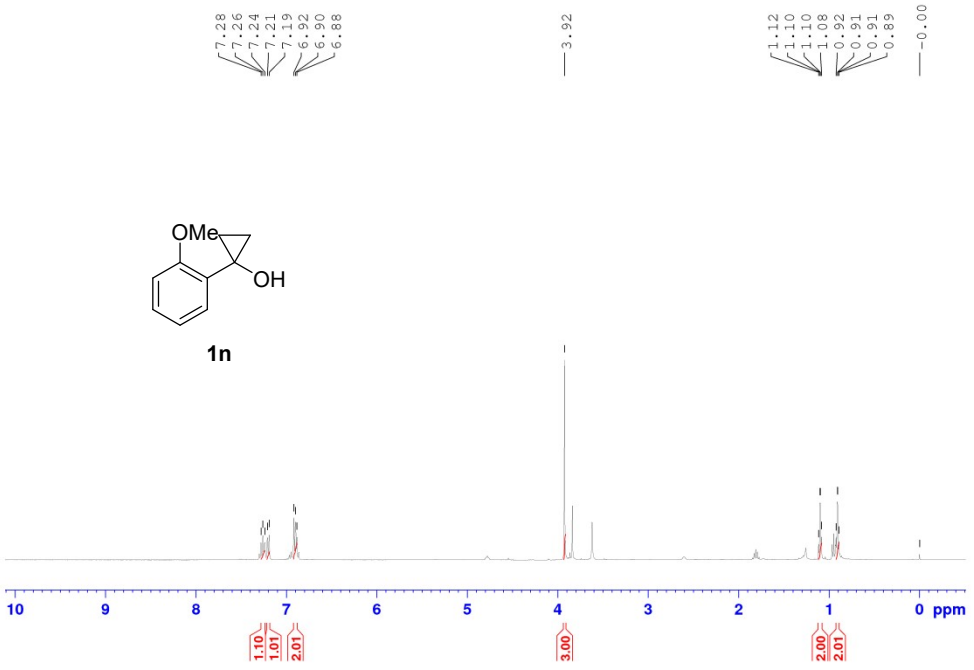

Cl
OH

1l

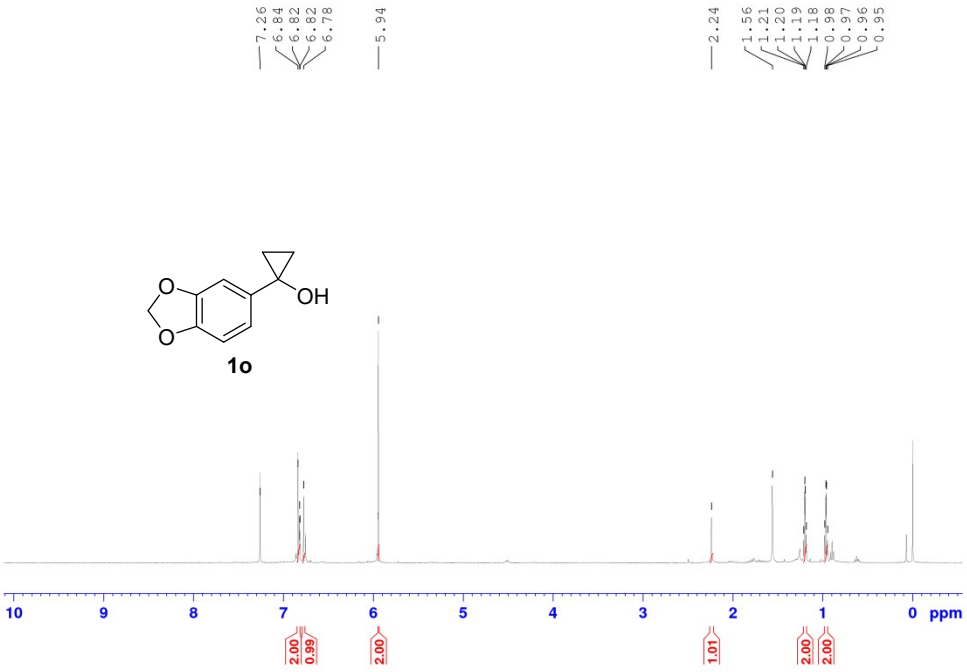

10
9
8
7
6
5
4
3
2
1
0 ppm
0.99
1.01
1.00
0.99
1.01
2.01
2.00

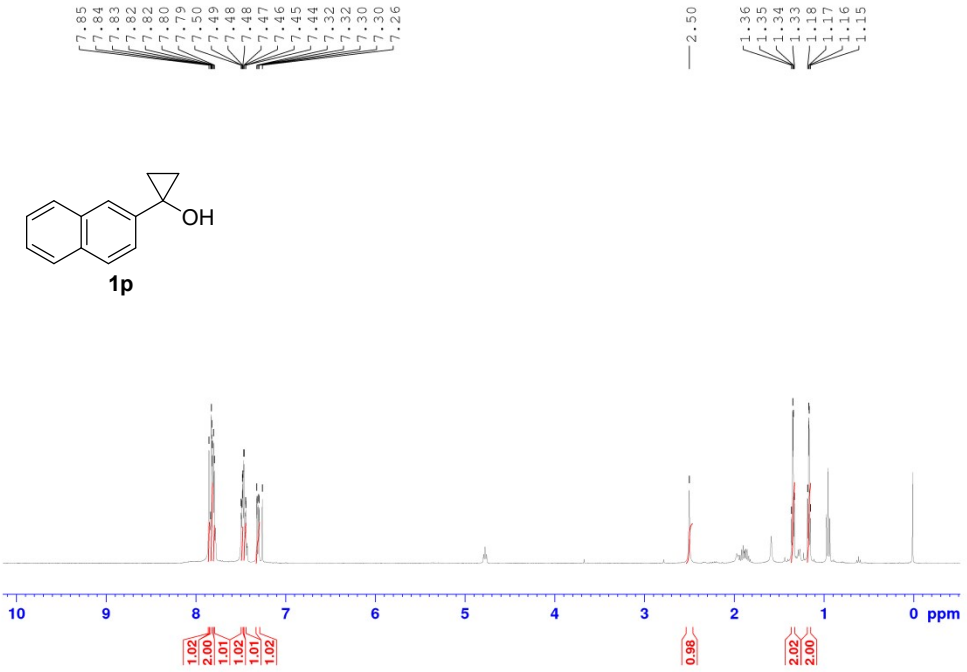

7.15
7.13
7.11
6.81
6.81
6.73
6.71
6.67
6.67
6.65
6.65
3.70
2.78
1.16
1.15
1.14
1.13
0.94
0.93
0.92
0.91
0.00
MeO
OH
10
9
8
7
6
5
4
3
2
1
0 ppm
1.10
1.01
1.03
1.02
3.02
0.99
2.00
2.03

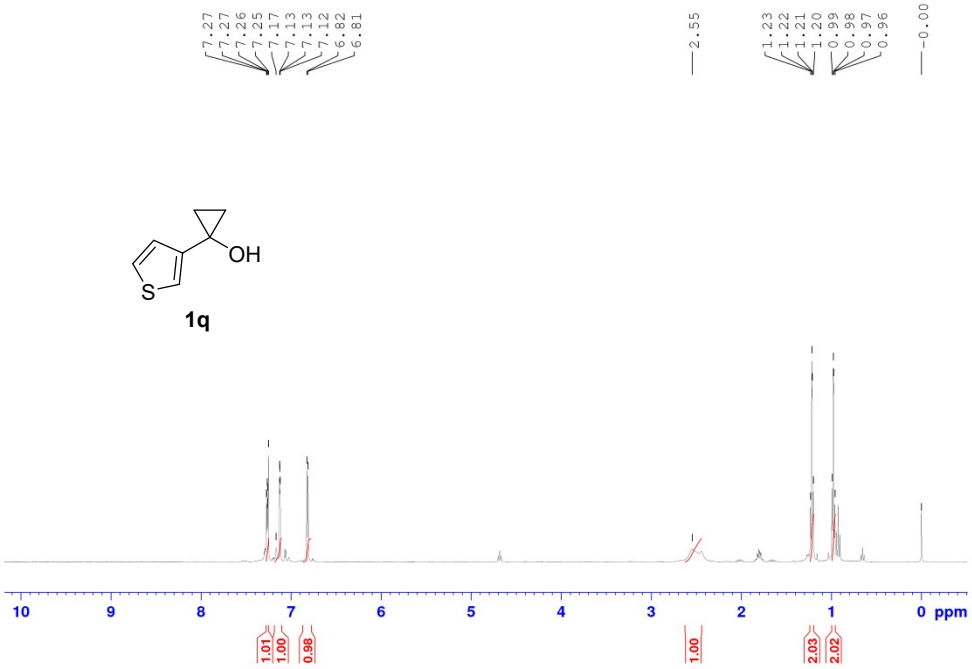
1m

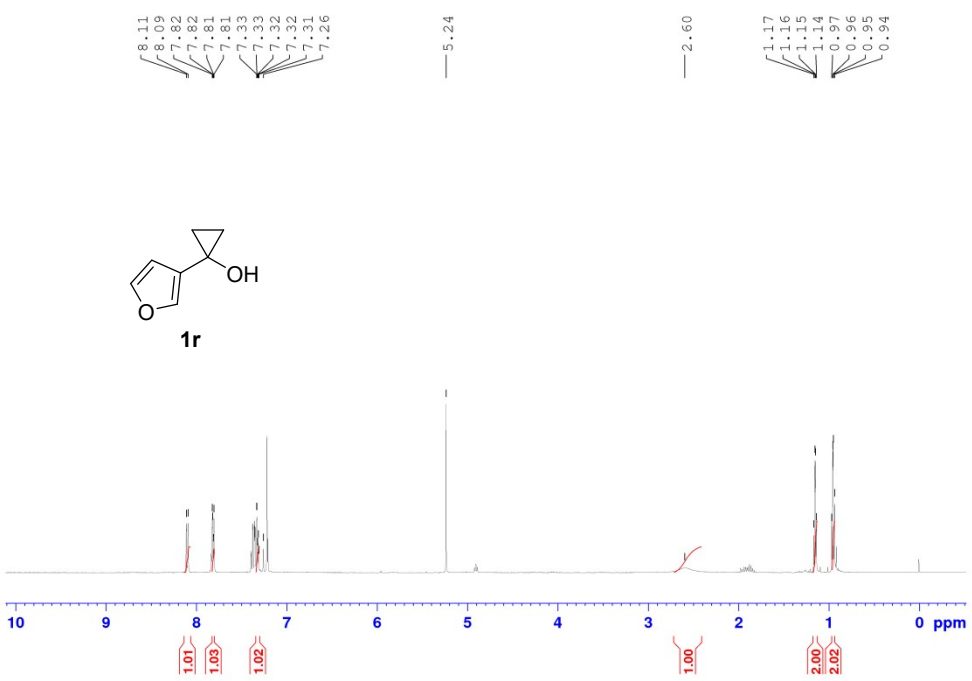

7.28
7.26
7.24
7.21
7.19
6.92
6.90
6.88
3.92
1.12
1.10
1.10
1.08
0.92
0.91
0.91
0.89
0.00
OMe
OH
10
9
8
7
6
5
4
3
2
1
0 ppm
1.10
1.01
2.01
3.00
2.00
2.01

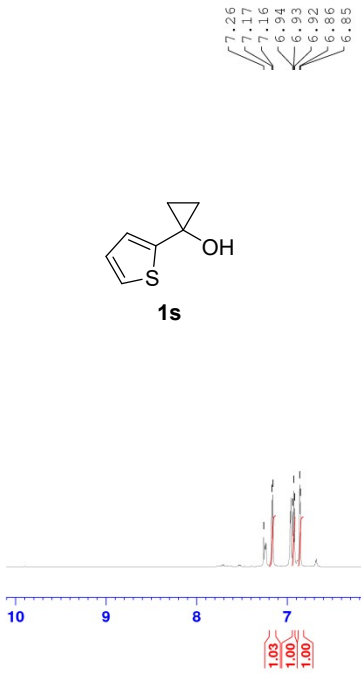
1n

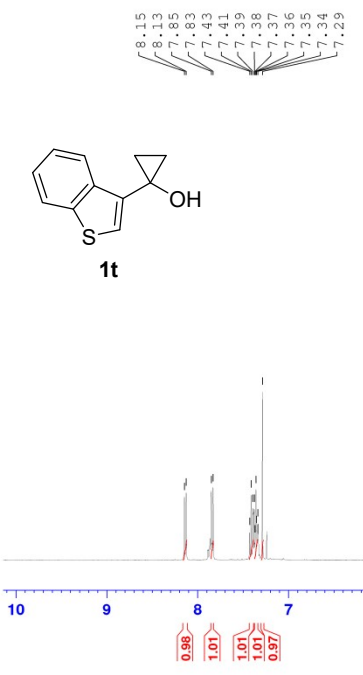

7.26
6.84
6.82
6.82
6.78
5.94
2.24
1.56
1.21
1.20
1.19
1.18
0.98
0.97
0.96
0.95
O
O
OH
1o
10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
0.99
2.00
1.01
2.00
2.00

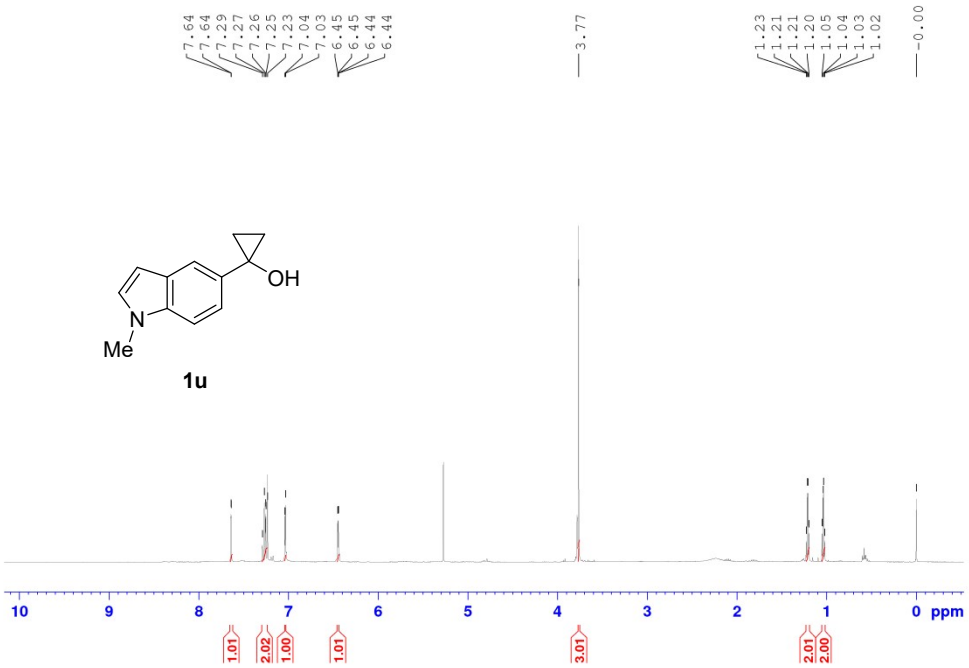

7.85
7.84
7.83
7.82
7.82
7.80
7.79
7.50
7.49
7.48
7.48
7.47
7.46
7.45
7.44
7.32
7.30
7.30
7.26
2.50
1.36
1.35
1.34
1.33
1.18
1.17
1.16
1.15
OH
1p
10
9
8
7
6
5
4
3
2
1
0 ppm
1.02
2.00
1.01
1.02
1.01
1.02
0.98
2.02
2.00

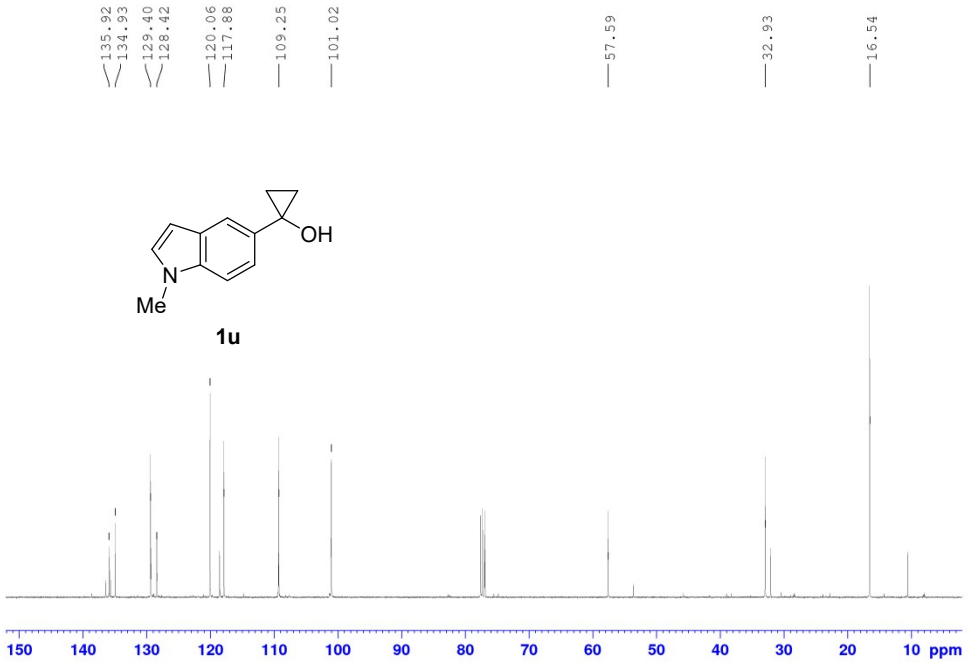

7.27
7.27
7.26
7.25
7.17
7.13
7.13
7.12
6.82
6.81
2.55
1.23
1.22
1.21
1.20
0.99
0.98
0.97
0.96
0.00
OH
S
1q
10
9
8
7
6
5
4
3
2
1
0 ppm
1.01
1.00
0.98
1.00
2.03
2.02


8.11
8.09
7.82
7.82
7.81
7.81
7.33
7.32
7.32
7.31
7.26
5.24
2.60
1.17
1.16
1.15
1.14
0.97
0.96
0.95
0.94
OH
O
1r
10
9
8
7
6
5
4
3
2
1
0 ppm
1.01
1.03
1.02
1.00
2.00
2.02

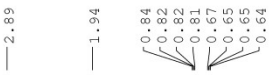

7.26
7.17
7.16
6.94
6.93
6.92
6.86
6.85
2.81
1.29
1.28
1.27
1.26
1.06
1.05
1.05
1.03
OH
S
1s
10
9
8
7
6
5
4
3
2
1
0 ppm
1.03
1.00
1.00
0.99
2.03
2.00

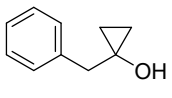

8.15
8.13
7.85
7.83
7.43
7.41
7.39
7.38
7.37
7.36
7.35
7.34
7.29
2.45
1.23
1.21
1.21
1.19
1.02
1.01
1.00
0.99
0.00
OH
S
1t
10
9
8
7
6
5
4
3
2
1
ppm
0.98
1.01
1.01
1.01
0.97
1.00
2.00
2.04


7.64
7.64
7.29
7.27
7.26
7.25
7.23
7.04
7.03
6.45
6.45
6.44
6.44
3.77
1.23
1.21
1.21
1.20
1.05
1.04
1.03
1.02
0.00
OH
N
Me
1u
10
9
8
7
6
5
4
3
2
1
0 ppm
1.01
2.02
1.00
1.01
3.01
2.01
2.00

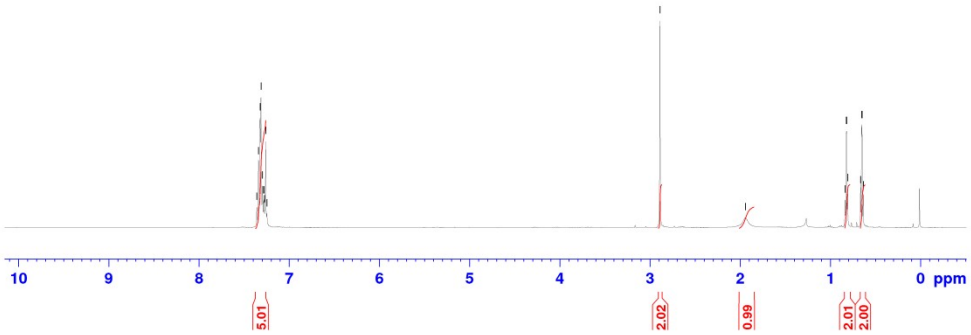

135.92
134.93
129.40
128.42
120.06
117.88
109.25
101.02
57.59
32.93
16.54
OH
N
Me
1u
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm


7.36
7.34
7.32
7.31
7.30
7.28
7.28
7.27
7.26
7.25


2.89
1.94
0.84
0.82
0.82
0.81
0.67
0.65
0.65
0.64

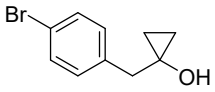

OH

1v

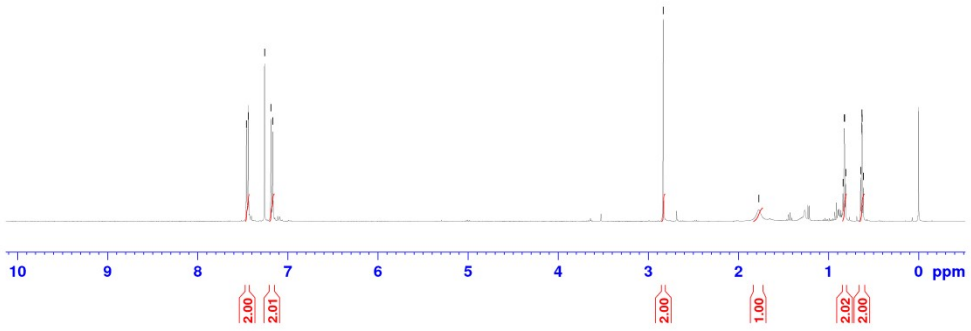

10
9
8
7
6
5
4
3
2
1
0 ppm
5.01
2.02
0.99
2.01
2.00

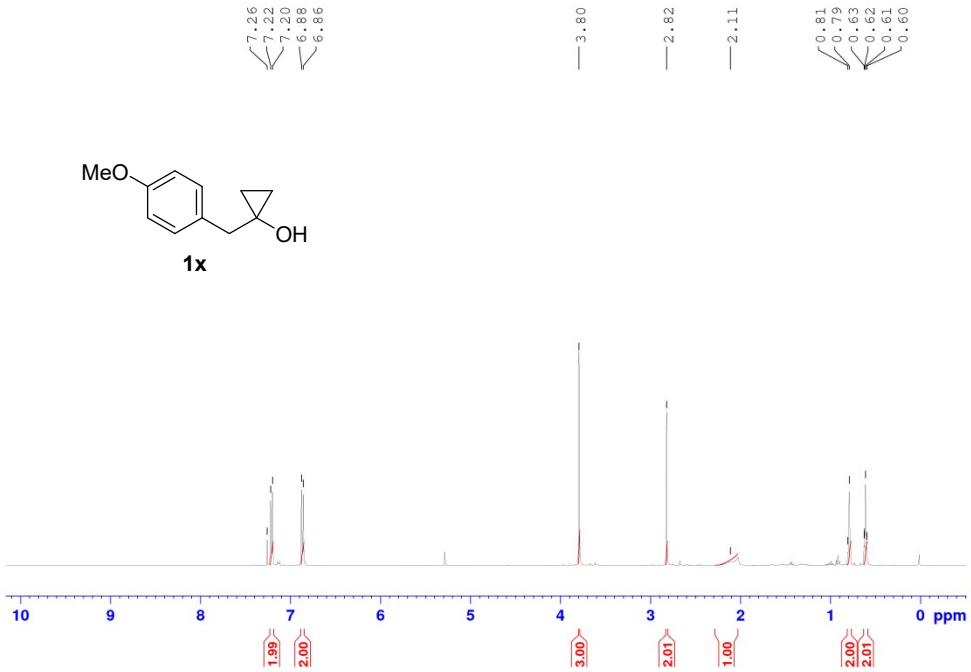

7.46
7.44
7.26
7.19
7.17


2.83
1.77
0.84
0.83
0.82
0.81
0.64
0.63
0.63
0.61

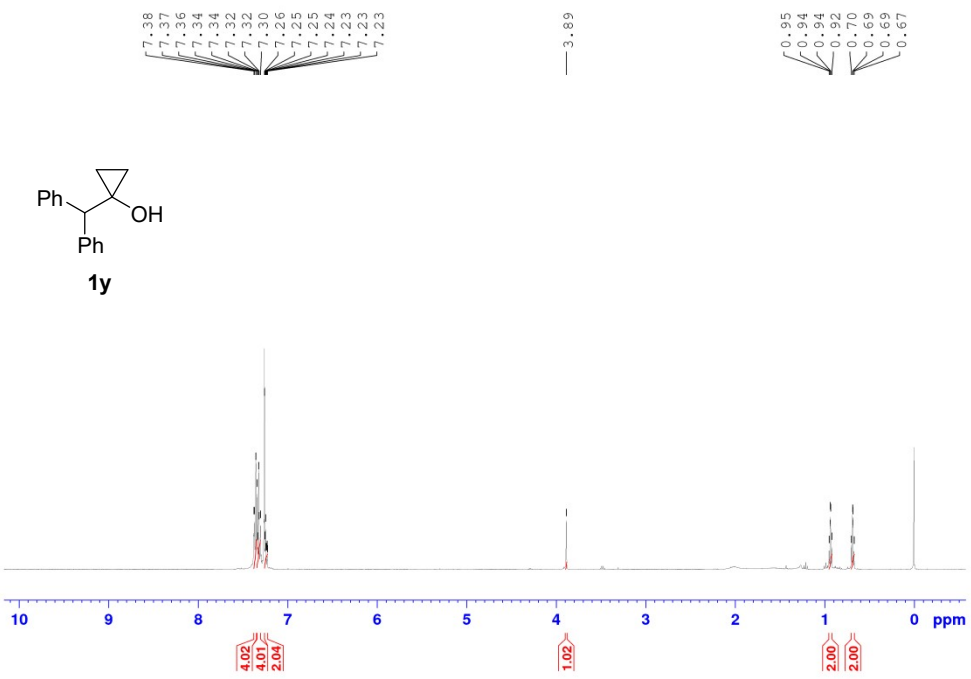

Br
OH

1w

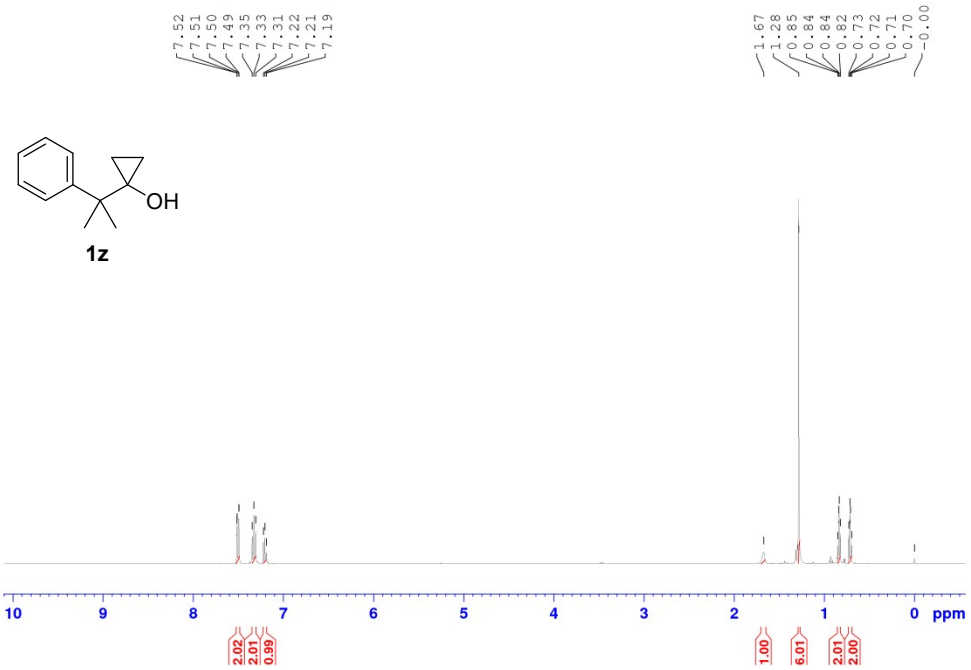

10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
2.01
2.00
1.00
2.02
2.00


7.26
7.22
7.20
6.88
6.86
3.80
2.82
2.11
0.81
0.79
0.63
0.62
0.61
0.60
MeO
OH
10
9
8
7
6
5
4
3
2
1
0 ppm
1.99
2.00
3.00
2.01
1.00
2.00
2.01

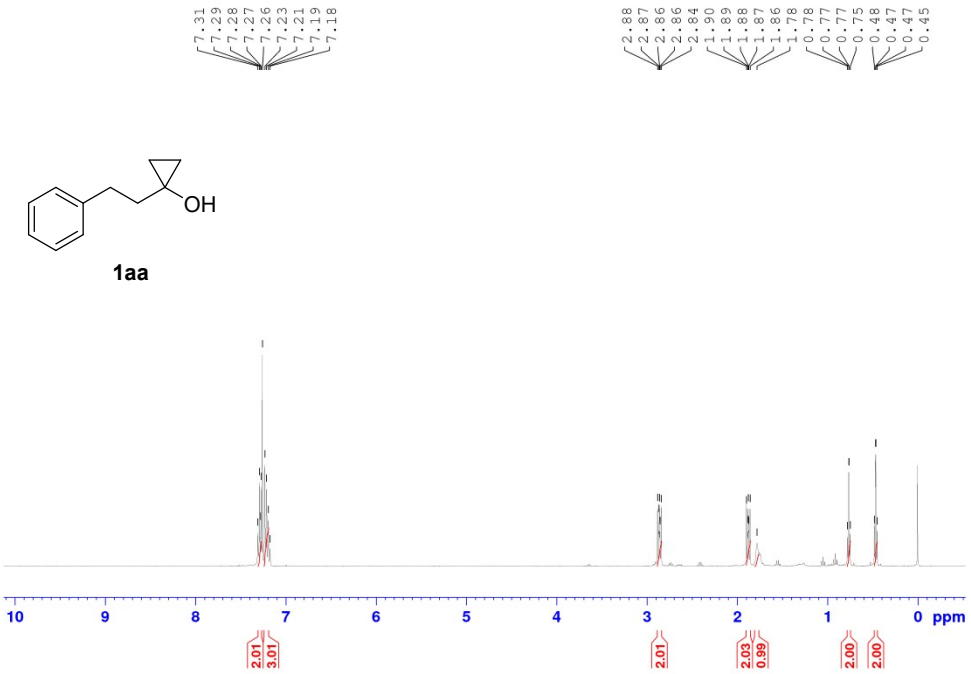
1x


7.38
7.37
7.36
7.34
7.34
7.32
7.32
7.30
7.26
7.25
7.25
7.24
7.23
7.23
7.23
3.89
0.95
0.94
0.94
0.92
0.70
0.69
0.69
0.67
Ph
OH
Ph
10
9
8
7
6
5
4
3
2
1
0 ppm
4.02
4.01
2.04
1.02
2.00
2.00

1y

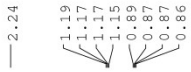

7.52
7.51
7.50
7.49
7.35
7.33
7.31
7.22
7.21
7.19
1.67
1.28
0.85
0.84
0.84
0.82
0.73
0.72
0.71
0.70
0.00
OH
10
9
8
7
6
5
4
3
2
1
0 ppm
2.02
2.01
0.99
1.00
6.01
2.01
2.00

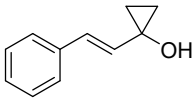
1z


7.31
7.29
7.28
7.27
7.26
7.23
7.21
7.19
7.18
2.88
2.87
2.86
2.86
2.84
1.90
1.89
1.88
1.87
1.86
1.78
0.78
0.77
0.77
0.75
0.48
0.47
0.47
0.45
OH
10
9
8
7
6
5
4
3
2
1
0 ppm
2.01
3.01
2.01
2.03
0.99
2.00
2.00

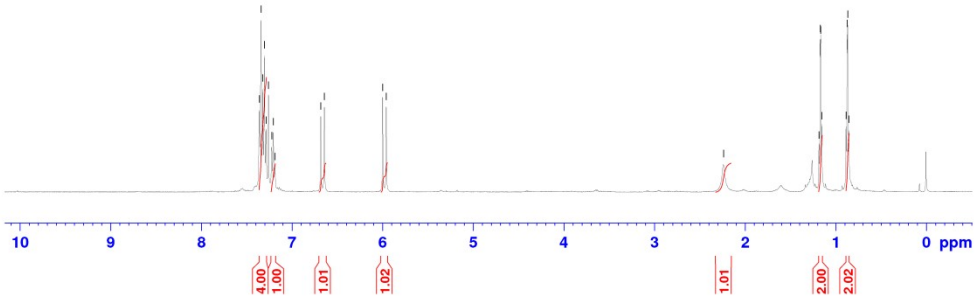
1aa

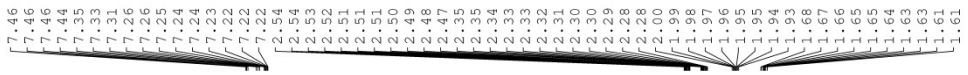

7.36
7.34
7.32
7.30
7.29
7.26
7.22
7.21
7.19
6.68
6.64
6.00
5.96

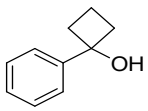

2.24
1.19
1.17
1.17
1.15
0.89
0.87
0.87
0.86


OH

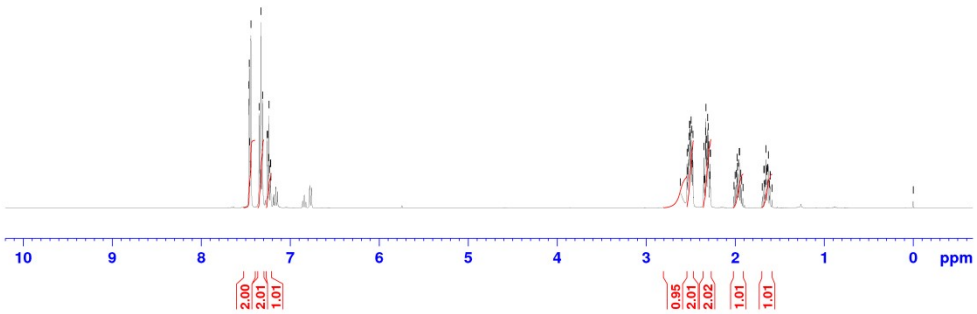
1ab


10
9
8
7
6
5
4
3
2
1
0 ppm
4.00
1.00
1.01
1.02
1.01
2.00
2.02

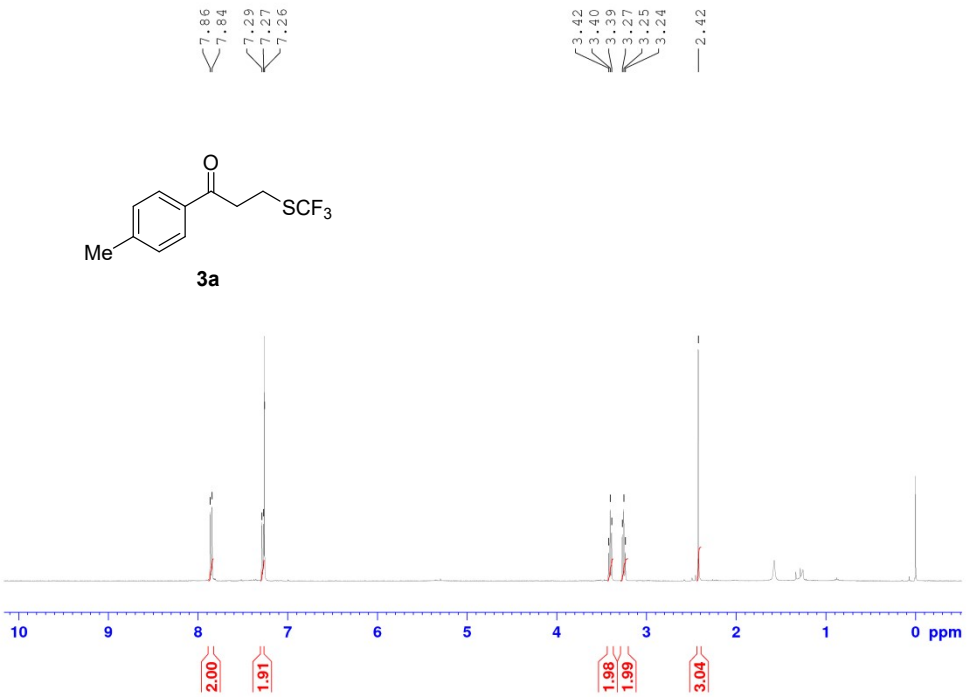

7.46
7.46
7.46
7.44
7.35
7.33
7.31
7.26
7.26
7.25
7.24
7.24
7.23
7.22
7.22
7.22
2.54
2.54
2.53
2.52
2.51
2.51
2.51
2.50
2.49
2.48
2.47
2.35
2.35
2.34
2.33
2.33
2.32
2.31
2.30
2.30
2.29
2.28
2.28
2.00
1.99
1.98
1.97
1.96
1.95
1.95
1.94
1.93
1.68
1.67
1.66
1.65
1.65
1.64
1.63
1.63
1.61
1.61

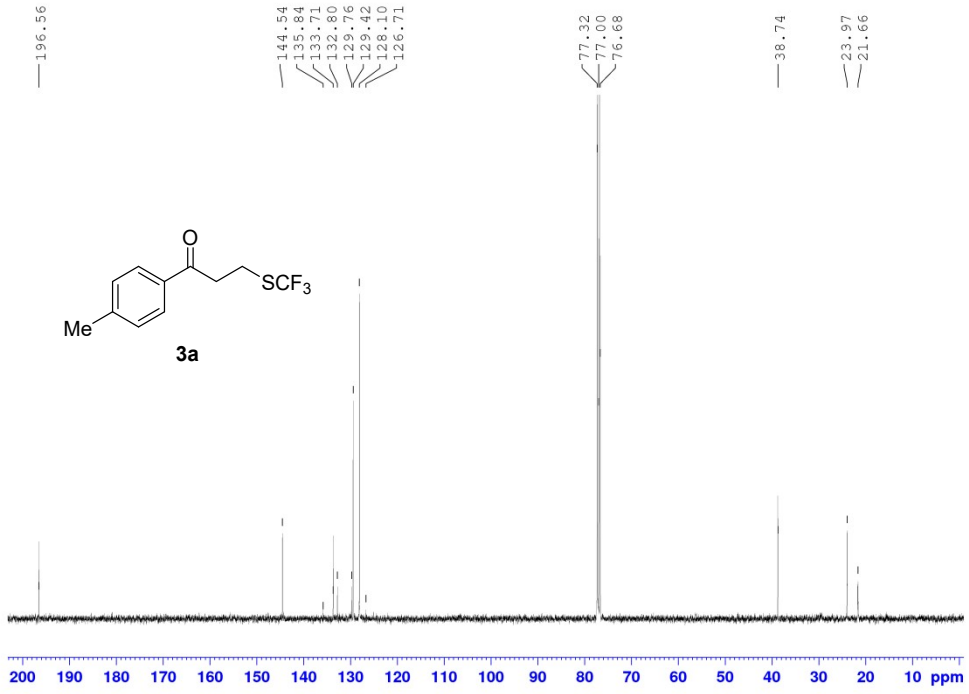

OH

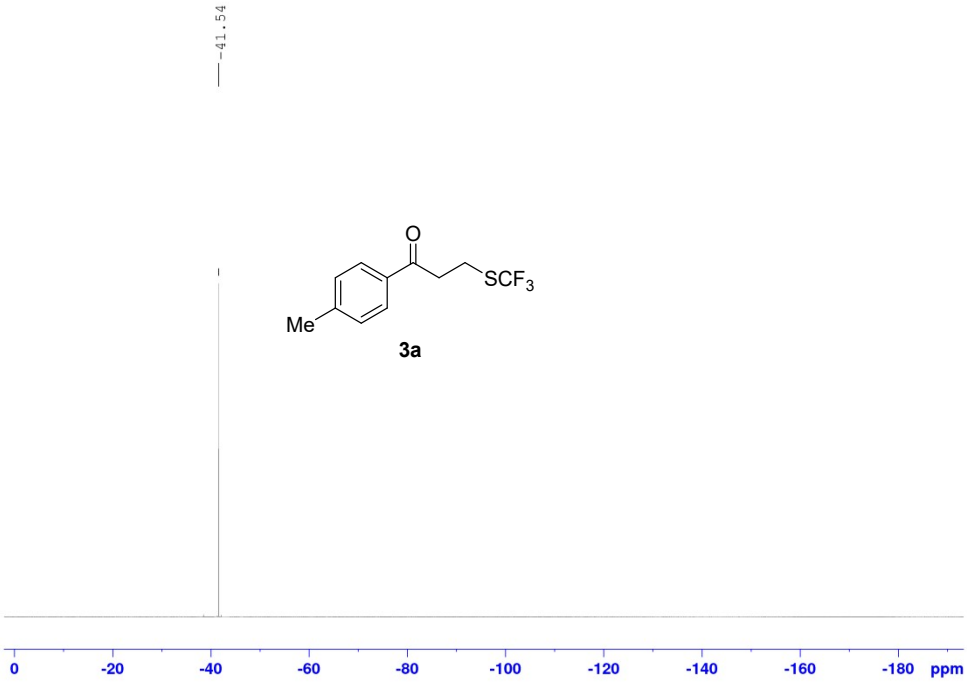
1ac


10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
2.01
1.01
0.95
2.01
2.02
1.01
1.01

5) Spectra for 3 and 4

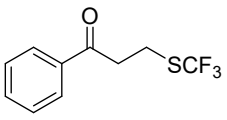




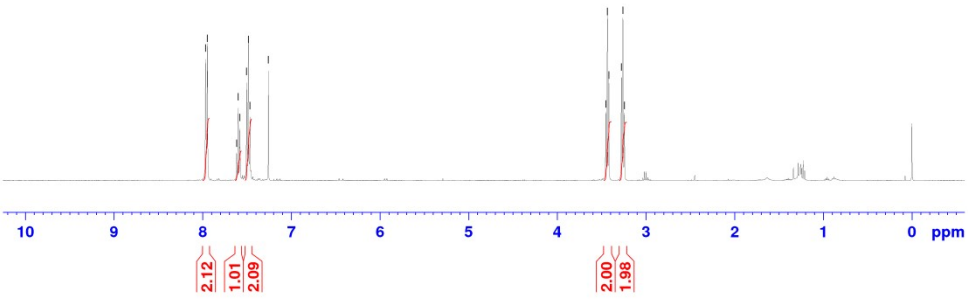

-41.54
O
SCF3
Me
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

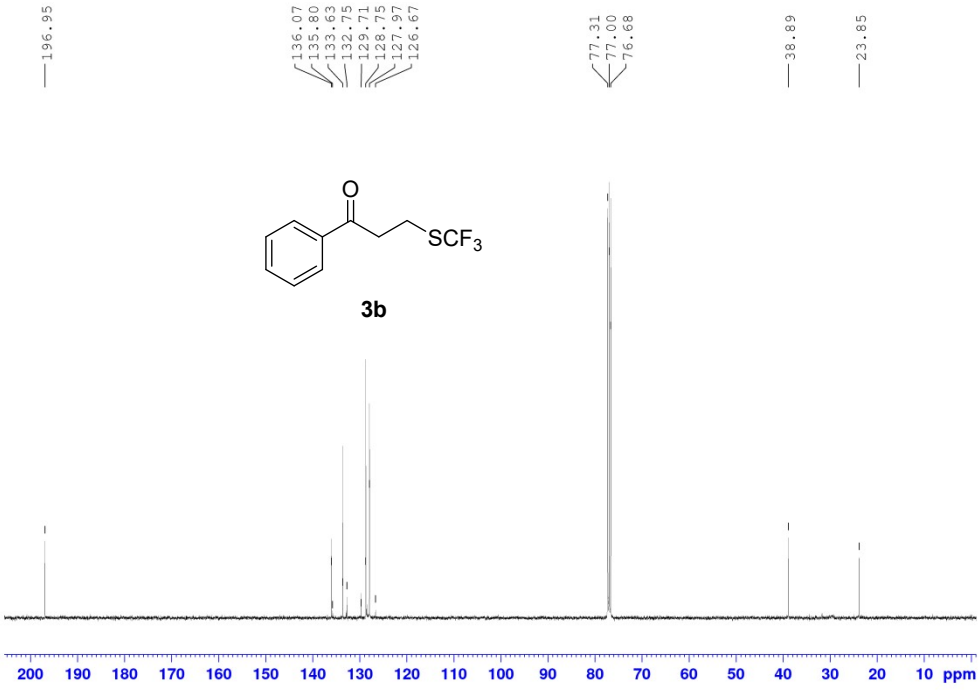
3a


7.97
7.95
7.62
7.60
7.58
7.51
7.49
7.47
7.26
3.45
3.44
3.42
3.28
3.26
3.24

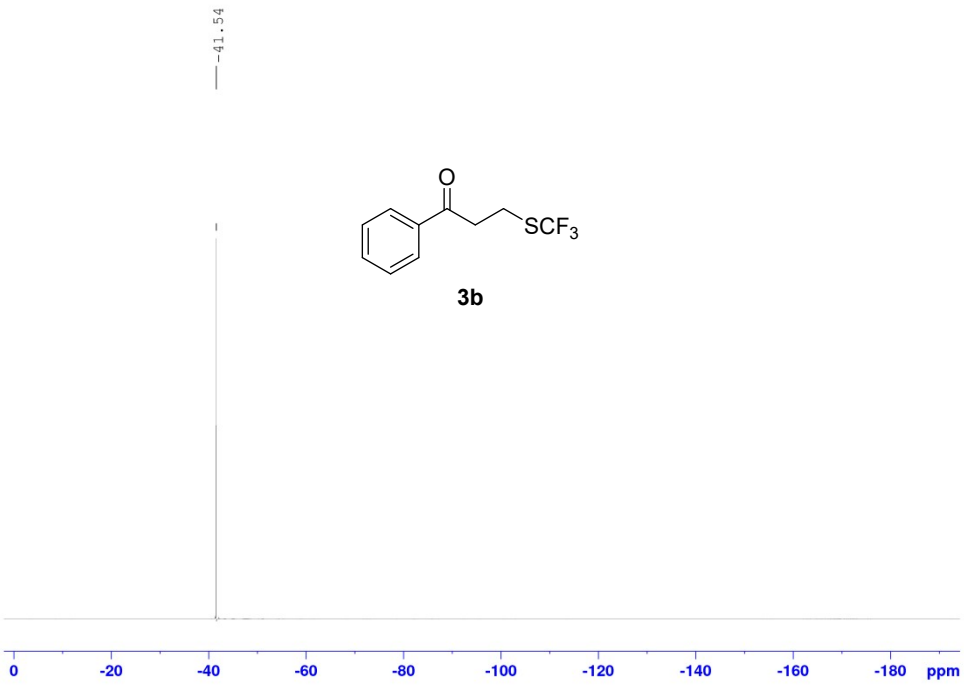

O
SCF3

3b

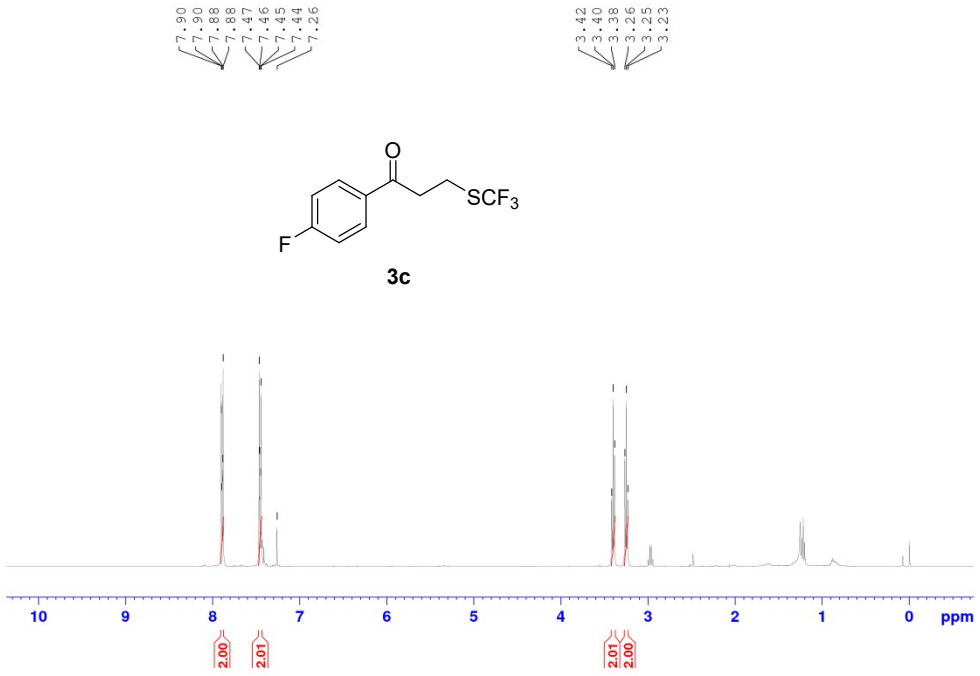

10
9
8
7
6
5
4
3
2
1
0
ppm
2.12
1.01
2.09
2.00
1.98

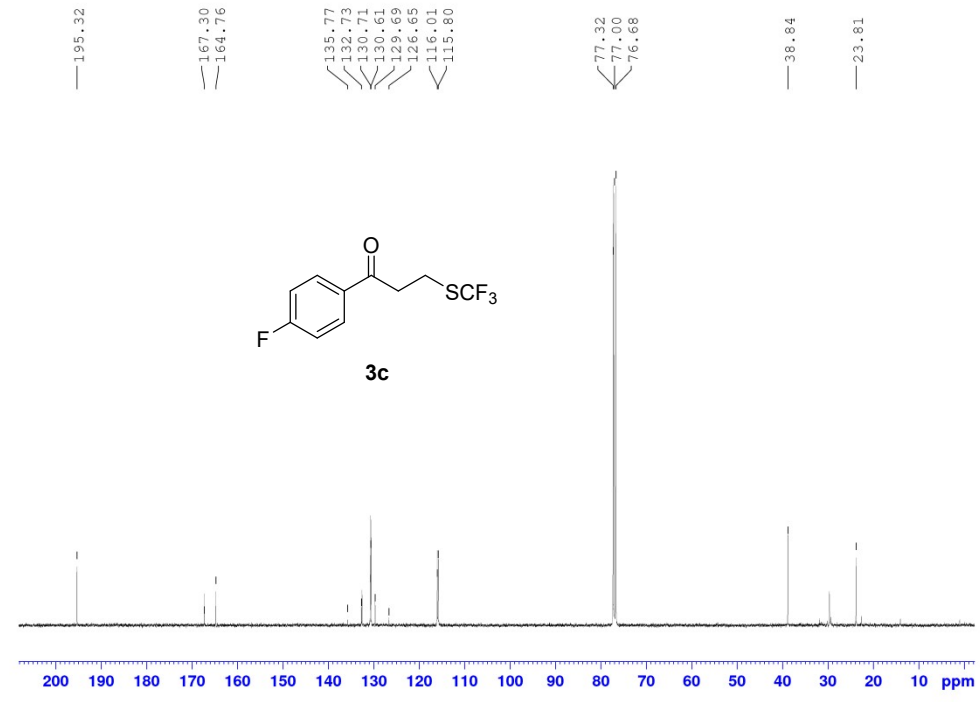

196.95
136.07
135.80
133.63
132.75
129.71
128.75
127.97
126.67
77.31
77.00
76.68
38.89
23.85
O
SCF3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

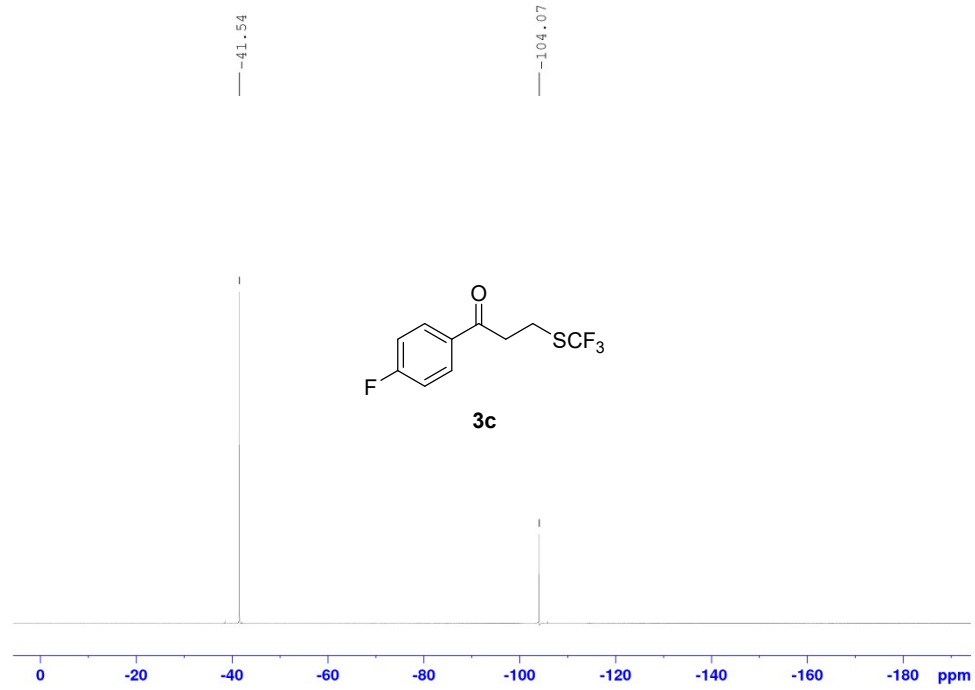
3b

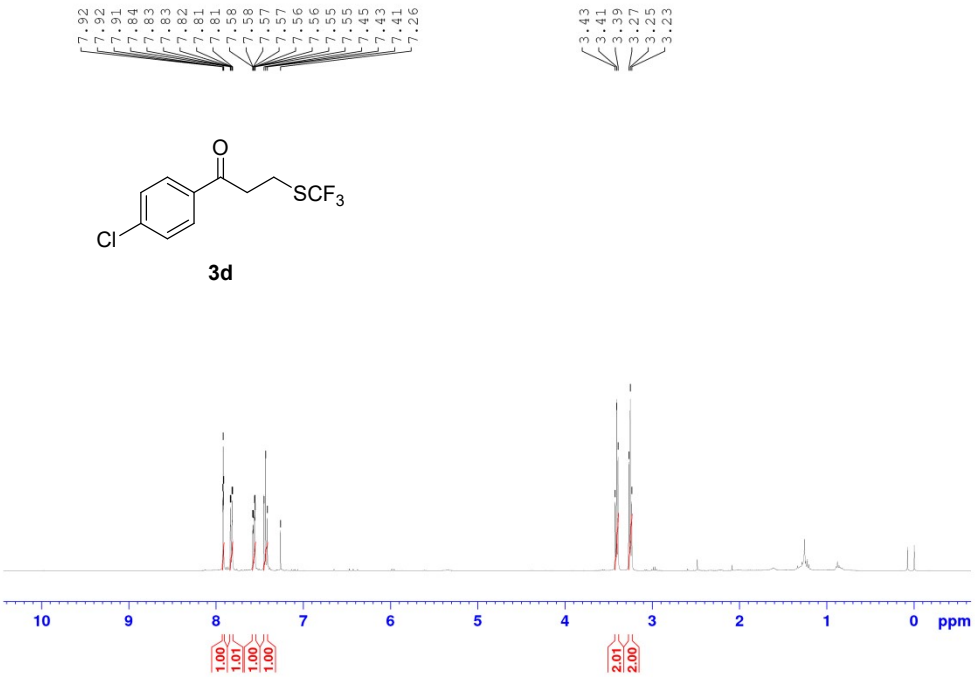

-41.54
O
SCF3
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

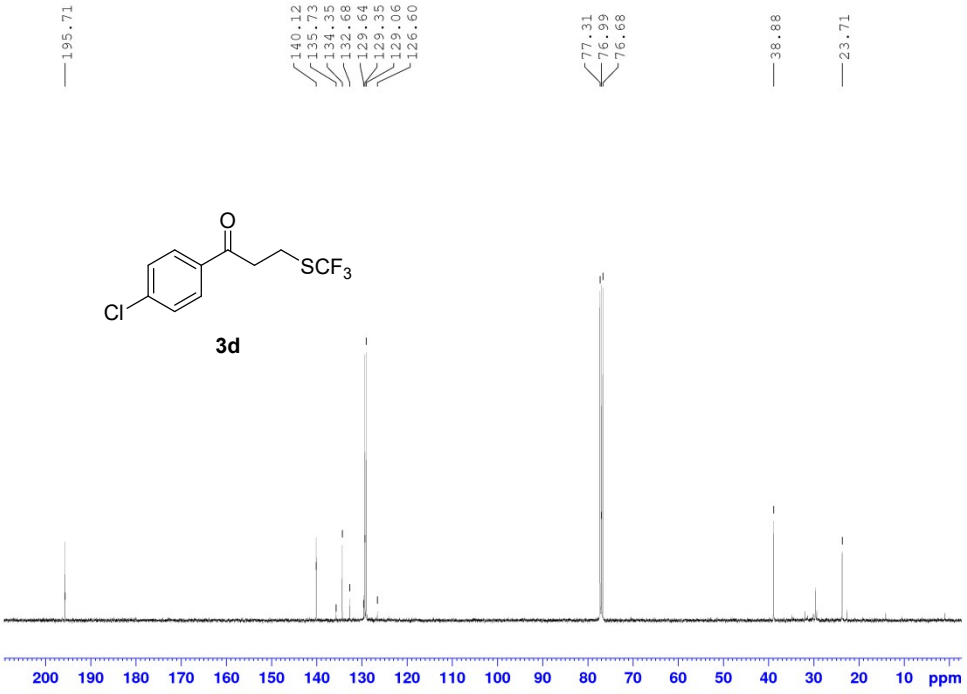
3b

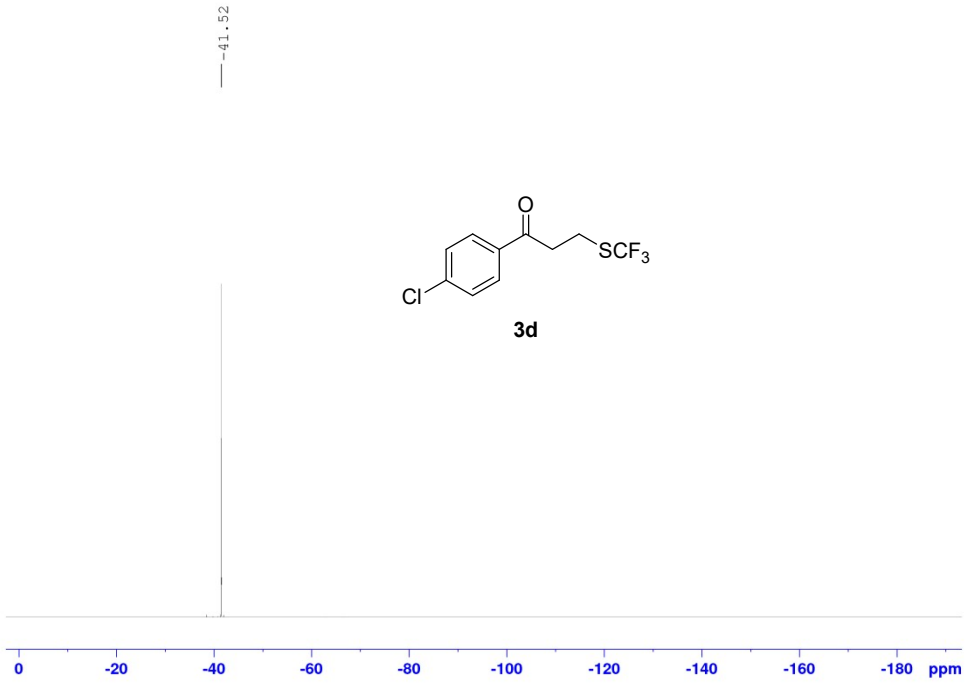

7.90
7.90
7.88
7.88
7.47
7.46
7.45
7.44
7.26
3.42
3.40
3.38
3.26
3.25
3.23
O
SCF3
F
3c
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.01
2.01
2.00

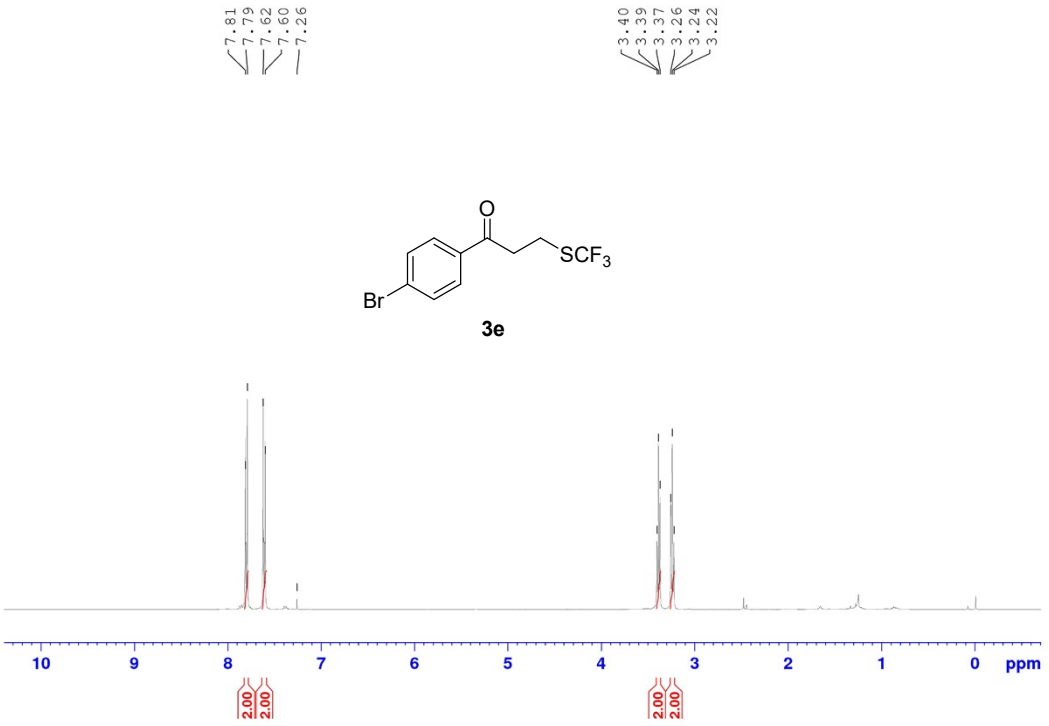

195.32
167.30
164.76
135.77
132.73
130.71
130.61
129.69
126.65
116.01
115.80
77.32
77.00
76.68
38.84
23.81
O
SCF3
F
3c
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

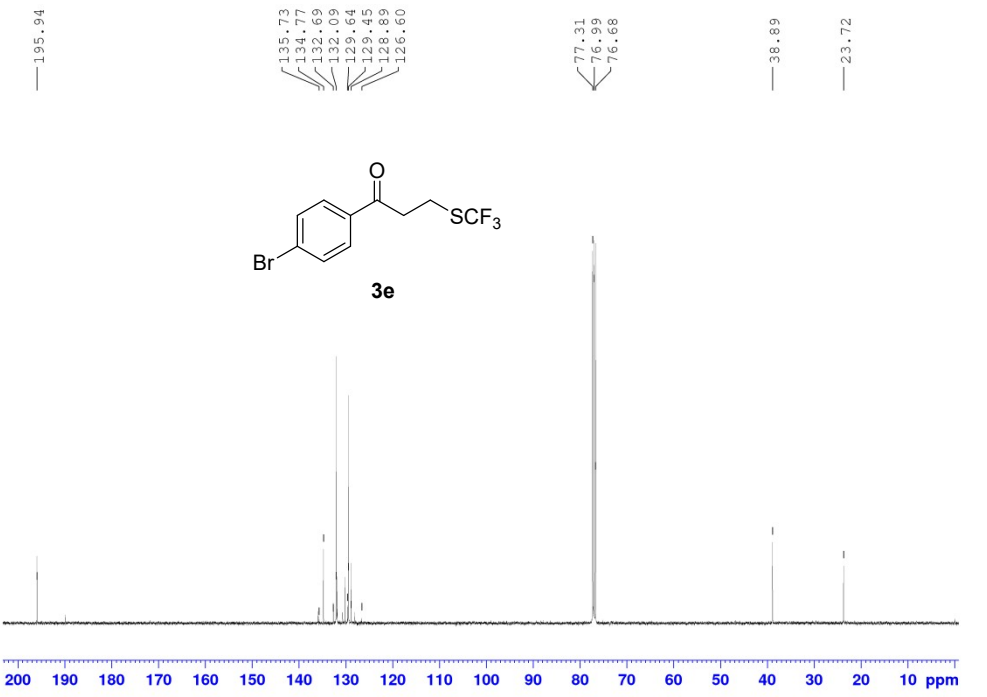

-41.54
-104.07
O
SCF3
F
3c
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

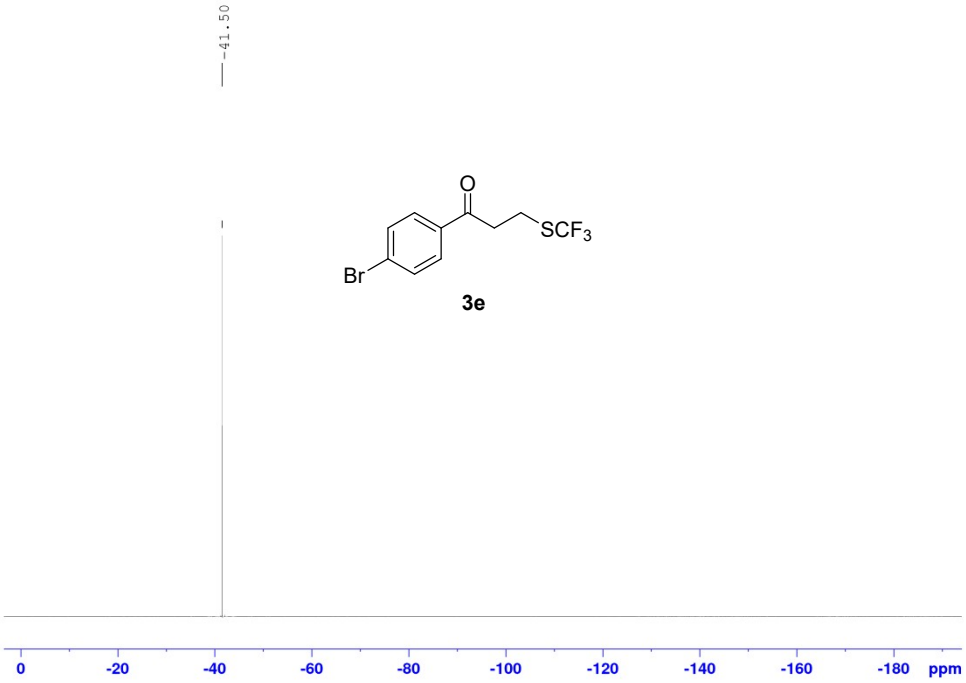

7.92
7.92
7.91
7.84
7.83
7.83
7.82
7.81
7.81
7.58
7.58
7.57
7.57
7.56
7.56
7.55
7.55
7.45
7.43
7.41
7.26
3.43
3.41
3.39
3.27
3.25
3.23
O
SCF3
Cl
3d
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.00
1.00
2.01
2.00


195.71
140.12
135.73
134.35
132.68
129.64
129.35
129.06
126.60
77.31
76.99
76.68
38.88
23.71
O
SCF3
Cl
3d
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

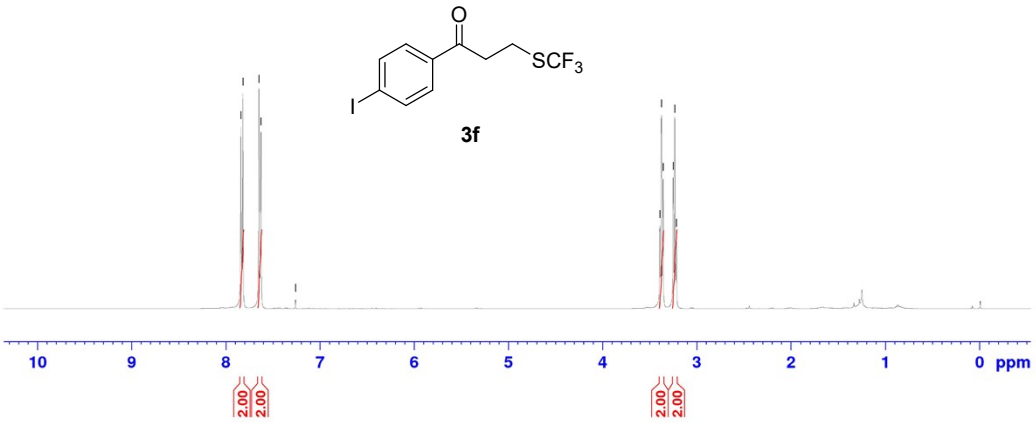

-41.52
O
SCF3
Cl
3d
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

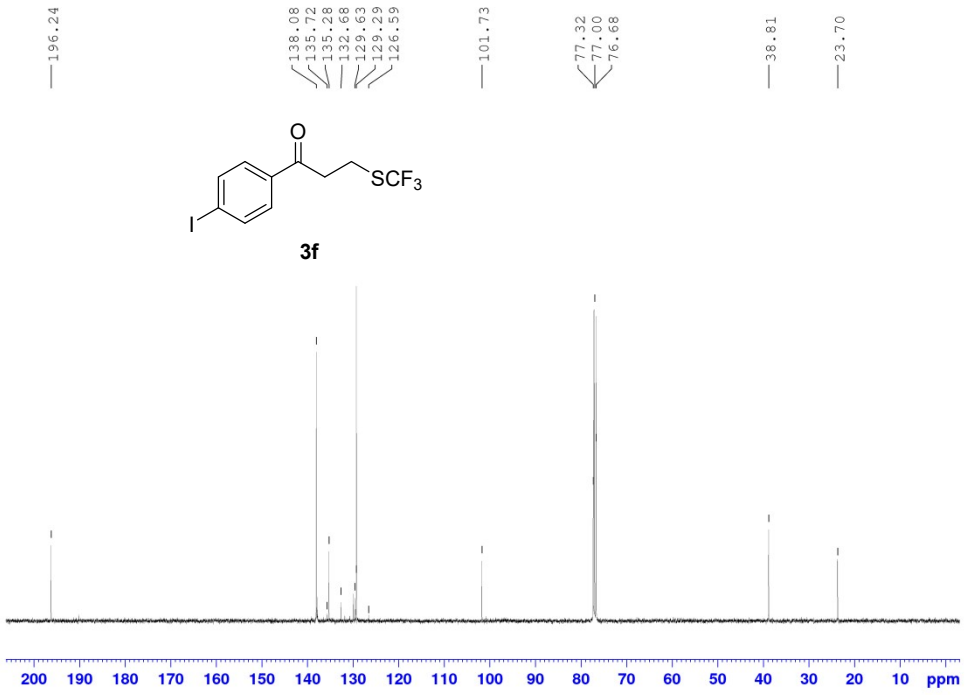

7.81
7.79
7.62
7.60
7.26
3.40
3.39
3.37
3.26
3.24
3.22
O
SCF3
Br
3e
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.00
2.00
2.00


195.94
135.73
134.77
132.69
132.09
129.64
129.45
128.89
126.60
77.31
76.99
76.68
38.89
23.72
O
SCF3
Br
3e
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

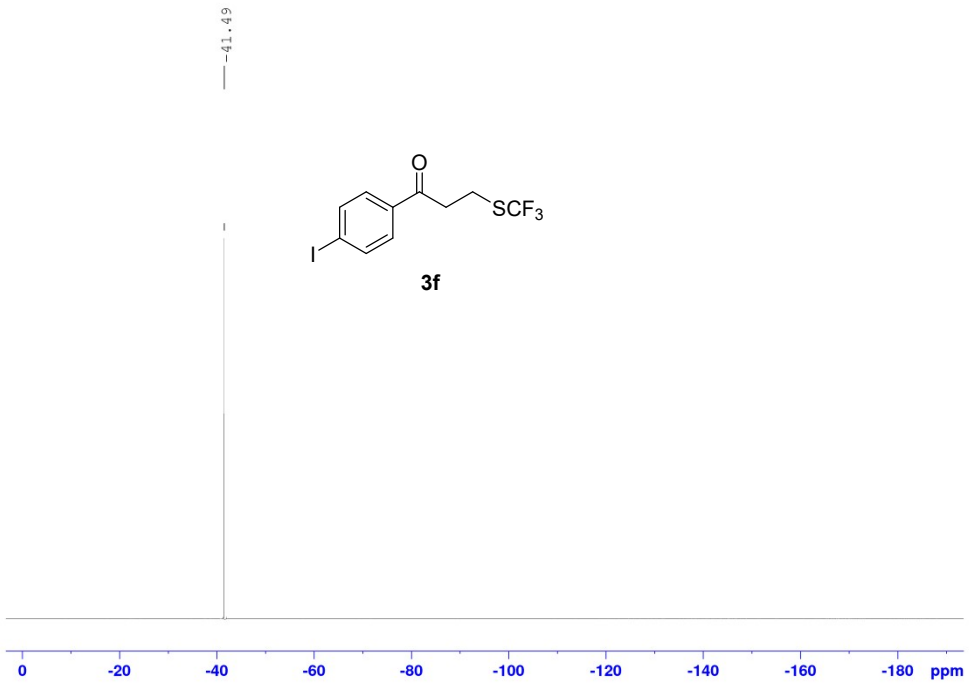

-41.50
O
SCF3
Br
3e
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm


7.84
7.82
7.65
7.63
7.26
3.39
3.37
3.36
3.25
3.23
3.22

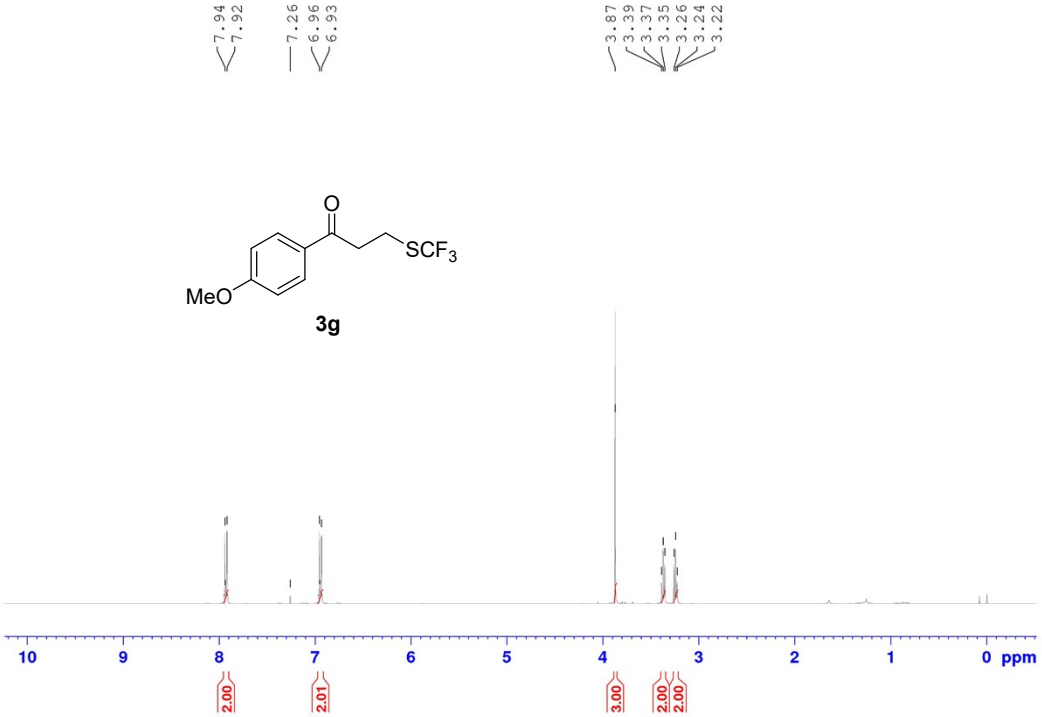

O
SCF3
I
3f
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.00
2.00
2.00

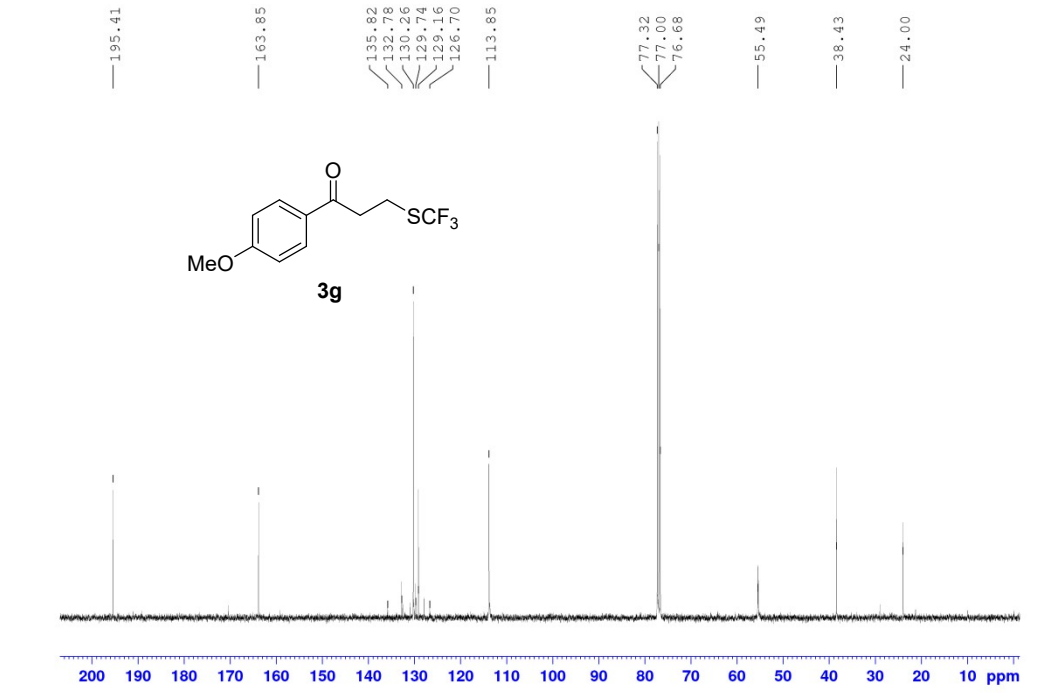

196.24
138.08
135.72
135.28
132.68
129.63
129.29
126.59
101.73
77.32
77.00
76.68
38.81
23.70
O
SCF3
I
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

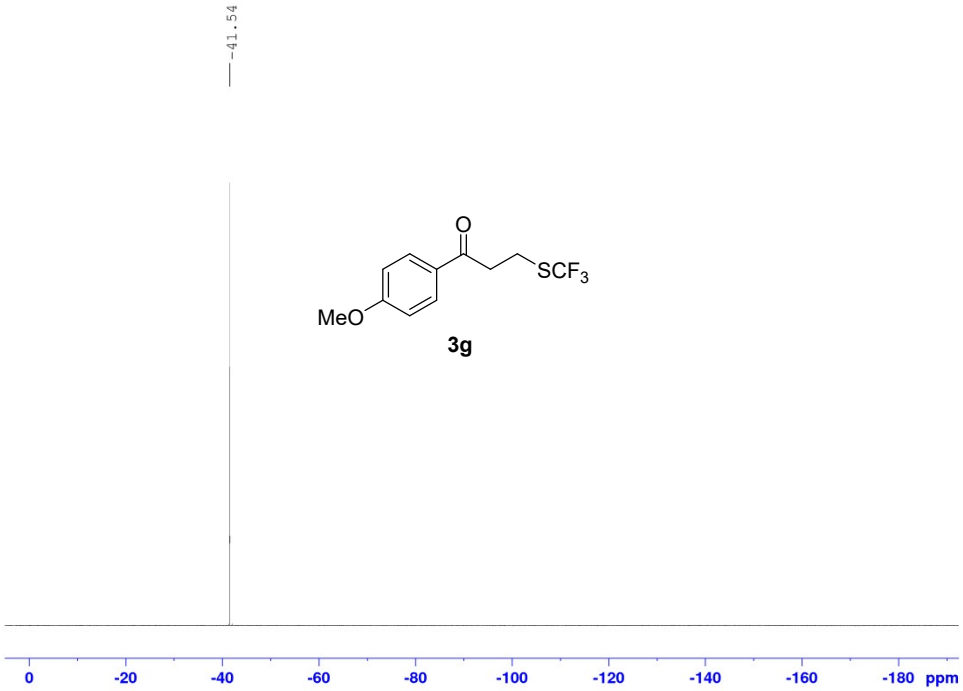
3f

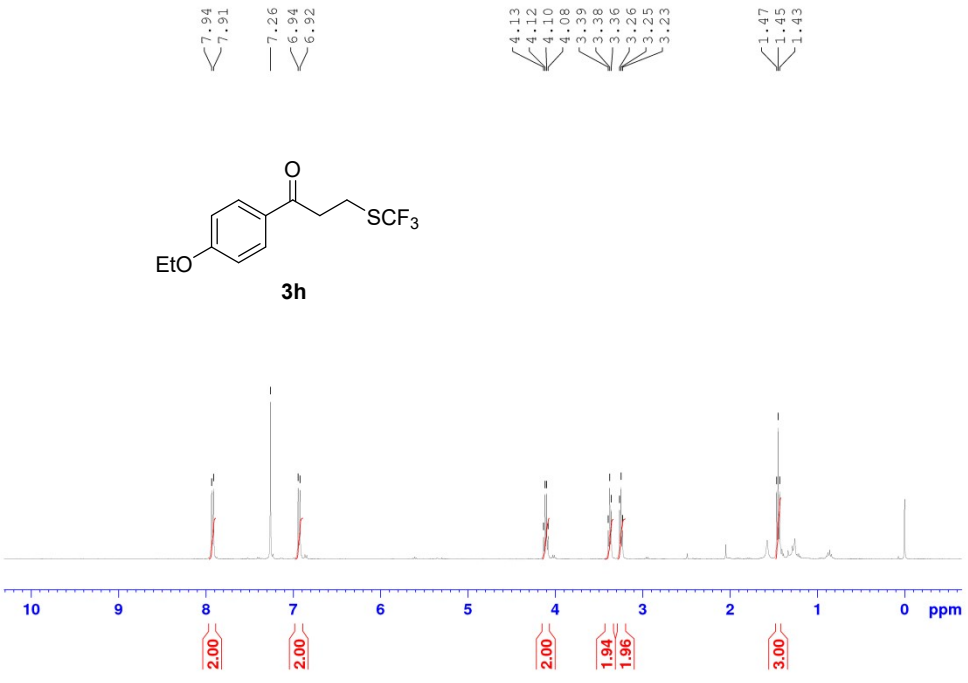

41.49
O
SCF3
I
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

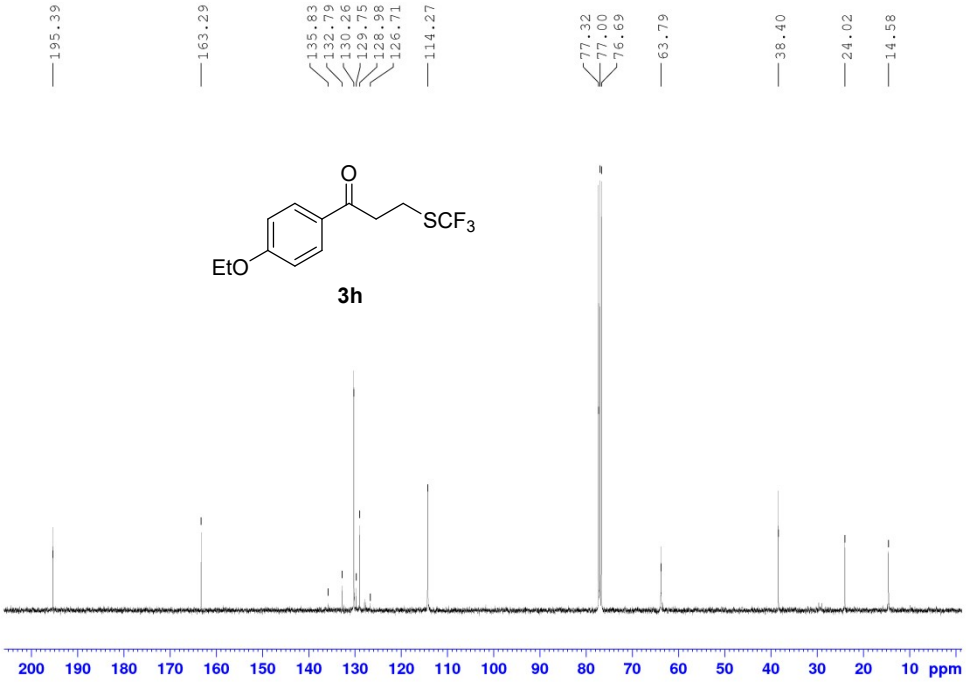
3f

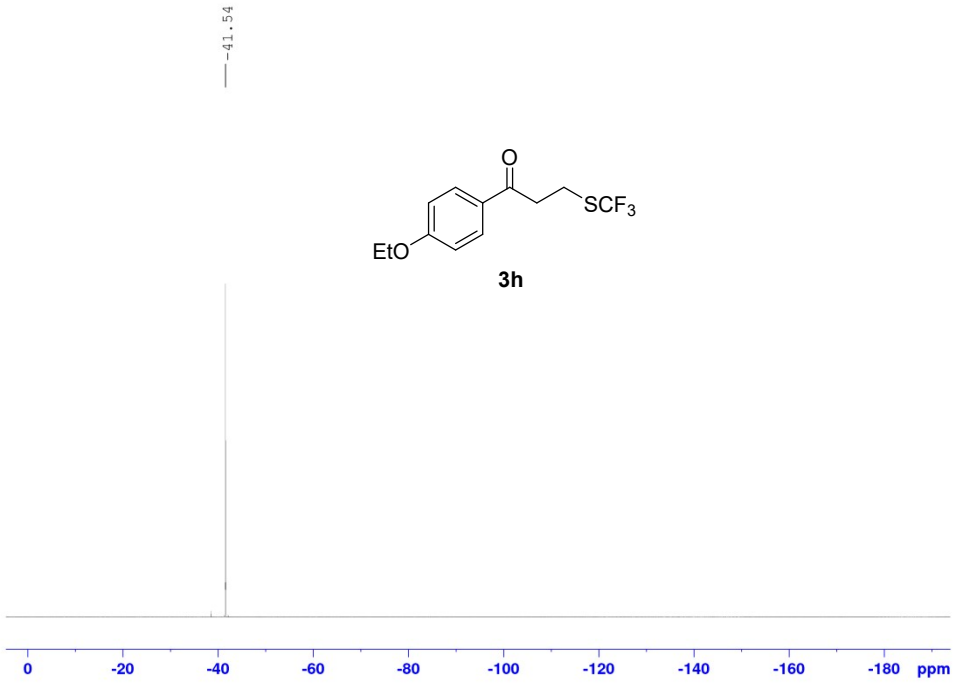

7.94
7.92
7.26
6.96
6.93
3.87
3.39
3.37
3.35
3.26
3.24
3.22
O
SCF3
MeO
3g
10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
2.01
3.00
2.00
2.00

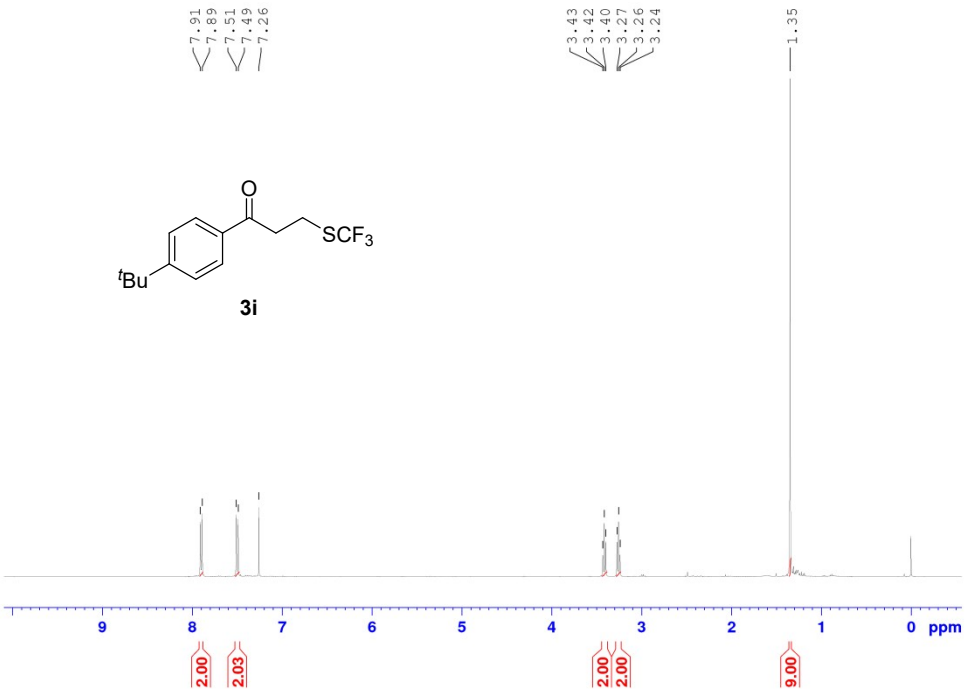

195.41
163.85
135.82
132.78
130.26
129.74
129.16
126.70
113.85
77.32
77.00
76.68
55.49
38.43
24.00
O
SCF3
MeO
3g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm


-41.54
O
SCF3
MeO
3g
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

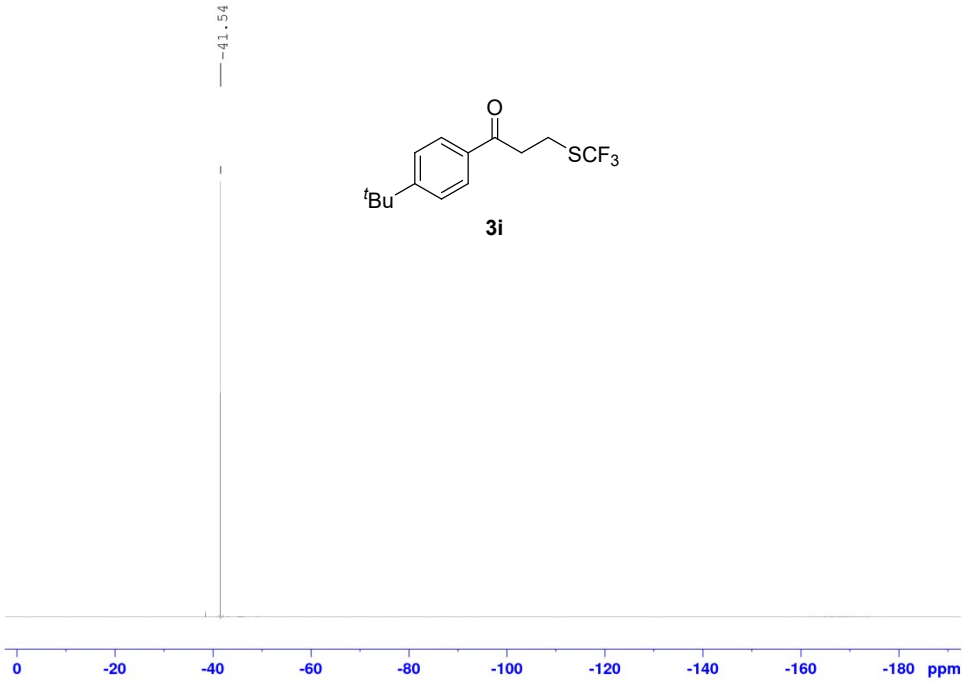

7.94
7.91
7.26
6.94
6.92
4.13
4.12
4.10
4.08
3.39
3.38
3.36
3.26
3.25
3.23
1.47
1.45
1.43
O
SCF3
EtO
3h
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.00
2.00
1.94
1.96
3.00

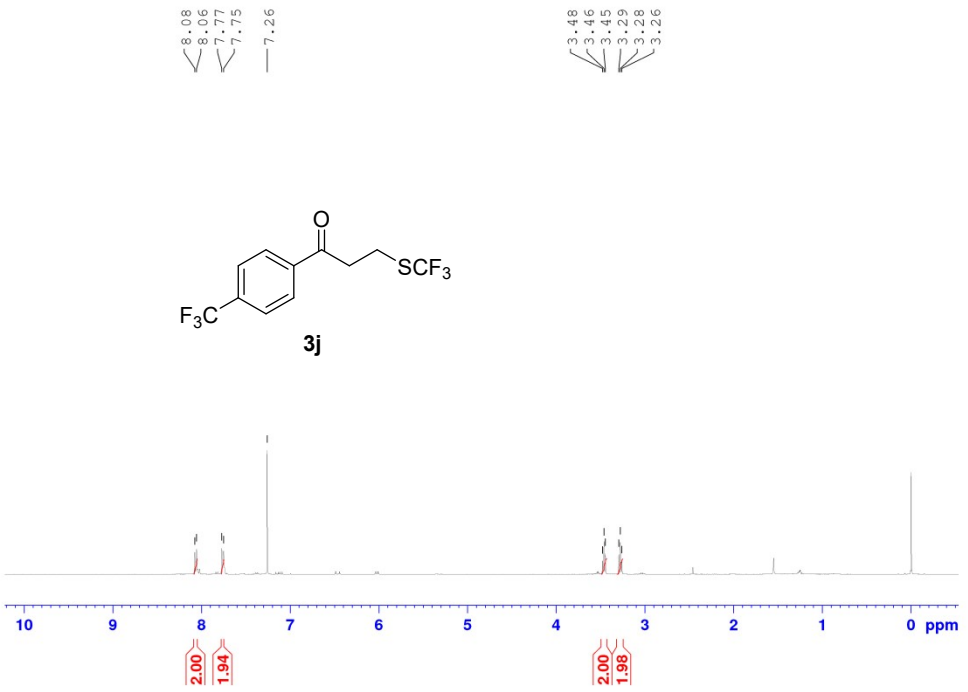

195.39
163.29
135.83
132.79
130.26
129.75
128.98
126.71
114.27
77.32
77.00
76.69
63.79
38.40
24.02
14.58
O
SCF3
EtO
3h
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

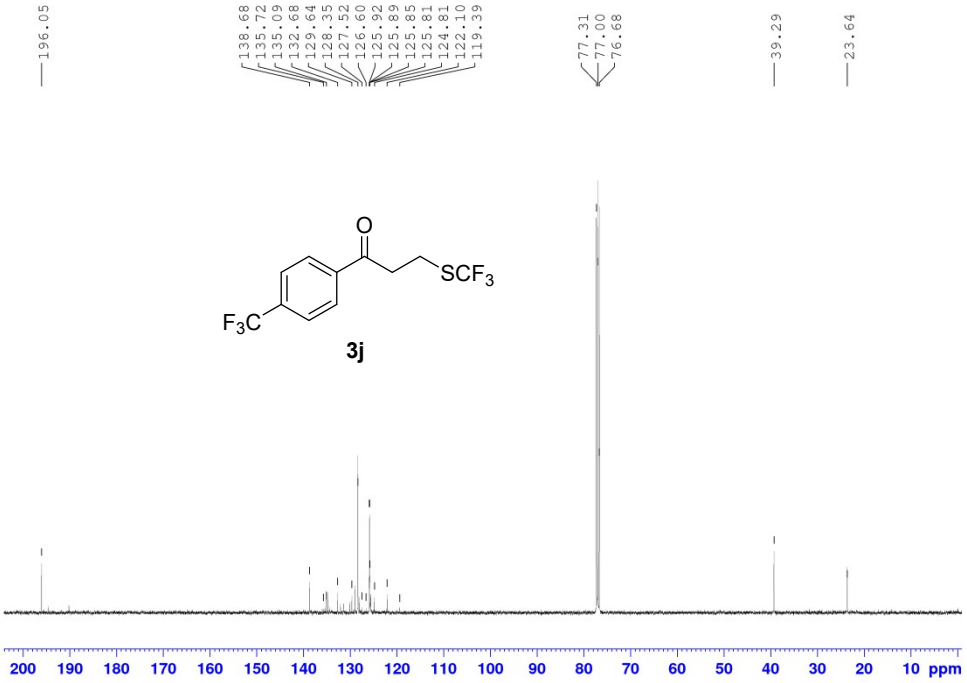

-41.54
O
SCF3
EtO
3h
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

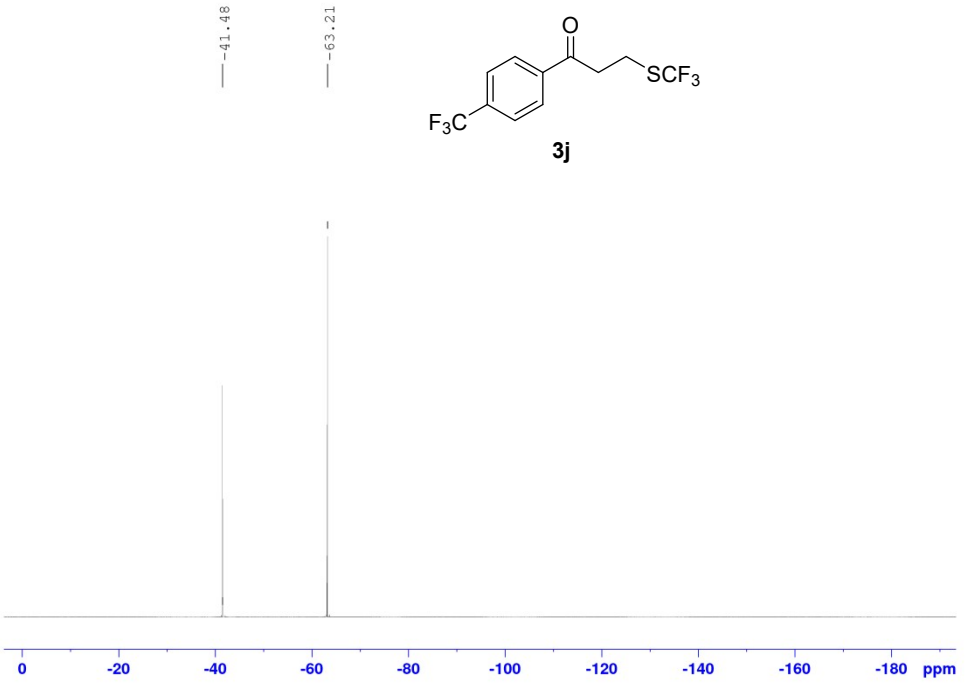

7.91
7.89
7.51
7.49
7.26
3.43
3.42
3.40
3.27
3.26
3.24
1.35
O
SCF3
tBu
3i
9
8
7
6
5
4
3
2
1
0 ppm
2.00
2.03
2.00
2.00
9.00

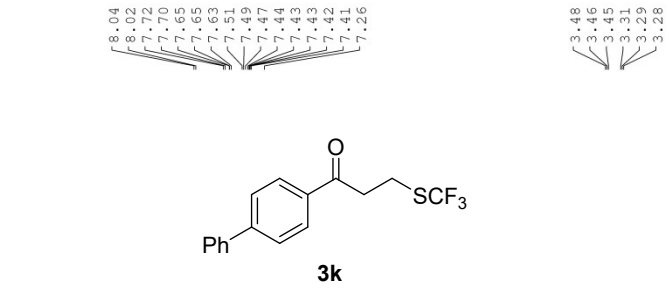

196.56
157.46
135.83
133.55
132.79
129.75
127.96
126.70
125.68
77.32
77.00
76.68
38.74
35.13
31.01
23.93
O
SCF3
tBu
3i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm


-41.54
O
SCF3
tBu
3i
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

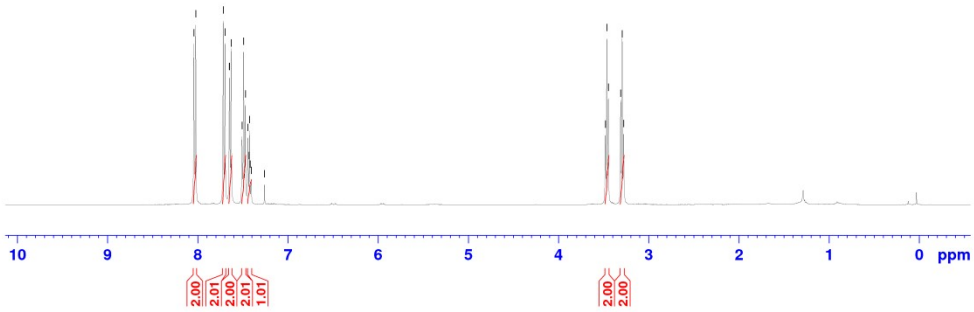

8.08
8.06
7.77
7.75
7.26
3.48
3.46
3.45
3.29
3.28
3.26
O
SCF3
F3C
3j
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
1.94
2.00
1.98

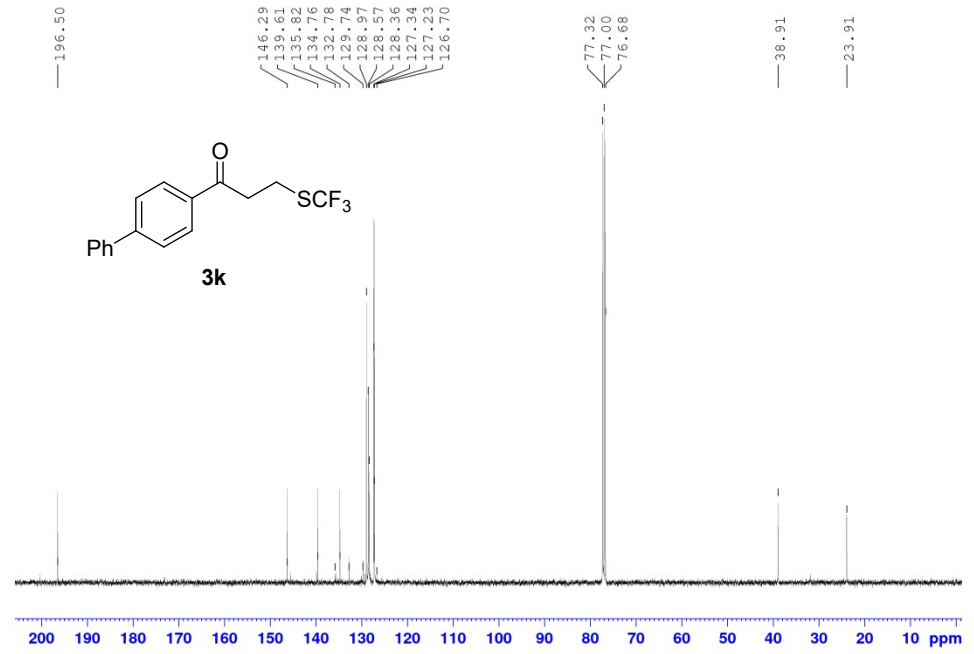

196.05
138.68
135.72
135.09
132.68
129.64
128.35
127.52
126.60
125.92
125.89
125.85
125.81
124.81
122.10
119.39
77.31
77.00
76.68
39.29
23.64
O
SCF3
F3C
3j
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


-41.48
-63.21
O
SCF3
F3C
3j
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

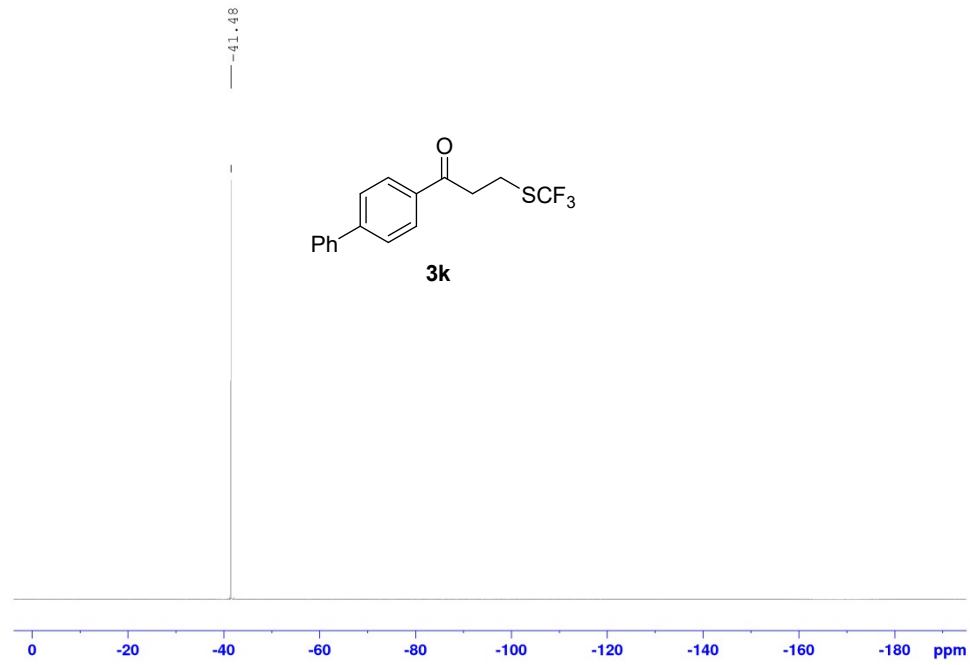

8.04
8.02
7.72
7.70
7.65
7.63
7.51
7.49
7.47
7.44
7.43
7.42
7.41
7.26
3.48
3.46
3.45
3.31
3.29
3.28
O
SCF3
Ph

3k

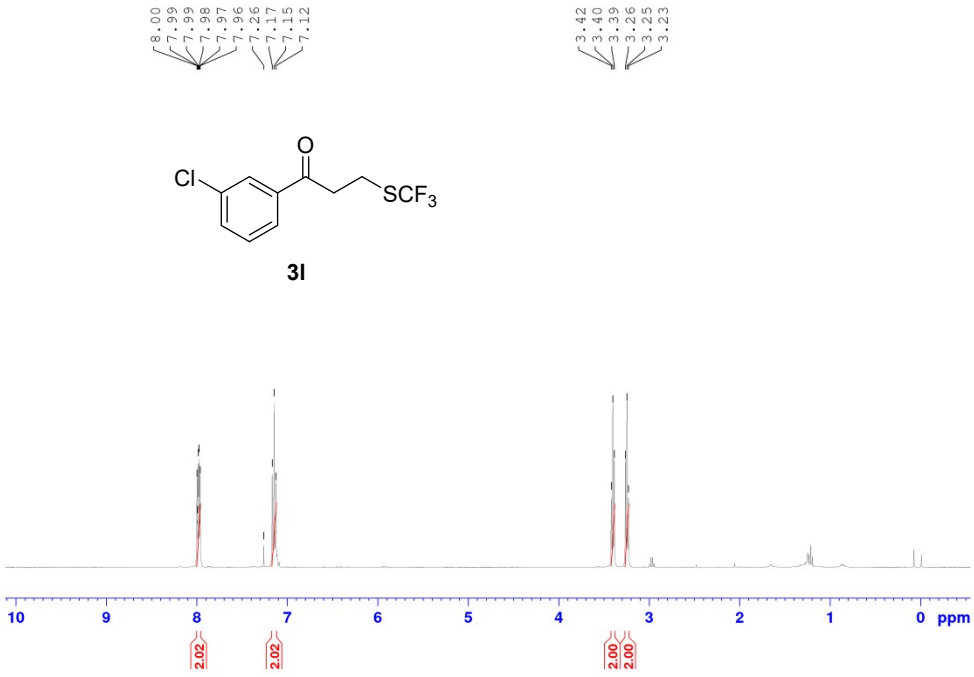

10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
2.01
2.00
2.01
1.01
2.00
2.00


196.50
146.29
139.61
135.82
134.76
132.78
129.74
128.97
128.57
128.36
127.34
127.23
126.70
77.32
77.00
76.68
38.91
23.91
O
SCF3
Ph
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

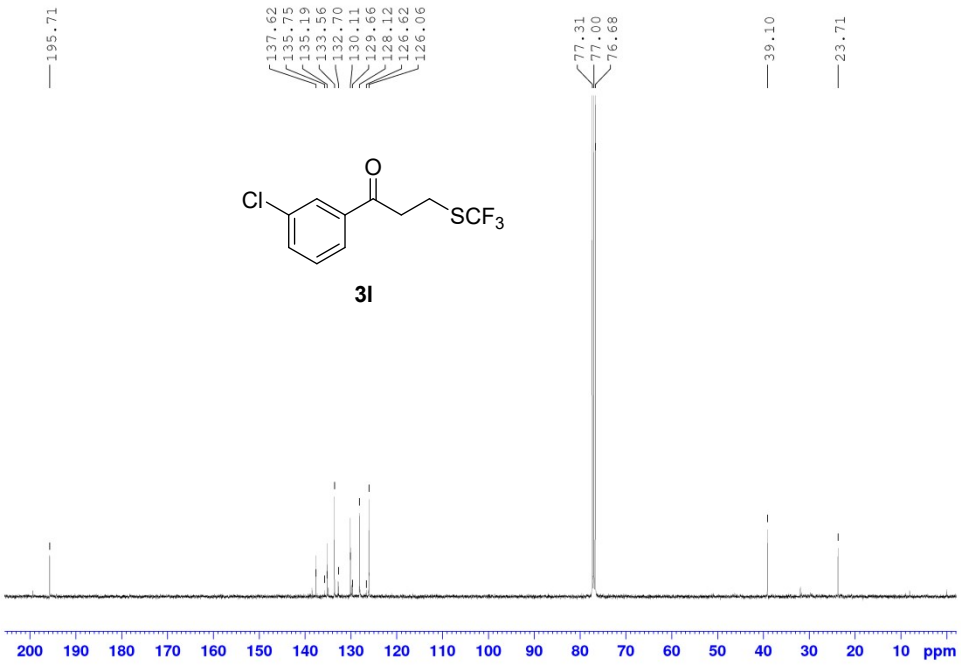
3k


-41.48
O
SCF3
Ph
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

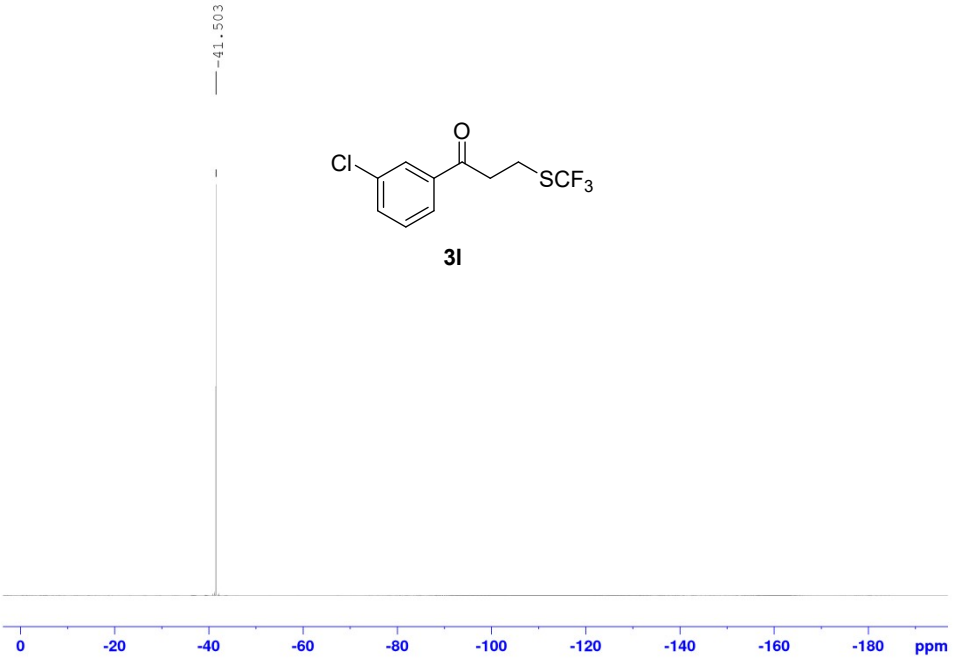
3k


8.00
7.99
7.99
7.98
7.97
7.96
7.26
7.17
7.15
7.12
3.42
3.40
3.39
3.26
3.25
3.23
O
Cl
SCF3
10
9
8
7
6
5
4
3
2
1
0
ppm
2.02
2.02
2.00
2.00

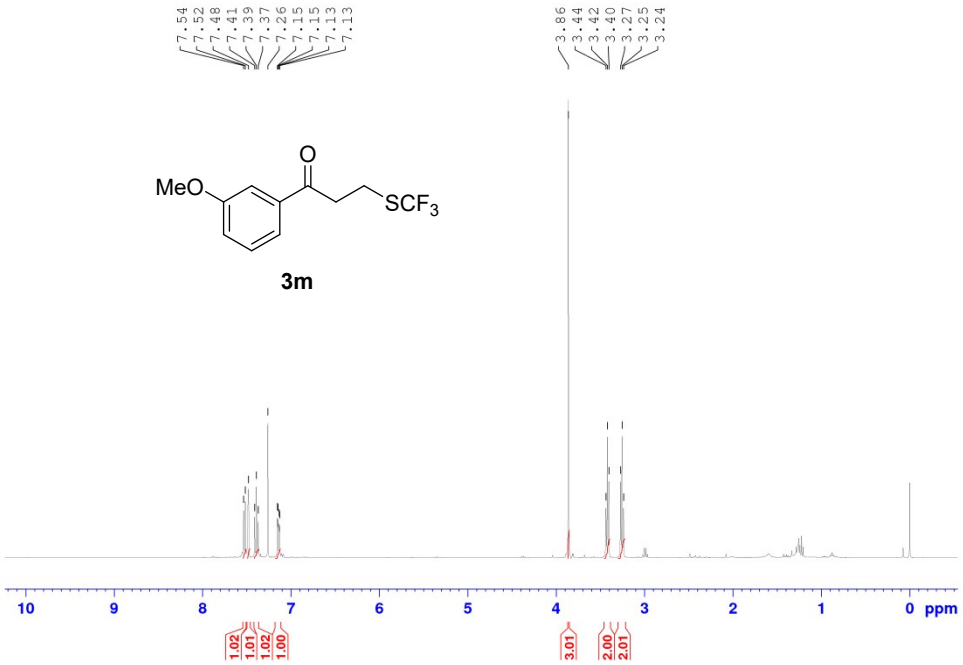
3l

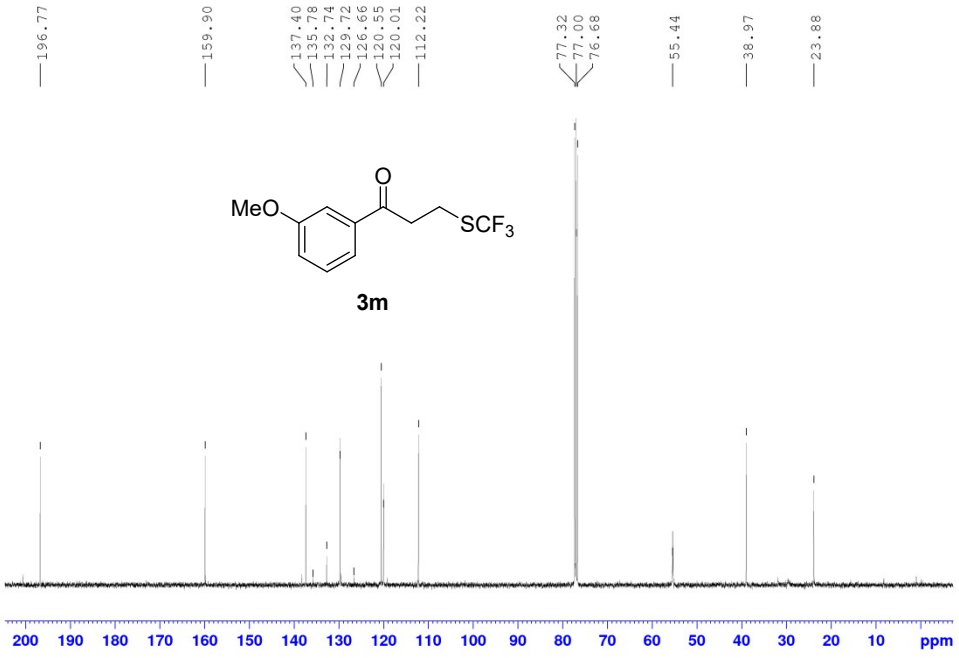

195.71
137.62
135.75
135.19
133.56
132.70
130.11
129.66
128.12
126.62
126.06
77.31
77.00
76.68
39.10
23.71
O
Cl
SCF3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

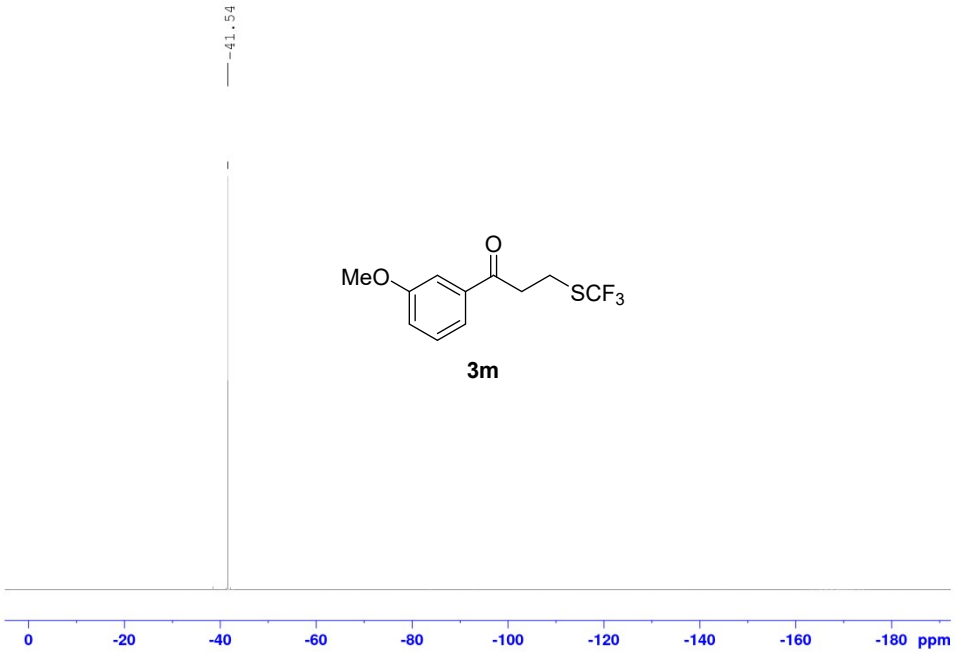
3l

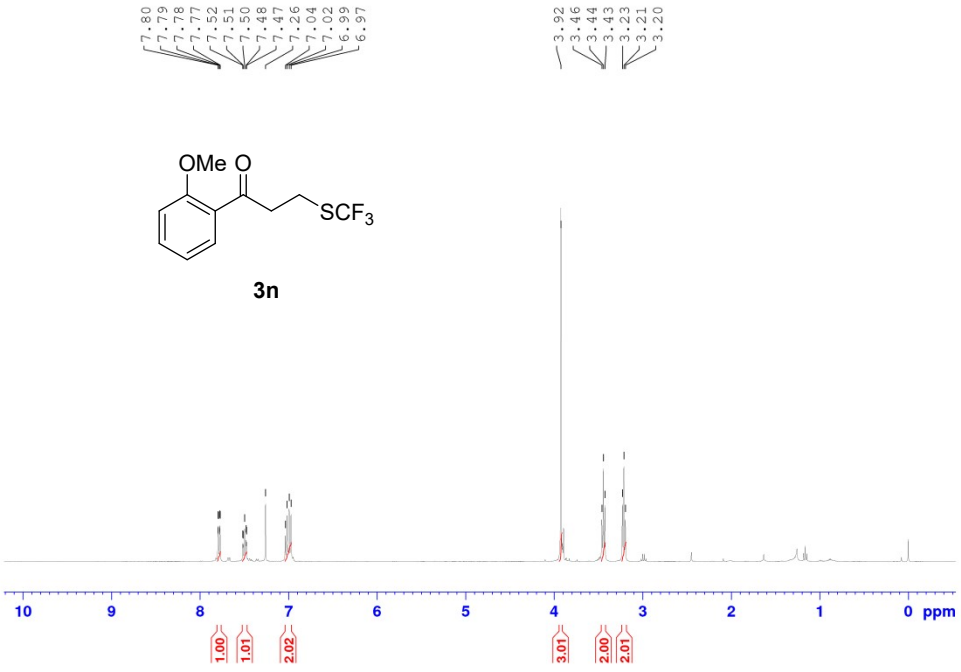

-41.503
O
Cl
SCF3
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

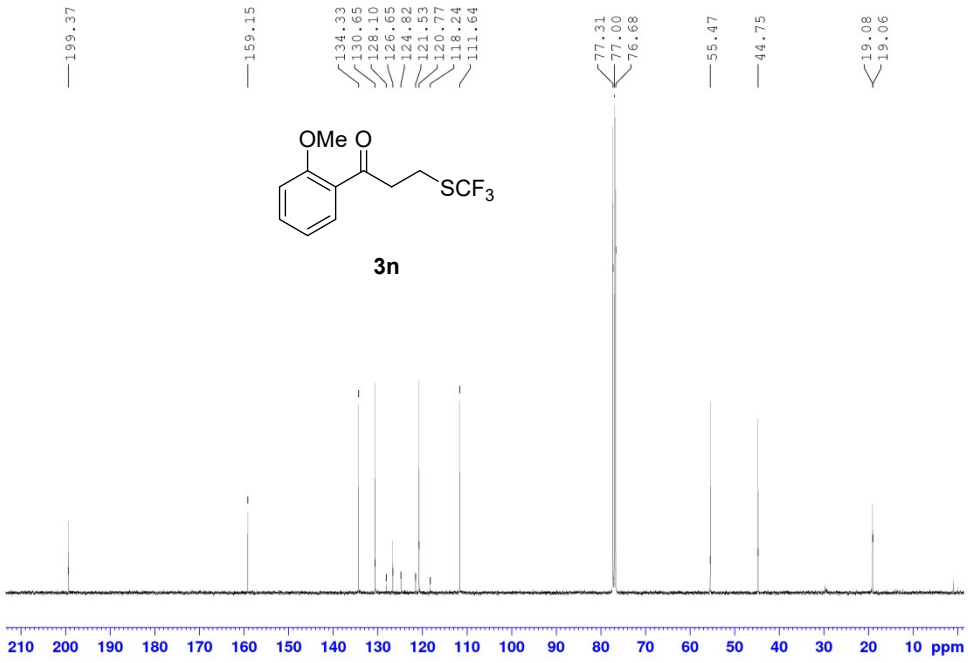
3l

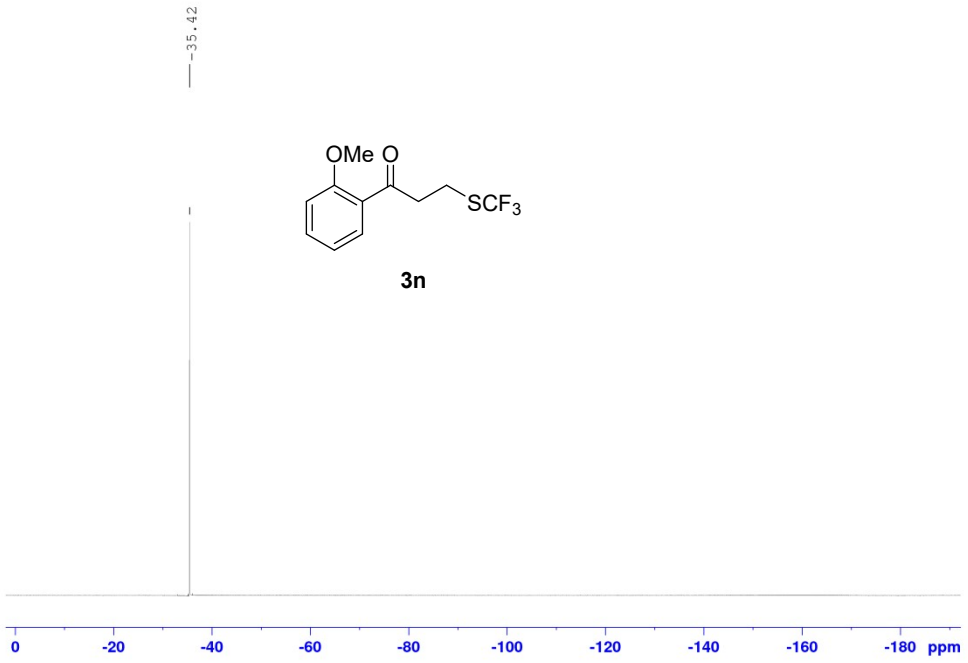

7.54
7.52
7.48
7.41
7.39
7.37
7.26
7.15
7.15
7.13
7.13
3.86
3.44
3.42
3.40
3.27
3.25
3.24
MeO
O
SCF3
3m
10
9
8
7
6
5
4
3
2
1
0 ppm
1.02
1.01
1.02
1.00
3.01
2.00
2.01

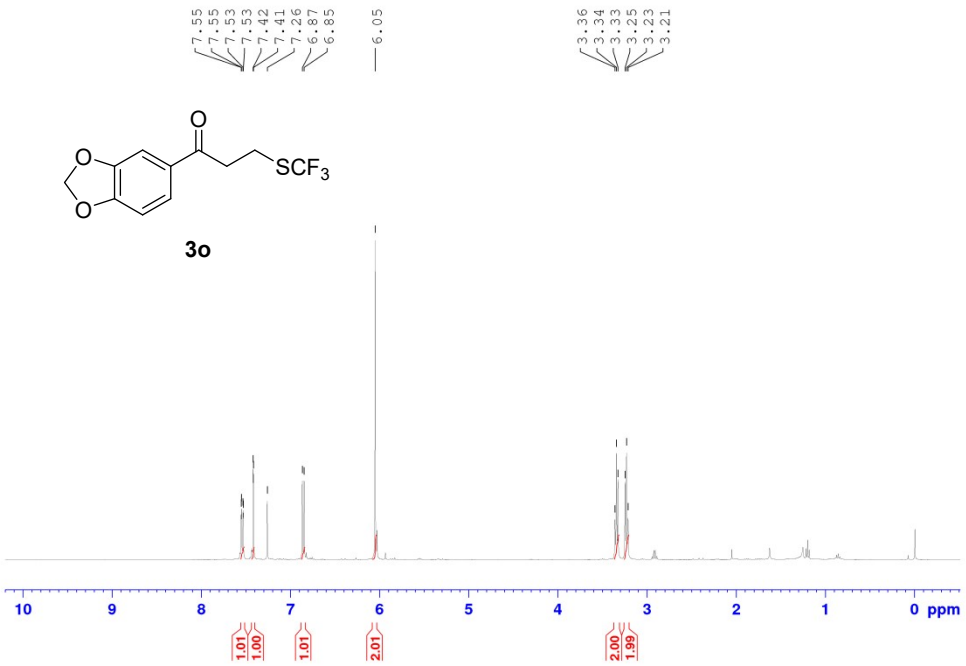

196.77
159.90
137.40
135.78
132.74
129.72
126.66
120.55
120.01
112.22
77.32
77.00
76.68
55.44
38.97
23.88
MeO
O
SCF3
3m
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-41.54
MeO
O
SCF3
3m
0
-20
-40
-60
-80
-100
-120
-140
-160
-180 ppm

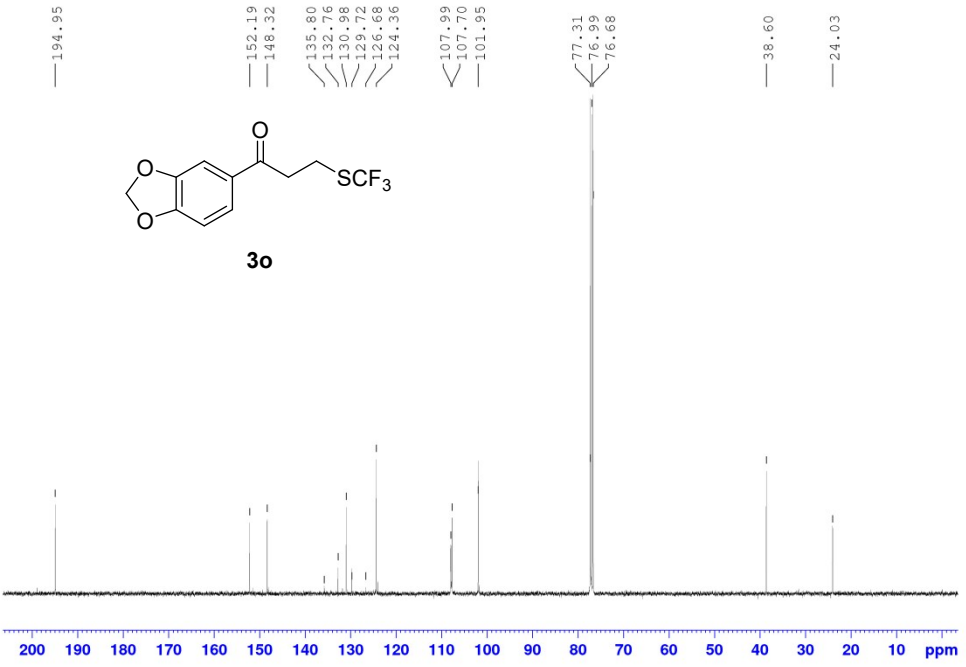

7.80
7.79
7.78
7.77
7.52
7.51
7.50
7.48
7.47
7.26
7.04
7.02
6.99
6.97
3.92
3.46
3.44
3.43
3.23
3.21
3.20
OMe O
SCF3
3n
10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.01
2.02
3.01
2.00
2.01


199.37
159.15
134.33
130.65
128.10
126.65
124.82
121.53
120.77
118.24
111.64
77.31
77.00
76.68
55.47
44.75
19.08
19.06
OMe O
SCF3
3n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

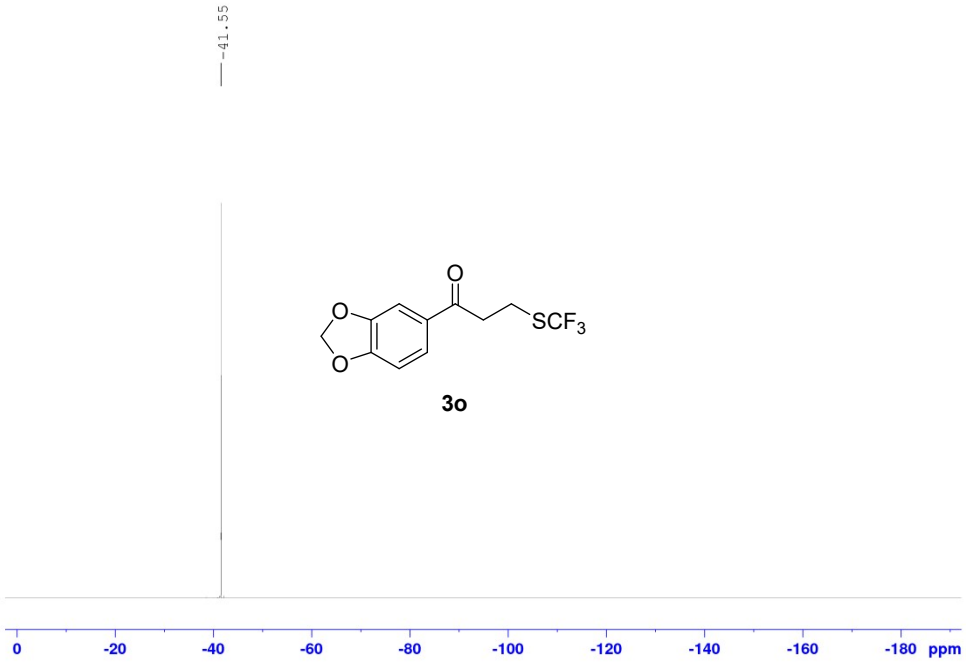

-35.42
OMe O
SCF3
3n
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm


7.55
7.55
7.53
7.53
7.42
7.41
7.26
6.87
6.85
6.05
3.36
3.34
3.33
3.25
3.23
3.21
O
O
O
SCF3
10
9
8
7
6
5
4
3
2
1
0 ppm
1.01
1.00
1.01
2.01
2.00
1.99

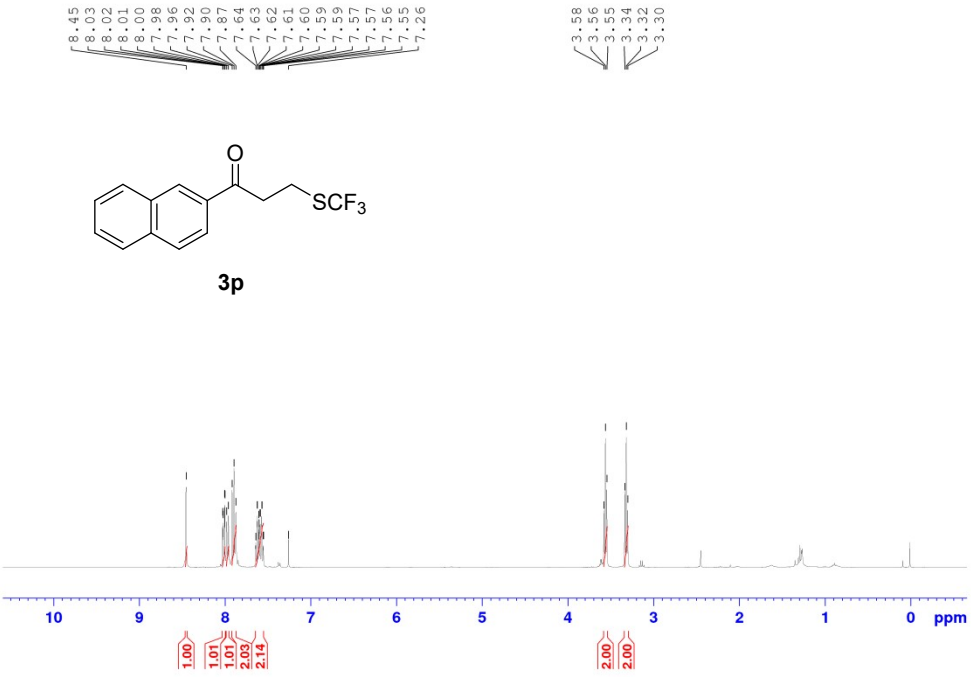
3o


194.95
152.19
148.32
135.80
132.76
130.98
129.72
126.68
124.36
107.99
107.70
101.95
77.31
76.99
76.68
38.60
24.03
O
O
O
SCF3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

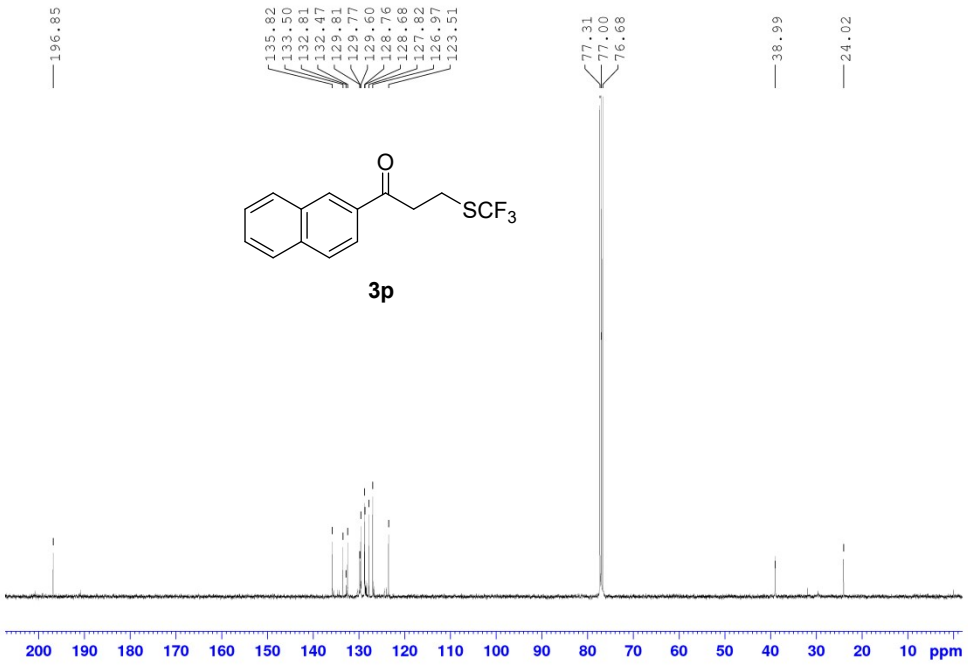
3o


-41.55
O
O
O
SCF3
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

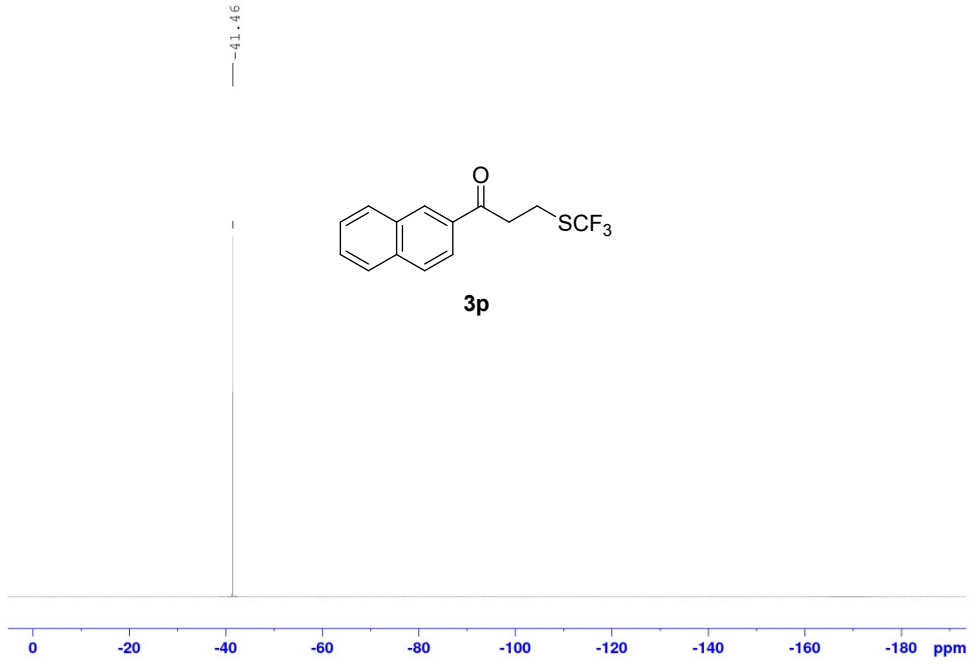
3o


8.45
8.03
8.02
8.01
8.00
7.98
7.96
7.92
7.90
7.87
7.64
7.63
7.62
7.61
7.60
7.59
7.59
7.57
7.57
7.56
7.55
7.26
3.58
3.56
3.55
3.34
3.32
3.30
O
SCF3
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.01
2.03
2.14
2.00
2.00

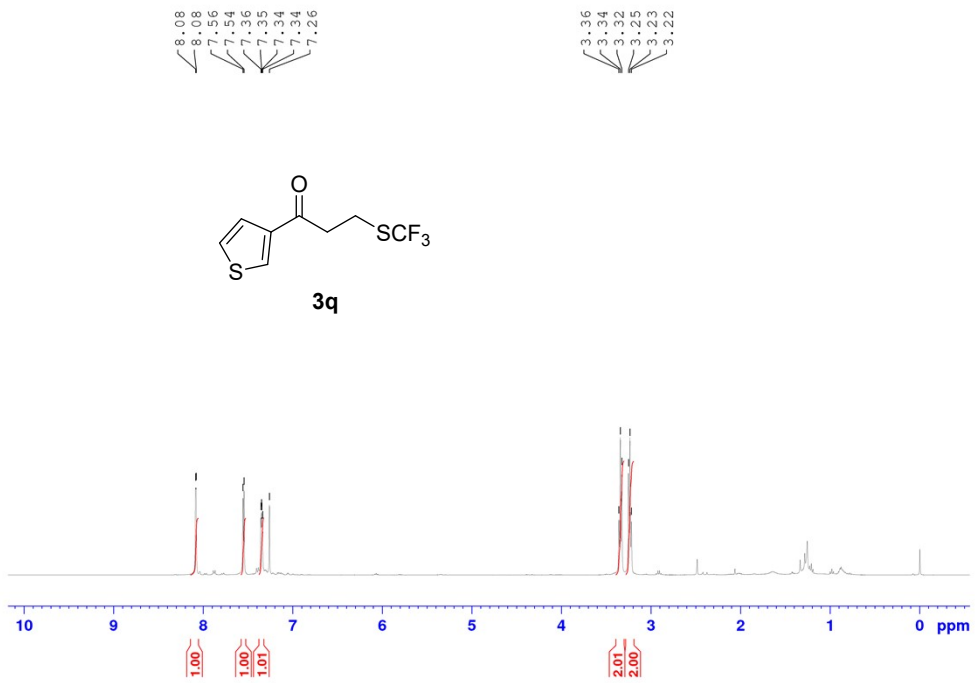
3p

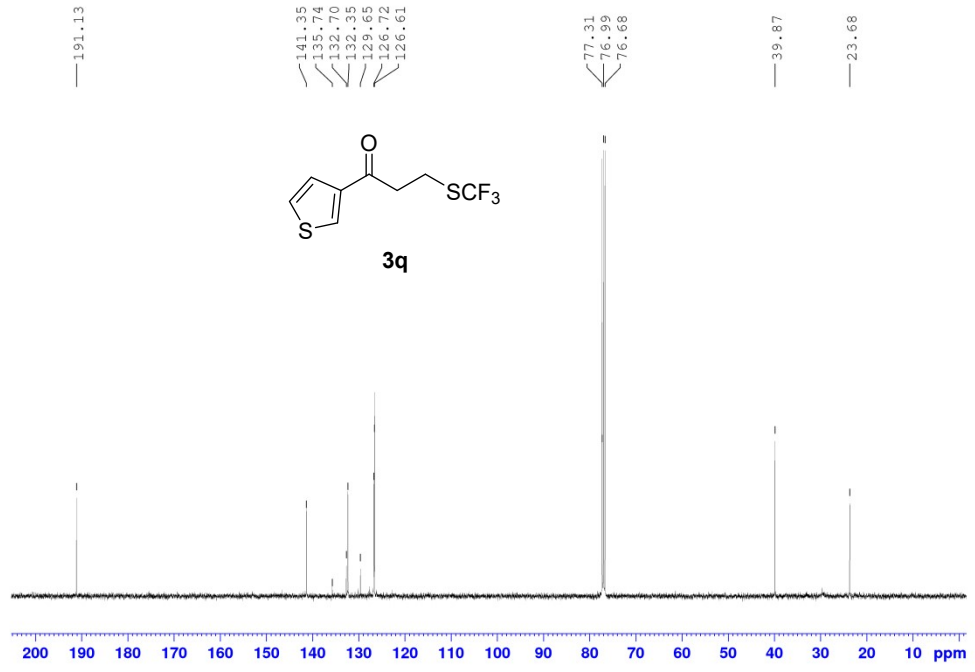

196.85
135.82
133.50
132.81
132.47
129.81
129.77
129.60
128.76
128.68
127.82
126.97
123.51
77.31
77.00
76.68
38.99
24.02
O
SCF3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

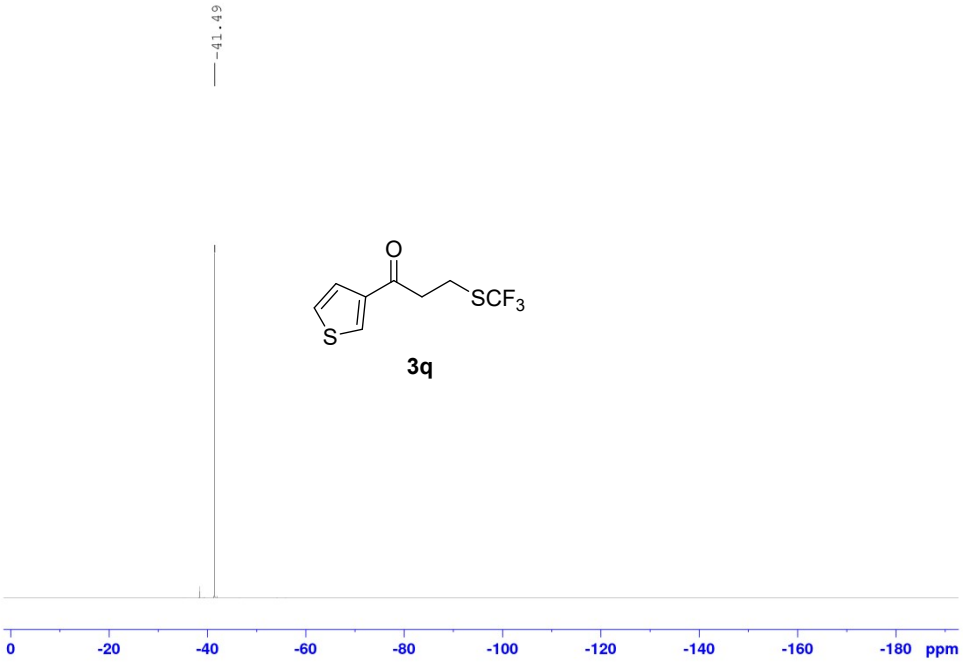
3p


41.46
O
SCF3
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

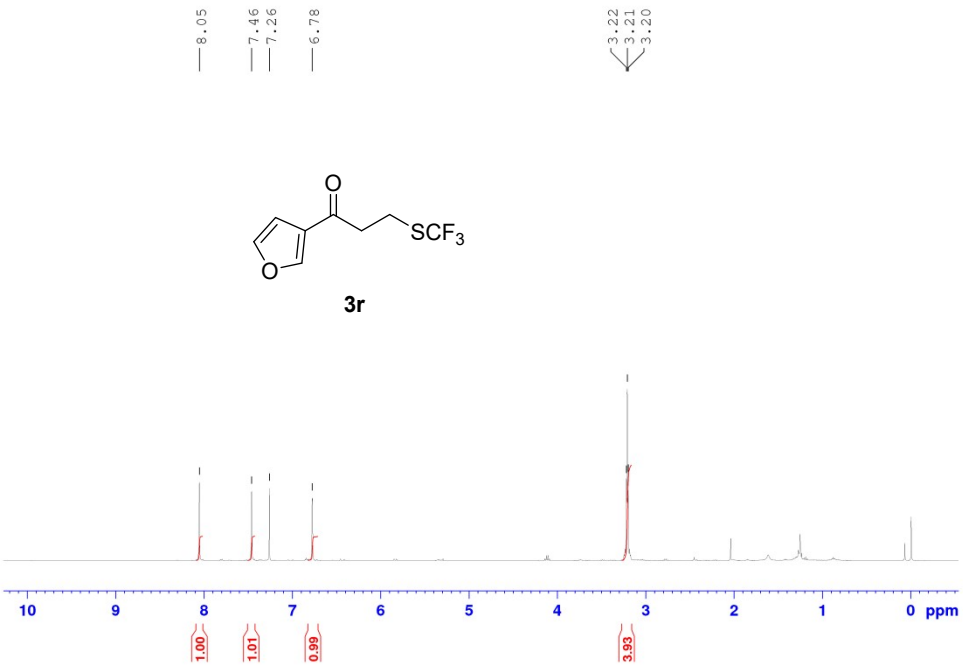
3p


8.08
8.08
7.56
7.54
7.36
7.35
7.34
7.34
7.26
3.36
3.34
3.32
3.25
3.23
3.22
O
SCF3
S
3q
10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.00
1.01
2.01
2.00

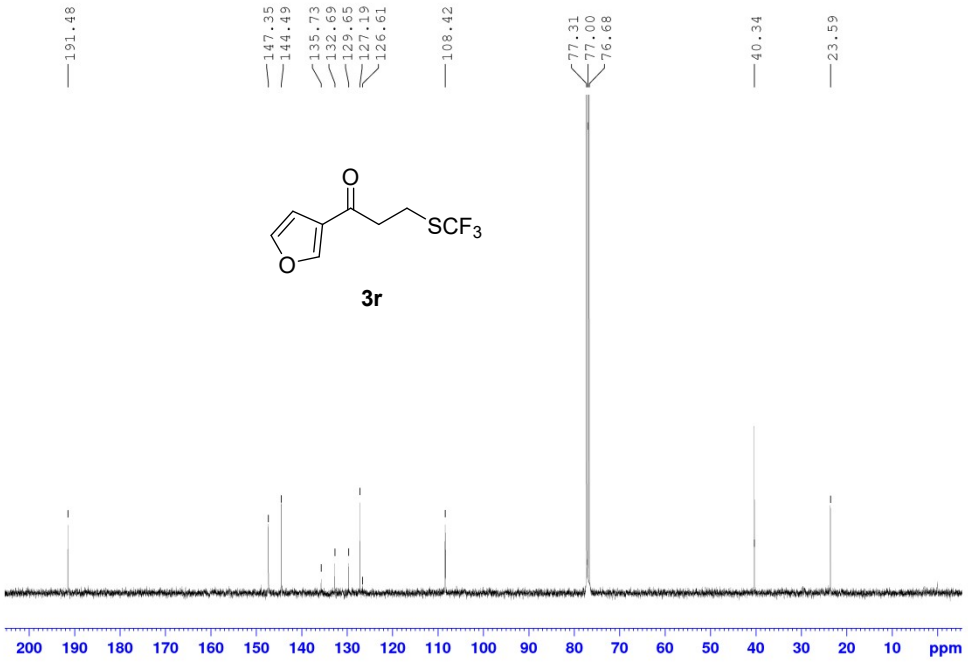

191.13
141.35
135.74
132.70
132.35
129.65
126.72
126.61
77.31
76.99
76.68
39.87
23.68
O
SCF3
S
3q
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

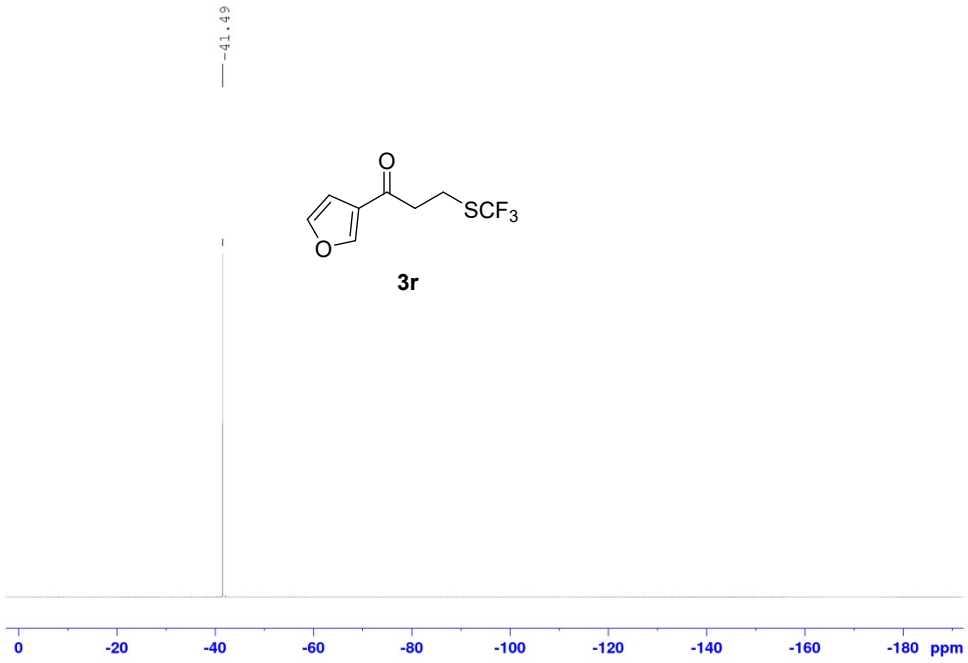

-41.49
O
SCF3
S
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

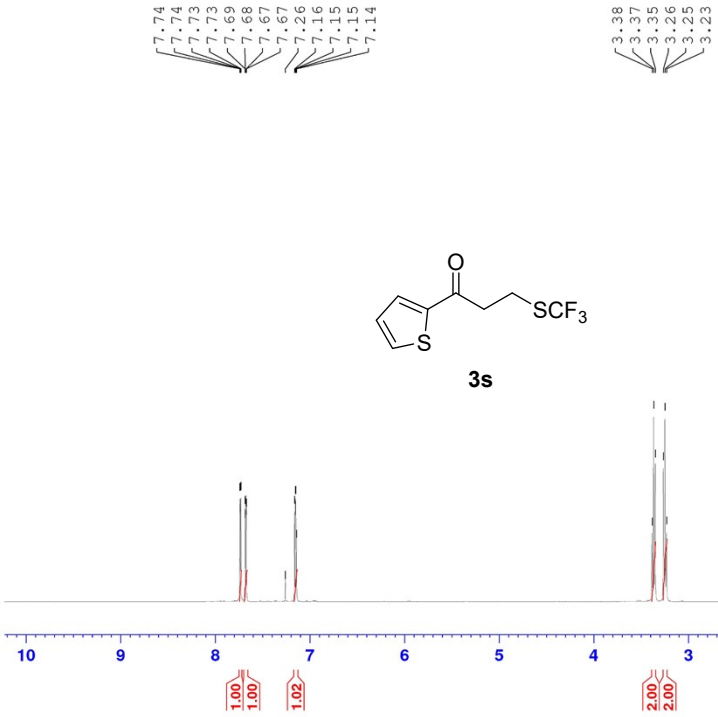
3q

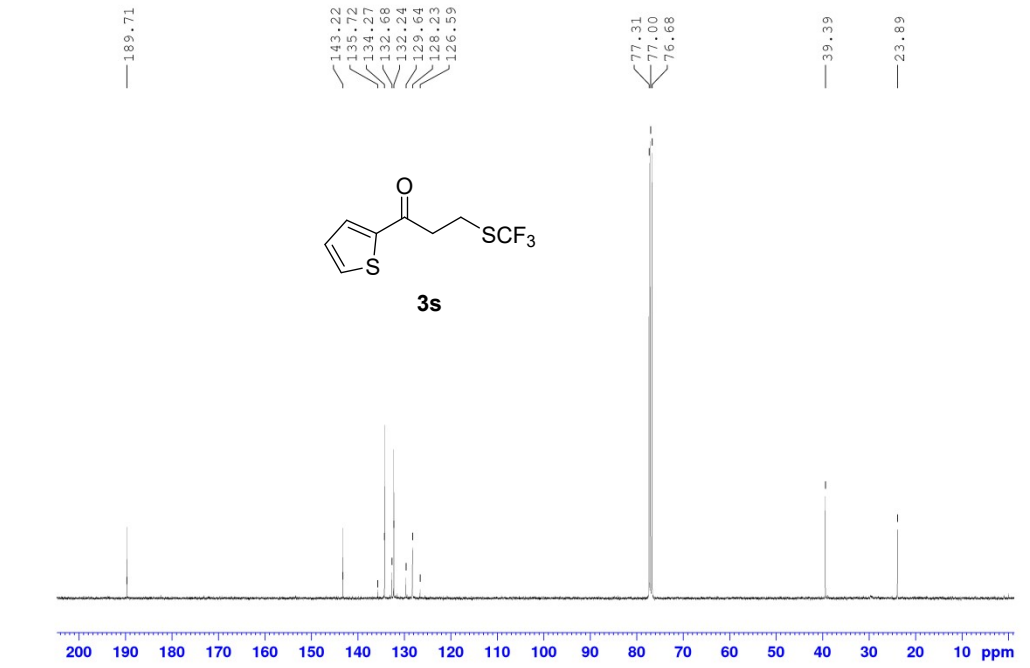

8.05
7.46
7.26
6.78
3.22
3.21
3.20
O
SCF3
O
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
0.99
3.93

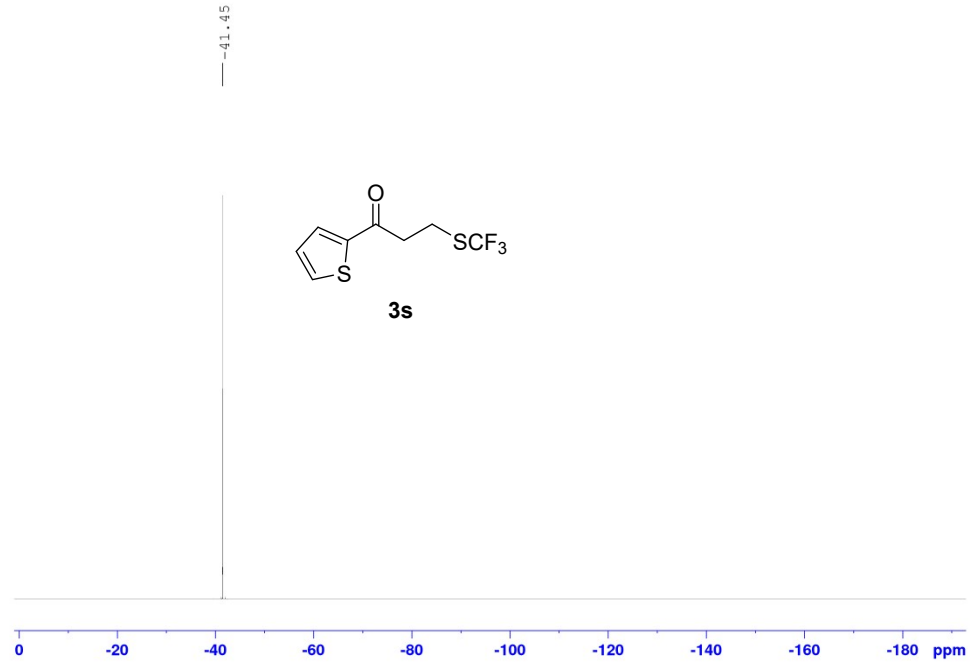
3r


191.48
147.35
144.49
135.73
132.69
129.65
127.19
126.61
108.42
77.31
77.00
76.68
40.34
23.59
O
SCF3
O
3r
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

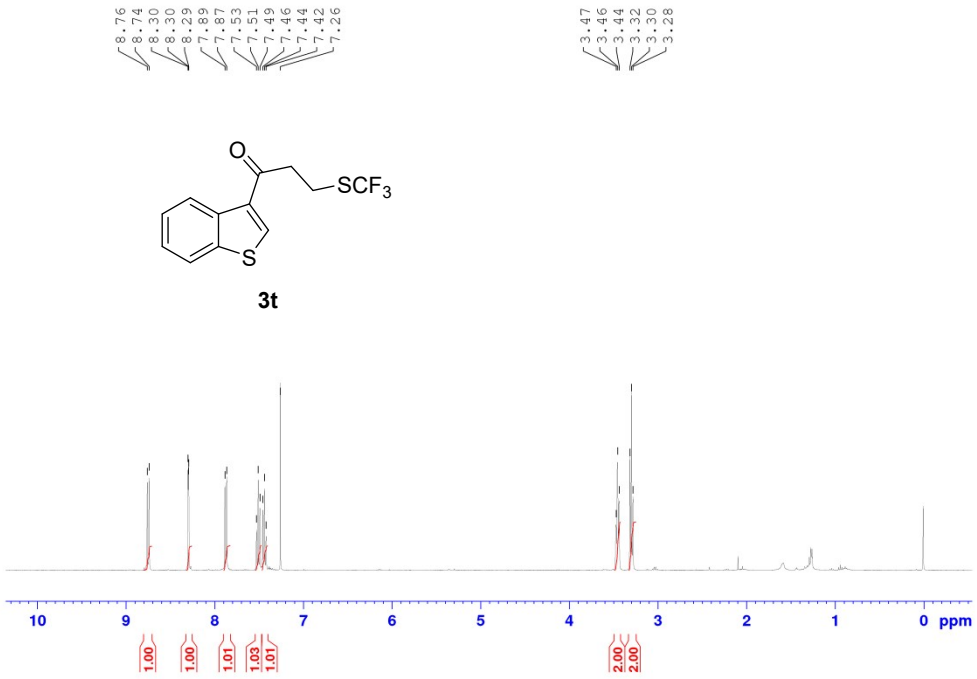

-41.49
O
SCF3
O
3r
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm


7.74
7.74
7.73
7.73
7.69
7.68
7.67
7.67
7.26
7.16
7.15
7.15
7.14
3.38
3.37
3.35
3.26
3.25
3.23
O
SCF3
S
3s
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
1.02
2.00
2.00

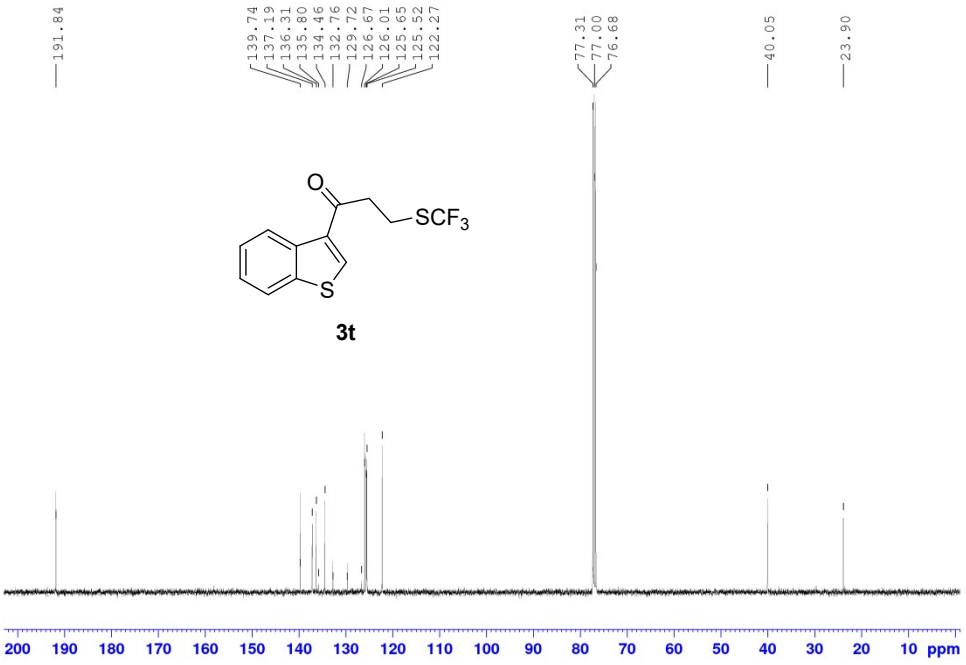

189.71
143.22
135.72
134.27
132.68
132.24
129.64
128.23
126.59
77.31
77.00
76.68
39.39
23.89
O
SCF3
S
3s
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-41.45
O
SCF3
S
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

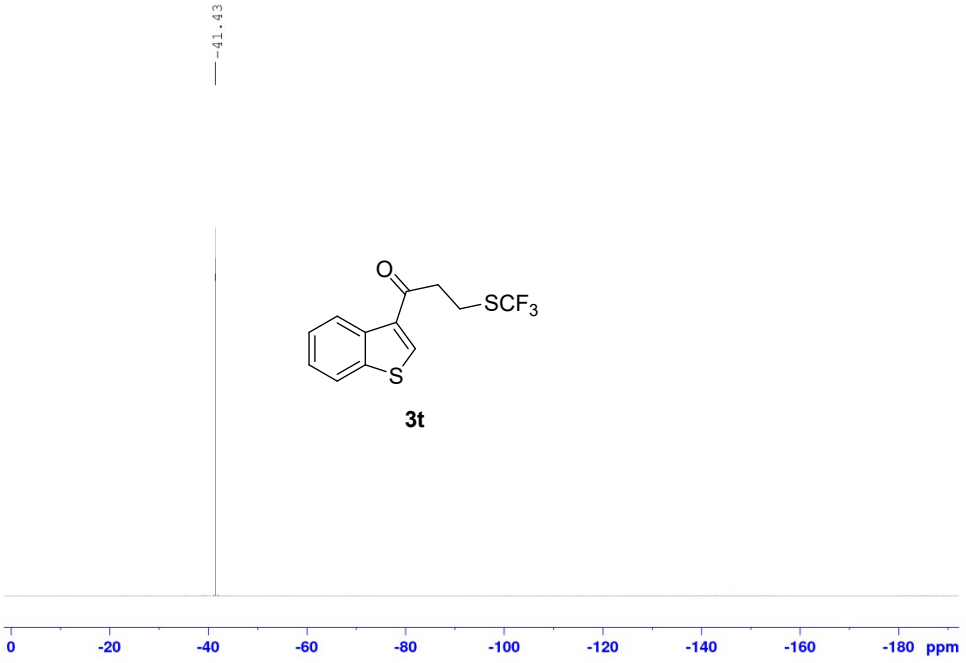
3s


8.76
8.74
8.30
8.29
7.89
7.87
7.53
7.51
7.49
7.46
7.44
7.42
7.26
3.47
3.46
3.44
3.32
3.30
3.28
O
SCF3
S
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
1.01
1.03
1.01
2.00
2.00

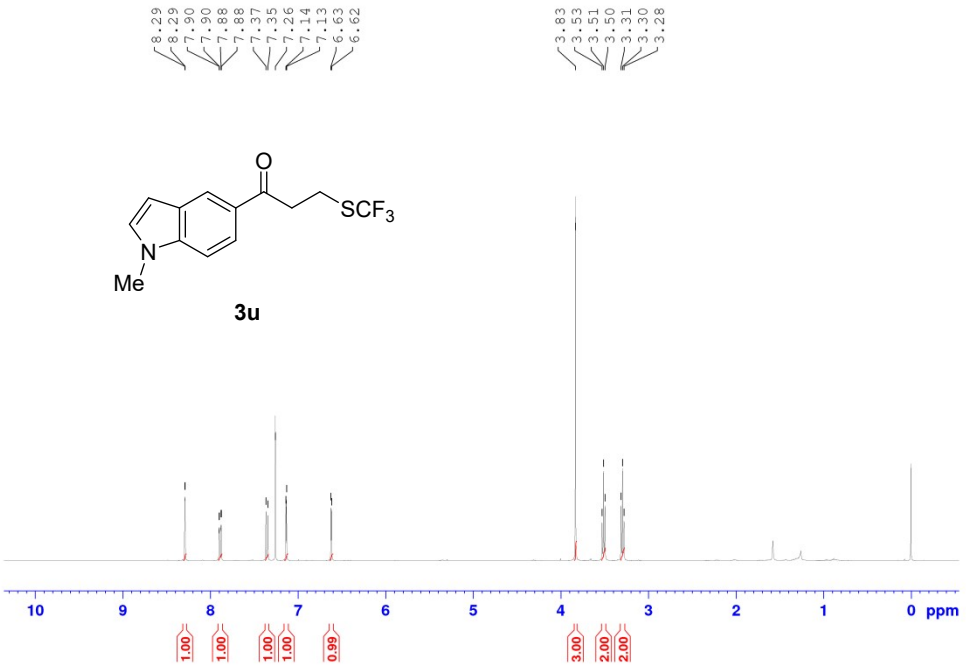
3t

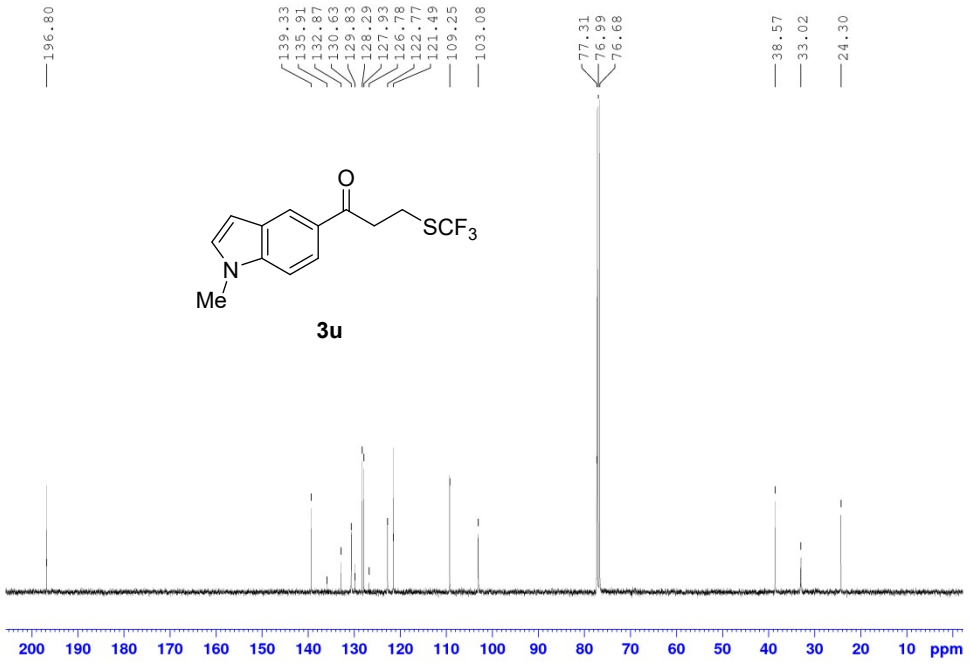

191.84
139.74
137.19
136.31
135.80
134.46
132.76
129.72
126.67
126.01
125.65
125.52
122.27
77.31
77.00
76.68
40.05
23.90
O
SCF3
S
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

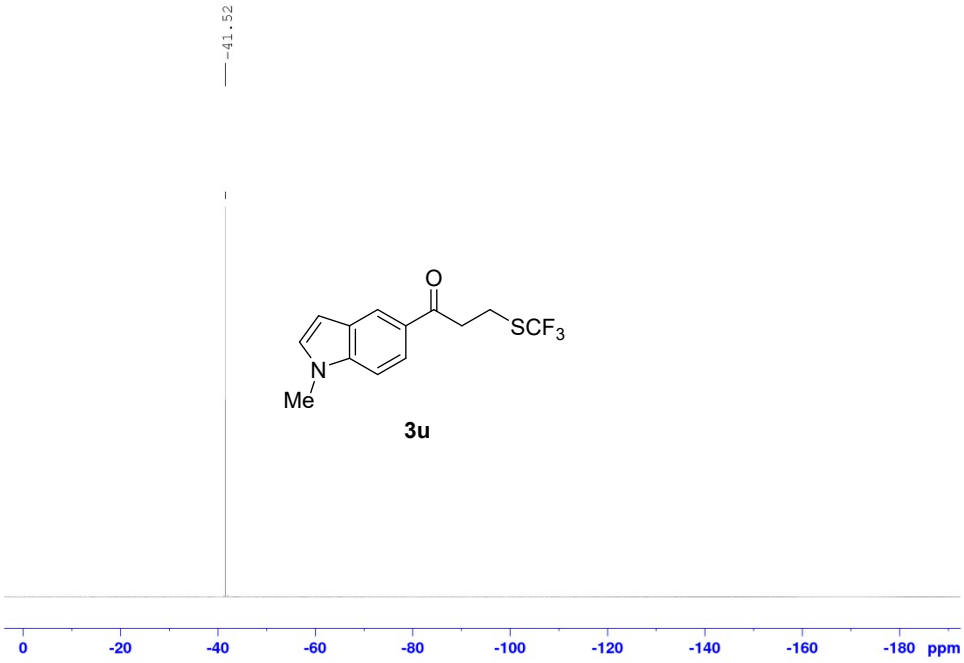
3t


-41.43
O
SCF3
S
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

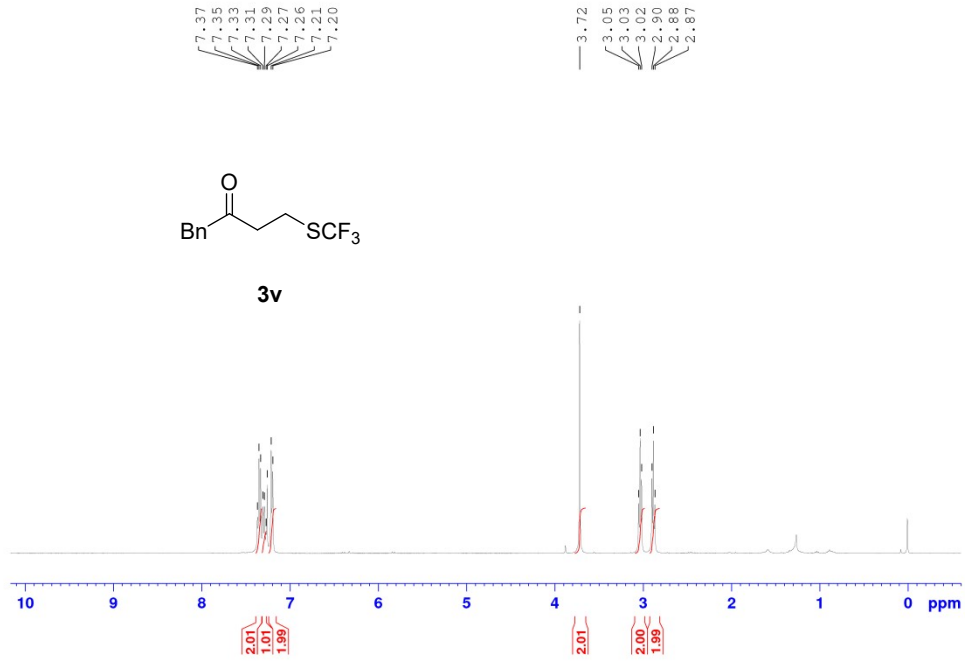
3t


8.29
8.29
7.90
7.90
7.88
7.88
7.37
7.35
7.26
7.14
7.13
6.63
6.62
3.83
3.53
3.51
3.50
3.31
3.30
3.28
O
SCF3
N
Me
3u
10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.00
1.00
1.00
0.99
3.00
2.00
2.00

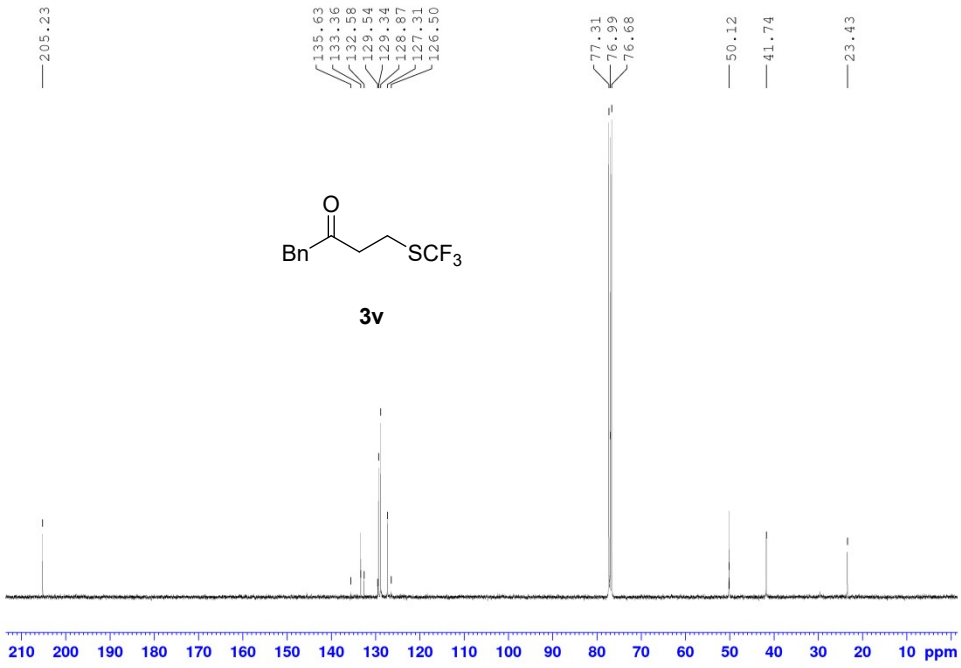

196.80
139.33
135.91
132.87
130.63
129.83
128.29
127.93
126.78
122.77
121.49
109.25
103.08
77.31
76.99
76.68
38.57
33.02
24.30
O
SCF3
N
Me
3u
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-41.52
O
SCF3
N
Me
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

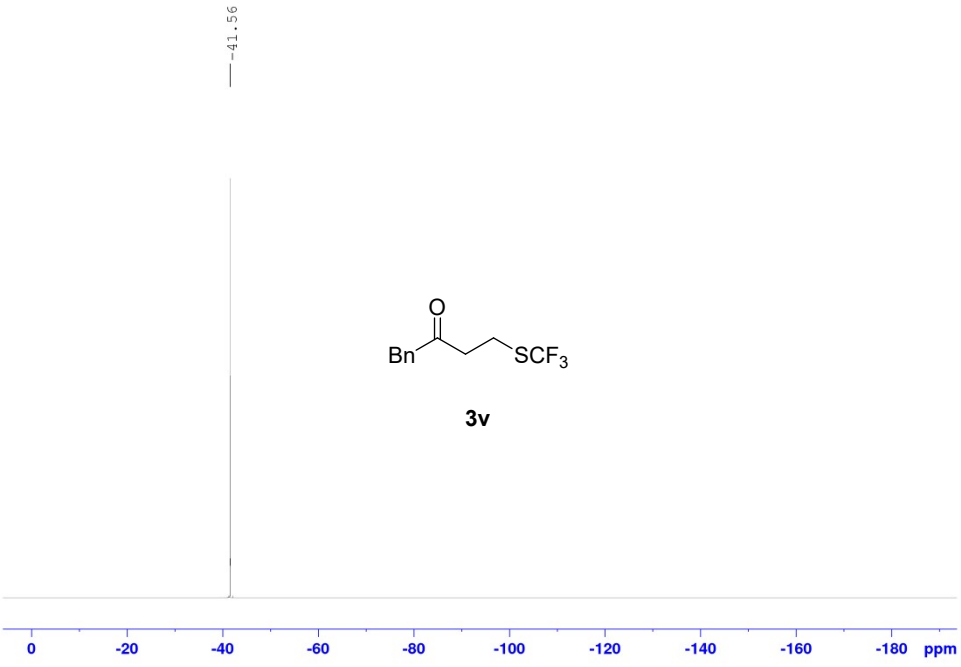
3u


7.37
7.35
7.33
7.31
7.29
7.27
7.26
7.21
7.20
3.72
3.05
3.03
3.02
2.90
2.88
2.87
O
Bn
SCF3
10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
1.01
1.99
2.01
2.00
1.99

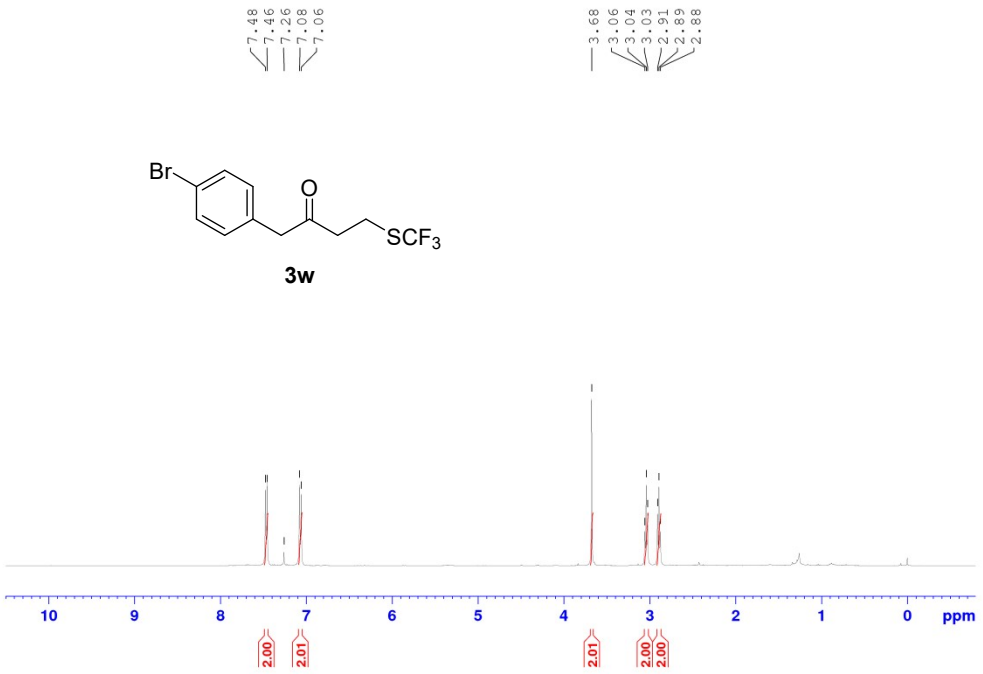
3v

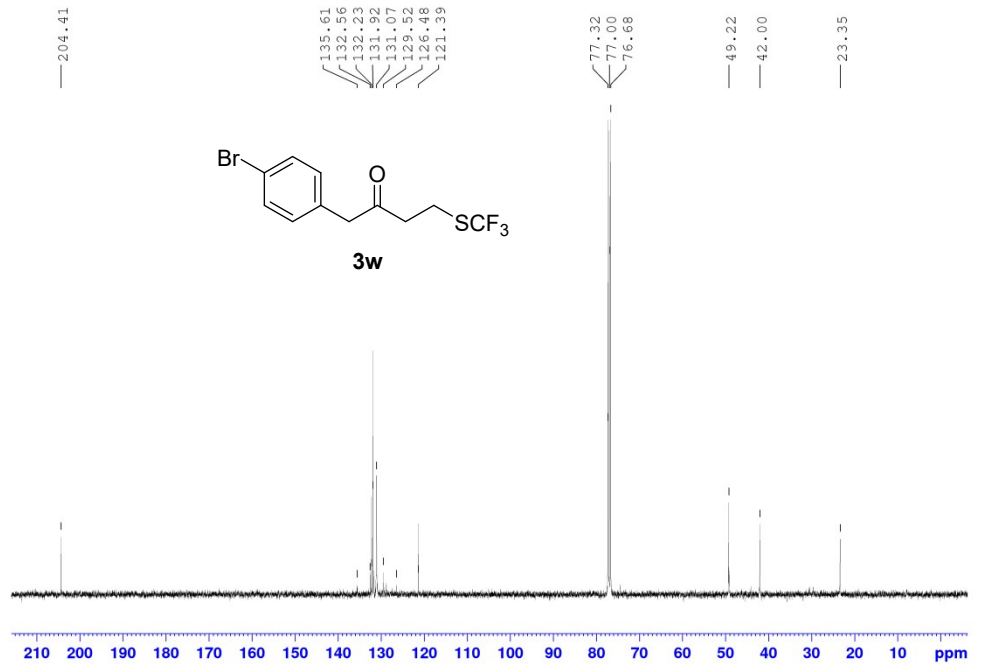

205.23
135.63
133.36
132.58
129.54
129.34
128.87
127.31
126.50
77.31
76.99
76.68
50.12
41.74
23.43
O
Bn
SCF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

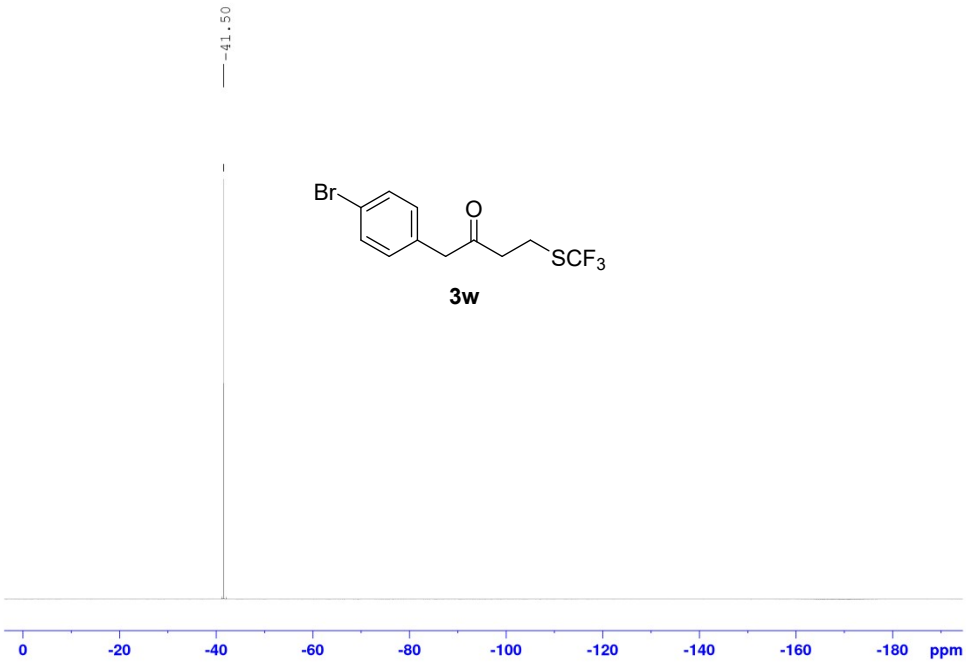
3v

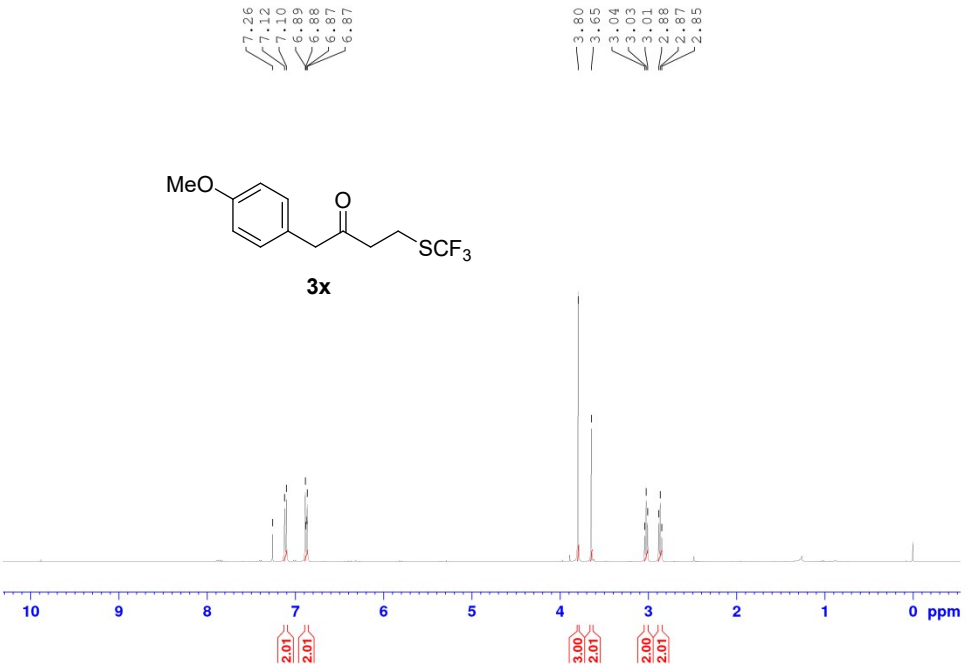

41.56
O
Bn
SCF3
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

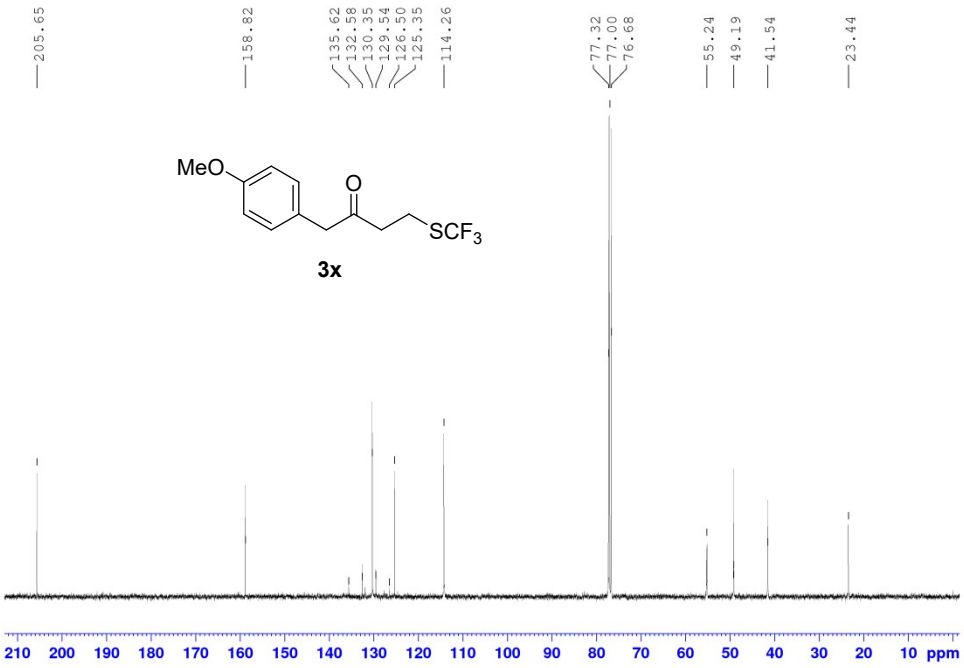
3v

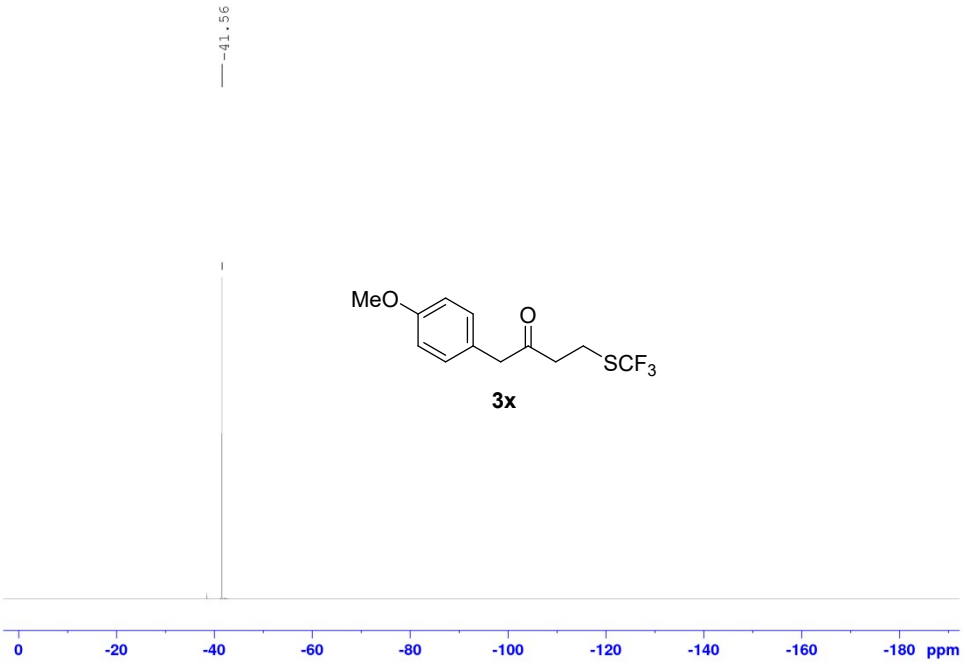

7.48
7.46
7.26
7.08
7.06
3.68
3.06
3.04
3.03
2.91
2.89
2.88
Br
O
SCF3
3w
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.01
2.01
2.00
2.00

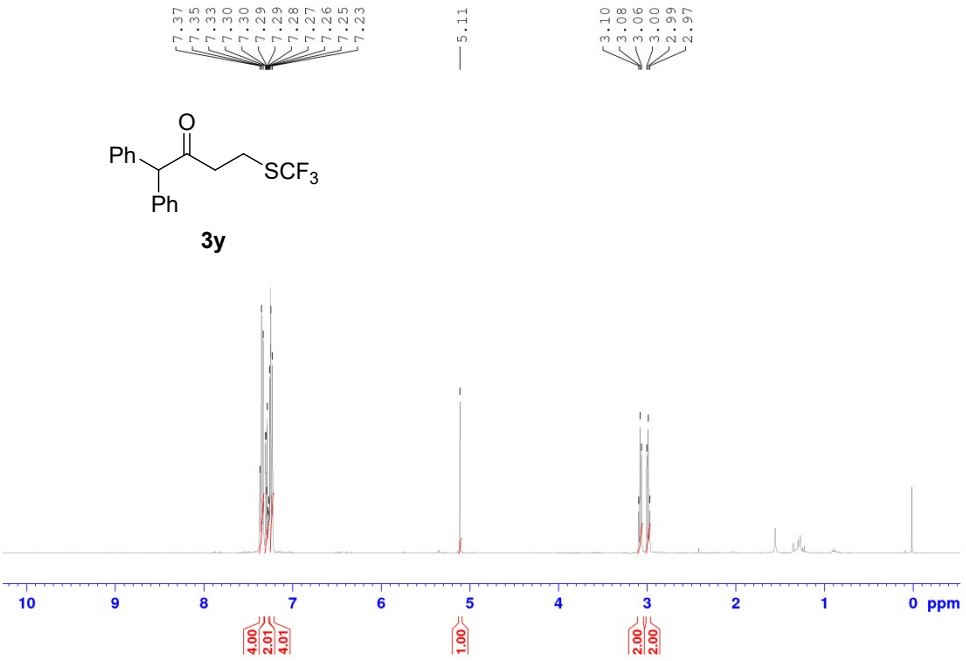

204.41
135.61
132.56
132.23
131.92
131.07
129.52
126.48
121.39
77.32
77.00
76.68
49.22
42.00
23.35
Br
O
SCF3
3w
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-41.50
Br
O
SCF3
3w
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

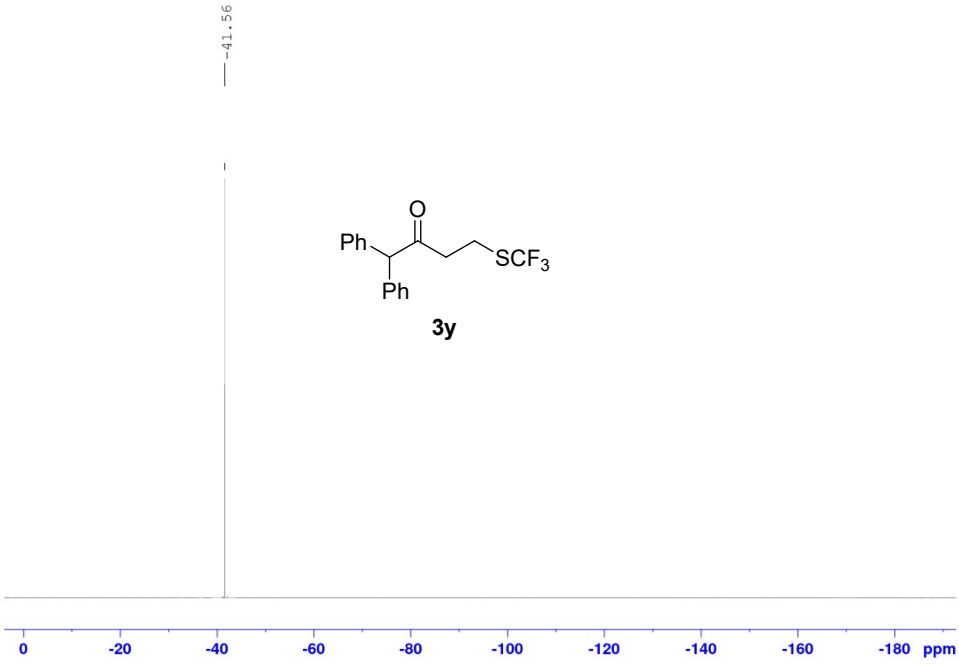

7.26
7.12
7.10
6.89
6.88
6.87
6.87
3.80
3.65
3.04
3.03
3.01
2.88
2.87
2.85
MeO
O
SCF3
3x
10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
2.01
3.00
2.01
2.00
2.01


205.65
158.82
135.62
132.58
130.35
129.54
126.50
125.35
114.26
77.32
77.00
76.68
55.24
49.19
41.54
23.44
MeO
O
SCF3
3x
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

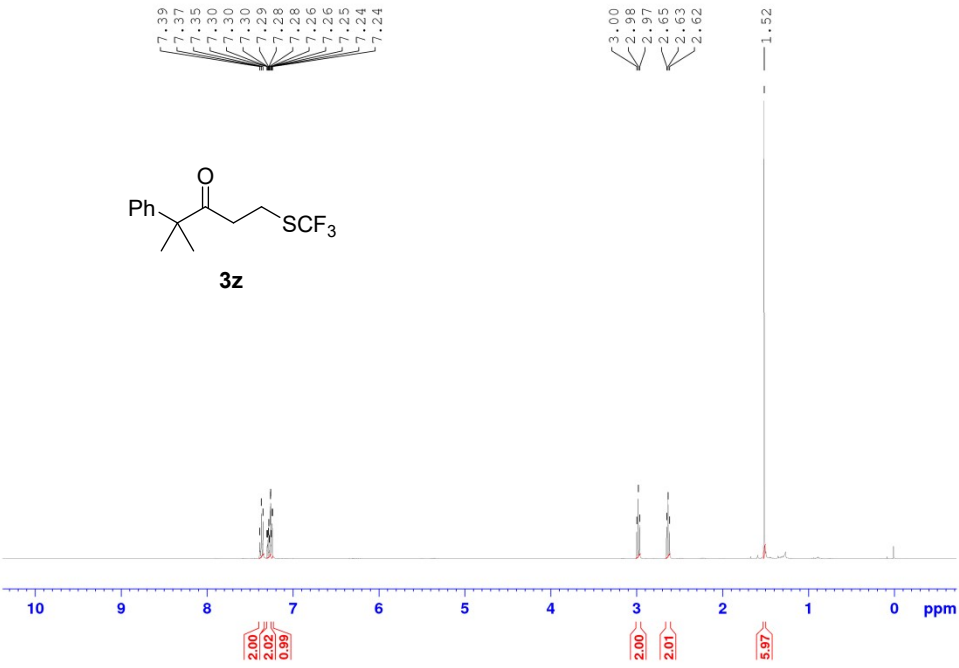

-41.56
MeO
O
SCF3
3x
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm


7.37
7.35
7.33
7.30
7.30
7.29
7.29
7.28
7.27
7.26
7.25
7.23
5.11
3.10
3.08
3.06
3.00
2.99
2.97
O
Ph
SCF3
Ph
3y
10
9
8
7
6
5
4
3
2
1
0 ppm
4.00
2.01
4.01
1.00
2.00
2.00

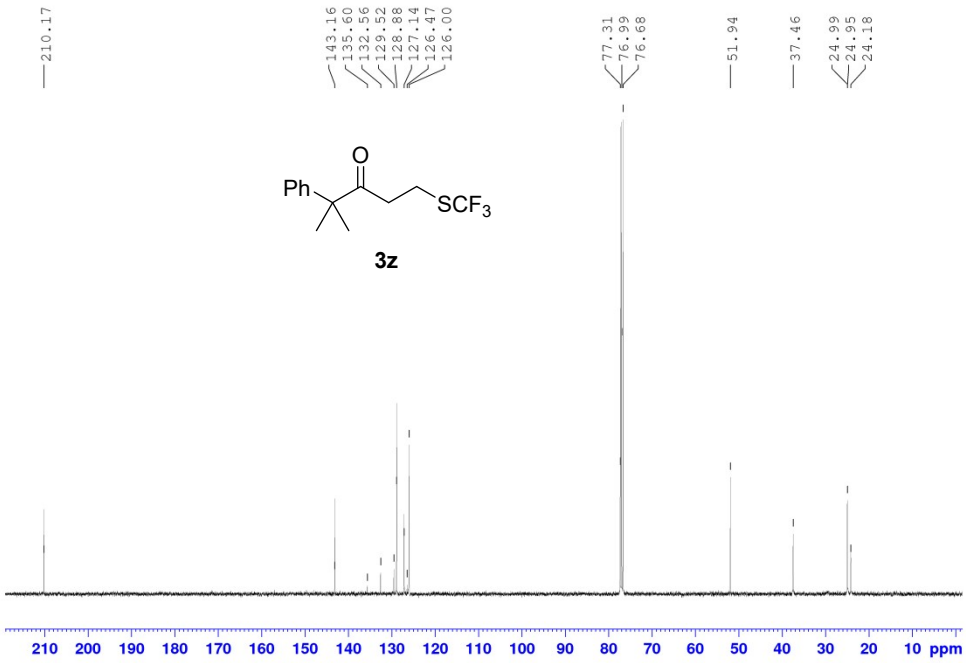

205.60
137.65
135.61
132.57
129.52
128.89
128.81
127.47
77.32
77.00
76.68
64.22
42.43
23.70
O
Ph
SCF3
Ph
3y
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

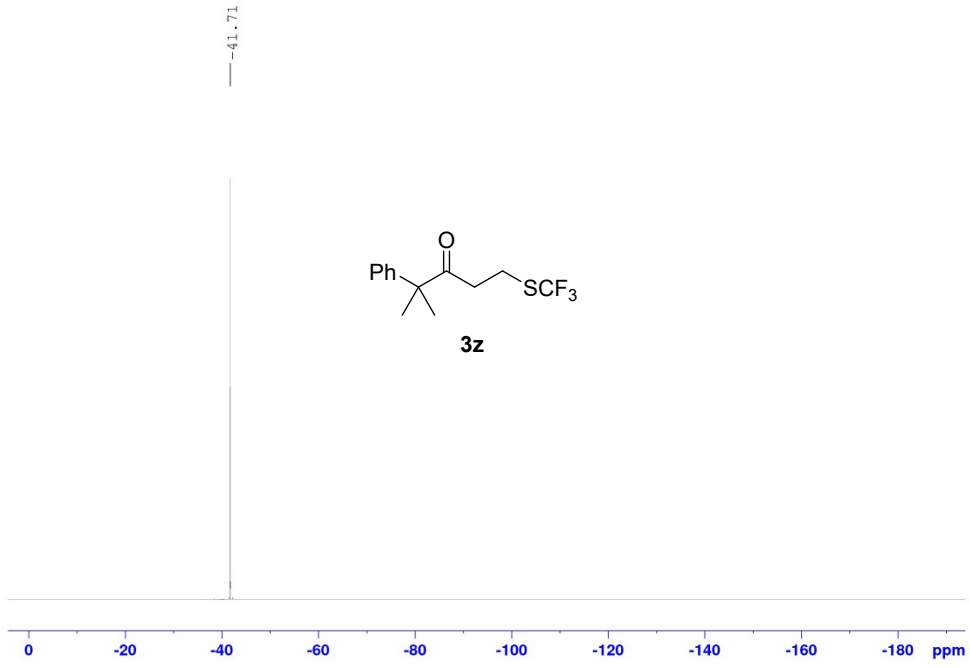

-41.56
O
Ph
Ph
SCF3
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

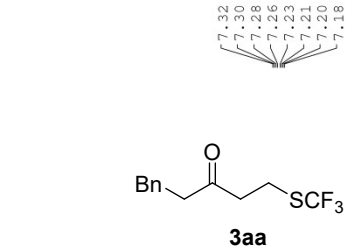
3y


7.39
7.37
7.35
7.30
7.30
7.30
7.29
7.28
7.28
7.26
7.26
7.25
7.24
7.24
3.00
2.98
2.97
2.65
2.63
2.62
1.52
O
Ph
SCF3
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.02
0.99
2.00
2.01
5.97

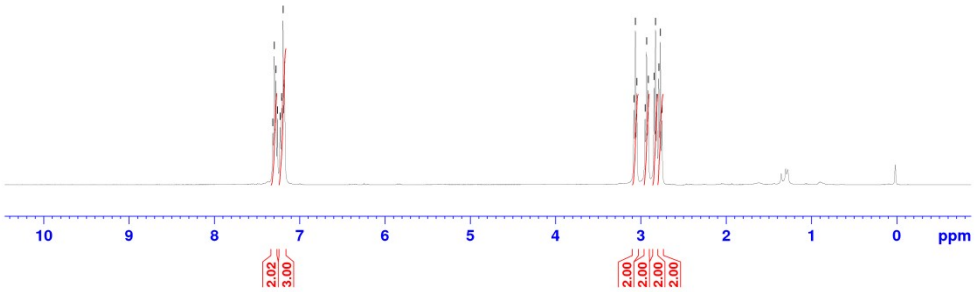
3z

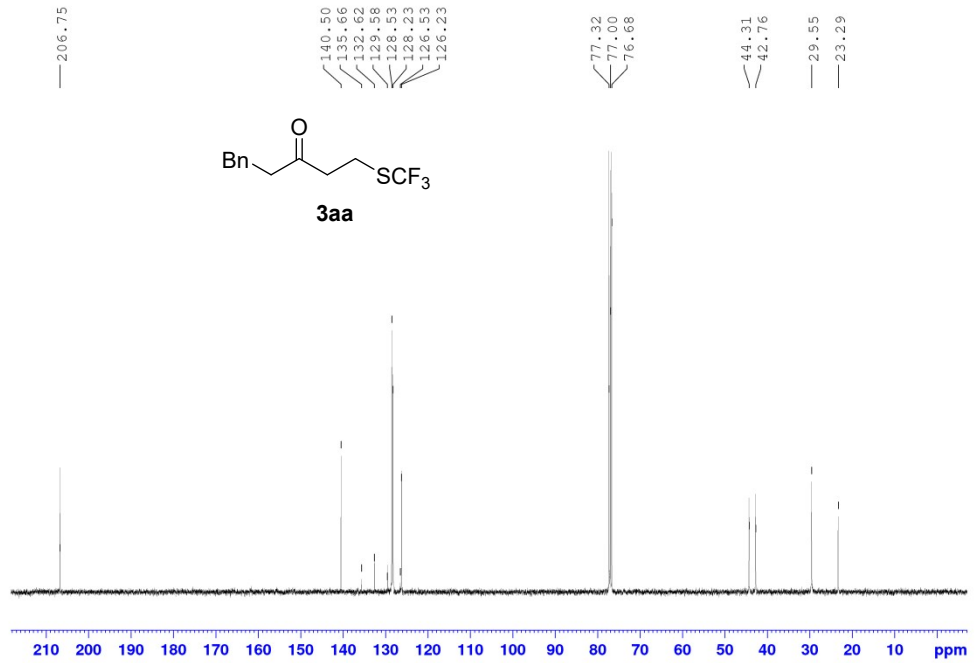

210.17
143.16
135.60
132.56
129.52
128.88
127.14
126.47
126.00
77.31
76.99
76.68
51.94
37.46
24.99
24.95
24.18
O
Ph
SCF3
3z
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


-41.71
O
Ph
SCF3
3z
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

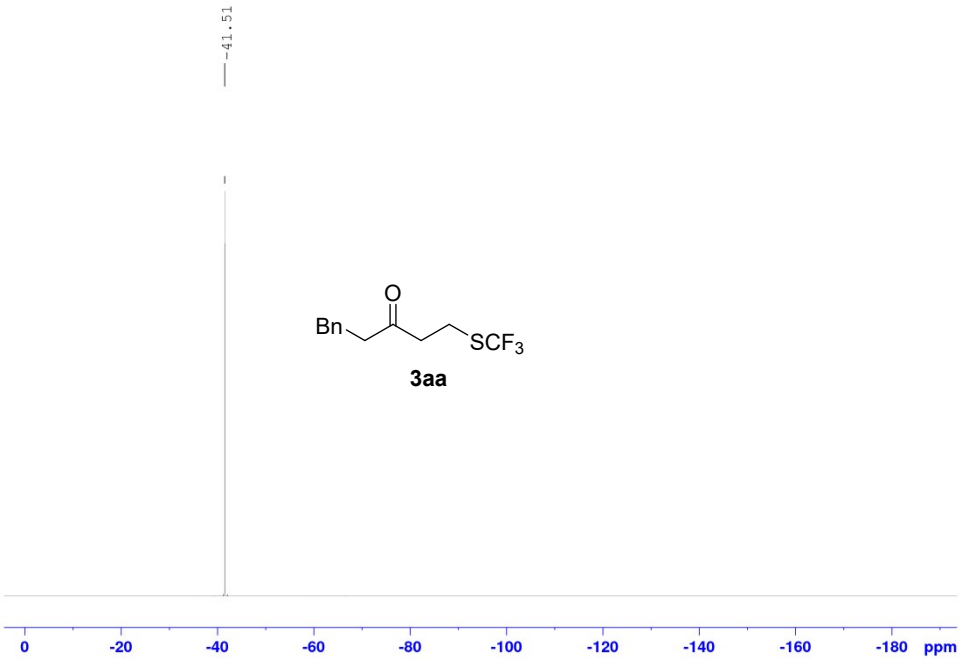

7.32
7.30
7.28
7.26
7.23
7.21
7.20
7.18
3.08
3.06
3.05
2.95
2.93
2.91
2.84
2.83
2.81
2.79
2.77
2.75
O
Bn
SCF3

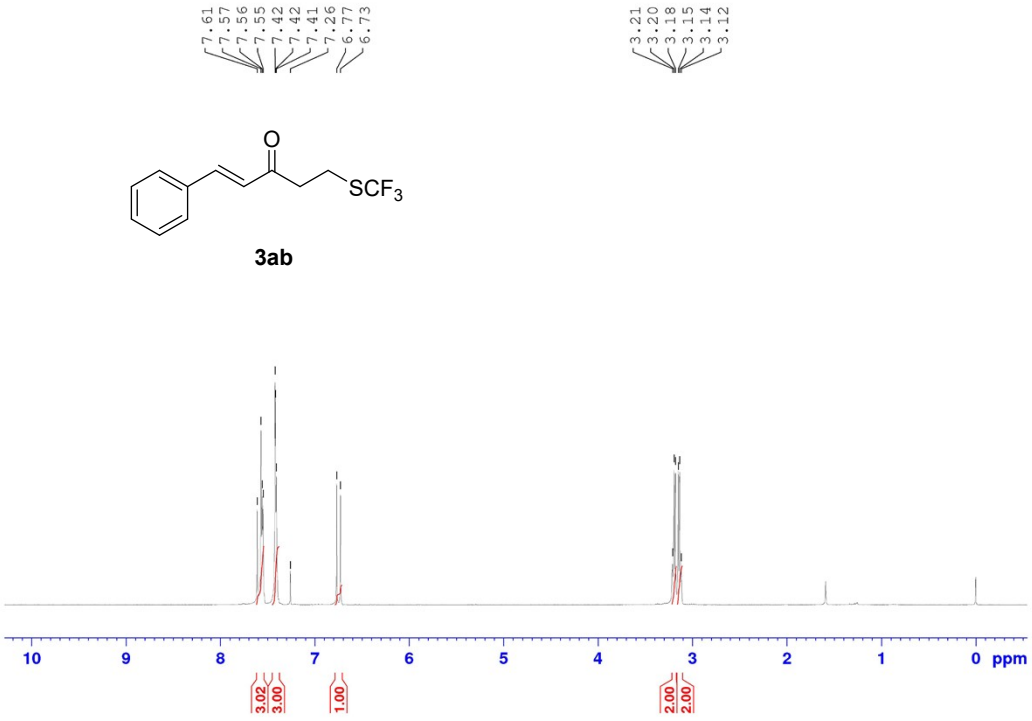
3aa

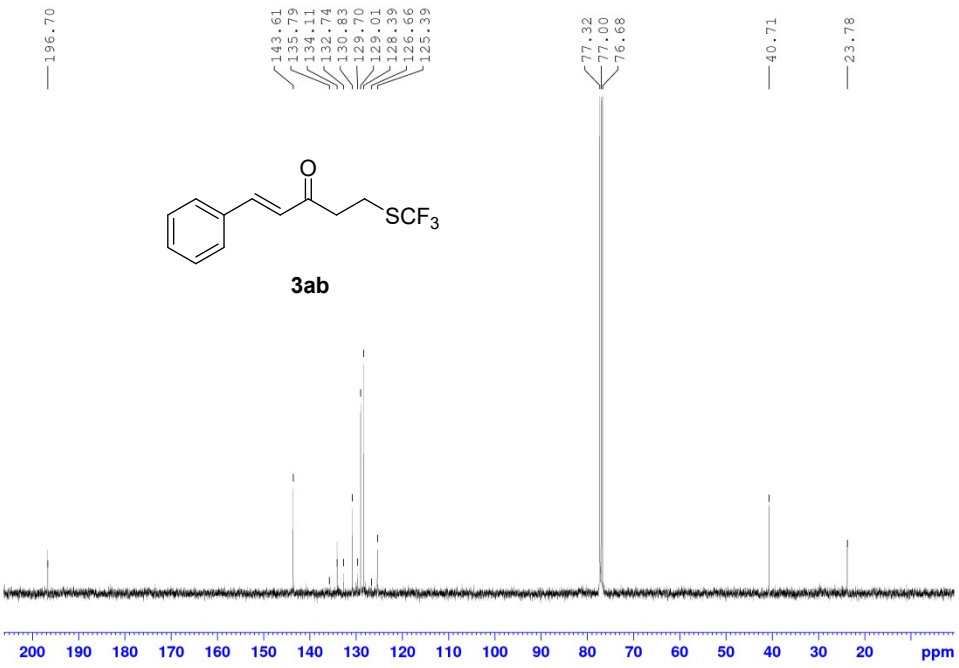

10
9
8
7
6
5
4
3
2
1
0
ppm
2.02
3.00
2.00
2.00
2.00
2.00


206.75
140.50
135.66
132.62
129.58
128.53
128.23
126.53
126.23
77.32
77.00
76.68
44.31
42.76
29.55
23.29
O
Bn
SCF3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

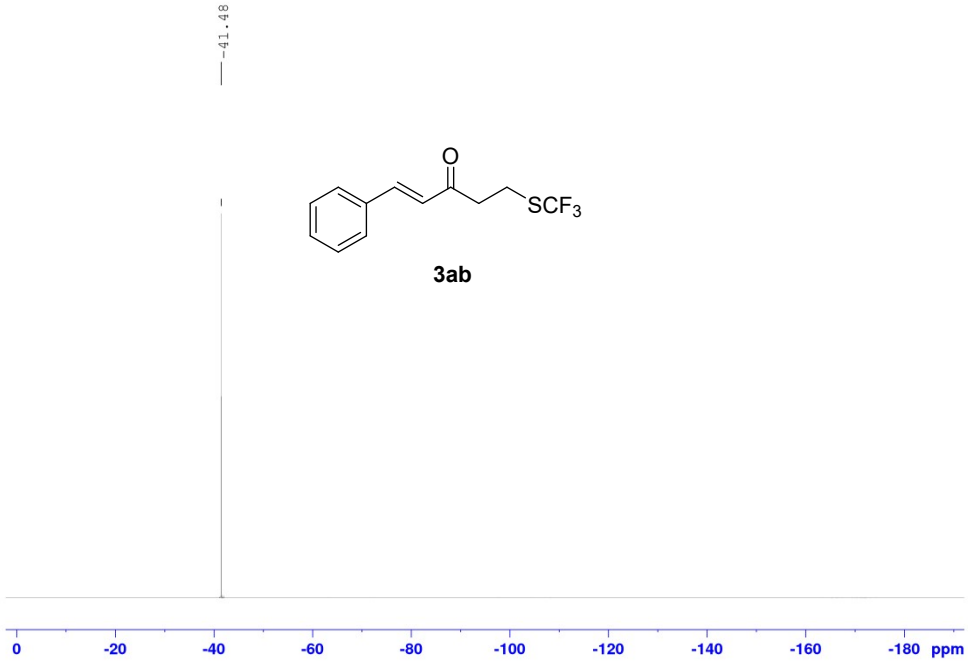
3aa


-41.51
O
Bn
SCF3
3aa
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

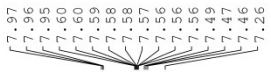

7.61
7.57
7.56
7.55
7.42
7.42
7.41
7.26
6.77
6.73
3.21
3.20
3.18
3.15
3.14
3.12
O
SCF3
3ab
10
9
8
7
6
5
4
3
2
1
0
ppm
3.02
3.00
1.00
2.00
2.00

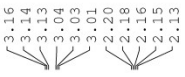

196.70
143.61
135.79
134.11
132.74
130.83
129.70
129.01
128.39
126.66
125.39
77.32
77.00
76.68
40.71
23.78
O
SCF3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

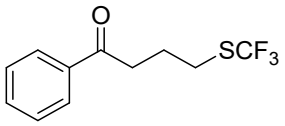
3ab


41.48
O
SCF3
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

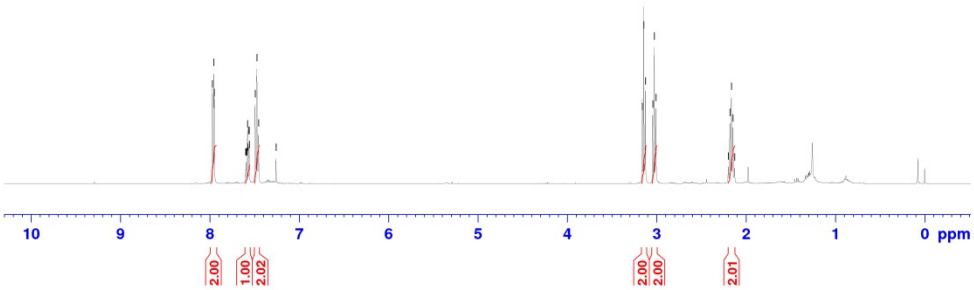
3ab


7.97
7.96
7.95
7.60
7.60
7.59
7.58
7.58
7.57
7.56
7.56
7.56
7.49
7.47
7.46
7.26

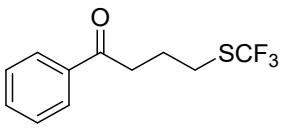

3.16
3.14
3.13
3.04
3.03
3.01
2.20
2.18
2.16
2.15
2.13


O
SCF3

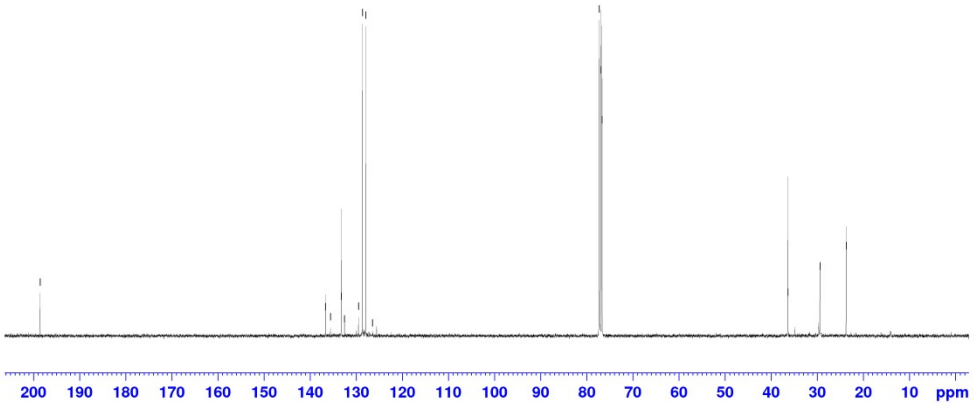
3ac

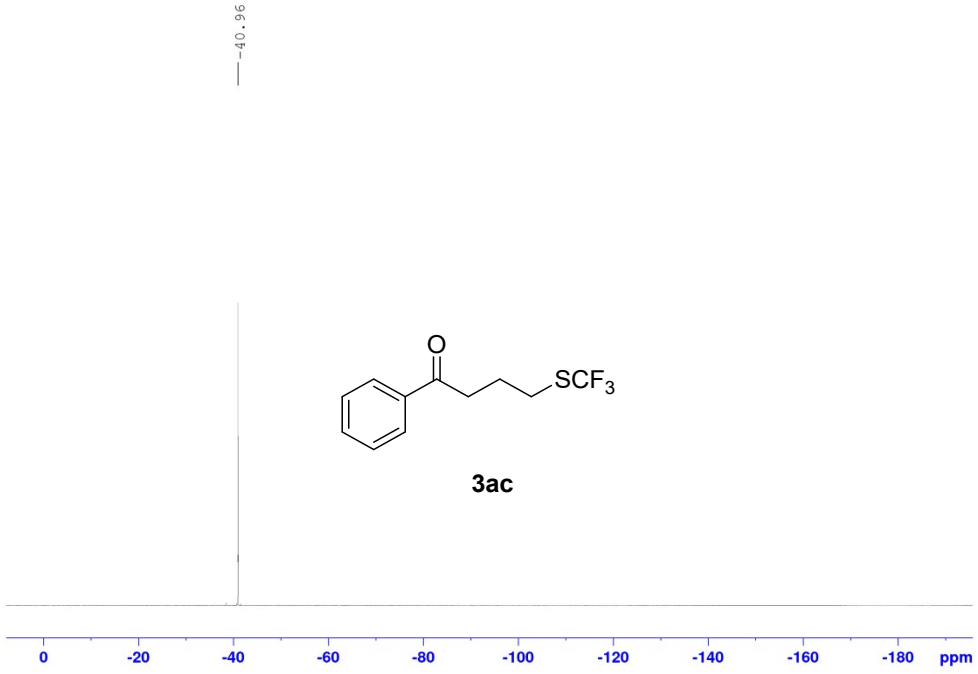

10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
1.00
2.02
2.00
2.00
2.01


198.56
136.68
135.59
133.25
132.55
129.51
128.66
127.95
126.47
77.32
77.00
76.68
36.36
29.41
23.74

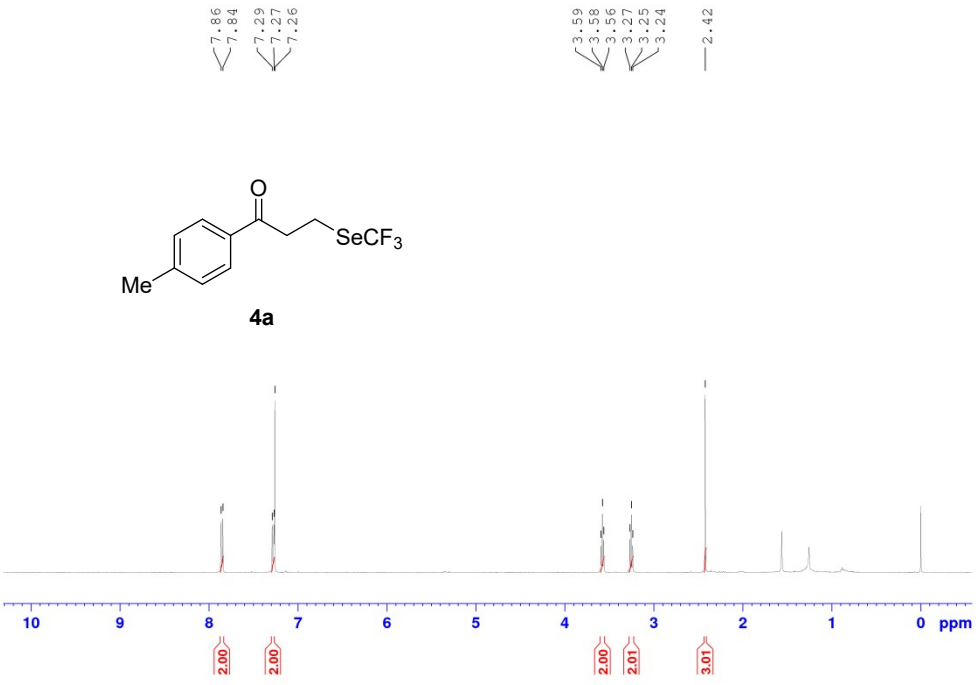

O
SCF3

3ac

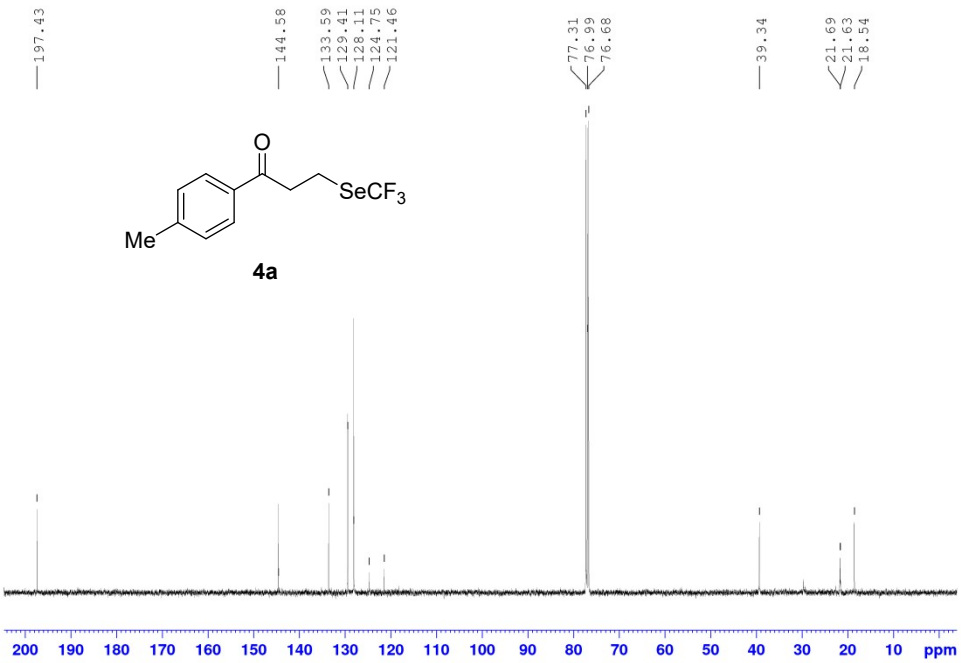

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-40.96
O
SCF3
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

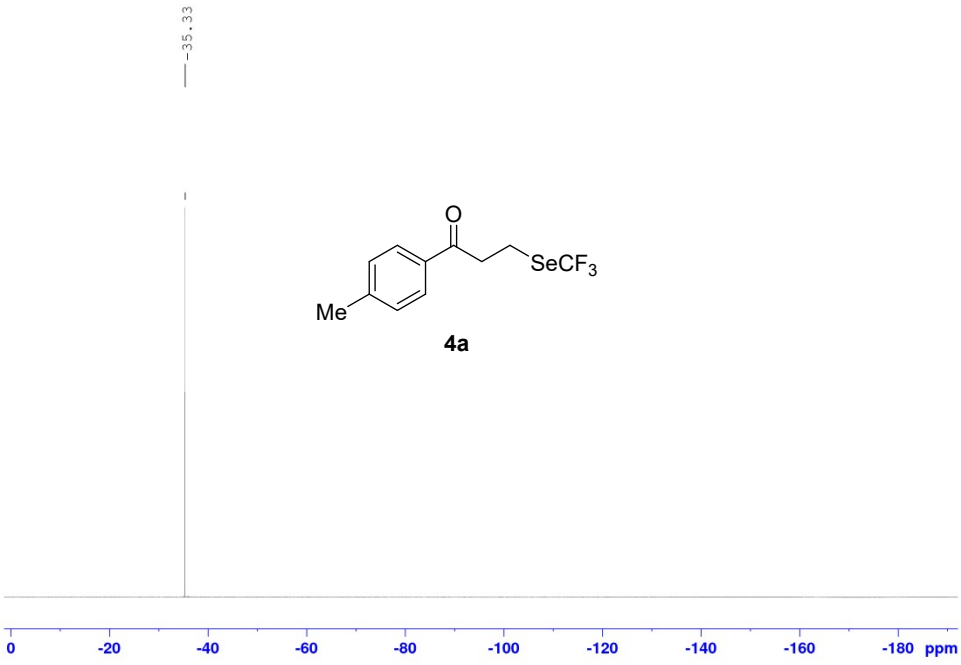
3ac


7.86
7.84
7.29
7.27
7.26
3.59
3.58
3.56
3.27
3.25
3.24
2.42
O
SeCF3
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.00
2.00
2.01
3.01

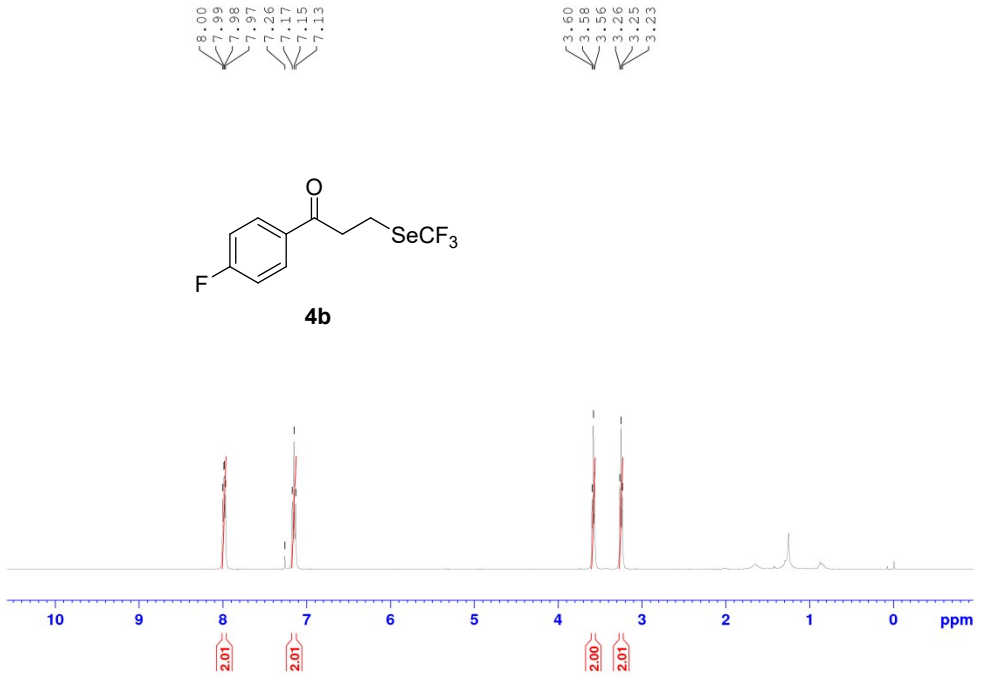
4a

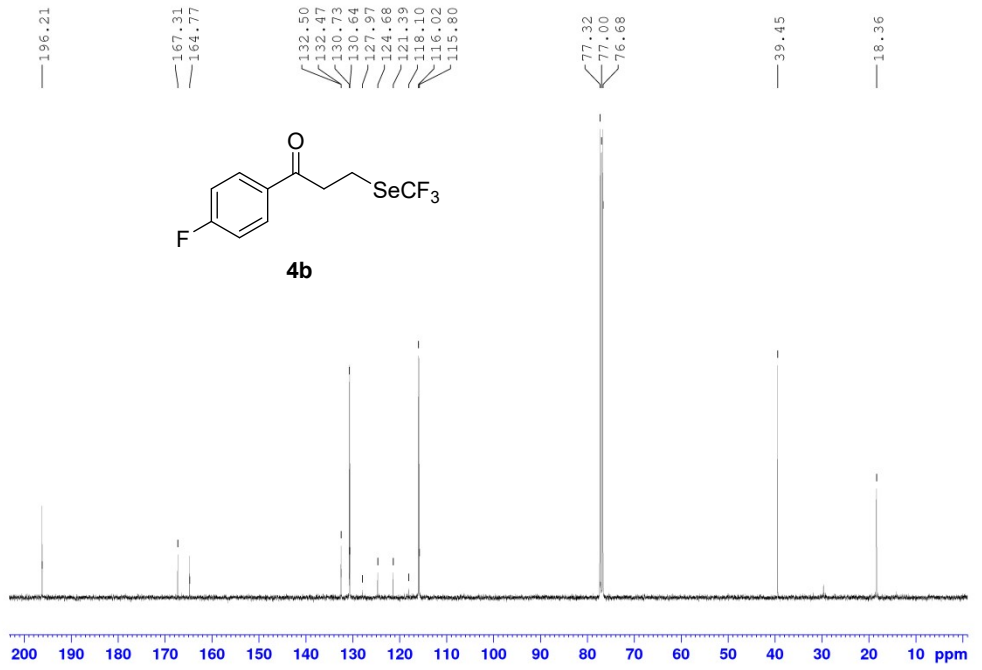

197.43
144.58
133.59
129.41
128.11
124.75
121.46
77.31
76.99
76.68
39.34
21.69
21.63
18.54
O
SeCF3
Me
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

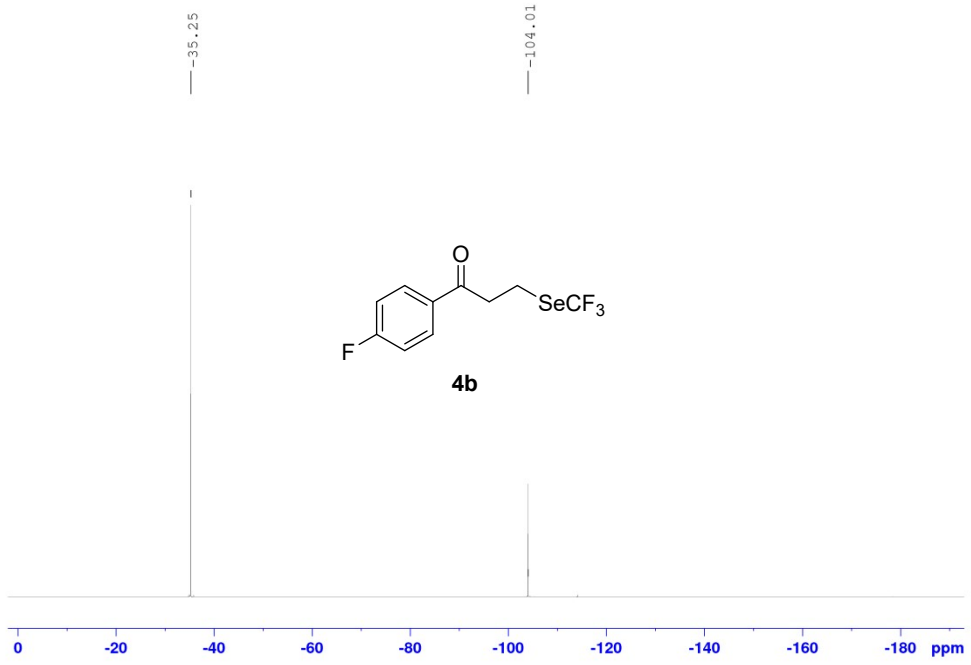
4a

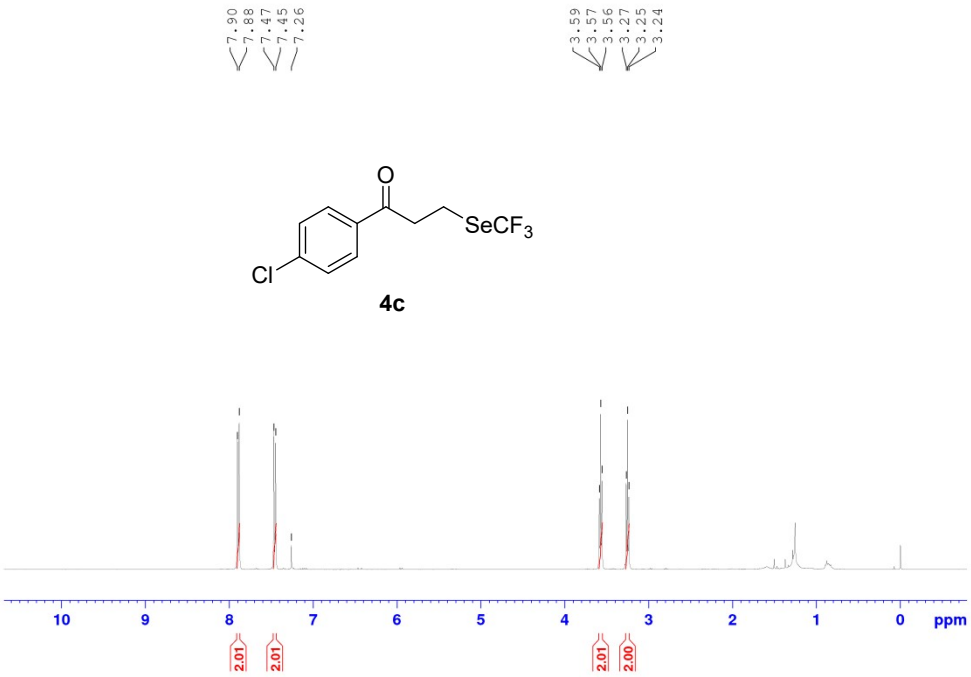

-35.33
O
SeCF3
Me
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

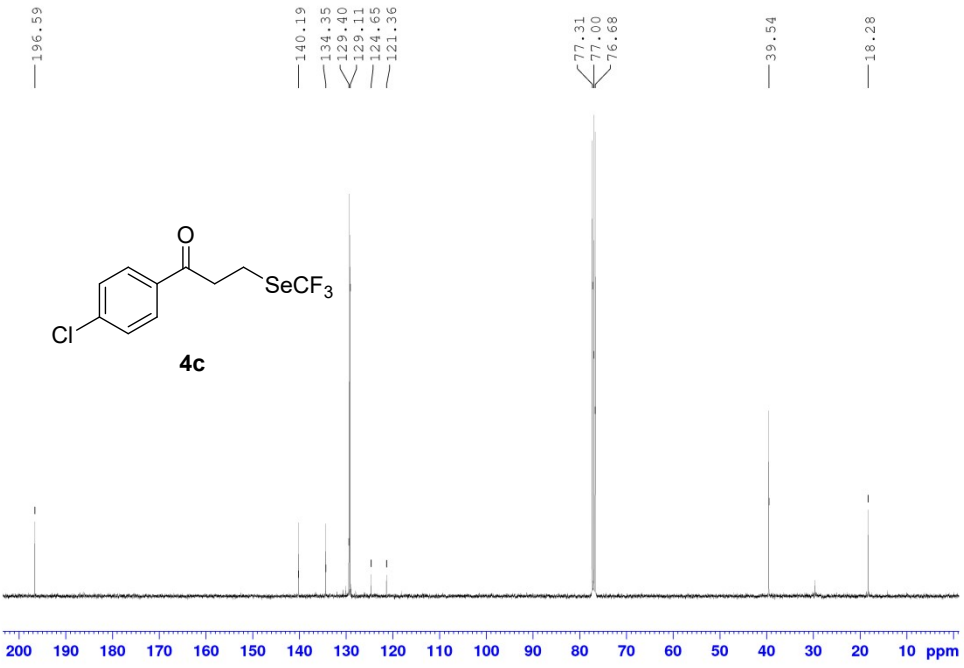
4a

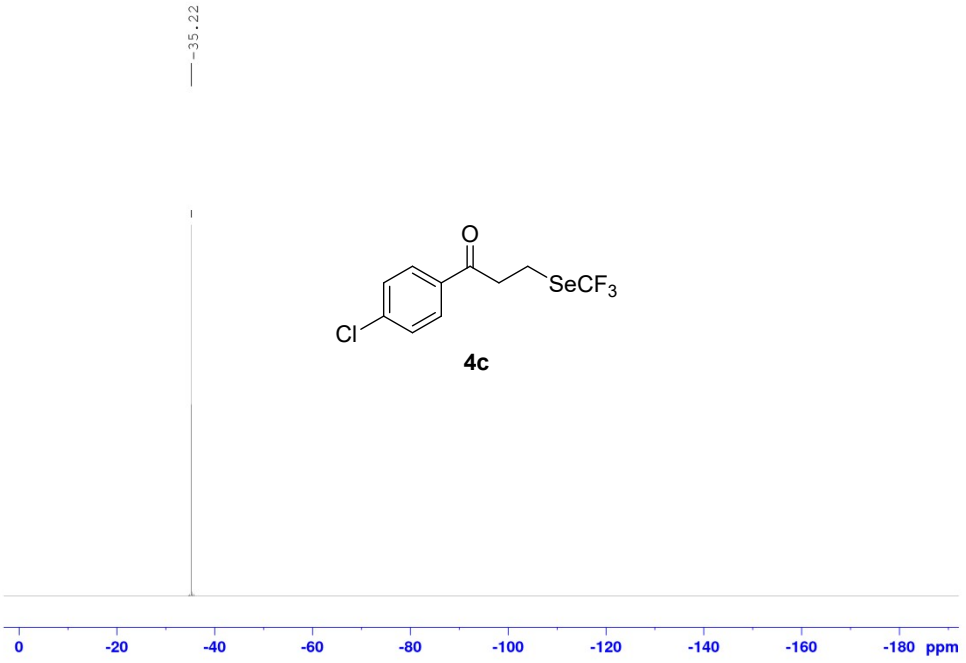

8.00
7.99
7.98
7.97
7.26
7.17
7.15
7.13
3.60
3.58
3.56
3.26
3.25
3.23
O
SeCF3
F
4b
10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
2.01
2.00
2.01


196.21
167.31
164.77
132.50
132.47
130.73
130.64
127.97
124.68
121.39
118.10
116.02
115.80
77.32
77.00
76.68
39.45
18.36
O
SeCF3
F
4b
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

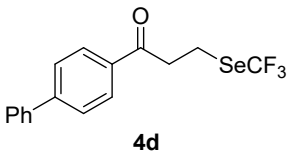

-35.25
-104.01
O
SeCF3
F
4b
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm


7.90
7.88
7.47
7.45
7.26
3.59
3.57
3.56
3.27
3.25
3.24
O
SeCF3
Cl
4c
10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
2.01
2.01
2.00

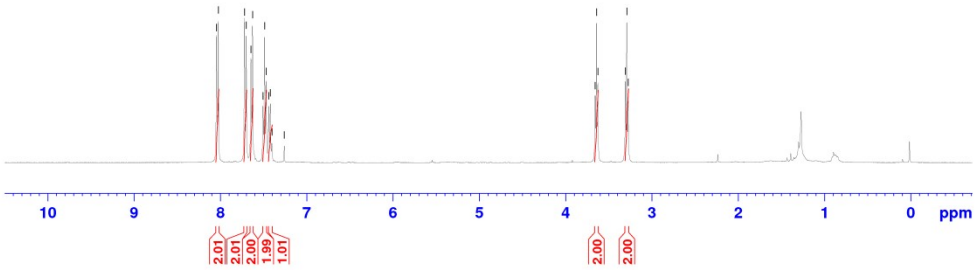

196.59
140.19
134.35
129.40
129.11
124.65
121.36
77.31
77.00
76.68
39.54
18.28
O
SeCF3
Cl
4c
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


-35.22
O
SeCF3
Cl
4c
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

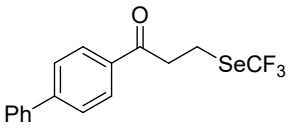

8.05
8.02
7.72
7.70
7.65
7.63
7.51
7.49
7.47
7.44
7.42
7.40
7.26
3.66
3.64
3.63
3.31
3.29
3.28


O
SeCF3
Ph

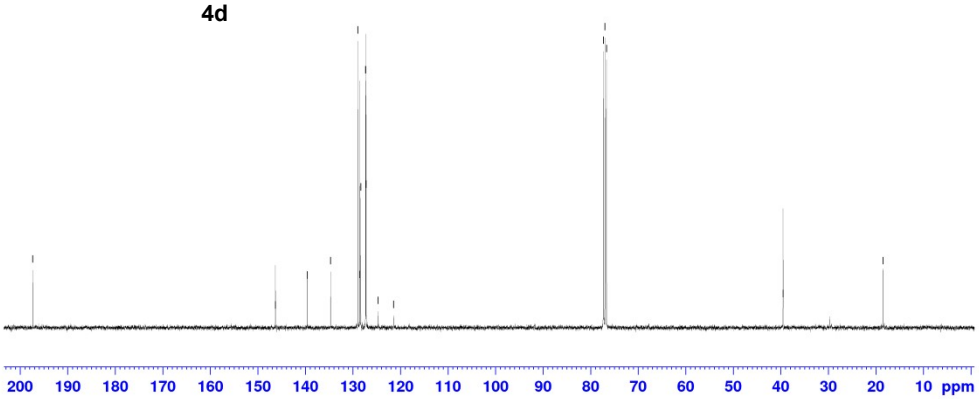
4d

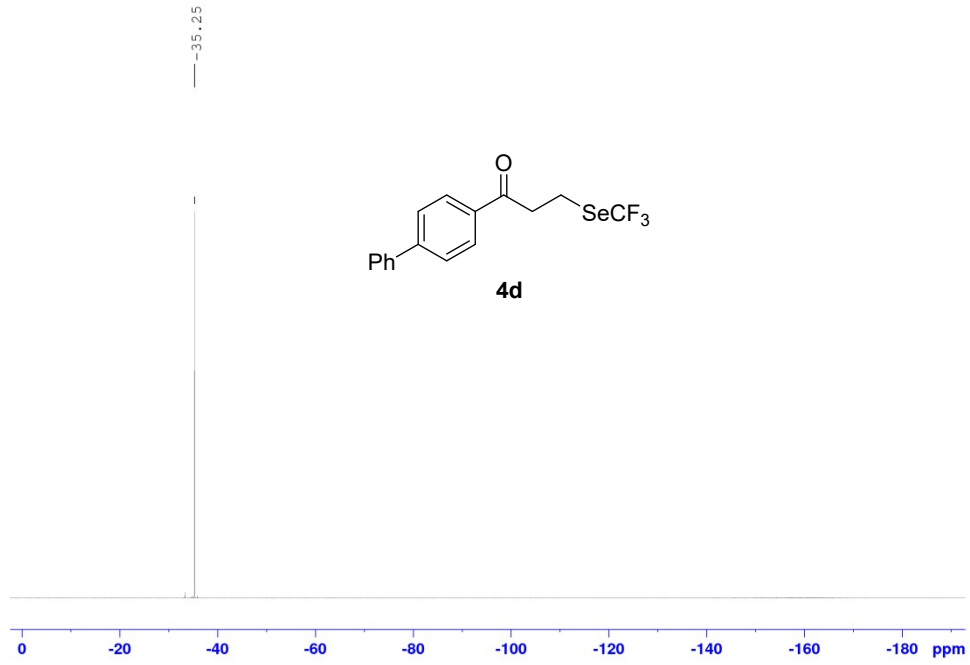

10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
2.01
2.00
1.99
1.01
2.00
2.00


197.38
146.33
139.63
134.70
128.98
128.60
128.37
127.35
127.24
124.74
121.45
77.31
77.00
76.68
39.54
18.51

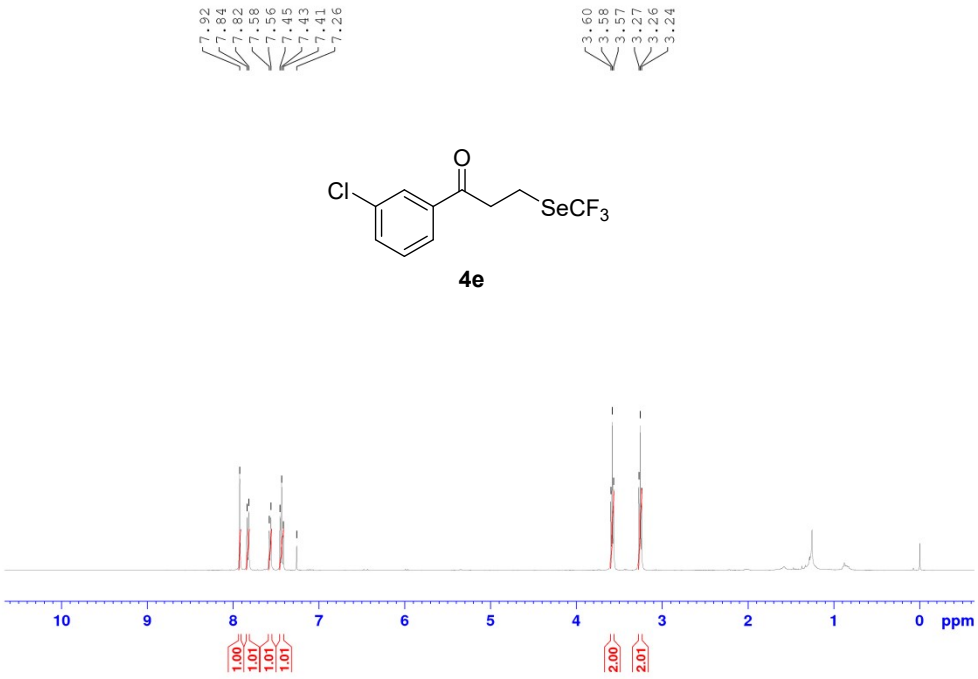

O
SeCF3
Ph

4d

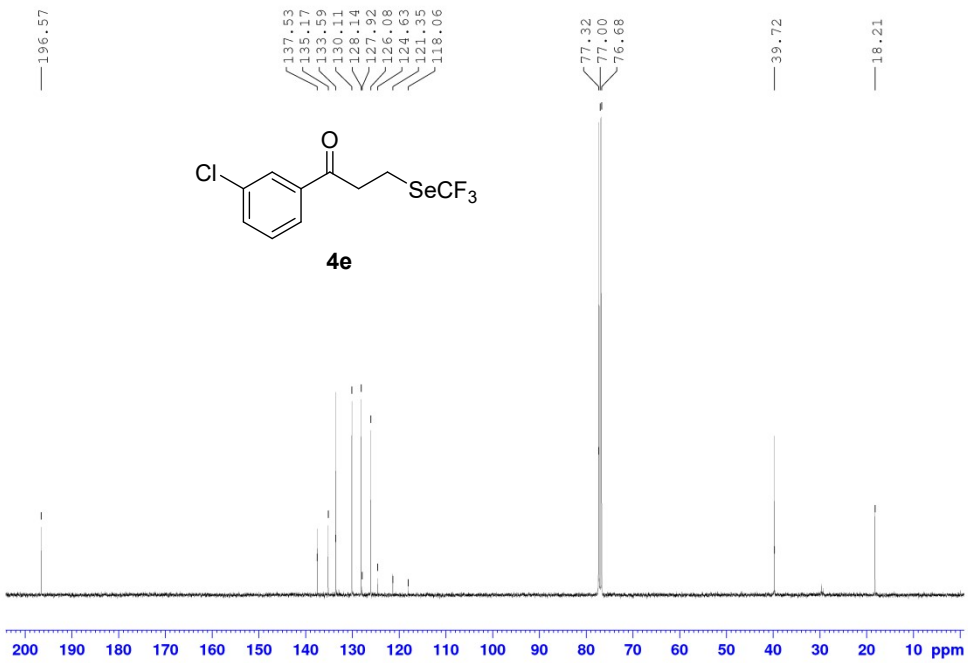

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

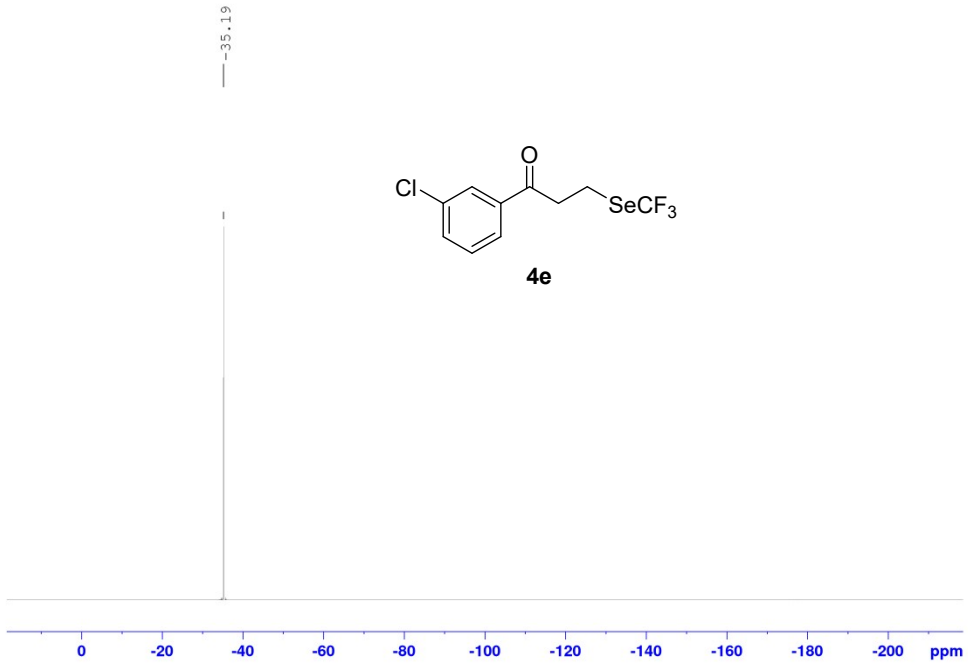

-35.25
O
SeCF3
Ph
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

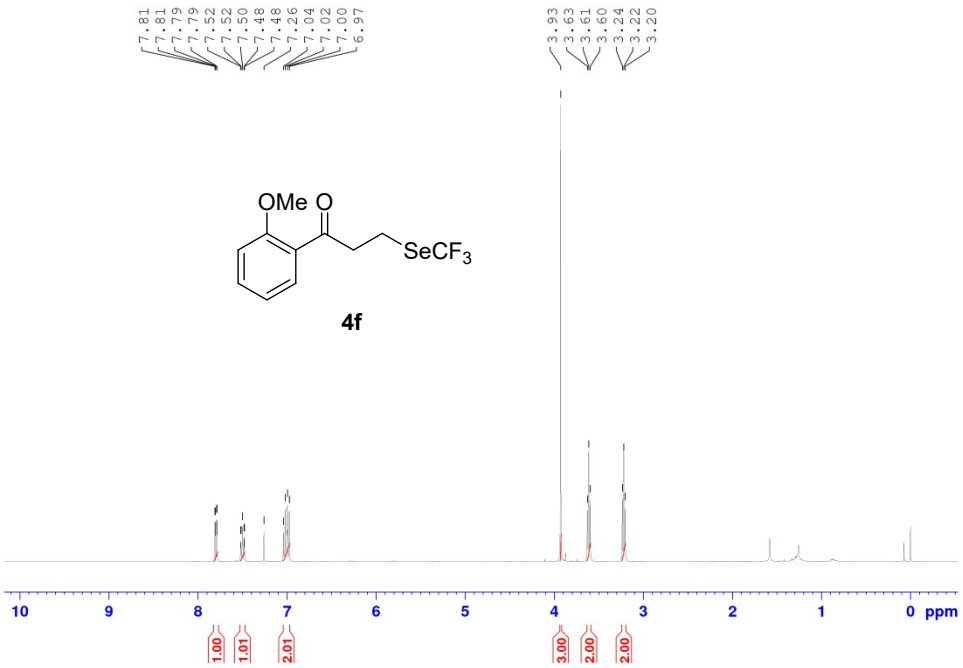
4d

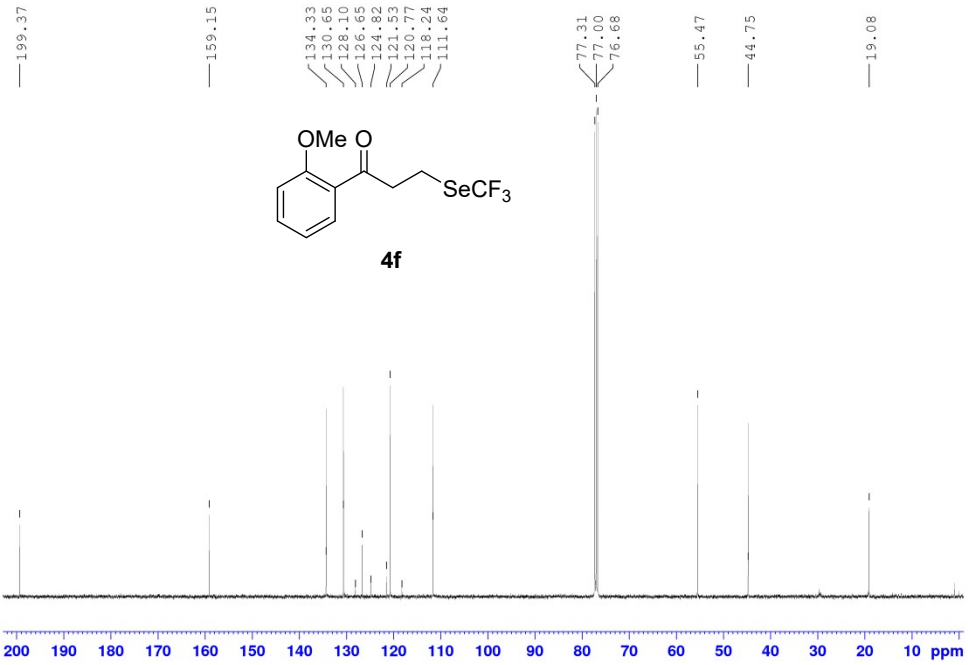

7.92
7.84
7.82
7.58
7.56
7.45
7.43
7.41
7.26
3.60
3.58
3.57
3.27
3.26
3.24
O
Cl
SeCF3
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.01
1.01
2.00
2.01

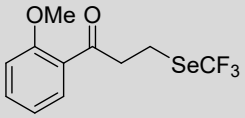
4e


196.57
137.53
135.17
133.59
130.11
128.14
127.92
126.08
124.63
121.35
118.06
77.32
77.00
76.68
39.72
18.21
Cl
O
SeCF3
4e
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


-35.19
Cl
O
SeCF3
4e
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm

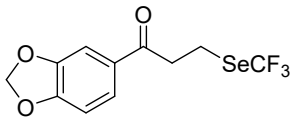

7.81
7.81
7.79
7.79
7.52
7.50
7.48
7.26
7.04
7.02
7.00
6.97
3.93
3.63
3.61
3.60
3.24
3.22
3.20
OMe O
SeCF3
4f
10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.01
2.01
3.00
2.00
2.00


199.37
159.15
134.33
130.65
128.10
126.65
124.82
121.53
120.77
118.24
111.64
77.31
77.00
76.68
55.47
44.75
19.08
OMe O
SeCF3
4f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

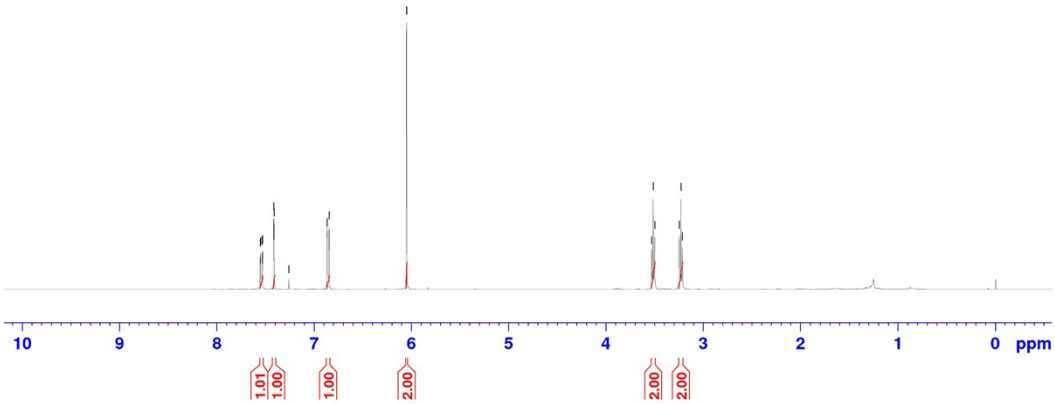

OMe
O
SeCF3

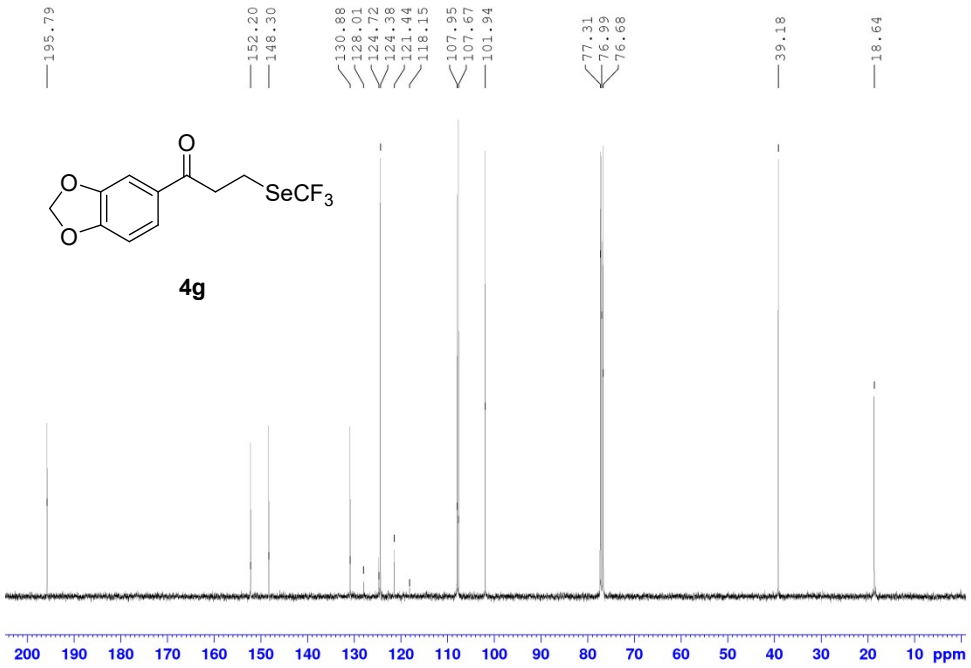
4f


7.55
7.55
7.53
7.53
7.41
7.41
7.26
6.87
6.85
6.05
3.53
3.51
3.50
3.25
3.23
3.21

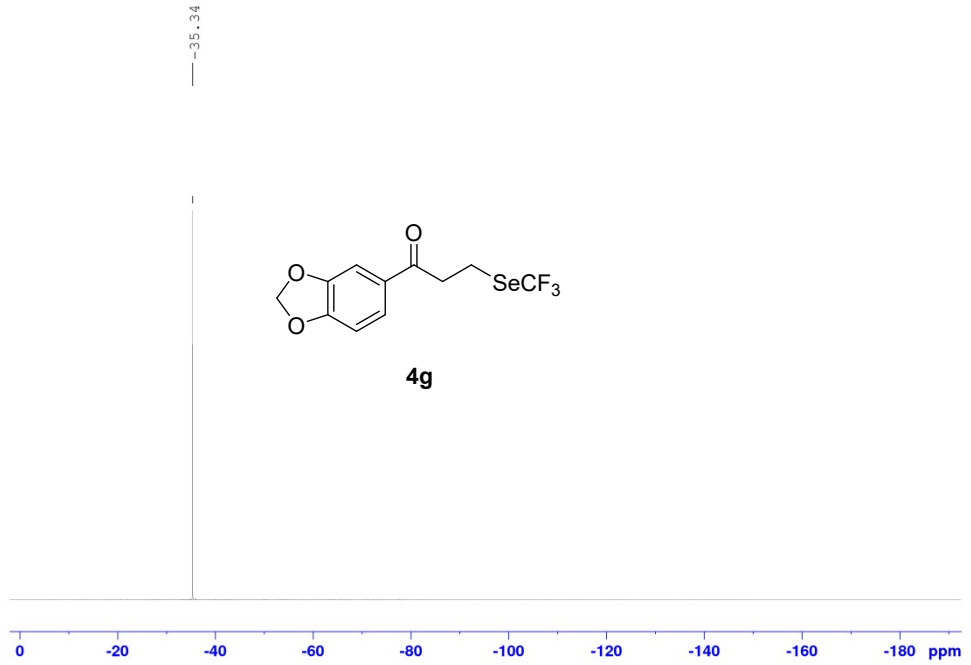

O
O
O
SeCF3

4g

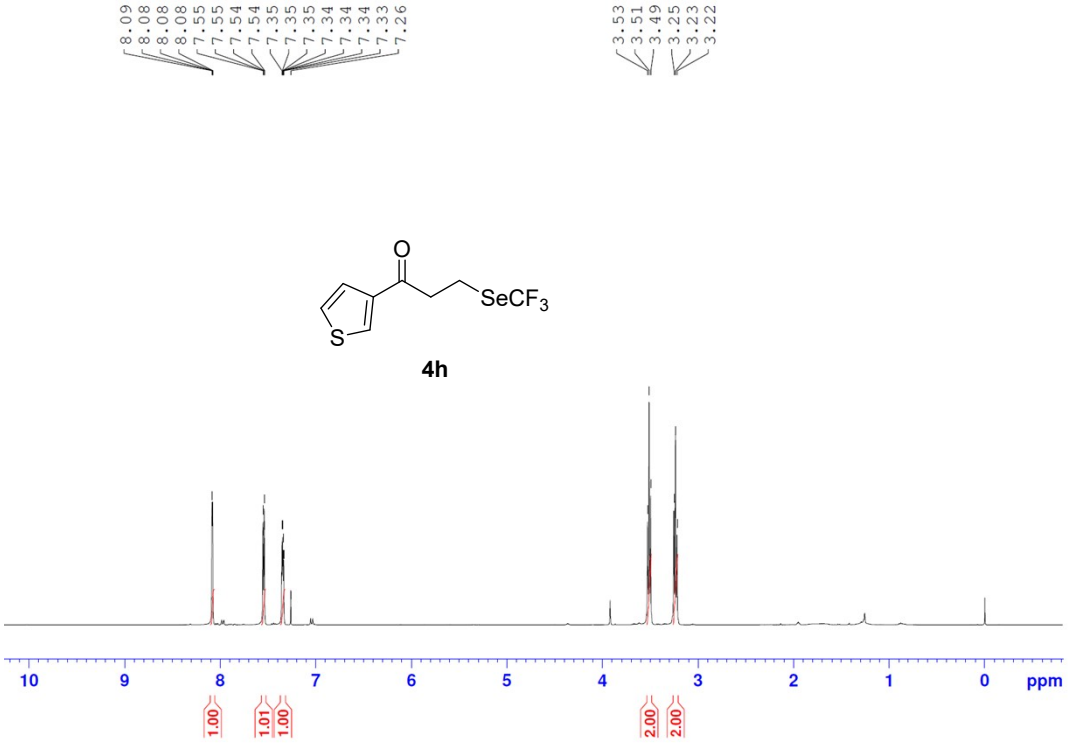

10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
1.00
1.00
2.00
2.00
2.00

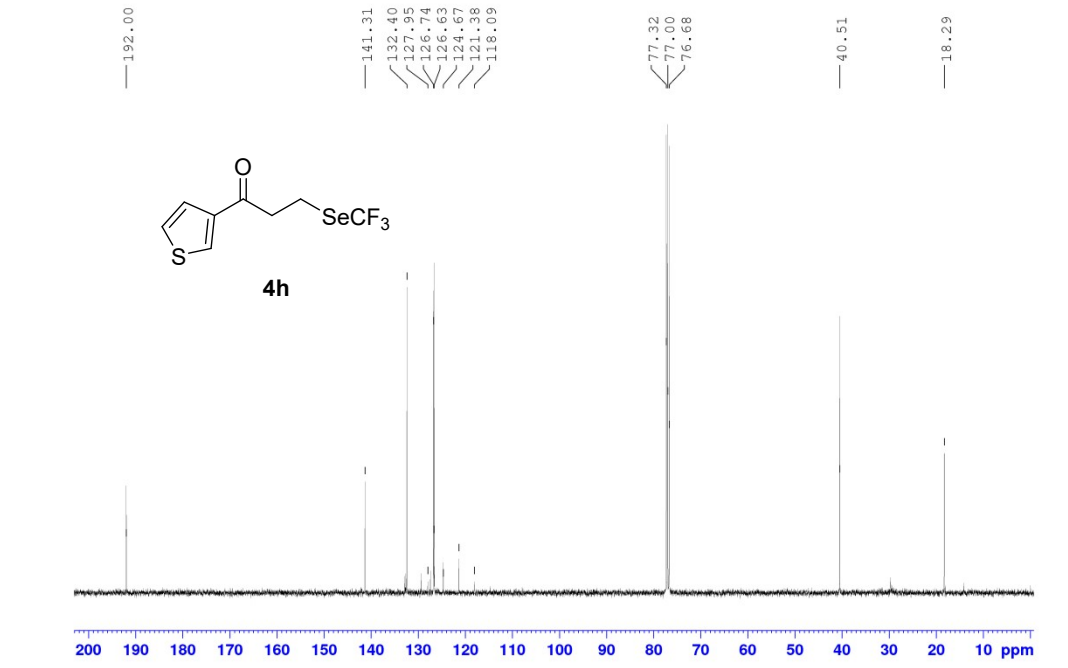

195.79
152.20
148.30
130.88
128.01
124.72
124.38
121.44
118.15
107.95
107.67
101.94
77.31
76.99
76.68
39.18
18.64
O
O
O
SeCF3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

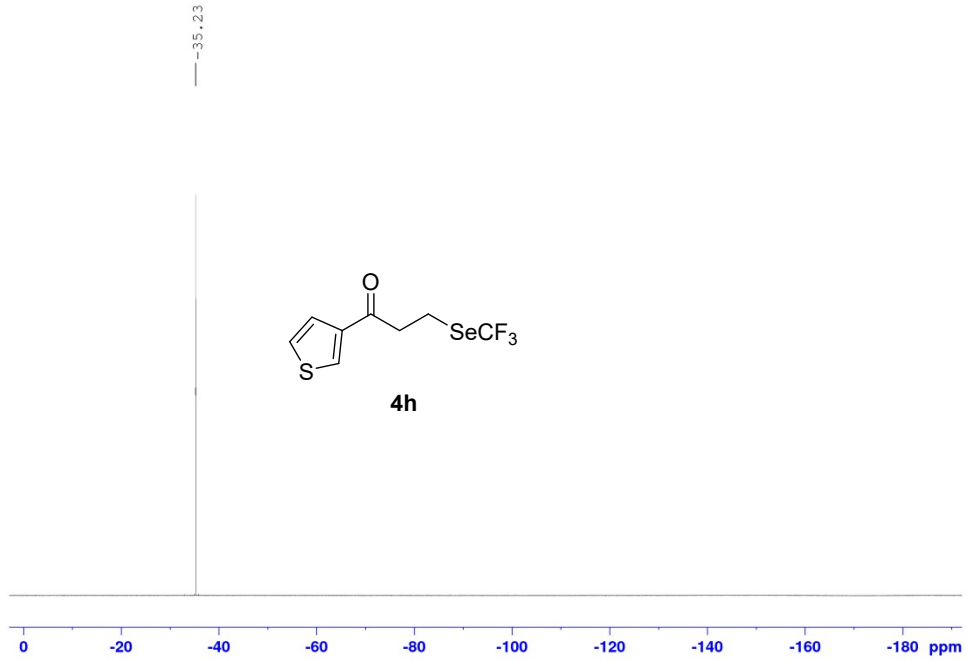
4g


-35.34
O
O
O
SeCF3
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

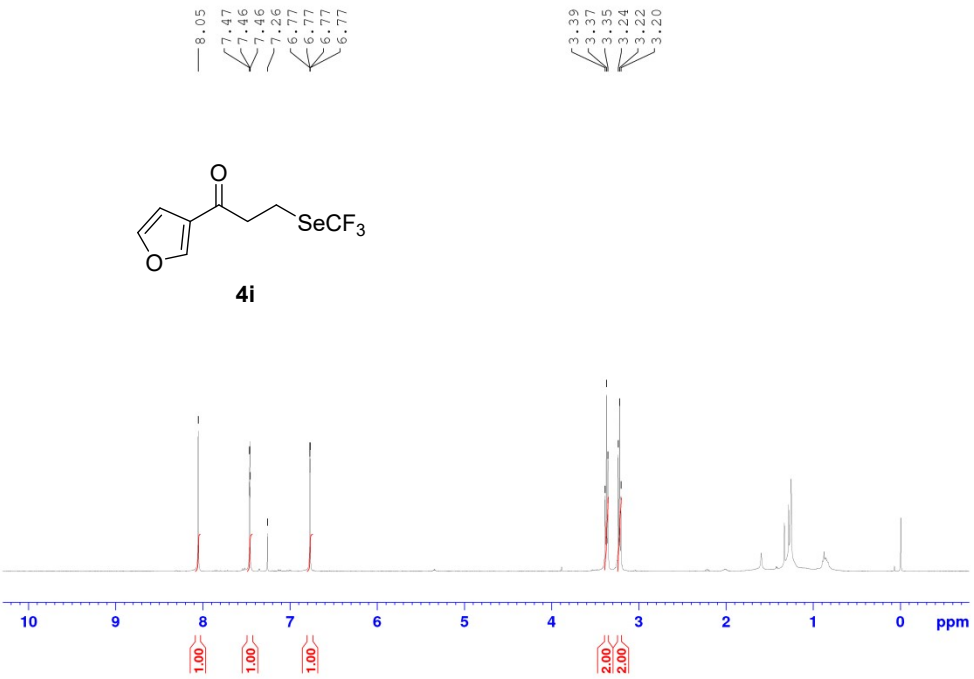
4g


8.09
8.08
8.08
8.08
7.55
7.55
7.54
7.54
7.35
7.35
7.35
7.34
7.34
7.34
7.33
7.26
3.53
3.51
3.49
3.25
3.23
3.22
O
SeCF3
S
4h
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.00
2.00
2.00

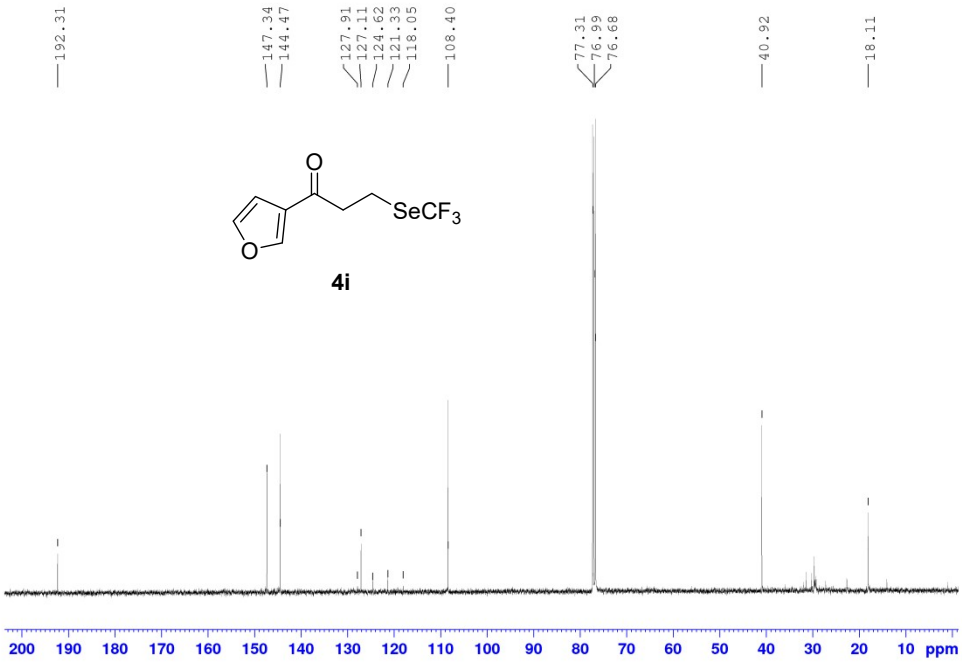

192.00
141.31
132.40
127.95
126.74
126.63
124.67
121.38
118.09
77.32
77.00
76.68
40.51
18.29
O
SeCF3
S
4h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-35.23
O
SeCF3
S
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

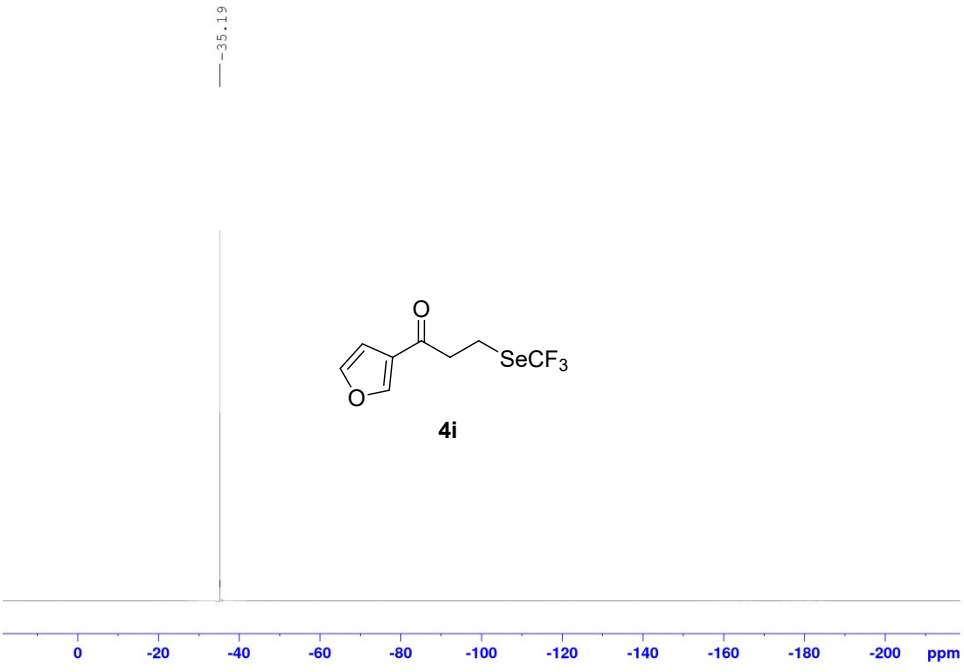
4h


8.05
7.47
7.46
7.46
7.26
6.77
6.77
6.77
6.77
3.39
3.37
3.35
3.24
3.22
3.20
O
SeCF3
O
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
1.00
2.00
2.00

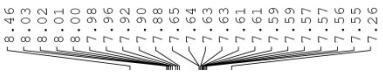
4i


192.31
147.34
144.47
127.91
127.11
124.62
121.33
118.05
108.40
77.31
76.99
76.68
40.92
18.11
O
SeCF3
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

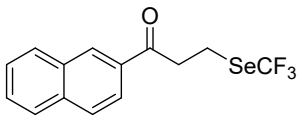
4i


-35.19
O
SeCF3
O
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm

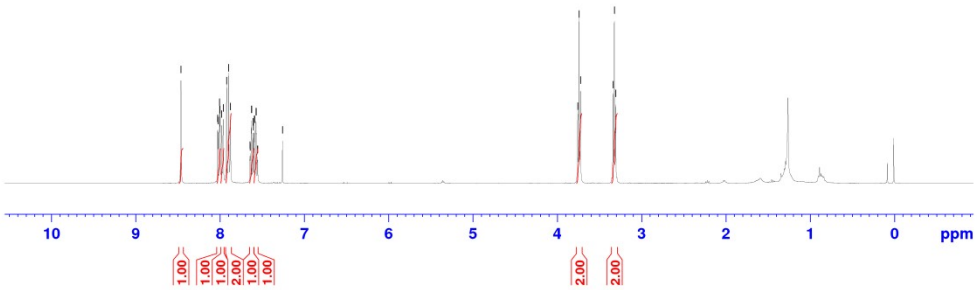
4i

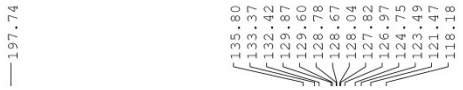

8.46
8.03
8.02
8.01
8.00
7.98
7.96
7.92
7.90
7.88
7.65
7.64
7.63
7.63
7.61
7.61
7.59
7.59
7.57
7.57
7.56
7.55
7.26

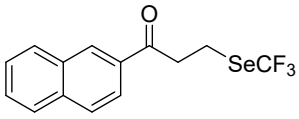

3.76
3.74
3.73
3.34
3.32
3.31


O
SeCF3

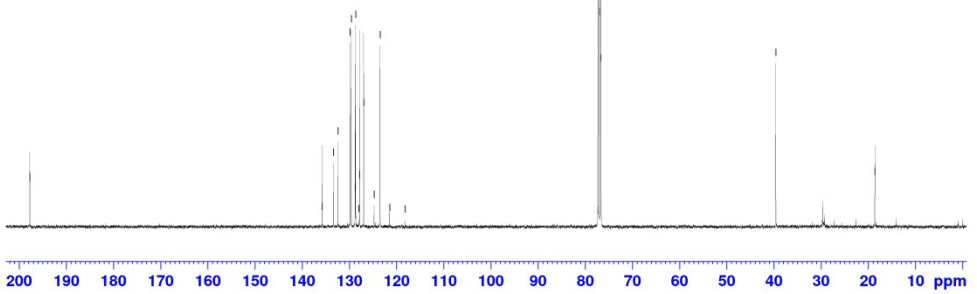
4j

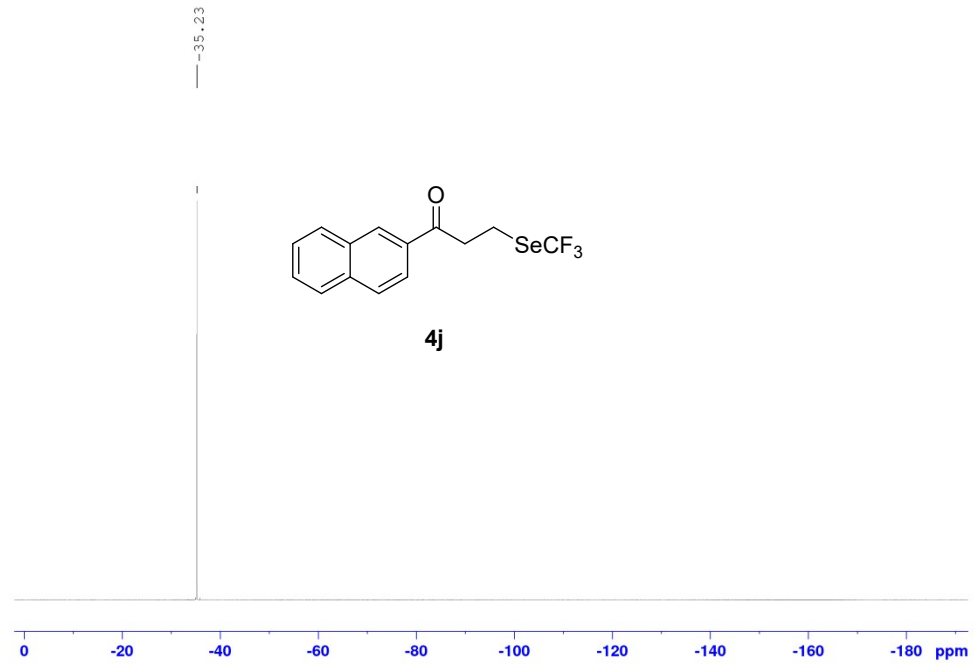

10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
1.00
2.00
1.00
1.00
2.00
2.00


197.74
135.80
133.37
132.42
129.87
129.60
128.78
128.67
128.04
127.82
126.97
124.75
123.49
121.47
118.18
77.32
77.00
76.68
39.59
18.61

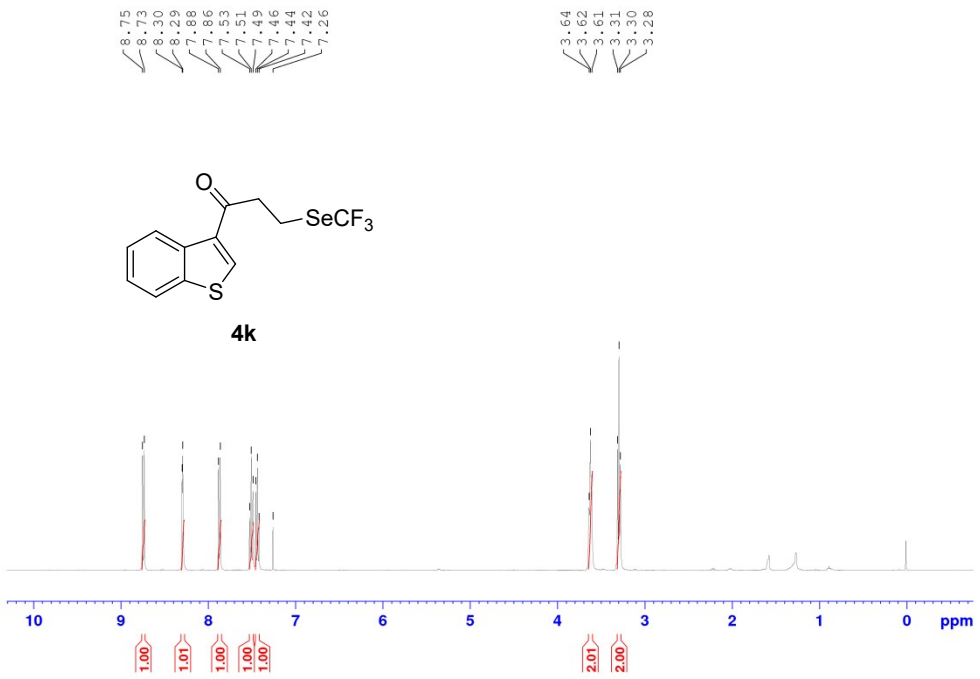

O
SeCF3

4j

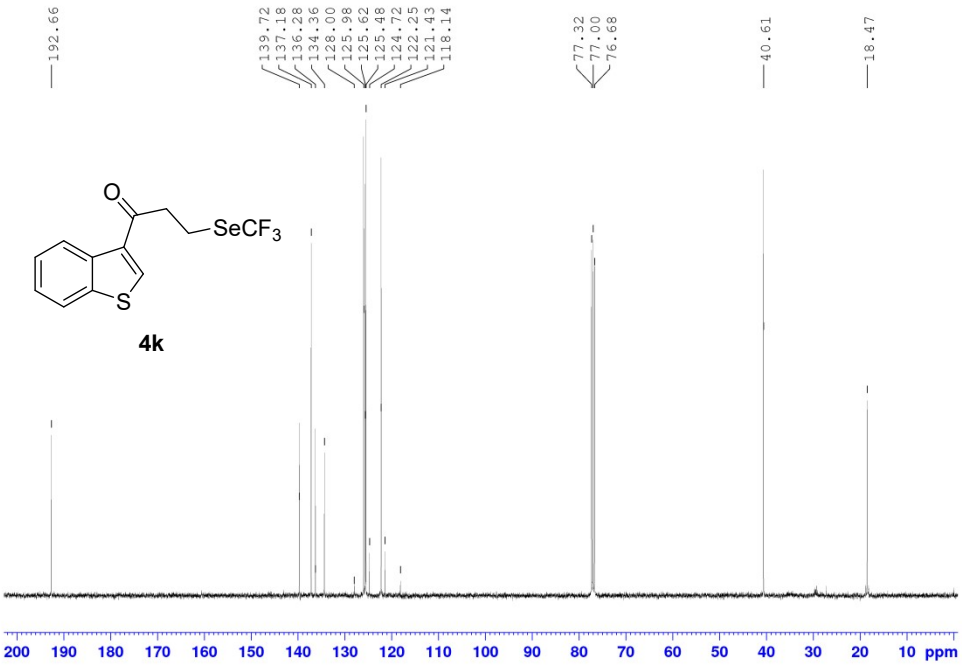

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-35.23
O
SeCF3
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

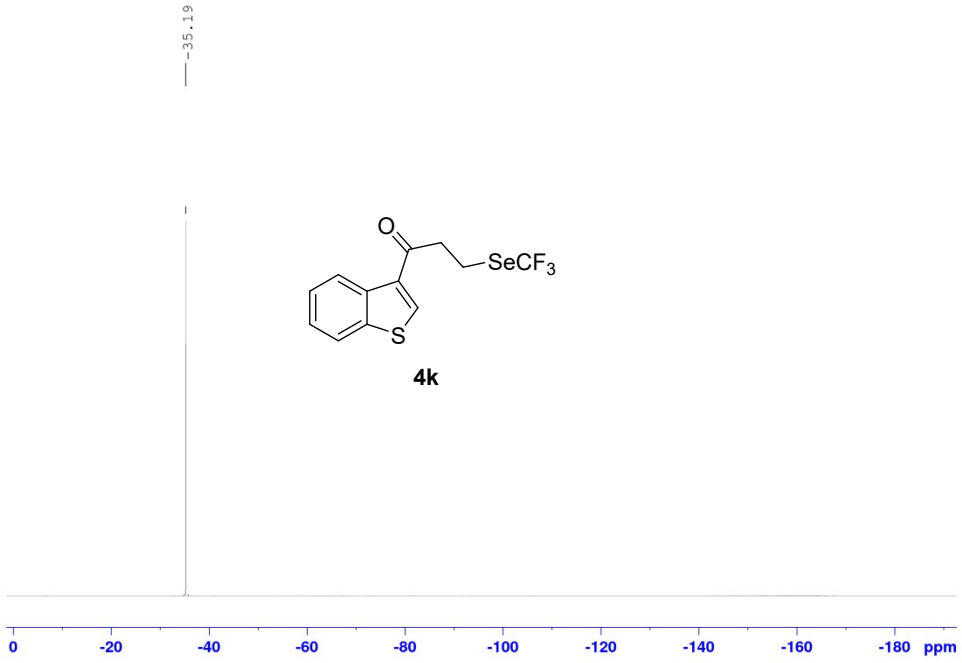
4j


8.75
8.73
8.30
8.29
7.88
7.86
7.53
7.51
7.49
7.46
7.44
7.42
7.26
3.64
3.62
3.61
3.31
3.30
3.28
O
SeCF3
S
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.00
1.00
1.00
2.01
2.00

4k

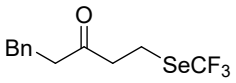

192.66
139.72
137.18
136.28
134.36
128.00
125.98
125.62
125.48
124.72
122.25
121.43
118.14
77.32
77.00
76.68
40.61
18.47
O
SeCF3
S
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

4k

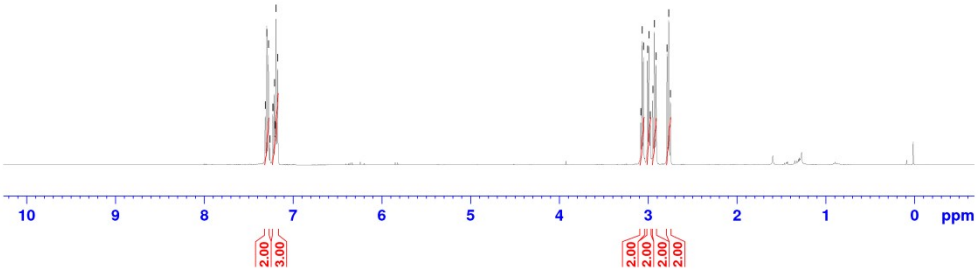

-35.19
O
SeCF3
S
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

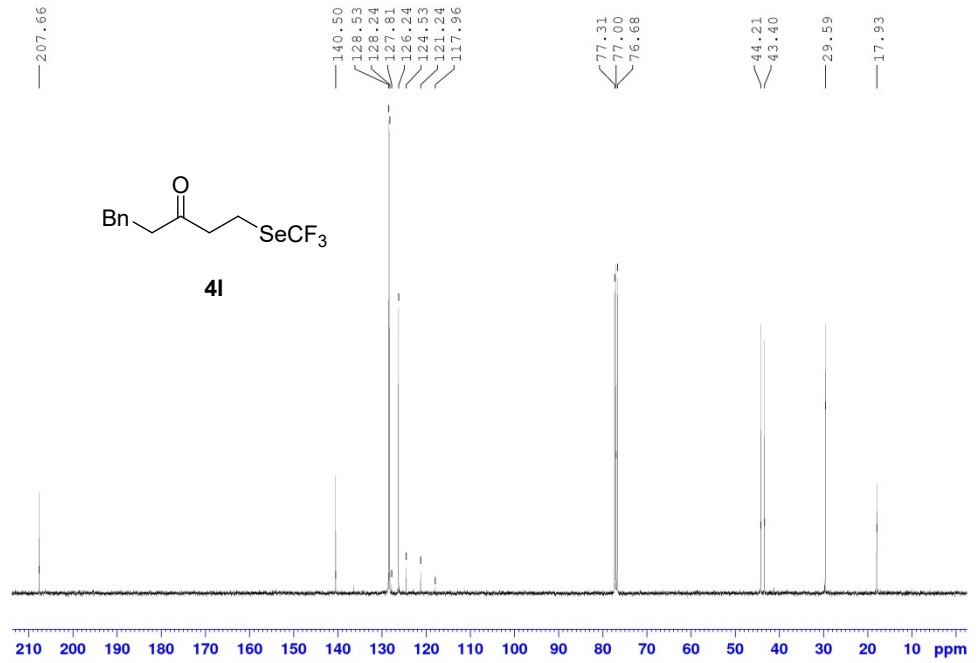
4k


7.31
7.30
7.28
7.26
7.23
7.23
7.21
7.20
7.19
7.17
3.08
3.07
3.05
3.01
2.99
2.98
2.95
2.93
2.91
2.79
2.77
2.75

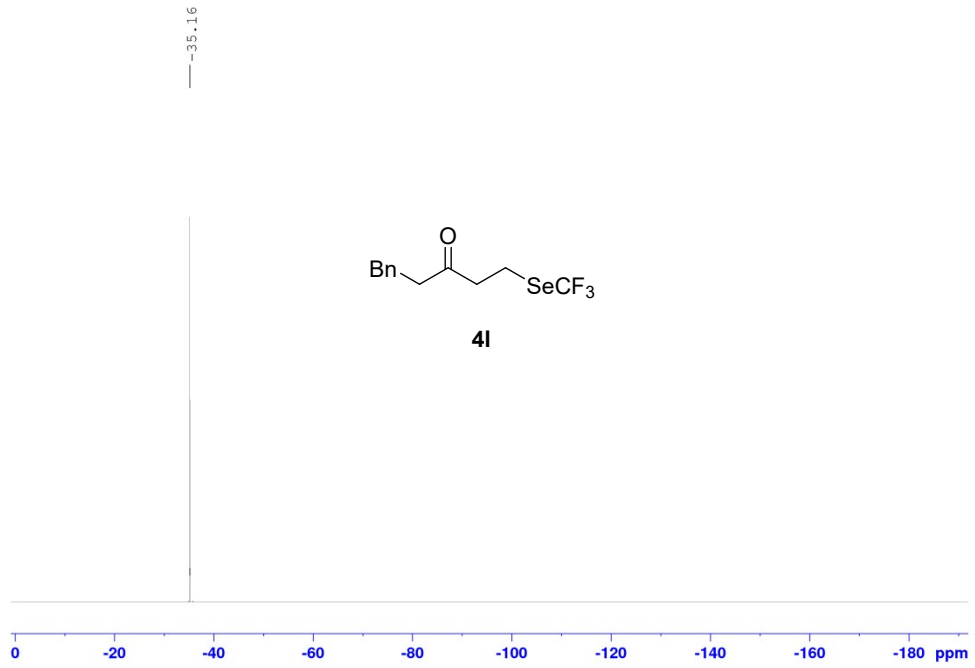

O
Bn
SeCF3

4l

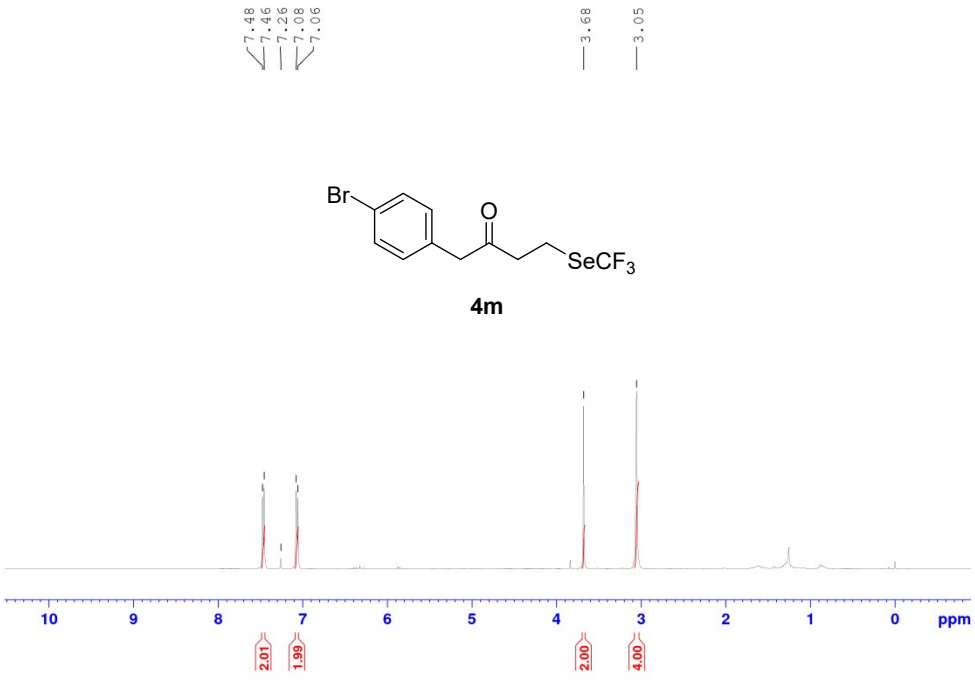

10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
3.00
2.00
2.00
2.00
2.00


207.66
140.50
128.53
128.24
127.81
126.24
124.53
121.24
117.96
77.31
77.00
76.68
44.21
43.40
29.59
17.93
O
Bn
SeCF3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

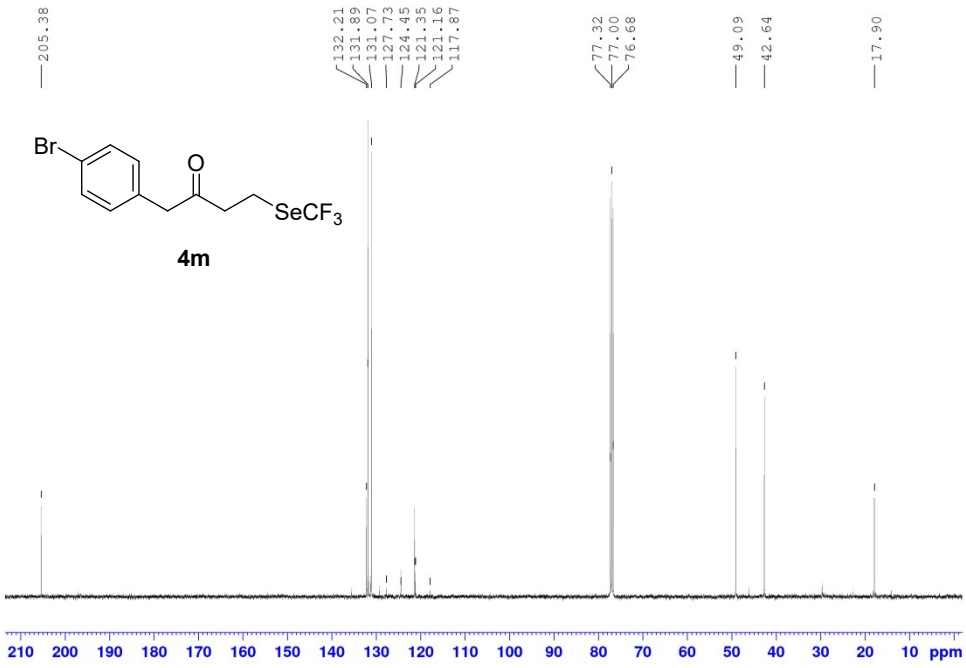
4l

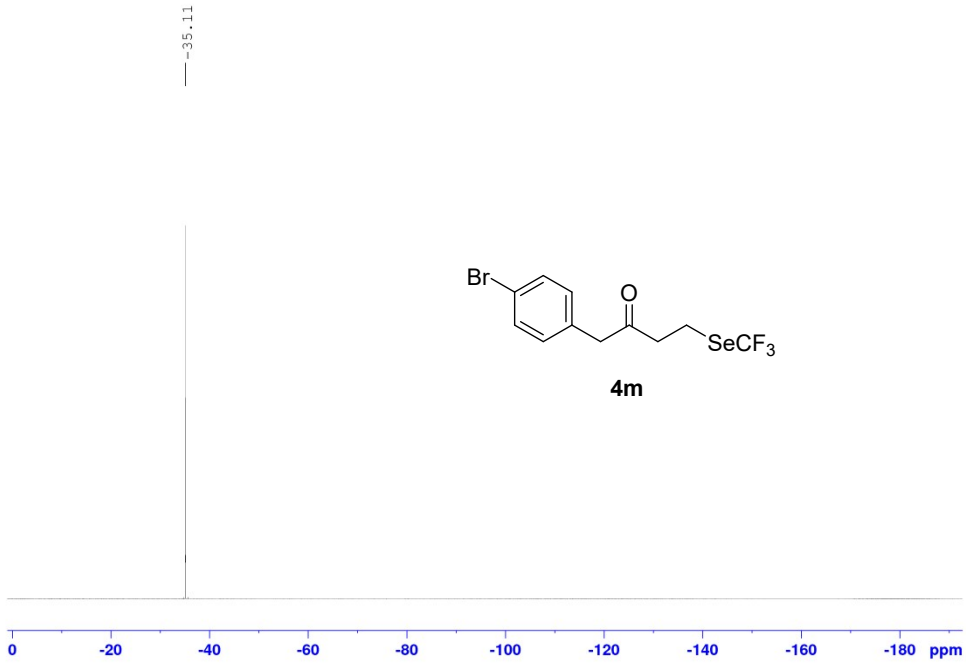

-35.16
Bn
O
SeCF3
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

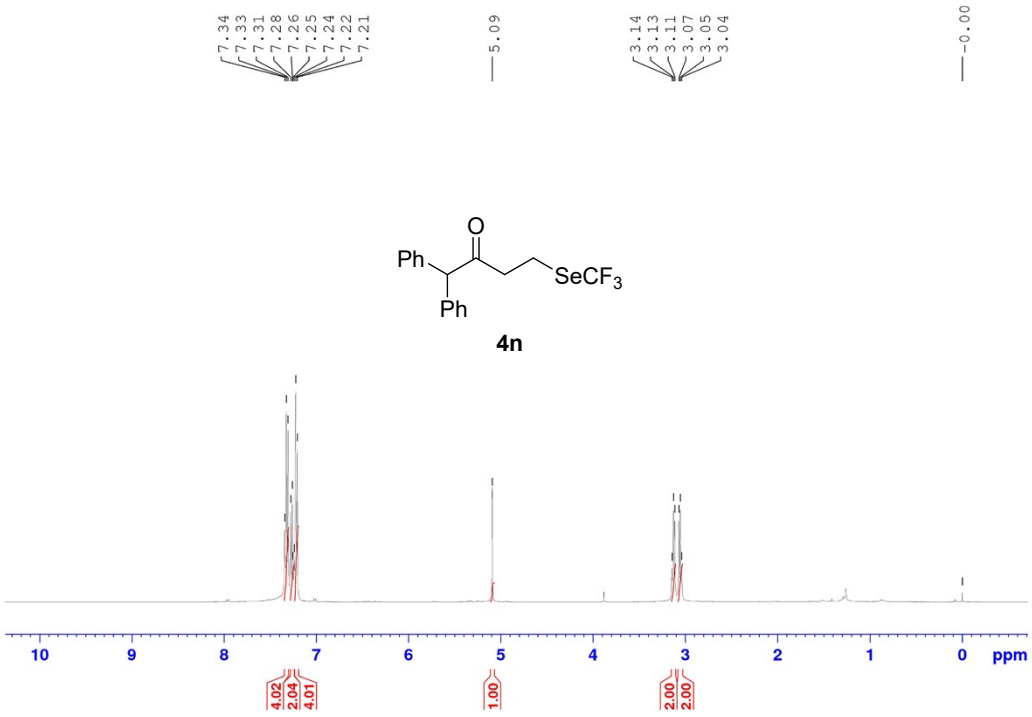
4l

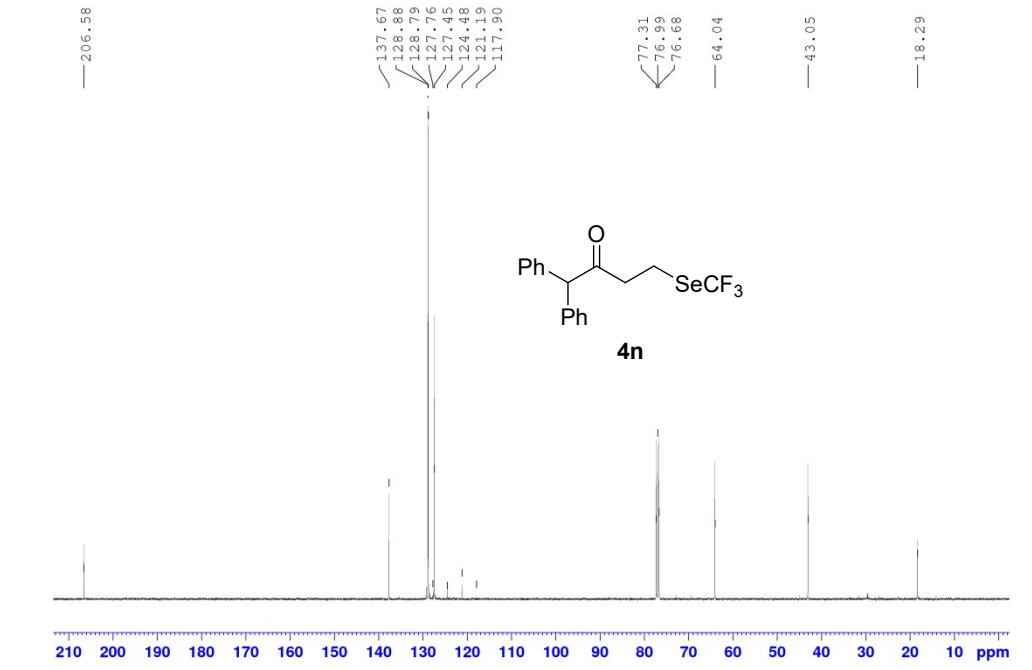

7.48
7.46
7.26
7.08
7.06
3.68
3.05
Br
O
SeCF3
10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
1.99
2.00
4.00

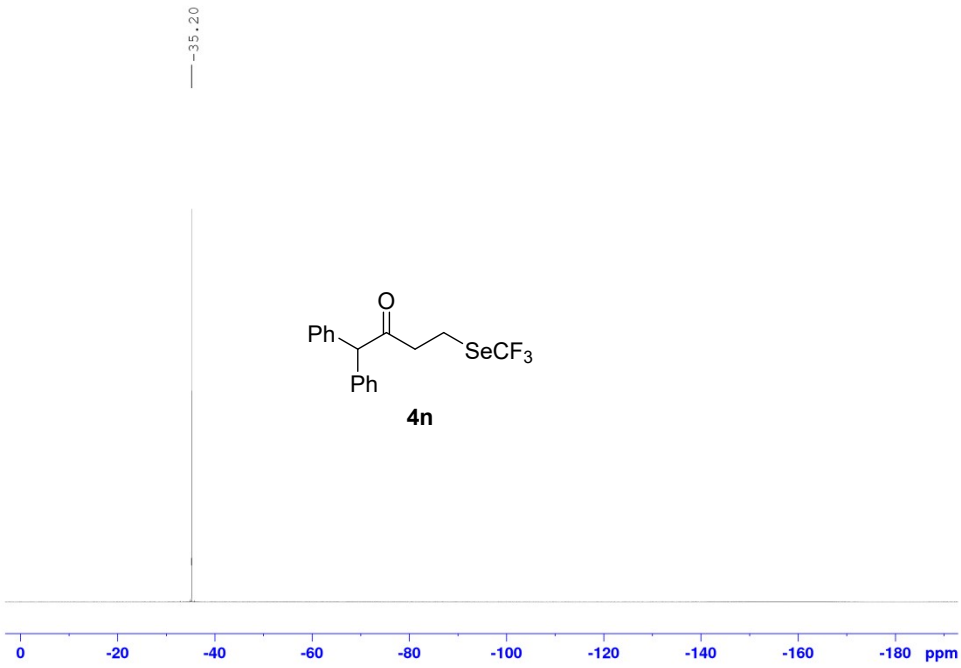
4m


205.38
132.21
131.89
131.07
127.73
124.45
121.35
121.16
117.87
77.32
77.00
76.68
49.09
42.64
17.90
Br
O
SeCF3
4m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

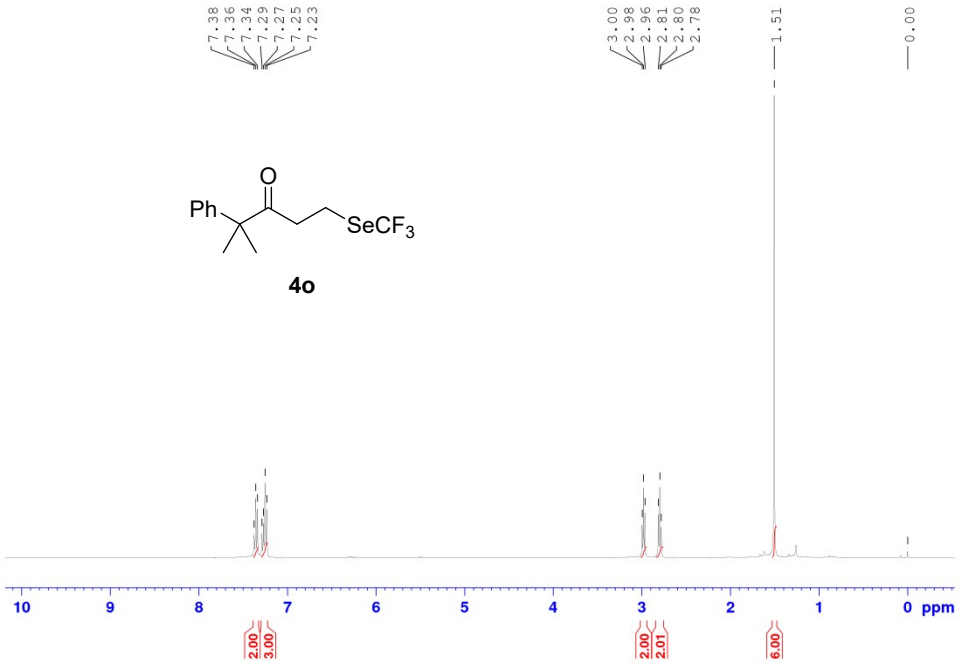

-35.11
Br
O
SeCF3
4m
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm


7.34
7.33
7.31
7.28
7.26
7.25
7.24
7.22
7.21
5.09
3.14
3.13
3.11
3.07
3.05
3.04
0.00
O
Ph
Ph
SeCF3
4n
10
9
8
7
6
5
4
3
2
1
0
ppm
4.02
2.04
4.01
1.00
2.00
2.00

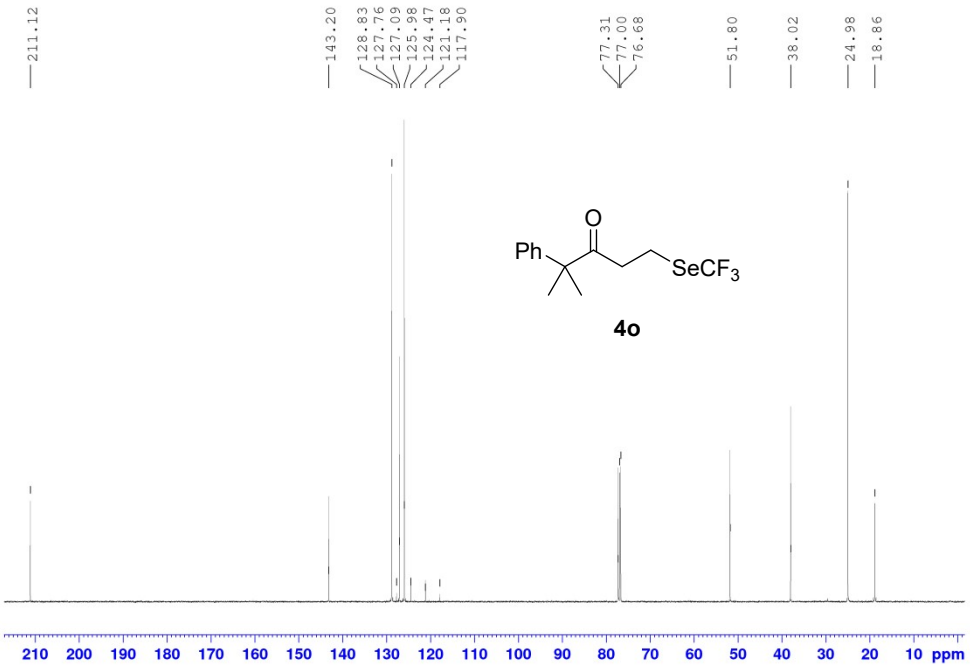

206.58
137.67
128.88
128.79
127.76
127.45
124.48
121.19
117.90
77.31
76.99
76.68
64.04
43.05
18.29
O
Ph
Ph
SeCF3
4n
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-35.20
O
Ph
Ph
SeCF3
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

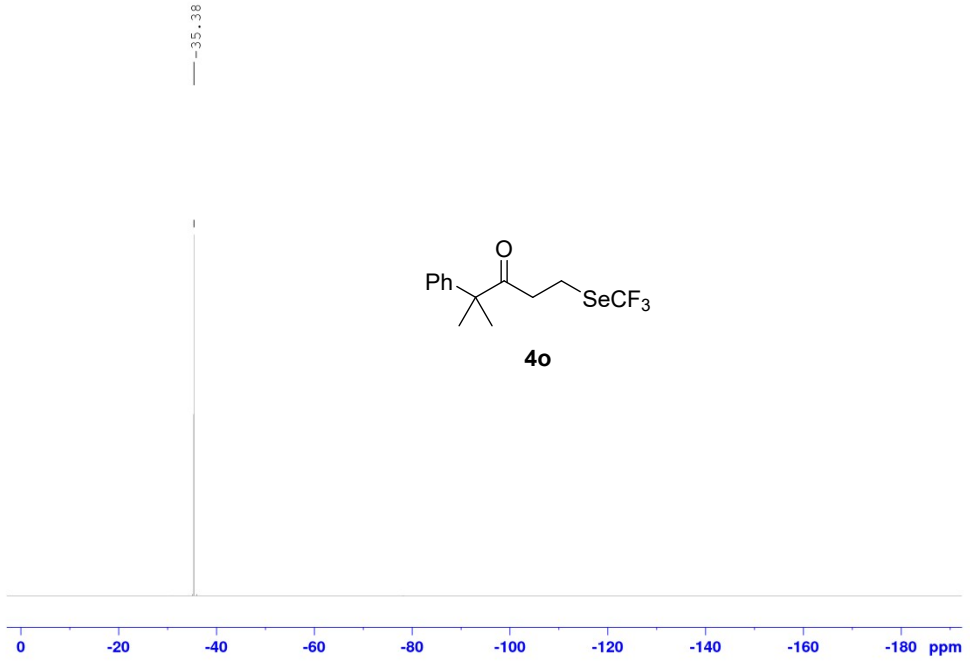
4n


7.38
7.36
7.34
7.29
7.27
7.25
7.23
3.00
2.98
2.96
2.81
2.80
2.78
1.51
0.00
O
Ph
SeCF3
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
3.00
2.00
2.01
6.00

4o


211.12
143.20
128.83
127.76
127.09
125.98
124.47
121.18
117.90
77.31
77.00
76.68
51.80
38.02
24.98
18.86
O
Ph
SeCF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

4o


-35.38
O
Ph
SeCF3
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

4o