Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

`

Influence of Sulfonyl Substituents on the Decomposition of *N*-Sulfonylhydrazones at Room Temperature

Zhaohong Liu,[a] Kaki Raveendra Babu,[a] Feng Wang,[c] Yang Yang,[a] and Xihe Bi*[ab]

[a]Jilin Province Key Laboratory of Organic Functional Molecular Design & Synthesis, Northeast Normal University, Changchun 130024, China.

[b] State Key Laboratory of Elemento-Organic Chemistry, Nankai University, Tianjin 300071, China.

[c] School of Chemical Engineering, Changchun University of Technology, Changchun 130012, China

E-mail: bixh507@nenu.edu.cn

Contents

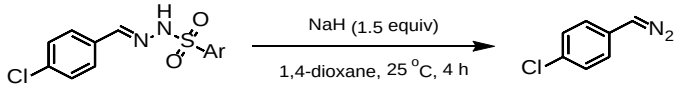
I. General information

Unless otherwise noted, all reactions were carried out in standard Schlenk techniques with magnetic stirring bar under air. All reagents were purchased from commercial sources and used without purification unless otherwise mentioned. The products were purified by column chromatography over silica gel (200-400 size). ^{1}H and ^{13}C Nuclear Magnetic Resonance (NMR) spectra were recorded at 25 °C on a Varian 600 MHz and 151 MHz, and TMS was used as internal standard. Chemical shifts are reported in ppm with the deuterium solvent as the internal standard (e.g. $CDCl_3$: 77.0 ppm). Mass spectra were recorded on BRUKER AutoflexIII Smartbeam MS-spectrometer. High resolution mass spectra (HRMS) were recorded on Bruck microTof by using ESI method.

II. Optimization of the decomposition of *N*-sulfonylhydrazone

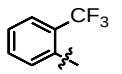
General procedure A (with 1aa as an example): In a rubber capped reaction vial, *N*'-(4-chlorobenzylidene)-2-trifluoromethylbenzenesulfonohydrazide **1aa** (181.4 mg, 0.5 mmol) 1,3,5-trimethyoxybenzene (42.05 mg, 0.25 mmol), and NaH (30.0 mg, 60 wt%, 0.75 mmol) were added. After sealed the tube was evacuated and backfilled with N2 for three times, followed by dry 1,4-dioxane (10 mL) addition via syringe. The reaction mixture was stirred at 25 ºC for 4 h. At the indicated reaction time, 200 ul reaction mixture was extracted with a syringe, which was dissolved in DMSO-d_6 for NMR analysis.

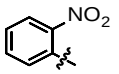
Table S1. Effect of substituent on the aryl ring of sulfonyl group[a]

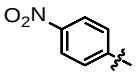


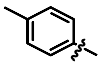
1aa-1ha **2aa**

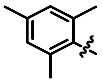
Ar =

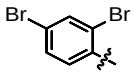

1aa

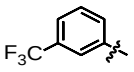

1ba

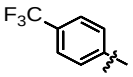

1ca


1da


1ea


1fa

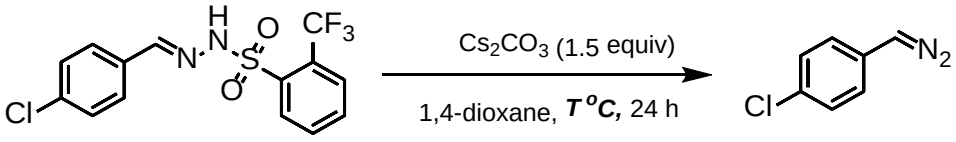

1ga


1ha

Time (min)	1aa	1ba	1ca	1da	1ea	1fa	1ga	1ha
0	0	0	0	0	0	0	0	0
10	45	18	0	0	13	0	0	0
20	60	27	0	0	25	24	0	0
30	70	33	1	1	36	32	2	2
60	80	44	1	2	46	37	4	3
120	82	60	2	3	39	33	8	4
180	85	69	3	4	35	33	8	6
240	89	75	4	5	33	20	6	4

[a] Reaction conditions: **1** (0.5 mmol), NaH (0.75 mmol), in 1,4-dioxane (10.0 mL) for 4 h under N_2 atmosphere. Yield calculated from ^{1}H-NMR spectroscopy with 1,3,5-trimethyoxybenzene as the internal standard and the yield is the average of three repeated experiments.

Table S2. Effect Effect of temperature on the decomposition of **1aa**[a]



1aa **2aa**

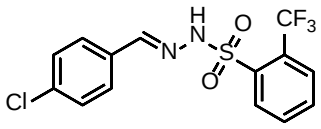
Time	-25 ºC	0 ºC	25 ºC	40 ºC
10 min	2	5	27	43
30 min	5	12	57	80
1 h	6	16	72	91
1.5 h	7	18	88	88

2 h	8	22	93	84
4 h	10	28	87	70
6 h	12	35	83	60
9 h	14	42	79	53
18 h	18	51	77	45
24 h	20	55	76	40

[a] Reaction conditions: 1 (0.5 mmol), Cs_2CO_3 (0.75 mmol), in 1,4-dioxane (10.0 mL) for 24 h under N_2 atmosphere. Yield calculated from ^{1}H-NMR spectroscopy with 1,3,5-trimethyoxybenzene as the internal standard and the yield is the average of three repeated experiments.

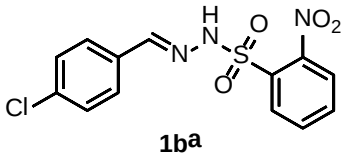
III. General procedure for the synthesis of *N*-sulfonylhydrazone

General procedure B: To a stirred solution of $ArSO_2NHNH_2$ (2.0 mmol, 1.0 equiv) in methanol (2 mL) were added carbonyl compounds (2.2 mmol, 1.1 equiv) and the mixture was stirred for 1-2 h at room temperature. The mixture was filtered and the resulting solid was washed with ice cold diethyl ether and dried under reduced pressure to give pure *N*-Sulfonylhydrazones. The yields were around 80% in general.



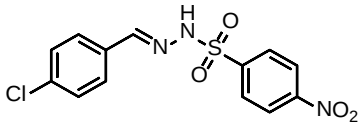
1aa

***N′*-(4-Chlorobenzylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1aa).** White solid, m.p. 151-152 ^oC; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 7.43 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 8.4 Hz, 2H), 7.86 (t, *J* = 7.8 Hz, 1H), 7.92 (t, *J* = 7.8 Hz, 1H), 8.01 (d, *J* = 7.2 Hz, 1H), 8.05 (s, 1H), 8.13 (d, *J* = 7.8 Hz, 1H), 12.19 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 123.2 (q, *J* = 272.0 Hz), 126.9 (q, *J* = 33.0 Hz), 128.91(q, *J* = 6.2 Hz), 128.92, 129.4, 131.7, 132.9, 133.8, 134.0, 135.1, 138.5, 146.1; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.23 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{14}H_{10}ClF_3N_2O_2SNa$ $[M+Na]^+$ 384.9996, found 384.9999.



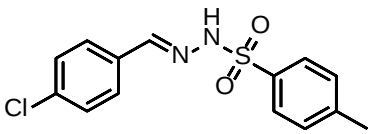
1ba

***N′*-(4-Chlorobenzylidene)-2-nitrobenzenesulfonohydrazide (1ba)**. White solid, m.p. 152-153 ^{o}C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 7.44 (d, *J* = 8.4 Hz, 2H), 7.60 (d, *J* = 8.4 Hz, 2H), 7.86-7.91 (m, 2H), 7.99-8.02 (m, 1H), 8.05-8.08 (m, 2H), 12.25 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 125.0, 129.0, 129.4, 131.0, 131.4, 132.8, 133.1, 135.28, 135.32, 146.9, 148.3; **HRMS** (ESI) m/z calculated for $C_{13}H_{10}ClN_3O_4SNa$ $[M+Na]^+$ 361.9973, found 361.9968.



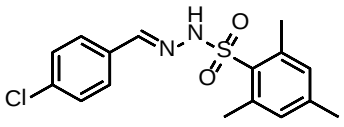
1ca

***N′*-(4-Chlorobenzylidene)-4-nitrobenzenesulfonohydrazide (1ca)**. Yellow solid, m.p. 175-176 ^{o}C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 7.45 (d, *J* = 8.4 Hz, 2H), 7.60 (d, *J* = 8.4 Hz, 2H), 7.97 (s, 1H), 8.14 (d, *J* = 8.4 Hz, 2H), 8.42 (d, *J* = 8.4 Hz, 2H), 11.97 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 125.1, 129.1, 129.3, 129.4, 132.8, 135.3, 144.7, 147.5, 151.5; **HRMS** (ESI) m/z calculated for $C_{13}H_{10}ClN_3O_4SNa$ $[M+Na]^+$ 361.9973, found 361.9965.



1da

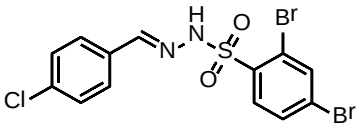
***N′*-(4-Chlorobenzylidene)-4-methylbenzenesulfonohydrazide (1da)**. White solid, m.p. 147-148 ^{o}C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 2.35 (s, 3H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.45 (d, *J* = 8.4 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.76 (d, *J* = 8.4 Hz, 2H), 7.90 (s, 1H), 11.54 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 21.5, 127.7, 128.9, 129.4, 130.2, 133.1, 135.0, 136.6, 144.0, 146.1; **HRMS** (ESI) m/z calculated for $C_{14}H_{13}ClN_2O_2SNa$ $[M+Na]^+$ 331.0278, found 331.0281.



1ea

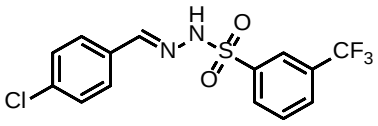
***N′*-(4-Chlorobenzylidene)-2,4,6-trimethylbenzenesulfonohydrazide (1ea)**. Yellow solid, m.p. 143-144 ^{o}C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 2.23 (s, 3H), 2.63 (s, 6H), 7.04 (s, 2H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.90 (s, 1H), 11.70 (s, 1H); **^{13}C-NMR** (151 MHz,

DMSO-d_6) δ 20.9, 23.2, 128.6, 129.4, 132.1, 133.2, 133.8, 134.8, 139.7, 142.8, 144.4; **HRMS** (ESI) m/z calculated for $C_{16}H_{17}ClN_2O_2SNa$ $[M+Na]^+$ 359.0591, found 359.0599.



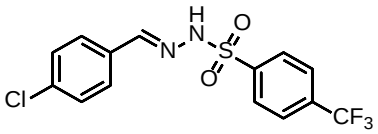
1fa

***N'*-(4-Chlorobenzylidene)-2,4-dibromo-benzenesulfonohydrazide (1fa).** Yellow solid, m.p. 143-144 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 7.42 (d, *J* = 8.4 Hz, 2H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.83-7.85 (m, 1H), 7.99 (d, *J* = 9.0 Hz, 1H), 8.03 (s, 1H), 8.12-8.13 (m, 1H), 12.25 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 120.9, 127.9, 128.9, 129.3, 131.9, 132.8, 133.5, 135.1, 137.7, 138.1, 145.8.



1ga

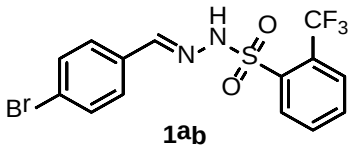
***N'*-(4-Chlorobenzylidene)-3-(trifluoromethyl)benzenesulfonohydrazide (1ga).** Whate solid, m.p. 152-153 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 7.44 (d, *J* = 8.4 Hz, 2H), 7.58 (d, *J* = 8.4 Hz, 2H), 7.88 (t, *J* = 7.8 Hz, 1H), 7.95 (s, 1H), 8.05 (d, *J* = 7.8 Hz, 1H), 8.13 (s, 1H), 8.20 (d, *J* = 7.8 Hz, 1H), 11.79 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 124.0 (q, *J* = 272.8 Hz), 124.2 (q, *J* = 3.8 Hz), 129.0, 129.4, 130.3 (q, *J* = 32.8 Hz), 130.4 (q, *J* = 3.6 Hz), 131.5, 131.8, 132.8, 135.4, 140.4, 147.5; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -61.55 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{14}H_{10}ClF_3N_2O_2SNa$ $[M+Na]^+$ 384.9996, found 384.9999.



1ha

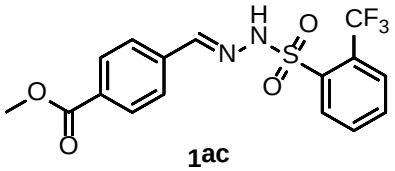
***N'*-(4-Chlorobenzylidene)-4-(trifluoromethyl)benzenesulfonohydrazide (1ha).** Yellow solid, m.p. 154-155°C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 7.37-7.45 (m, 2H), 7.59 (d, *J* = 7.8 Hz, 2H), 7.95-7.99 (m, 3H), 8.11 (d, *J* = 7.8 Hz, 2H), 11.90 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ

123.8 (q, *J* = 272.0 Hz), 126.9 (q, *J* = 3.2 Hz), 128.7, 129.0, 129.3, 132.8, 133.3 (q, *J* = 32.5 Hz), 135.3, 143.3, 147.2; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -61.82 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{14}H_{10}ClF_3N_2O_2SNa$ $[M+Na]^+$ 384.9996, found 384.9999.



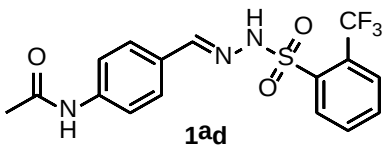
1ab

***N′*-(4-Bromobenzylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1ab).** White solid, m.p. 158-159 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 7.50 (d, *J* = 8.4 Hz, 2H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.88 (t, *J* = 7.8 Hz, 1H), 7.93 (t, *J* = 7.8 Hz, 1H), 8.02 (d, *J* = 7.8 Hz, 1H), 8.04 (s, 1H), 8.14 (d, *J* = 7.8 Hz, 1H), 12.21 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 123.2 (q, *J* = 273.0 Hz), 123.9, 126.9 (q, *J* = 33.0 Hz), 128.9 (q, *J* = 6.0 Hz), 129.2, 131.7, 132.3, 133.3, 133.8, 134.0, 138.5, 146.2; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.22 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{14}H_{10}BrF_3N_2O_2SNa$ $[M+Na]^+$ 428.9491, found 428.9499.



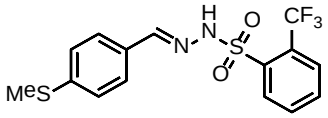
1ac

Methyl 4-((2-((2-(trifluoromethyl)phenyl)sulfonyl)hydrazono)methyl)benzoate (1ac). White solid, m.p. 156-157 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 3.83 (s, 3H), 7.68 (d, *J* = 8.4 Hz, 2H), 7.86 (t, *J* = 7.8 Hz, 1H), 7.91-7.95 (m, 3H), 8.01 (d, *J* = 7.8 Hz, 1H), 8.12 (s, 1H), 8.14 (d, *J* = 7.8 Hz, 1H), 12.36 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 52.7, 123.2 (q, *J* = 274.5 Hz), 126.8 (q, *J* = 33.0 Hz), 127.5, 128.9 (q, *J* = 6.2 Hz), 130.1, 131.0, 131.7, 133.9, 134.1, 138.3, 138.5, 146.0, 166.2; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.25 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{16}H_{13}F_3N_2O_4SNa$ $[M+Na]^+$ 409.0440, found 409.0447.



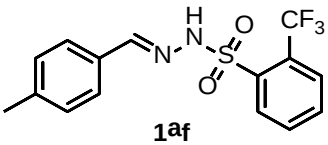
1ad

***N*-(4-((2-((2-(trifluoromethyl)phenyl)sulfonyl)hydrazono)methyl)phenyl)acetamide (1ad).** Yellow solid, m.p. 156-157 ^{o}C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 2.04 (s, 3H), 7.47 (d, *J* = 8.4 Hz, 2H), 7.60 (d, *J* = 8.4 Hz, 2H), 7.85 (t, *J* = 7.8 Hz, 1H), 7.92 (t, *J* = 7.8 Hz, 1H), 7.98-8.01 (m, 2H), 8.12 (d, *J* = 7.8 Hz, 1H), 10.10 (s, 1H), 11.94 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 24.6, 119.3, 123.3 (q, *J* = 273.0 Hz), 126.9 (q, *J* = 32.8 Hz), 128.1, 128.6, 128.9 (q, *J* = 6.2 Hz), 131.7, 133.8, 133.9, 138.7, 141.6, 147.4, 169.0; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.19 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{16}H_{14}F_3N_3O_3SNa$ $[M+Na]^+$ 408.0600, found 408.0606.



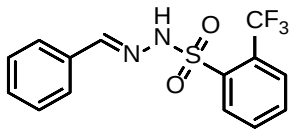
1ae

***N'*-(4-(Methylthio)benzylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1ae)**. Yellow solid, m.p. 118-119 ^{o}C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 2.46 (s, 3H), 7.24 (d, *J* = 7.8 Hz, 2H), 7.46 (d, *J* = 7.8 Hz, 2H), 7.85 (t, *J* = 7.8 Hz, 1H), 7.91 (t, *J* = 7.8 Hz, 1H), 7.99-8.01 (m, 2H), 8.13 (d, *J* = 7.8 Hz, 1H), 12.03 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 14.7, 123.3 (q, *J* = 273.6 Hz), 126.1, 126.9 (q, *J* = 32.7 Hz), 127.7, 128.9 (q, *J* = 6.2 Hz), 130.4, 131.7, 133.8, 133.9, 138.6, 141.7, 147.1; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.20 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{15}H_{13}F_3N_2O_2S_2Na$ $[M+Na]^+$ 397.0263, found 397.0270.



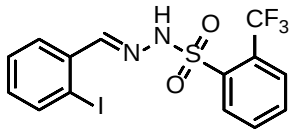
1af

***N'*-(4-Methylbenzylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1af)**. Yellow solid, m.p. 110-111^{o}C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 2.27 (s, 3H), 7.17 (d, *J* = 7.8 Hz, 2H), 7.42 (d, *J* = 7.8 Hz, 2H), 7.84 (t, *J* = 7.8 Hz, 1H), 7.91 (t, *J* = 7.8 Hz, 1H), 7.99 (d, *J* = 7.8 Hz, 1H), 8.02 (s, 1H), 8.13 (d, *J* = 7.8 Hz, 1H), 11.99 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 21.4, 123.3 (q, *J* = 274.4 Hz), 126.9 (q, *J* = 33.1 Hz), 127.3, 128.9 (q, *J* = 6.1 Hz), 129.9, 131.3, 131.7, 133.7, 133.9, 138.6, 140.5, 147.6; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.22 (s, 3F); **HRMS**(ESI) m/z calculated for $C_{15}H_{13}F_3N_2O_2SNa$ $[M+Na]^+$ 365.0542, found 365.0548.



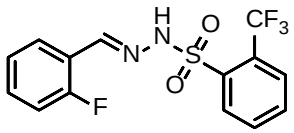
1ag

***N′*-Benzylidene-2-(trifluoromethyl)benzenesulfonohydrazide (1ag)**. White solid, m.p. 119-120 ^{o}C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 7.36-7.38 (m, 3H), 7.52-7.54 (m, 2H), 7.85 (t, *J* = 7.8 Hz, 1H), 7.92 (t, *J* = 7.8 Hz, 1H), 8.00 (d, *J* = 7.8 Hz, 1H), 8.06 (s, 1H), 8.15 (d, *J* = 7.8 Hz, 1H), 12.10 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 123.3 (q, *J* = 274.0 Hz), 126.9 (q, *J* = 32.9 Hz), 127.3, 128.9 (q, *J* = 6.3 Hz), 129.3, 130.7, 131.8, 133.8, 133.96, 134.01, 138.6, 147.5; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.23 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{14}H_{11}F_3N_2O_2SNa$ $[M+Na]^+$ 351.0386, found 351.0390.



1ah

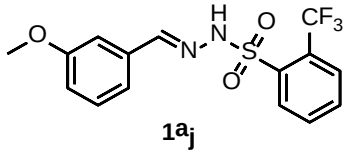
***N′*-(2-iodobenzylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1ah).** Yellow solid, m.p. 152-153 ^{o}C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 7.11-7.14 (m, 1H), 7.37 (t, *J* = 7.8 Hz, 1H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.85-7.88 (m, 2H), 7.94 (t, *J* = 7.8 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 8.15 (d, *J* = 7.8 Hz, 1H), 8.27 (s, 1H), 12.33 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 100.2, 123.2 (q, *J* = 274.3 Hz), 126.8 (q, *J* = 32.8 Hz), 127.1, 128.9 (q, *J* = 6.3 Hz), 129.1, 131.8, 132.4, 133.9, 134.1, 135.5, 138.3, 140.1, 151.2; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.26 (s, 3F); **HRMS**(ESI) m/z calculated for $C_{14}H_{10}F_3IN_2O_2SNa$ $[M+Na]^+$ 476.9352, found 476.9358.



1ai

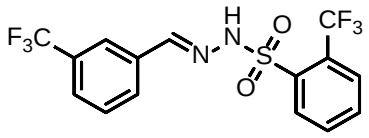
***N′*-(2-Fluorobenzylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1ai)**. White solid, m.p. 137-138 ^{o}C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 7.20 (t, *J* = 7.2 Hz, 1H), 7.25 (t, *J* = 9.0 Hz, 1H), 7.42-7.46 (m, 1H), 7.63 (t, *J* = 7.2 Hz, 1H), 7.87 (t, *J* = 7.8 Hz, 1H), 7.93 (t, *J* = 7.8 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 8.15 (d, *J* = 7.8 Hz, 1H), 8.24 (s, 1H), 12.24 (s, 1H); **^{13}C-NMR** (151 MHz,

DMSO-d_6) δ 116.5 (d, *J* = 20.8 Hz), 121.5 (d, *J* = 10.0 Hz), 123.2 (q, *J* = 274.0 Hz), 125.4 (d, *J* = 3.0 Hz), 126.5 (d, *J* = 3.0 Hz), 126.9 (q, *J* = 32.9 Hz), 128.9 (q, *J* = 6.0 Hz), 131.9, 132.6 (d, *J* = 8.5 Hz), 133.9, 134.1, 138.4, 140.1 (d, *J* = 4.5 Hz), 161.0 (d, *J* = 250.0 Hz); **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.27 (s, 3F), -120.94 – -120.92 (m, 1F); **HRMS** (ESI) m/z calculated for $C_{14}H_{10}F_4N_2O_2SNa$ $[M+Na]^+$ 369.0297, found 369.0301.



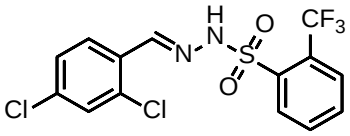
1a$_j$

***N′*-(3-Methoxybenzylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1aj).** **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 3.74 (s, 3H), 6.96 (dd, *J* = 2.4 Hz, 7.8 Hz, 1H), 7.06-7.07 (m, 1H), 7.11 (d, *J* = 7.8 Hz, 1H), 7.29 (t, *J* = 7.8 Hz, 1H), 7.86 (t, *J* = 7.8 Hz, 1H), 7.93 (t, *J* = 7.8 Hz, 1H), 8.00-8.02 (m, 2H), 8.14 (d, *J* = 8.4 Hz, 1H), 12.09 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 55.6, 112.0, 116.6, 119.8, 123.2 (q, *J* = 273.0 Hz), 126.9 (q, *J* = 31.5 Hz), 128.8 (q, *J* = 6.0 Hz), 130.4, 131.9, 133.8, 134.0, 135.4, 138.5, 147.2, 159.9; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.20 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{15}H_{13}F_3N_2O_3SNa$ $[M+Na]^+$ 381.0491, found 381.0494.



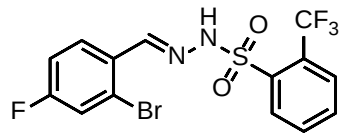
1ak

2-(Trifluoromethyl)-*N′*-(3-(trifluoromethyl)benzylidene)benzenesulfonohydrazide (1ak). White solid, m.p. 103-104 ^{o}C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 7.61 (t, *J* = 7.8 Hz, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.83-7.87 (m, 3H), 7.92 (t, *J* = 7.8 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 8.14 (s, 1H), 8.16 (d, *J* = 7.8 Hz, 1H), 12.36 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 123.4 (q, *J* = 272.4 Hz, CF_3), 123.7 (q, *J* = 3.8 Hz), 123.8 (q, *J* = 274.2 Hz, CF_3), 126.8 (d, *J* = 3.6 Hz), 126.9 (q, *J* = 32.1 Hz), 128.9 (q, *J* = 6.2 Hz), 130.1 (q, *J* = 32.1 Hz), 130.5, 130.9, 131.7, 133.8, 134.1, 135.2, 138.5, 145.7; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.26 (s, 3F), -61.47 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{15}H_{10}F_6N_2O_2SNa$ $[M+Na]^+$ 419.0260, found 419.0268.



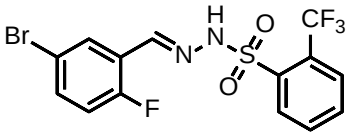
1al

***N′*-(2,4-Dichlorobenzylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1al)**. White solid, m.p. 153-154 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 7.41 (dd, *J* = 1.2 Hz, 8.4 Hz, 1H), 7.63-7.68 (m, 2H), 7.87 (t, *J* = 7.2 Hz, 1H), 7.93 (t, *J* = 7.2 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 8.15 (d, *J* = 7.8 Hz, 1H), 8.36 (s, 1H), 12.41 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 123.2 (q, *J* = 274.0 Hz), 126.8 (q, *J* = 33.0 Hz), 128.2, 128.5, 128.9 (q, *J* = 6.4 Hz), 129.8, 130.3, 131.8, 133.9, 134.15, 134.16, 135.7, 138.3, 142.1; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.30 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{14}H_9Cl_2F_3N_2O_2SNa$ $[M+Na]^+$ 418.9606, found 418.9608.



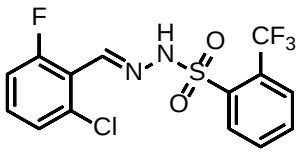
1am

***N′*-(2-Bromo-4-fluorobenzylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1am)**. White solid, m.p. 162-163 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 7.24 (td, *J* = 2.4 Hz, 8.4 Hz, 1H), 7.59 (dd, *J* = 2.4 Hz, 8.4 Hz, 1H), 7.68 (dd, *J* = 6.0 Hz, 8.4 Hz, 1H), 7.86 (t, *J* = 7.8 Hz, 1H), 7.93 (t, *J* = 7.8 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 8.16 (d, *J* = 7.8 Hz, 1H), 8.34 (s, 1H), 12.35 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 116.2 (d, *J* = 22.0 Hz), 120.5 (d, *J* = 25.0 Hz), 122.5 (d, *J* = 272.2 Hz), 124.1 (d, *J* = 9.9 Hz), 126.8 (q, *J* = 32.9 Hz), 128.9 (q, *J* = 6.2 Hz), 129.5 (d, *J* = 3.3 Hz), 131.9, 133.9, 134.1, 138.3, 144.6, 163.1 (d, *J* = 252.8 Hz); **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.32 (s, 3F), -108.36 – -108.41 (m, 1F); **HRMS** (ESI) m/z calculated for $C_{14}H_9BrF_4N_2O_2SNa$ $[M+Na]^+$ 446.9397, found 446.9402.



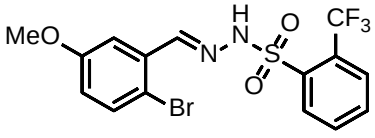
1an

***N'*- (5-Bromo-2-fluorobenzylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1an)**. White solid, m.p. 159-161 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 7.22-7.28 (m, 1H), 7.57-7.61 (m, 1H), 7.66-7.69 (m, 1H), 7.87 (t, *J* = 7.8 Hz, 1H), 7.94 (t, *J* = 7.8 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 8.14-8.17 (m, 2H), 12.41 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 117.2 (d, *J* = 2.7 Hz), 119.1 (d, *J* = 22.6 Hz), 122.5 (q, *J* = 274.0 Hz), 123.8 (d, *J* = 11.6 Hz), 126.8 (q, *J* = 32.9 Hz), 128.5 (d, *J* = 2.2 Hz), 129.0 (d, *J* = 6.2 Hz), 131.8, 133.9, 134.2, 134.9 (d, *J* = 8.6 Hz), 138.3, 138.6 (d, *J* = 3.8 Hz), 160.0 (d, *J* = 251.1 Hz); **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.30 (d, 3F), -122.23 – -122.20 (m, 1F); **HRMS** (ESI) m/z calculated for $C_{14}H_9BrF_4N_2O_2SNa$ $[M+Na]^+$ 446.9397, found 446.9402.



1ao

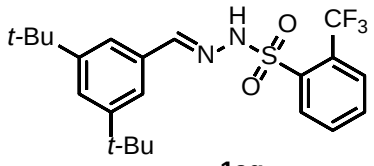
***N'*-(2-Chloro-6-fluorobenzylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1ao)**. White solid, m.p. 160-161 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 7.23 (t, *J* = 7.8 Hz, 1H), 7.34 (t, *J* = 7.8 Hz, 1H), 7.39-7.44 (m, 1H), 7.87 (t, *J* = 7.2 Hz, 1H), 7.92 (d, *J* = 7.2 Hz, 1H), 8.01 (d, *J* = 8.4 Hz, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 8.22 (s, 1H), 12.37 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 115.9 (d, *J* = 21.8 Hz), 120.4 (d, *J* = 13.6 Hz), 123.2 (q, *J* = 274.1 Hz), 126.5 (d, *J* = 3.4 Hz), 126.8 (q, *J* = 32.8 Hz), 128.8 (q, *J* = 6.2 Hz), 132.2, 132.3 (d, *J* = 10.0 Hz), 133.7, 134.0 (d, *J* = 4.3 Hz), 134.1, 138.1, 140.1, 160.5 (d, *J* = 256.5 Hz); **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.37 (d, 3F), -110.73 – -110.76 (m, 1F); **HRMS** (ESI) m/z calculated for $C_{14}H_9ClF_4N_2O_2SNa$ $[M+Na]^+$ 402.9902, found 402.9916.



1ap

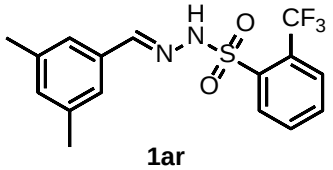
***N'*-(2-Bromo-5-methoxybenzylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1ap)**. White solid, m.p. 157-158 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 3.70 (s, 3H), 6.88-6.93 (m, 1H), 7.10 (d, *J* = 9.0 Hz, 1H), 7.46-7.51 (m, 1H), 7.84-7.88 (m, 1H), 7.94 (t, *J* = 7.8 Hz, 1H), 7.99 (s,

1H), 8.19-8.22 (m, 1H), 8.30 (s, 1H), 12.32 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 55.8, 111.6, 114.4, 118.8, 123.2 (q, *J* = 273.1 Hz), 126.9 (q, *J* = 32.9 Hz), 128.9 (), 132.2, 133.4, 133.8, 134.2, 134.4, 138.2, 145.4, 159.0; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.30 (s, 3F).



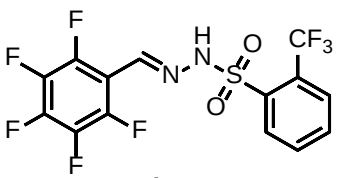
1aq

***N′*-(2,4-Dichlorobenzylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1aq)**. White solid, m.p. 162-163 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 1.24 (s, 18H), 7.35 (d, *J* = 7.8 Hz, 2H), 7.41 (t, *J* = 7.8 Hz, 1H), 7.85 (t, *J* = 7.8 Hz, 1H), 7.91 (t, *J* = 7.8 Hz, 1H), 7.99 (d, *J* = 7.8 Hz, 1H), 8.01 (s, 1H), 8.16 (d, *J* = 7.8 Hz, 1H), 11.95 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 31.5, 34.9, 121.4, 123.2 (q, *J* = 273.6 Hz), 124.6, 127.0 (q, *J* = 32.8 Hz), 128.7 (q, *J* = 6.2 Hz), 132.1, 133.4, 133.6, 134.0, 138.6, 148.2, 151.3; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.16 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{22}H_{27}Cl_2F_3N_2O_2SNa$ $[M+Na]^+$ 463.1638, found 463.1630.



1ar

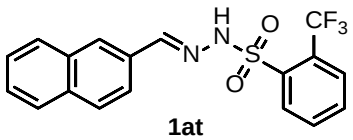
***N′*- (3,5-Dimethylbenzylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1ar)**. White solid, m.p. 149-150 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 2.24 (s, 6H), 7.01 (s, 1H), 7.14 (s, 2H), 7.85 (t, *J* = 7.8 Hz, 1H), 7.92 (t, *J* = 7.8 Hz, 1H), 7.99 (s, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 8.10 (d, *J* = 7.8 Hz, 1H), 12.04 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 21.2, 123.2 (q, *J* = 274.1 Hz), 125.0, 126.8 (q, *J* = 32.8 Hz), 128.9 (q, *J* = 6.2 Hz), 131.5, 132.2, 133.8, 133.88, 133.89, 138.4, 138.7, 147.8; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.21 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{16}H_{15}F_3N_2O_2SNa$ $[M+Na]^+$ 379.0699, found 379.0704.



1as

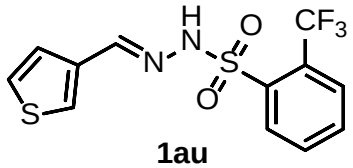
`

***N'*-((Perfluorophenyl)methylene)-2-(trifluoromethyl)benzenesulfonohydrazide (1as)**. White solid, m.p. 164-166 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 7.87 (t, *J* = 7.8 Hz, 1H), 7.93 (t, *J* = 7.8 Hz, 1H), 7.99 (d, *J* = 7.8 Hz, 1H), 8.04 (s, 1H), 8.14 (d, *J* = 7.8 Hz, 1H), 12.52 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 109.5 (t, *J* = 10.9 Hz), 123.2 (q, *J* = 272.6 Hz, CF_3), 126.8 (q, *J* = 32.9 Hz), 128.9 (q, *J* = 6.0 Hz), 132.4, 133.8, 134.3, 135.0, 137.7, 137.8 (dt, *J* = 14.8 Hz, 249.8 Hz), 141.4 (dt, *J* = 14.4 Hz, 255.0 Hz), 144.9 (d, *J* = 253.6 Hz); **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.53 (s, 3F), -142.48 (dd, *J* = 24.0 Hz, *J* = 7.8 Hz, 2F), -153.19 (t, *J* = 24.0 Hz, 1F), -162.73 (td, *J* = 24.0 Hz, 8.4 Hz, 2F); **HRMS** (ESI) m/z calculated for $C_{14}H_6F_8N_2O_2SNa$ $[M+Na]^+$ 440.9915, found 440.9921.



1at

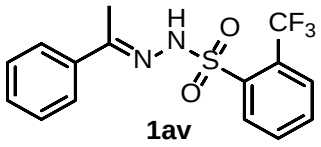
***N'*-(Naphthalen-2-ylmethylene)-2-(trifluoromethyl)benzenesulfonohydrazide (1at)**. White solid, m.p. 162-163 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 7.51-7.56 (m, 2H), 7.71 (dd, *J* = 1.2 Hz, 8.4 Hz, 1H), 7.84-7.91 (m, 3H), 7.92-7.96 (m, 2H), 8.01 (d, *J* = 7.8 Hz, 1H), 8.04 (s, 1H), 8.19 (d, *J* = 8.4 Hz, 1H), 8.22 (s, 1H), 12.20 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 122.6, 123.3 (q, *J* = 274.2 Hz), 126.9 (q, *J* = 32.4 Hz), 127.3, 127.7, 128.2, 128.8, 128.9 (q, *J* = 6.2 Hz), 129.0, 129.3, 131.68, 131.73, 133.2, 133.8, 134.0, 134.2, 138.6, 147.5; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.18 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{18}H_{13}F_3N_2O_2SNa$ $[M+Na]^+$ 401.0542, found 401.0546.



1au

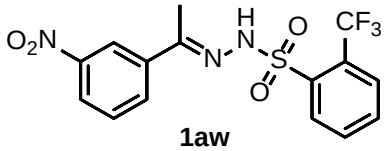
***N'*-(Thiophen-3-ylmethylene)-2-(trifluoromethyl)benzenesulfonohydrazide (1au).** Brown solid, m.p. 135-136 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 7.23 (dd, *J* = 1.2 Hz, 5.4 Hz, 1H), 7.54 (dd, *J* = 3.0 Hz, 5.4 Hz, 1H), 7.82-7.87 (m, 2H), 7.92 (t, *J* = 7.2 Hz, 1H), 8.00 (d, *J* = 7.2 Hz, 1H), 8.08 (s, 1H), 8.11 (d, *J* = 8.4 Hz, 1H), 11.91 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 123.2 (q, *J* = 271.5 Hz), 124.7, 126.8 (q, *J* = 31.5 Hz), 128.2, 128.8 (q, *J* = 6.0 Hz), 129.0, 131.7, 133.8,

133.9, 137.1, 138.6, 143.2; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.20 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{12}H_9F_3N_2O_2S_2Na$ $[M+Na]^+$ 356.9950, found 356.9944.



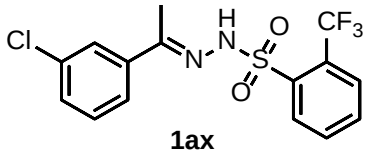
1av

***N'*-(1-Phenylethylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1av).** White solid, m.p. 111-112 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 2.29 (s, 3H), 7.32-7.37 (m, 3H), 7.57 (dd, *J* = 2.4 Hz, 7.8 Hz, 2H), 7.85 (t, *J* = 7.8 Hz, 1H), 7.92 (t, *J* = 7.8 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 8.09 (d, *J* = 7.8 Hz, 1H), 11.21 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 15.1, 123.3 (q, *J* = 274.0 Hz), 126.6, 127.1 (q, *J* = 32.9 Hz), 128.7 (q, *J* = 6.4 Hz), 128.8, 130.0, 131.4, 133.6, 133.8, 137.8, 138.8, 153.9; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.05 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{15}H_{14}F_3N_2O_2S$ $[M+H]^+$ 343.0723, found 343.0722.



1aw

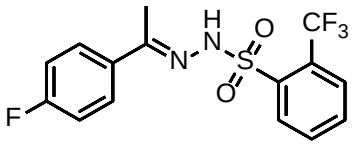
***N'*-(1-(3-Nitrophenyl)ethylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1aw).** Yellow solid, m.p. 153-154 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 2.35 (s, 3H), 7.64 (t, *J* = 7.8 Hz, 1H), 7.87 (t, *J* = 7.8 Hz, 1H), 7.92 (t, *J* = 7.8 Hz, 1H), 8.01 (t, *J* = 7.8 Hz, 2H), 8.13 (d, *J* = 7.8 Hz, 1H), 8.18 (dd, *J* = 1.8 Hz, 7.8 Hz, 1H), 8.31 (t, *J* = 1.8 Hz, 1H), 11.50 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 15.0, 120.9, 123.3 (q, *J* = 274.0 Hz), 124.3, 127.2 (q, *J* = 32.8 Hz), 128.8 (q, *J* = 6.2 Hz), 130.5, 131.6, 132.8, 133.7, 134.0, 138.6, 139.4, 148.4, 151.3; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.10 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{15}H_{12}F_3N_3O_4SNa$ $[M+Na]^+$ 410.0398, found 410.0403.



1ax

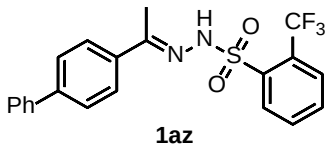
***N'*-(1-(3-Chlorophenyl)ethylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1ax).** Yellow solid, m.p. 118-119 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 2.28 (s, 3H), 7.38 (t, *J* = 7.8 Hz,

1H), 7.43 (d, *J* = 7.8 Hz, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.57 (s, 1H), 7.86 (t, *J* = 7.8 Hz, 1H), 7.92 (t, *J* = 7.2 Hz, 1H), 8.02 (d, *J* = 7.2 Hz, 1H), 8.09 (d, *J* = 7.8 Hz, 1H), 11.36 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 15.0, 123.3 (q, *J* = 274.1 Hz), 125.2, 126.2, 127.2 (q, *J* = 32.8 Hz), 128.8 (q, *J* = 6.2 Hz), 129.7, 130.7, 131.5, 133.66, 133.75, 133.85, 138.8, 139.9, 152.2; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.08 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{15}H_{12}ClF_3N_2O_2SNa$ $[M+Na]^+$ 399.0152, found 399.0157.



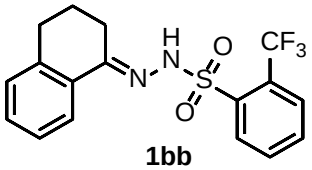
1ay

***N'*-(1-(4-fluorophenyl)ethylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1ay).** White solid, m.p. 162-163 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 2.28 (s, 3H), 7.17 (t, *J* = 8.4 Hz, 2H), 7.62 (dd, *J* = 5.4 Hz, 8.4 Hz, 2H), 7.84 (t, *J* = 7.8 Hz, 1H), 7.91 (t, *J* = 7.8 Hz, 1H), 8.00 (d, *J* = 7.8 Hz, 1H), 8.10 (d, *J* = 7.8 Hz, 1H), 11.23 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 15.1, 115.7 (d, *J* = 21.6 Hz), 123.3 (q, *J* = 274.2 Hz), 127.2 (q, *J* = 32.8 Hz), 128.77 (q, *J* = 6.3 Hz), 128.80 (d, *J* = 8.6 Hz), 131.4, 133.6, 133.8, 134.3 (d, *J* = 2.9 Hz), 138.8, 153.0, 163.4 (d, *J* = 247.1 Hz); **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.05 (s, 3F), -112.02 – -111.95 (m, 1F); **HRMS** (ESI) m/z calculated for $C_{15}H_{12}F_4N_2O_2SNa$ $[M+Na]^+$ 383.0453, found 383.0459.



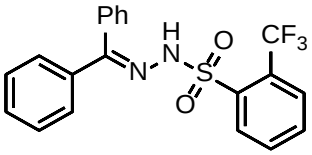
1az

***N'*-(1-([1,1'-Biphenyl]-4-yl)ethylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1az)**. Yellow solid, m.p. 131-132 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 2.32 (s, 3H), 7.37 (t, *J* = 7.8 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.64-7.69 (m, 6H), 7.86 (t, *J* = 7.8 Hz, 1H), 7.93 (t, *J* = 7.8 Hz, 1H), 8.02 (d, *J* = 7.8 Hz, 1H), 8.11 (d, *J* = 7.8 Hz, 1H), 11.25 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 15.0, 123.3 (q, *J* = 274.2 Hz), 127.05, 127.10, 127.14, 127.2 (q, *J* = 32.0 Hz), 128.3, 128.8 (q, *J* = 6.2 Hz), 129.5, 131.4, 133.7, 133.8, 136.8, 138.9, 139.7, 141.5, 153.4; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.02 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{21}H_{17}F_3N_2O_2SNa$ $[M+Na]^+$ 441.0855, found 441.0857.



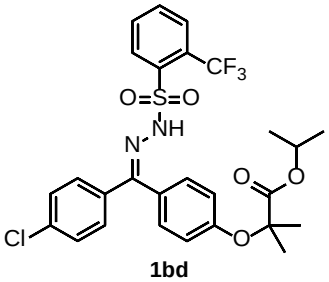
1bb

***N′*-(3,4-Dihydronaphthalen-1(2H)-ylidene)-2-(trifluoromethyl)benzenesulfonohydrazide (1bb).** Yellow solid, m.p. 177-178 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 1.78-1.83 (m, 2H), 2.65 (t, *J* = 6.6 Hz, 2H), 2.72 (t, *J* = 6.0 Hz, 2H), 7.13 (t, *J* = 7.8 Hz, 1H), 7.16 (d, *J* = 7.8 Hz, 1H), 7.25 (t, *J* = 7.8 Hz, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.85 (t, *J* = 7.8 Hz, 1H), 7.91 (t, *J* = 7.8 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 8.10 (d, *J* = 7.8 Hz, 1H), 11.10 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 21.7, 26.7, 29.2, 123.4 (q, *J* = 274.2 Hz), 124.6, 126.7, 127.3 (q, *J* = 32.8 Hz), 128.7 (q, *J* = 6.2 Hz), 129.1, 129.9, 131.6, 132.0, 133.6, 133.7, 139.0, 140.5, 153.5; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.00 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{17}H_{15}F_3N_2O_2SNa$ $[M+Na]^+$ 391.0699, found 391.0698.



1bc

***N′*-(Diphenylmethylene)-2-(trifluoromethyl)benzenesulfonohydrazide (1bc).** White solid, m.p. 134-135 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 7.22-7.24 (m, 2H), 7.28-7.33 (m, 4H), 7.37 (t, *J* = 7.8 Hz, 1H), 7.54-7.59 (m, 3H), 7.88 (t, *J* = 7.8 Hz, 1H), 7.95 (t, *J* = 7.8 Hz, 1H), 8.03 (d, *J* = 7.8 Hz, 1H), 8.11 (d, *J* = 7.8 Hz, 1H), 10.92 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 123.3 (q, *J* = 274.1 Hz), 127.2 (q, *J* = 32.8 Hz), 127.7, 128.7 (q, *J* = 6.2 Hz), 128.8, 129.2, 129.5, 130.1, 130.3, 131.4, 132.9, 133.7, 133.8, 137.4, 138.8, 155.4; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.03 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{20}H_{15}F_3N_2O_2SNa$ $[M+Na]^+$ 427.0699, found 427.0701.

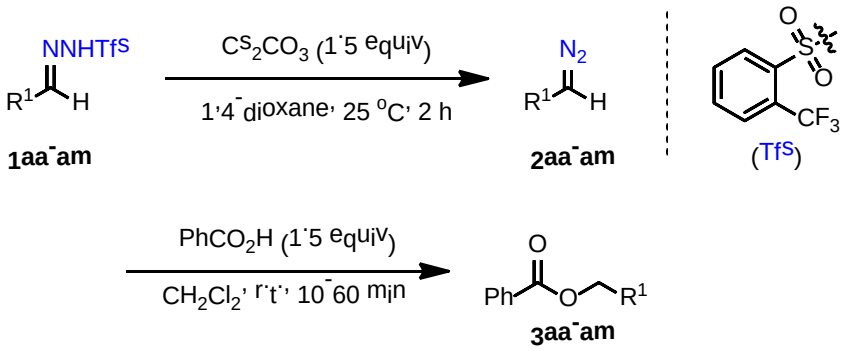


1bd

Isopropyl 2-(4-((4-chlorophenyl)(2-((2-(trifluoromethyl)phenyl)sulfonyl)hydrazono)methyl) phenoxy)-2-methylpropanoate (1bd). Yellow solid, m.p. 177-178 °C; **^{1}H-NMR** (600 MHz, DMSO-d_6) δ 1.12 (d, *J* = 6.6 Hz, 6H), 1.50 (s, 6H), 4.89-4.96 (m, 1H), 6.71 (d, *J* = 9.0 Hz, 2H), 7.16 (d, *J* = 9.0 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.87 (t, *J* = 7.8 Hz, 1H), 7.92 (t, *J* = 7.8 Hz, 1H), 8.01-8.05 (m, 2H), 11.02 (s, 1H); **^{13}C-NMR** (151 MHz, DMSO-d_6) δ 21.7, 25.4, 69.2, 79.2, 118.2, 123.3 (q, *J* = 274.0 Hz), 127.2 (q, *J* = 32.8 Hz), 128.7 (q, *J* = 6.0 Hz), 128.8, 129.7, 130.4, 131.2, 131.3, 131.9, 133.7, 134.7, 138.9, 153.5, 157.2, 172.8; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -56.02 (s, 3F).

IV. Synthetic procedures and characterization for benzyl esters

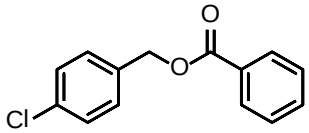
CAUTION! Although we did not have any incidents by handling, it is known that diazoalkanes are presumed to be highly toxic and potentially explosive. All manipulations should be carried out in a fume cupboard .



General procedure C (with **3aa** as an example): In a screw capped reaction vial, *N*-tfsylhydrazone **1aa** (181.4 mg, 0.5 mmol) and Cs_2CO_3 (244.4 mg, 0.75 mmol) were added. After sealed the tube was evacuated and backfilled with N_2 for three times, followed by dry 1,4-dioxane (10 mL) addition *via* syringe. The reaction mixture was stirred at 25 °C for 2 h. The reaction mixture was quenched by 5 mL saturated sodium chloride solution, the organic layer was separated. The aqueous phase was extracted with dichloromethane (3 x 10 mL). The organic

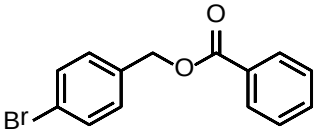
phases were combined, washed with saturated ammonium chloride solution (10 mL), dried by $MgSO_4$ and filtered through a short pad of silica gel to provide a clear, intensely colored solution.

Then, the benzoic acid (0.75 mmol) was added, and stirred at room temperature until the gas evolution ceased and the colour of diazo compound disappeared. The mixture was dried with Na_2SO_4 and filtered. The solvent was removed under reduced pressure, and the final product was purified by column chromatography to afford the desired product **3aa** colorless oil.



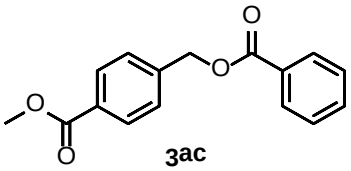
3aa

4-Chlorobenzyl benzoate (3aa).[2] Colorless oil; **^{1}H-NMR** (500 MHz, $CDCl_3$) δ 5.30 (s, 2H), 7.31-7.37 (m, 4H), 7.41 (t, *J* = 7.5 Hz, 2H), 7.53 (t, *J* = 7.5 Hz, 1H), 8.03-8.07 (m, 2H); **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 65.7, 128.3, 128.7, 129.5, 129.6, 129.8, 133.0, 134.0, 134.5, 166.1; **HRMS** (ESI) m/z calculated for $C_{14}H_{11}ClO_2Na$ $[M+Na]^+$ 269.0340, found 269.0347.



3ab

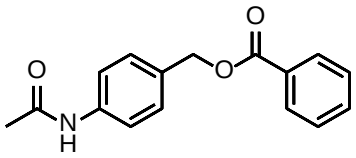
4-Bromobenzyl benzoate (3ab).[2] Colorless oil; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 5.32 (s, 2H), 7.33 (d, *J* = 8.4 Hz, 2H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.57 (t, *J* = 7.8 Hz, 1H), 8.06-8.09 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 65.8, 122.2, 128.4, 129.6, 129.80, 129.84, 131.7, 133.1, 135.0, 166.2; **HRMS** (ESI) m/z calculated for $C_{14}H_{11}BrO_2Na$ $[M+Na]^+$ 312.9835, found 312.9826.



3ac

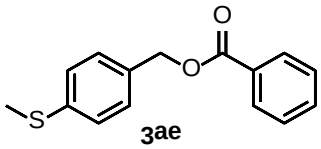
Methyl 4-((benzoyloxy)methyl)benzoate (3ac). Colorless oil; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 3.91 (s, 3H), 5.41 (s, 2H), 7.44 (t, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.55-7.58 (m, 1H),

8.06 (d, *J* = 8.4 Hz, 2H), 8.07-8.10 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 52.1, 65.8, 127.5, 128.4, 129.6, 129.7, 129.81, 129.85, 133.1, 141.0, 166.1, 166.6; **HRMS** (ESI) m/z calculated for $C_{16}H_{14}O_4Na$ $[M+Na]^+$ 293.0784, found 293.0786.



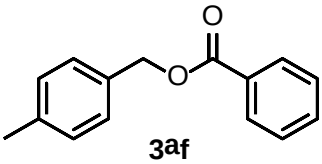
3ad

4-Acetamidobenzyl benzoate (3ad). Yellow solid；**^{1}H-NMR** (600 MHz, $CDCl_3$) δ 2.16 (s, 3H), 5.31 (s, 2H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.52-7.56 (m, 3H), 7.71 (s, 1H), 8.05 (d, *J* = 7.8 Hz, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 24.5, 66.3, 119.9, 128.4, 129.1, 129.6, 130.0, 131.8, 133.0, 138.0, 166.5, 168.6; **HRMS** (ESI) m/z calculated for $C_{16}H_{15}NO_3Na$ $[M+Na]^+$ 292.0944, found 292.0946.



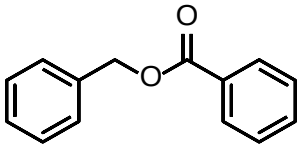
3ae

4-(Methylthio)benzyl benzoate (3ae). Yellow oil; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 2.47 (s, 3H), 5.31 (s, 2H), 7.26 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.42 (t, *J* = 7.8 Hz, 2H), 7.54 (t, *J* = 7.8 Hz, 1H), 8.05-8.07 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 15.7, 66.3, 126.5, 128.3, 128.8, 129.6, 130.0, 132.7, 133.0, 138.7, 166.3; **HRMS** (ESI) m/z calculated for $C_{15}H_{14}O_2SNa$$[M+Na]^+$ 281.0607, found 281.0602.



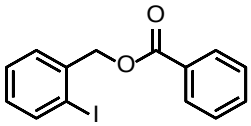
3af

4-Methylbenzyl benzoate (3af).[2] Colorless oil; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 2.36 (s, 3H), 5.33 (s, 2H), 7.19 (d, *J* = 7.8 Hz, 2H), 7.34 (d, *J* = 7.8 Hz, 2H), 7.42 (t, *J* = 7.8 Hz, 2H), 7.55 (t, *J* = 7.8 Hz, 1H), 8.03-8.08 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 21.2, 66.6, 128.29, 128.31, 129.2, 129.7, 130.2, 132.9, 133.0, 138.0, 166.4; **HRMS** (ESI) m/z calculated for $C_{15}H_{14}O_2Na$ $[M+Na]^+$ 249.0886, found 249.0903.



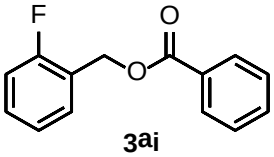
3ag

Benzyl benzoate (3ag). Colorless oil; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 5.36 (s, 2H), 7.33 (t, *J* = 7.2 Hz, 1H), 7.38 (t, *J* = 7.8 Hz, 2H), 7.40-7.45 (m, 4H), 7.52-7.55 (m, 1H), 8.06-8.09 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 66.6, 128.1, 128.2, 128.3, 128.5, 129.7, 130.1, 133.0, 136.0, 166.4; **HRMS** (ESI) m/z calculated for $C_{14}H_{12}O_2Na$ $[M+Na]^+$ 235.0730, found 235.0728.



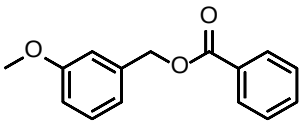
3ah

2-Iodobenzyl benzoate (3ah). Yellow oil; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 5.38 (s, 2H), 7.04 (td, *J* = 1.8 Hz, 7.8 Hz, 1H), 7.37 (td, *J* = 1.2 Hz, 7.8 Hz, 1H), 7.44-7.48 (m, 3H), 7.58 (t, *J* = 7.8 Hz, 1H), 7.89 (dd, *J* = 1.2 Hz, 7.8 Hz, 1H), 8.10-8.13 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 70.4, 98.4, 128.35, 128.42, 129.6, 129.8, 129.9, 133.1, 138.5, 139.6, 166.1; **HRMS** (ESI) m/z calculated for $C_{14}H_{11}IO_2Na$ $[M+Na]^+$ 360.9696, found 360.9701.



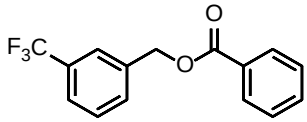
3ai

2-Fluorobenzyl benzoate (3ai).[2] Yellow oil; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 5.43 (s, 2H), 7.09 (t, *J* = 9.0 Hz, 1H), 7.15 (t, *J* = 7.8 Hz, 1H), 7.30-7.35 (m, 1H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.48 (td, *J* = 1.8 Hz, 7.8 Hz, 1H), 7.55 (t, *J* = 7.8 Hz, 1H), 8.05-8.08 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 60.6 (d, *J* = 4.2 Hz), 115.5 (d, *J* = 21.2 Hz), 123.2 (d, *J* = 14.6 Hz), 124.1 (d, *J* = 3.7 Hz), 128.3, 129.7, 129.9, 130.2 (d, *J* = 8.2 Hz), 130.5 (d, *J* = 3.7 Hz), 133.1, 161.0 (d, *J* = 248.6 Hz), 166.3; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -117.89 – -117.85 (m, 1F); **HRMS** (ESI) m/z calculated for $C_{14}H_{11}FO_2Na$ $[M+Na]^+$ 253.0635, found 263.0646.



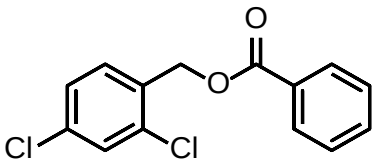
3a$_j$

3-Methoxybenzyl benzoate (3aj). Colorless oil; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 3.80 (s, 3H), 5.33 (s, 2H), 6.87 (dd, *J* = 2.4 Hz, 8.4 Hz, 1H), 6.98-6.99 (m, 1H), 7.02 (d, *J* = 7.8 Hz, 1H), 7.29 (t, *J* = 7.8 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 2H), 7.52-7.55 (m, 1H), 8.06-8.09 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 55.2, 66.4, 113.5, 113.6, 120.2, 128.3, 129.58, 129.63, 130.0, 133.0, 137.5, 159.7, 166.3; **HRMS** (ESI) m/z calculated for $C_{15}H_{14}O_3Na$ $[M+Na]^+$ 265.0835, found 265.0835.



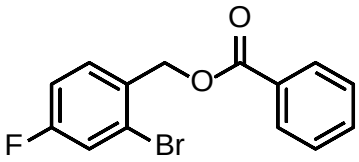
3ak

3-(Trifluoromethyl)benzyl benzoate (3ak). Colorless oil; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 5.40 (s, 2H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.50 (t, *J* = 7.8 Hz, 1H), 7.57 (t, *J* = 7.8 Hz, 1H), 7.59 (d, *J* = 7.8 Hz, 1H), 7.63 (d, *J* = 7.8 Hz, 1H), 7.71 (s, 1H), 8.06-8.09 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 65.7, 124.5 (q, *J* = 272.3 Hz), 124.8 (q, *J* = 3.7 Hz), 125.0 (q, *J* = 3.7 Hz), 128.4, 129.1, 129.68, 129.72, 131.0 (q, *J* = 32.8 Hz), 131.4, 133.2, 137.0, 166.2; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -62.61 (s, 3F); **HRMS** (ESI) m/z calculated for $C_{15}H_{11}F_3O_2Na$ $[M+Na]^+$ 303.0604, found 303.0608.



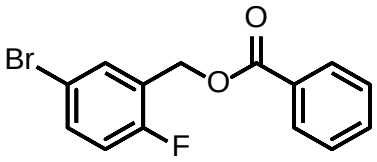
3al

2,4-Dichlorobenzyl benzoate (3al). Colorless oil; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 5.43 (s, 2H), 7.27 (dd, *J* = 1.8 Hz, 8.4 Hz, 1H), 7.44-7.47 (m, 4H), 7.58 (t, *J* = 7.8 Hz, 1H), 8.06-8.09 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 63.4, 127.2, 128.5, 129.5, 129.7, 130.7, 132.4, 133.3, 134.5, 134.7, 166.1; **HRMS** (ESI) m/z calculated for $C_{14}H_{10}Cl_2O_2Na$ $[M+Na]^+$ 302.9950, found 302.9961.



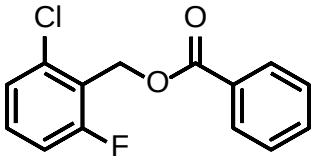
3am

2-Bromo-4-fluorobenzyl benzoate (3am). Colorless oil；**^{1}H-NMR** (600 MHz, $CDCl_3$) δ 5.40 (s, 2H), 7.05 (td, *J* = 2.4 Hz, 8.4 Hz, 1H), 7.35 (dd, *J* = 2.4 Hz, 8.4 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.49 (dd, *J* = 6.0 Hz, 8.4 Hz, 1H), 7.57 (t, *J* = 7.2 Hz, 1H), 8.06-8.09 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 65.5, 114.6 (d, *J* = 21.0 Hz), 120.2 (d, *J* = 24.6 Hz), 123.9 (d, *J* = 9.7 Hz), 128.4, 129.7, 129.8, 131.3 (d, *J* = 8.6 Hz), 131.4 (d, *J* = 3.4 Hz), 133.2, 162.1 (d, *J* = 252.1 Hz), 166.1; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -111.36 – -111.40 (m, 1F); **HRMS** (ESI) m/z calculated for $C_{14}H_{10}BrFO_2Na$ $[M+Na]^+$ 330.9741, found 330.9738.



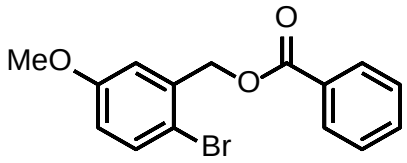
3an

5-Bromo-2-fluorobenzyl benzoate (3an). Colorless oil；**^{1}H-NMR** (600 MHz, $CDCl_3$) δ 5.38 (s, 2H), 6.99 (t, *J* = 9.0 Hz, 1H), 7.42-7.47 (m, 3H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.61 (dd, *J* = 2.4 Hz, 6.6 Hz, 1H), 8.07 (d, *J* = 7.8 Hz, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 59.8 (d, *J* = 4.1 Hz), 116.6 (d, *J* = 3.5 Hz), 117.3 (d, *J* = 22.9 Hz), 125.5 (d, *J* = 16.0 Hz), 128.4, 129.6, 129.7, 132.9 (d, *J* = 8.3 Hz), 133.0 (d, *J* = 3.9 Hz), 133.2, 159.9 (d, *J* = 249.2 Hz), 166.1; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -119.75 – -119.78 (m, 1F); **HRMS** (ESI) m/z calculated for $C_{14}H_{10}BrFO_2Na$ $[M+Na]^+$ 330.9741, found 330.9738.



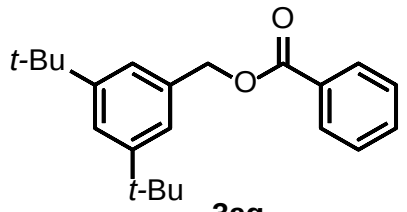
3ao

2-Chloro-6-fluorobenzyl benzoate (3ao). Colorless oil; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 5.52 (s, 2H), 7.05 (t, *J* = 8.4 Hz, 1H), 7.25 (d, *J* = 7.8 Hz, 1H), 7.28-7.32 (m, 1H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.54 (t, *J* = 7.8 Hz, 1H), 8.02-8.05 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 57.70 (d, *J* = 4.3 Hz), 114.3 (d, *J* = 22.6 Hz), 121.8 (d, *J* = 17.3 Hz), 125.5 (d, *J* = 3.5 Hz), 128.3, 129.7, 129.8, 130.8 (d, *J* = 9.8 Hz) 133.0, 136.5 (d, *J* = 4.9 Hz), 162.0 (d, *J* = 252.5 Hz), 166.2; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -112.69 – -112.71 (m, 1F).



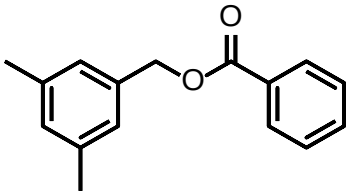
3ap

2-Bromo-5-methoxybenzyl benzoate (3ap). Colorless oil; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 3.79 (s, 3H), 5.40 (s, 2H), 6.76 (dd, *J* = 3.0 Hz, 8.4 Hz, 1H), 7.05 (d, *J* = 9.0 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.48 (d, *J* = 9.0 Hz, 1H), 7.57 (t, *J* = 7.8 Hz, 1H), 8.09-9.11 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 55.5, 66.1, 113.5, 115.0, 115.7, 128.4, 129.7, 129.9, 133.1, 133.4, 136.3, 159.0, 166.1; **HRMS** (ESI) m/z calculated for $C_{15}H_{13}BrO_3Na$ $[M+Na]^+$ 342.9941, found 342.9942.



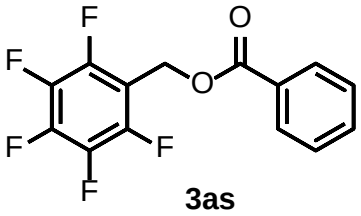
3aq

3,5-Di-tert-butylbenzyl benzoate (3aq). Colorless oil; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 1.35 (s, 18H), 5.36 (s, 2H), 7.30 (d, *J* = 1.2 Hz, 2H), 7.40-7.44 (m, 3H), 7.53 (t, *J* = 7.2 Hz, 1H), 8.06-8.11 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 31.4, 34.8, 67.4, 122.3, 122.6, 128.3, 129.7, 130.3, 132.9, 135.1, 151.1, 166.5; **HRMS** (ESI) m/z calculated for $C_{22}H_{28}O_2Na$ $[M+Na]^+$ 347.1982, found 347.1986.



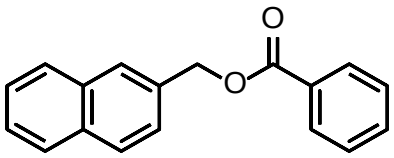
3ar

3,5-Dimethylbenzyl benzoate (3ar). Colorless oil；**^{1}H-NMR** (600 MHz, $CDCl_3$) δ 2.35 (s, 6H), 5.31 (s, 2H), 7.00 (s, 1H), 7.08 (s, 2H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.57 (t, *J* = 7.8 Hz, 1H), 8.10 (t, *J* = 7.8 Hz, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 21.2, 66.8, 126.0, 128.3, 129.7, 129.9, 130.2, 132.9, 135.9, 138.2, 166.5; **HRMS** (ESI) m/z calculated for $C_{16}H_{16}O_2K$ $[M+K]^+$ 279.0782, found 279.0785.



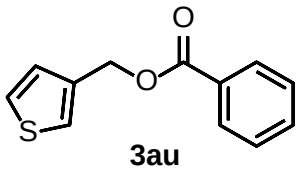
3as

(Perfluorophenyl)methyl benzoate (3as). Colorless oil；**^{1}H-NMR** (600 MHz, $CDCl_3$) δ 5.45 (s, 2H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.57 (t, *J* = 7.8 Hz, 1H), 8.00-8.04 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 53.8, 109.5 (td, *J* = 3.8 Hz, 17.4 Hz), 128.4, 129.2, 129.7, 133.4, 136.6-138.5 (m), 140.8-142.7 (m), 144.8-146.7 (m), 165.8; **^{19}F-NMR** (564 MHz, DMSO-d_6) δ -114.72 (dd, *J* = 9.8 Hz, *J* = 23.8 Hz, 2F), -152.58 (t, *J* = 3.8 Hz, 1F), -161.53 – -161.63 (m, 2F) **HRMS** (ESI) m/z calculated for $C_{14}H_7F_5O_2Na$ $[M+Na]^+$ 325.0619, found 325.0622.



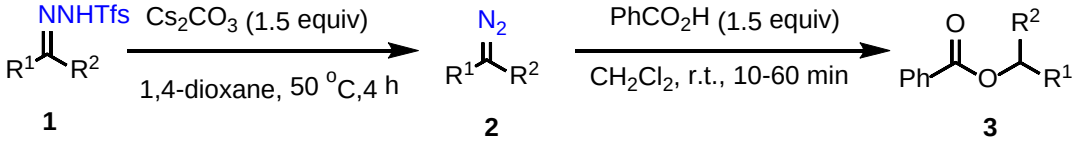
3at

Naphthalen-2-ylmethyl benzoate (3at).[2] Colorless oil；**^{1}H-NMR** (600 MHz, $CDCl_3$) δ 5.52 (s, 2H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.47-7.51 (m, 2H), 7.54-7.57 (m, 2H), 7.83-7.88 (m, 3H), 7.91 (s, 1H), 8.08-8.12 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 66.9, 125.9, 126.26, 126.30, 127.3, 127.7, 128.0, 128.38, 128.41, 129.7, 130.1, 133.0, 133.1, 133.2, 133.5, 166.5; **HRMS** (ESI) m/z calculated for $C_{18}H_{14}O_2Na$ $[M+Na]^+$ 285.0886, found 285.0892.



3au

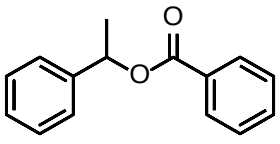
Thiophen-3-ylmethyl benzoate (3au). Yellow oil; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 5.36 (s, 2H), 7.17 (dd, *J* = 1.2 Hz, 5.4 Hz, 1H), 7.31-7.33 (m, 1H), 7.36-7.37 (m, 1H), 7.42 (t, *J* = 7.8 Hz, 2H), 7.54 (t, *J* = 7.8 Hz, 1H), 8.05-8.07 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 61.8, 124.2, 126.2, 127.6, 128.3, 129.6, 130.1, 133.0, 136.8 166.3; **HRMS** (ESI) m/z calculated for $C_{12}H_{10}O_2SNa$ $[M+Na]^+$ 241.0299, found 241.0301.



1 **2** **3**

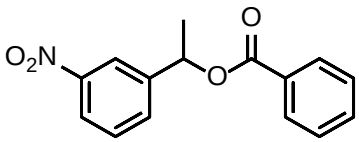
General procedure D (with **3av** as an example): In a screw capped reaction vial, *N*-Tfsylhydrazone **1av** (171.2 mg, 0.5 mmol) and Cs_2CO_3 (244.4 mg, 0.75 mmol) were added. After sealed the tube was evacuated and backfilled with argon for three times, followed by dry 1,4-dioxane (10 mL) addition *via* syringe. The reaction mixture was stirred at 50 °C for 4 h. The reaction mixture was quenched by 5 mL saturated sodium chloride solution, the organic layer was separated. The aqueous phase was extracted with dichloromethane (3 x 10 mL). The organic phases were combined, washed with saturated ammonium chloride solution (10 mL), dried by $MgSO_4$ and filtered through a short pad of silica gel to provide a clear, intensely colored solution.

Then, the benzoic acid (0.75 mmol) was added, and stirred at room temperature until the gas evolution ceased and the colour of diazo compound disappeared.. The mixture was dried with Na_2SO_4 and filtered. The solvent was removed under reduced pressure, and the final product was purified by column chromatography to afford the desired product **3av** yellow oil.



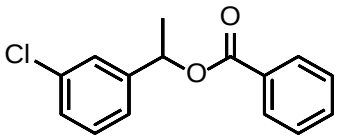
3av

1-Phenylethyl benzoate (3av).[2] Yellow oil; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 1.67 (d, *J* = 6.6 Hz, 3H), 6.14 (q, *J* = 6.6 Hz, 1H), 7.29 (t, *J* = 7.8 Hz, 1H), 7.36 (t, *J* = 7.8 Hz, 2H), 7.41-7.45 (m, 4H), 7.54 (t, *J* = 7.8 Hz, 1H), 8.06-8.10 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 22.4, 72.9, 126.0, 127.8, 128.3, 128.5, 129.6, 130.5, 132.9, 141.8, 165.8; **HRMS** (ESI) m/z calculated for $C_{15}H_{14}O_2Na$ $[M+Na]^+$ 249.0886, found 249.0900.



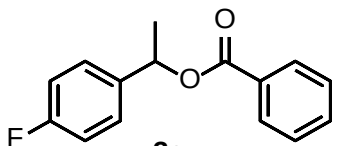
3aw

1-(3-Nitrophenyl)ethyl benzoate (3aw). Yellow solid, m.p. 64-65 °C; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 1.72 (d, *J* = 6.6 Hz, 3H), 6.19 (q, *J* = 6.6 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.55 (t, *J* = 7.8 Hz, 1H), 7.59 (t, *J* = 7.8 Hz, 1H), 7.77 (d, *J* = 7.8 Hz, 1H), 8.08 (d, *J* = 7.8 Hz, 2H), 8.16 (dd, *J* = 1.2 Hz, 7.8 Hz, 1H), 8.32 (s, 1H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 22.3, 71.7, 121.0, 122.9, 128.5, 129.61, 129.63, 129.8, 132.2, 133.3, 143.9, 148.4, 165.6; **HRMS** (ESI) m/z calculated for $C_{15}H_{13}NO_4Na$ $[M+Na]^+$ 294.0737, found 294.0735.



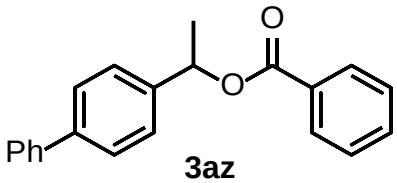
3ax

1-(3-Chlorophenyl)ethyl benzoate (3ax). Yellow oil; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 1.66 (d, *J* = 6.6 Hz, 3H), 6.09 (q, *J* = 6.6 Hz, 1H), 7.26-7.33 (m, 3H), 7.43 (s, 1H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.55-7.59 (m, 1H), 8.06-8.09 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 22.4, 72.1, 124.3, 126.2, 128.0, 128.4, 129.7, 129.9, 130.2, 133.1, 134.4, 143.8, 165.7; **HRMS** (ESI) m/z calculated for $C_{15}H_{13}ClO_2Na$ $[M+Na]^+$ 283.0496, found 283.0497.



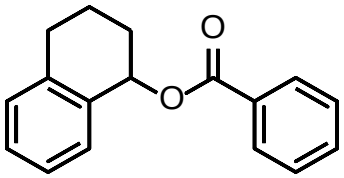
3ay

1-(4-Fluorophenyl)ethyl benzoate (3ay). Yellow oil; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 1.65 (d, *J* = 6.6 Hz, 3H), 6.11 (q, *J* = 6.6 Hz, 1H), 7.04 (t, *J* = 8.4 Hz, 2H), 7.41-7.45 (m, 4H), 7.55 (t, *J* = 7.8 Hz, 1H), 8.06 (d, *J* = 7.8 Hz, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 22.3, 72.2, 115.4 (d, *J* = 21.6 Hz), 127.8 (d, *J* = 8.2 Hz), 128.3, 129.6, 130.4, 133.0, 137.6 (d, *J* = 3.1 Hz), 162.3 (d, *J* = 246.0 Hz), 165.7; **HRMS** (ESI) m/z calculated for $C_{15}H_{13}FO_2Na$ $[M+Na]^+$ 267.0792, found 267.0801.



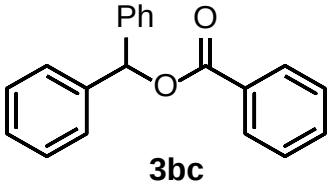
3az

1-([1,1'-Biphenyl]-4-yl)ethyl benzoate (3az). Yellow oil; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 1.71 (d, *J* = 6.6 Hz, 3H), 6.18 (q, *J* = 6.6 Hz, 1H), 7.32-7.35 (m, 1H), 7.41-7.46 (m, 4H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.54-760 (m, 5H), 8.08-8.11 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 22.3, 72.7, 126.5, 127.1, 127.3, 128.3, 128.7, 129.6, 130.5, 132.9, 140.74, 140.75, 140.9, 165.8; **HRMS**(ESI) m/z calculated For$C_{21}H_{18}O_2Na$$[M+Na]^+$ 325.1199, found 325.1203.



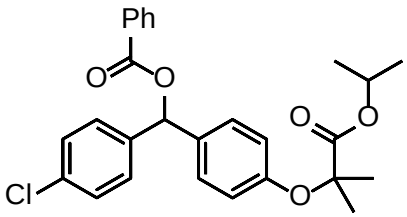
3bb

1,2,3,4-Tetrahydronaphthalen-1-yl benzoate (3bb). Yellow oil; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 1.85-1.90 (m, 1H), 2.03-2.13 (m, 3H), 2.77-2.82 (m, 1H), 2.89-2.94 (m, 1H), 6.26 (t, *J* = 4.2 Hz, 1H), 7.15-7.18 (m, 2H), 7.23 (t, *J* = 7.2 Hz, 1H), 7.36 (d, *J* = 7.2 Hz, 1H), 7.40 (t, *J* = 7.2 Hz, 2H), 7.52 (t, *J* = 7.2 Hz, 1H), 8.05 (d, *J* = 7.2 Hz, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 19.0, 29.0, 29.2, 70.6, 126.1, 128.0, 128.3, 129.0, 129.5, 129.7, 130.6, 132.8, 134.6, 138.0, 166.2; **HRMS** (ESI) m/z calculated for $C_{17}H_{16}O_2Na$ $[M+Na]^+$ 275.1043, found 275.1047.



3bc

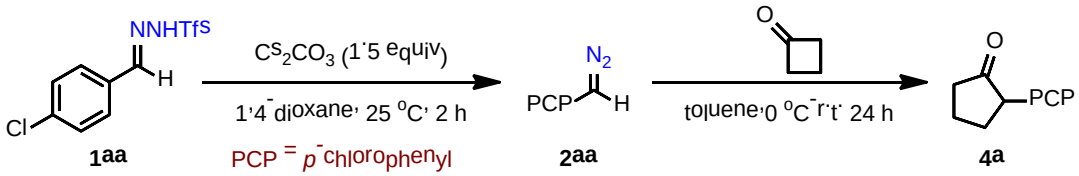
Benzhydryl benzoate (3bc).[3] White solid m.p. 88-89 °C; **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 7.13 (s, 1H), 7.28 (t, *J* = 7.2 Hz, 2H), 7.34 (t, *J* = 7.8 Hz, 4H), 7.42-7.45 (m, 6H), 7.53-7.57 (m, 1H), 8.12-8.16 (m, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 77.4, 127.1, 127.9, 128.4, 128.5, 129.8, 130.2, 133.1, 140.2, 165.5; **HRMS** (ESI) m/z calculated for $C_{20}H_{16}O_2Na$ $[M+Na]^+$ 311.1043, found 311.1048.



3bd

(4-Chlorophenyl)(4-((1-isopropoxy-2-methyl-1-oxopropan-2-yl)oxy)phenyl)methyl benzoate (3bd). ^{1}H-NMR (600 MHz, $CDCl_3$) δ 1.19 (dd, *J* = 2.4 Hz, 6.6 Hz, 6H), 1.57 (s, 3H), 1.58 (s, 3H), 5.03-5.09 (m, 1H), 6.82 (d, *J* = 8.4 Hz, 2H), 7.04 (s, 1H), 7.26 (d, *J* = 8.4 Hz, 2H), 7.30-7.34 (m, 4H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.56 (t, *J* = 7.8 Hz, 1H), 8.11 (d, *J* = 7.2 Hz, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 21.5, 25.31, 25.35, 68.9, 76.3, 79.1, 118.7, 128.1, 128.39, 128.41, 128.6, 129.7, 130.0, 132.9, 133.2, 133.7, 138.9, 155.5, 165.4, 173.5.

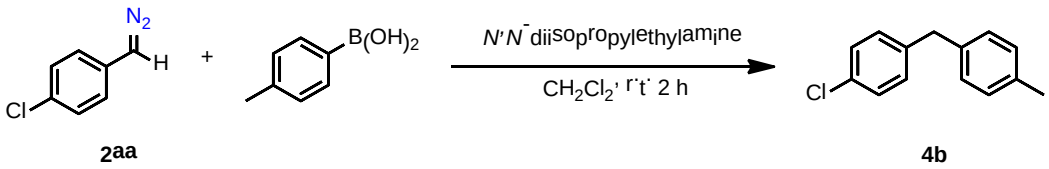
V. Synthetic applications



In a screw capped reaction vial, *N*-tfsylhydrazone **1aa** (199.5 mg, 0.6 mmol) and Cs_2CO_3 (269.8 mg, 0.83 mmol) were added. After sealed the tube was evacuated and backfilled with argon for three times, followed by dry 1,4-dioxane (10 mL) addition *via* syringe. The reaction mixture was stirred at 25 °C for 2 h. The reaction mixture was quenched by 5 mL saturated sodium chloride solution, the organic layer was separated. The aqueous phase was extracted with toluene (3 x 10 mL). The organic phases were combined, washed with saturated ammonium chloride solution (10

mL), and the benzoic acid (0.75 mmol) was added. Nitrogen evolution occurred, and the resulting mixture was stirred for 30-60 min at room temperature. The mixture was dried with Na_2SO_4 and filtered. The solvent was removed under reduced pressure, and the final product was purified by column chromatography to afford the desired product **4a** yellow oil.

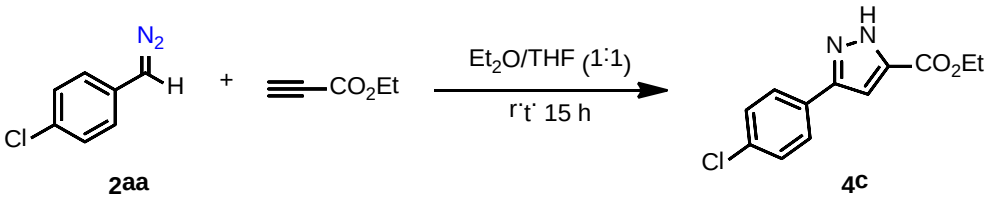
2-(4-Chlorophenyl)cyclopentan-1-one (4a).[4] **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 1.88-1.97 (m, 1H), 2.03-2.10 (m, 1H), 2.13-2.18 (m, 1H), 2.24-2.30 (m, 1H), 2.44-2.52 (m, 2H), 3.29 (dd, *J* = 8.4, 11.4 Hz, 1H), 7.13 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 20.7, 31.4, 38.2, 54.5, 128.6, 129.4, 132.6, 136.7, 217.3.



2aa **4b**

The solution of **2aa**/CH_2Cl_2 (0.75 mmol, obtained by general procedure C in 90% yield) was added to a mixture of 4-tolylboronic acid (0.5 mmol) and *N*,*N*-diisopropylethylamine (1.0 mmol) in 2 mL CH_2Cl_2. The resulting mixture was stirred at room temperature for additional 15 min after the colour of diazo compound disappeared. After evaporation of organic layer, the desired product **4b** was obtained by silica gel chromatography.

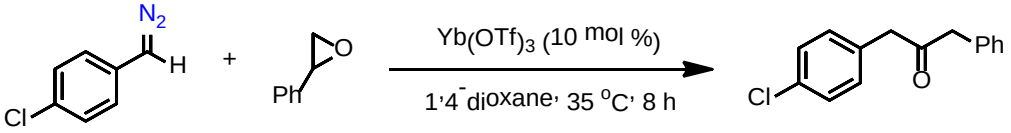
1-Chloro-4-(4-methylbenzyl)benzene (4b).[5] **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 2.32 (s, 3H), 3.90 (s, 2H), 7.05 (d, *J* = 7.8 Hz, 2H), 7.09-7.11 (m, 4H), 7.23 (d, *J* = 8.4 Hz, 2H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 21.00, 40.8, 128.5, 128.7, 129.2, 130.2, 131.8, 135.8, 137.5, 139.9.



2aa **4c**

The solution of **2aa**/Et_2O (0.6 mmol, obtained by general procedure C in 90% yield) was added to a mixture of ethyl propiolate (0.5 mmol) in 10 mL THF. The resulting mixture was stirred at room temperature for 15 h. After evaporation of organic layer, the desired product **4c** was obtained by silica gel chromatography.

Ethyl 3-(4-chlorophenyl)-1H-pyrazole-5-carboxylate (4c).[6] **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 1.35 (t, *J* = 7.2 Hz, 3H), 4.35 (q, *J* = 7.2 Hz, 2H), 7.05 (s, 1H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.70 (d, *J* = 8.4 Hz, 2H), 12.11 (s, 1H); **^{13}C-NMR** (151 MHz, $CDCl_3$) δ 14.0, 61.2, 105.1, 126.8, 129.0, 134.3, 139.6, 147.0, 160.6; **HRMS** (ESI) m/z calculated for $C_{12}H_{12}ClN_2O_2$ $[M+H]^+$ 251.0587, found 251.0592.



2aa **4d**

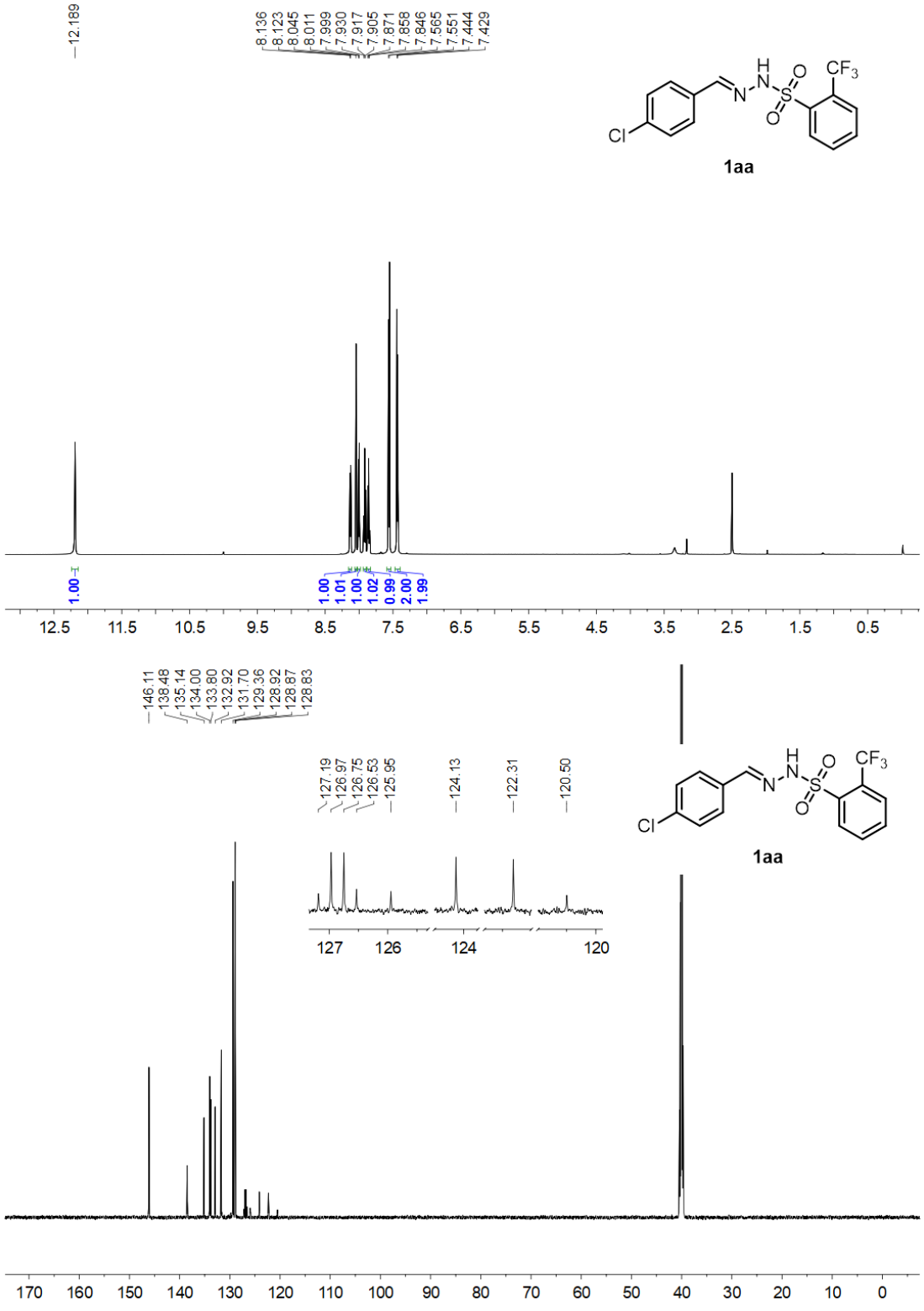
In a dried glass tube, styrene oxide (0.45 mmol), $Yb(OTf)_3$, and 1,4-dioxane (2 mL) was added sequentially at room temperature. After being stirred at 35 °C for 5 min, **2aa** (0.3 mmol) in 5 mL 1,4-dioxane was added dropwise for 30 min. The resulting mixture was allowed to stir at 40 °C for 8 h. After the reaction was completed, the reaction mixture was evaporated under reduced pressure to leave a crude mixture, which was purified by column chromatography on silica gel to afford **4d** as a white solid.

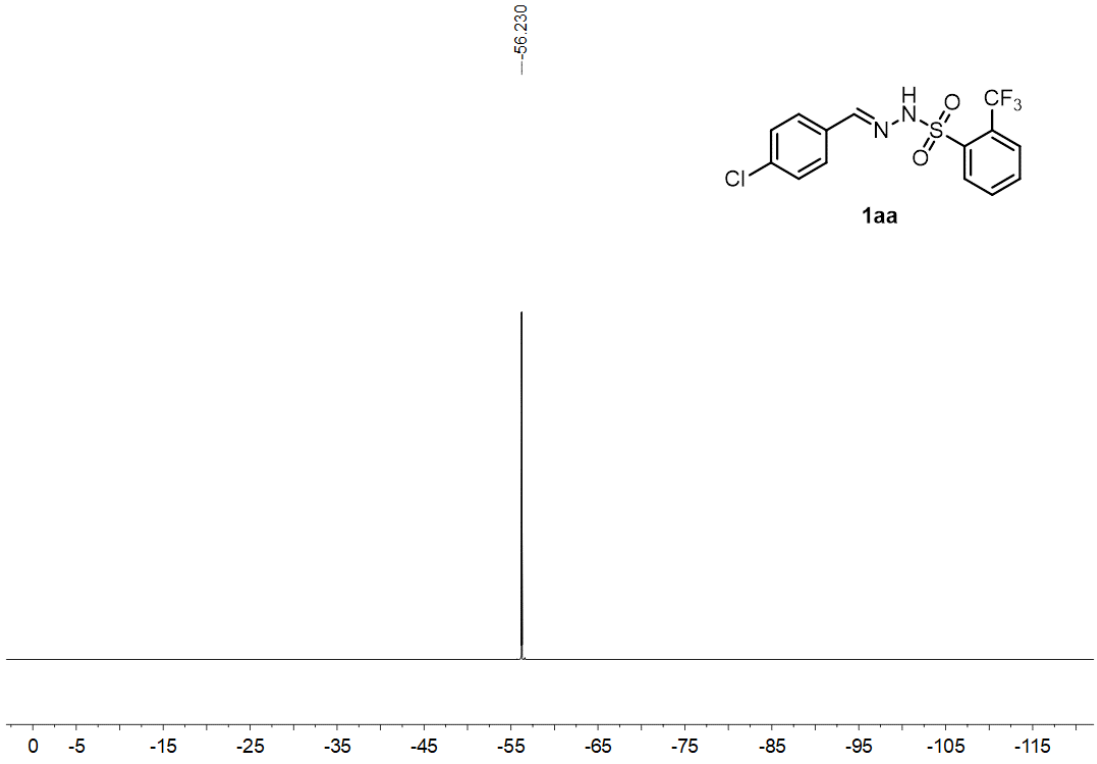
1-(4-Chlorophenyl)-3-phenylpropan-2-one (4d). White solid; m.p. 36-37 °C; **^{1}H-NMR** (500 MHz, $CDCl_3$) δ 3.69 (s, 2H), 3.72 (s, 2H), 7.05 (d, *J* = 7.0 Hz, 2H), 7.16 (d, *J* = 7.0 Hz, 2H), 7.26-7.29 (m, 3H), 7.33 (t, *J* = 7.0 Hz, 2H); **^{13}C-NMR** (125 MHz, $CDCl_3$) δ 48.0, 49.4, 127.2, 128.76, 128.80, 129.4, 130.8, 132.3, 133.0, 133.7, 205.1; **HRMS** (ESI) m/z calculated for $C_{15}H_{13}ClNaO$ $[M+Na]^+$ 267.0548, found 267.0552.

References

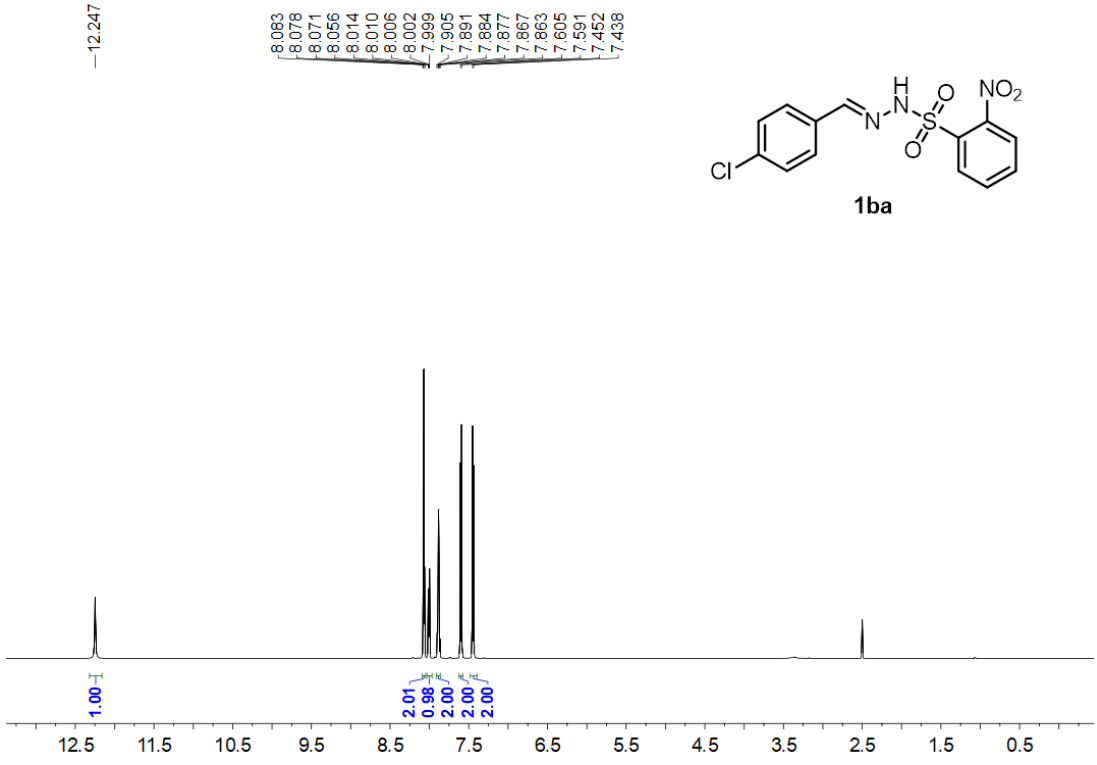
1. (*a*) Z. Liu, Q. Li, P. Liao, X. Bi, *Chem. Eur. J.*, 2017, **23**, 4756–4760; (*b*) Z. Liu, Q. Li, Y. Yang, X. Bi, *Chem. Commun.*, 2017, **53**, 2503–2506.
2. B. Lu, F. Zhu, H. Sun, Q. Shen, *Org. Lett.*, 2017, **19,** 1132-1135.
3. C. Zhang, P. Feng, N. Jiao, *J. Am. Chem. Soc.*, 2013, **135**, 15257−15262.
4. L. Zhou, X. Liu, J. Ji, Y. Zhang, W. Wu, Y. Liu, L. Lin, . X. Feng, *Org. Lett.*, 2014, **16**, 3938−3941.
5. F. Zhao, Q. Tan, F. Xiao, S. Zhang, G. Deng, *Org. Lett.*, 2013, **15**, 1520–1523.
6. N. S. Goulioukina, N. N. Makukhin, E. D. Shinkarev, Y. K. Grishin, V. A. Roznyatovsky, I. P. Beletskaya, *Org. Biomol. Chem.*, 2016, **14**, 10000–10010.

VI. ^{1}H, ^{13}C, and ^{19}F NMR spectral copies

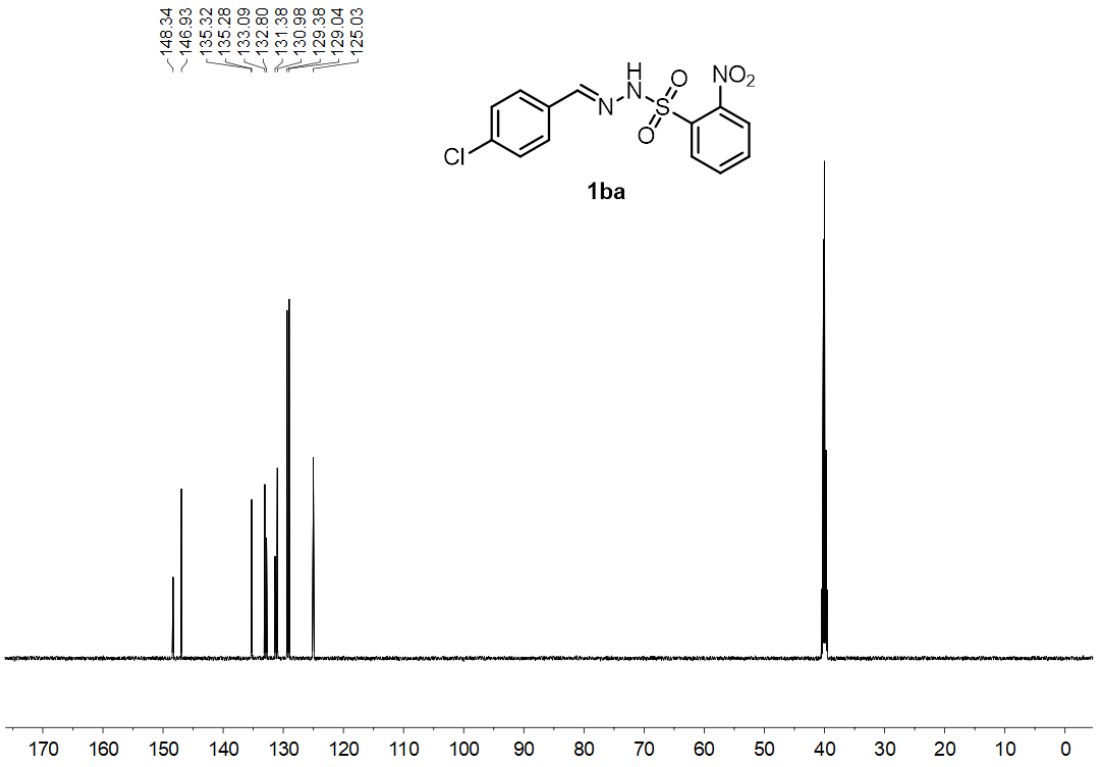


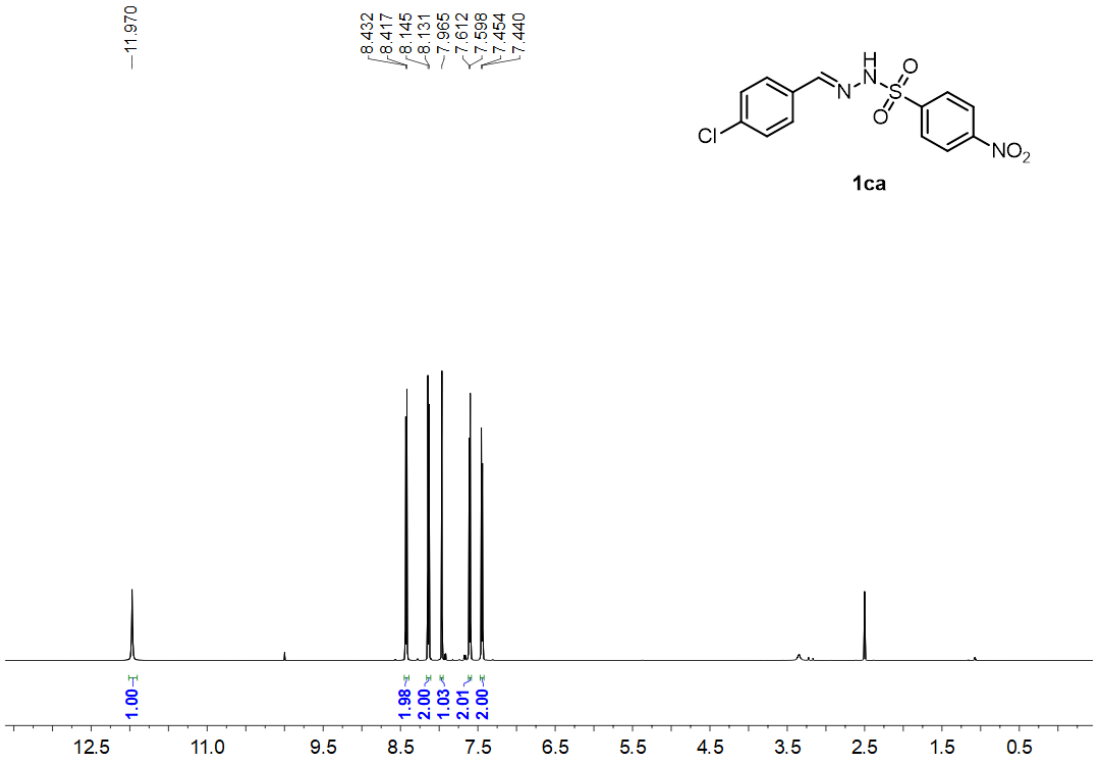

-56.230
0
-5
-15
-25
-35
-45
-55
-65
-75
-85
-95
-105
-115

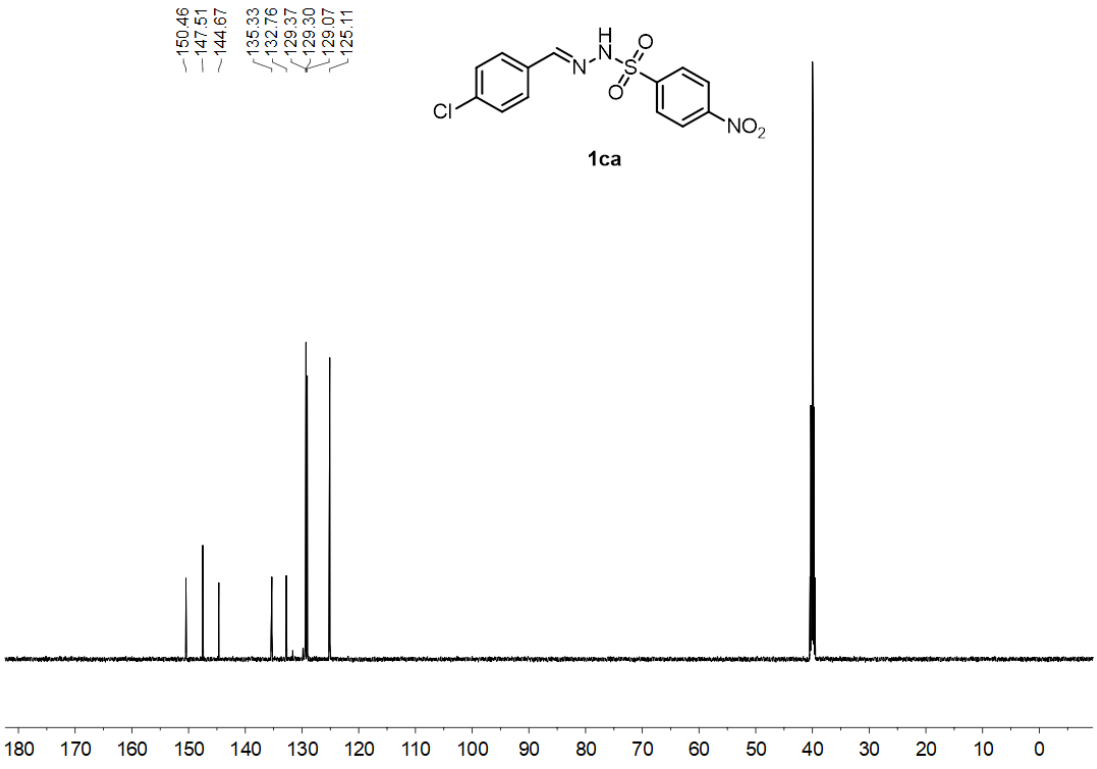
1aa

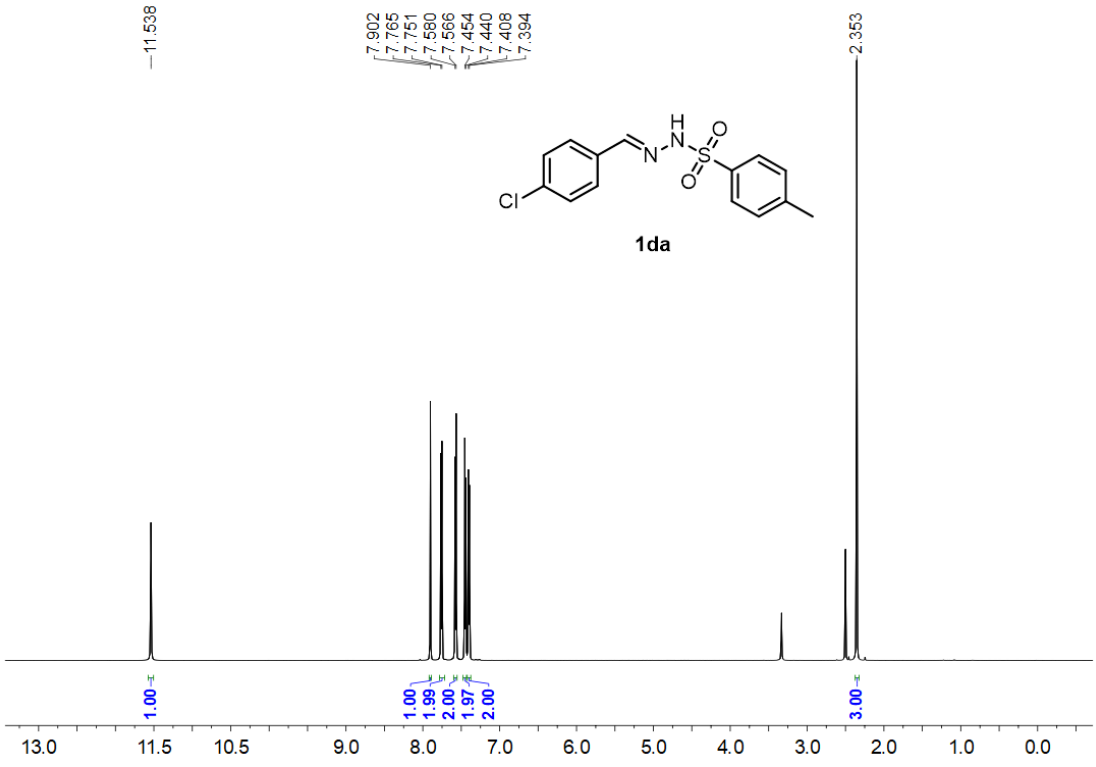

12.247
8.083
8.078
8.071
8.056
8.014
8.010
8.006
8.002
7.999
7.905
7.891
7.884
7.877
7.867
7.863
7.605
7.591
7.452
7.438
1.00
2.01
0.98
2.00
2.00
2.00
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5

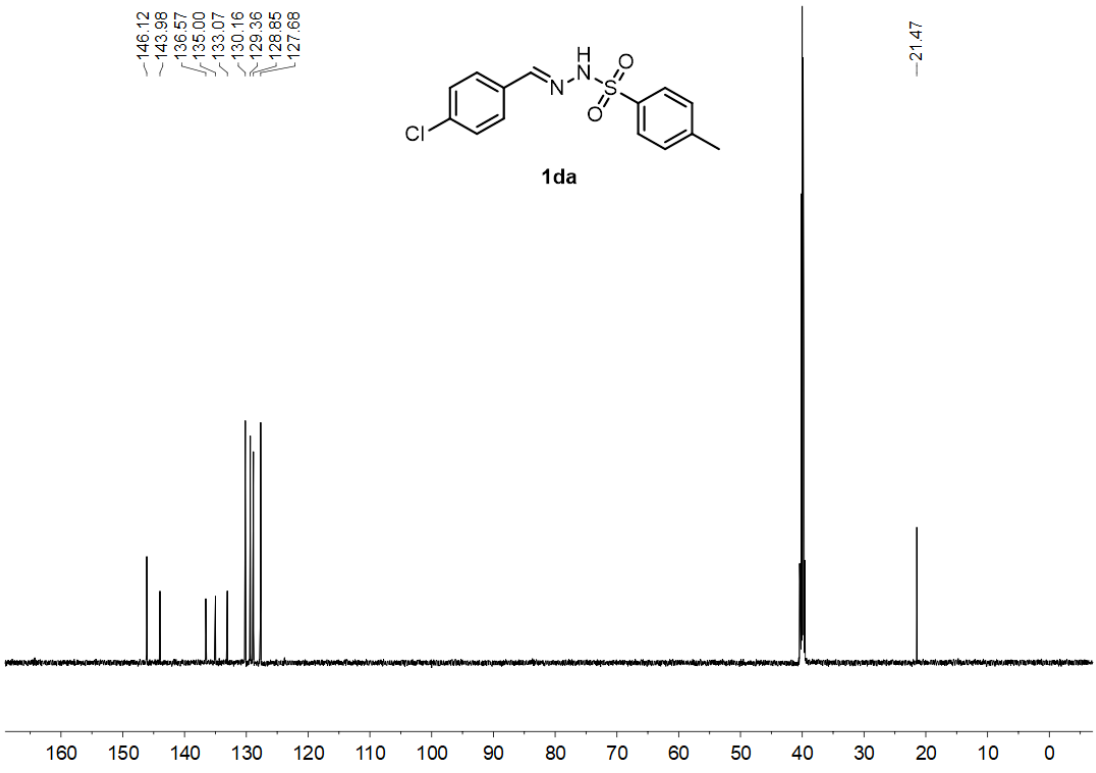
1ba

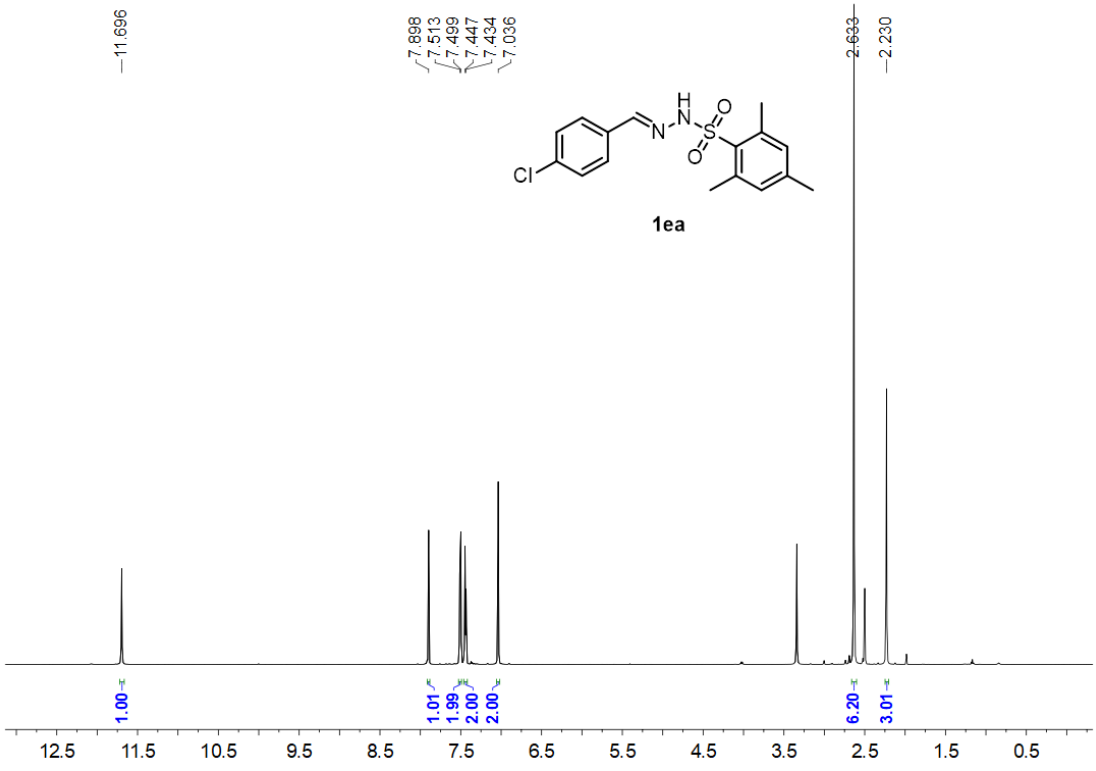

148.34
146.93
135.32
135.28
133.09
132.80
131.38
130.98
129.38
129.04
125.03
Cl
N
H
N
S
O
O
NO2
1ba
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

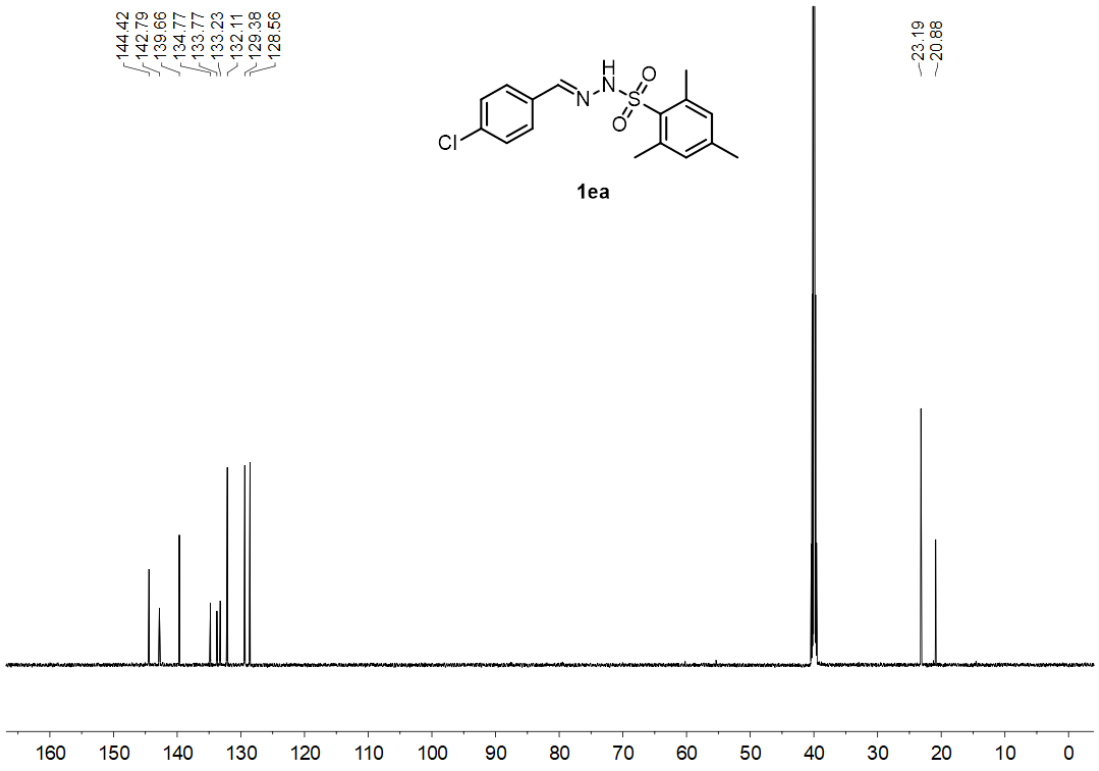

11.970
8.432
8.417
8.145
8.131
7.965
7.612
7.598
7.454
7.440
Cl
N
H
N
S
O
O
NO2
1ca
1.00
1.98
2.00
1.03
2.01
2.00
12.5
11.0
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5


150.46
147.51
144.67
135.33
132.76
129.37
129.30
129.07
125.11
Cl
NO2
1ca
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

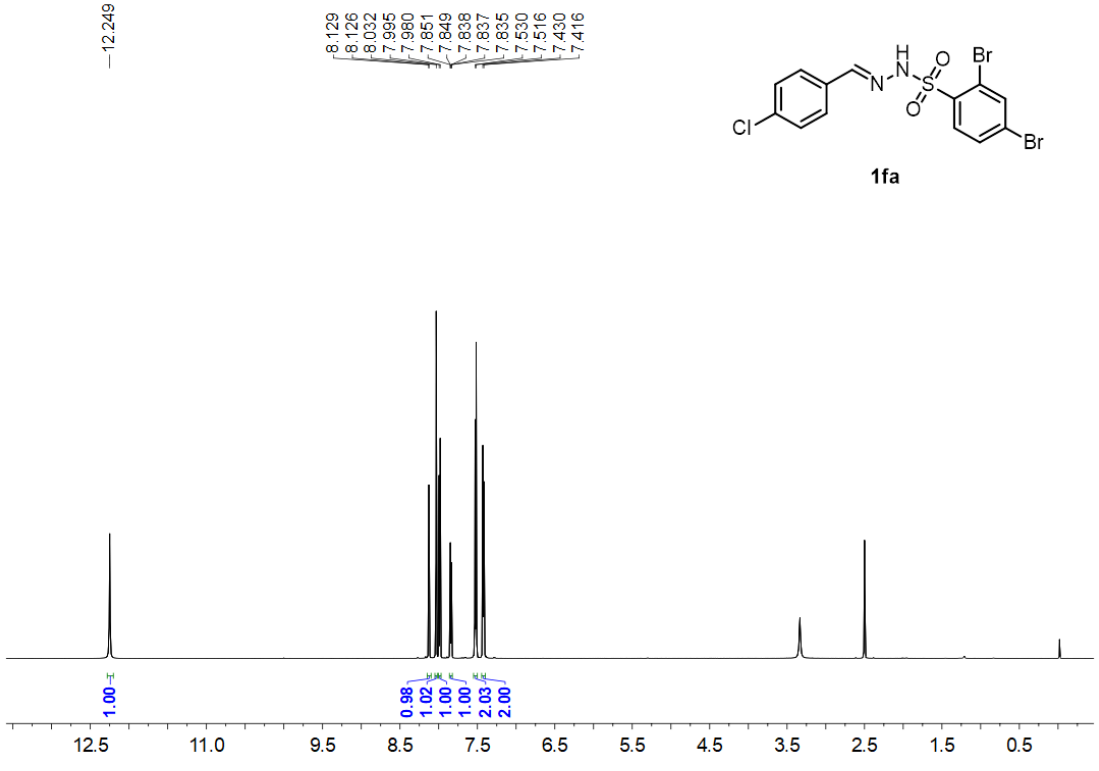

11.538
7.902
7.765
7.751
7.580
7.566
7.454
7.440
7.408
7.394
2.353
Cl
1da
1.00
1.00
1.99
2.00
1.97
2.00
3.00
13.0 11.5 10.5 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0


146.12
143.98
136.57
135.00
133.07
130.16
129.36
128.85
127.68
21.47
Cl
1da
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

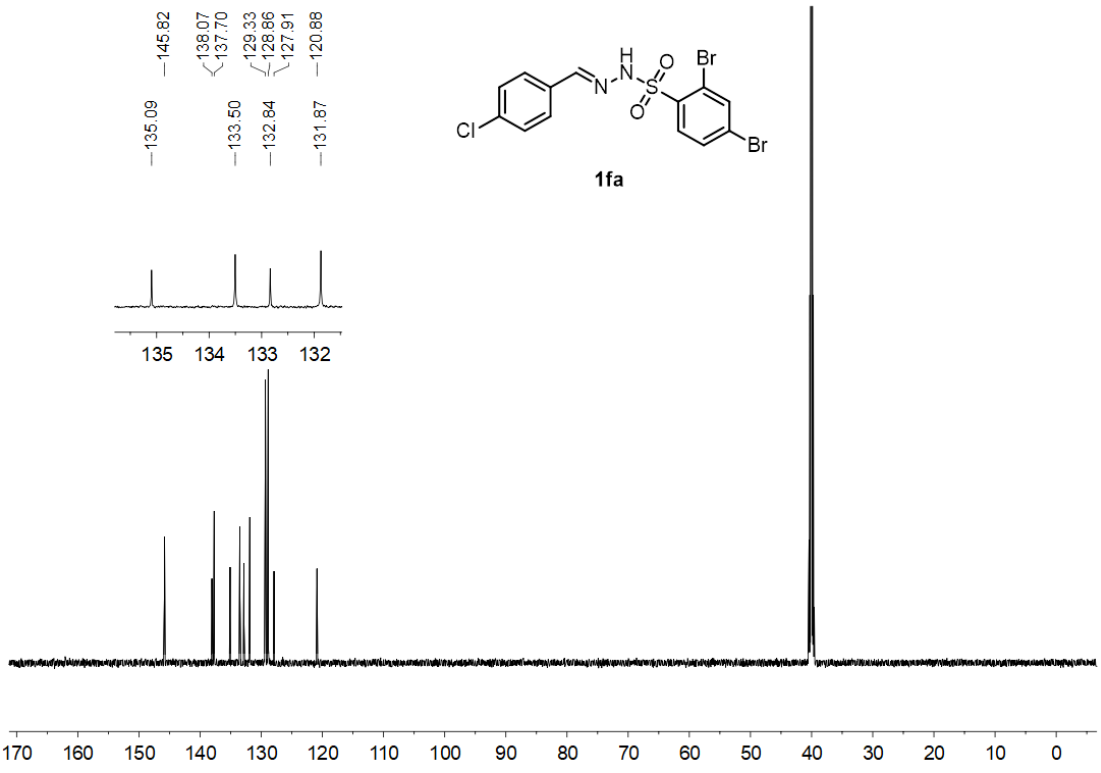

11.696
7.898
7.513
7.499
7.447
7.434
7.036
2.633
2.230
Cl
1ea
1.00
1.01
1.99
2.00
2.00
6.20
3.01
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5

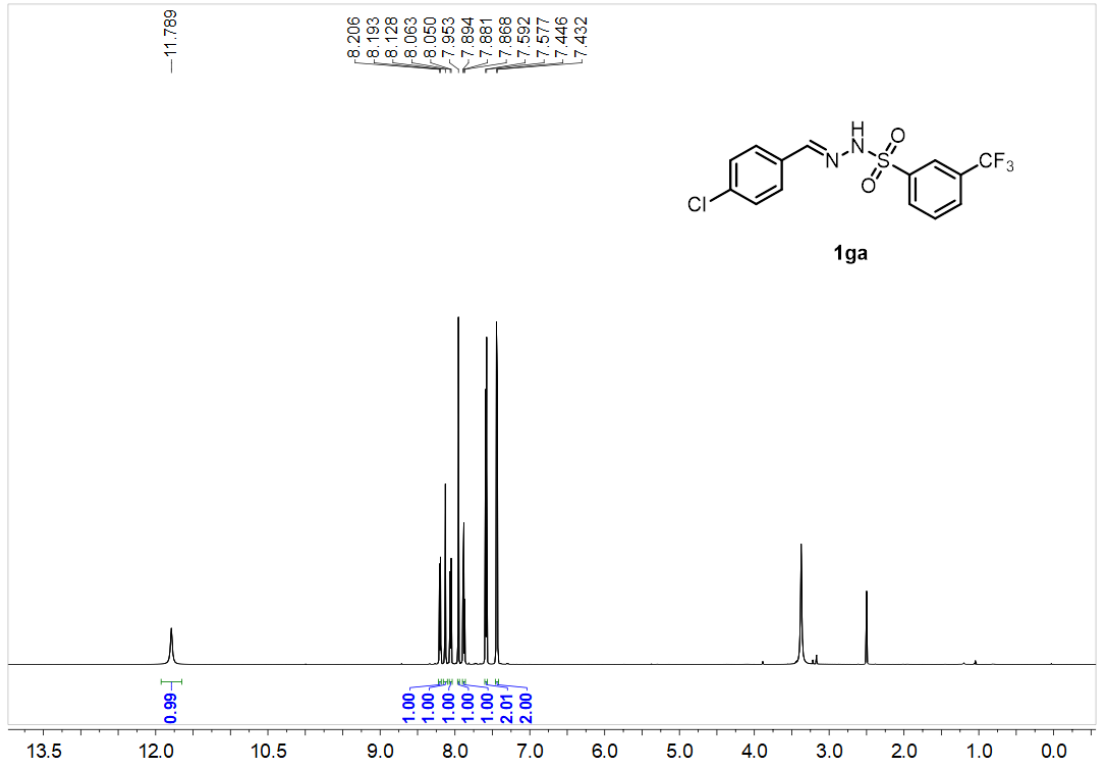

144.42
142.79
139.66
134.77
133.77
133.23
132.11
129.38
128.56
23.19
20.88
Cl
N
H
S
O
O
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

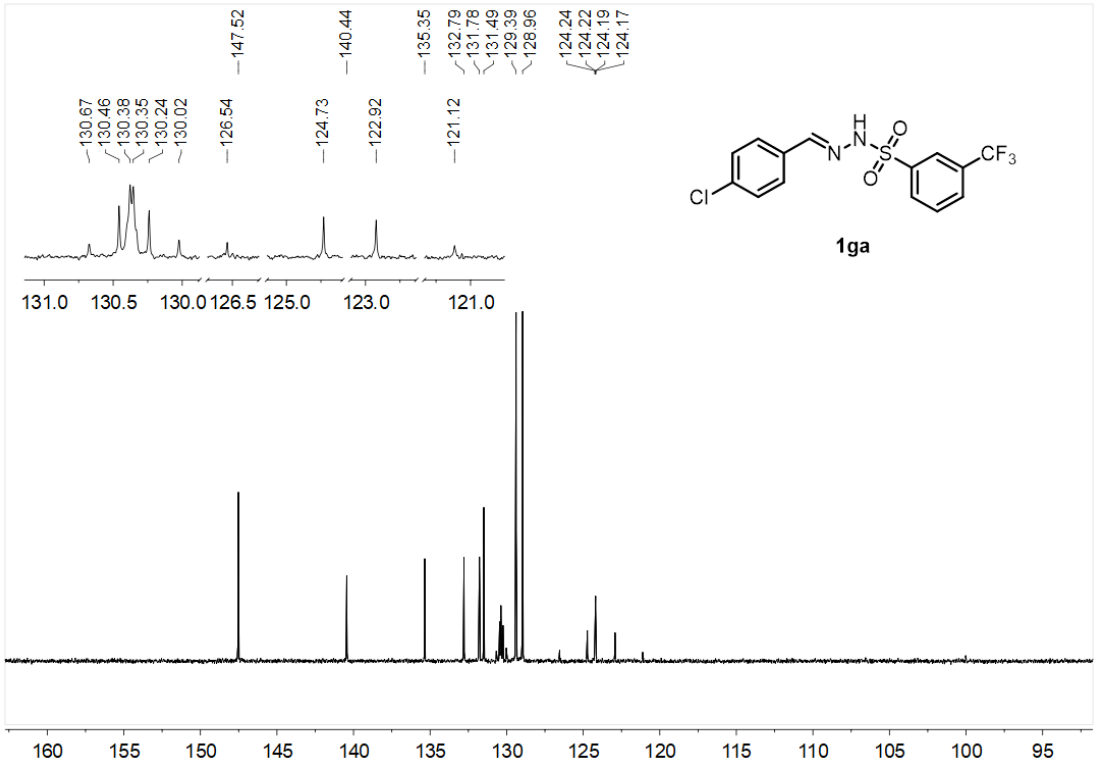
1ea


12.249
8.129
8.126
8.032
7.995
7.980
7.851
7.849
7.838
7.837
7.835
7.530
7.516
7.430
7.416
Cl
N
H
S
O
O
Br
Br
1.00
0.98
1.02
1.00
1.00
2.03
2.00
12.5 11.0 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5

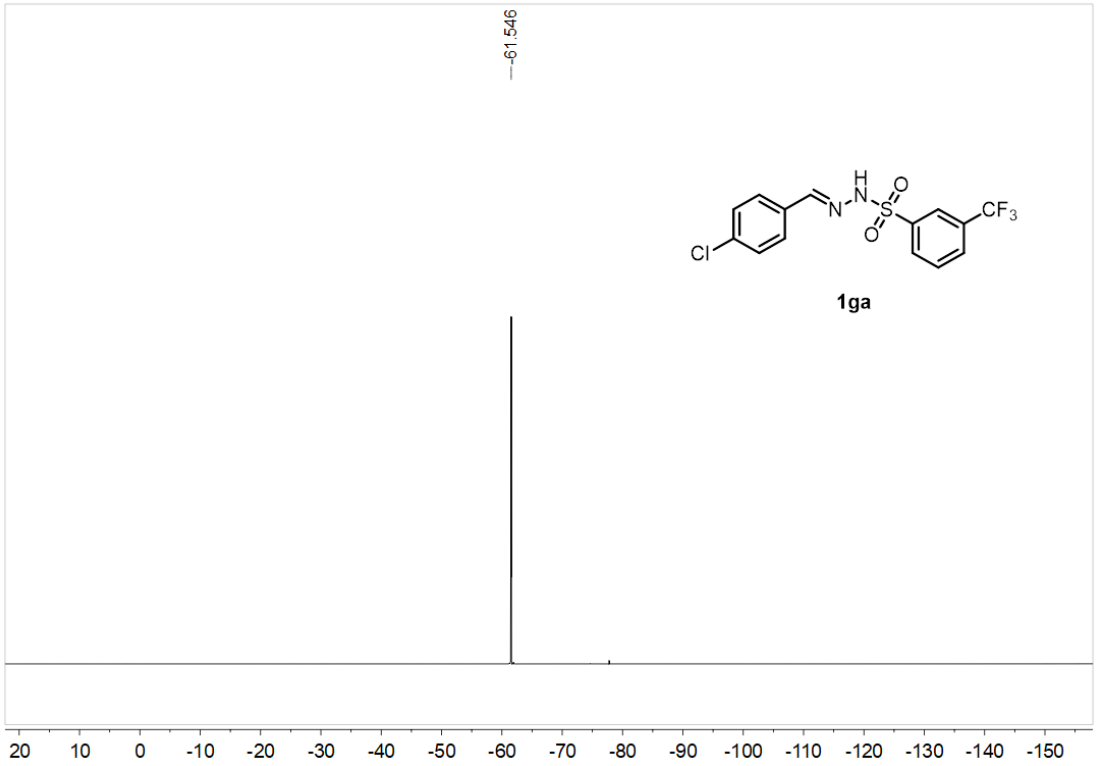
1fa


145.82
138.07
137.70
129.33
128.86
127.91
120.88
135.09
133.50
132.84
131.87
135
134
133
132
Cl
N
H
N
S
O
O
Br
Br
1fa
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

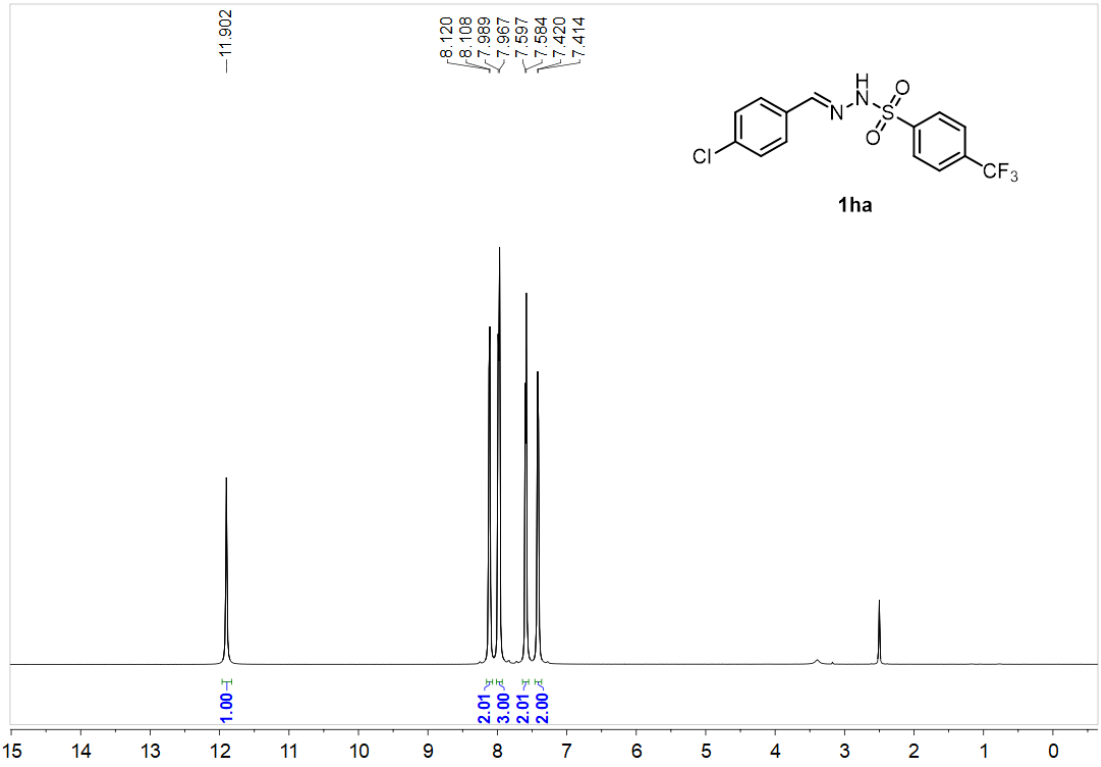

11.789
8.206
8.193
8.128
8.063
8.050
7.953
7.894
7.881
7.868
7.592
7.577
7.446
7.432
Cl
N
H
N
S
O
O
CF3
1ga
0.99
1.00
1.00
1.00
1.00
1.00
2.01
2.00
13.5
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

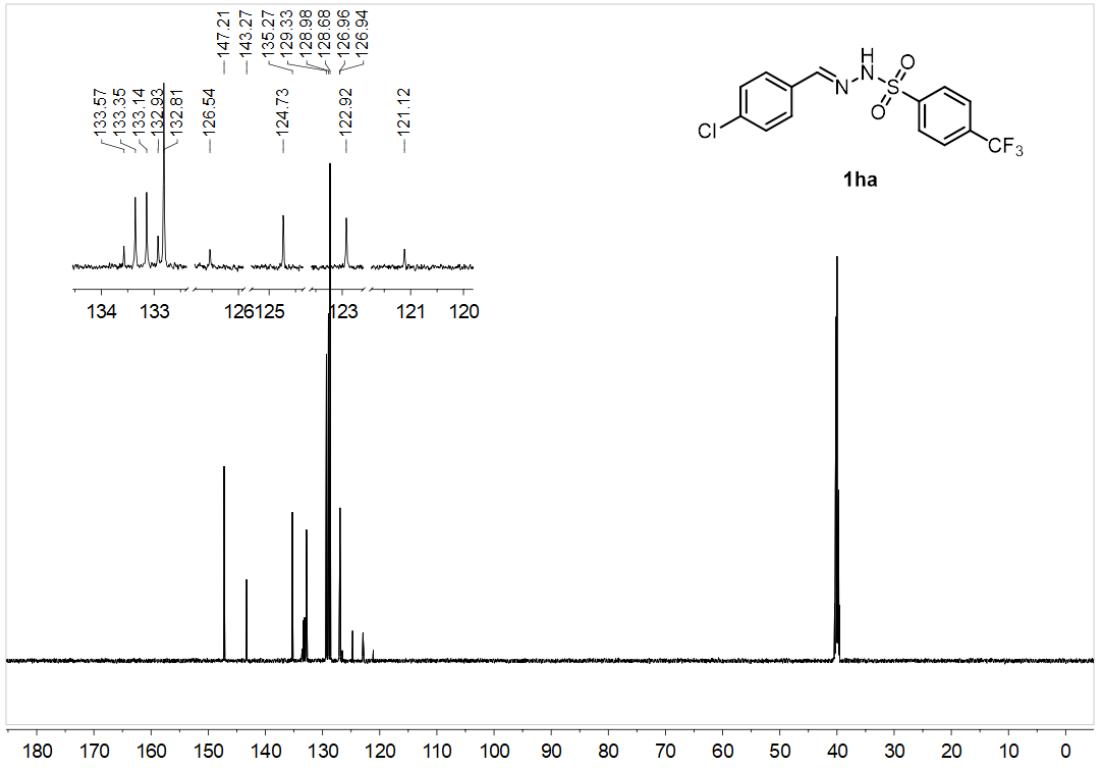

147.52
140.44
135.35
132.79
131.78
131.49
129.39
128.96
124.24
124.22
124.19
124.17
130.67
130.46
130.38
130.35
130.24
130.02
126.54
124.73
122.92
121.12
131.0
130.5
130.0
126.5
125.0
123.0
121.0
160
155
150
145
140
135
130
125
120
115
110
105
100
95
Cl
N
H
N
S
O
O
CF3

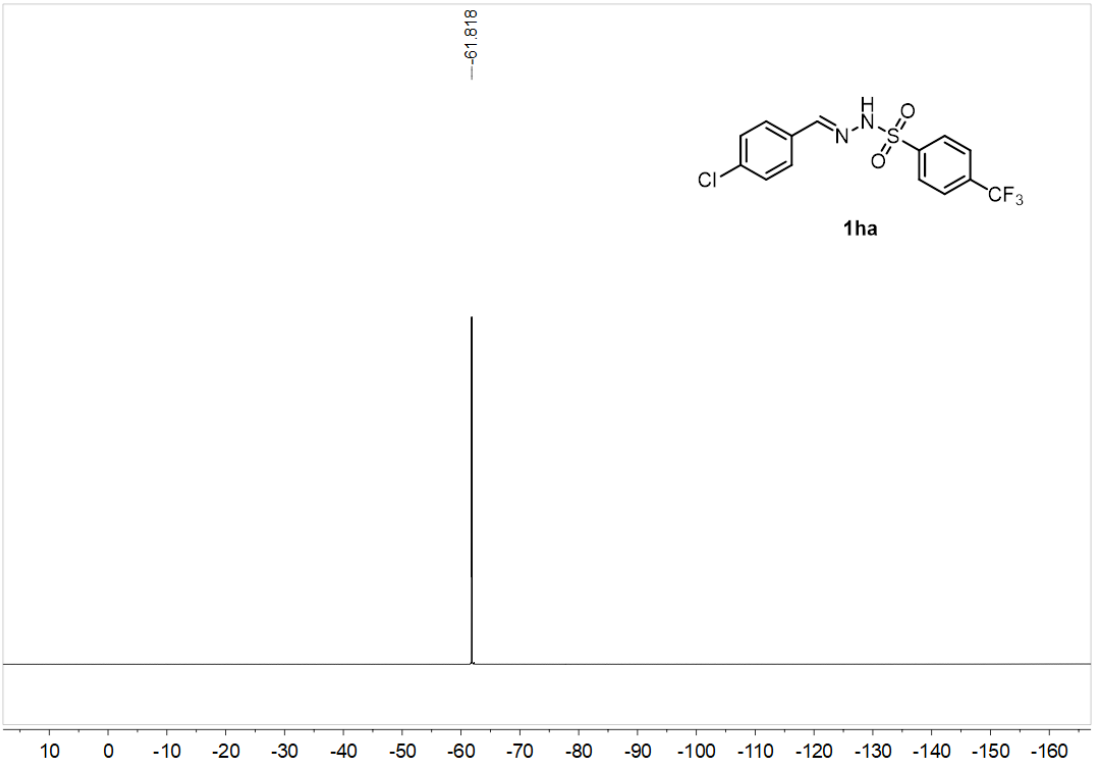
1ga

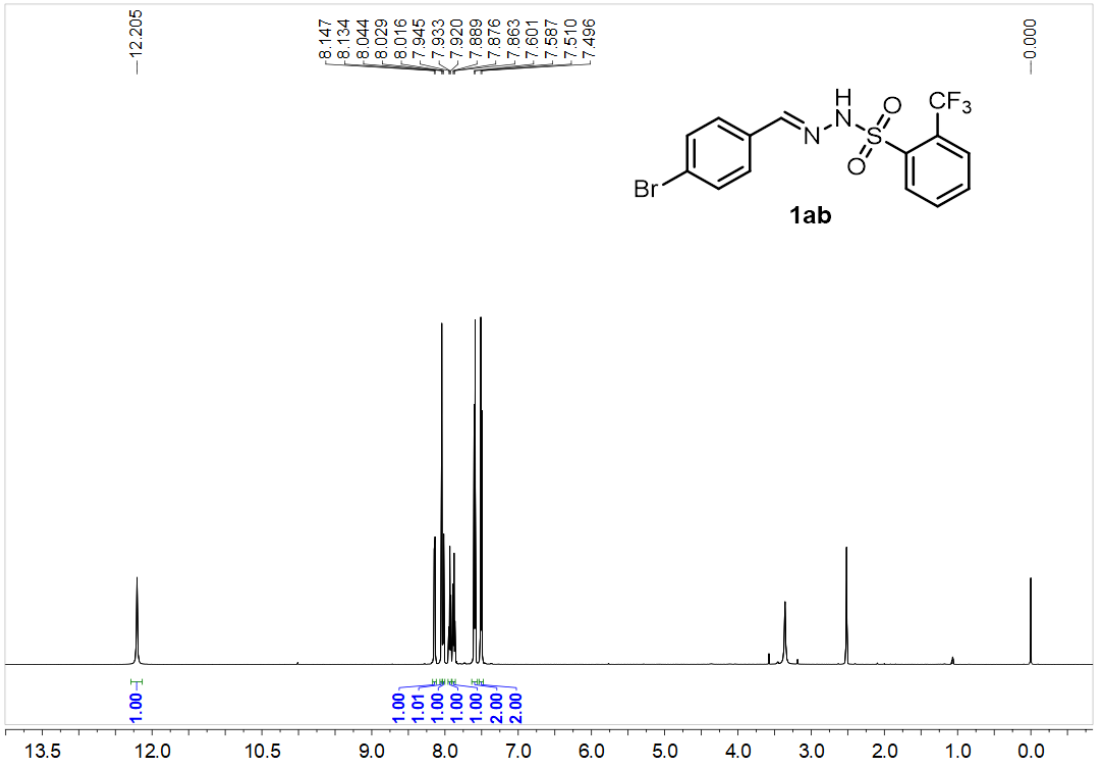

-61.546
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
Cl
N
H
N
S
O
O
CF3

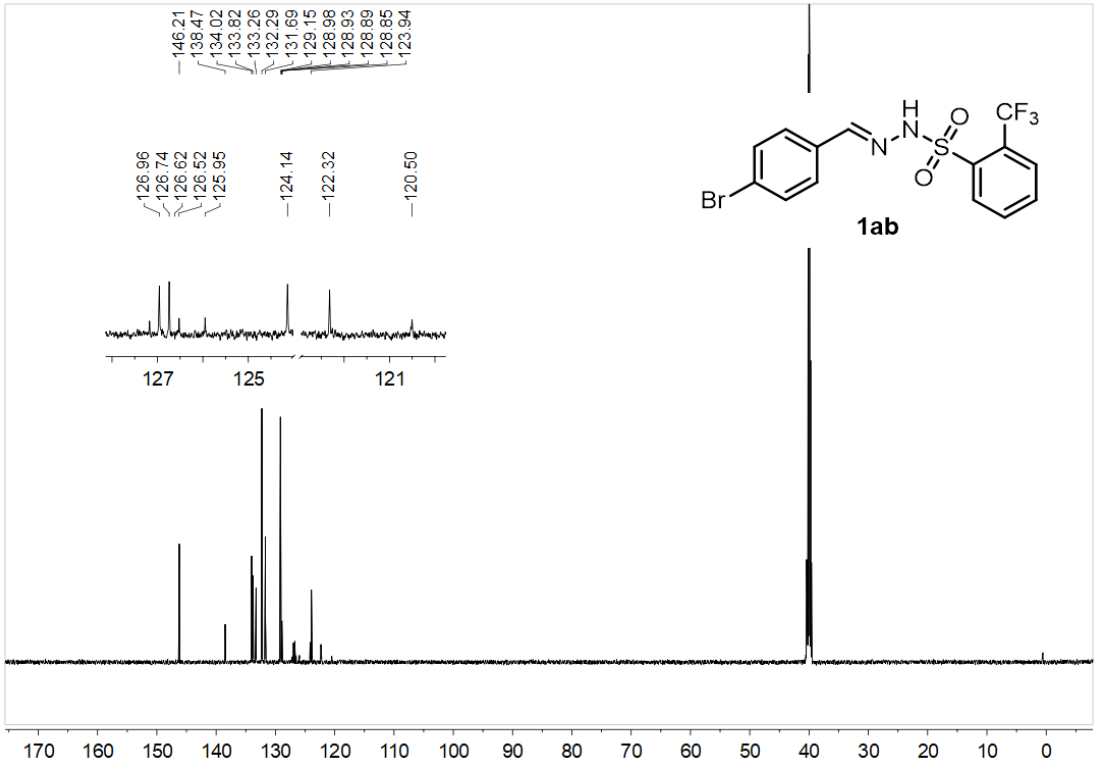
1ga

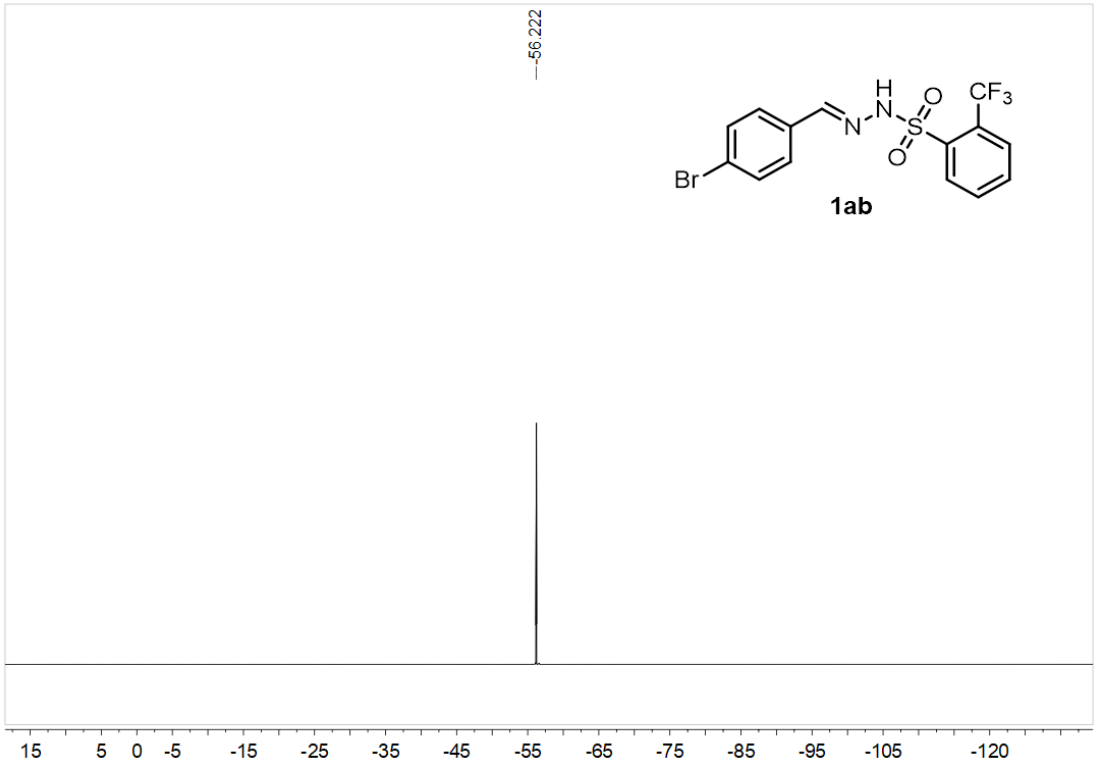

11.902
8.120
8.108
7.989
7.967
7.597
7.584
7.420
7.414
Cl
N
H
N
S
O
O
CF3
1ha
1.00
2.01
3.00
2.01
2.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0

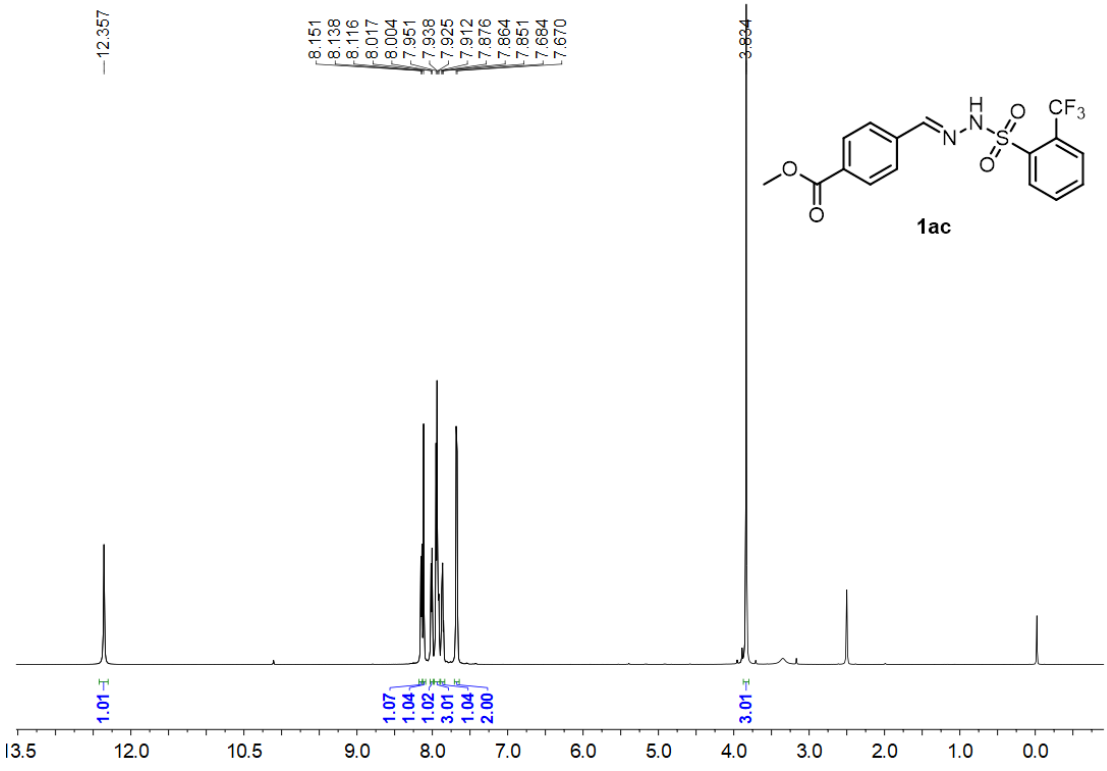

147.21
143.27
135.27
129.33
128.98
128.68
126.96
126.94
133.57
133.35
133.14
132.93
132.81
126.54
124.73
122.92
121.12
Cl
N
H
N
S
O
O
CF3
1ha
134 133 126125 123 121 120
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

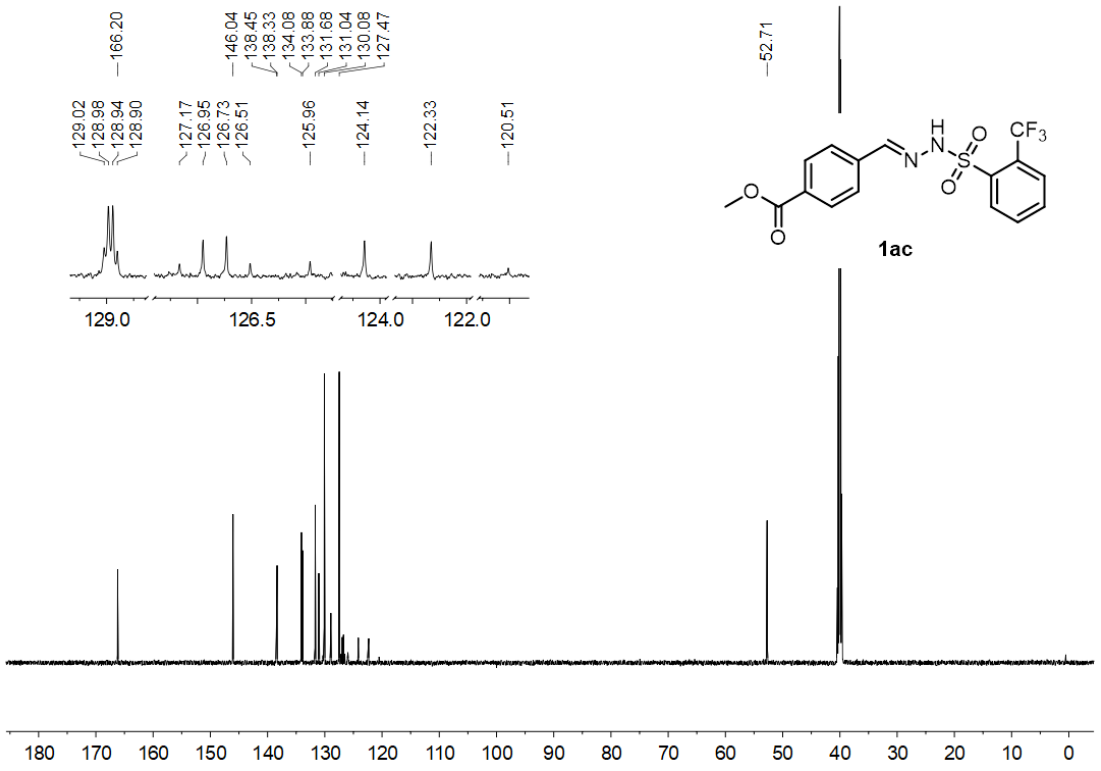

-61.818
Cl
N
H
N
S
O
O
CF3
1ha
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160

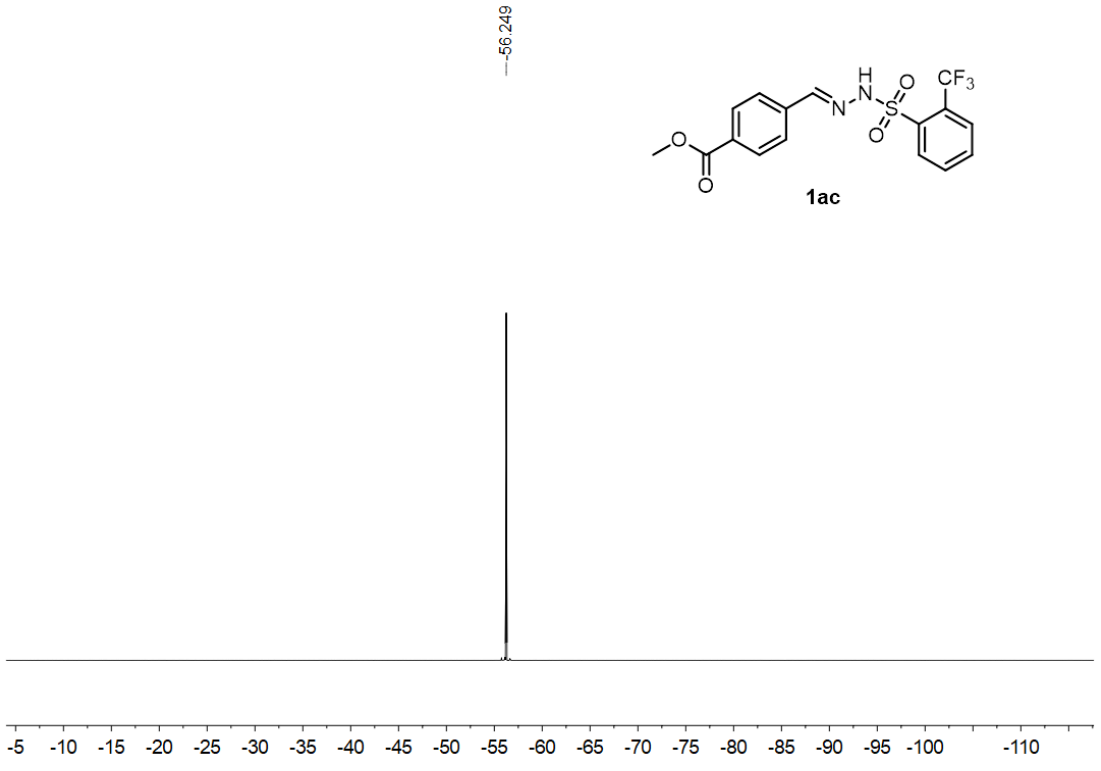

12.205
8.147
8.134
8.044
8.029
8.016
7.945
7.933
7.920
7.889
7.876
7.863
7.601
7.587
7.510
7.496
0.000
Br
N
H
N
S
O
O
CF3
1ab
1.00
1.00
1.01
1.00
1.00
1.00
2.00
2.00
13.5
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

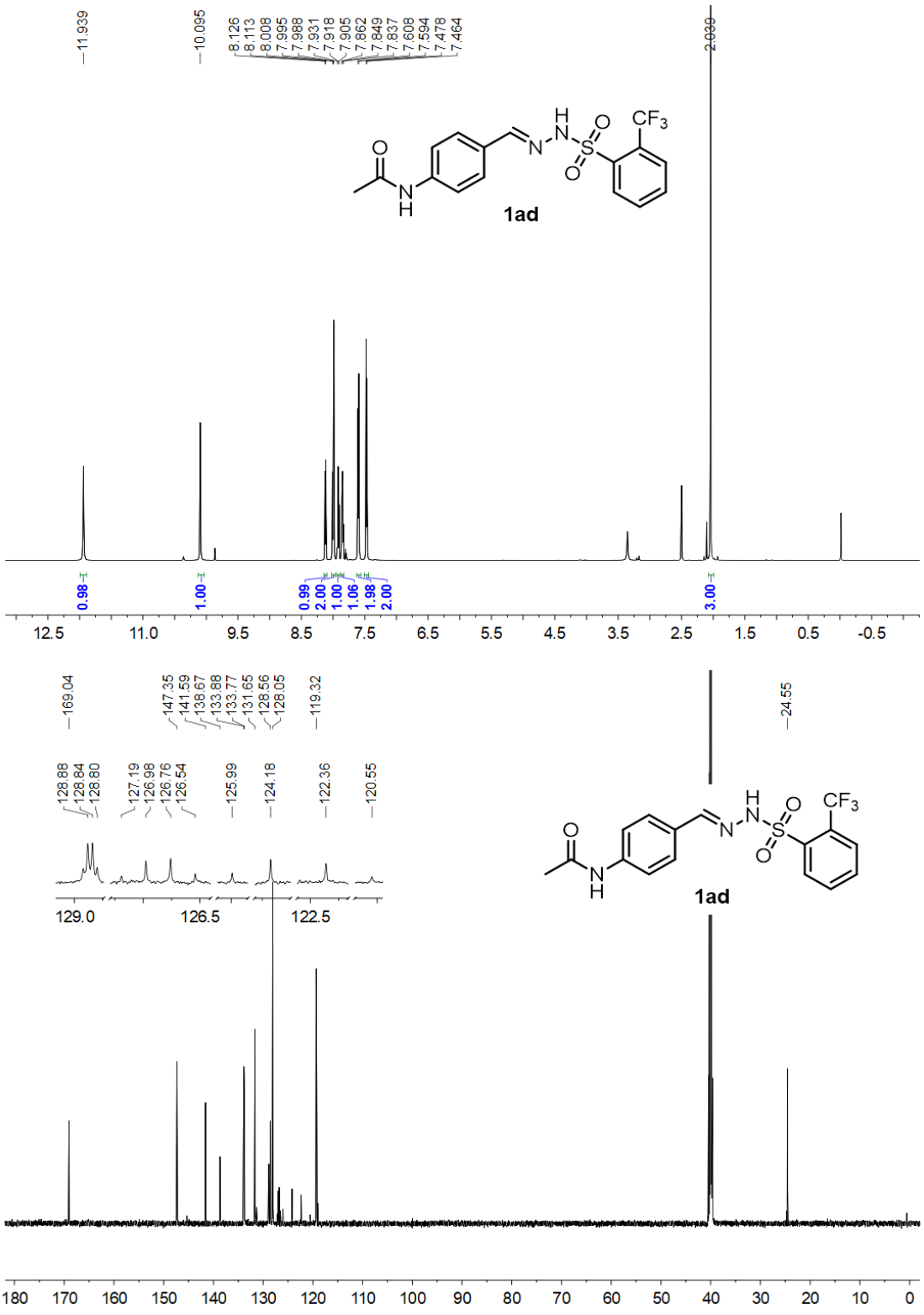

146.21
138.47
134.02
133.82
133.26
132.29
131.69
129.15
128.98
128.93
128.89
128.85
123.94
126.96
126.74
126.62
126.52
125.95
124.14
122.32
120.50
127
125
121
Br
N
H
N
S
O
O
CF3
1ab
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

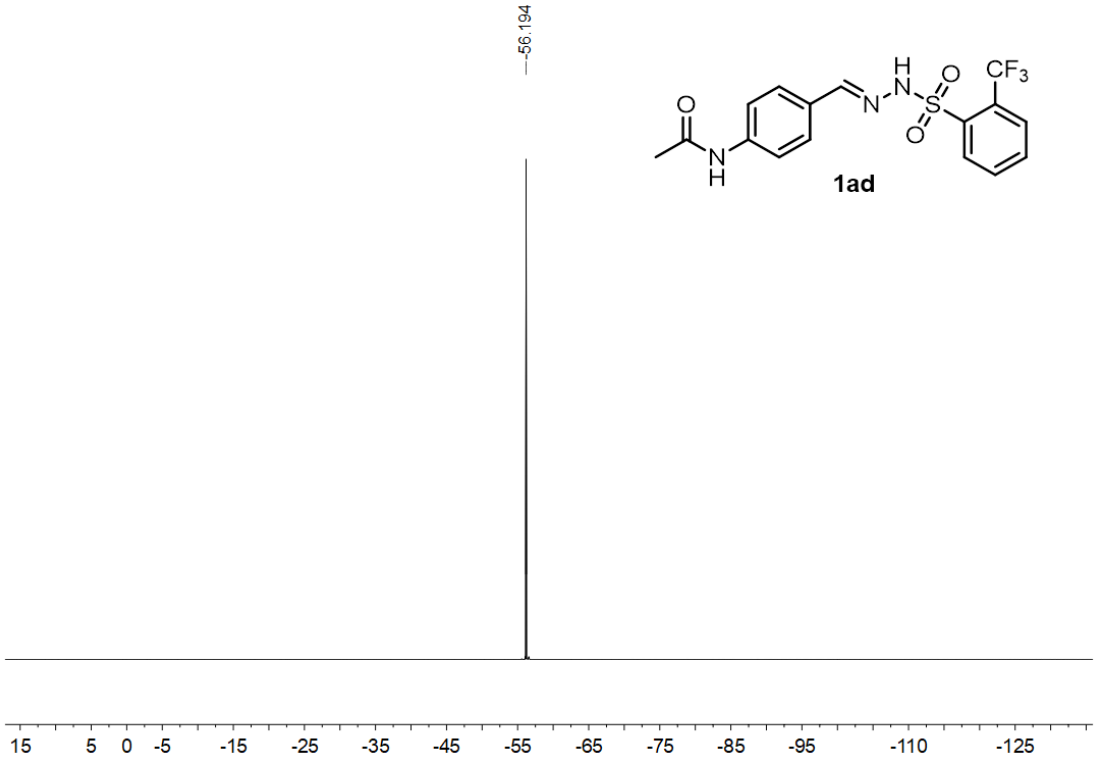

-56.222
Br
1ab
15
5
0
-5
-15
-25
-35
-45
-55
-65
-75
-85
-95
-105
-120

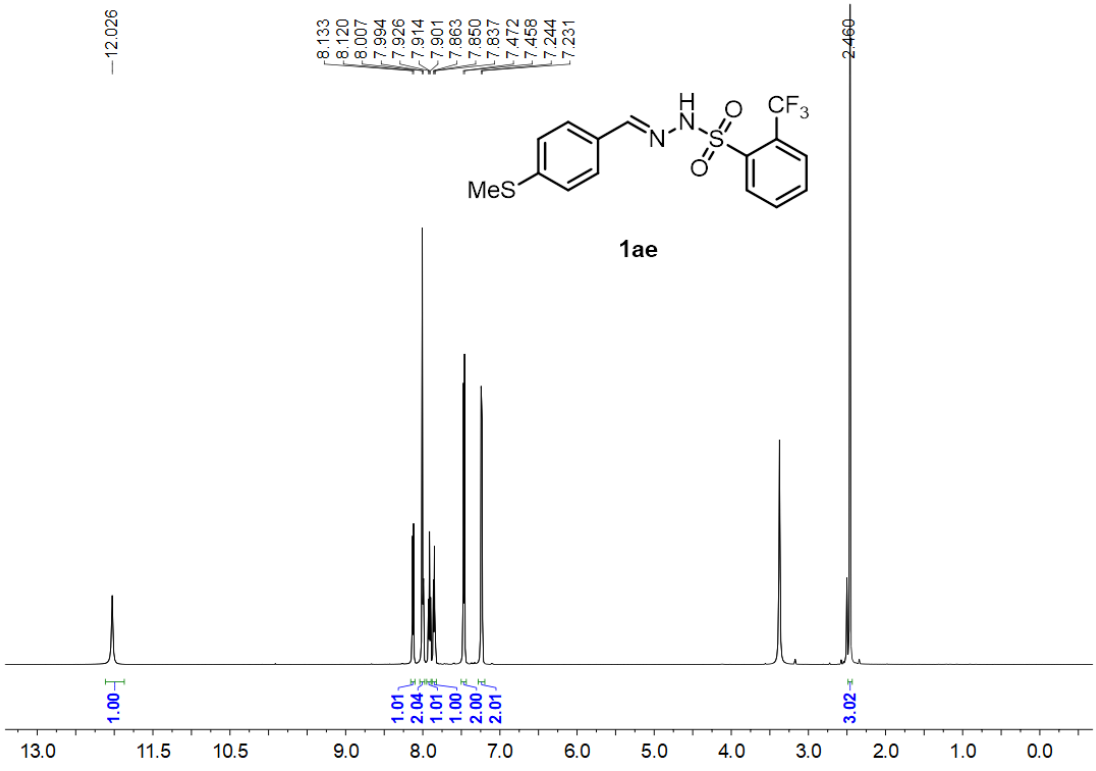

12.357
8.151
8.138
8.116
8.017
8.004
7.951
7.938
7.925
7.912
7.876
7.864
7.851
7.684
7.670
3.834
1ac
1.01
1.07
1.04
1.02
3.01
1.04
2.00
3.01
13.5
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

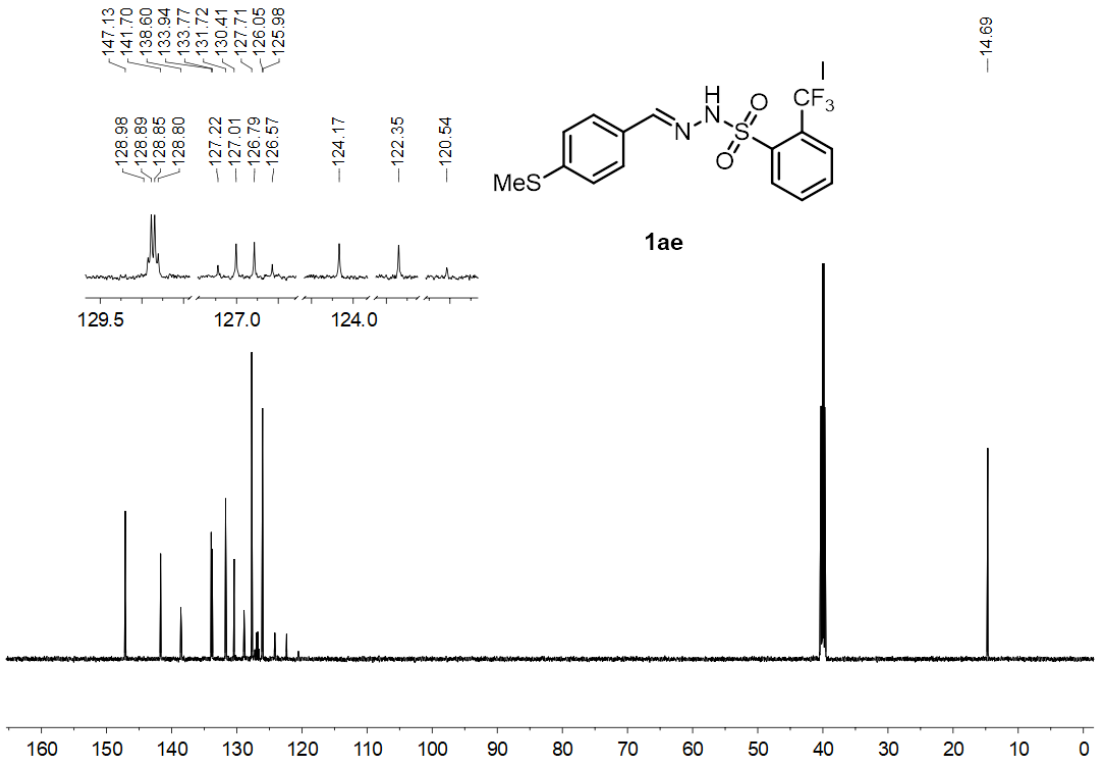

166.20
146.04
138.45
138.33
134.08
133.88
131.68
131.04
130.08
127.47
129.02
128.98
128.94
128.90
127.17
126.95
126.73
126.51
125.96
124.14
122.33
120.51
52.71
129.0
126.5
124.0
122.0
CF3
1ac

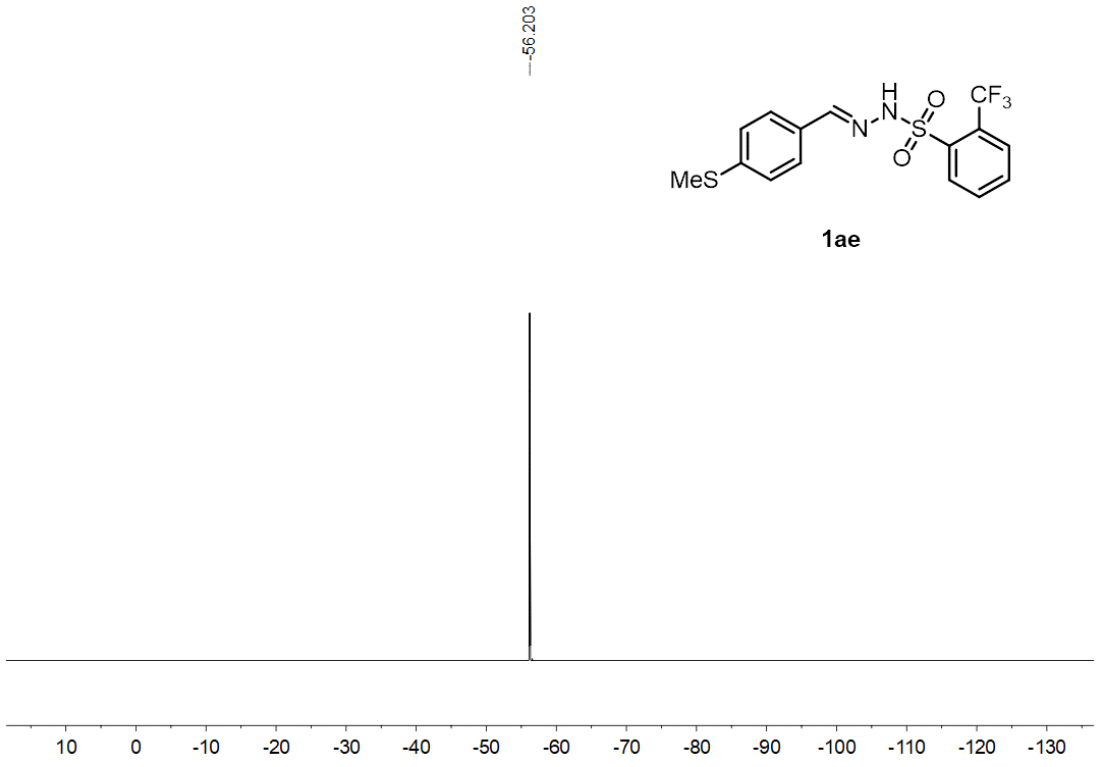

56.249
CF3
1ac

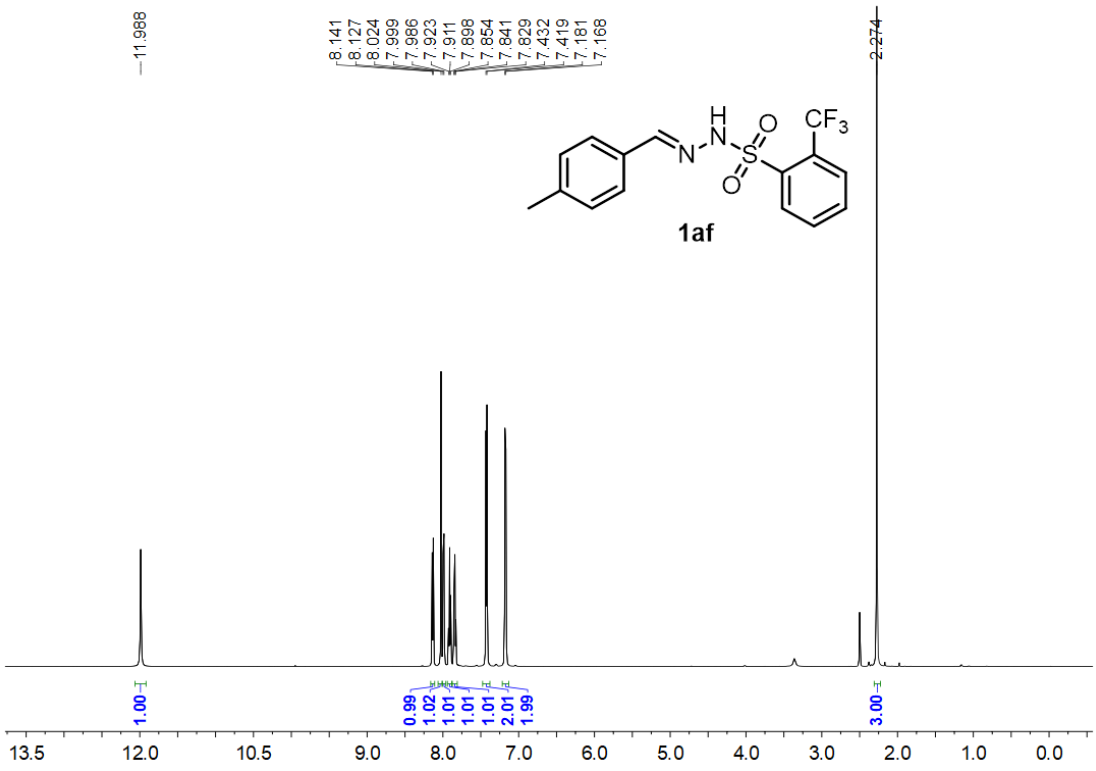

11.939
10.095
8.126
8.113
8.008
7.995
7.988
7.931
7.918
7.905
7.862
7.849
7.837
7.608
7.594
7.478
7.464
2.039
1ad
0.98
1.00
0.99
2.00
1.00
1.06
1.98
2.00
3.00
12.5
11.0
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
169.04
147.35
141.59
138.67
133.88
133.77
131.65
128.56
128.05
119.32
128.88
128.84
128.80
127.19
126.98
126.76
126.54
125.99
124.18
122.36
120.55
24.55
129.0
126.5
122.5
1ad
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

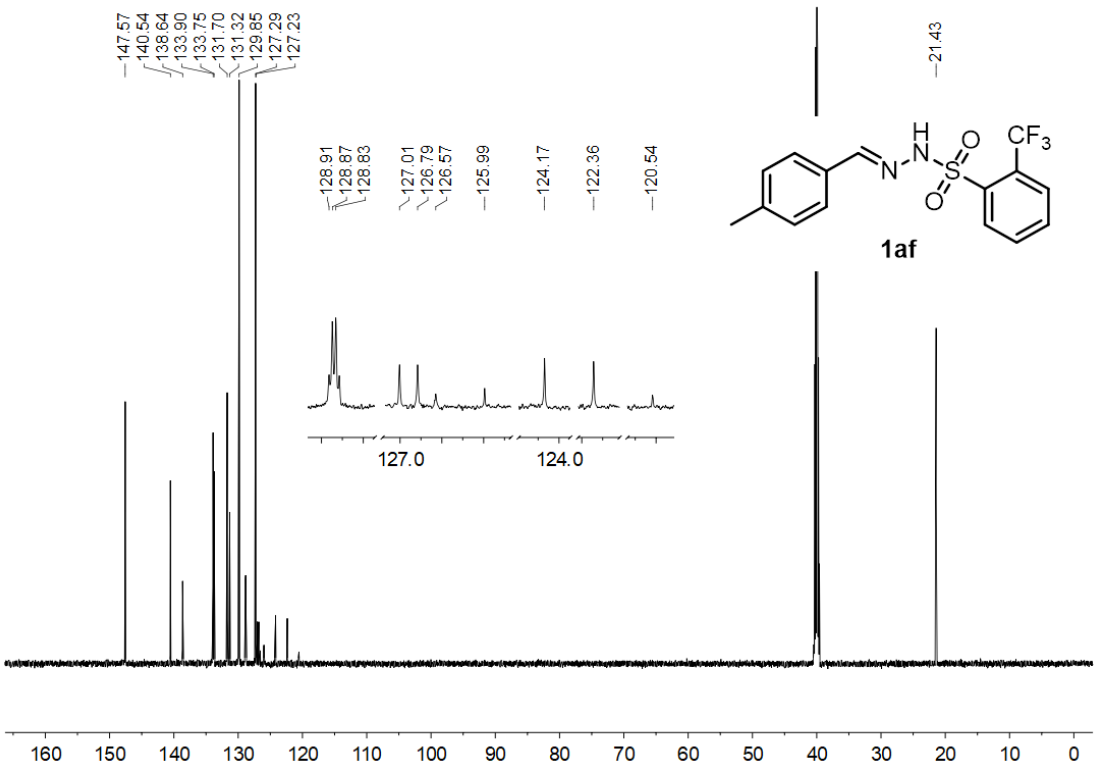

-56.194
1ad
15
5
0
-5
-15
-25
-35
-45
-55
-65
-75
-85
-95
-110
-125

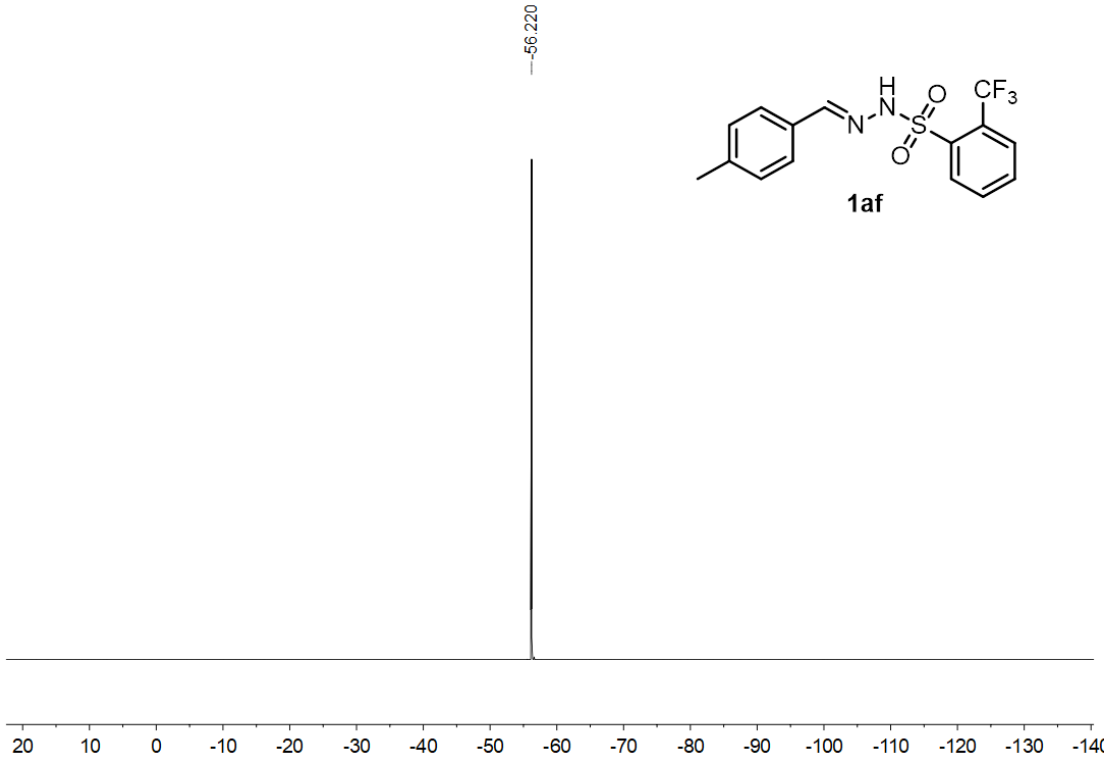

12.026
8.133
8.120
8.007
7.994
7.926
7.914
7.901
7.863
7.850
7.837
7.472
7.458
7.244
7.231
2.460
MeS
1ae
1.00
1.01
2.04
1.01
1.00
2.00
2.01
3.02
13.0
11.5
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


147.13
141.70
138.60
133.94
133.77
131.72
130.41
127.71
126.05
125.98
128.98
128.89
128.85
128.80
127.22
127.01
126.79
126.57
124.17
122.35
120.54
14.69
MeS
CF3
1ae
129.5
127.0
124.0
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

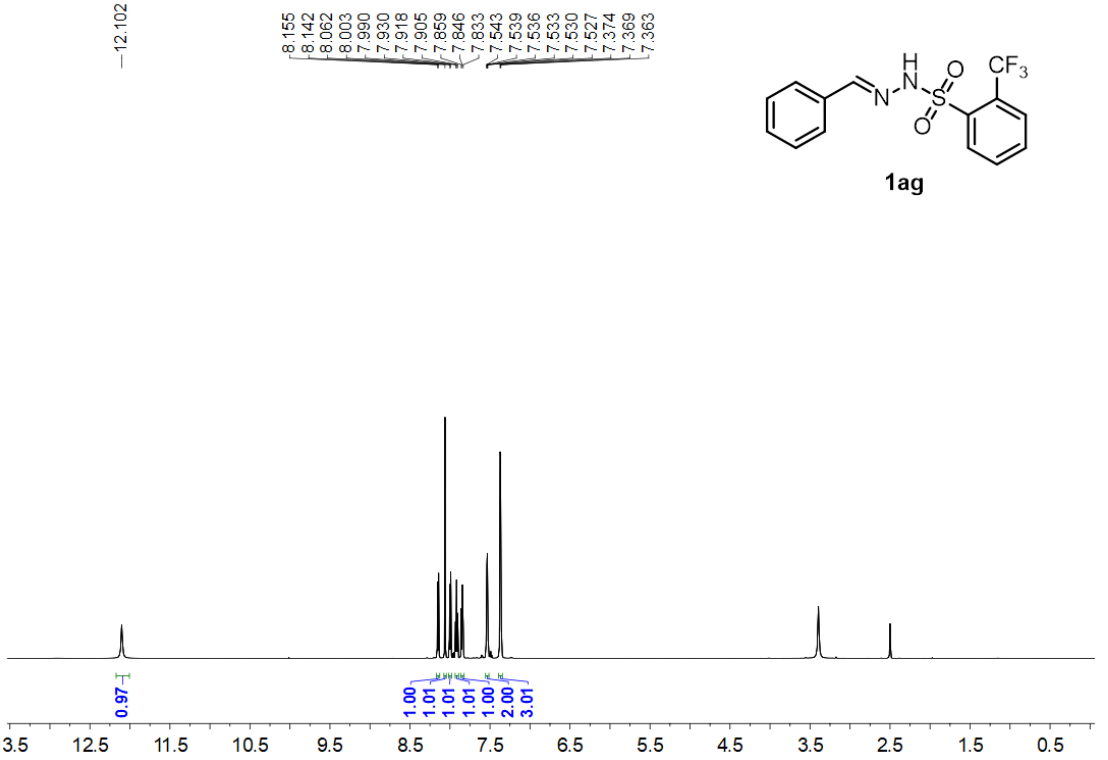

-56.203
MeS
CF3
1ae
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130


11.988
8.141
8.127
8.024
7.999
7.986
7.923
7.911
7.898
7.854
7.841
7.829
7.432
7.419
7.181
7.168
2.274
1af
1.00
0.99
1.02
1.01
1.01
1.01
2.01
1.99
3.00
13.5
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

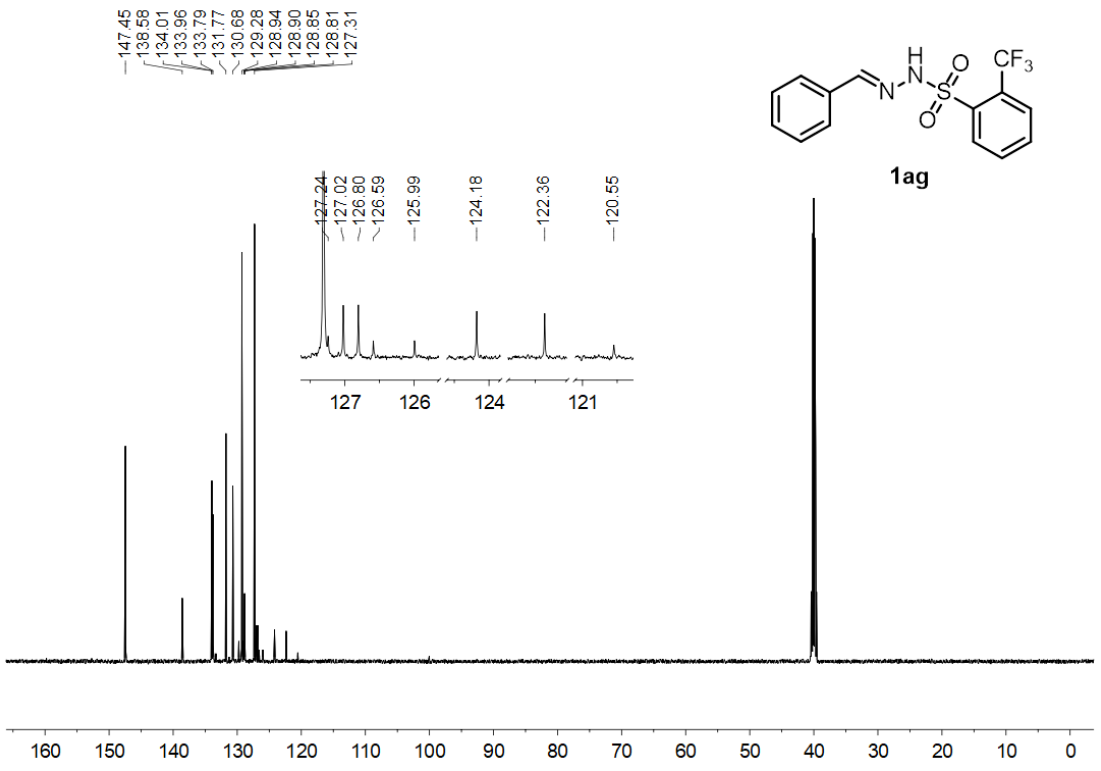

147.57
140.54
138.64
133.90
133.75
131.70
131.32
129.85
127.29
127.23
128.91
128.87
128.83
127.01
126.79
126.57
125.99
124.17
122.36
120.54
21.43
1af
127.0
124.0
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

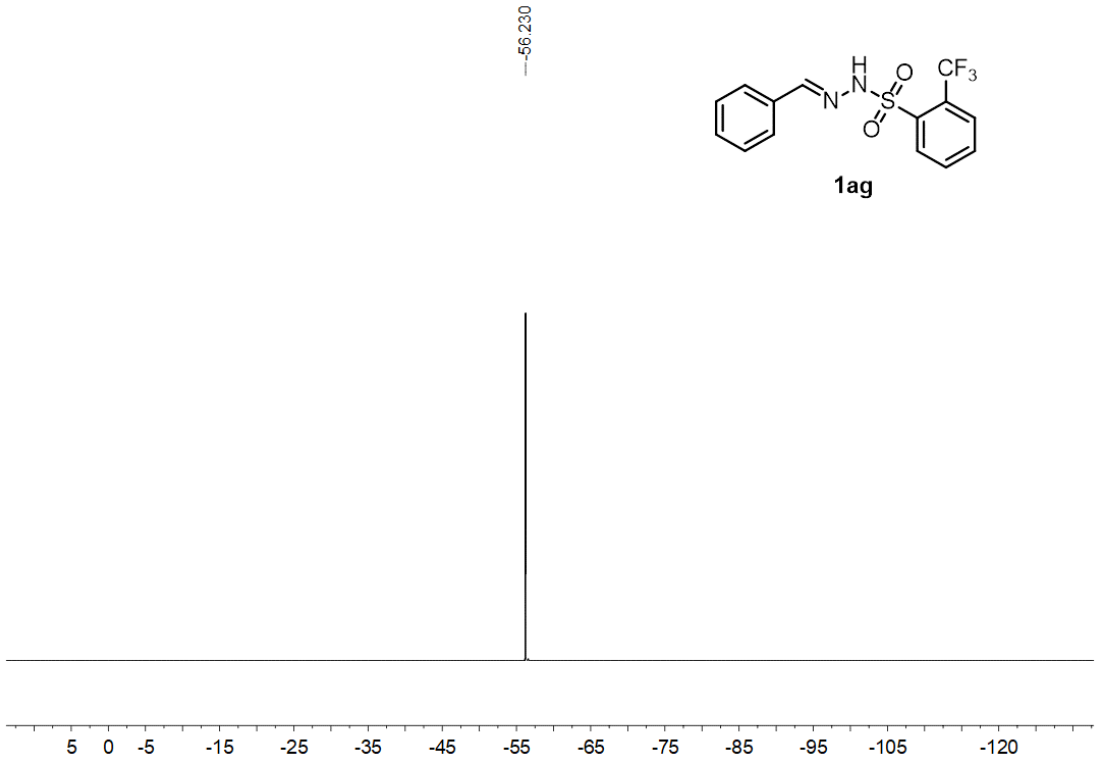

-56.220
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140

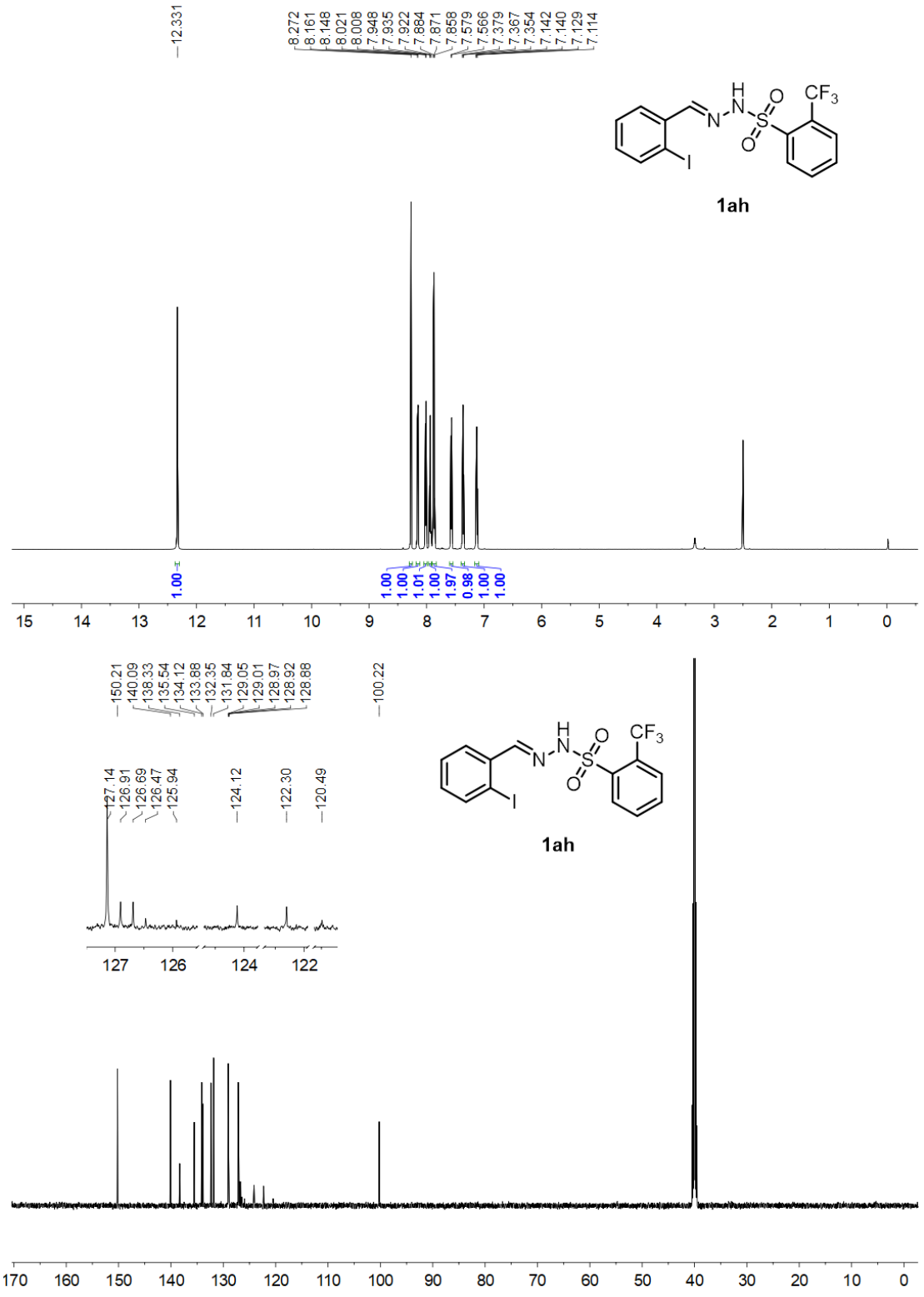
1af

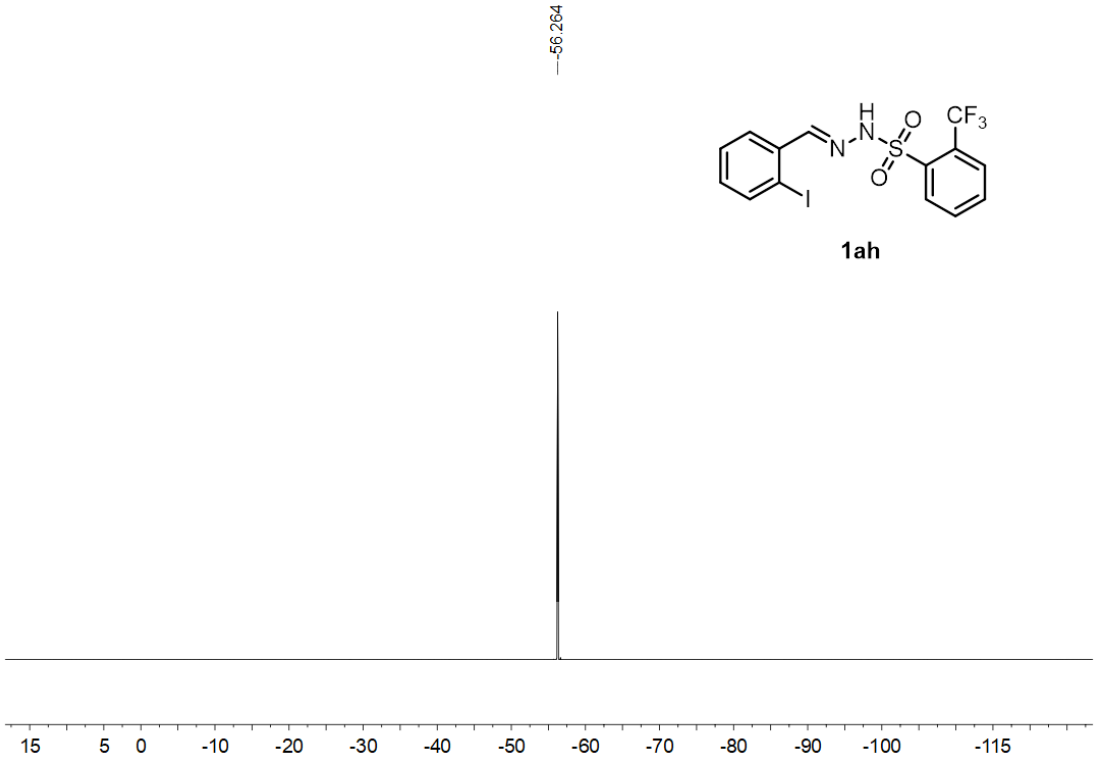

12.102
8.155
8.142
8.062
8.003
7.990
7.930
7.918
7.905
7.859
7.846
7.833
7.543
7.539
7.536
7.533
7.530
7.527
7.374
7.369
7.363
0.97
1.00
1.01
1.01
1.01
1.00
2.00
3.01
13.5
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5

1ag

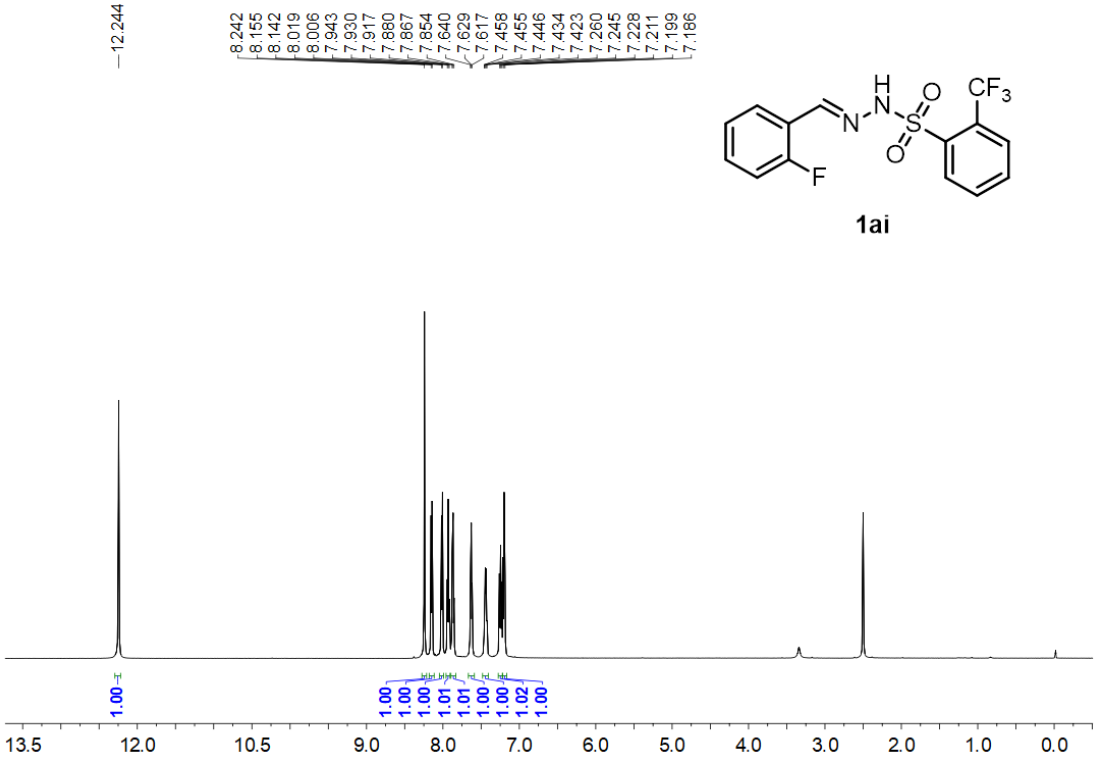

147.45
138.58
134.01
133.96
133.79
131.77
130.68
129.28
128.94
128.90
128.85
128.81
127.31
127.24
127.02
126.80
126.59
125.99
124.18
122.36
120.55
127
126
124
121
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
1ag


56.230
5
0
-5
-15
-25
-35
-45
-55
-65
-75
-85
-95
-105
-120
1ag

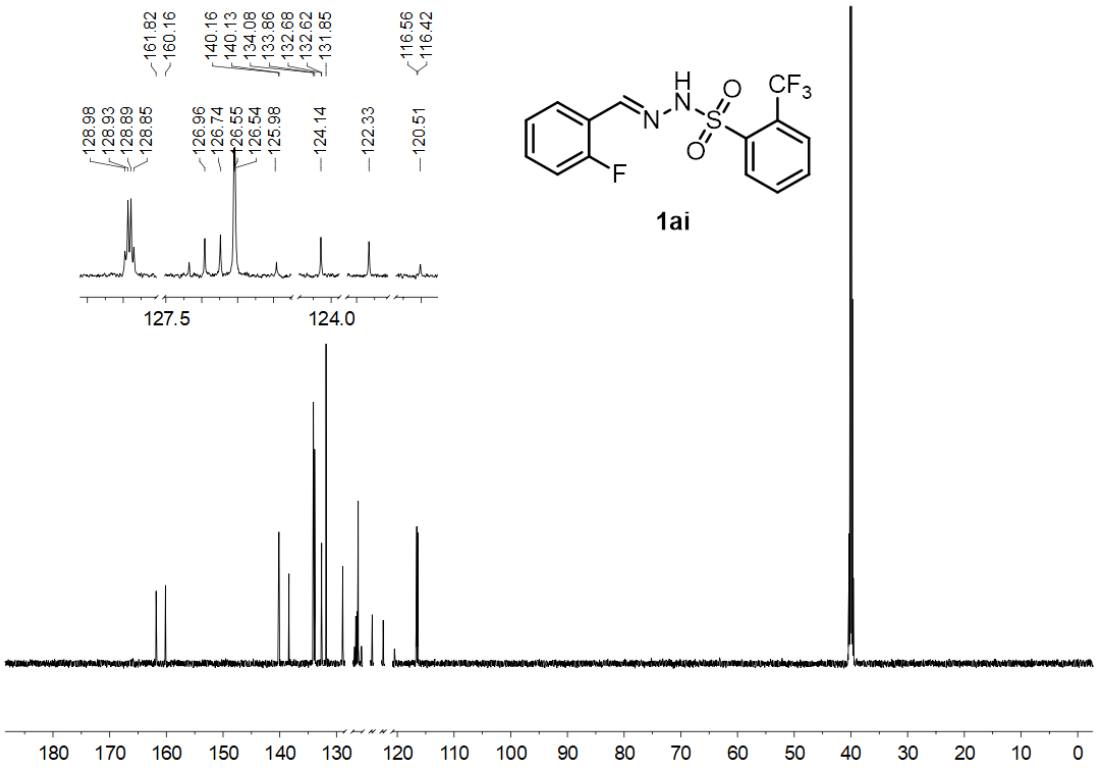

12.331
8.272
8.161
8.148
8.021
8.008
7.948
7.935
7.922
7.884
7.871
7.858
7.579
7.566
7.379
7.367
7.354
7.142
7.140
7.129
7.114
1ah
1.00
1.00
1.00
1.01
1.00
1.97
0.98
1.00
1.00
150.21
140.09
138.33
135.54
134.12
133.88
132.35
131.84
129.05
129.01
128.97
128.92
128.88
100.22
127.14
126.91
126.69
126.47
125.94
124.12
122.30
120.49
1ah

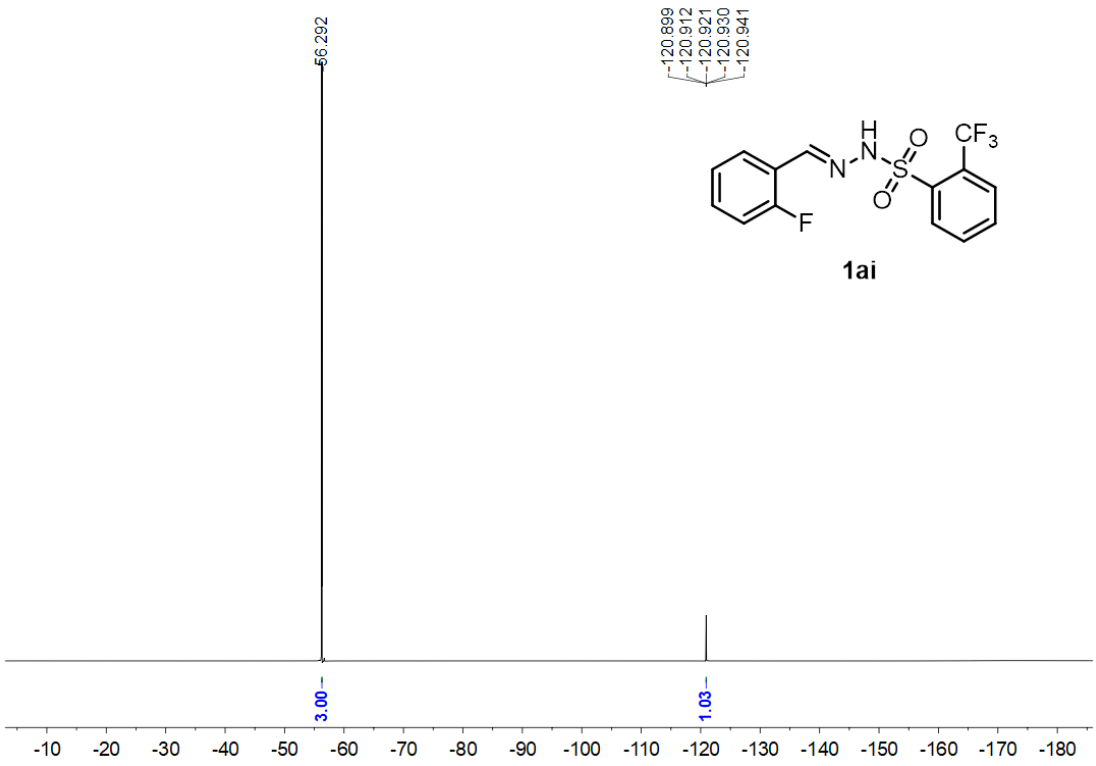

-56.264
15
5
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-115

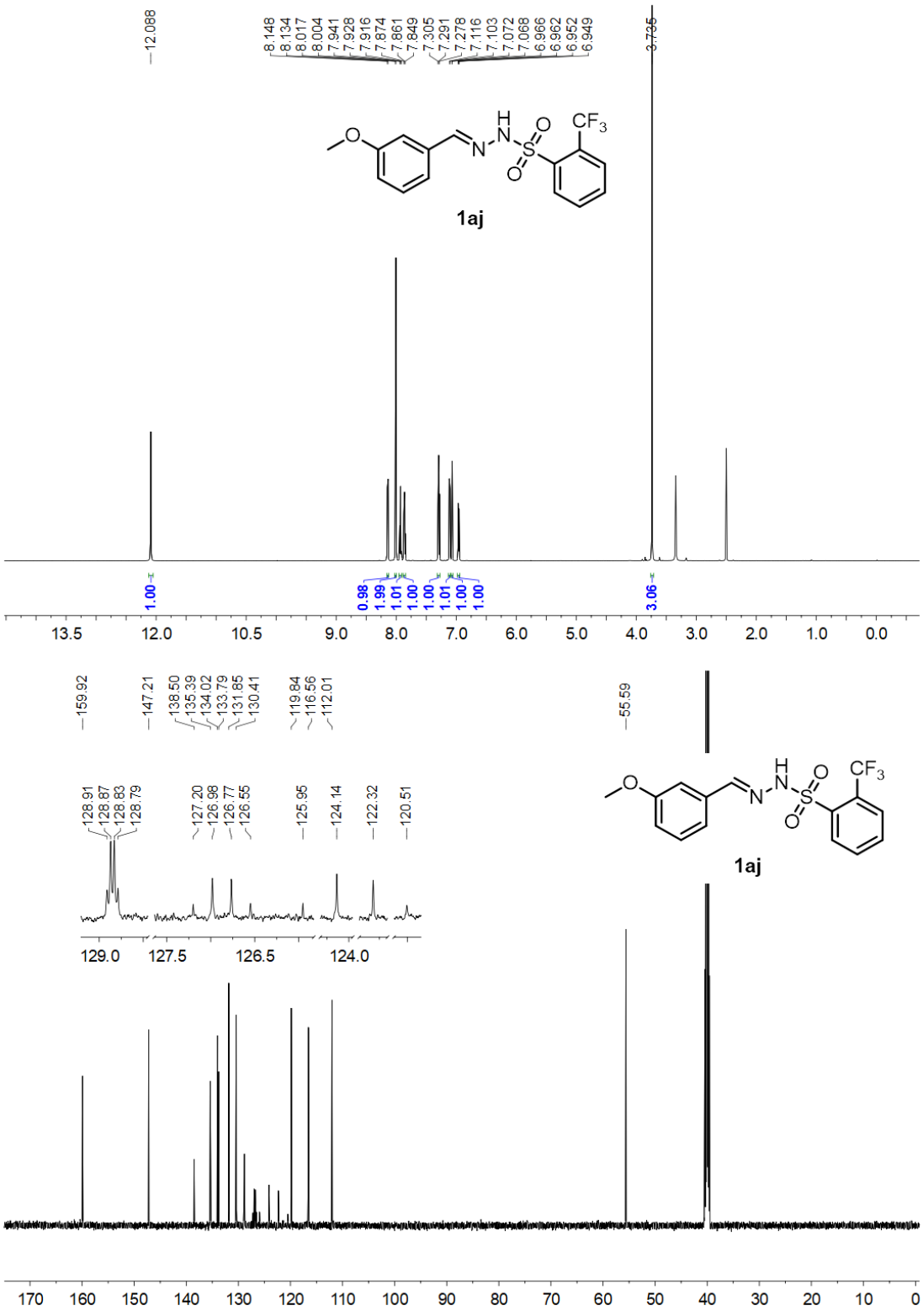
1ah

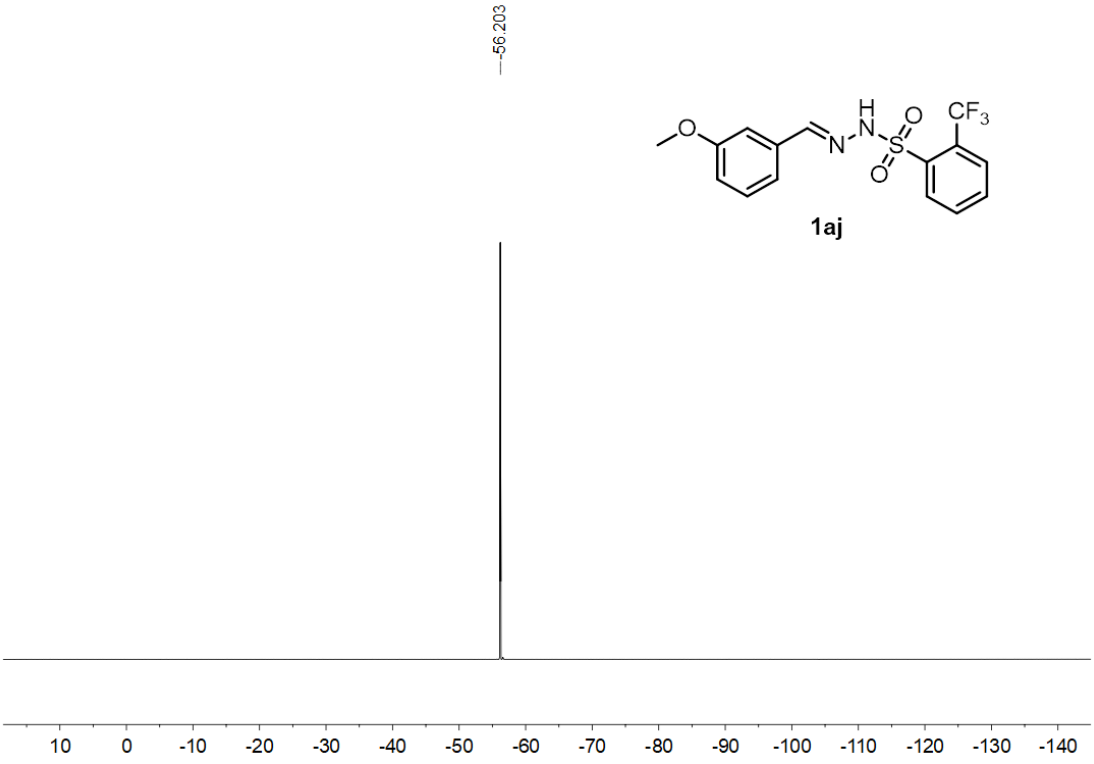

12.244
8.242
8.155
8.142
8.019
8.006
7.943
7.930
7.917
7.880
7.867
7.854
7.640
7.629
7.617
7.458
7.455
7.446
7.434
7.423
7.260
7.245
7.228
7.211
7.199
7.186
1.00
1.00
1.00
1.00
1.01
1.01
1.00
1.00
1.02
1.00
13.5
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

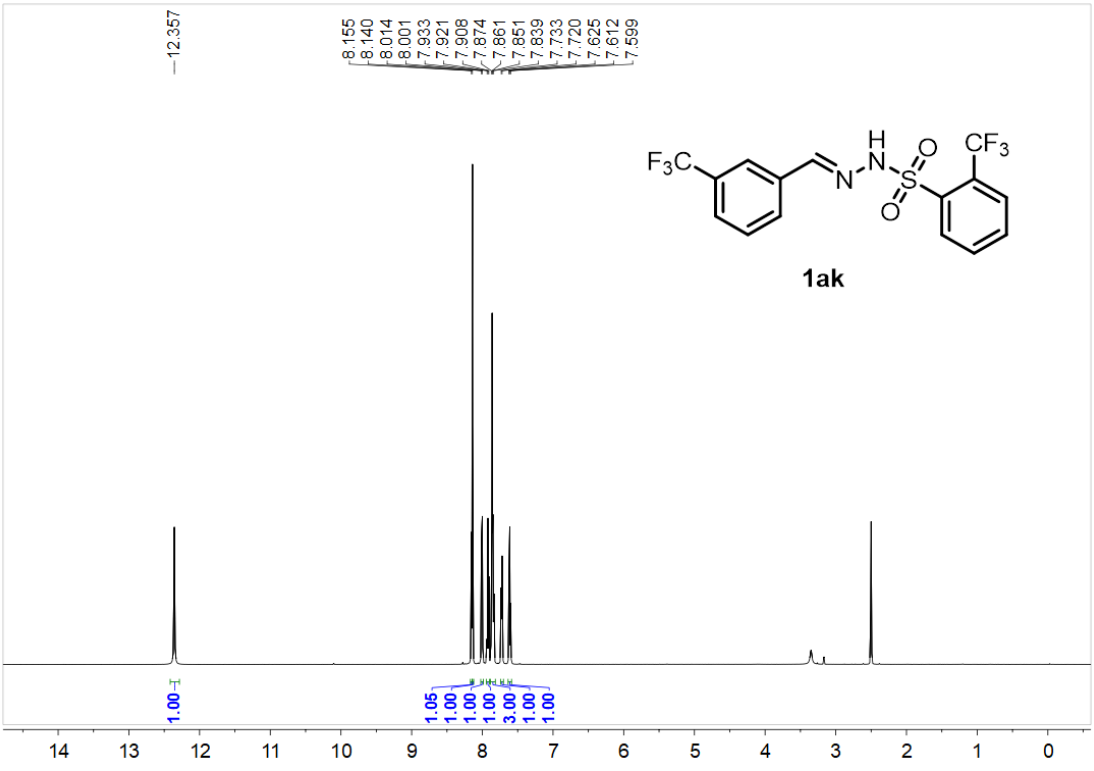
1ai

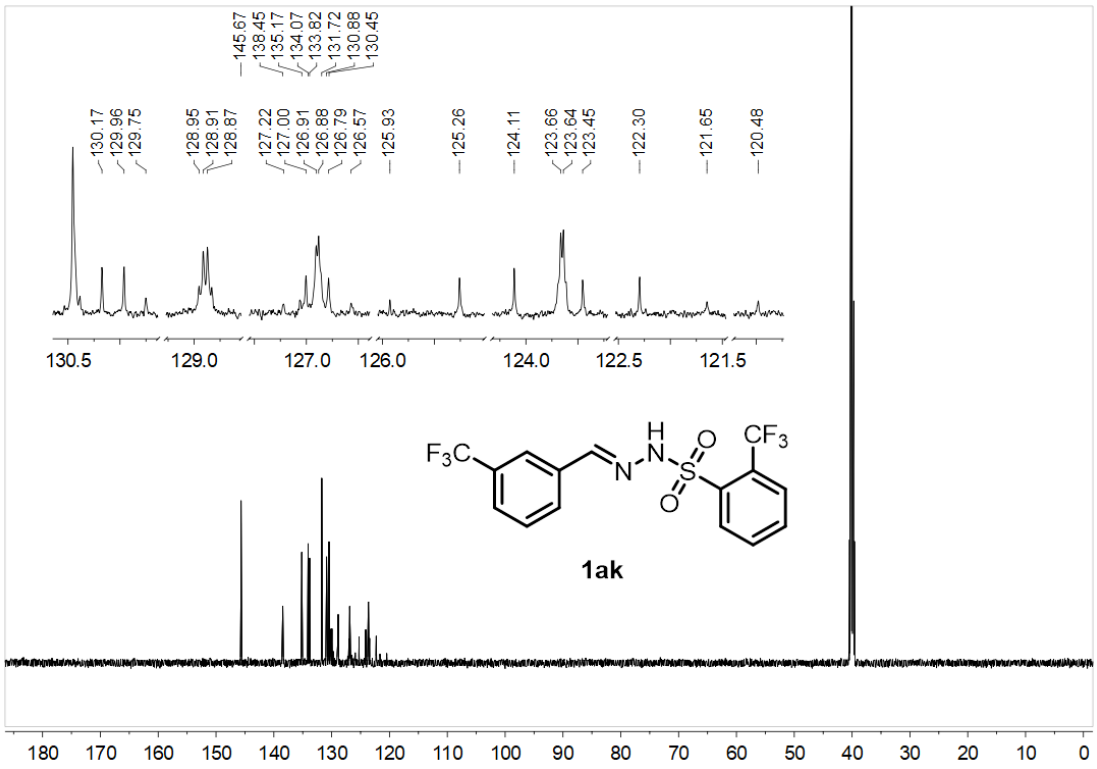

161.82
160.16
140.16
140.13
134.08
133.86
132.68
132.62
131.85
116.56
116.42
128.98
128.93
128.89
128.85
126.96
126.74
126.55
126.54
125.98
124.14
122.33
120.51
127.5
124.0
1ai
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

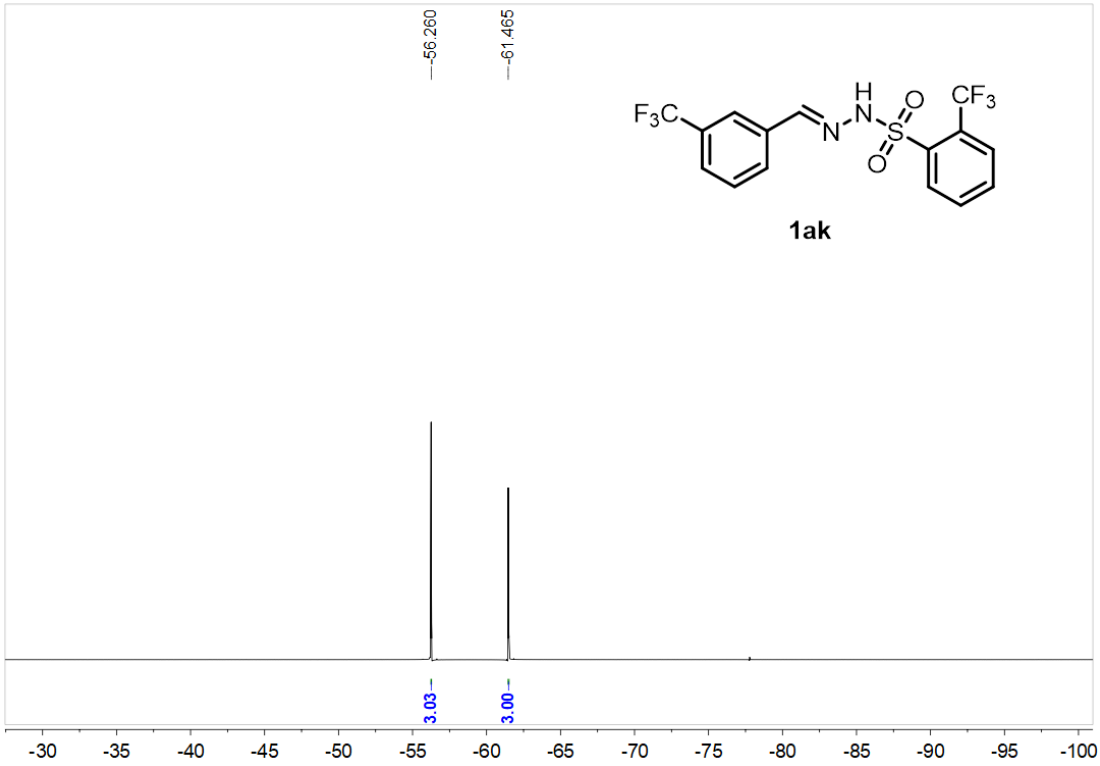

66.292
120.899
120.912
120.921
120.930
120.941
1ai
3.00
1.03
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180

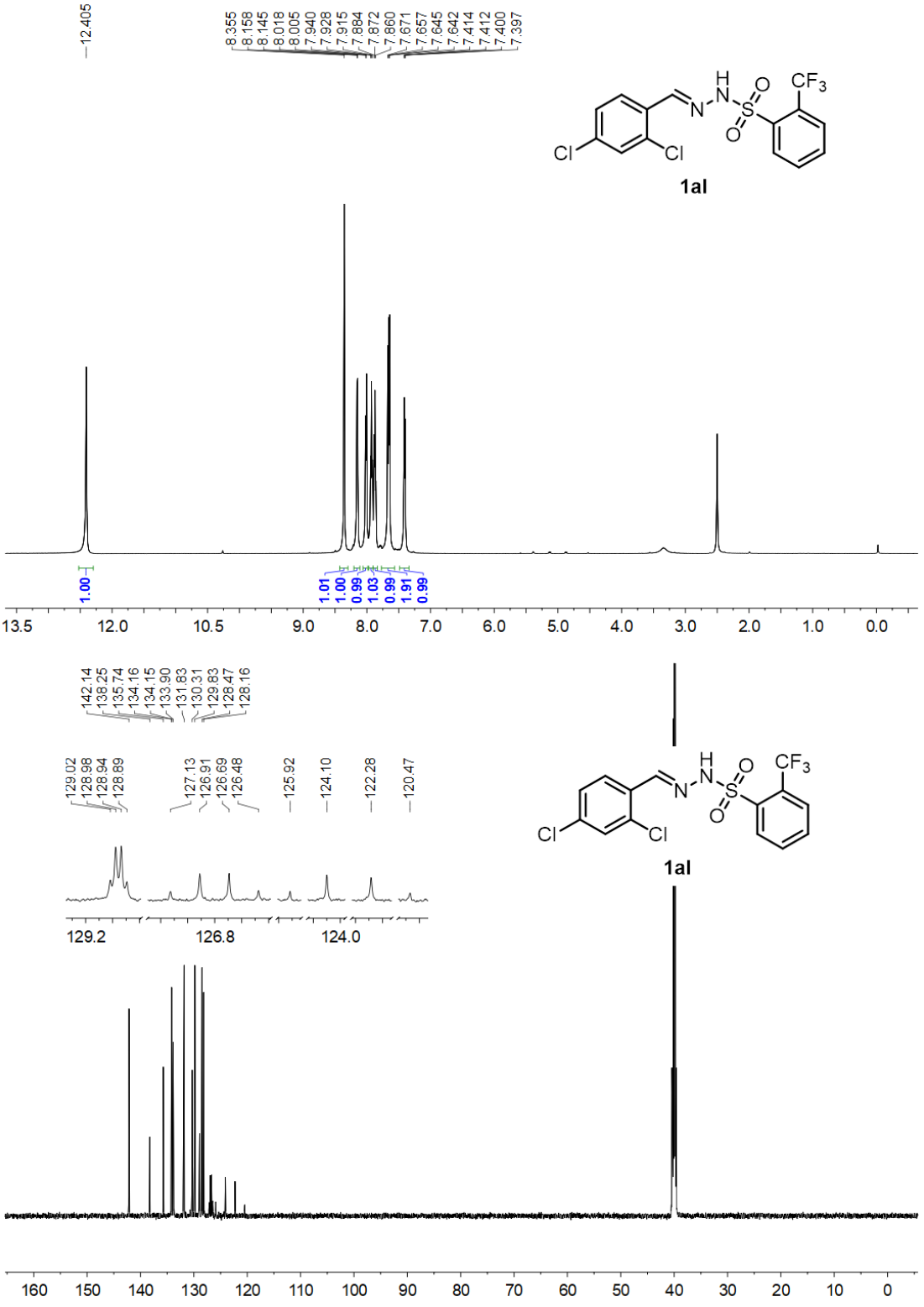

12.088
8.148
8.134
8.017
8.004
7.941
7.928
7.916
7.874
7.861
7.849
7.305
7.291
7.278
7.116
7.103
7.072
7.068
6.966
6.962
6.952
6.949
3.735
1aj
1.00
0.98
1.99
1.01
1.00
1.00
1.01
1.00
1.00
3.06
13.5
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
159.92
147.21
138.50
135.39
134.02
133.79
131.85
130.41
119.84
116.56
112.01
128.91
128.87
128.83
128.79
127.20
126.98
126.77
126.55
125.95
124.14
122.32
120.51
55.59
1aj
129.0
127.5
126.5
124.0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

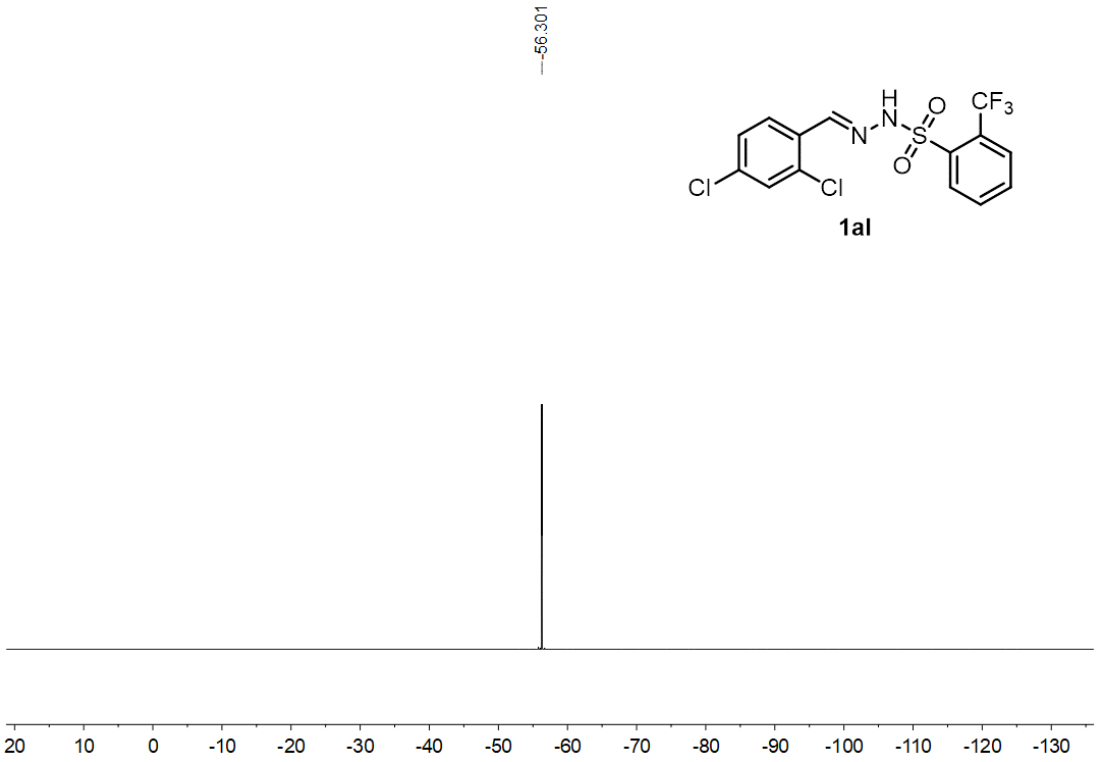

-56.203
1aj
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140


12.357
8.155
8.140
8.014
8.001
7.933
7.921
7.908
7.874
7.861
7.851
7.839
7.733
7.720
7.625
7.612
7.599
1ak
1.00
1.05
1.00
1.00
1.00
3.00
1.00
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0

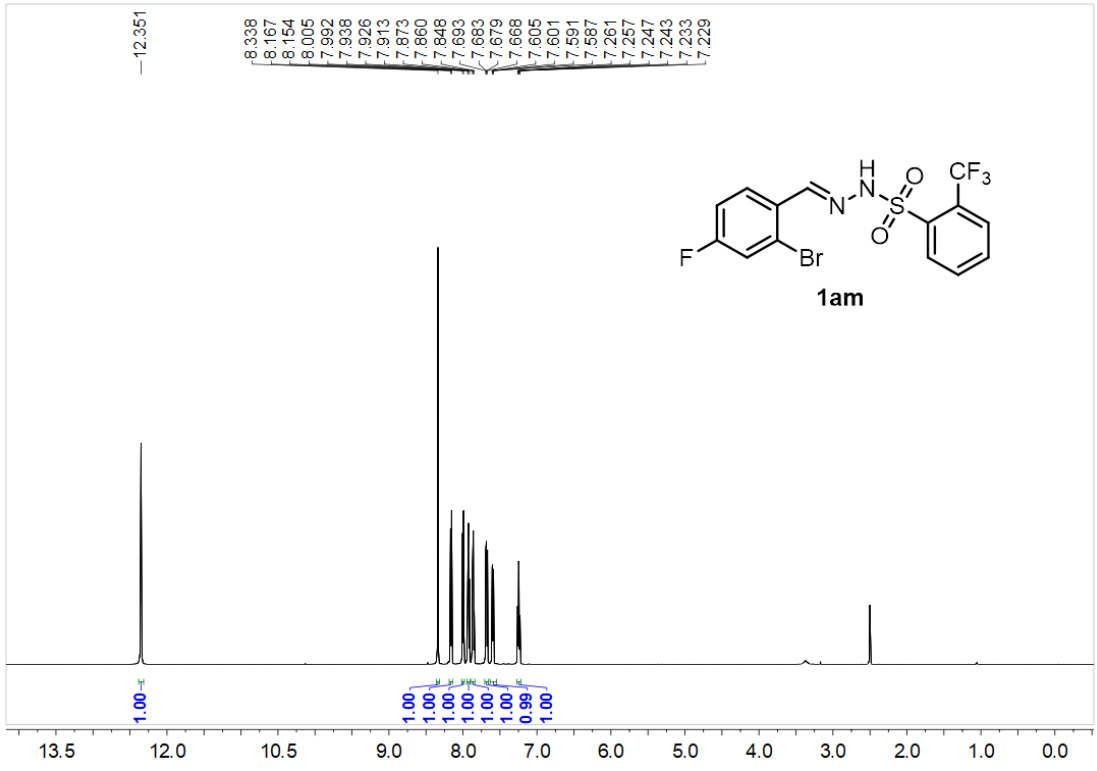

145.67
138.45
135.17
134.07
133.82
131.72
130.88
130.45
130.17
129.96
129.75
128.95
128.91
128.87
127.22
127.00
126.91
126.88
126.79
126.57
125.93
125.26
124.11
123.66
123.64
123.45
122.30
121.65
120.48
130.5
129.0
127.0
126.0
124.0
122.5
121.5
F3C
CF3
1ak
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


56.260
61.465
F3C
CF3
1ak
3.03
3.00
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100

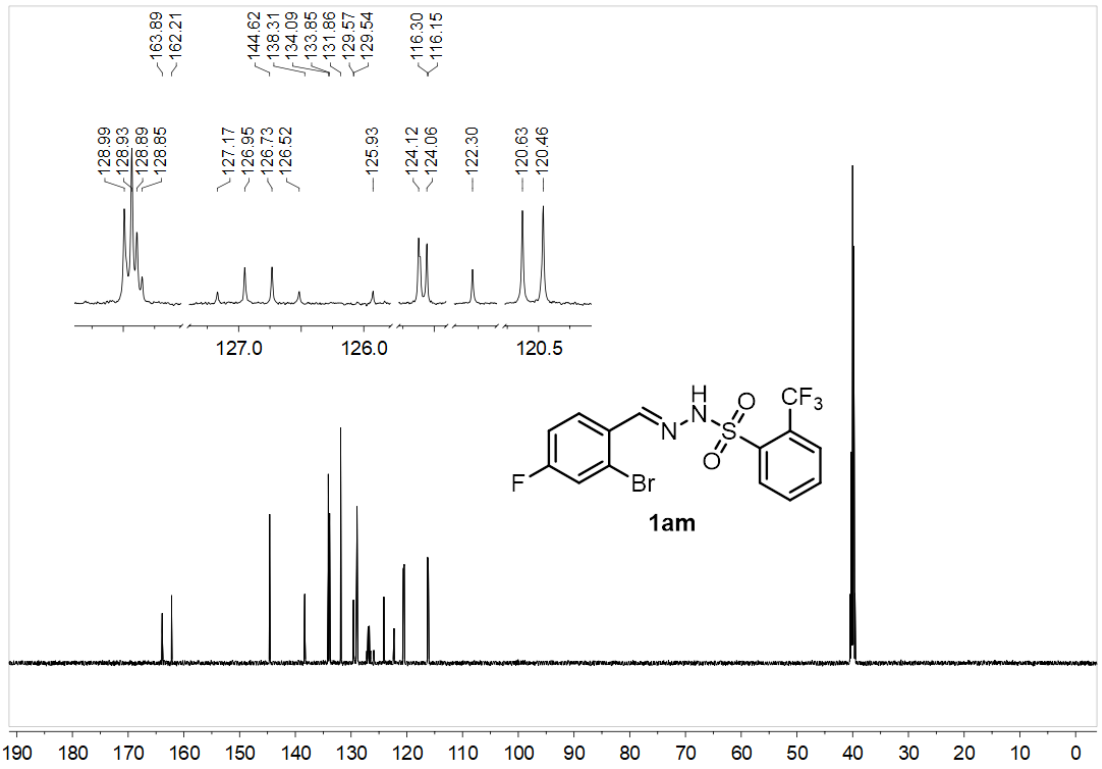

12.405
8.355
8.158
8.145
8.018
8.005
7.940
7.928
7.915
7.884
7.872
7.860
7.671
7.657
7.645
7.642
7.414
7.412
7.400
7.397
1al
1.00
1.01
1.00
0.99
1.03
0.99
1.91
0.99
142.14
138.25
135.74
134.16
134.15
133.90
131.83
130.31
129.83
128.47
128.16
129.02
128.98
128.94
128.89
127.13
126.91
126.69
126.48
125.92
124.10
122.28
120.47
1al

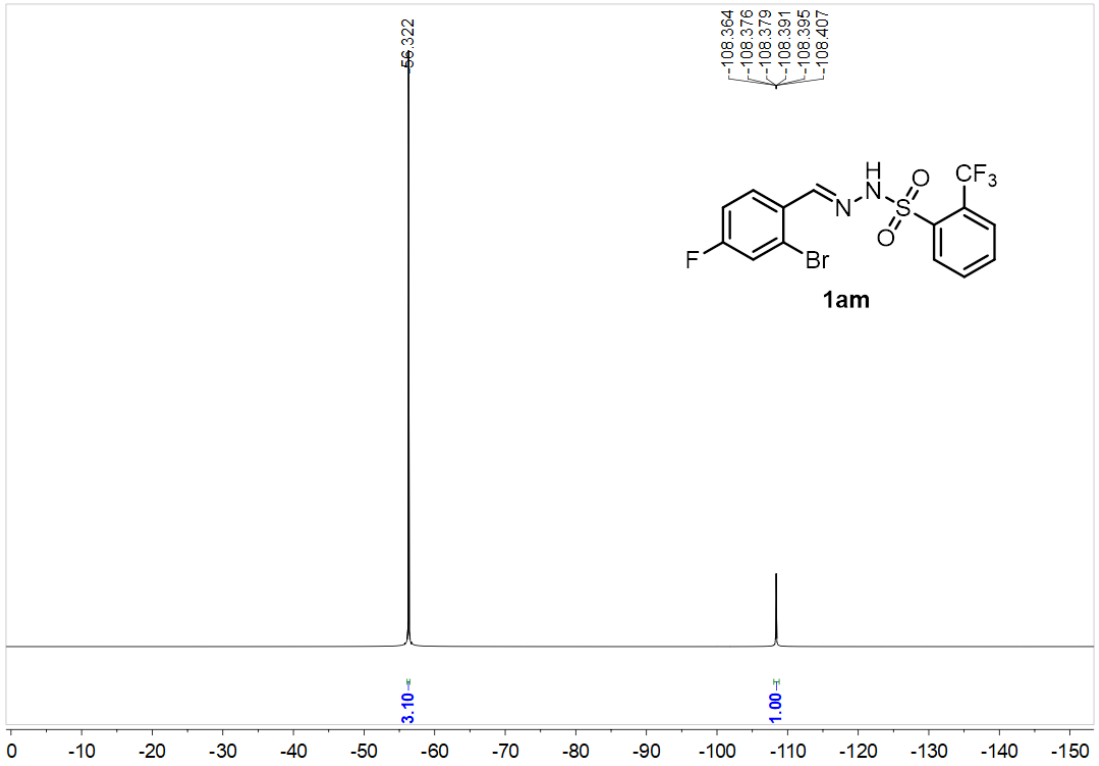

-56.301
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130

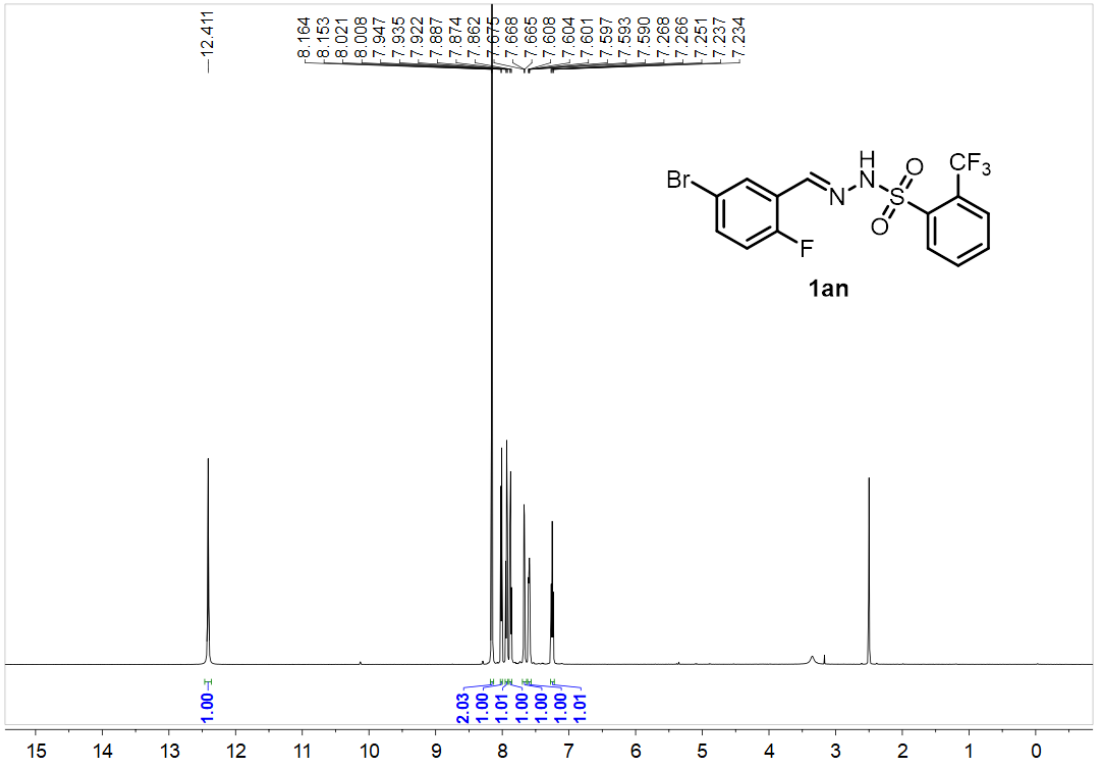
1al

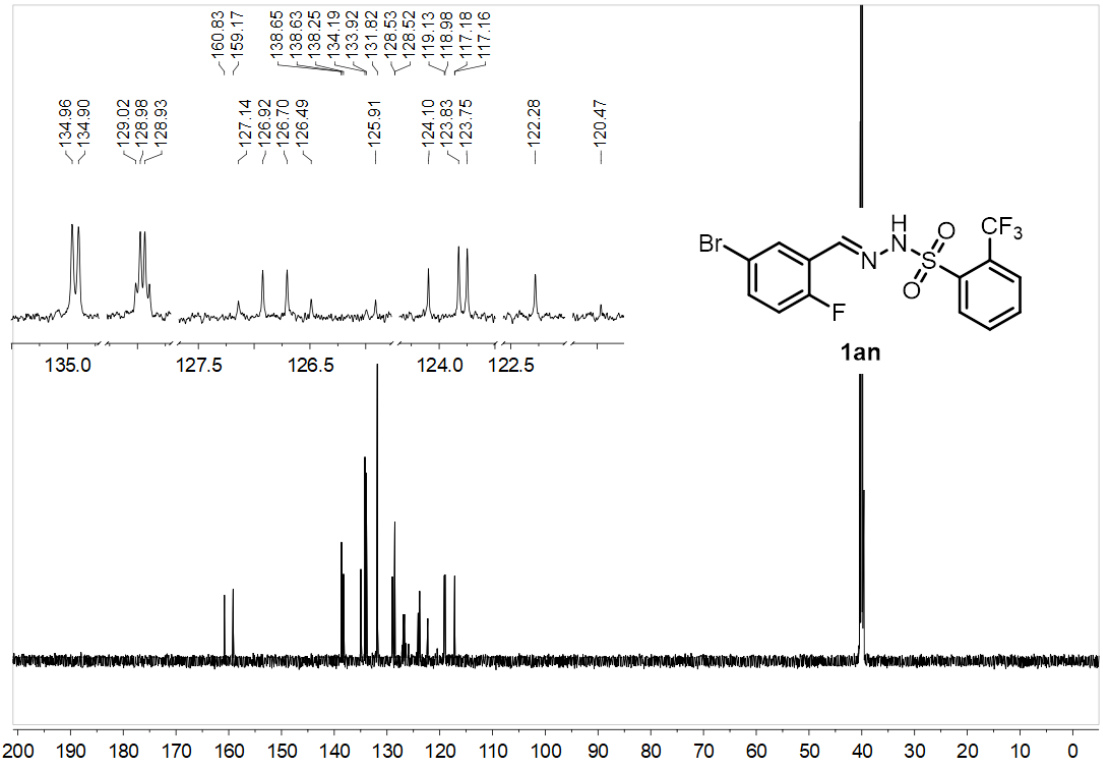

12.351
8.338
8.167
8.154
8.005
7.992
7.938
7.926
7.913
7.873
7.860
7.848
7.693
7.683
7.679
7.668
7.605
7.601
7.591
7.587
7.261
7.257
7.247
7.243
7.233
7.229
1.00
1.00
1.00
1.00
1.00
1.00
0.99
1.00
13.5
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

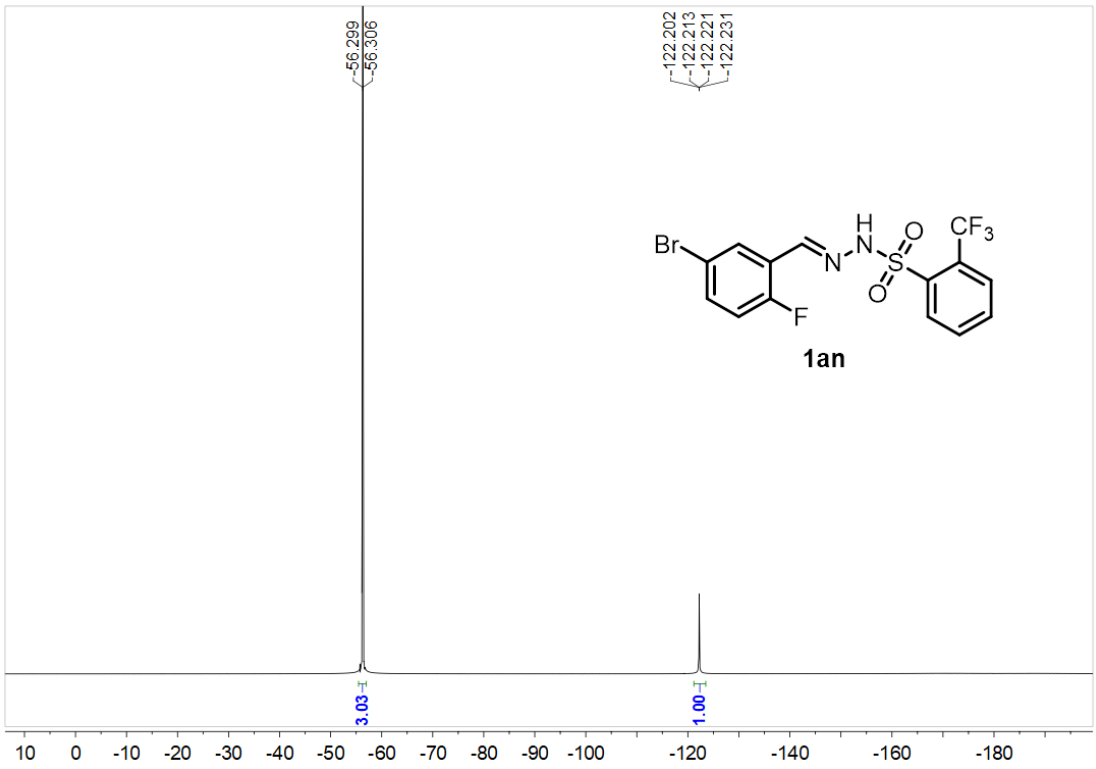
1am

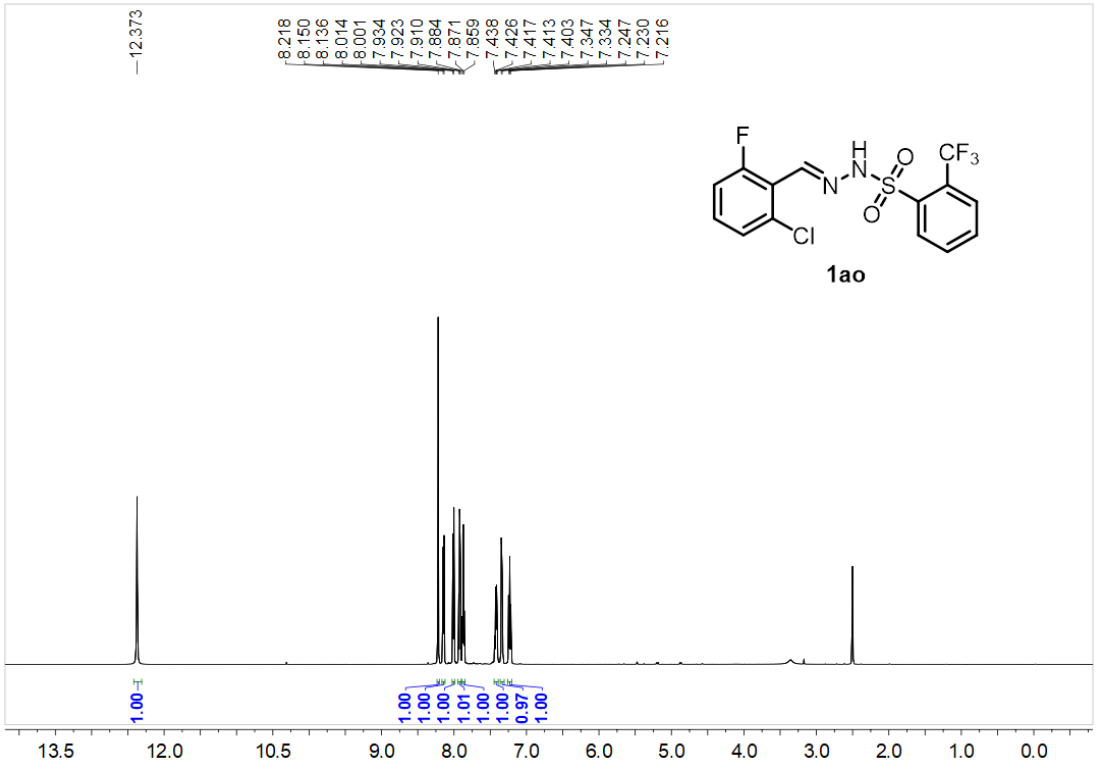

163.89
162.21
144.62
138.31
134.09
133.85
131.86
129.57
129.54
116.30
116.15
128.99
128.93
128.89
128.85
127.17
126.95
126.73
126.52
125.93
124.12
124.06
122.30
120.63
120.46
127.0
126.0
120.5
F
Br
N
H
N
O
S
O
O
CF3
1am
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

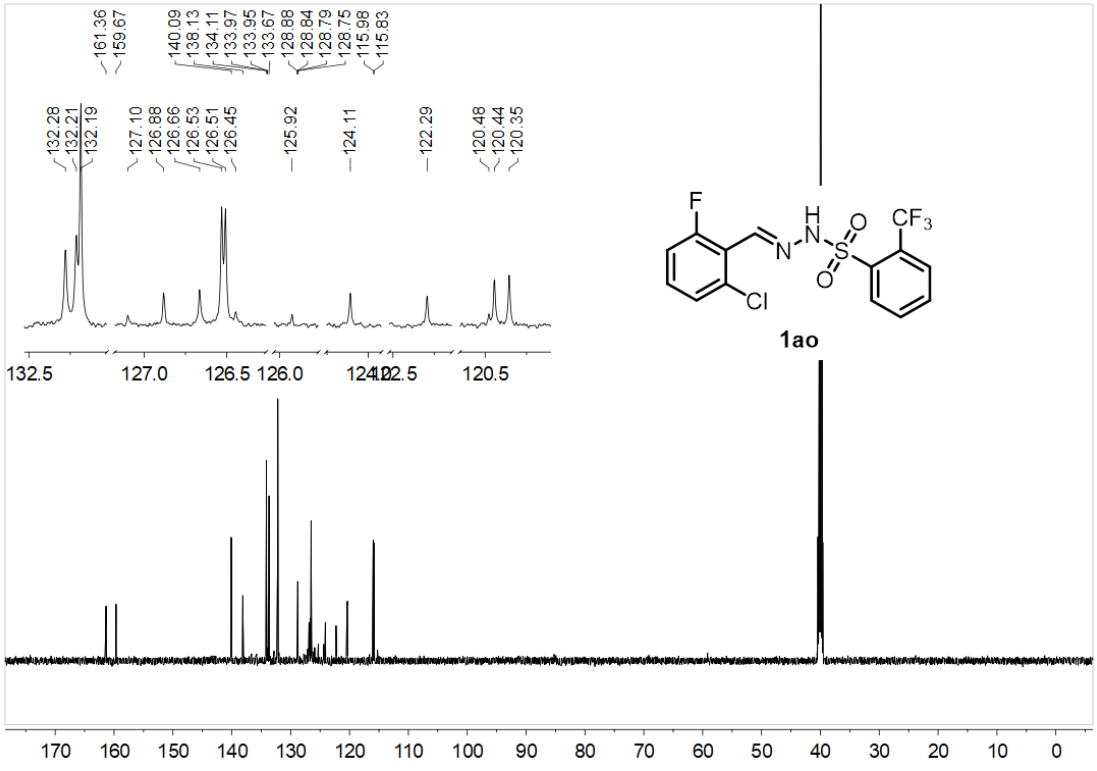

56.322
108.364
108.376
108.379
108.391
108.395
108.407
F
Br
N
H
N
O
S
O
O
CF3
1am
3.10
1.00
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150

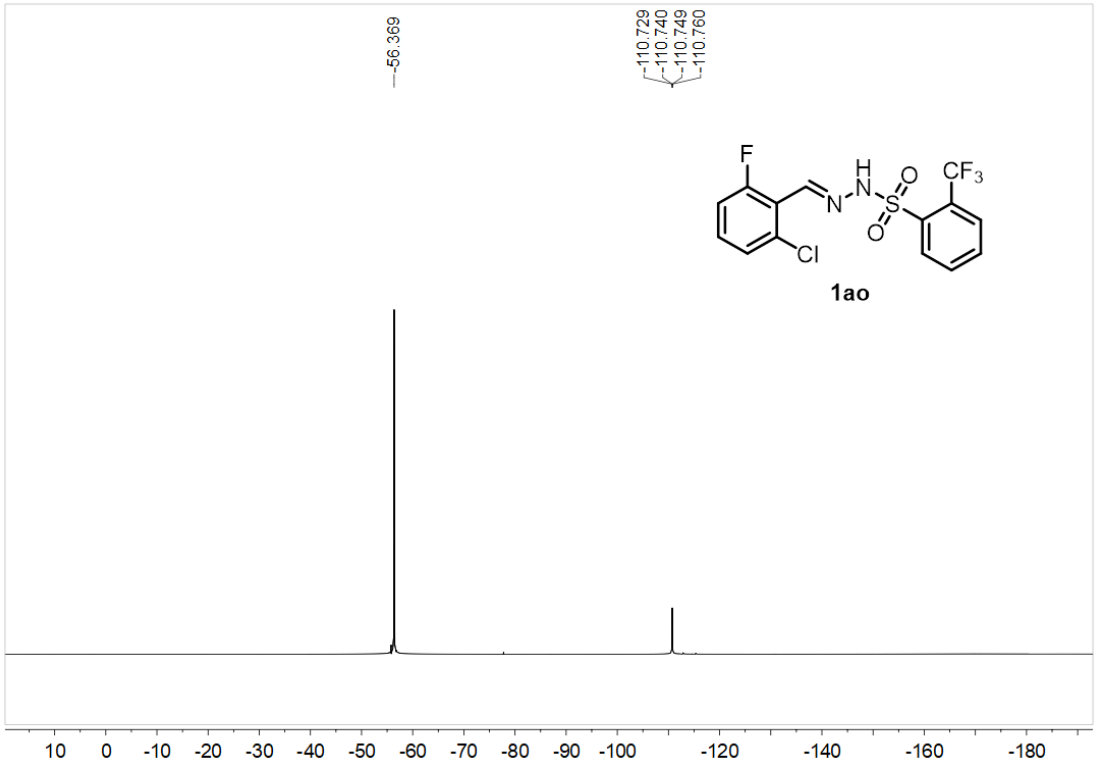

12.411
8.164
8.153
8.021
8.008
7.947
7.935
7.922
7.887
7.874
7.862
7.675
7.668
7.665
7.608
7.604
7.601
7.597
7.593
7.590
7.268
7.266
7.251
7.237
7.234
Br
F
N
H
N
O
S
O
O
CF3
1an
1.00
2.03
1.00
1.01
1.00
1.00
1.00
1.01
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0

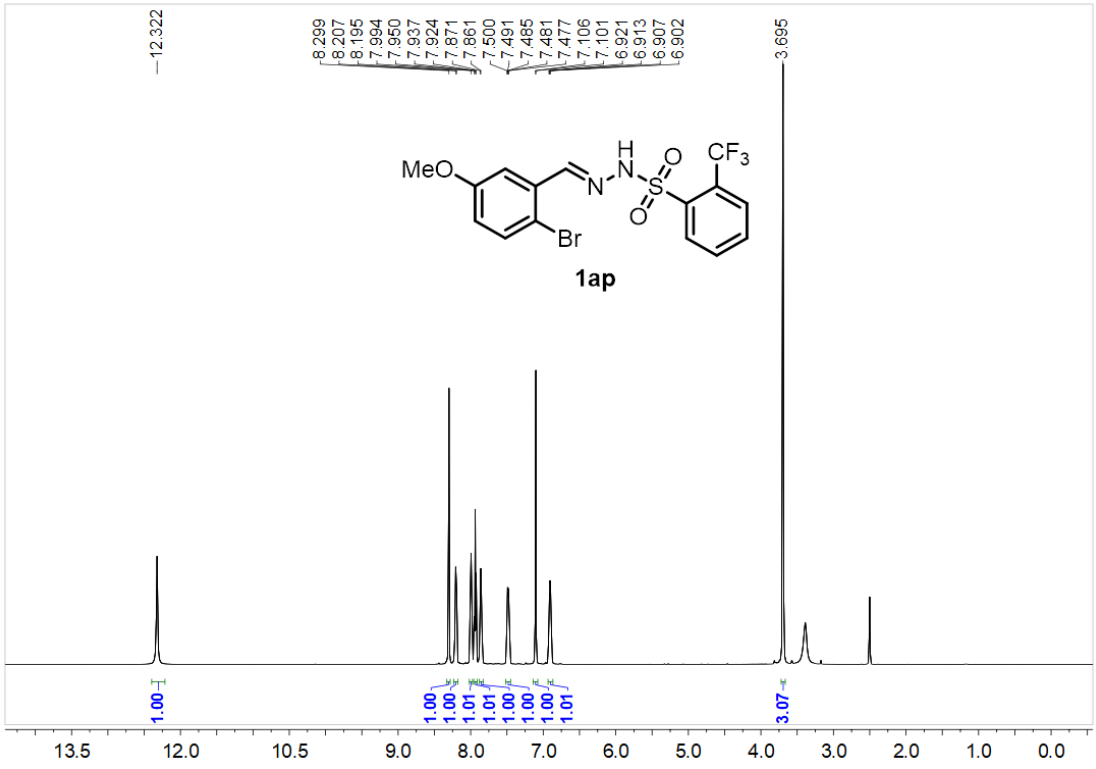

160.83
159.17
138.65
138.63
138.25
134.19
133.92
131.82
128.53
128.52
119.13
118.98
117.18
117.16
134.96
134.90
129.02
128.98
128.93
127.14
126.92
126.70
126.49
125.91
124.10
123.83
123.75
122.28
120.47
Br
F
N
H
N
O
S
O
O
CF3
1an
135.0
127.5
126.5
124.0
122.5
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

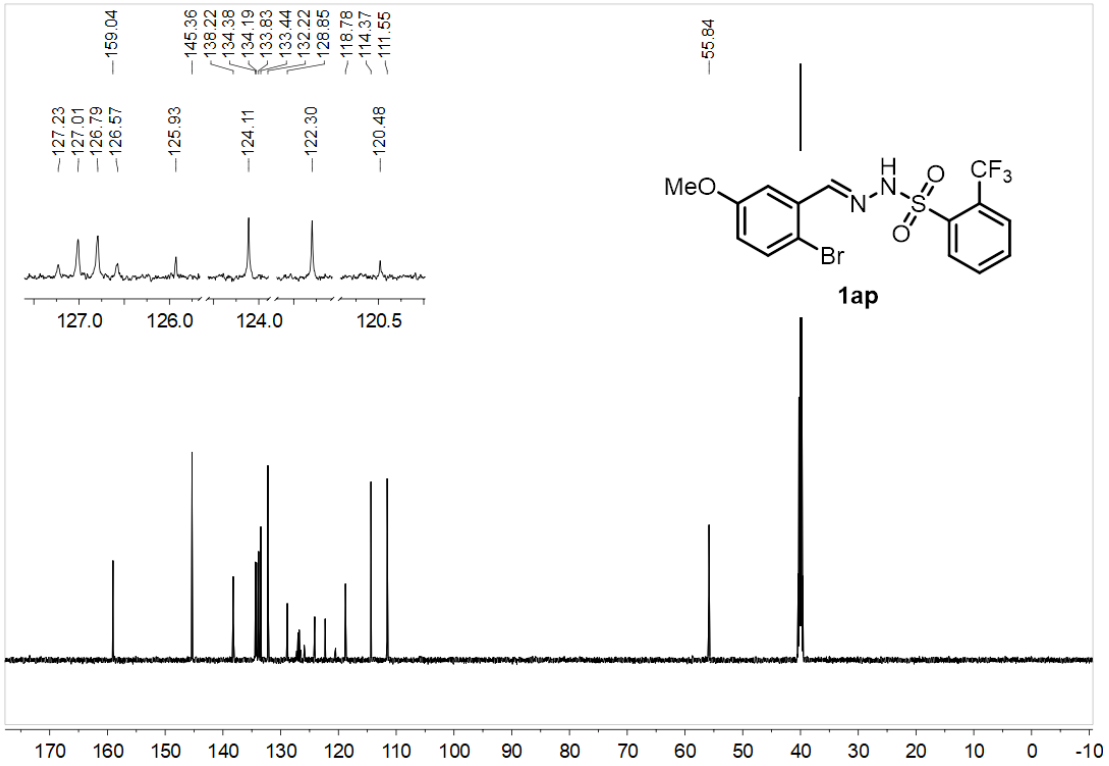

-56.299
-56.306
-122.202
-122.213
-122.221
-122.231
Br
F
N
H
O
S
O
CF3
1an
3.03
1.00
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180

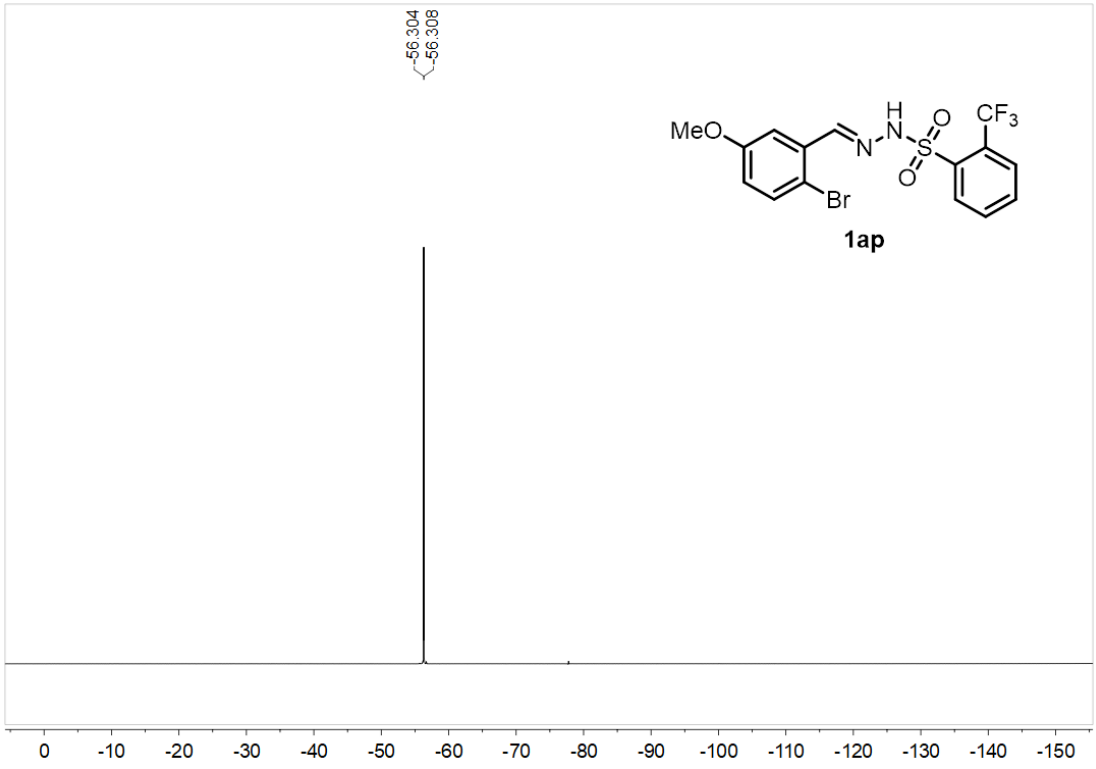

12.373
8.218
8.150
8.136
8.014
8.001
7.934
7.923
7.910
7.884
7.871
7.859
7.438
7.426
7.417
7.413
7.403
7.347
7.334
7.247
7.230
7.216
F
Cl
N
H
O
S
O
CF3
1ao
1.00
1.00
1.00
1.00
1.01
1.00
1.00
0.97
1.00
13.5 12.0 10.5 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0

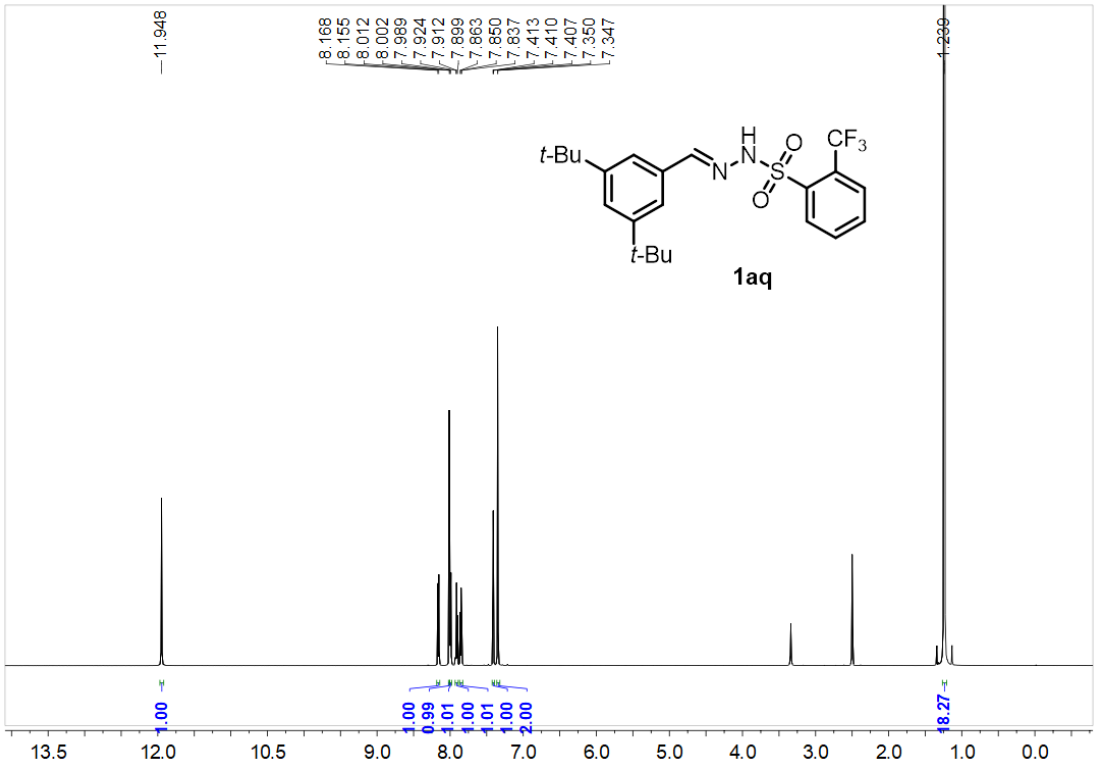

161.36
159.67
140.09
138.13
134.11
133.97
133.95
133.67
128.88
128.84
128.79
128.75
115.98
115.83
132.28
132.21
132.19
127.10
126.88
126.66
126.53
126.51
126.45
125.92
124.11
122.29
120.48
120.44
120.35
132.5
127.0
126.5
126.0
120.5
F
H
N
N
O
S
O
CF3
Cl
1ao
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

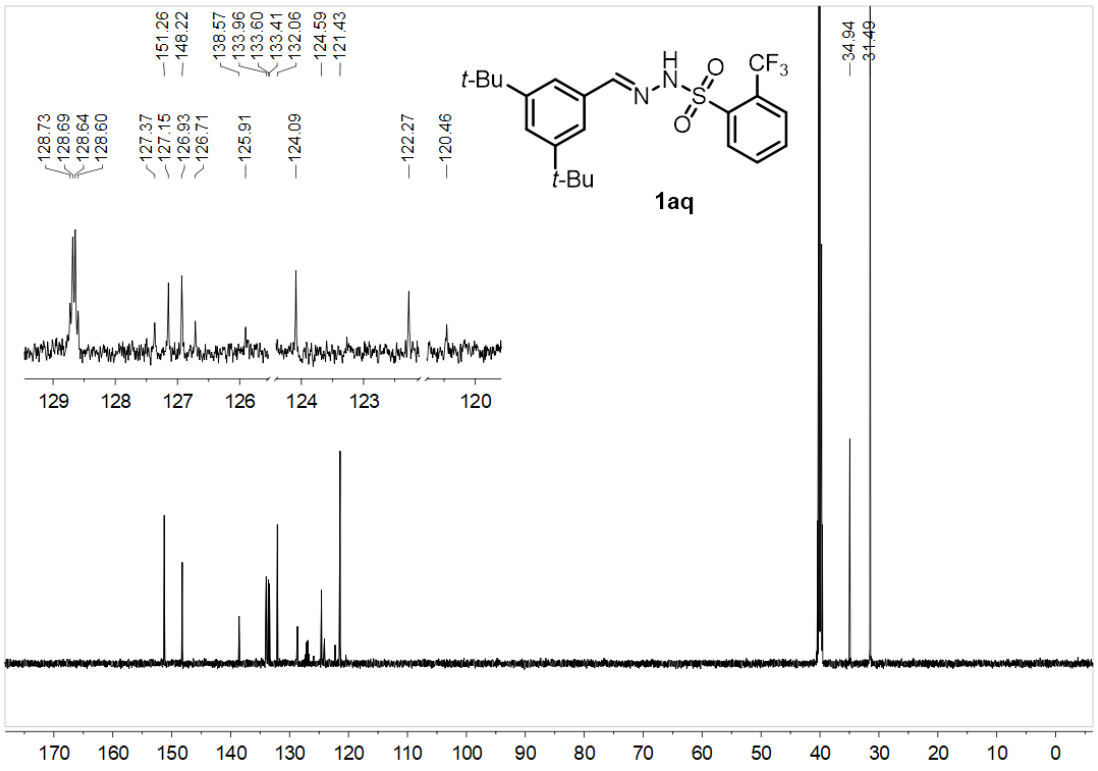

-56.369
110.729
110.740
110.749
110.760
F
H
N
N
O
S
O
CF3
Cl
1ao
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180

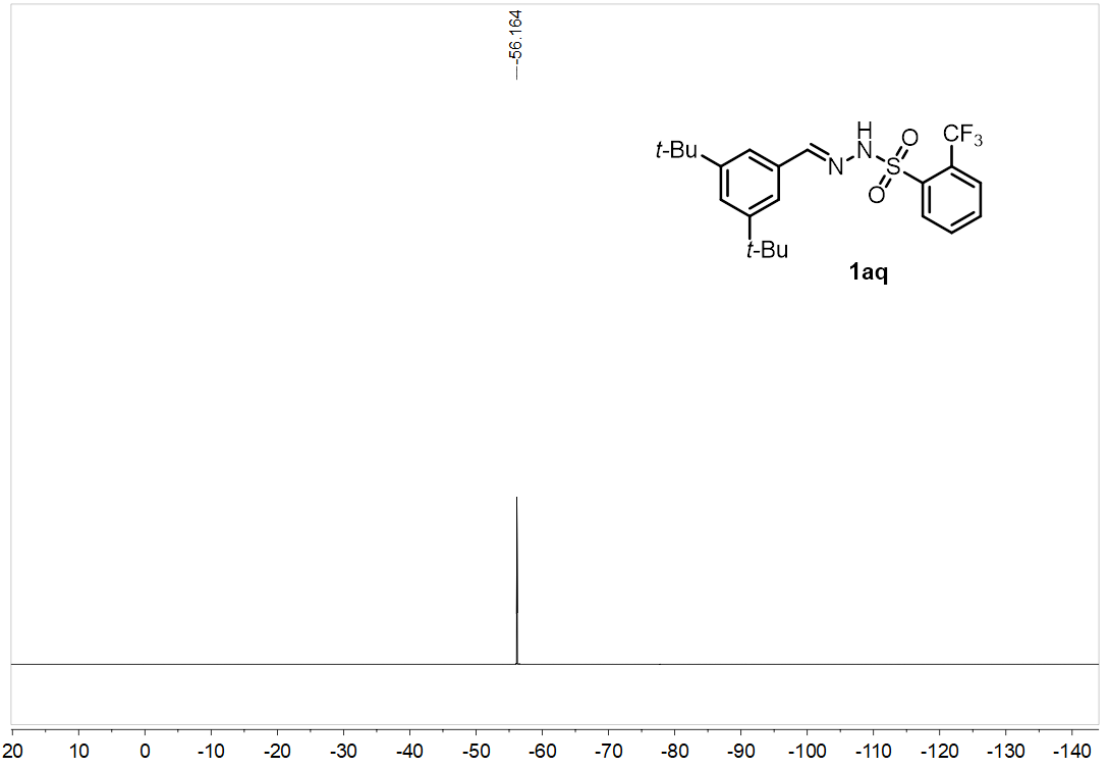

12.322
8.299
8.207
8.195
7.994
7.950
7.937
7.924
7.871
7.861
7.500
7.491
7.485
7.481
7.477
7.106
7.101
6.921
6.913
6.907
6.902
3.695
MeO
Br
CF3
1ap
1.00
1.00
1.00
1.01
1.01
1.00
1.00
1.00
1.01
3.07
13.5
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

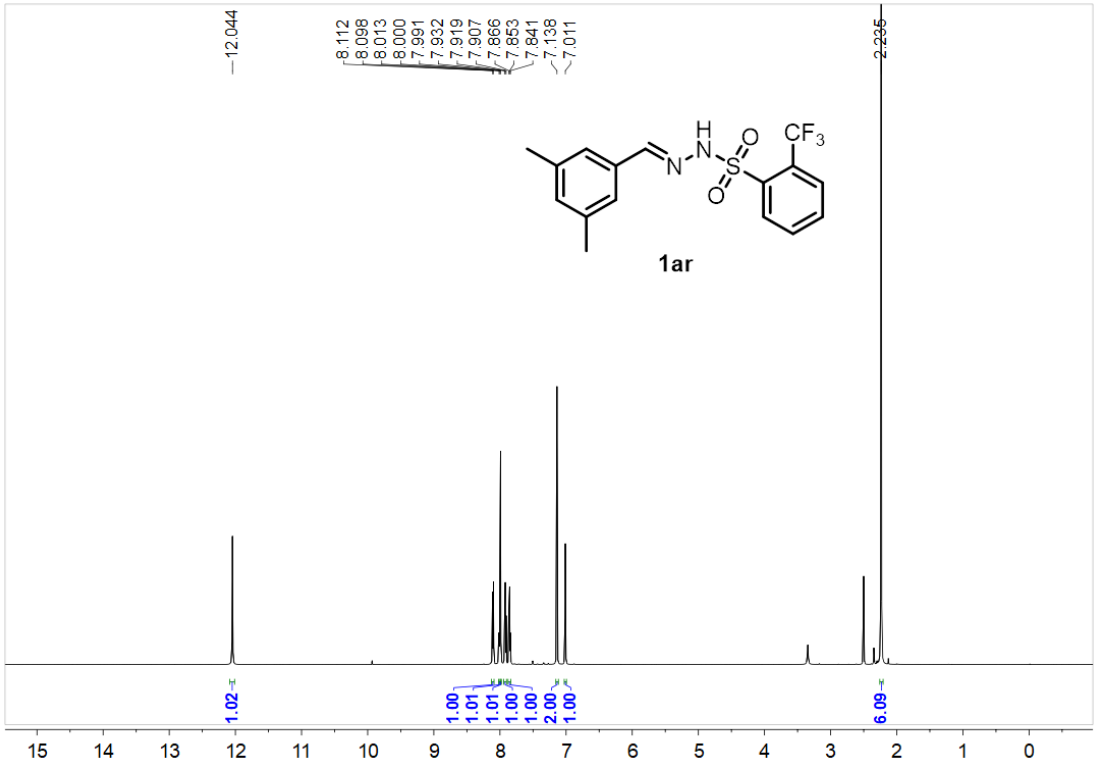

159.04
145.36
138.22
134.38
134.19
133.83
133.44
132.22
128.85
118.78
114.37
111.55
127.23
127.01
126.79
126.57
125.93
124.11
122.30
120.48
55.84
MeO
Br
CF3
1ap
127.0
126.0
124.0
120.5
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

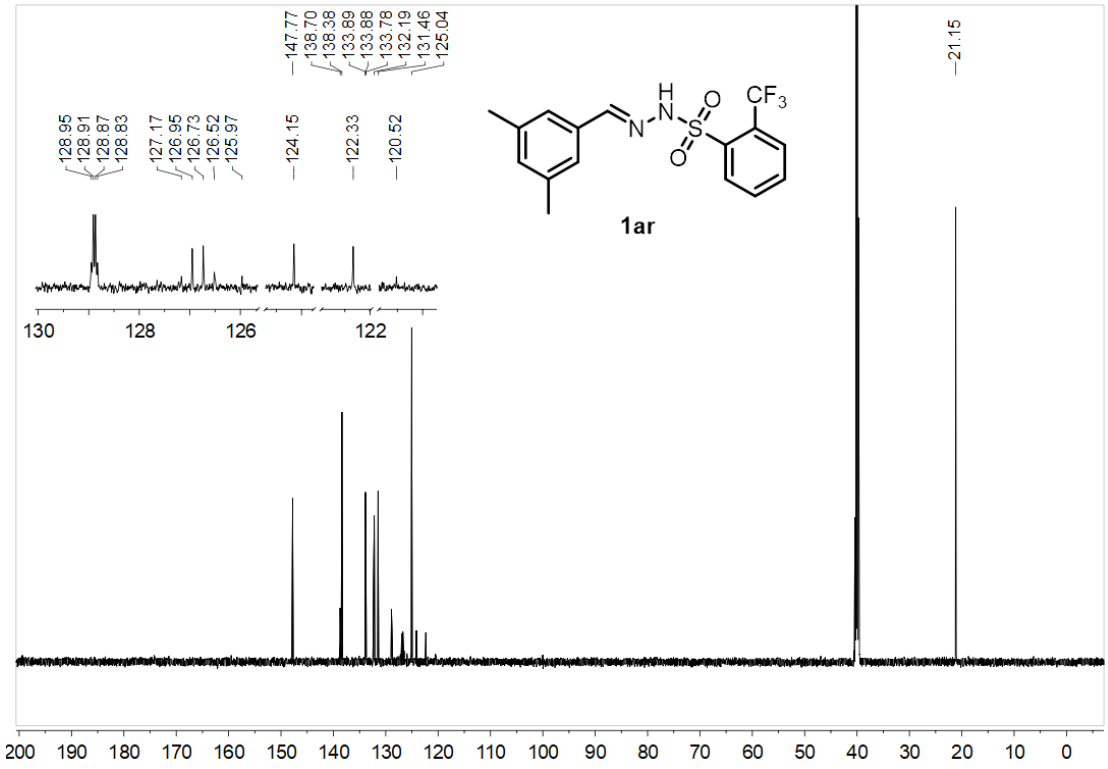

-56.304
-56.308
MeO
Br
N
H
N
S
O
O
CF3
1ap
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150

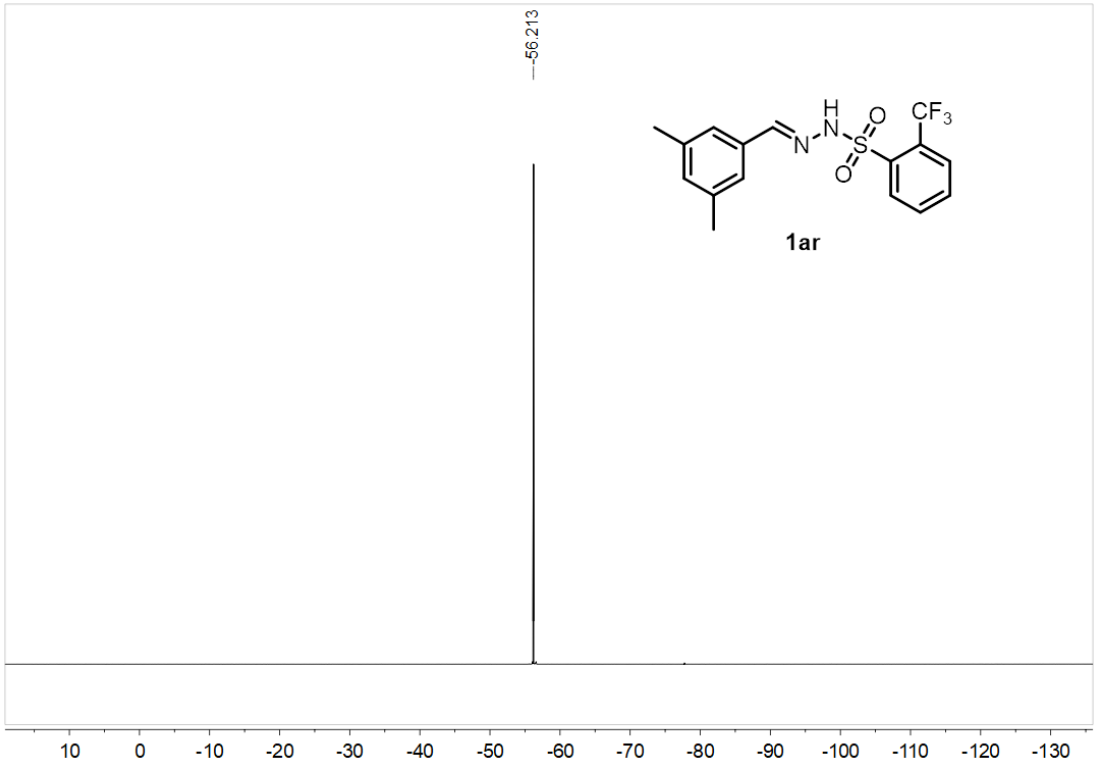

11.948
8.168
8.155
8.012
8.002
7.989
7.924
7.912
7.899
7.863
7.850
7.837
7.413
7.410
7.407
7.350
7.347
1.239
t-Bu
t-Bu
N
H
N
S
O
O
CF3
1aq
1.00
1.00
0.99
1.01
1.00
1.01
1.00
2.00
18.27
13.5
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

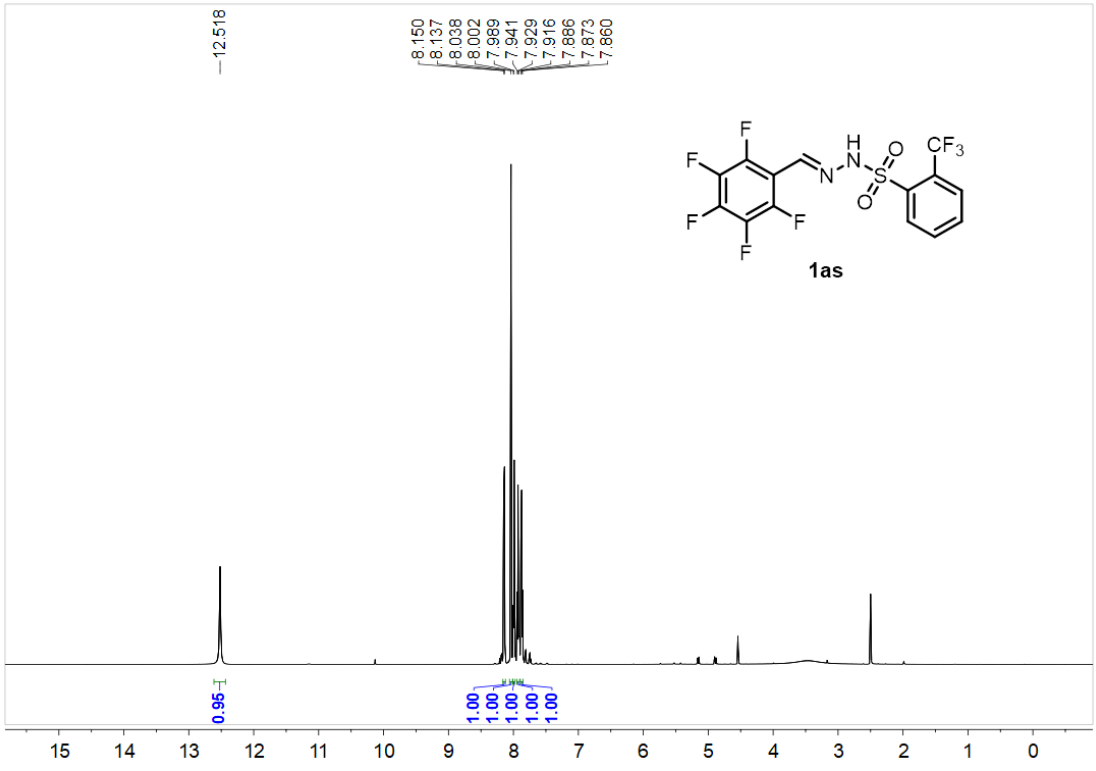

151.26
148.22
138.57
133.96
133.60
133.41
132.06
124.59
121.43
128.73
128.69
128.64
128.60
127.37
127.15
126.93
126.71
125.91
124.09
122.27
120.46
34.94
31.49
t-Bu
t-Bu
CF3
1aq
129
128
127
126
124
123
120
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

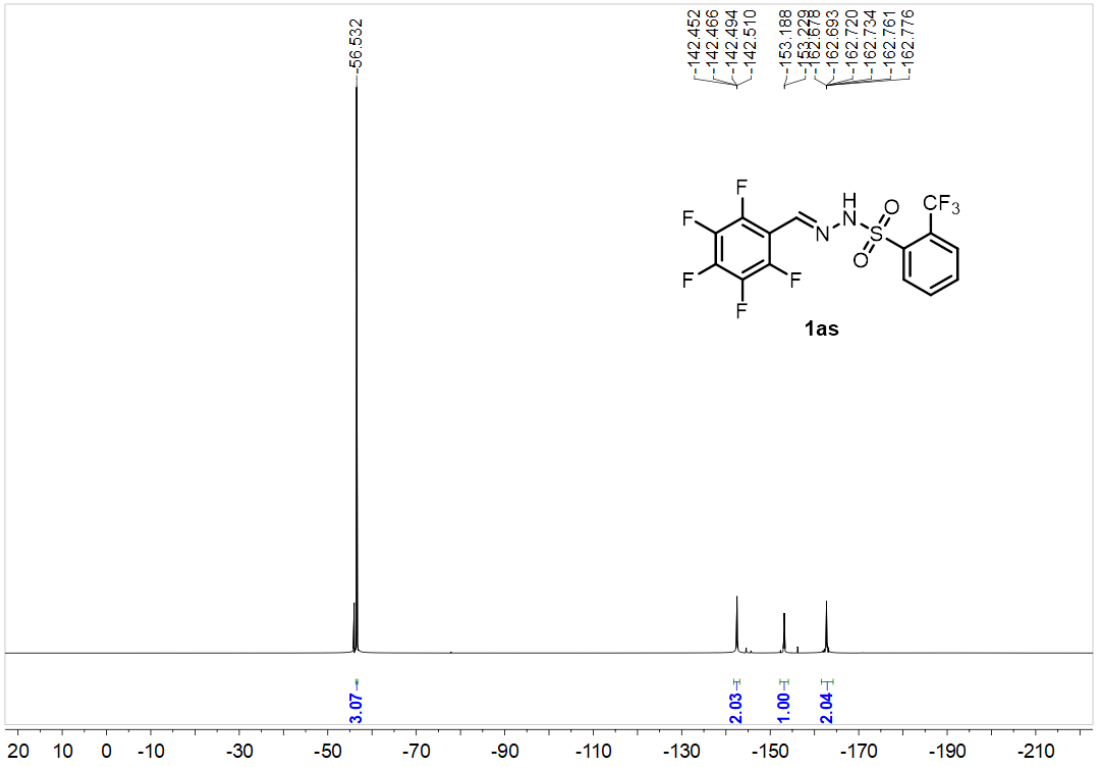

56.164
t-Bu
t-Bu
CF3
1aq
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140

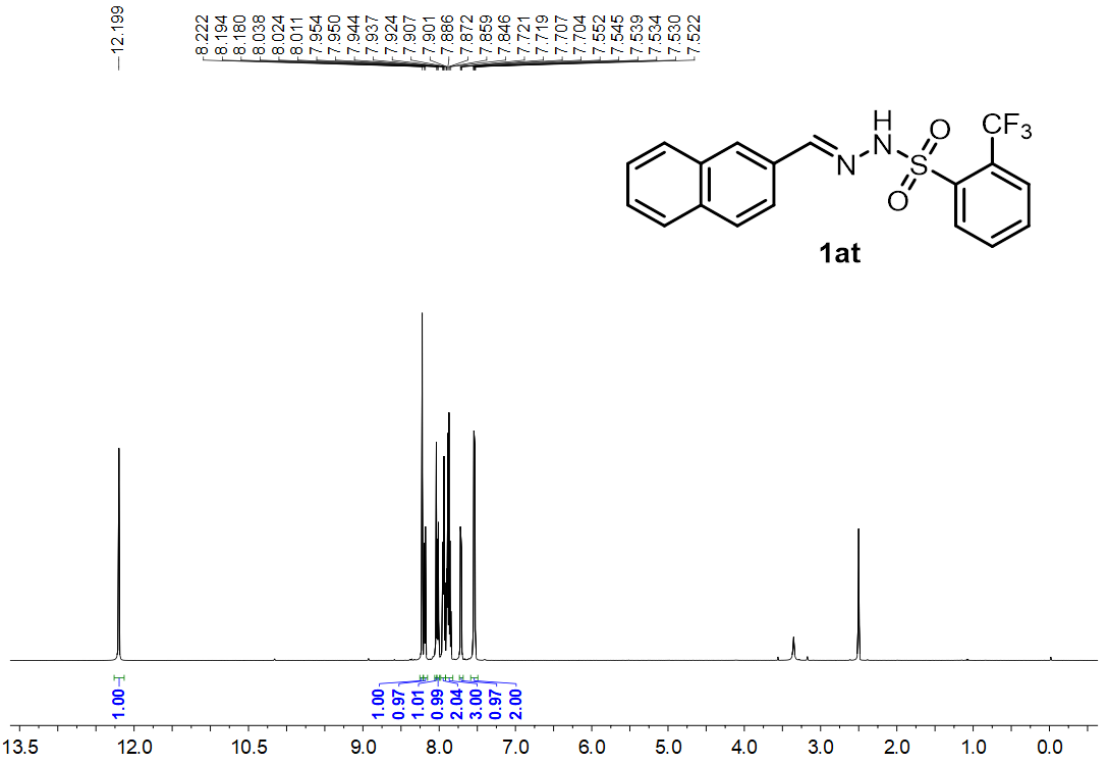

12.044
8.112
8.098
8.013
8.000
7.991
7.932
7.919
7.907
7.866
7.853
7.841
7.138
7.011
2.235
1ar
1.02
1.00
1.01
1.01
1.00
1.00
2.00
1.00
6.09

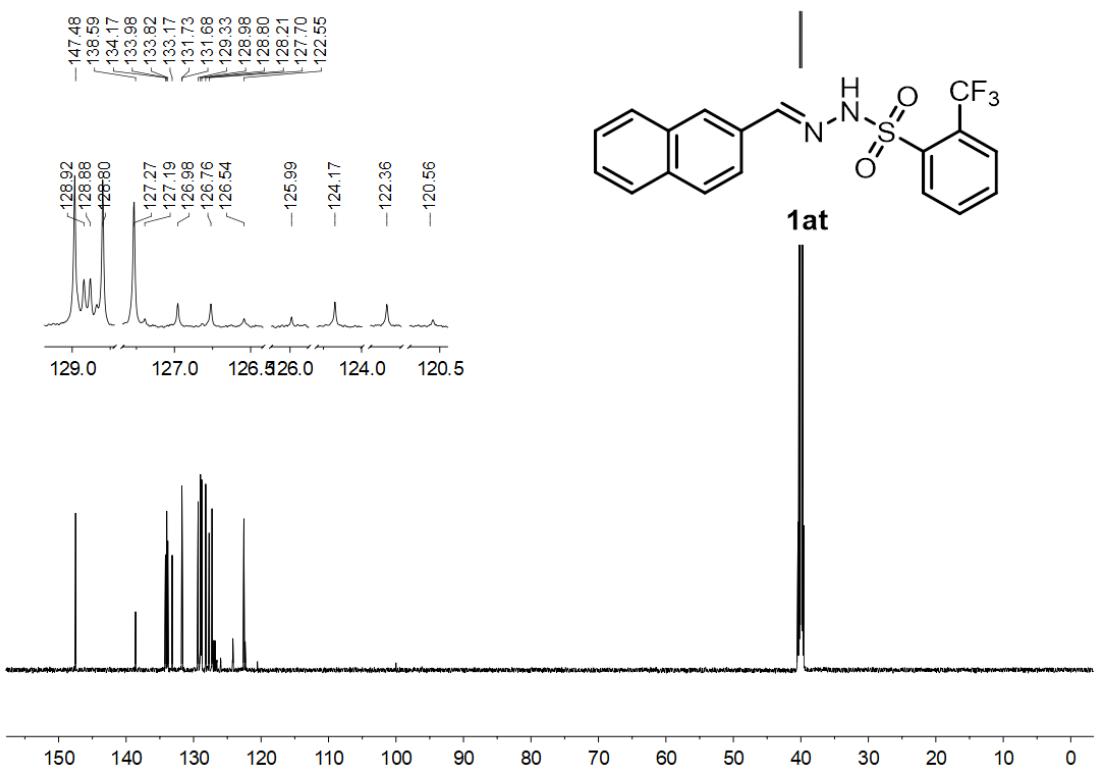

147.77
138.70
138.38
133.89
133.88
133.78
132.19
131.46
125.04
128.95
128.91
128.87
128.83
127.17
126.95
126.73
126.52
125.97
124.15
122.33
120.52
21.15
1ar

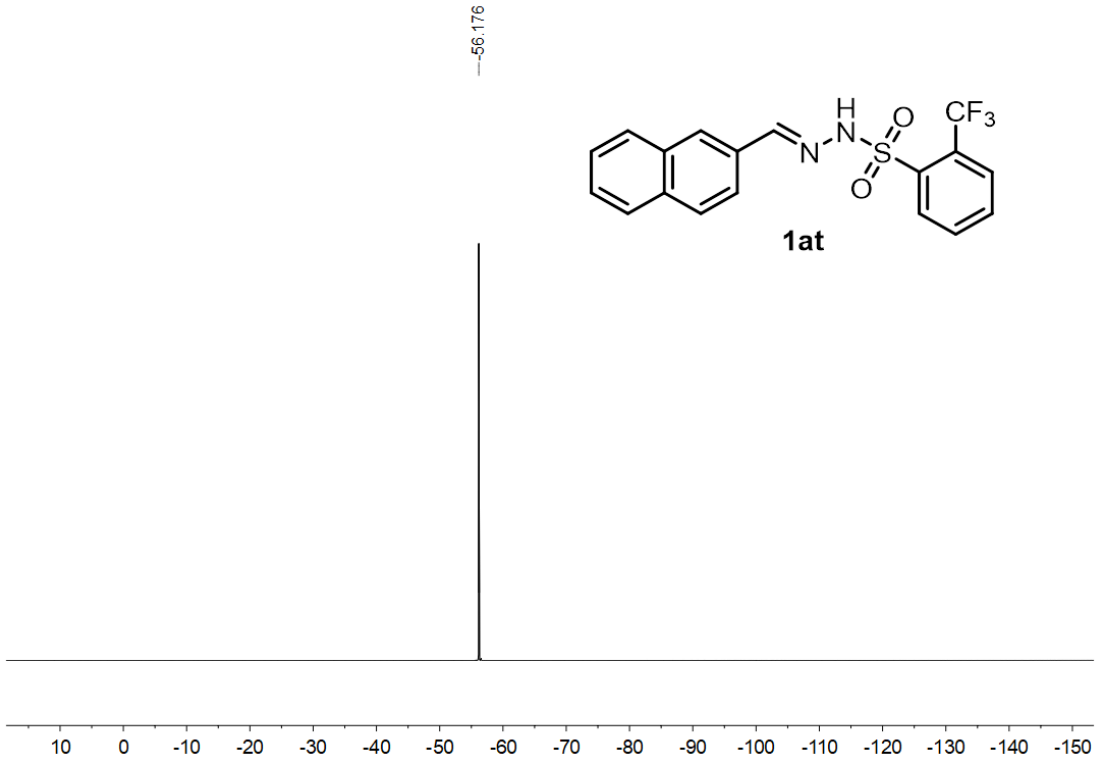

-56.213
1ar
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130

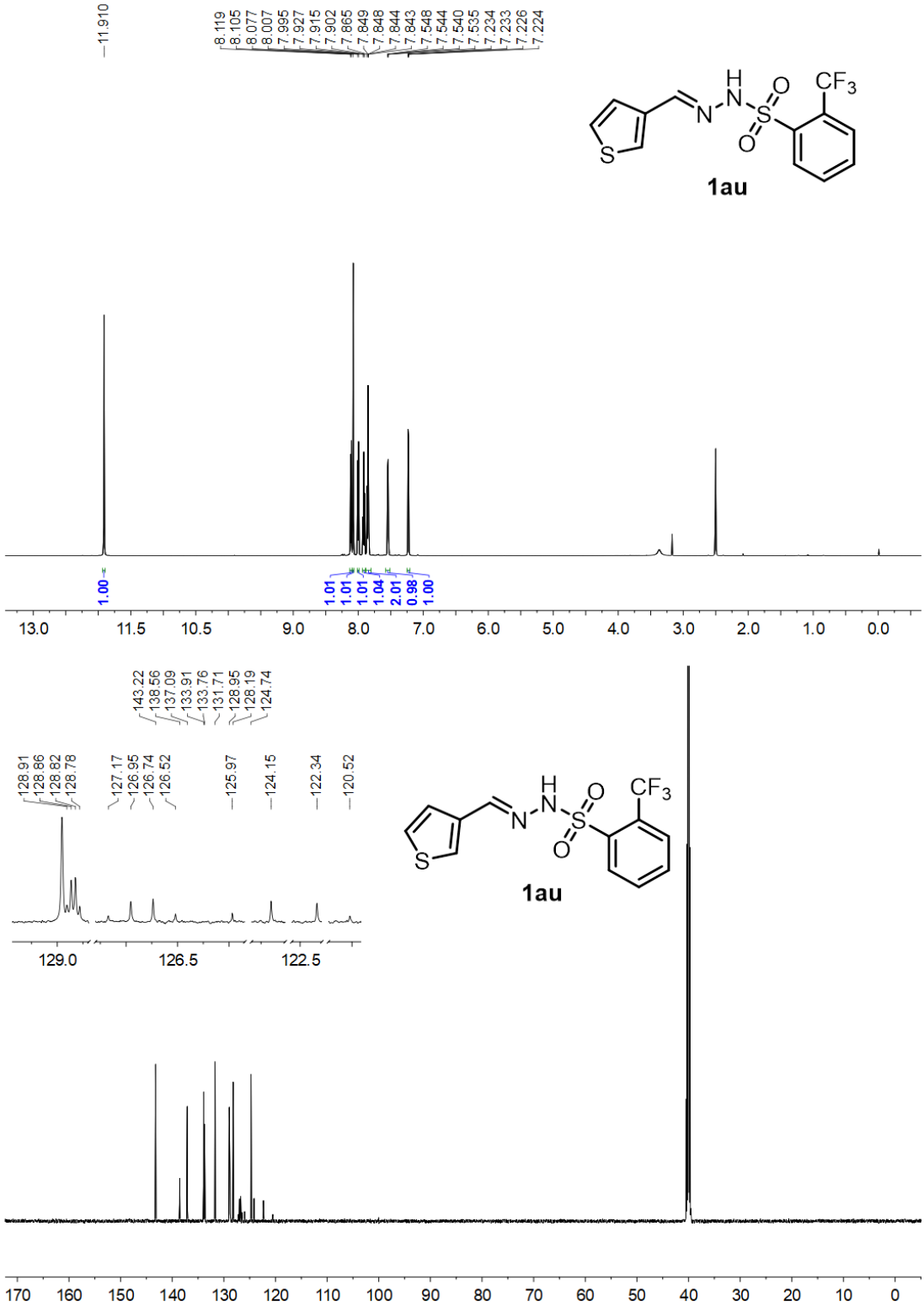

12.518
8.150
8.137
8.038
8.002
7.989
7.941
7.929
7.916
7.886
7.873
7.860
1as
0.95
1.00
1.00
1.00
1.00
1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0

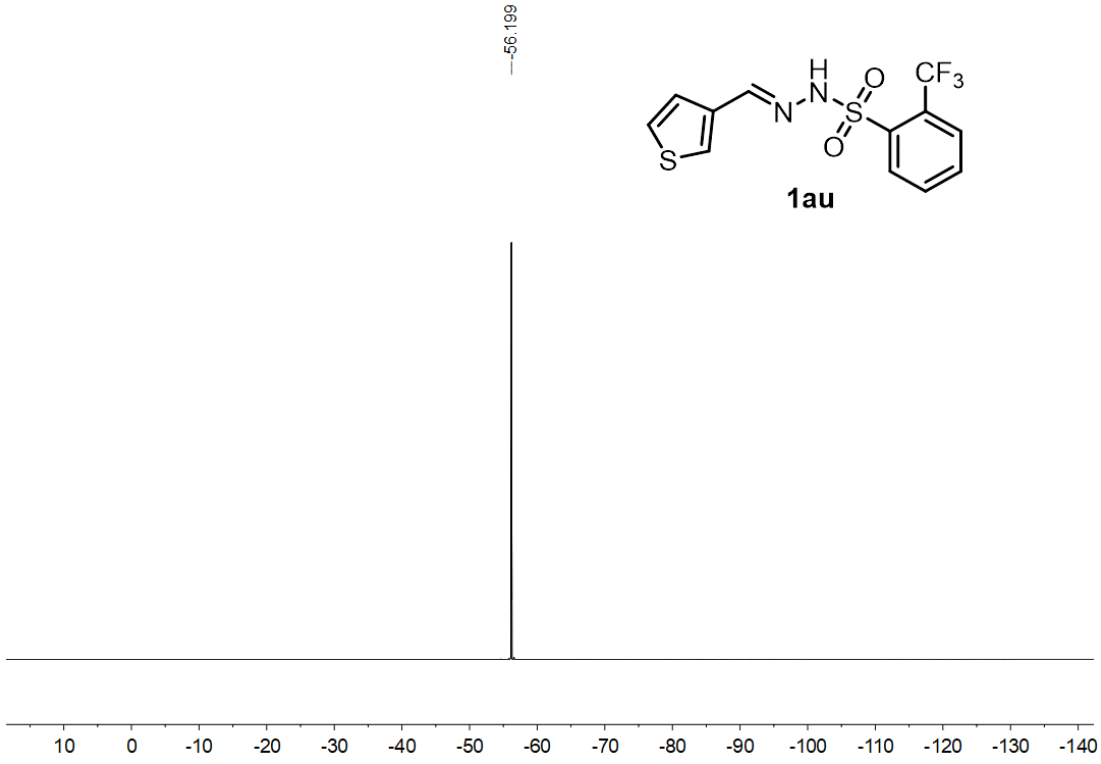

-56.532
-142.452
-142.466
-142.494
-142.510
-153.188
-153.229
-153.678
-162.693
-162.720
-162.734
-162.761
-162.776
F
F
F
F
F
H
N
N
O
S
O
CF3
1as
3.07
2.03
1.00
2.04
20 10 0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210

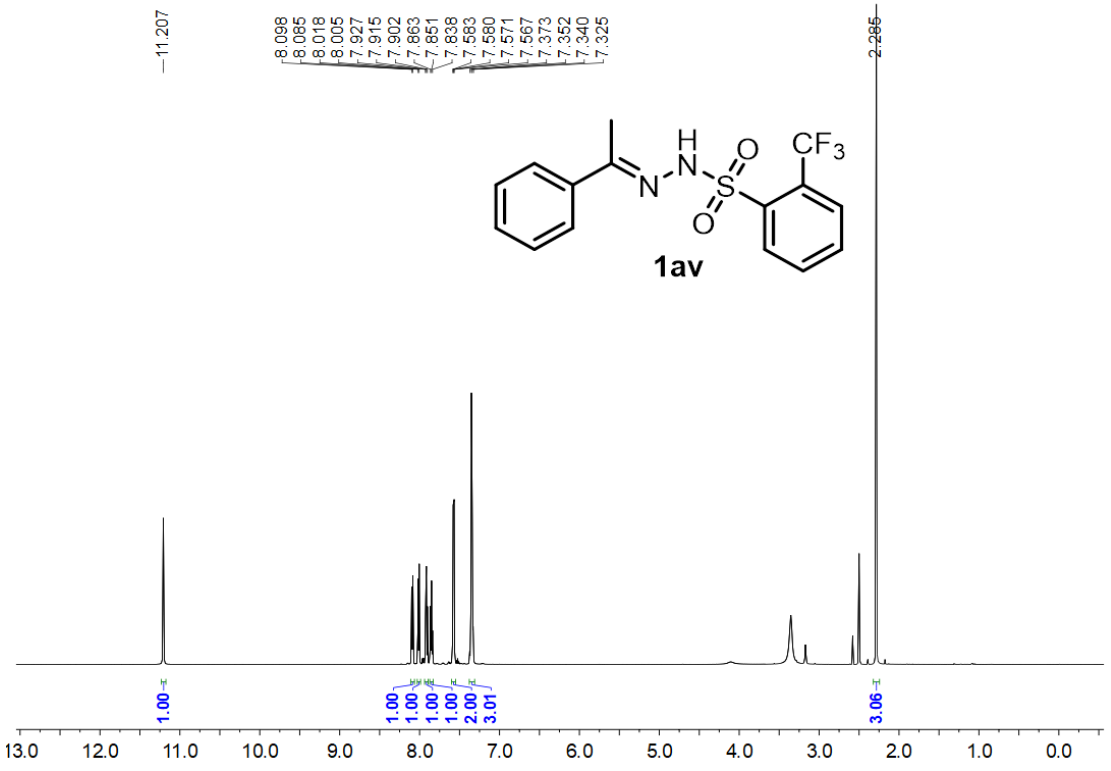

12.199
8.222
8.194
8.180
8.038
8.024
8.011
7.954
7.950
7.944
7.937
7.924
7.907
7.901
7.886
7.872
7.859
7.846
7.721
7.719
7.707
7.704
7.552
7.545
7.539
7.534
7.530
7.522
H
N
N
O
S
O
CF3
1at
1.00
1.00
0.97
1.01
0.99
2.04
3.00
0.97
2.00
13.5 12.0 10.5 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0

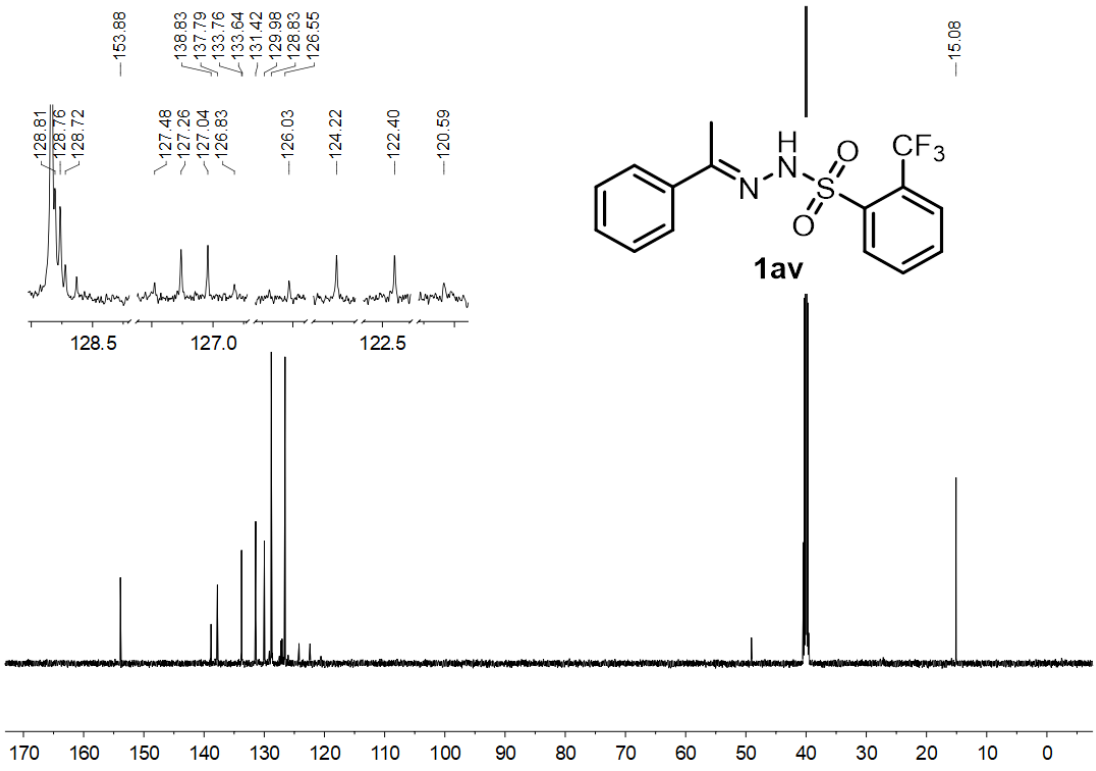

147.48
138.59
134.17
133.98
133.82
133.17
131.73
131.68
129.33
128.98
128.80
128.21
127.70
122.55
128.92
128.88
128.80
127.27
127.19
126.98
126.76
126.54
125.99
124.17
122.36
120.56
129.0
127.0
126.5
126.0
124.0
120.5
1at
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

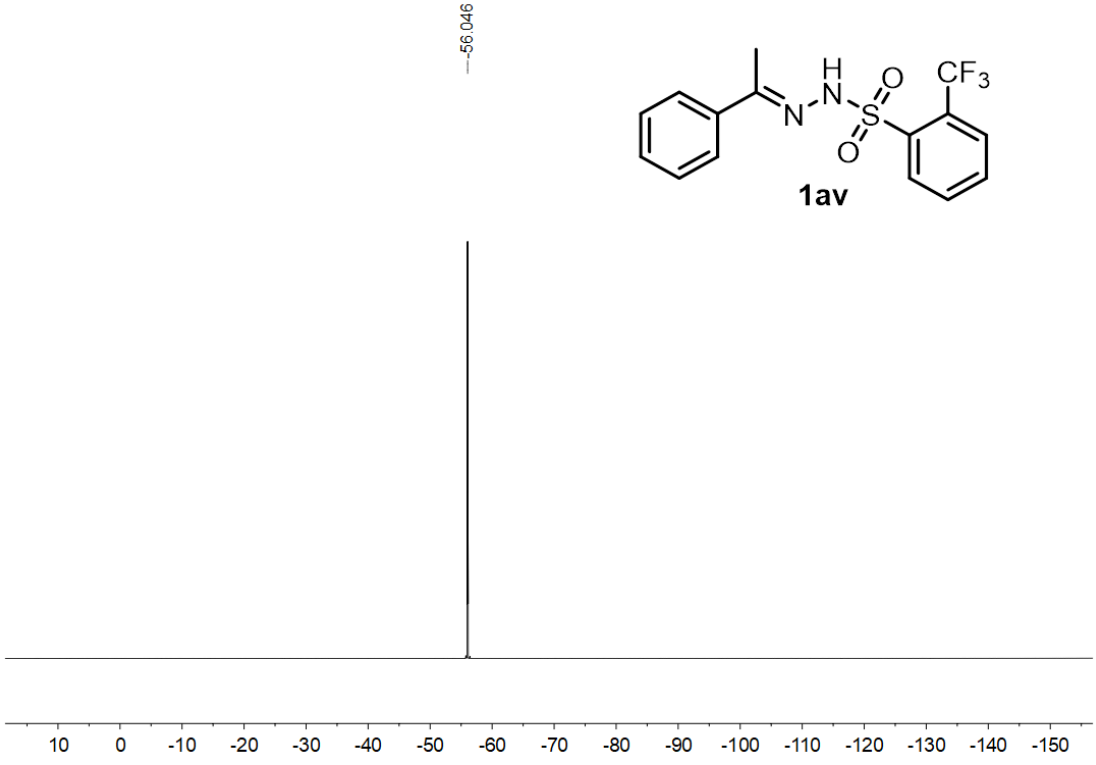

56.176
1at
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150

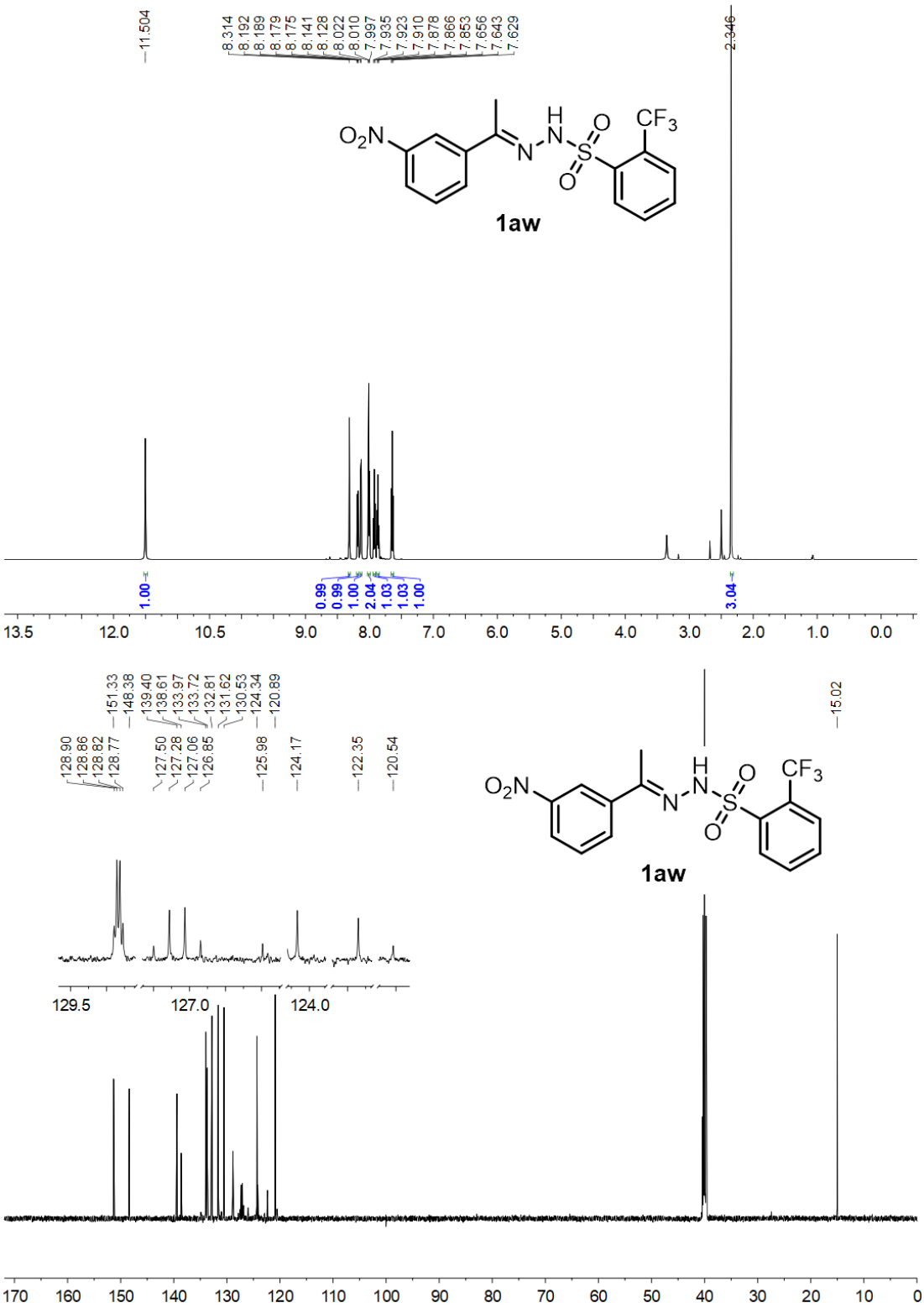

11.910
8.119
8.105
8.077
8.007
7.995
7.927
7.915
7.902
7.865
7.849
7.848
7.844
7.843
7.548
7.544
7.540
7.535
7.234
7.233
7.226
7.224
1au
1.00
1.01
1.01
1.01
1.04
2.01
0.98
1.00
13.0
11.5
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
143.22
138.56
137.09
133.91
133.76
131.71
128.95
128.19
124.74
128.91
128.86
128.82
128.78
127.17
126.95
126.74
126.52
125.97
124.15
122.34
120.52
1au
129.0
126.5
122.5
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

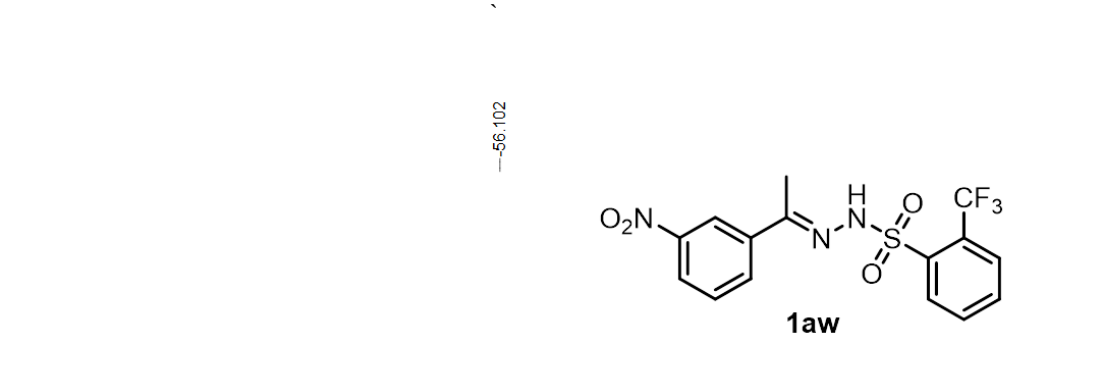

-56.199
1au
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140


11.207
8.098
8.085
8.018
8.005
7.927
7.915
7.902
7.863
7.851
7.838
7.583
7.580
7.571
7.567
7.373
7.352
7.340
7.325
2.285
1av
1.00
1.00
1.00
1.00
2.00
3.01
3.06
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

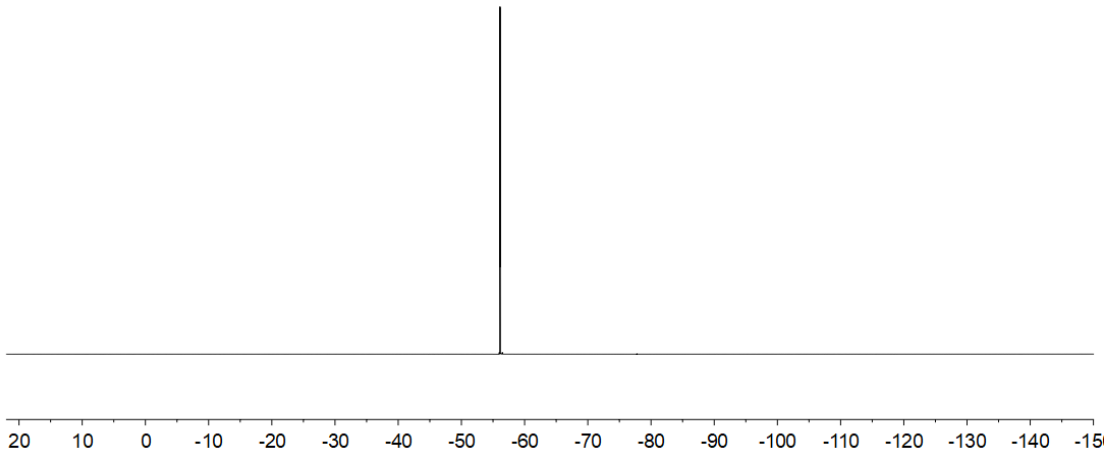

153.88
138.83
137.79
133.76
133.64
131.42
129.98
128.83
126.55
128.81
128.76
128.72
127.48
127.26
127.04
126.83
126.03
124.22
122.40
120.59
128.5
127.0
122.5
15.08
1av
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

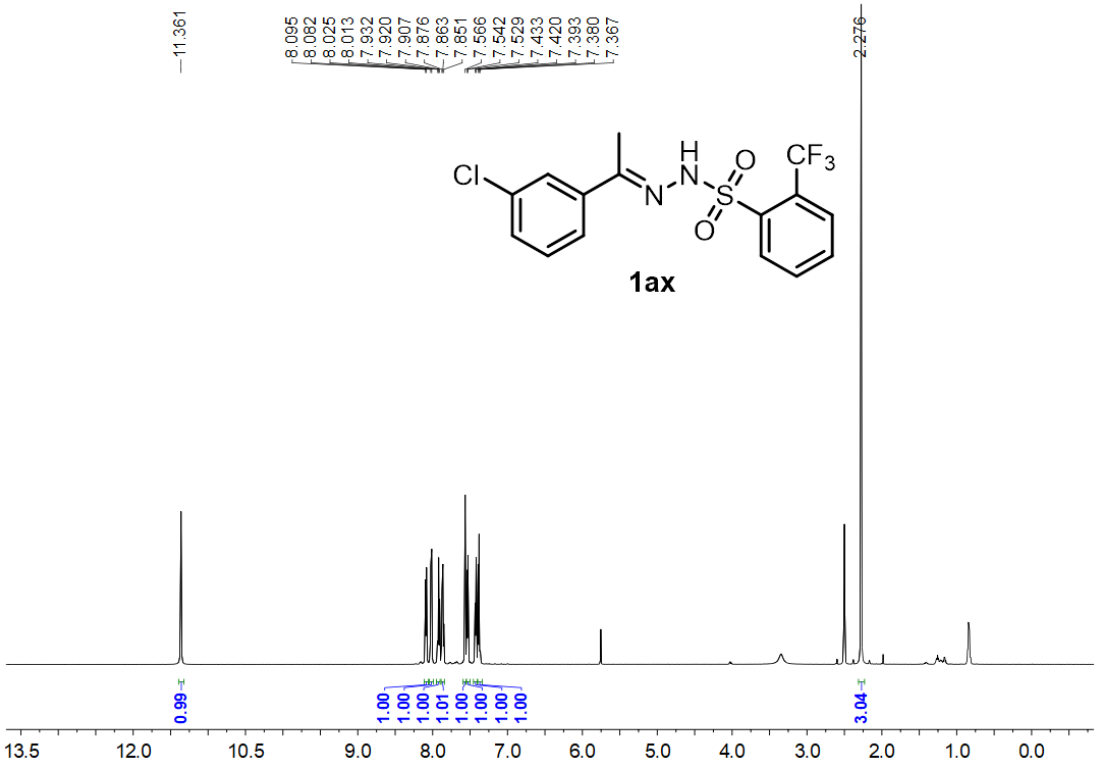

56.046
1av
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150


11.504
8.314
8.192
8.189
8.179
8.175
8.141
8.128
8.022
8.010
7.997
7.935
7.923
7.910
7.878
7.866
7.853
7.656
7.643
7.629
2.346
O2N
H
N
N
O
S
O
O
CF3
1aw
1.00
0.99
0.99
1.00
2.04
1.03
1.03
1.00
3.04
13.5
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
151.33
148.38
139.40
138.61
133.97
133.72
132.81
131.62
130.53
124.34
120.89
128.90
128.86
128.82
128.77
127.50
127.28
127.06
126.85
125.98
124.17
122.35
120.54
15.02
O2N
H
N
N
O
S
O
O
CF3
1aw
129.5
127.0
124.0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

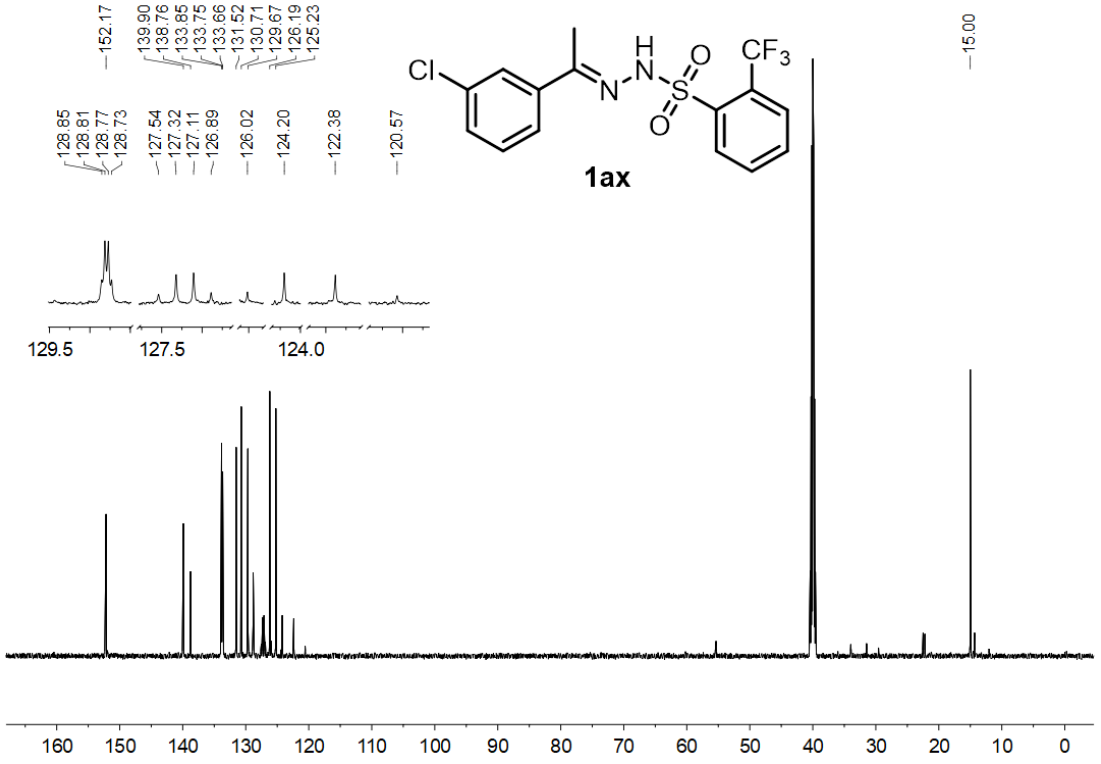

-56.102
O_2N
H
N
N
O
S
O
CF_3

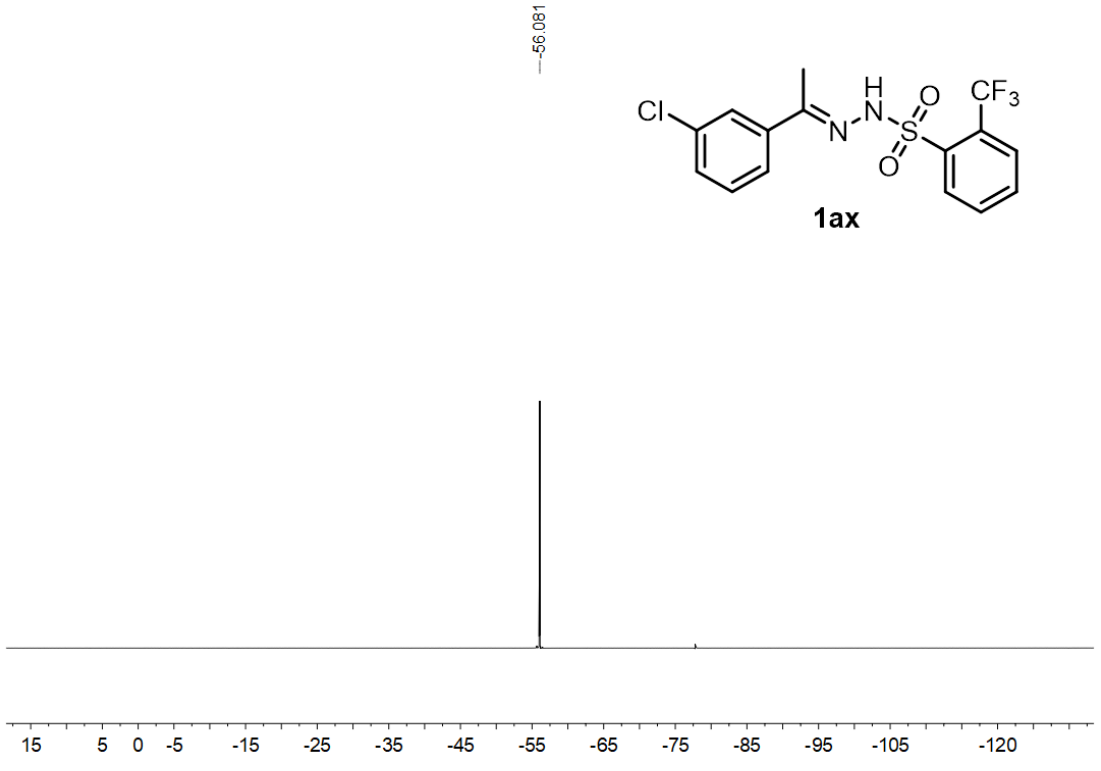
1aw

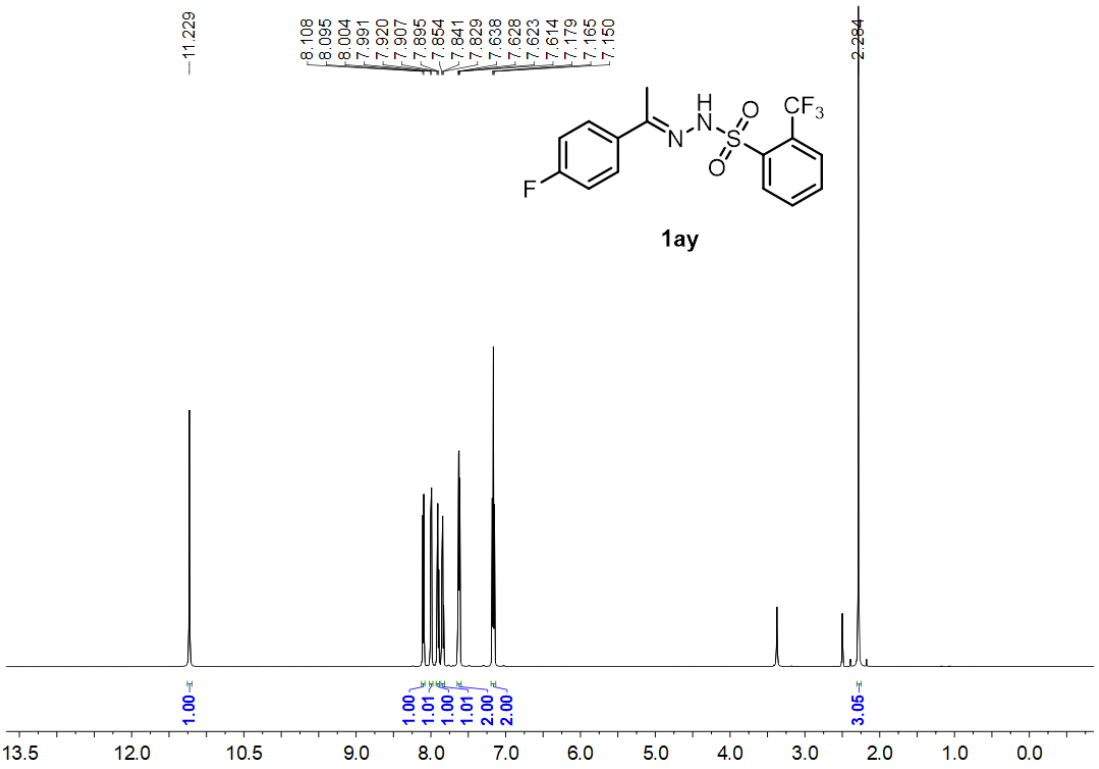

20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-15

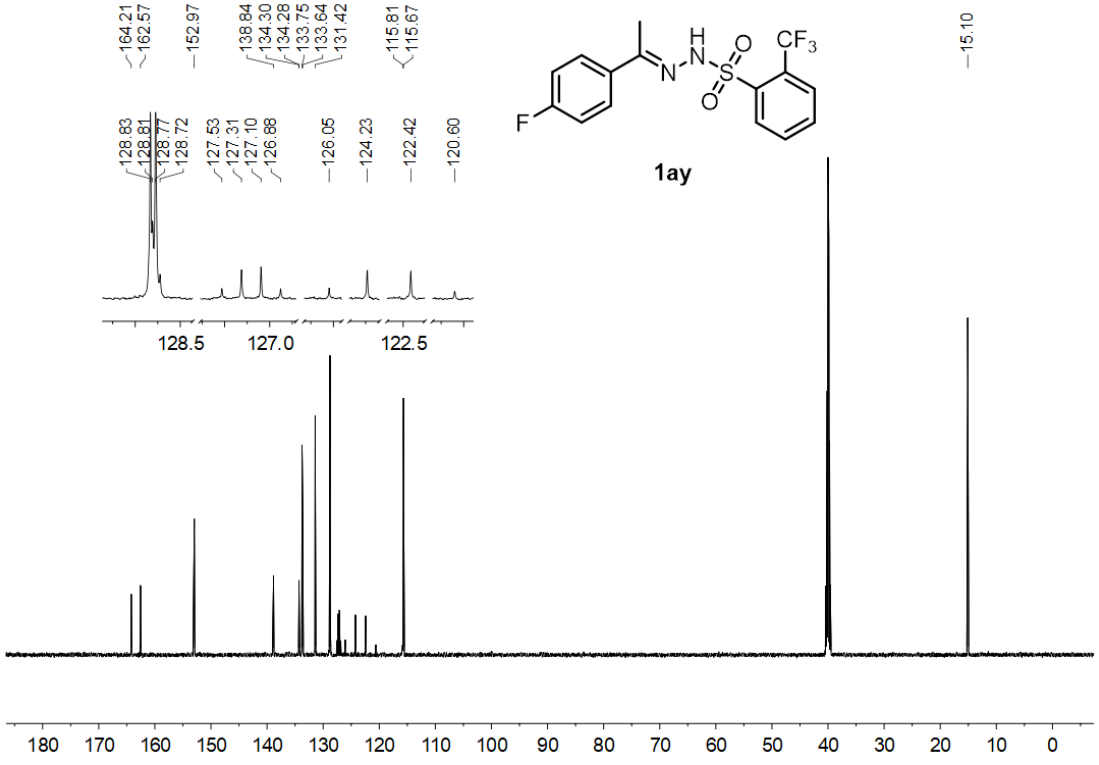

11.361
8.095
8.082
8.025
8.013
7.932
7.920
7.907
7.876
7.863
7.851
7.566
7.542
7.529
7.433
7.420
7.393
7.380
7.367
2.276
Cl
H
N
N
O
S
O
CF_3
0.99
1.00
1.00
1.00
1.01
1.00
1.00
1.00
3.04
13.5
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

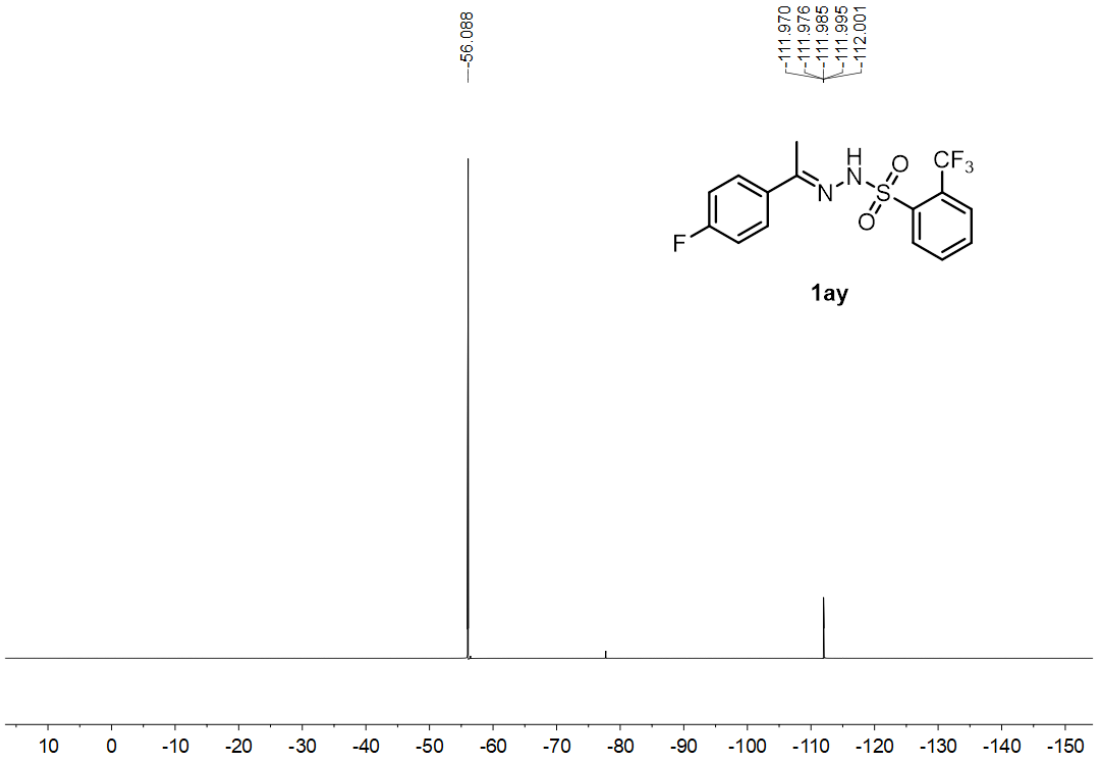
1ax

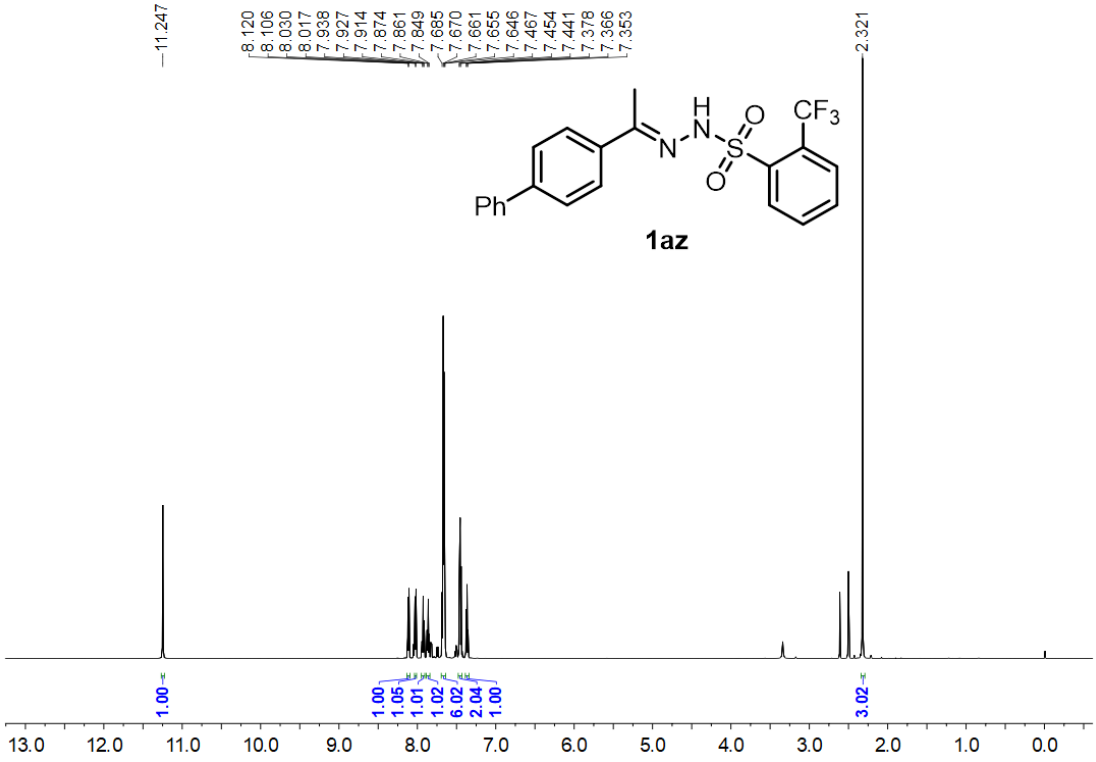

152.17
139.90
138.76
133.85
133.75
133.66
131.52
130.71
129.67
126.19
125.23
128.85
128.81
128.77
128.73
127.54
127.32
127.11
126.89
126.02
124.20
122.38
120.57
15.00
Cl
N
H
N
O
S
O
CF3
1ax
129.5
127.5
124.0
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

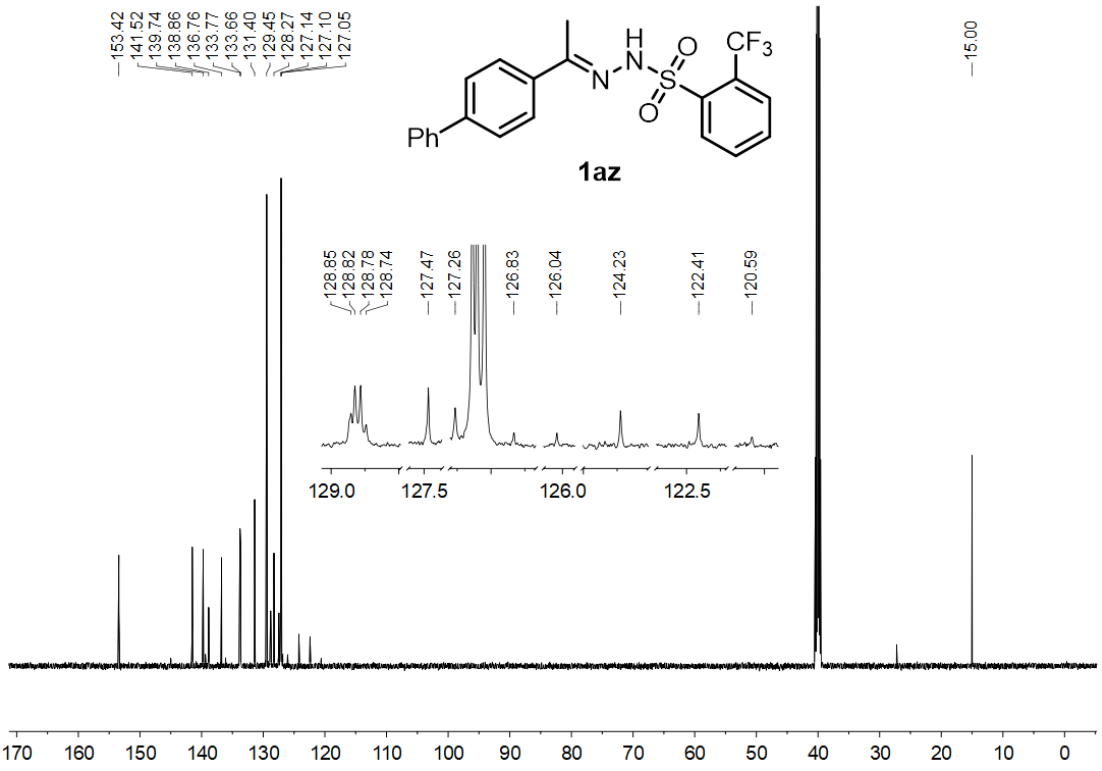

-56.081
Cl
N
H
N
O
S
O
CF3
1ax
15
5
0
-5
-15
-25
-35
-45
-55
-65
-75
-85
-95
-105
-120

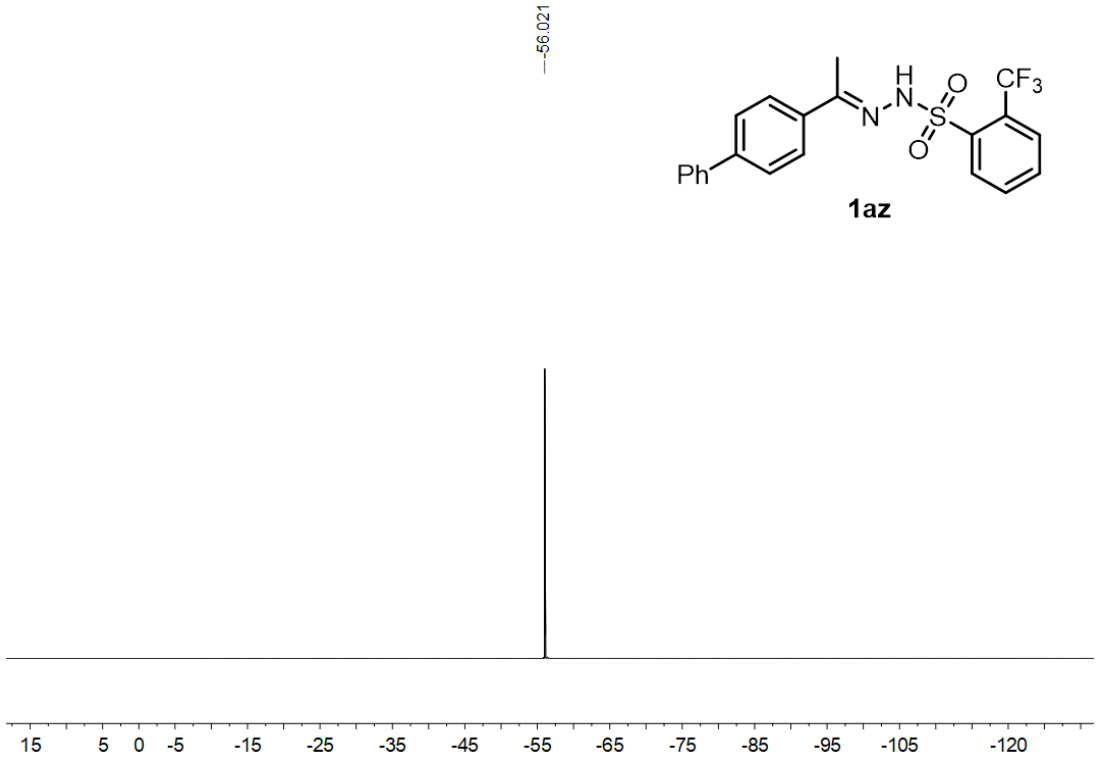

11.229
8.108
8.095
8.004
7.991
7.920
7.907
7.895
7.854
7.841
7.829
7.638
7.628
7.623
7.614
7.179
7.165
7.150
2.284
1ay
1.00
1.00
1.01
1.00
1.01
2.00
2.00
3.05
13.5
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

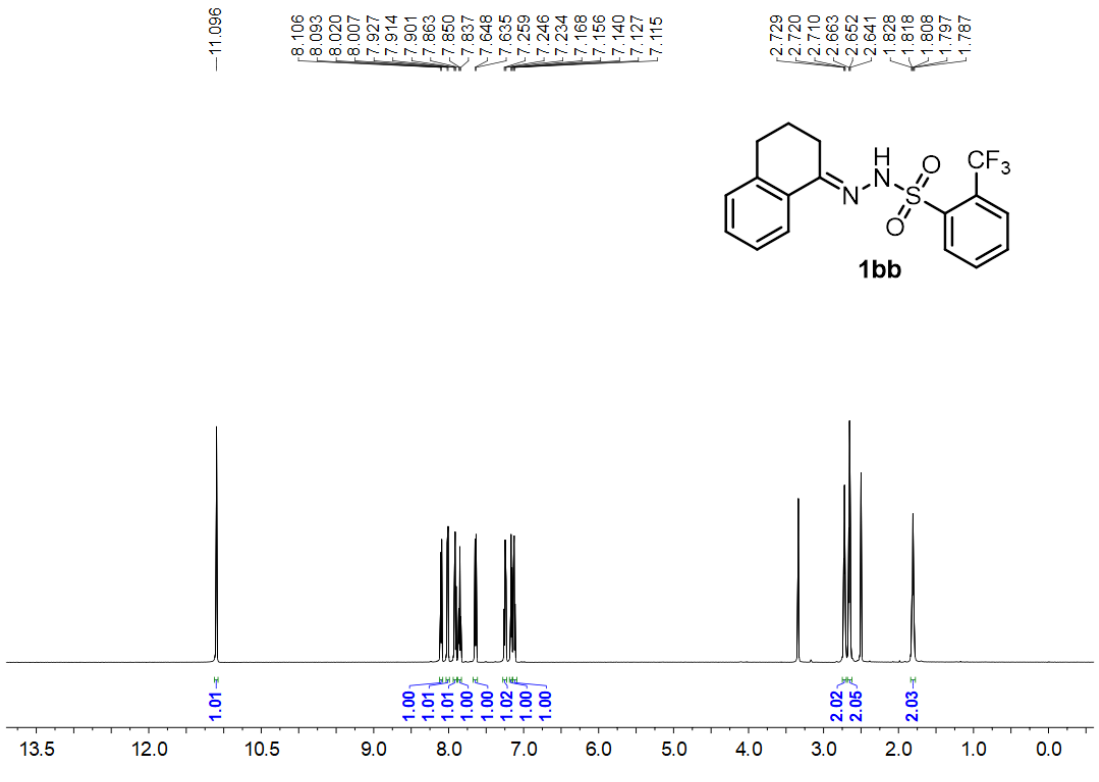

164.21
162.57
152.97
138.84
134.30
134.28
133.75
133.64
131.42
115.81
115.67
128.83
128.81
128.77
128.72
127.53
127.31
127.10
126.88
126.05
124.23
122.42
120.60
15.10
1ay
128.5
127.0
122.5
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

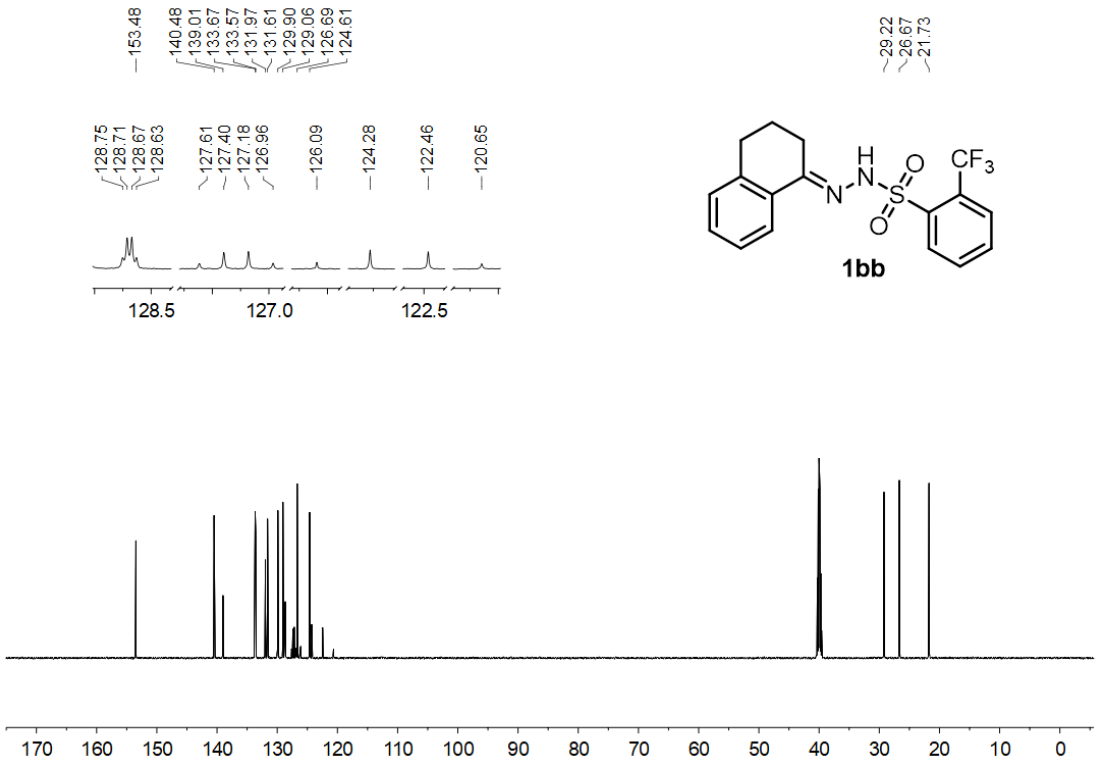

-56.088
-111.970
-111.976
-111.985
-111.995
-112.001
F
N
H
N
S
O
O
CF3
1ay
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150

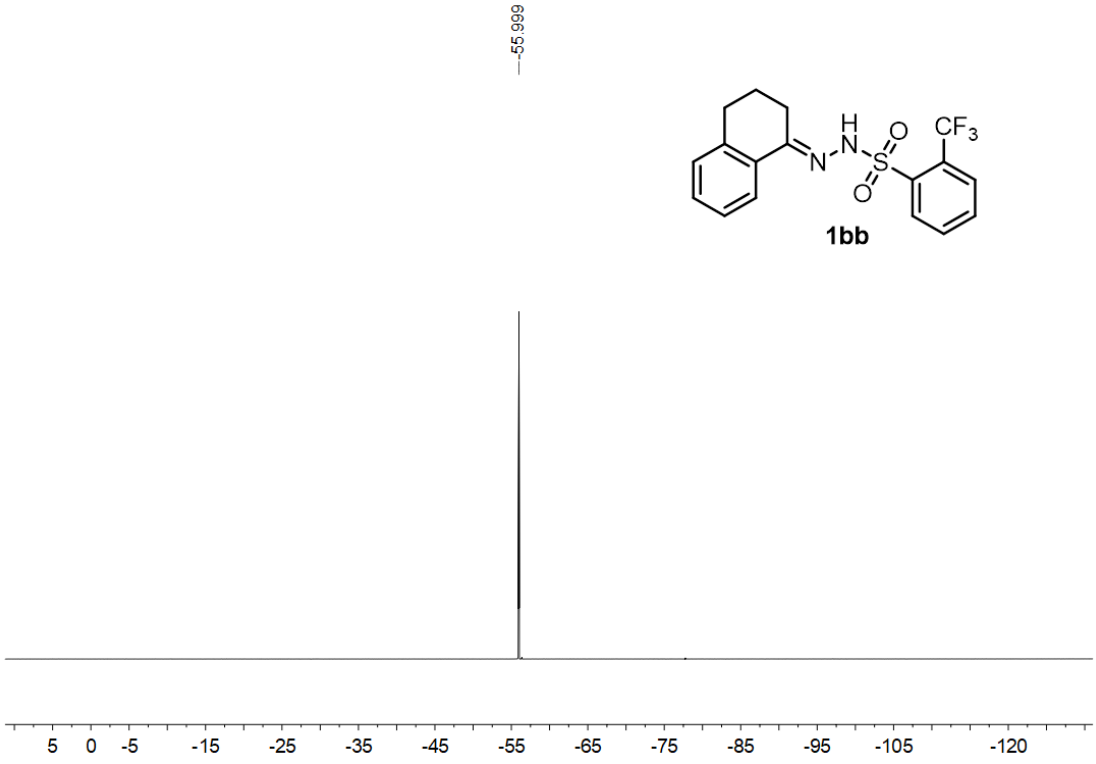

11.247
8.120
8.106
8.030
8.017
7.938
7.927
7.914
7.874
7.861
7.849
7.685
7.670
7.661
7.655
7.646
7.467
7.454
7.441
7.378
7.366
7.353
2.321
Ph
N
H
N
S
O
O
CF3
1az
1.00
1.00
1.05
1.01
1.02
6.02
2.04
1.00
3.02
13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0

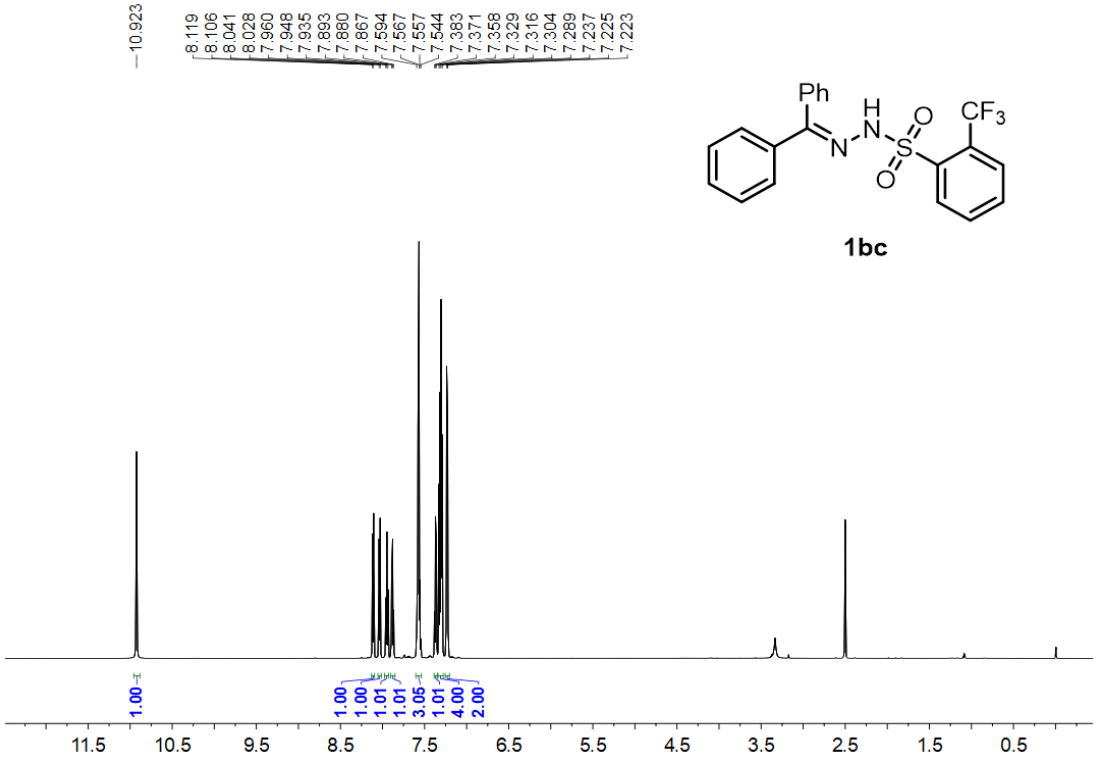

153.42
141.52
139.74
138.86
136.76
133.77
133.66
131.40
129.45
128.27
127.14
127.10
127.05
15.00
Ph
N
H
N
S
O
O
CF3
1az
128.85
128.82
128.78
128.74
127.47
127.26
126.83
126.04
124.23
122.41
120.59
129.0
127.5
126.0
122.5
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

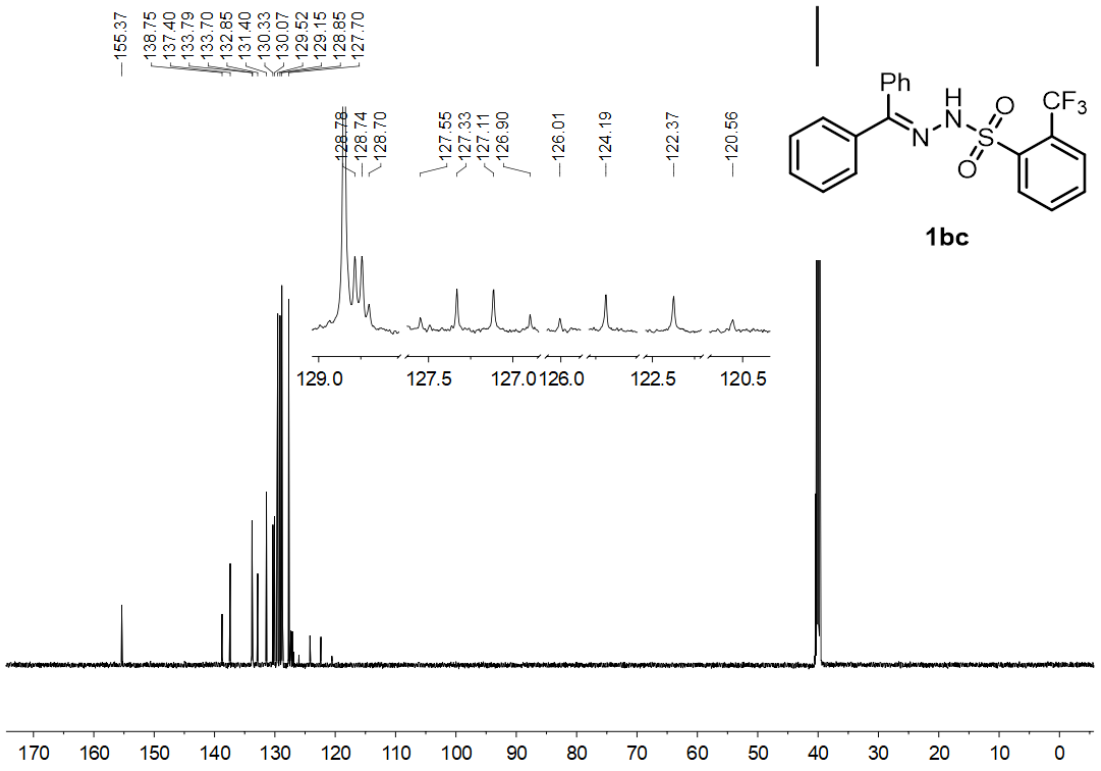

-56.021
Ph
N
H
N
S
O
O
CF3
1az
15
5
0
-5
-15
-25
-35
-45
-55
-65
-75
-85
-95
-105
-120

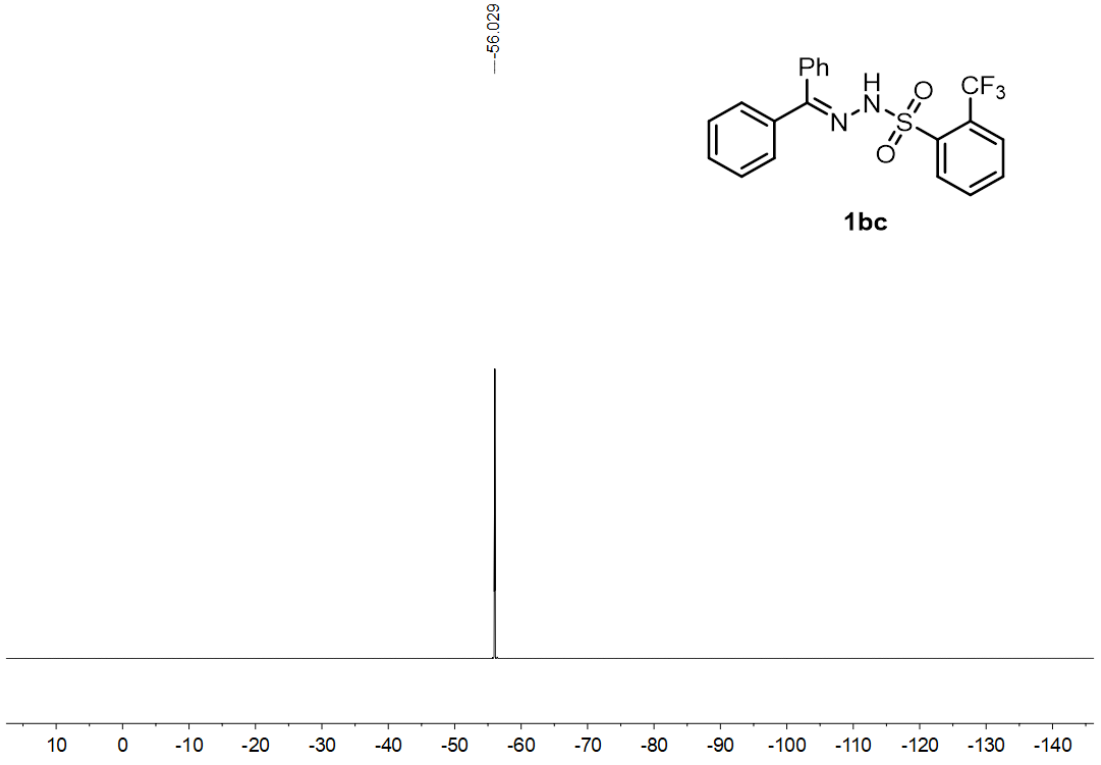

11.096
8.106
8.093
8.020
8.007
7.927
7.914
7.901
7.863
7.850
7.837
7.648
7.635
7.259
7.246
7.234
7.168
7.156
7.140
7.127
7.115
2.729
2.720
2.710
2.663
2.652
2.641
1.828
1.818
1.808
1.797
1.787
CF3
1bb
1.01
1.00
1.01
1.01
1.00
1.00
1.02
1.00
1.00
2.02
2.05
2.03
13.5
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

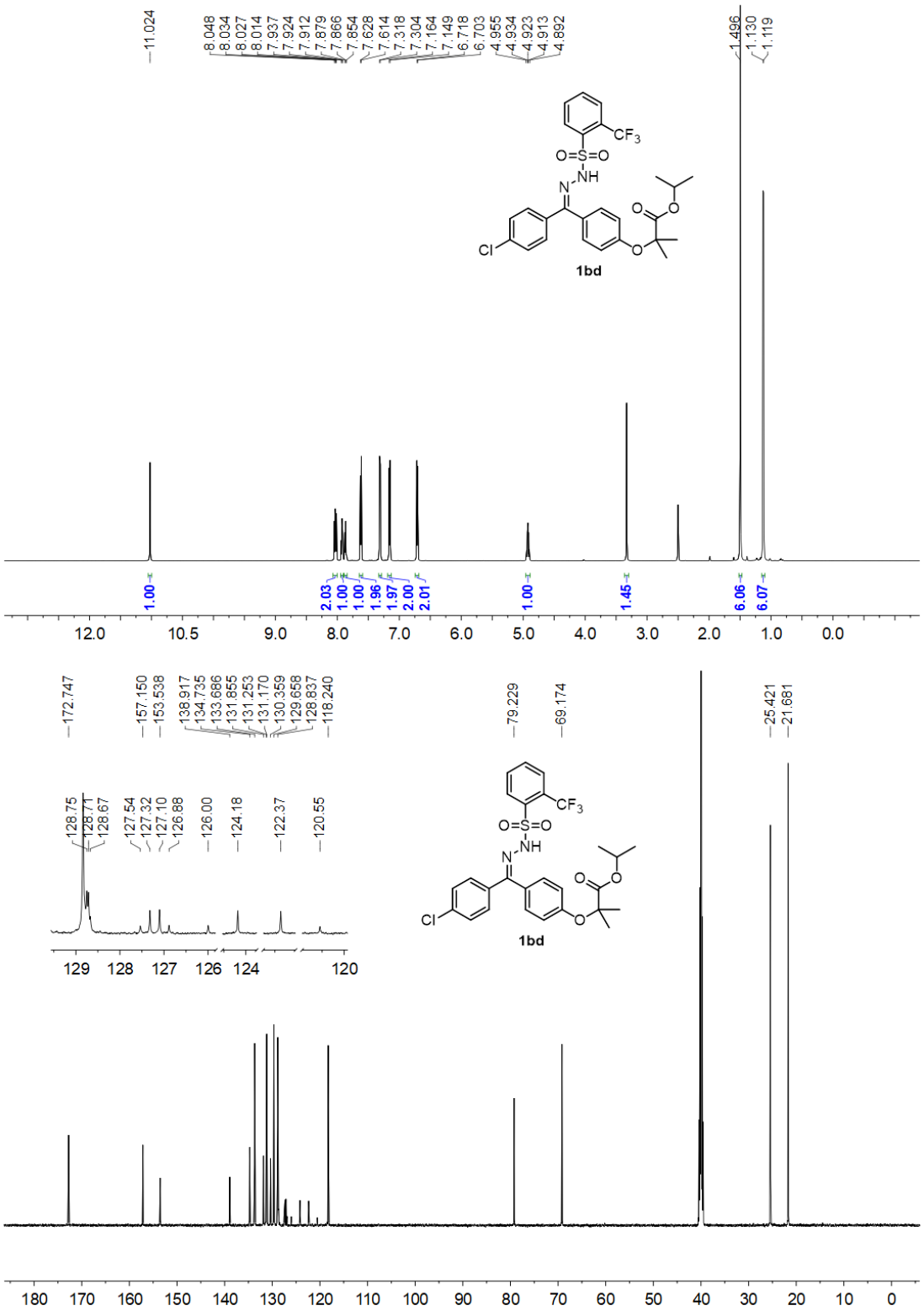

153.48
140.48
139.01
133.67
133.57
131.97
131.61
129.90
129.06
126.69
124.61
29.22
26.67
21.73
128.75
128.71
128.67
128.63
127.61
127.40
127.18
126.96
126.09
124.28
122.46
120.65
CF3
1bb
128.5
127.0
122.5
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

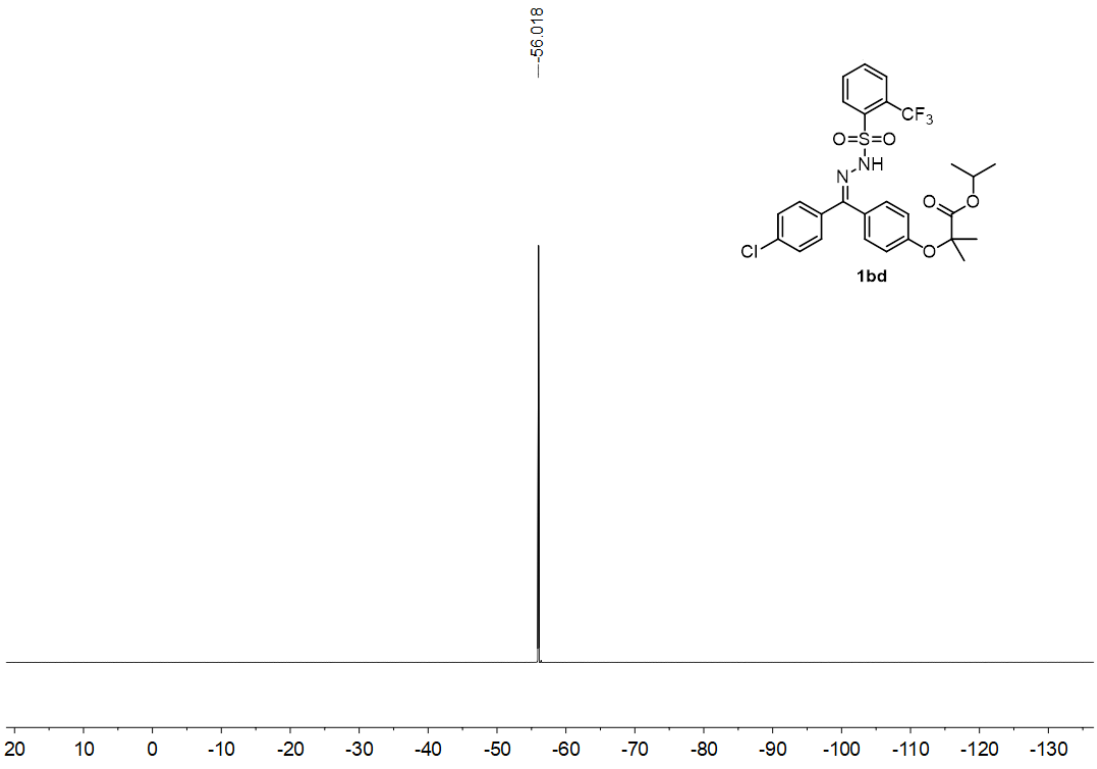

-55.999
1bb
5 0 -5 -15 -25 -35 -45 -55 -65 -75 -85 -95 -105 -120

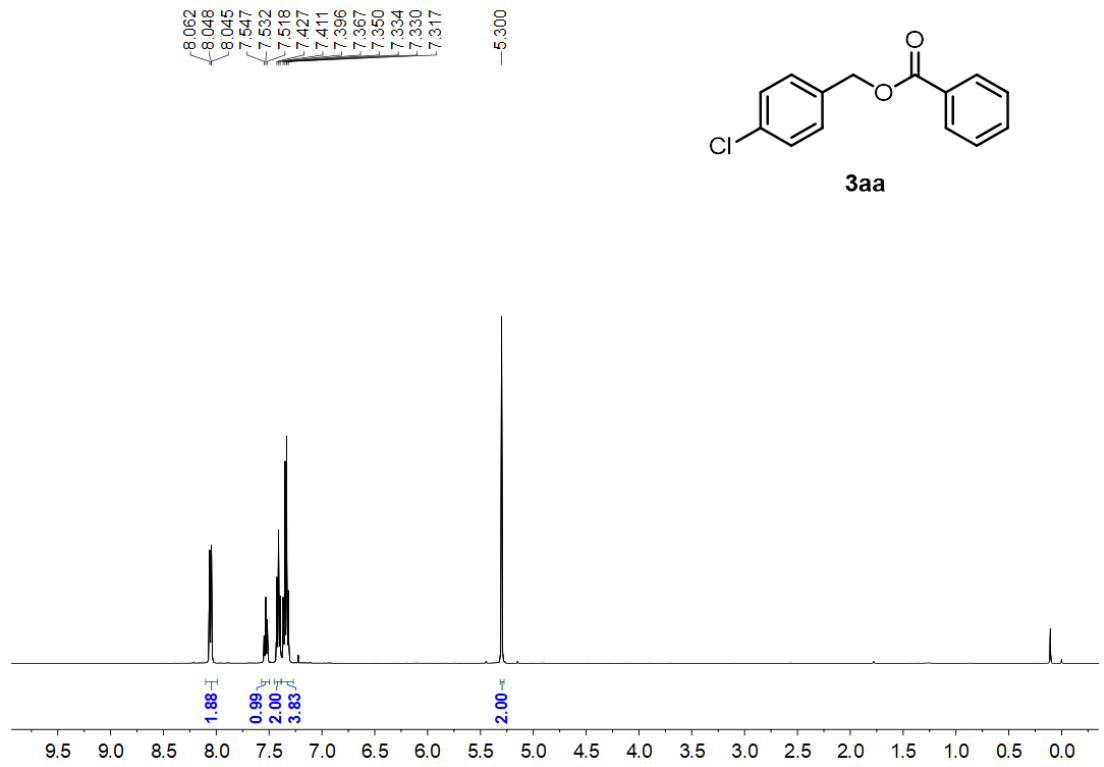

10.923
8.119
8.106
8.041
8.028
7.960
7.948
7.935
7.893
7.880
7.867
7.594
7.567
7.557
7.544
7.383
7.371
7.358
7.329
7.316
7.304
7.289
7.237
7.225
7.223
Ph
1bc
1.00 1.00 1.01 1.01 3.05 1.01 4.00 2.00
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5

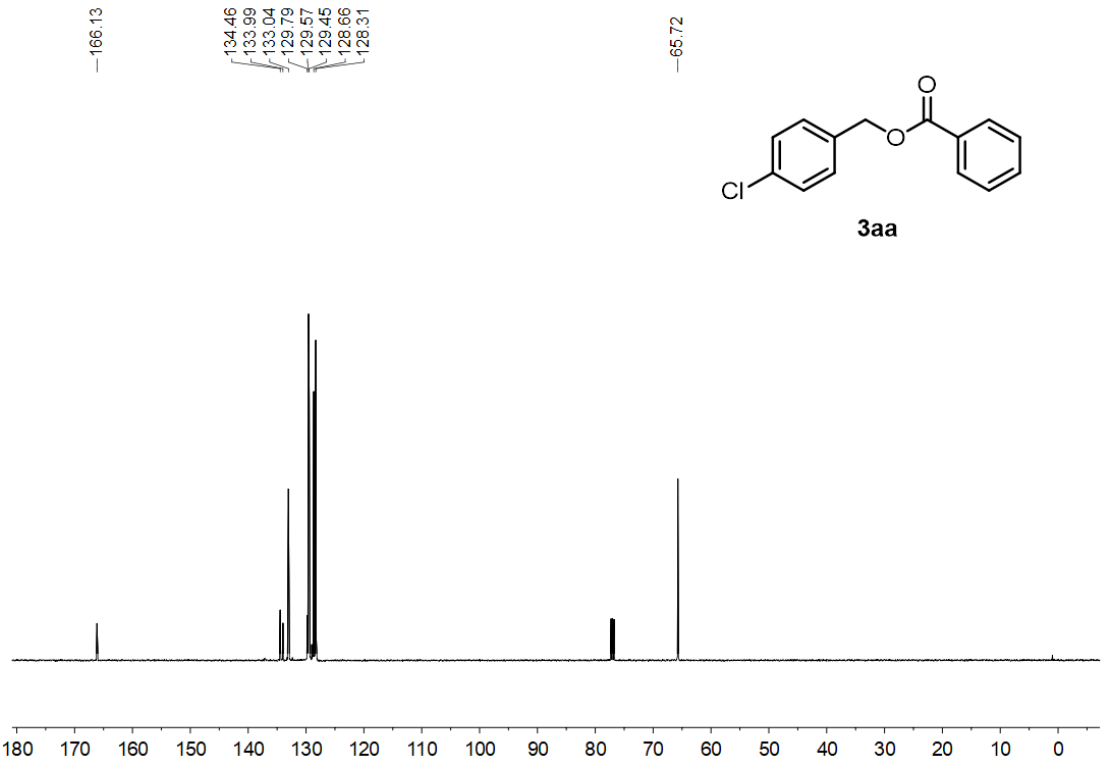

155.37
138.75
137.40
133.79
133.70
132.85
131.40
130.33
130.07
129.52
129.15
128.85
127.70
128.78
128.74
128.70
127.55
127.33
127.11
126.90
126.01
124.19
122.37
120.56
Ph
H
N
N
O
S
O
CF3
1bc
129.0
127.5
127.0
126.0
122.5
120.5
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

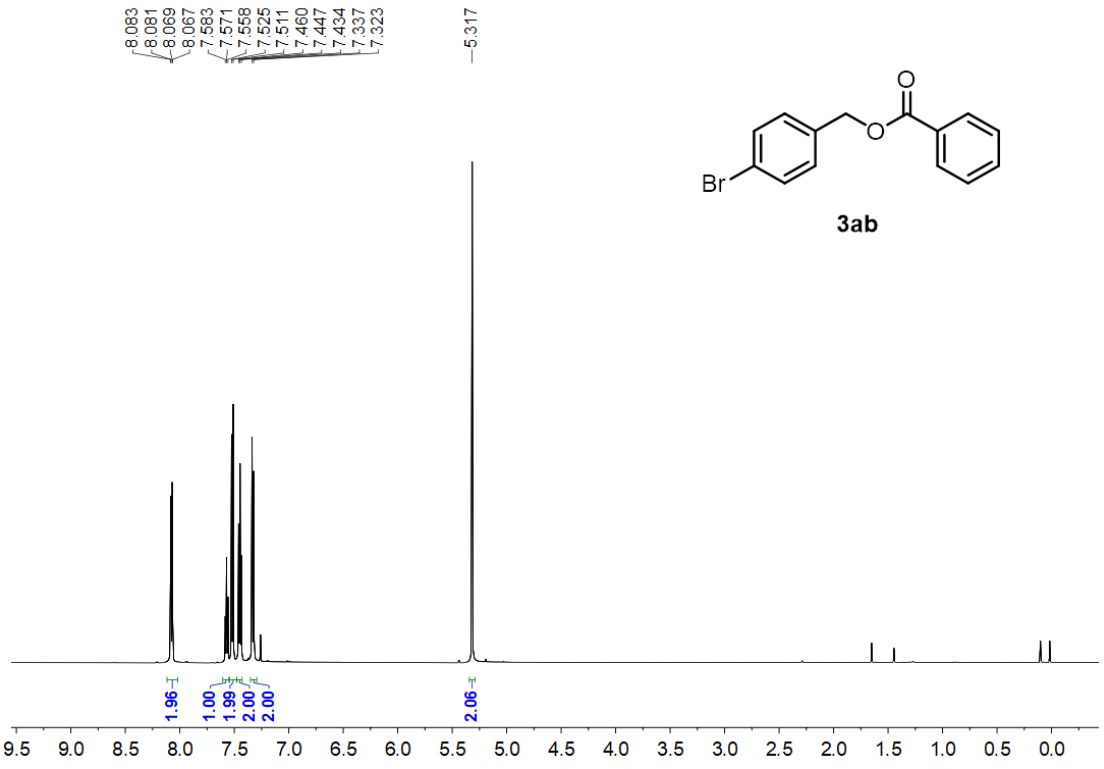

56.029
Ph
H
N
N
O
S
O
CF3
1bc
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140

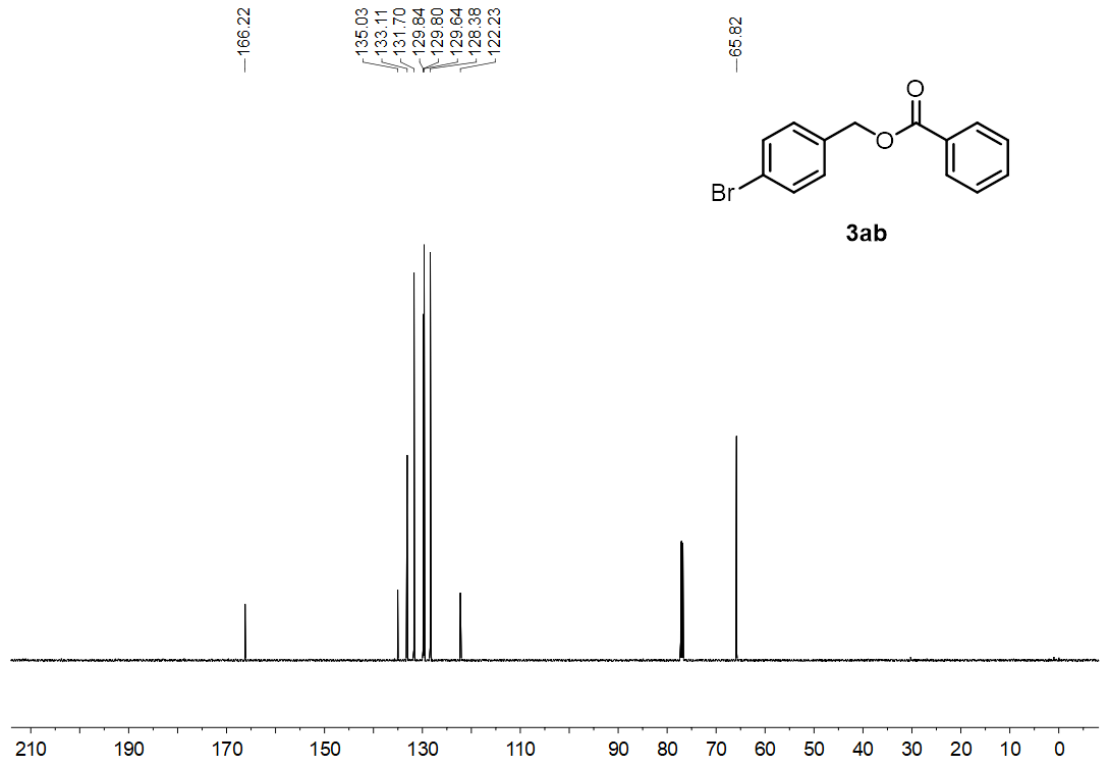

11.024
8.048
8.034
8.027
8.014
7.937
7.924
7.912
7.879
7.866
7.854
7.628
7.614
7.318
7.304
7.164
7.149
6.718
6.703
4.955
4.934
4.923
4.913
4.892
1.496
1.130
1.119
1bd
1.00
2.03
1.00
1.00
1.96
1.97
2.00
2.01
1.00
1.45
6.06
6.07
172.747
157.150
153.538
138.917
134.735
133.686
131.855
131.253
131.170
130.359
129.658
128.837
118.240
79.229
69.174
25.421
21.681
128.75
128.71
128.67
127.54
127.32
127.10
126.88
126.00
124.18
122.37
120.55
1bd

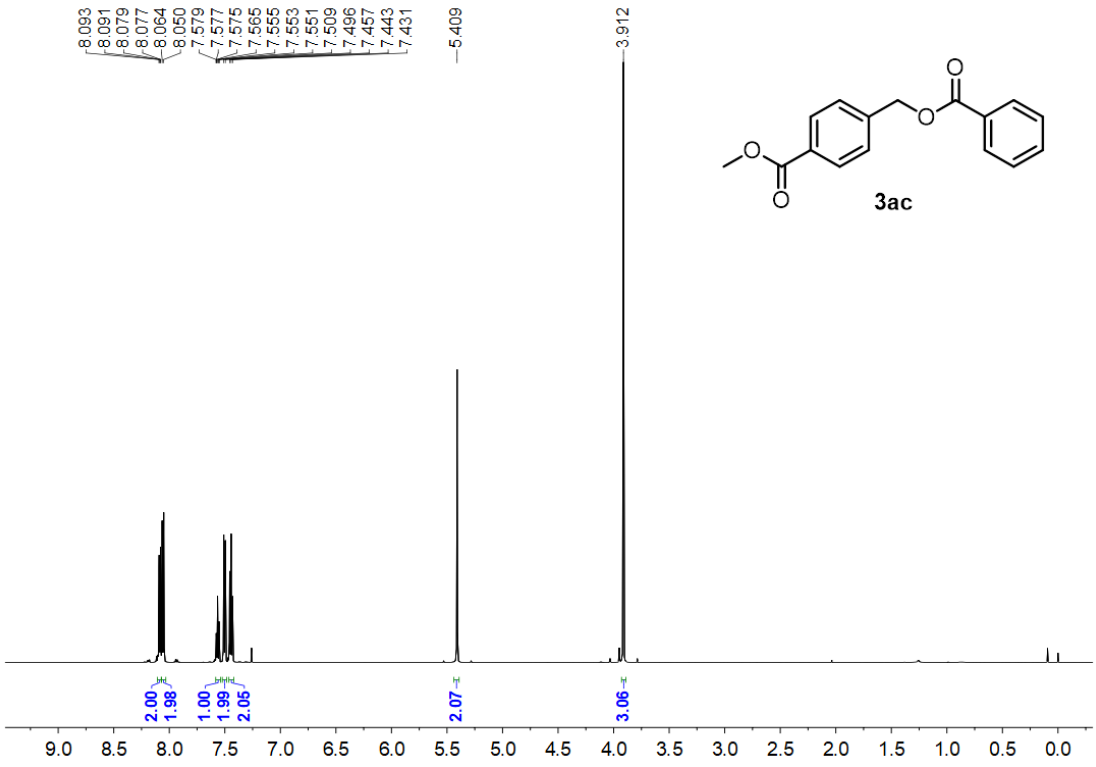

-56.018
CF3
O=S=O
NH
N
O
O
Cl
O
1bd
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130

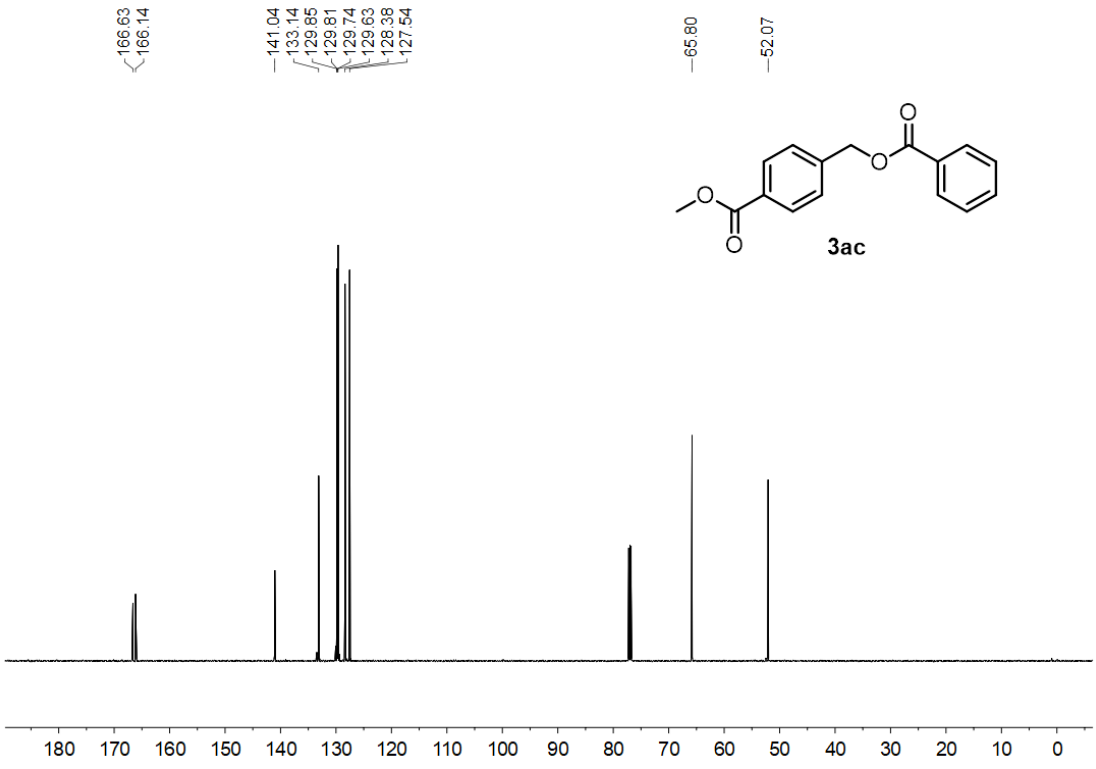

8.062
8.048
8.045
7.547
7.532
7.518
7.427
7.411
7.396
7.367
7.350
7.334
7.330
7.317
5.300
Cl
O
O
3aa
1.88
0.99
2.00
3.83
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

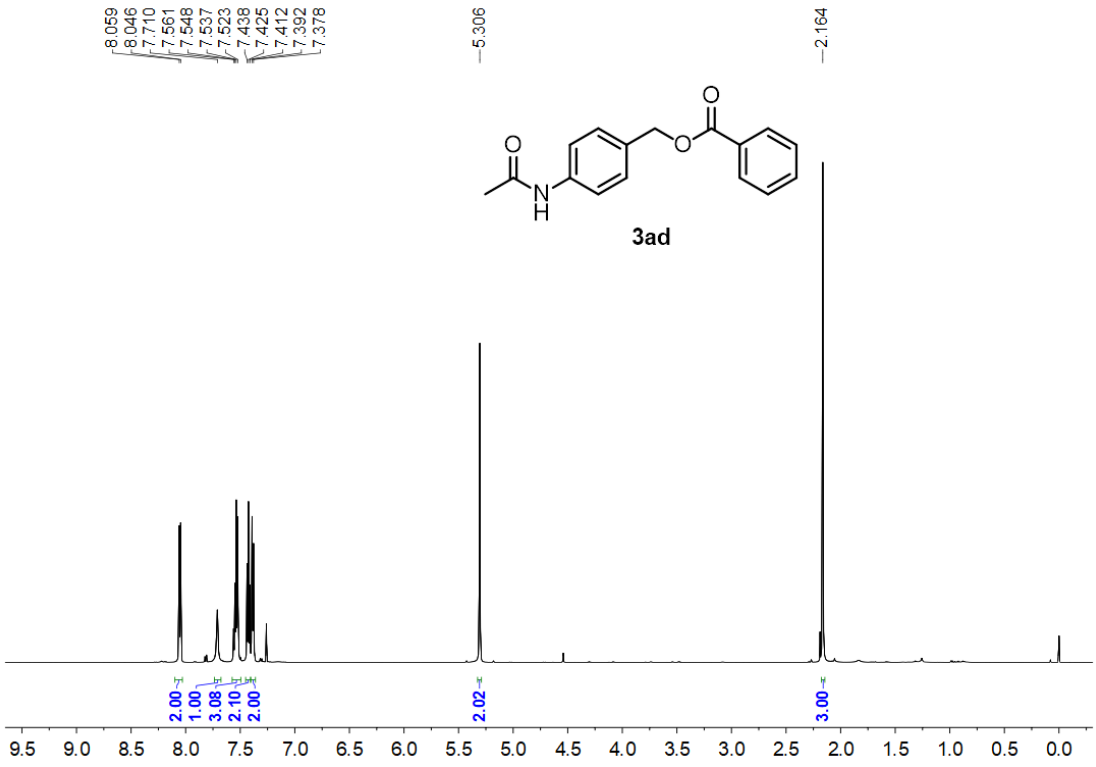

166.13
134.46
133.99
133.04
129.79
129.57
129.45
128.66
128.31
65.72
Cl
O
O
3aa
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

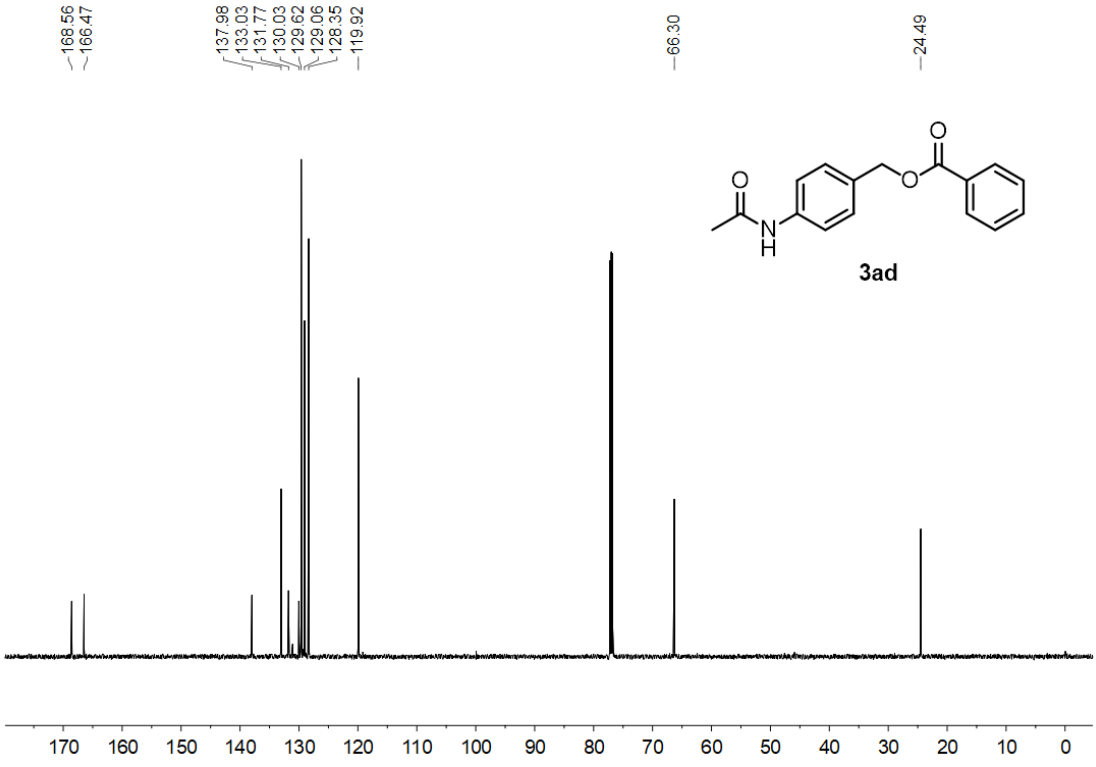

8.083
8.081
8.069
8.067
7.583
7.571
7.558
7.525
7.511
7.460
7.447
7.434
7.337
7.323
5.317
Br
O
O
3ab
1.96
1.00
1.99
2.00
2.00
2.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

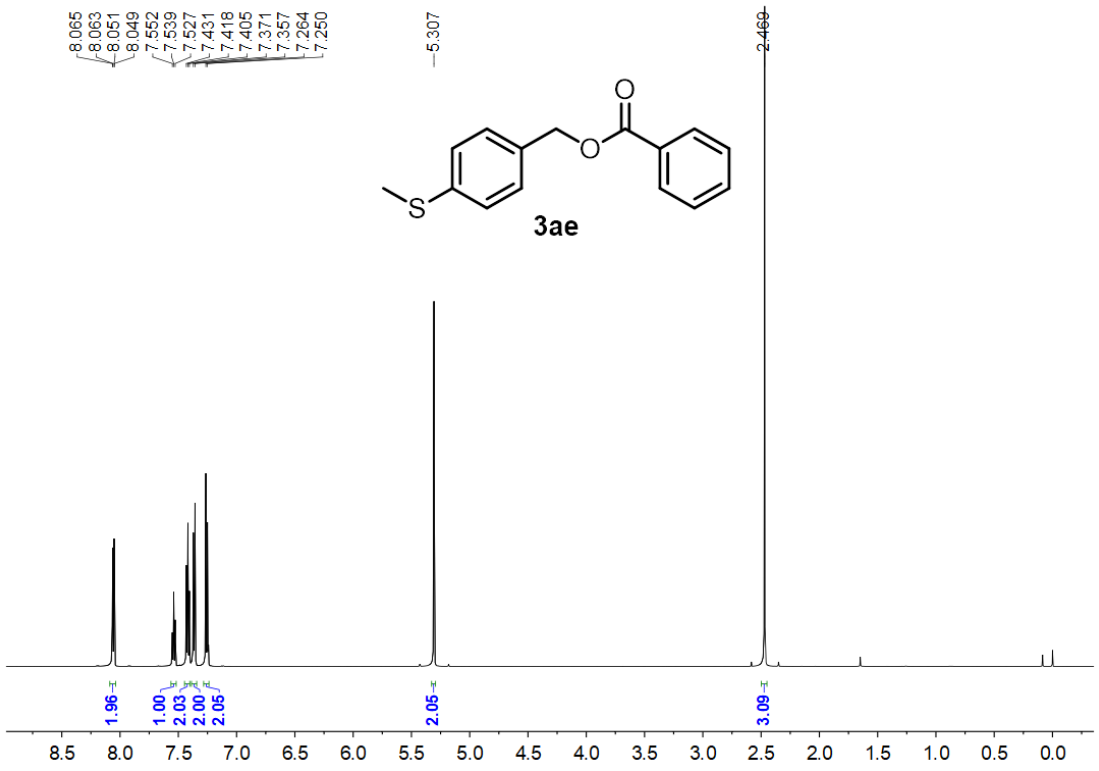

166.22
135.03
133.11
131.70
129.84
129.80
129.64
128.38
122.23
65.82
Br
O
O
3ab
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0

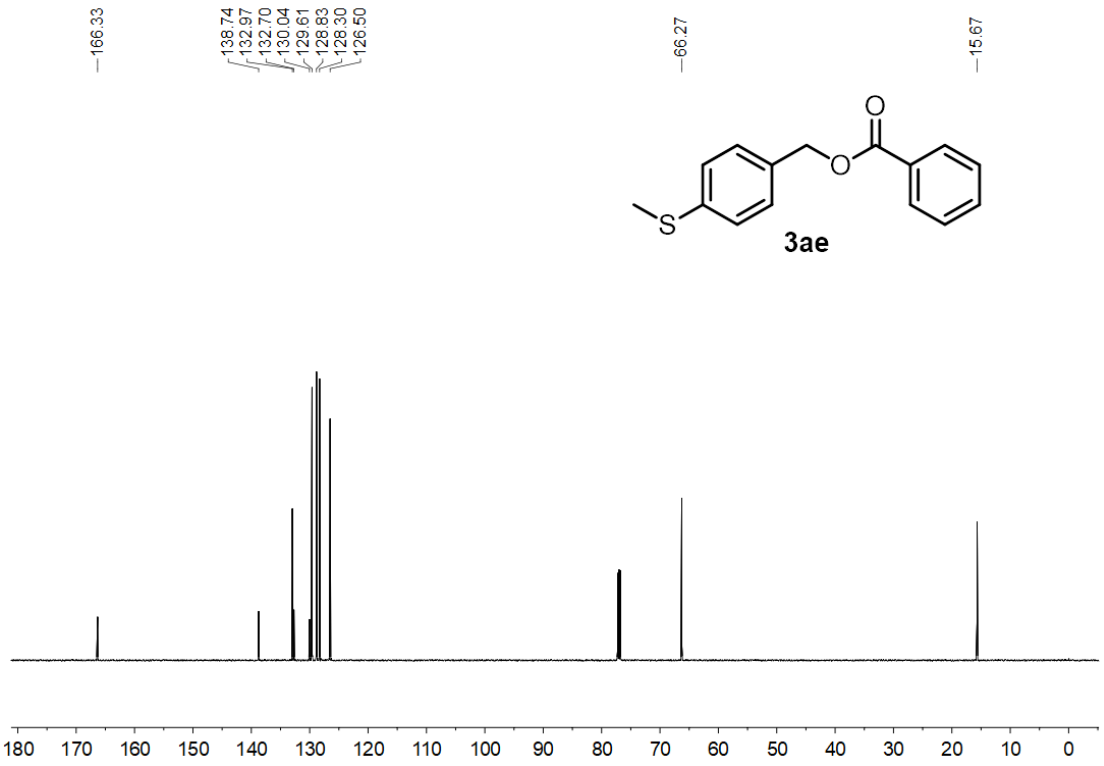

8.093
8.091
8.079
8.077
8.064
8.050
7.579
7.577
7.575
7.565
7.555
7.553
7.551
7.509
7.496
7.457
7.443
7.431
5.409
3.912
2.00
1.98
1.00
1.99
2.05
2.07
3.06
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
3ac

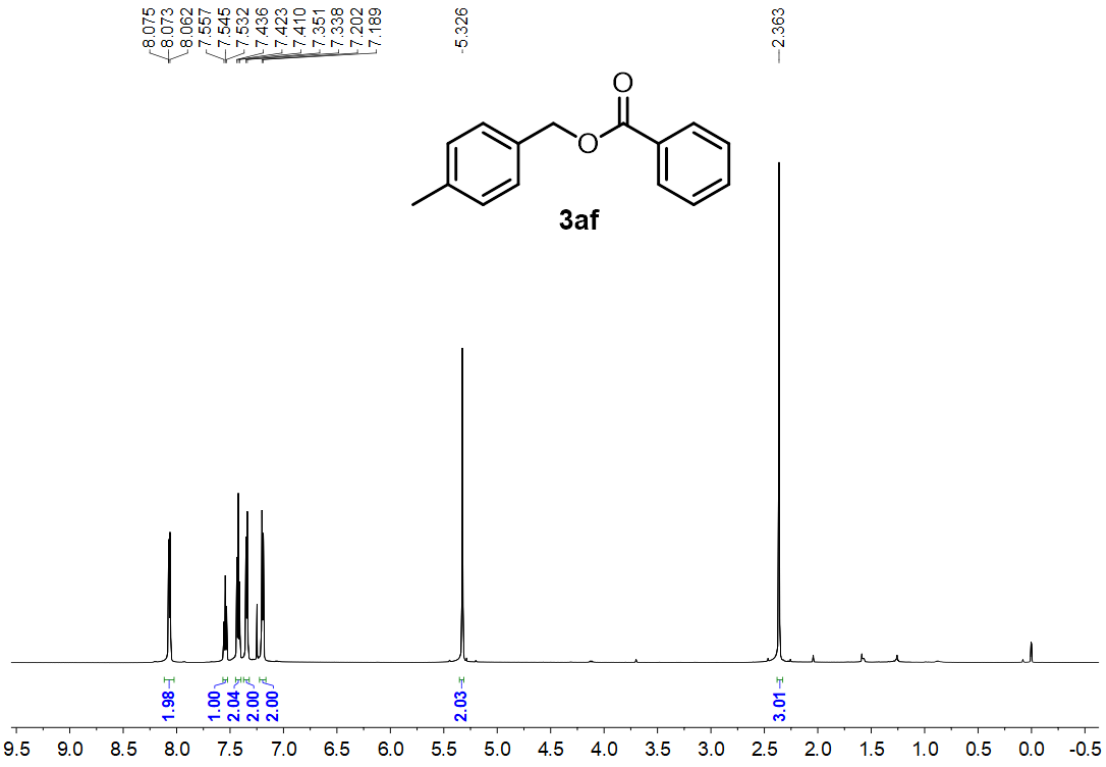

166.63
166.14
141.04
133.14
129.85
129.81
129.74
129.63
128.38
127.54
65.80
52.07
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
3ac

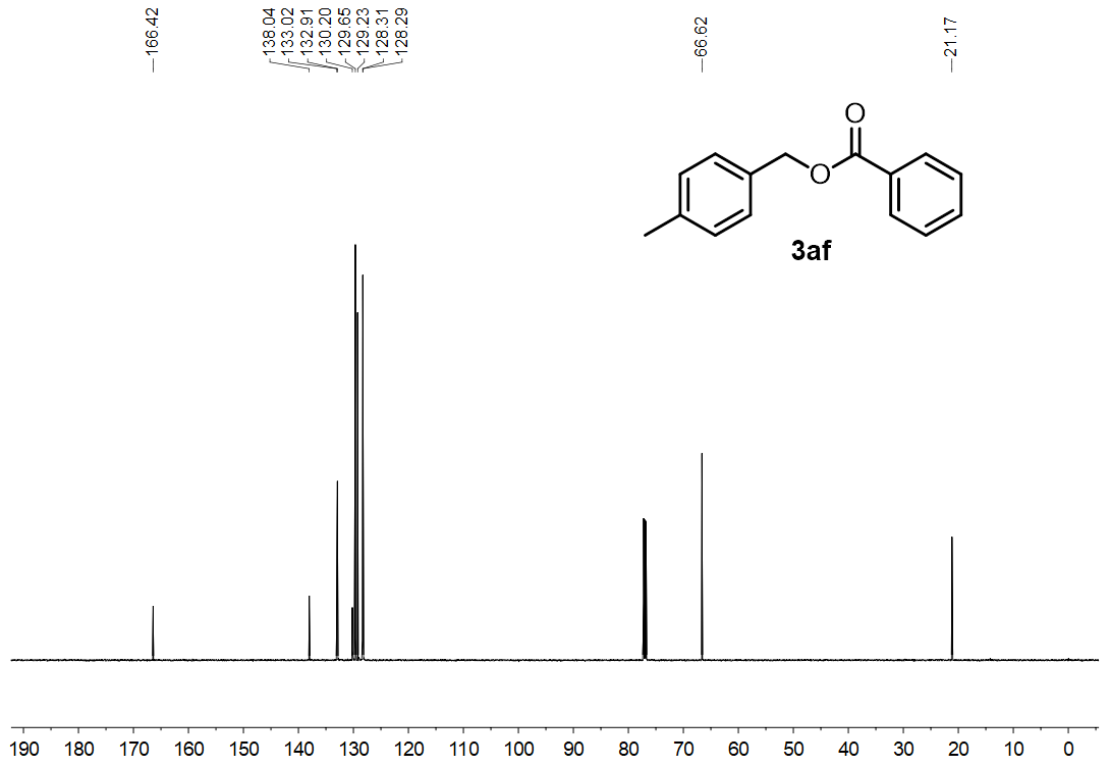

8.059
8.046
7.710
7.561
7.548
7.537
7.523
7.438
7.425
7.412
7.392
7.378
5.306
2.164
3ad
2.00
1.00
3.08
2.10
2.00
2.02
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

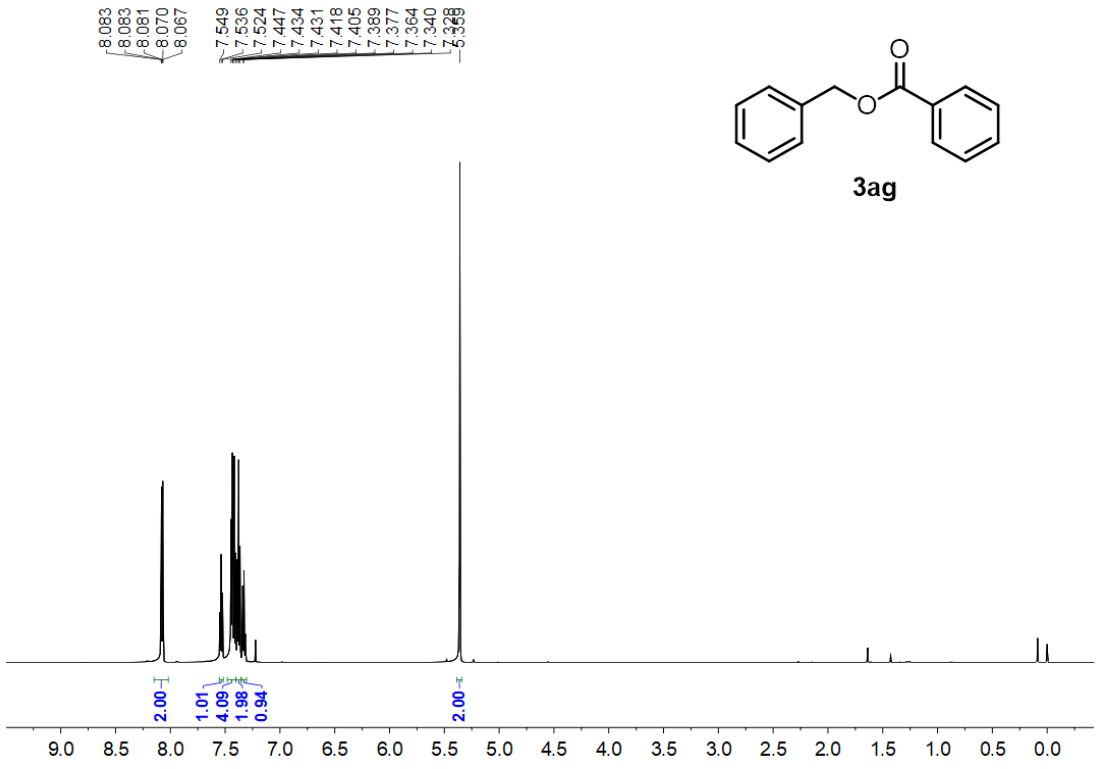

168.56
166.47
137.98
133.03
131.77
130.03
129.62
129.06
128.35
119.92
66.30
24.49
3ad
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

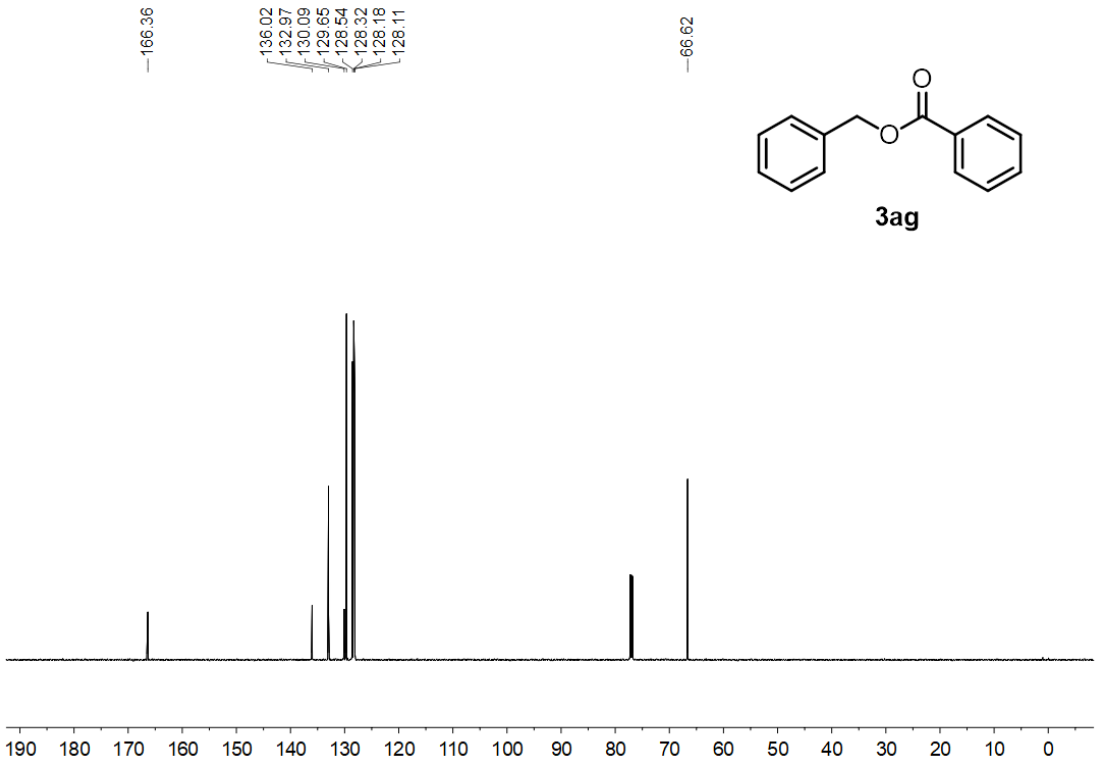

8.065
8.063
8.051
8.049
7.552
7.539
7.527
7.431
7.418
7.405
7.371
7.357
7.264
7.250
5.307
2.469
O
O
S
3ae
1.96
1.00
2.03
2.00
2.05
2.05
3.09
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

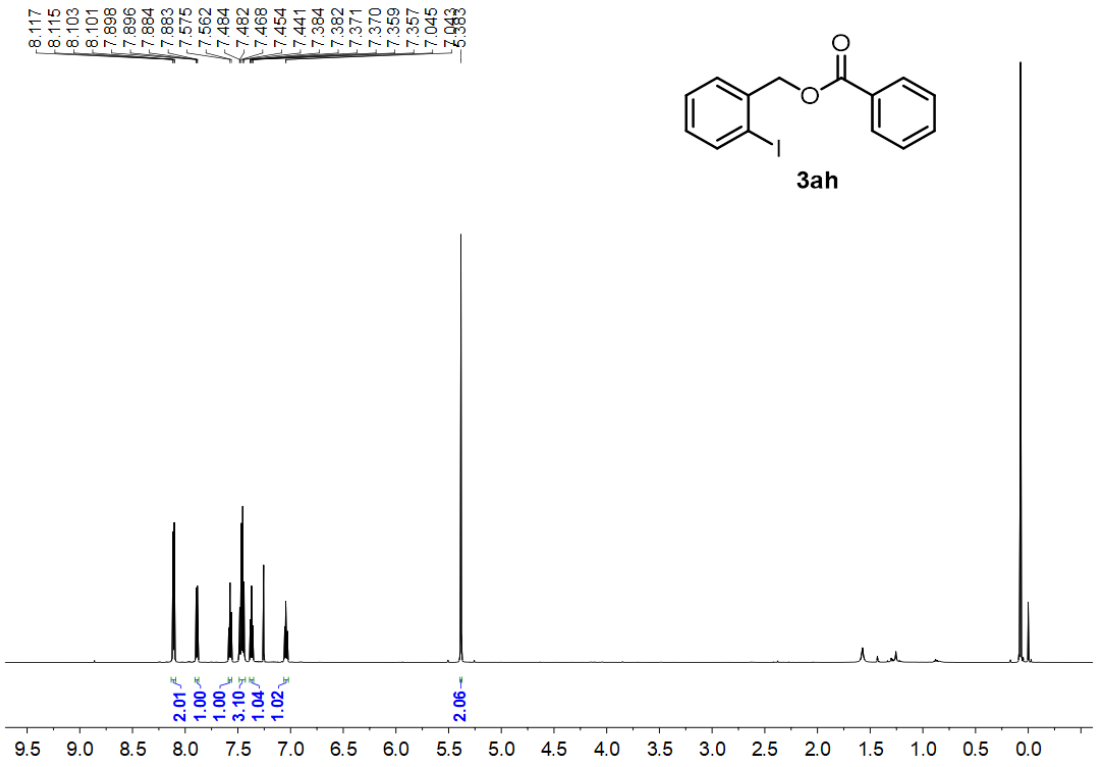

166.33
138.74
132.97
132.70
130.04
129.61
128.83
128.30
126.50
66.27
15.67
O
O
S
3ae
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

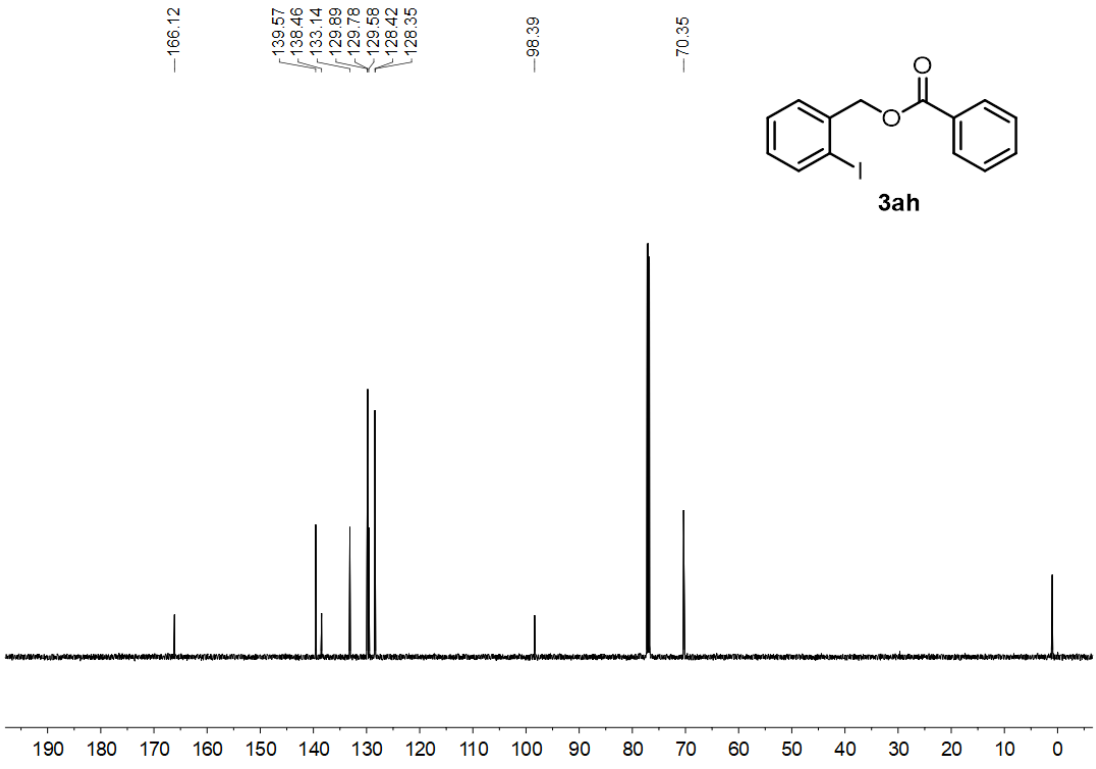

8.075
8.073
8.062
7.557
7.545
7.532
7.436
7.423
7.410
7.351
7.338
7.202
7.189
5.326
2.363
O
O
3af
1.98
1.00
2.04
2.00
2.00
2.03
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

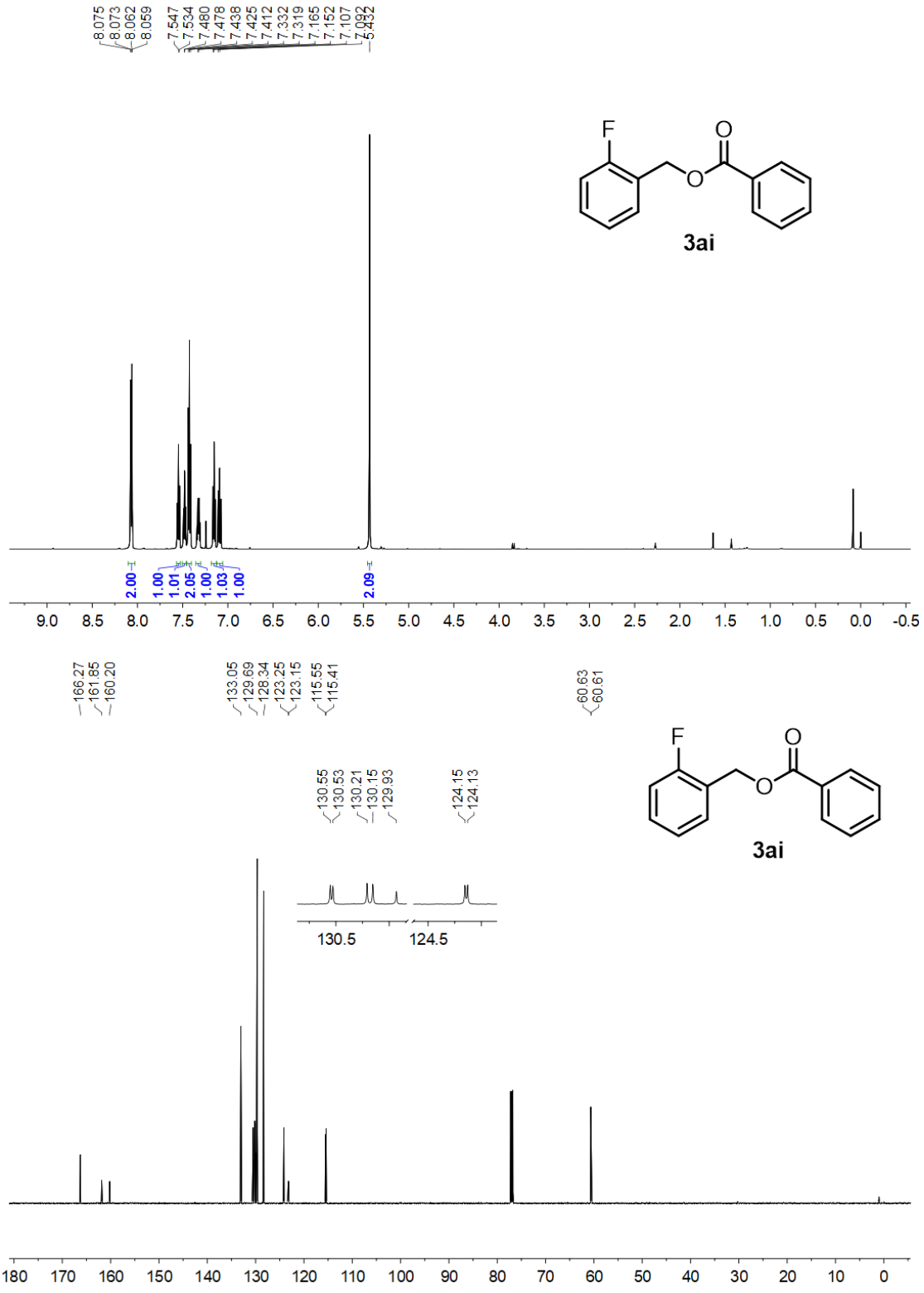

166.42
138.04
133.02
132.91
130.20
129.65
129.23
128.31
128.29
66.62
21.17
O
O
3af
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

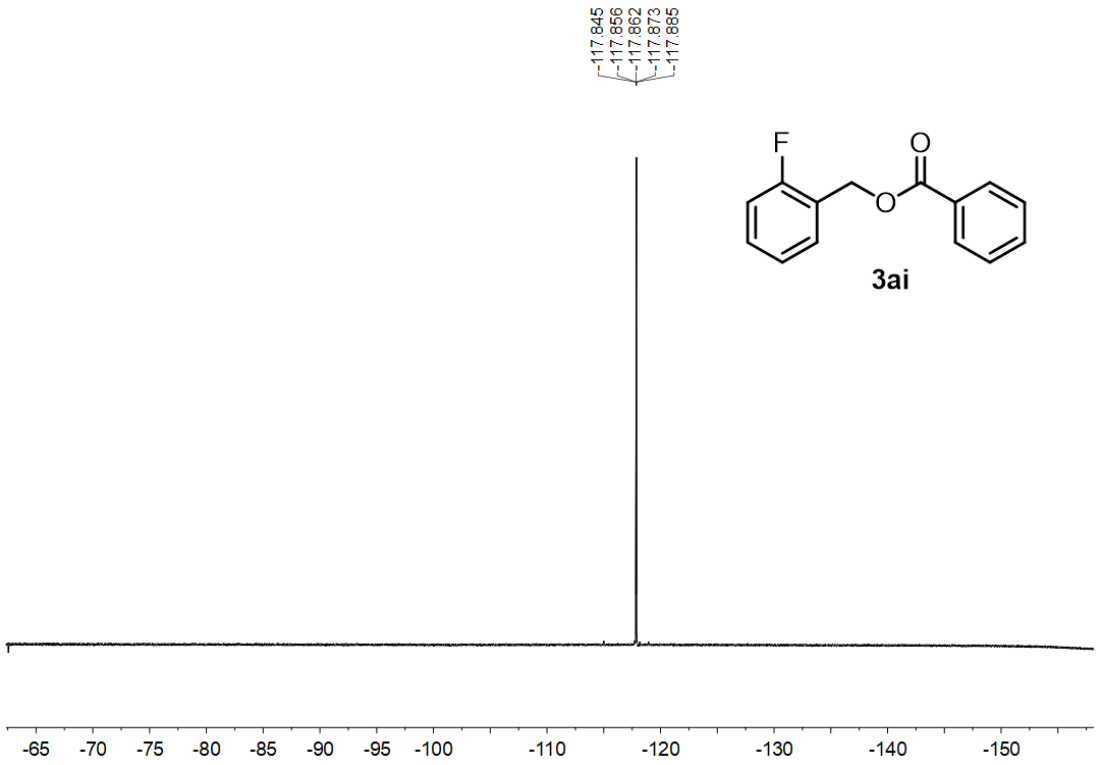

8.083
8.083
8.081
8.070
8.067
7.549
7.536
7.524
7.447
7.434
7.431
7.418
7.405
7.389
7.377
7.364
7.340
5.359
2.00
1.01
4.09
1.98
0.94
2.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
3ag

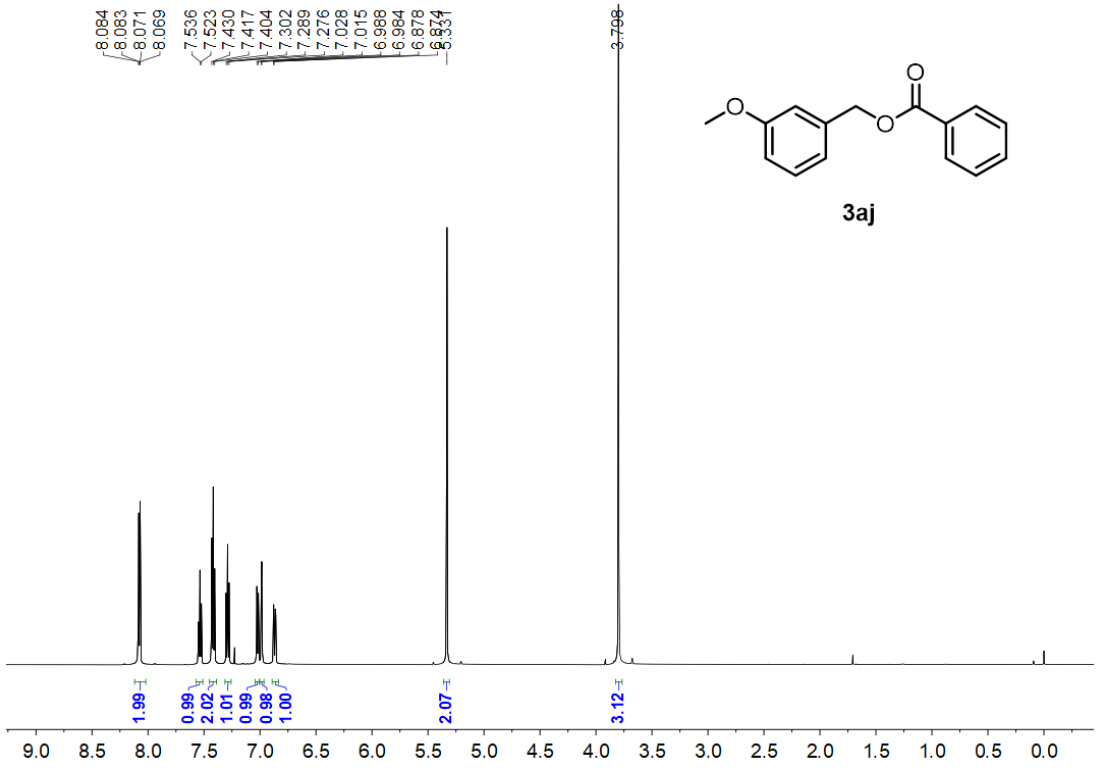

166.36
136.02
132.97
130.09
129.65
128.54
128.32
128.18
128.11
66.62
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
3ag

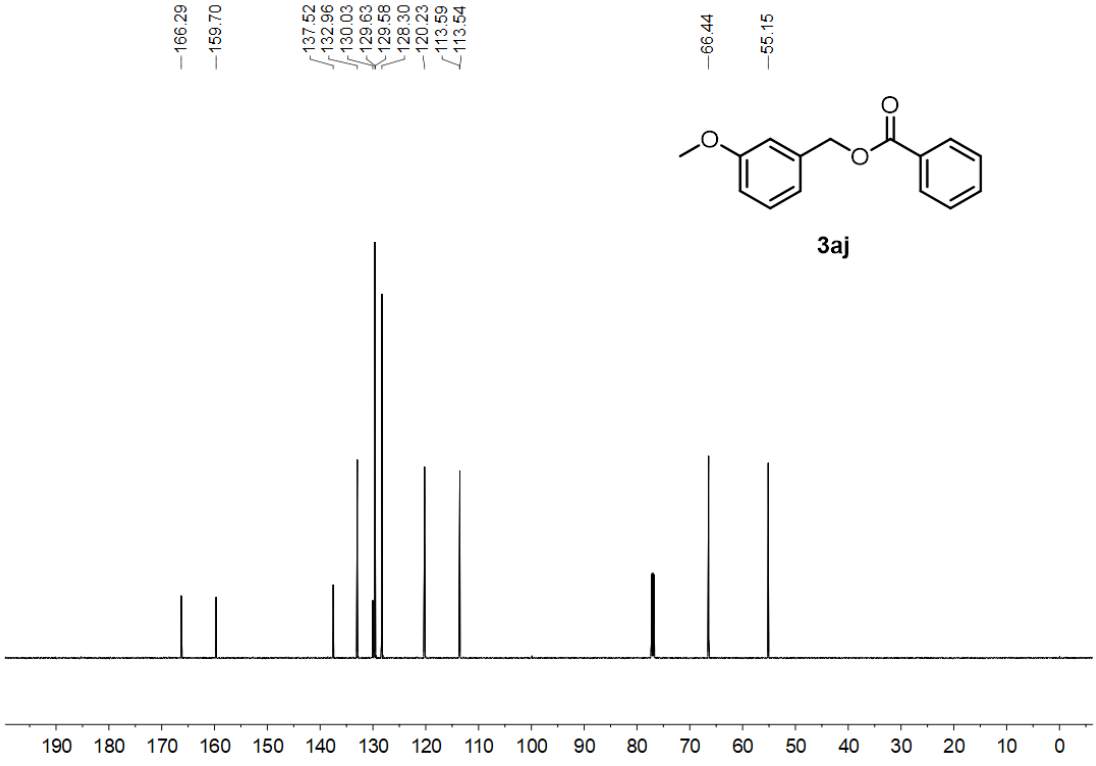

8.117
8.115
8.103
8.101
7.898
7.896
7.884
7.883
7.575
7.562
7.484
7.482
7.468
7.454
7.441
7.384
7.382
7.371
7.370
7.359
7.357
7.045
7.043
5.383
3ah
2.01
1.00
1.00
3.10
1.04
1.02
2.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

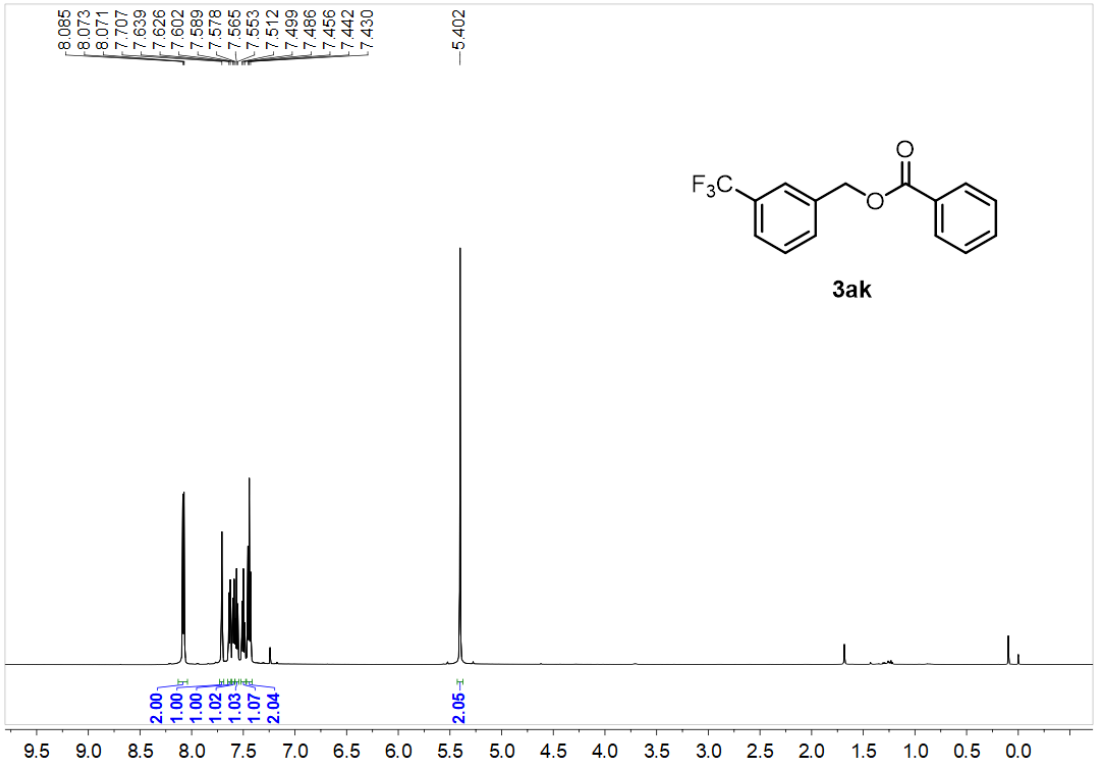

166.12
139.57
138.46
133.14
129.89
129.78
129.58
128.42
128.35
98.39
70.35
3ah
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

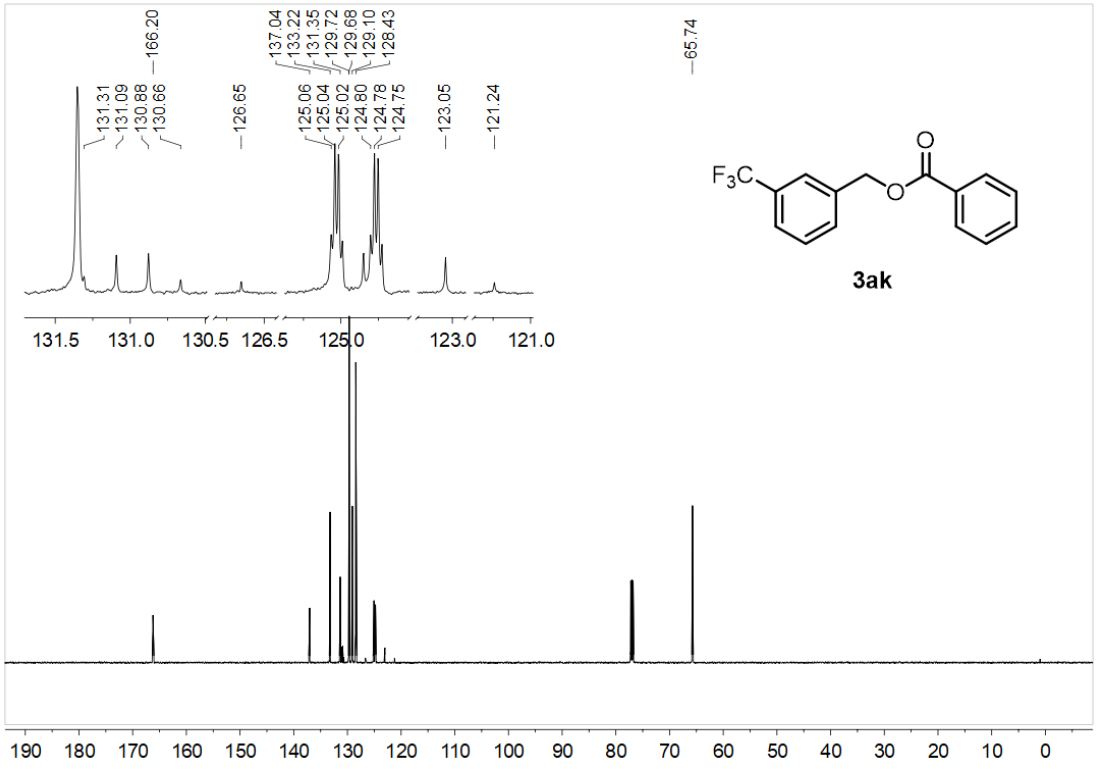

8.075
8.073
8.062
8.059
7.547
7.534
7.480
7.478
7.438
7.425
7.412
7.332
7.319
7.165
7.152
7.107
5.432
F
O
O
3ai
2.00
1.00
1.01
2.05
1.00
1.03
1.00
2.09
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
166.27
161.85
160.20
133.05
129.69
128.34
123.25
123.15
115.55
115.41
60.63
60.61
130.55
130.53
130.21
130.15
129.93
124.15
124.13
F
O
O
3ai
130.5
124.5
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

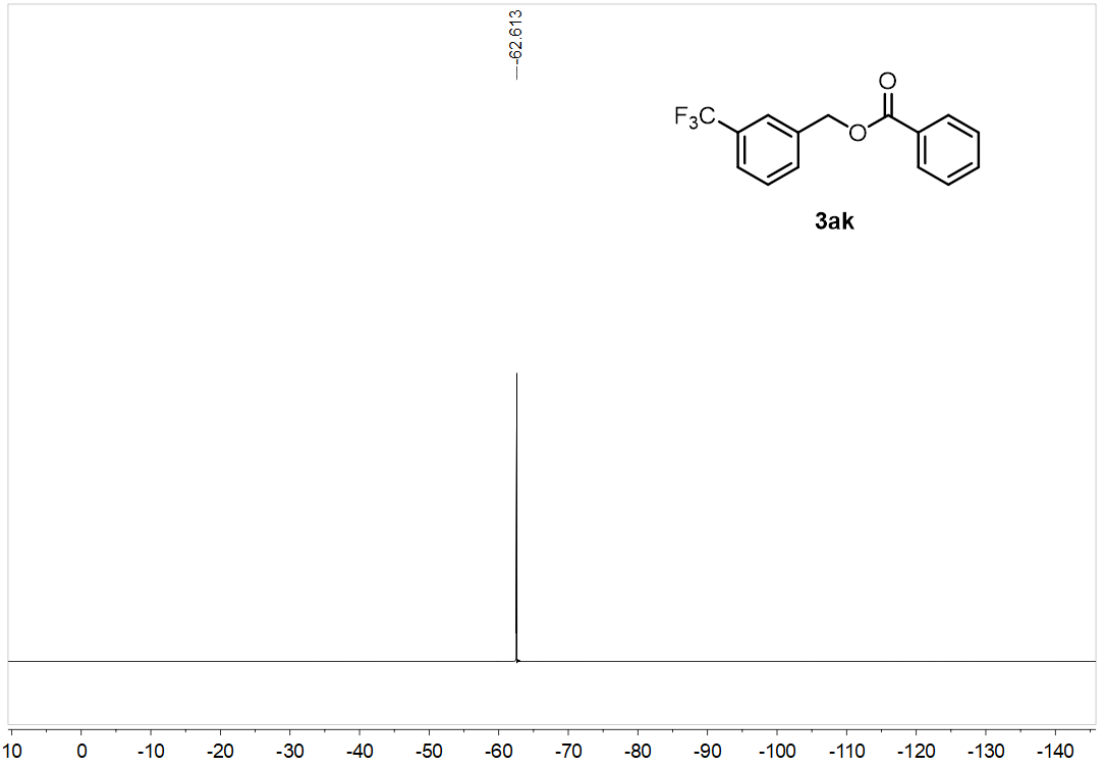

-117.845
-117.856
-117.862
-117.873
-117.885
F
O
O
3ai
-65
-70
-75
-80
-85
-90
-95
-100
-110
-120
-130
-140
-150

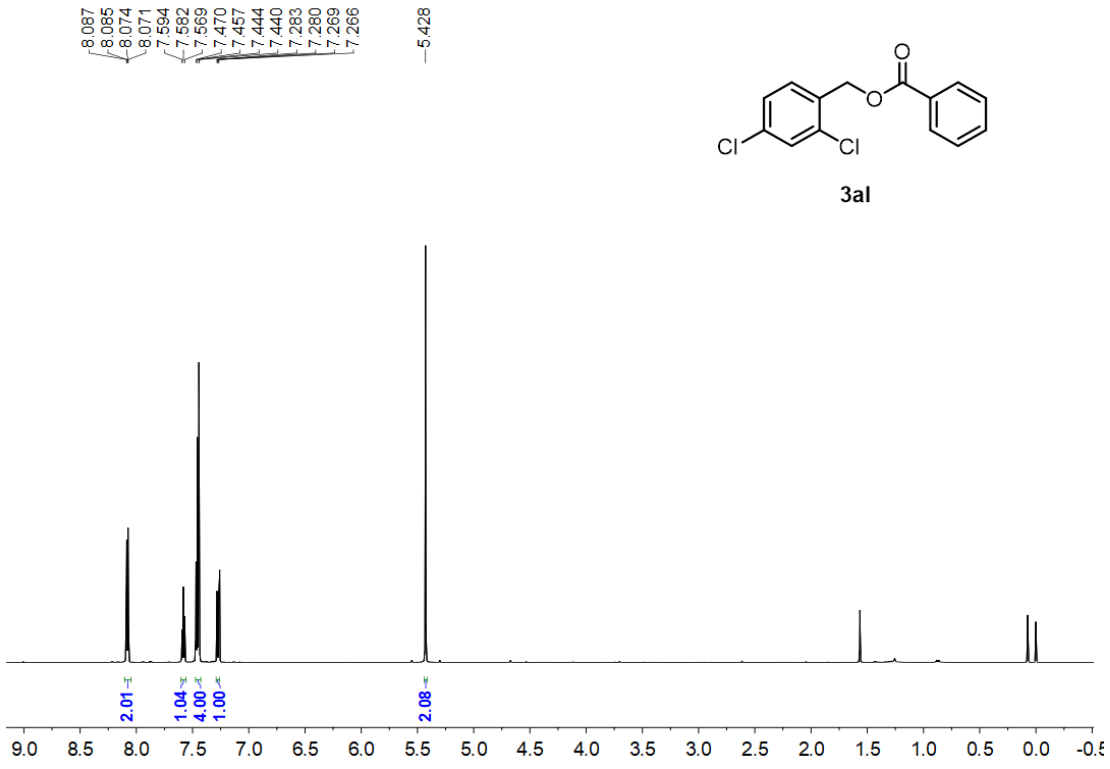

8.084
8.083
8.071
8.069
7.536
7.523
7.430
7.417
7.404
7.302
7.289
7.276
7.028
7.015
6.988
6.984
6.878
6.874
5.331
3.798
O
O
O
3aj
1.99
0.99
2.02
1.01
0.99
0.98
1.00
2.07
3.12
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

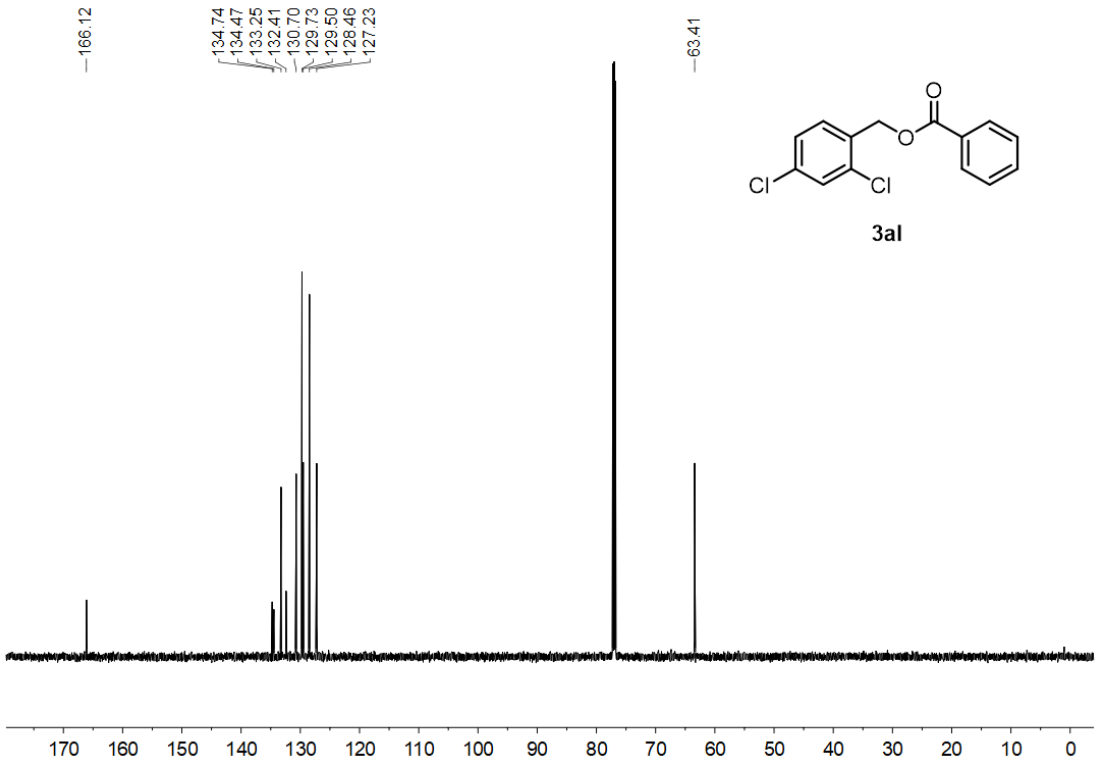

166.29
159.70
137.52
132.96
130.03
129.63
129.58
128.30
120.23
113.59
113.54
66.44
55.15
O
O
O
3aj
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

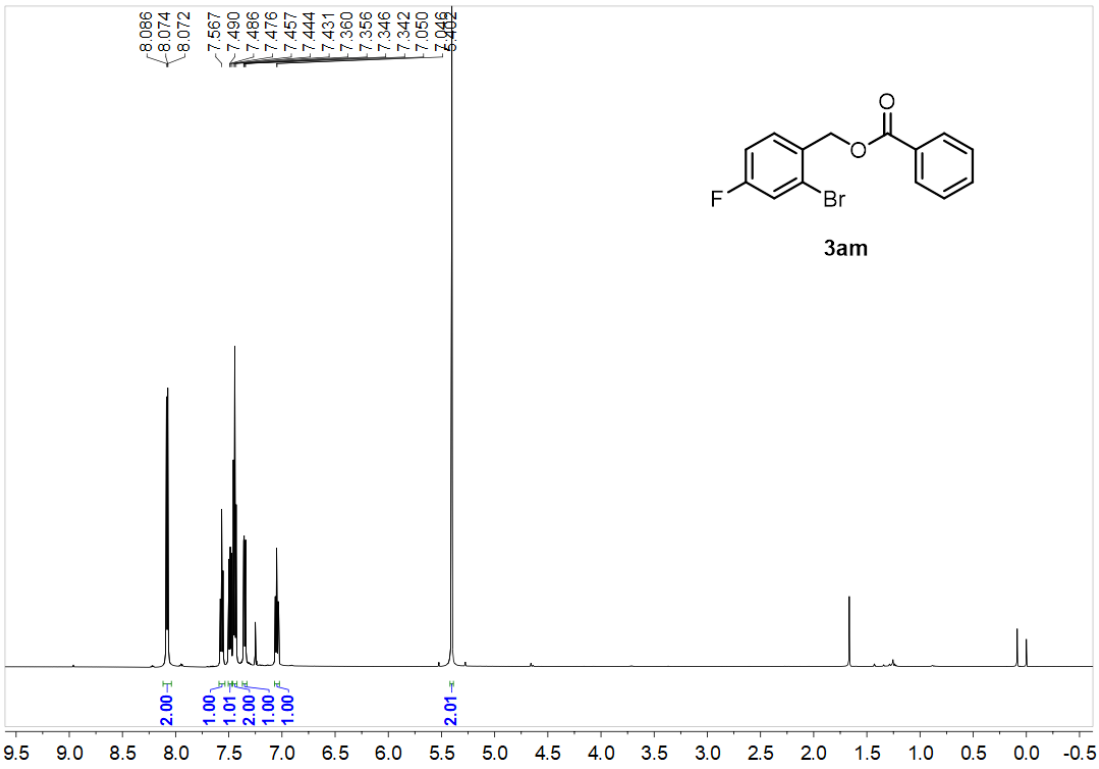

8.085
8.073
8.071
7.707
7.639
7.626
7.602
7.589
7.578
7.565
7.553
7.512
7.499
7.486
7.456
7.442
7.430
5.402
F3C
O
O
3ak
2.00
1.00
1.00
1.02
1.03
1.07
2.04
2.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

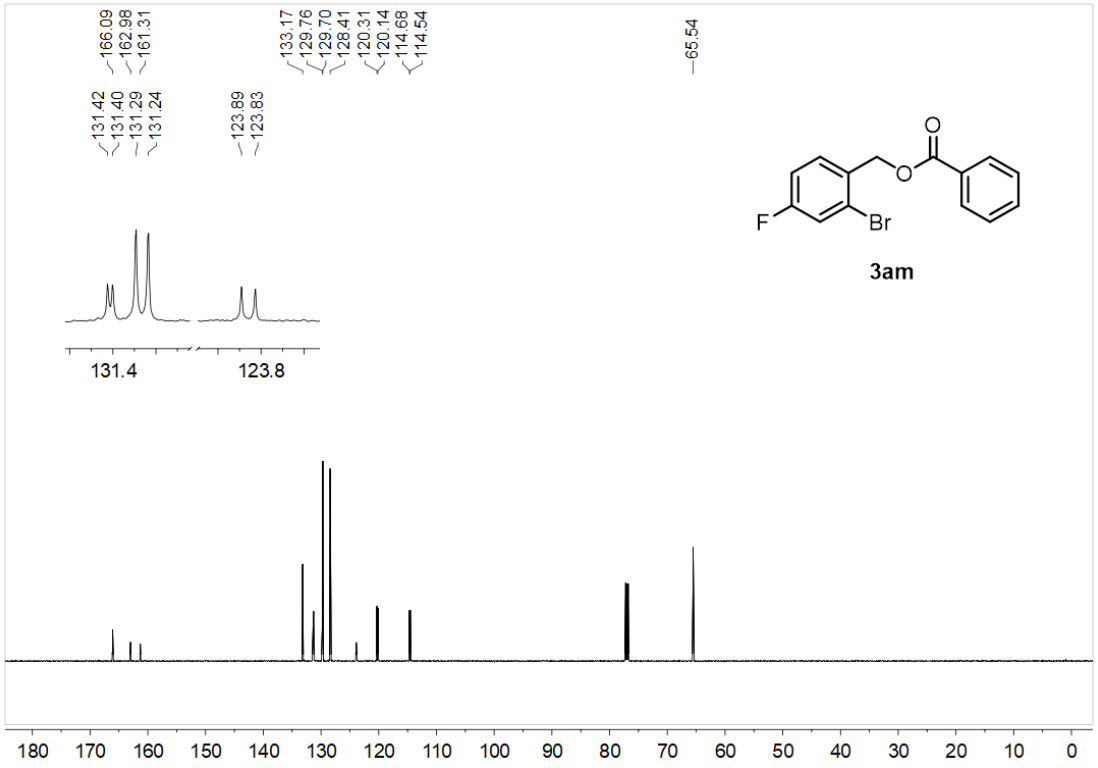

166.20
137.04
133.22
131.35
129.72
129.68
129.10
128.43
131.31
131.09
130.88
130.66
126.65
125.06
125.04
125.02
124.80
124.78
124.75
123.05
121.24
65.74
F3C
O
O
3ak
131.5
131.0
130.5
126.5
125.0
123.0
121.0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

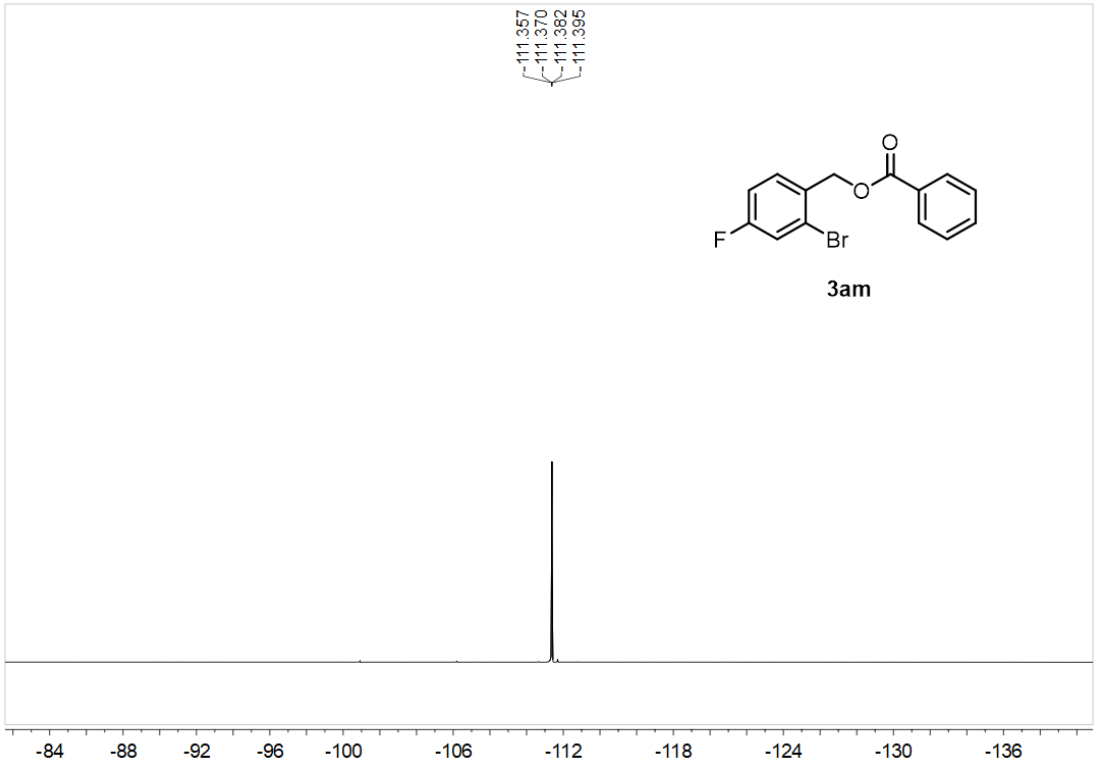

62.613
F3C
O
O
3ak
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140

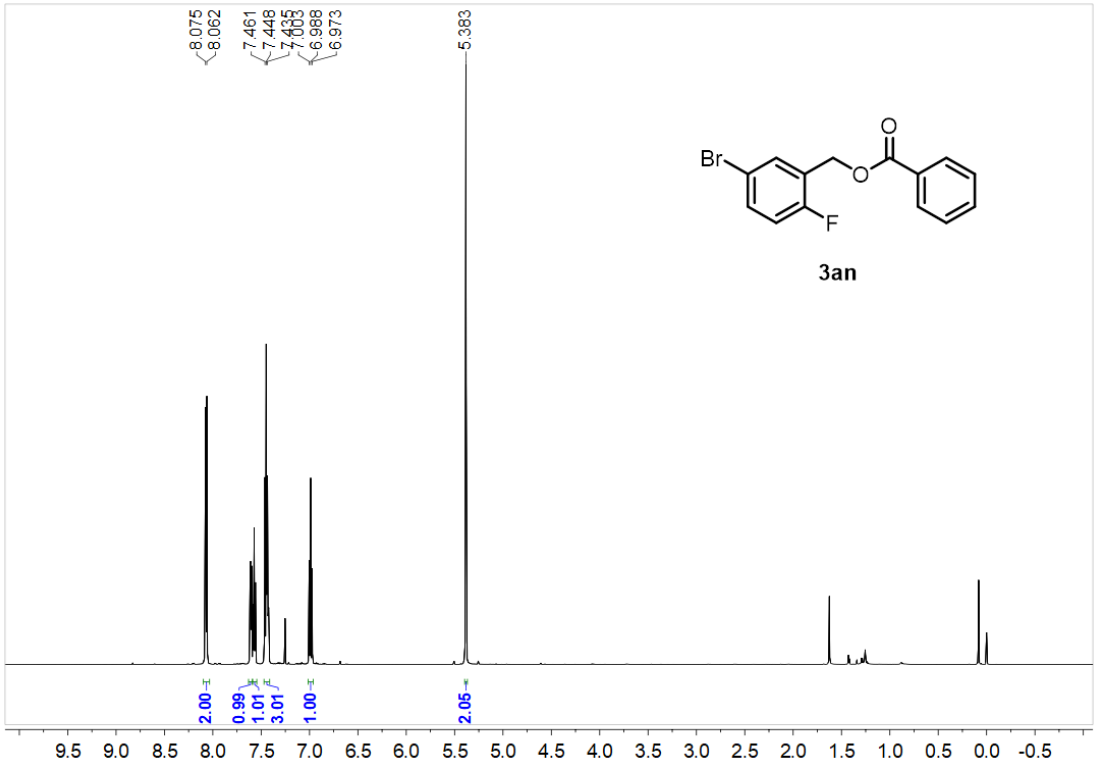

8.087
8.085
8.074
8.071
7.594
7.582
7.569
7.470
7.457
7.444
7.440
7.283
7.280
7.269
7.266
5.428
Cl
Cl
O
O
3al
2.01
1.04
4.00
1.00
2.08
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

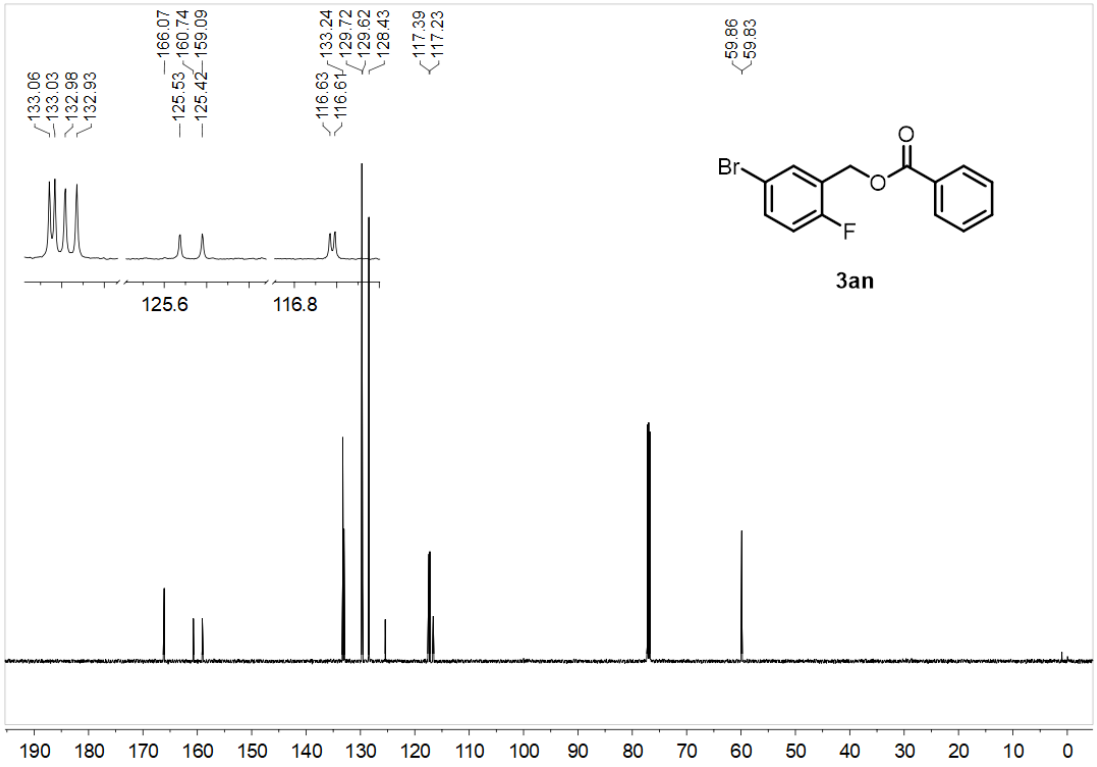

166.12
134.74
134.47
133.25
132.41
130.70
129.73
129.50
128.46
127.23
63.41
Cl
Cl
O
O
3al
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

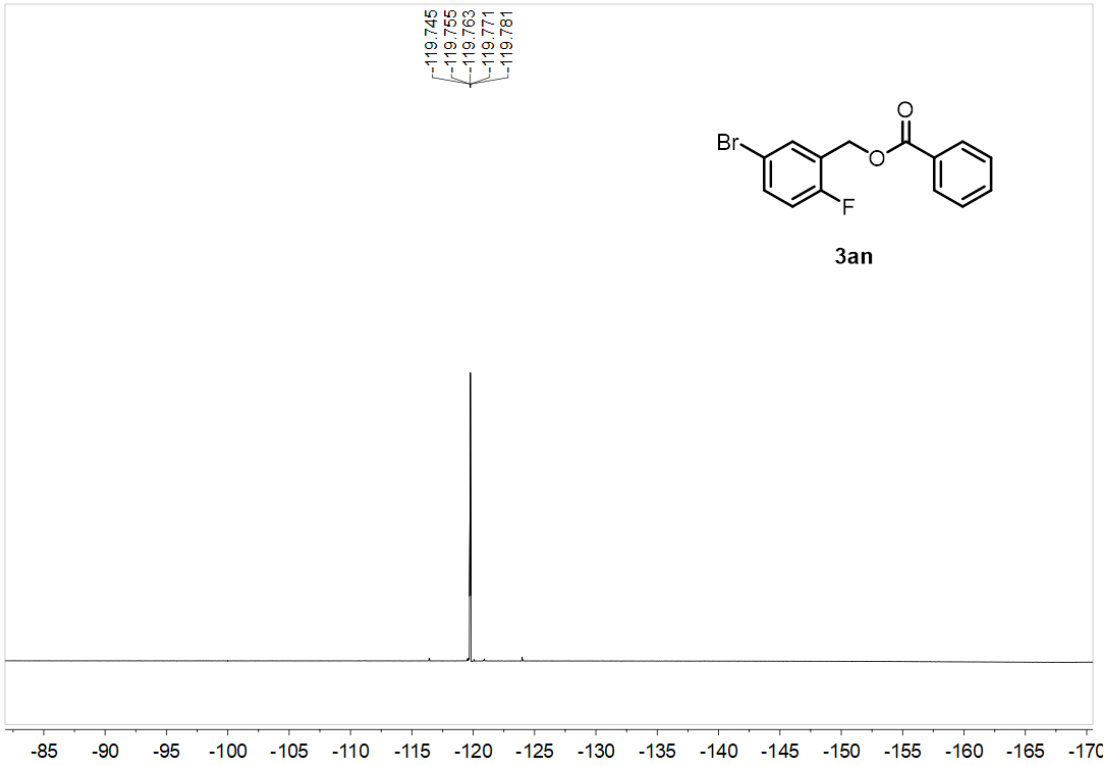

8.086
8.074
8.072
7.567
7.490
7.486
7.476
7.457
7.444
7.431
7.360
7.356
7.346
7.342
7.050
7.046
5.402
2.00
1.00
1.01
2.00
1.00
1.00
2.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
O
O
F
Br
3am

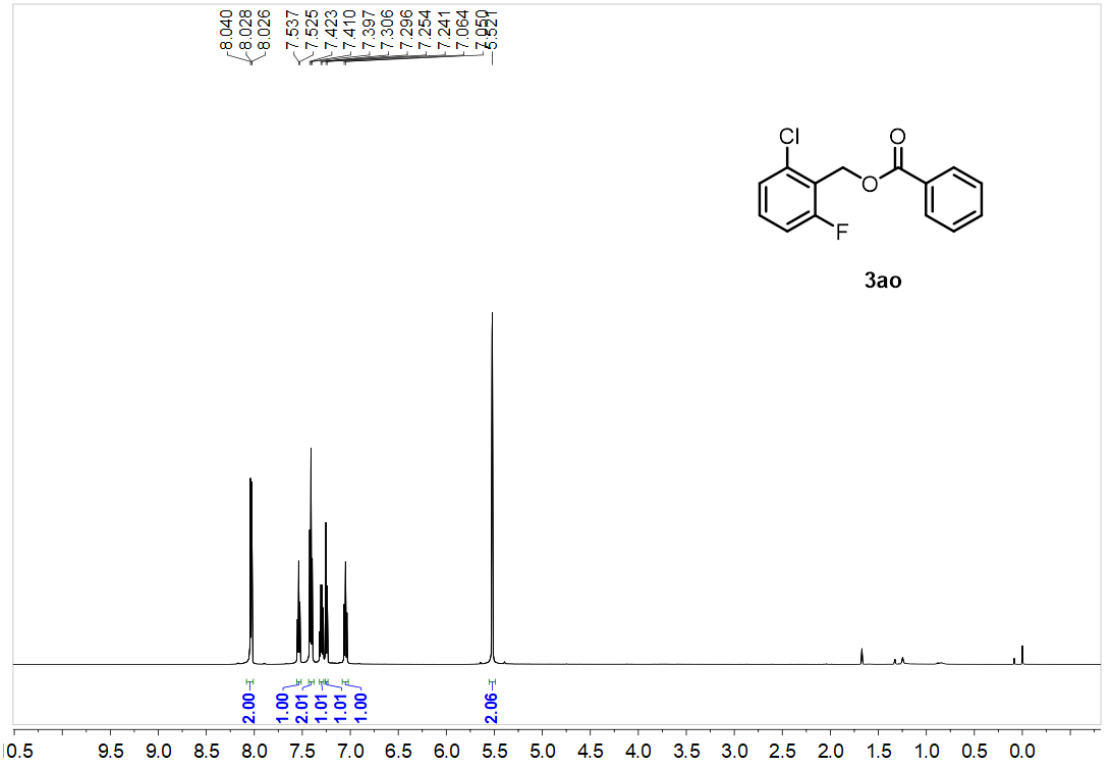

166.09
162.98
161.31
131.42
131.40
131.29
131.24
123.89
123.83
133.17
129.76
129.70
128.41
120.31
120.14
114.68
114.54
65.54
131.4
123.8
O
O
F
Br
3am
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

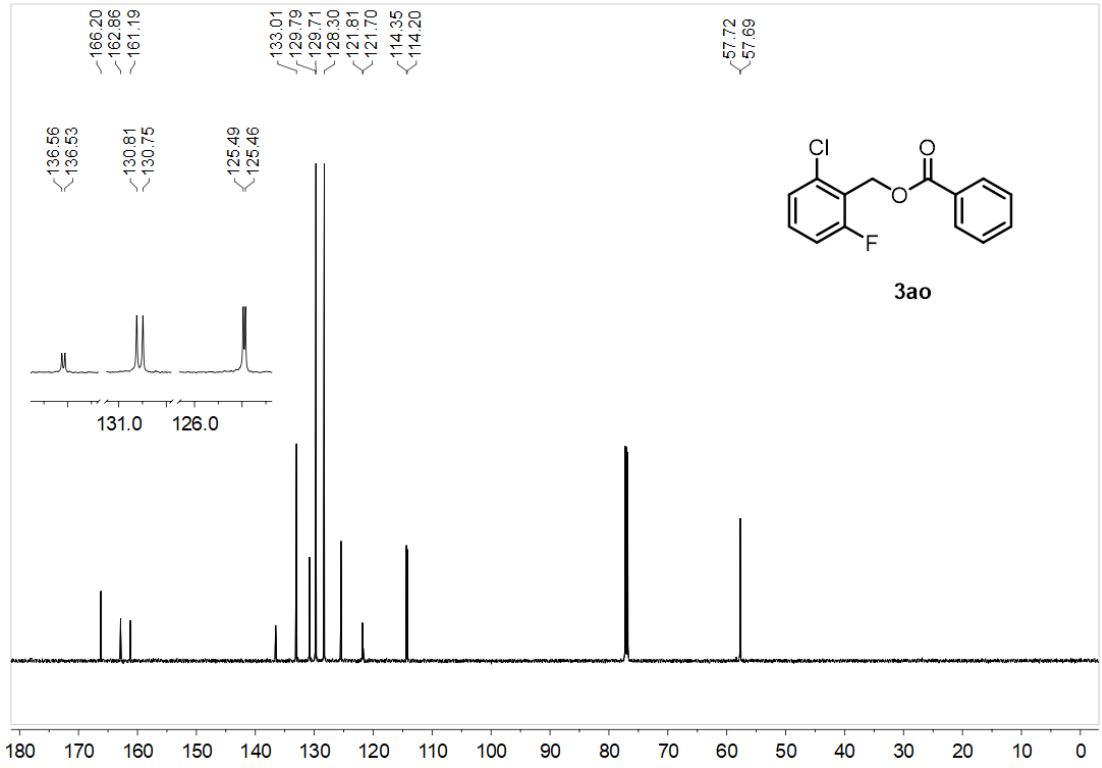

-111.357
-111.370
-111.382
-111.395
F
Br
O
O
3am
-84
-88
-92
-96
-100
-106
-112
-118
-124
-130
-136

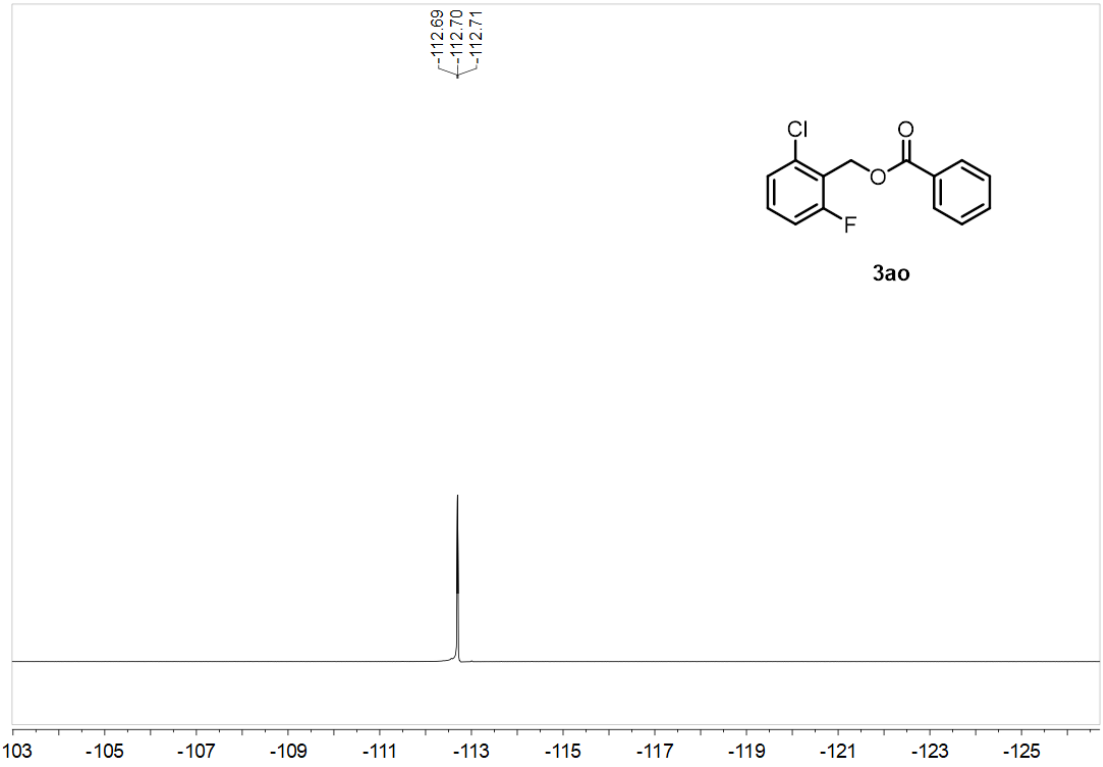

8.075
8.062
7.461
7.448
7.435
7.003
6.988
6.973
5.383
Br
F
O
O
3an
2.00
0.99
1.01
3.01
1.00
2.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

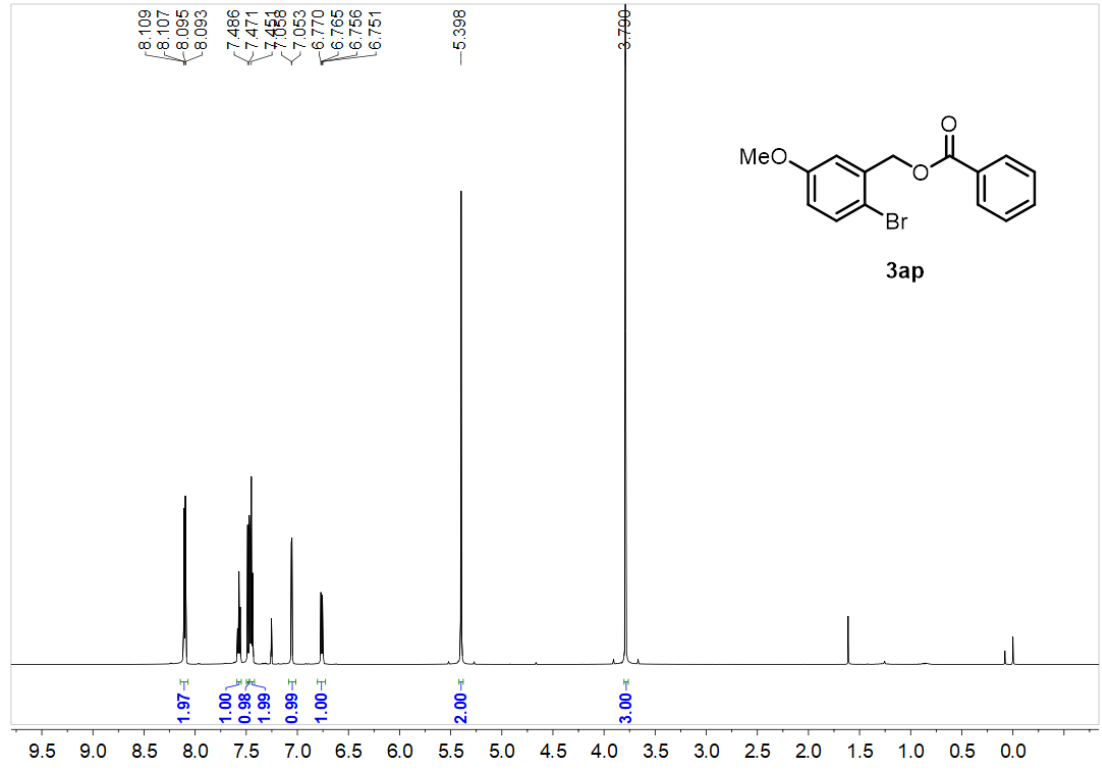

133.06
133.03
132.98
132.93
166.07
160.74
159.09
125.53
125.42
116.63
116.61
133.24
129.72
129.62
128.43
117.39
117.23
59.86
59.83
125.6
116.8
Br
O
O
F
3an
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

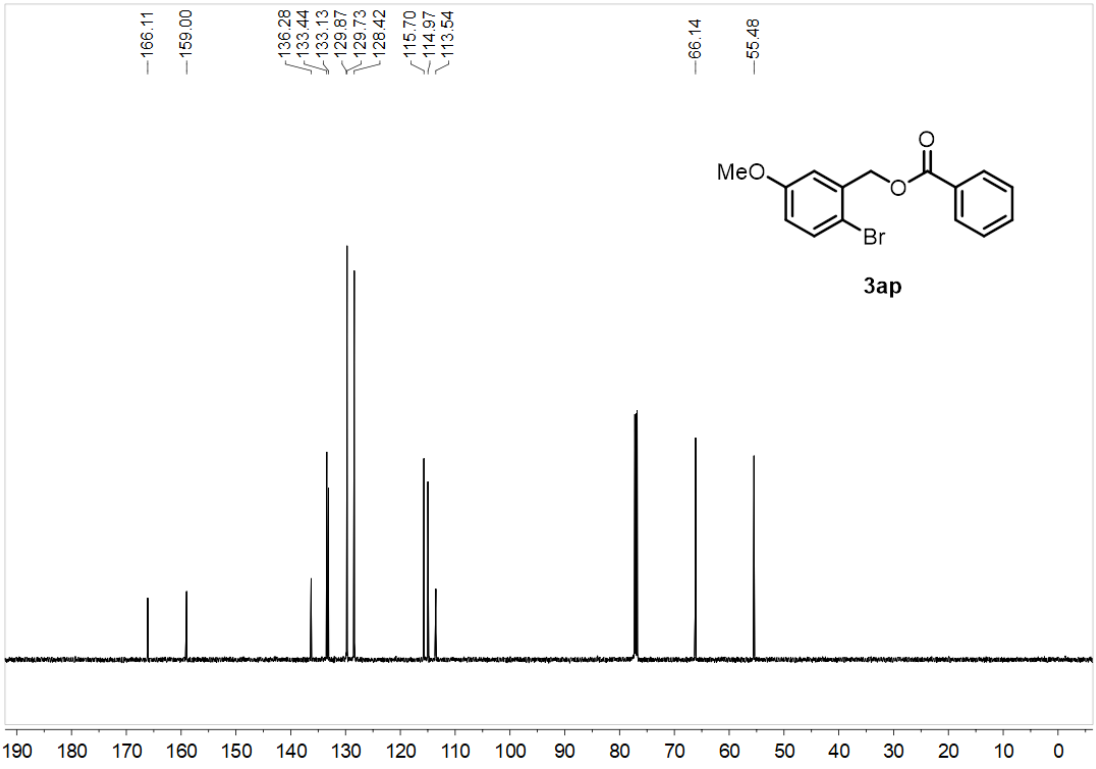

119.745
119.755
119.763
119.771
119.781
Br
O
O
F
3an
-85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150 -155 -160 -165 -170

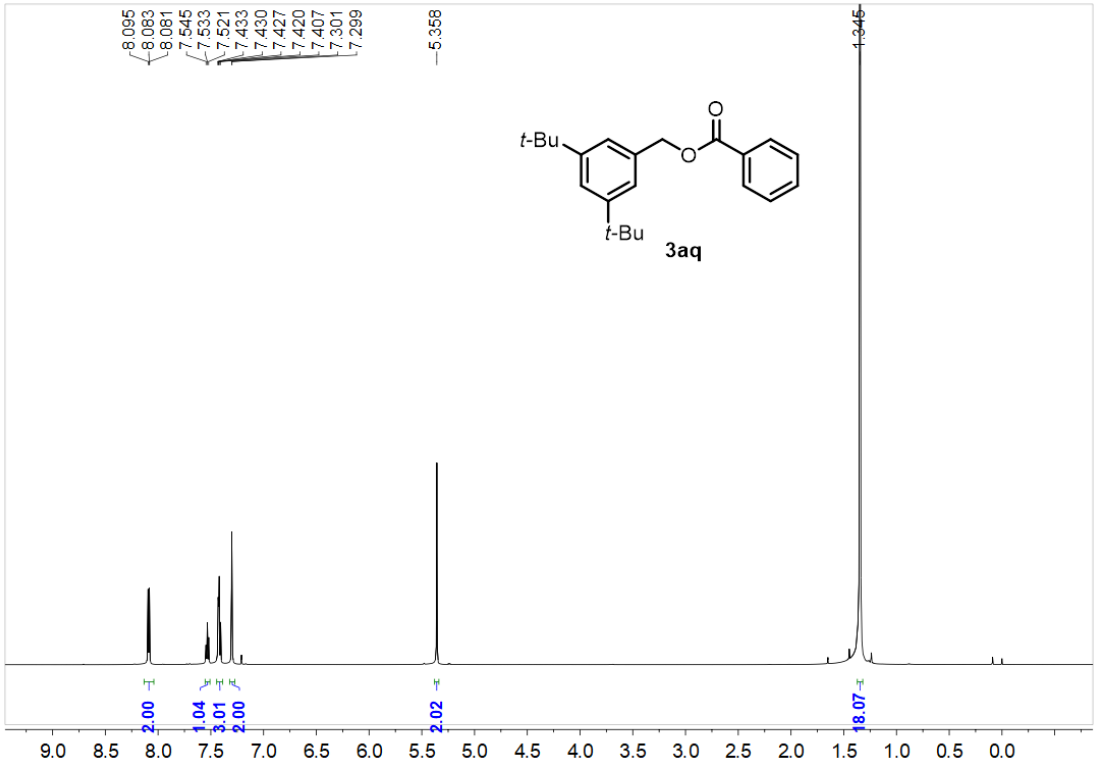

8.040
8.028
8.026
7.537
7.525
7.423
7.410
7.397
7.306
7.296
7.254
7.241
7.064
5.521
Cl
O
O
F
3ao
2.00
1.00
2.01
1.01
1.01
1.00
2.06
0.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

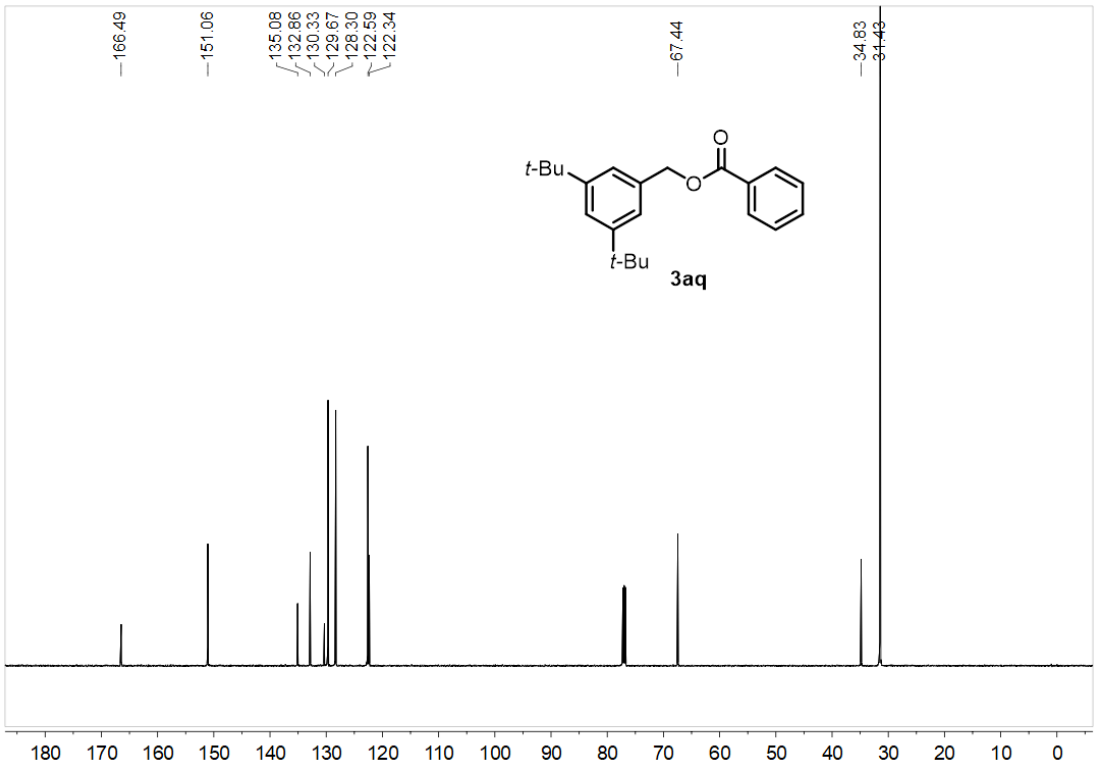

166.20
162.86
161.19
133.01
129.79
129.71
128.30
121.81
121.70
114.35
114.20
57.72
57.69
136.56
136.53
130.81
130.75
125.49
125.46
131.0
126.0
Cl
O
O
F
3ao
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

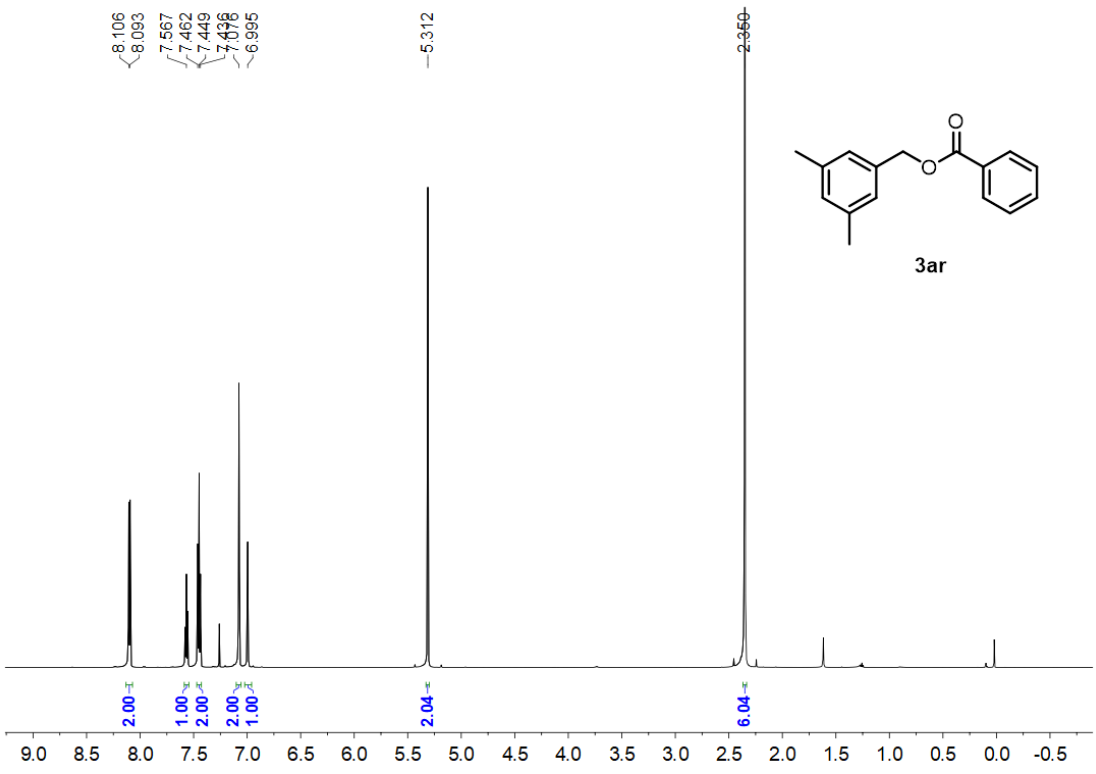

-112.69
-112.70
-112.71
Cl
O
O
F
3ao
103
-105
-107
-109
-111
-113
-115
-117
-119
-121
-123
-125

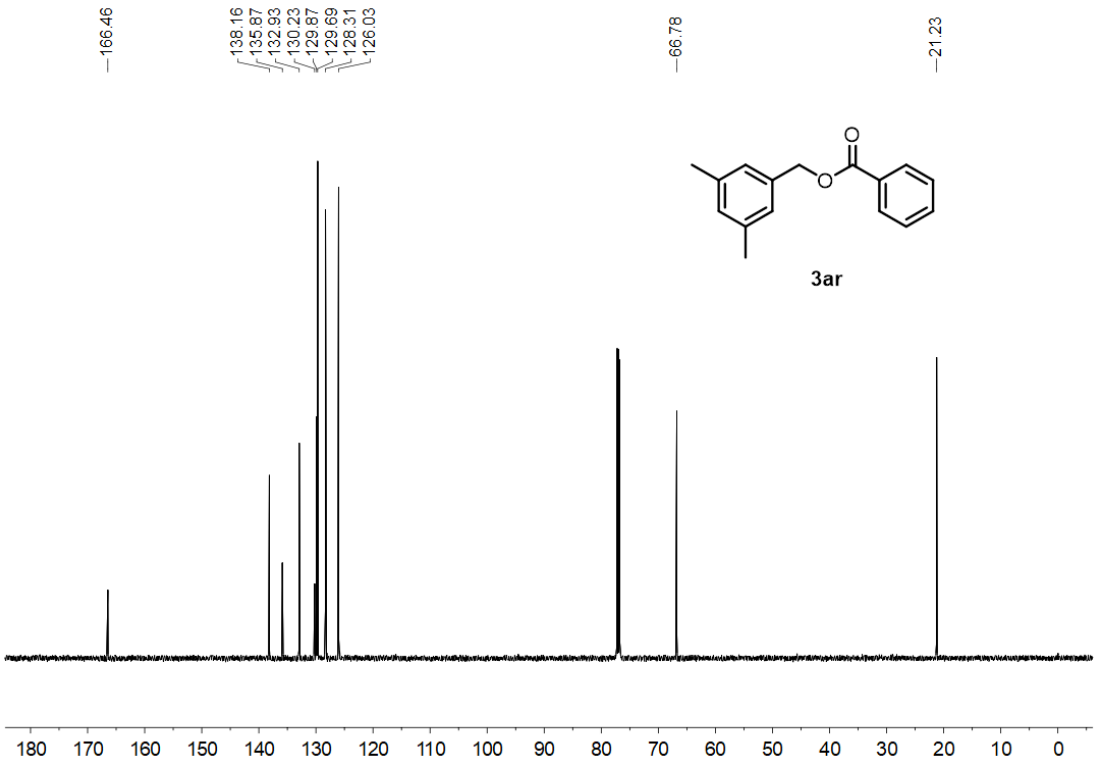

8.109
8.107
8.095
8.093
7.486
7.471
7.454
7.058
7.053
6.770
6.765
6.756
6.751
5.398
3.799
MeO
O
O
Br
3ap
1.97
1.00
0.98
1.99
0.99
1.00
2.00
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

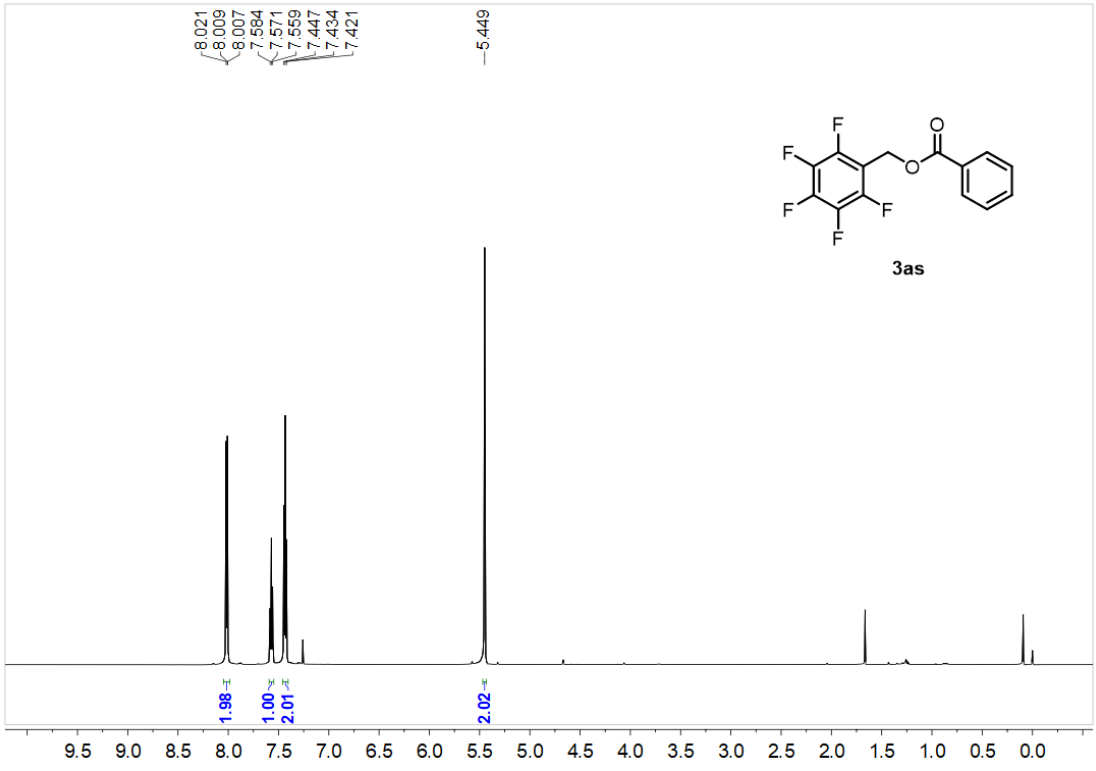

166.11
159.00
136.28
133.44
133.13
129.87
129.73
128.42
115.70
114.97
113.54
66.14
55.48
MeO
O
O
Br
3ap

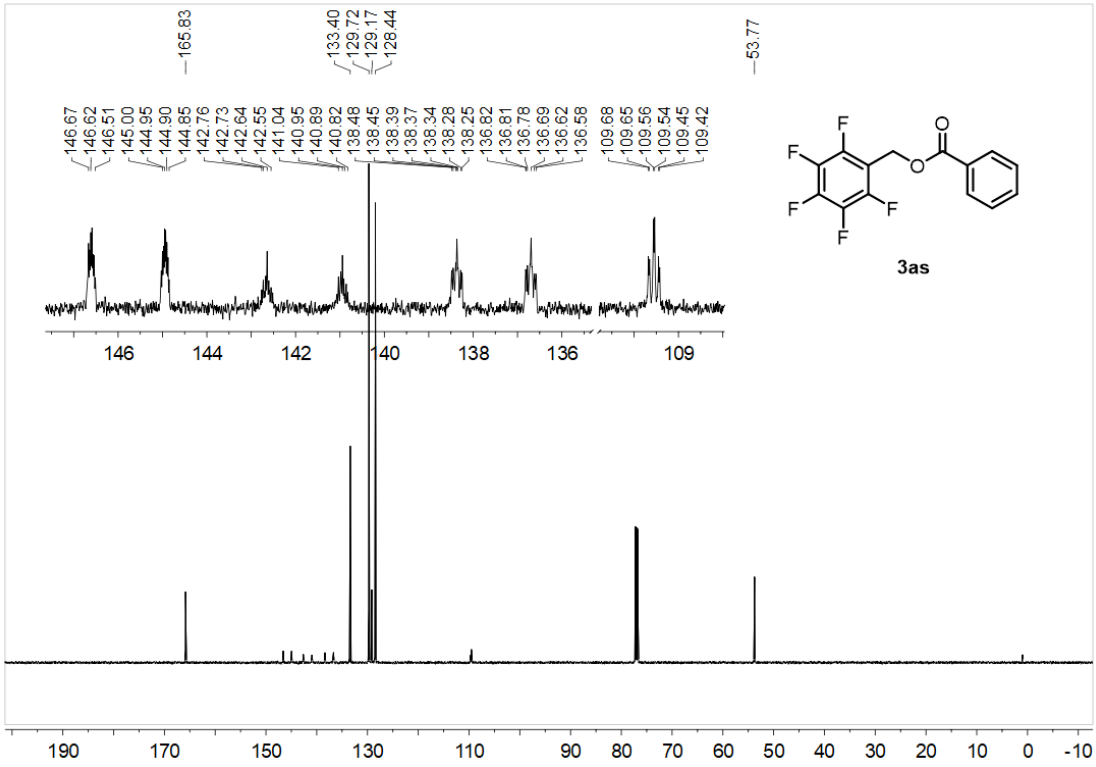

8.095
8.083
8.081
7.545
7.533
7.521
7.433
7.430
7.427
7.420
7.407
7.301
7.299
5.358
1.345
t-Bu
t-Bu
O
O
3aq
2.00
1.04
3.01
2.00
2.02
18.07

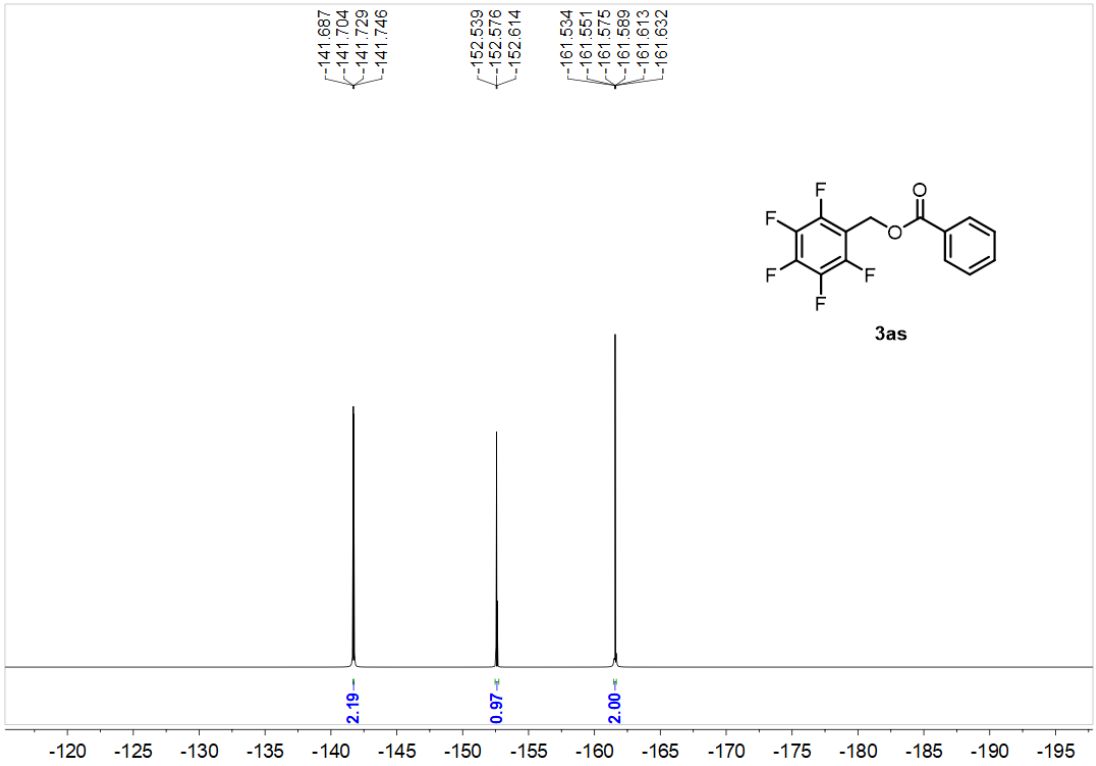

166.49
151.06
135.08
132.86
130.33
129.67
128.30
122.59
122.34
67.44
34.83
31.43
t-Bu
t-Bu
3aq
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

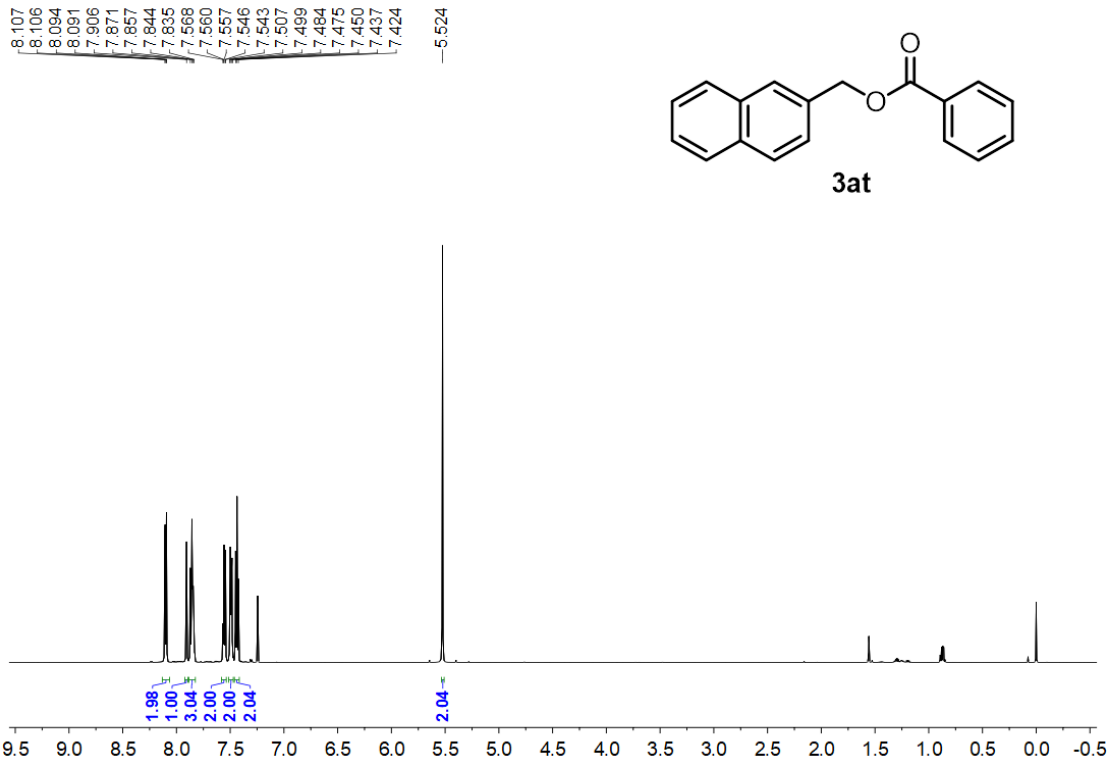

8.106
8.093
7.567
7.462
7.449
7.436
7.078
6.995
5.312
2.350
3ar
2.00
1.00
2.00
2.00
1.00
2.04
6.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


166.46
138.16
135.87
132.93
130.23
129.87
129.69
128.31
126.03
66.78
21.23
3ar
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

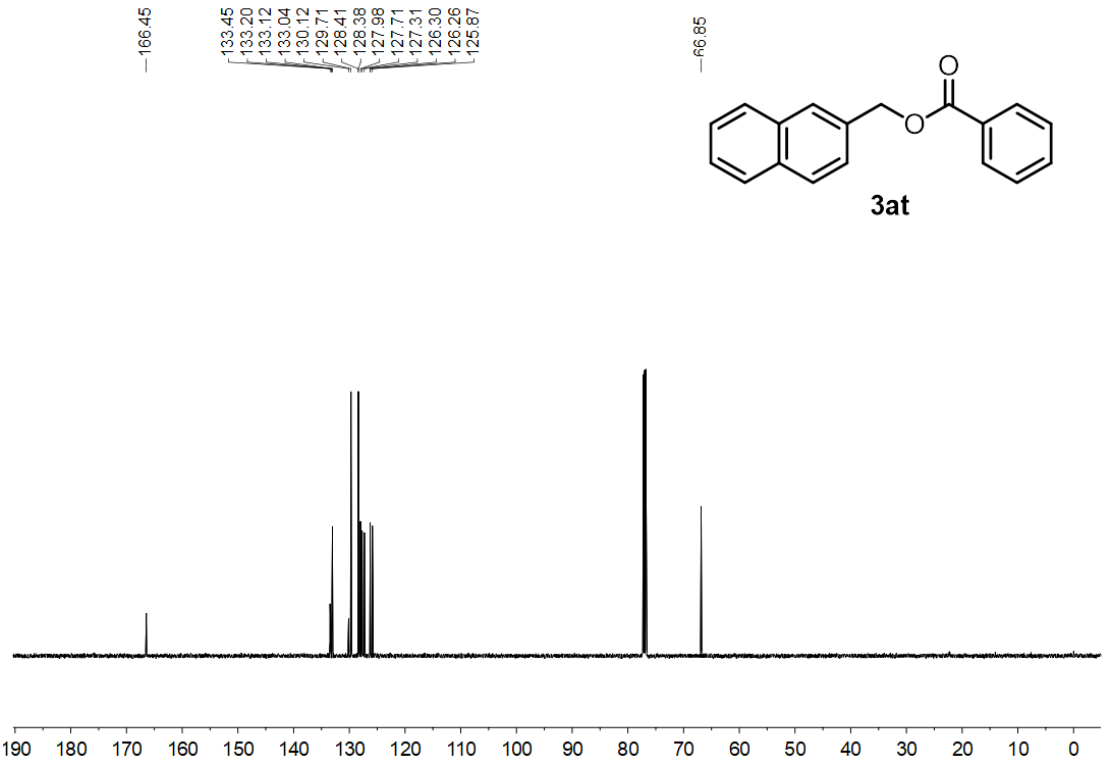

8.021
8.009
8.007
7.584
7.571
7.559
7.447
7.434
7.421
5.449
3as
1.98
1.00
2.01
2.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


165.83
133.40
129.72
129.17
128.44
53.77
146.67
146.62
146.51
145.00
144.95
144.90
144.85
142.76
142.73
142.64
142.55
141.04
140.95
140.89
140.82
138.48
138.45
138.39
138.37
138.34
138.28
138.25
136.82
136.81
136.78
136.69
136.62
136.58
109.68
109.65
109.56
109.54
109.45
109.42
3as

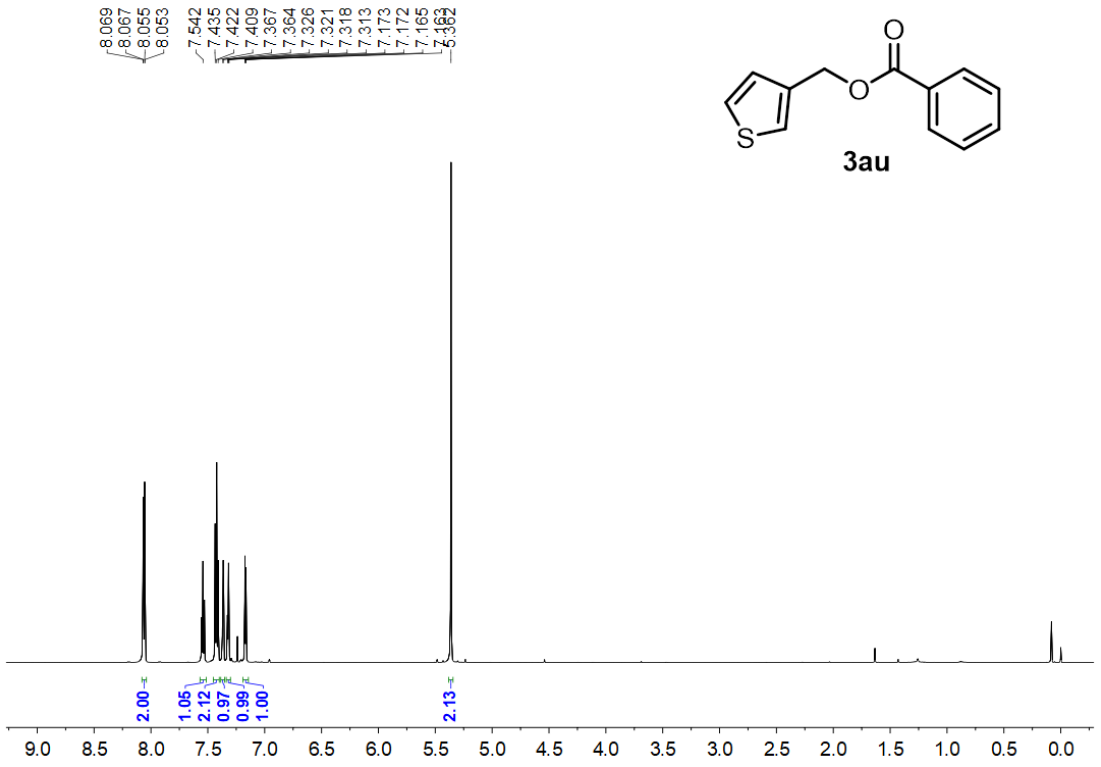

141.687
141.704
141.729
141.746
152.539
152.576
152.614
161.534
161.551
161.575
161.589
161.613
161.632
3as
2.19
0.97
2.00

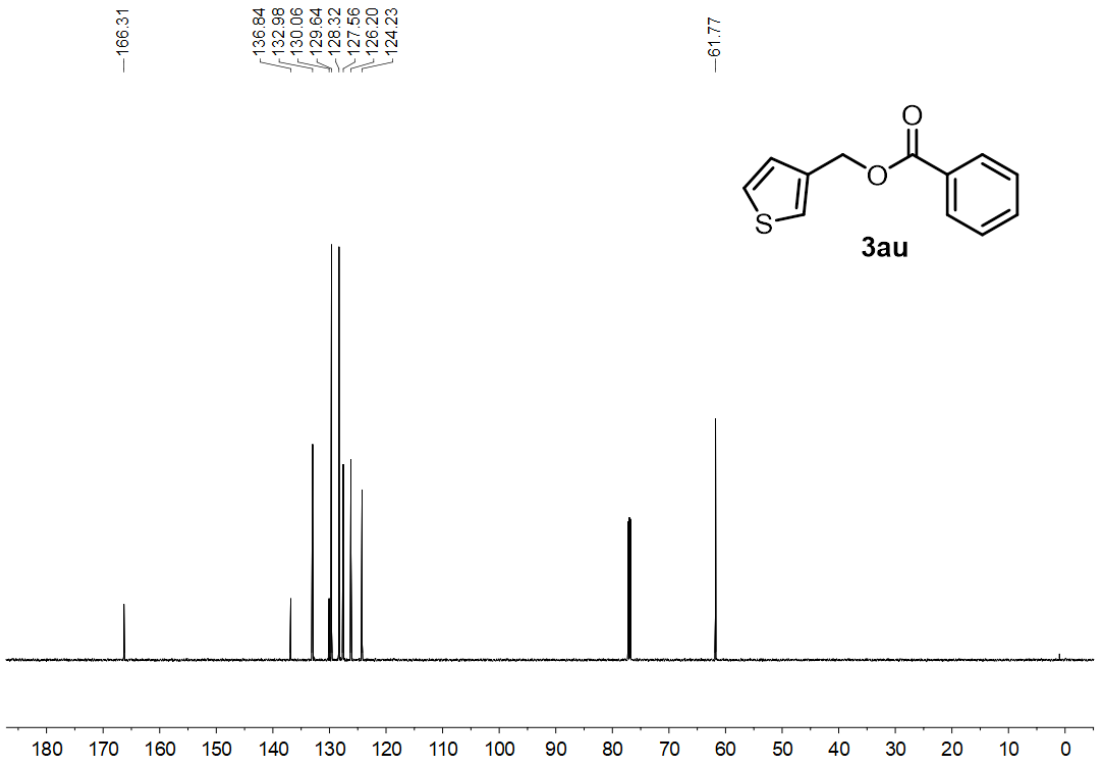

8.107
8.106
8.094
8.091
7.906
7.871
7.857
7.844
7.835
7.568
7.560
7.557
7.546
7.543
7.507
7.499
7.484
7.475
7.450
7.437
7.424
5.524
1.98
1.00
3.04
2.00
2.00
2.04
2.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

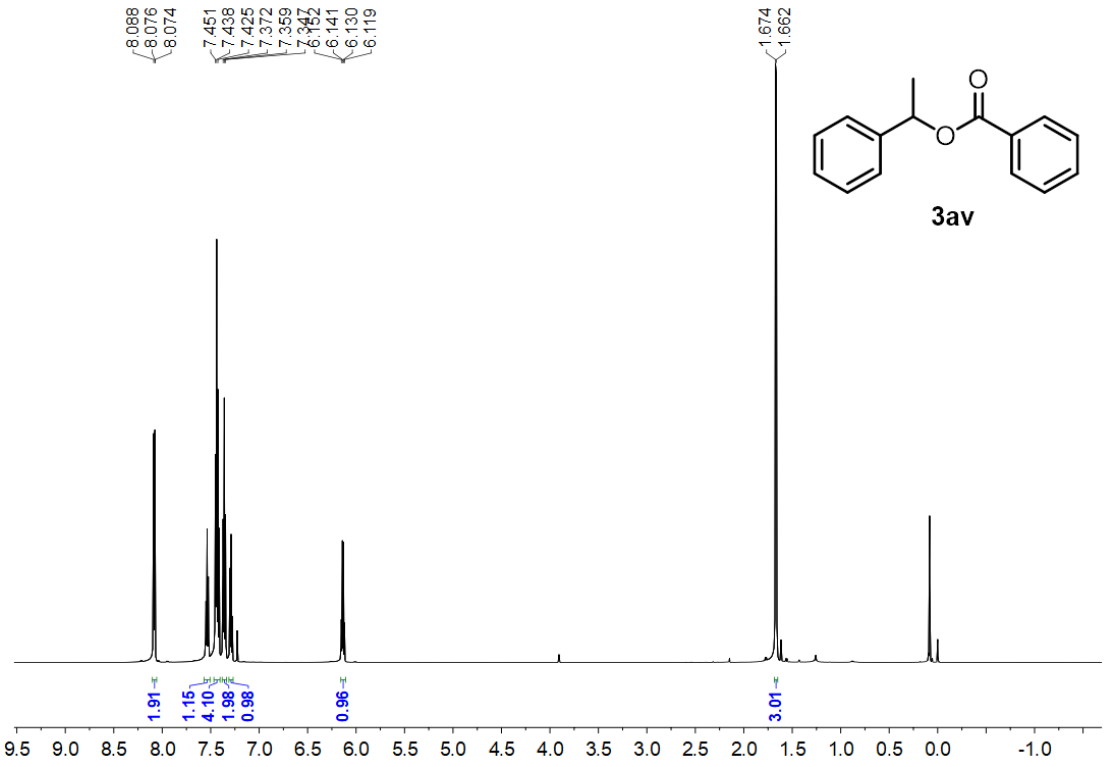
3at

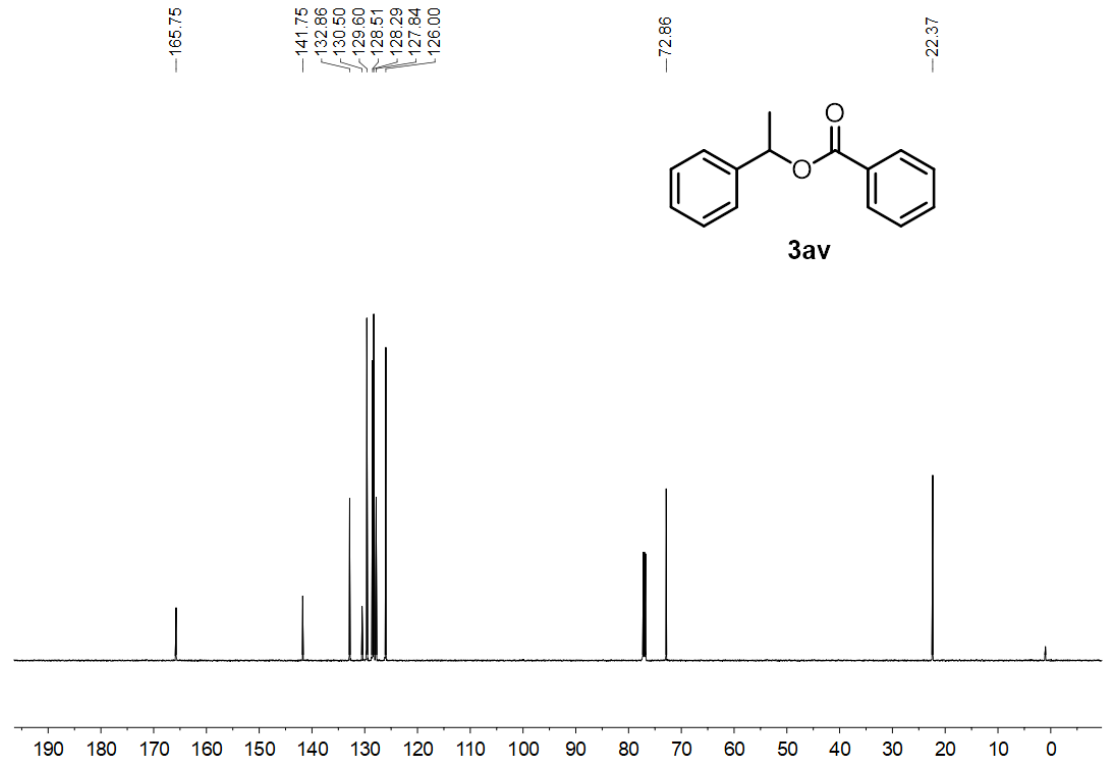

166.45
133.45
133.20
133.12
133.04
130.12
129.71
128.41
128.38
127.98
127.71
127.31
126.30
126.26
125.87
66.85
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

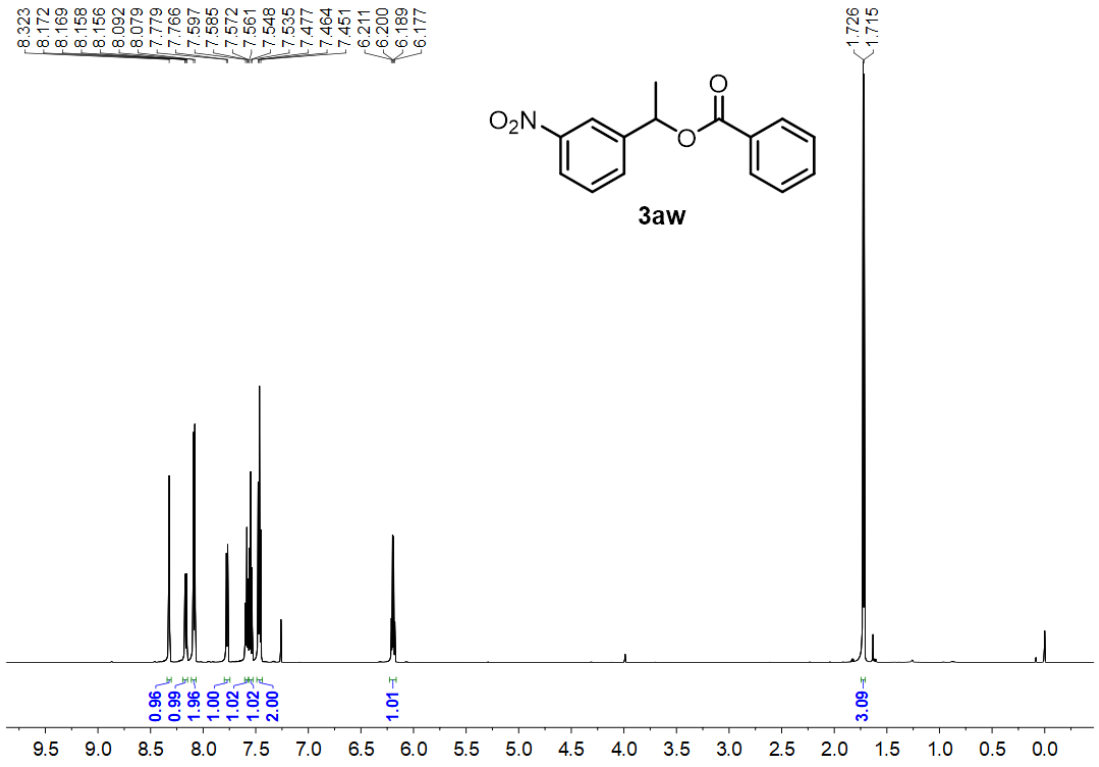
3at

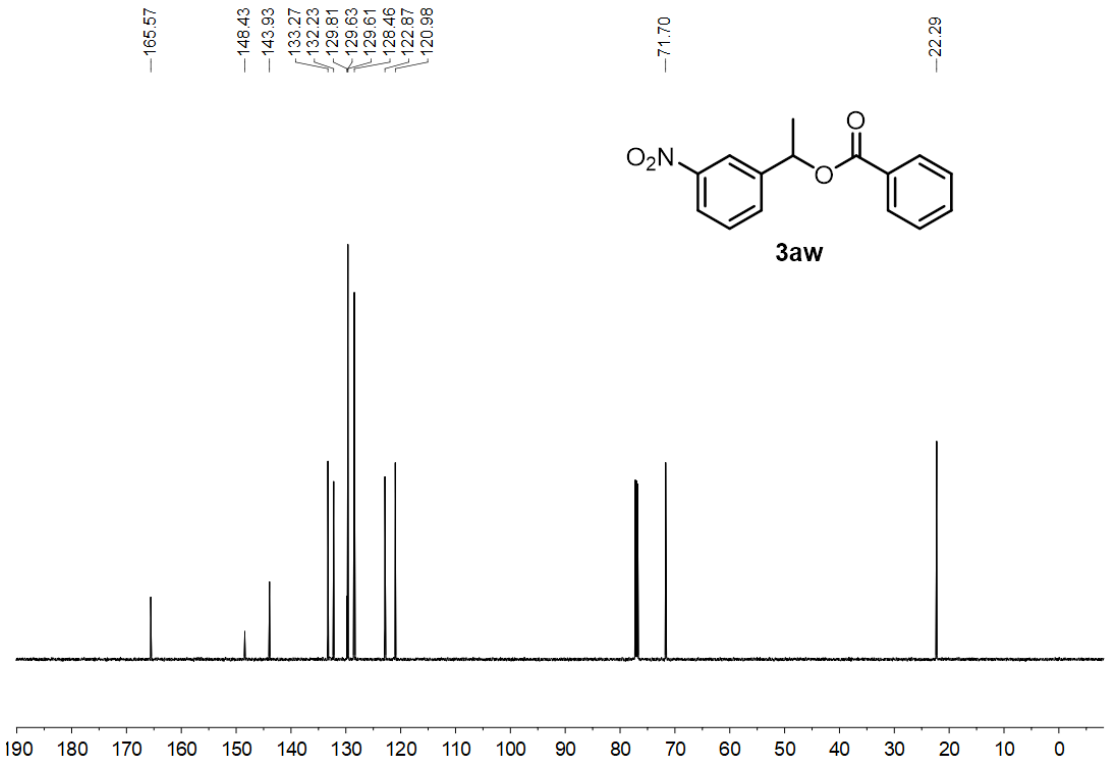

8.069
8.067
8.055
8.053
7.542
7.435
7.422
7.409
7.367
7.364
7.326
7.321
7.318
7.313
7.173
7.172
7.165
7.163
5.382
O
O
S
3au
2.00
1.05
2.12
0.97
0.99
1.00
2.13
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

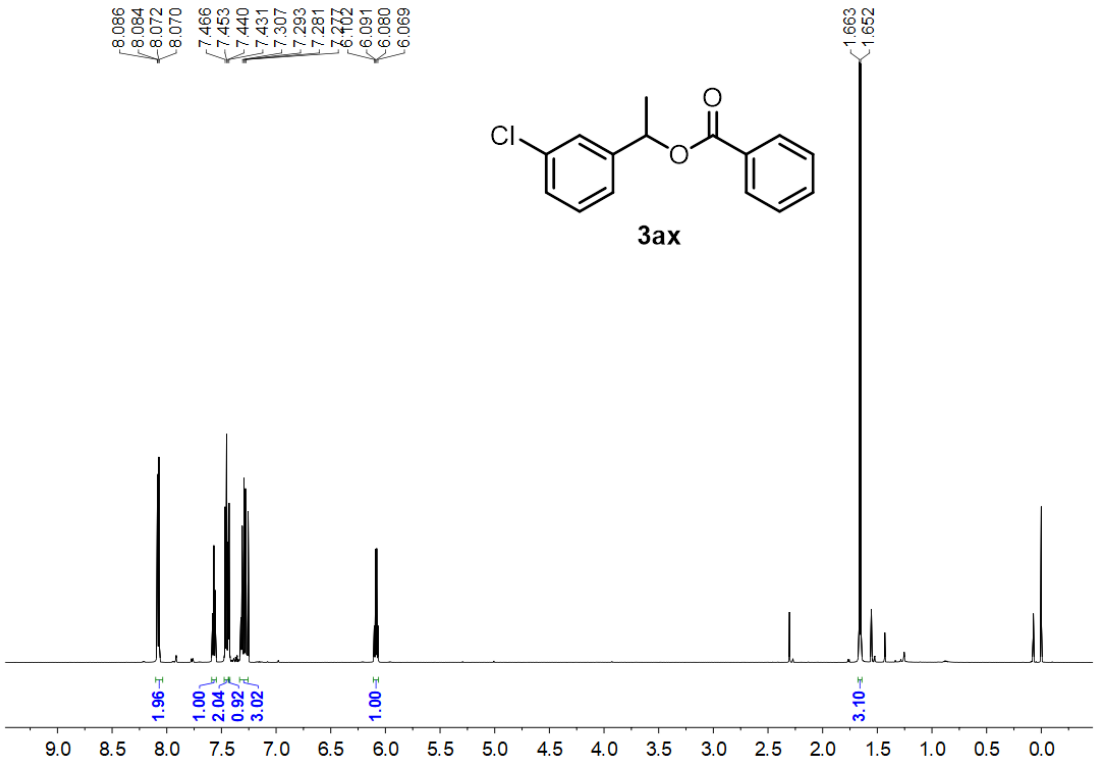

166.31
136.84
132.98
130.06
129.64
128.32
127.56
126.20
124.23
61.77
O
O
S
3au
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

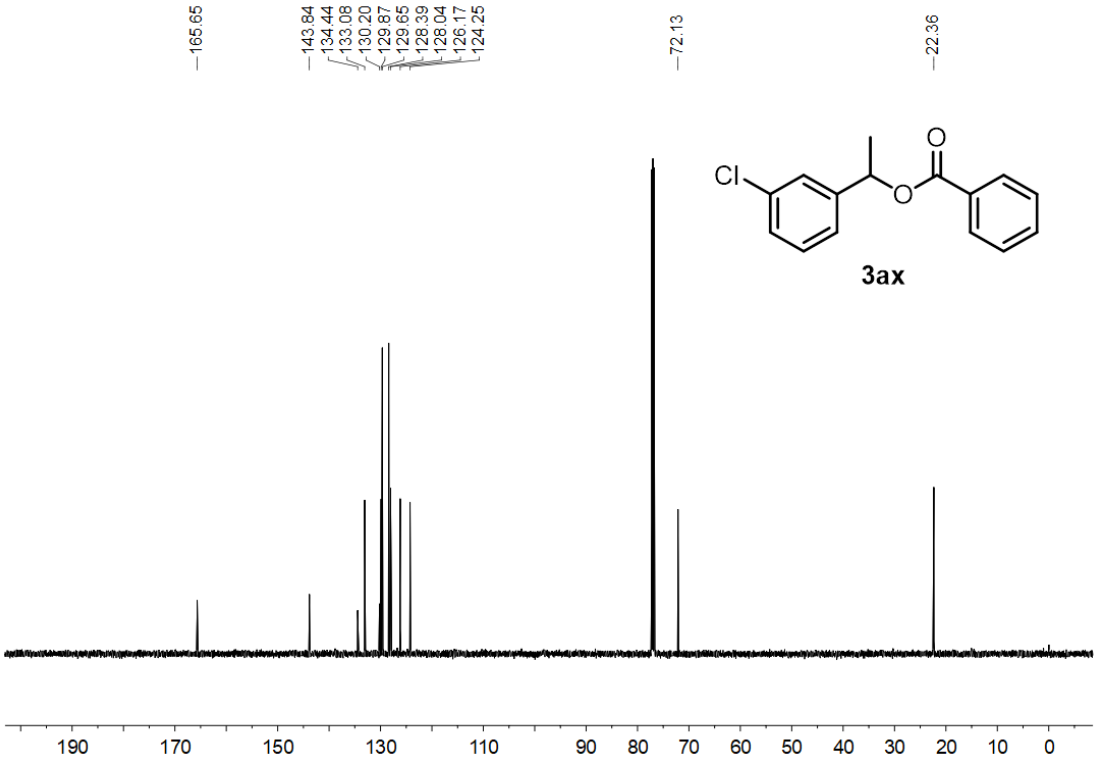

8.088
8.076
8.074
7.451
7.438
7.425
7.372
7.359
7.347
6.152
6.141
6.130
6.119
1.674
1.662
3av
1.91
1.15
4.10
1.98
0.98
0.96
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0

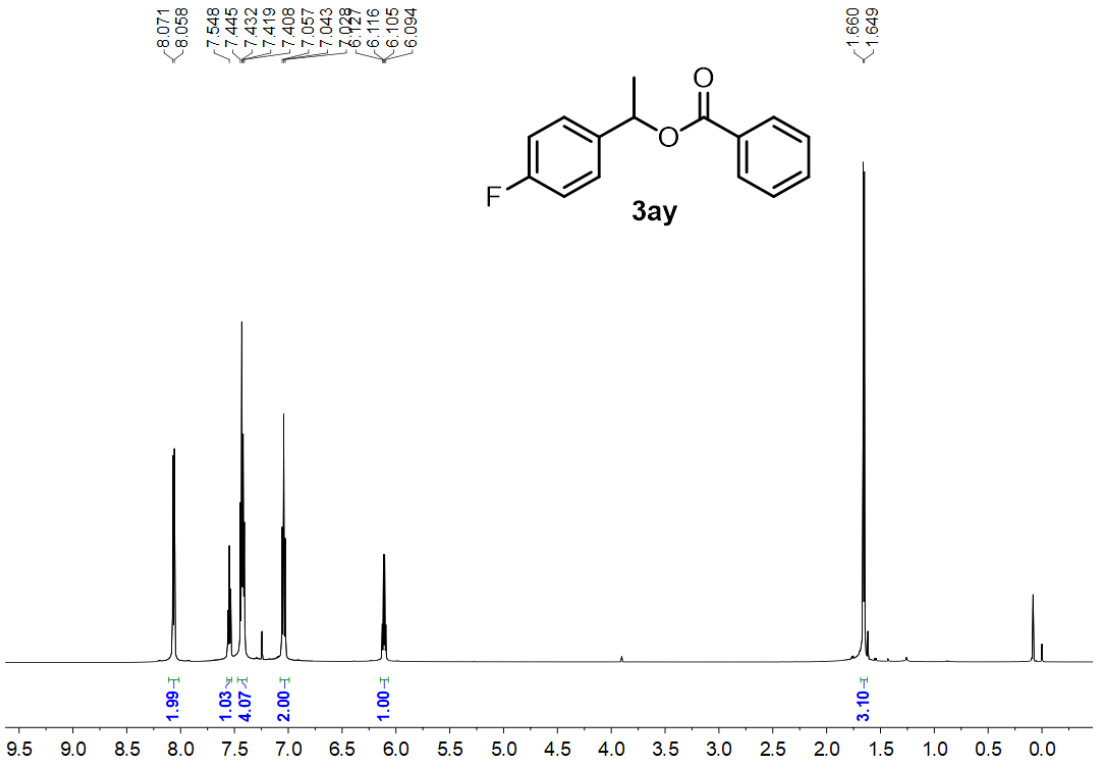

165.75
141.75
132.86
130.50
129.60
128.51
128.29
127.84
126.00
72.86
22.37
3av
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

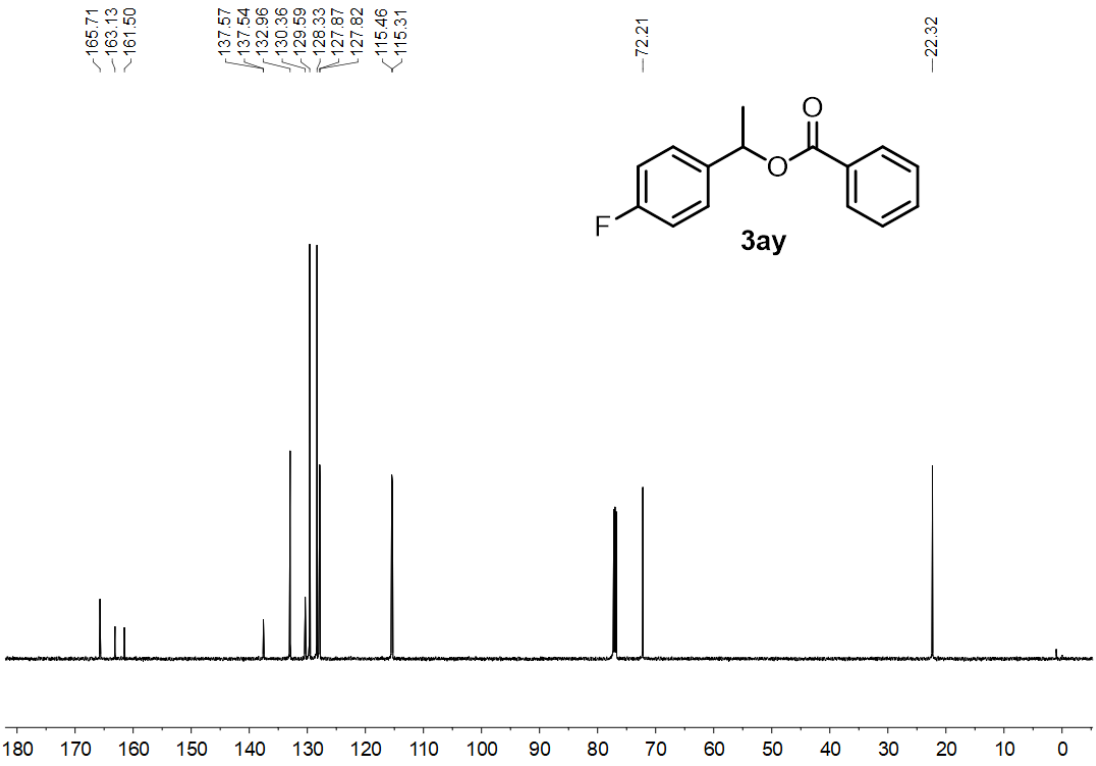

8.323
8.172
8.169
8.158
8.156
8.092
8.079
7.779
7.766
7.597
7.585
7.572
7.561
7.548
7.535
7.477
7.464
7.451
6.211
6.200
6.189
6.177
1.726
1.715
O2N
O
O
3aw
0.96
0.99
1.96
1.00
1.02
1.02
2.00
1.01
3.09
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

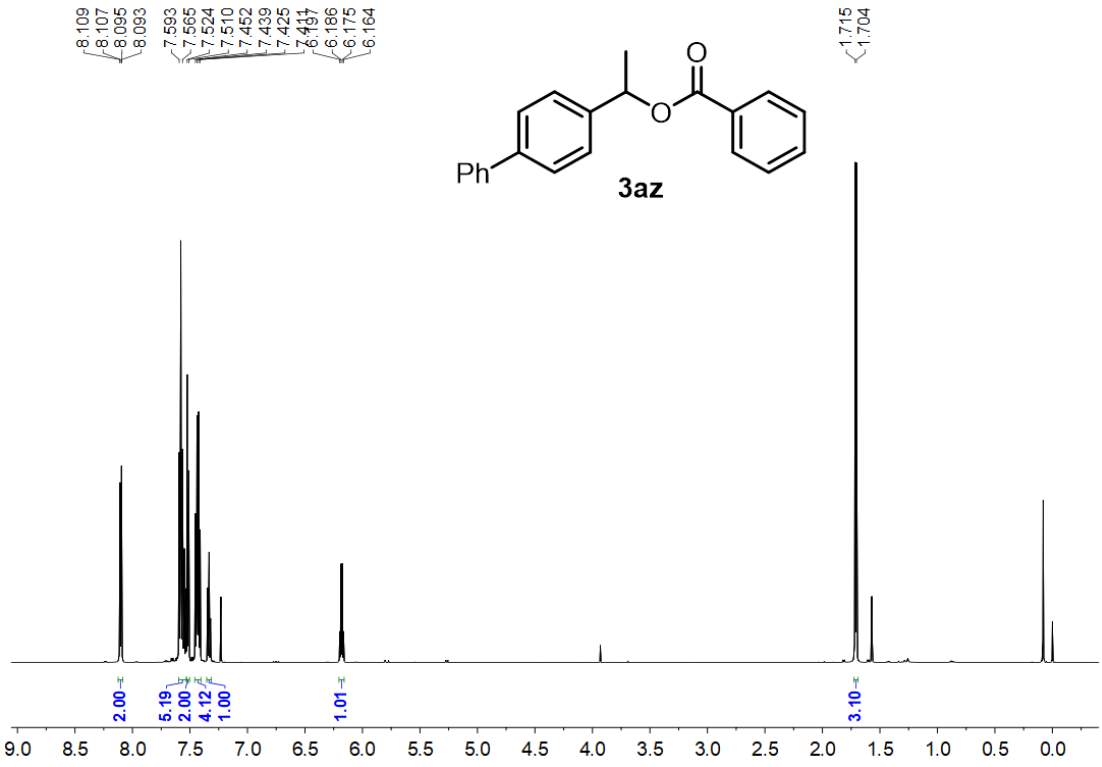

165.57
148.43
143.93
133.27
132.23
129.81
129.63
129.61
128.46
122.87
120.98
71.70
22.29
O2N
O
O
3aw
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

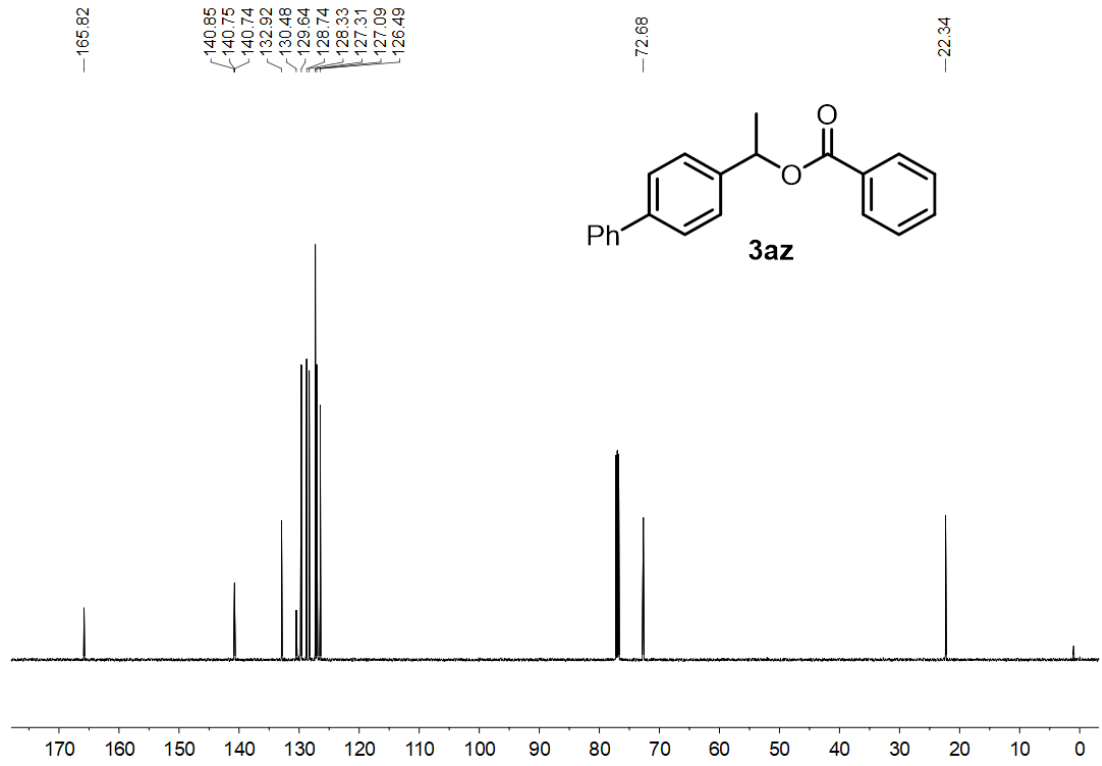

8.086
8.084
8.072
8.070
7.466
7.453
7.440
7.431
7.307
7.293
7.281
6.091
6.080
6.069
1.663
1.652
Cl
O
O
3ax
1.96
1.00
2.04
0.92
3.02
1.00
3.10
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

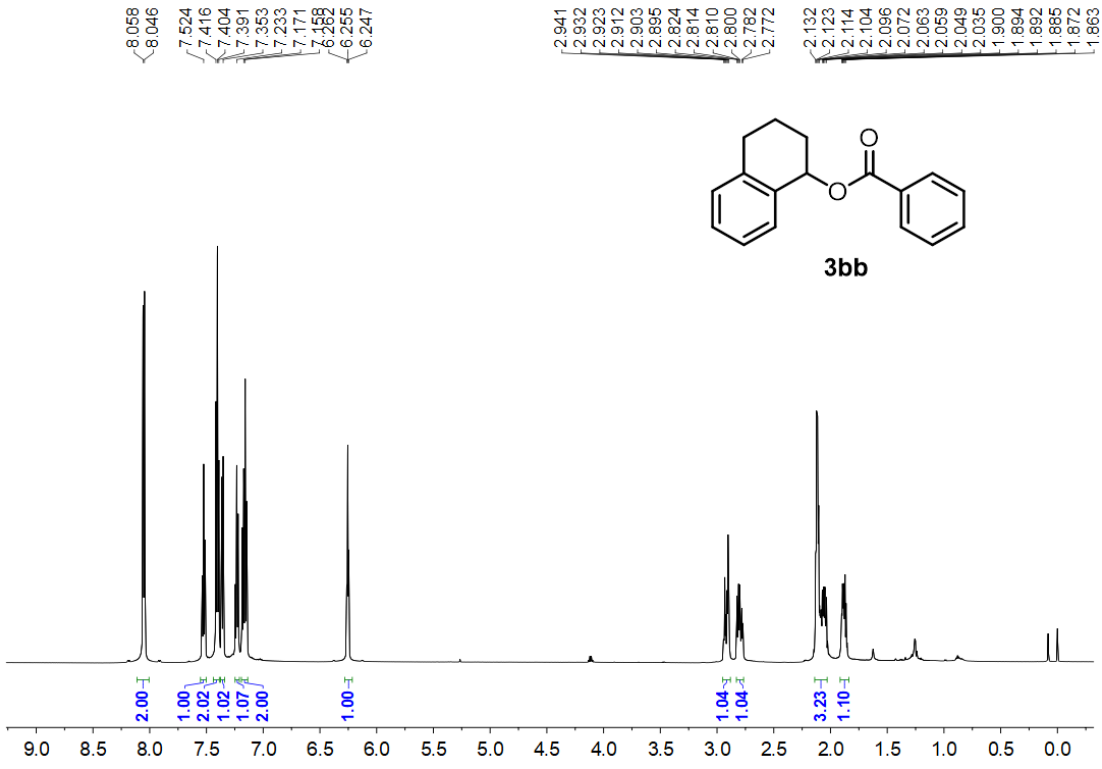

165.65
143.84
134.44
133.08
130.20
129.87
129.65
128.39
128.04
126.17
124.25
72.13
22.36
Cl
O
O
3ax
190 170 150 130 110 90 80 70 60 50 40 30 20 10 0

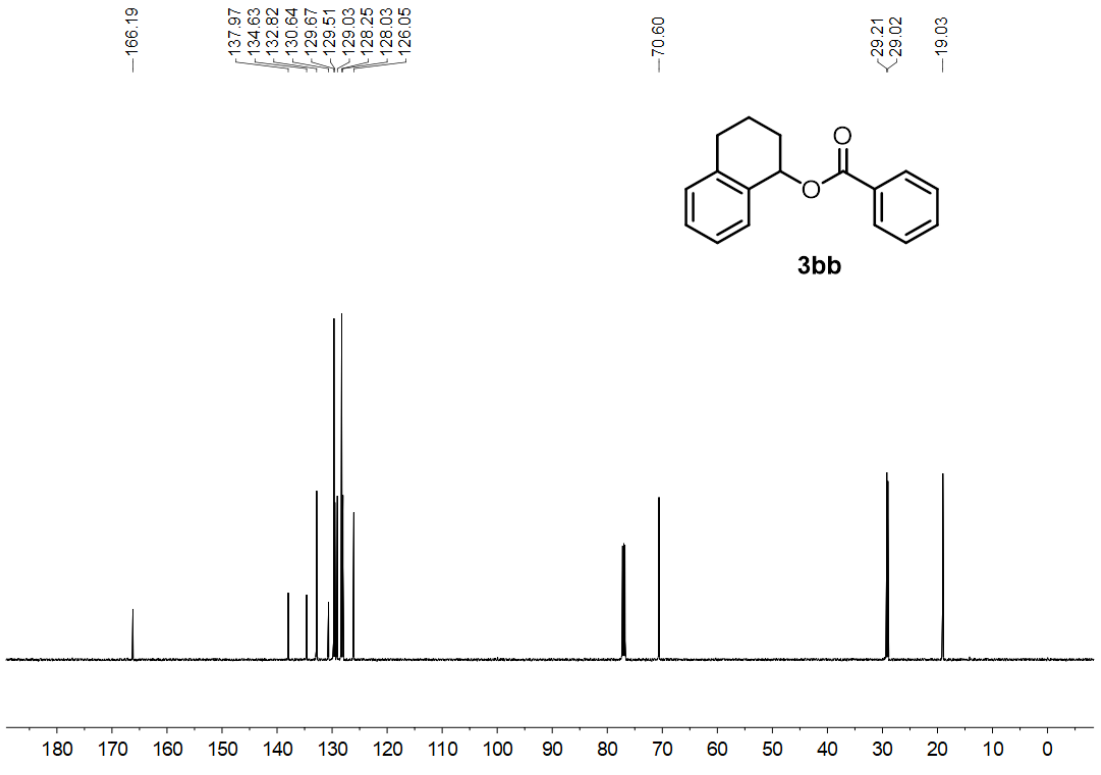

8.071
8.058
7.548
7.445
7.432
7.419
7.408
7.057
7.043
6.116
6.105
6.094
1.660
1.649
O
O
F
3ay
1.99
1.03
4.07
2.00
1.00
3.10
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

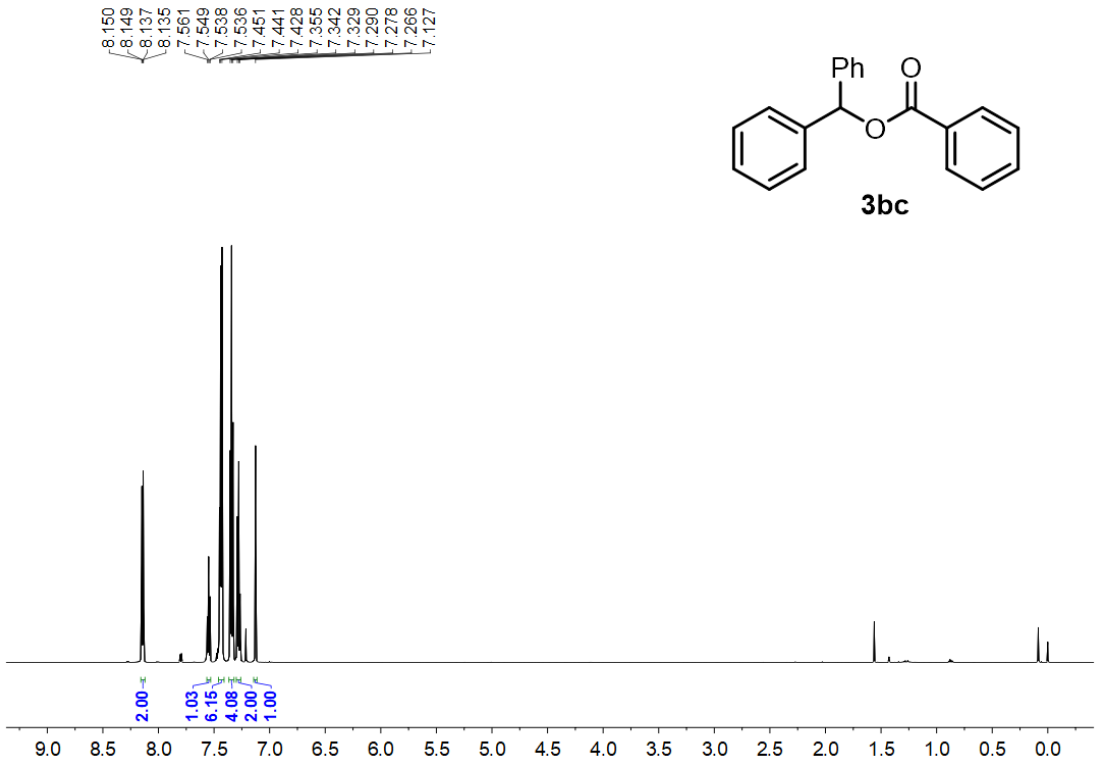

165.71
163.13
161.50
137.57
137.54
132.96
130.36
129.59
128.33
127.87
127.82
115.46
115.31
72.21
22.32
O
O
F
3ay
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

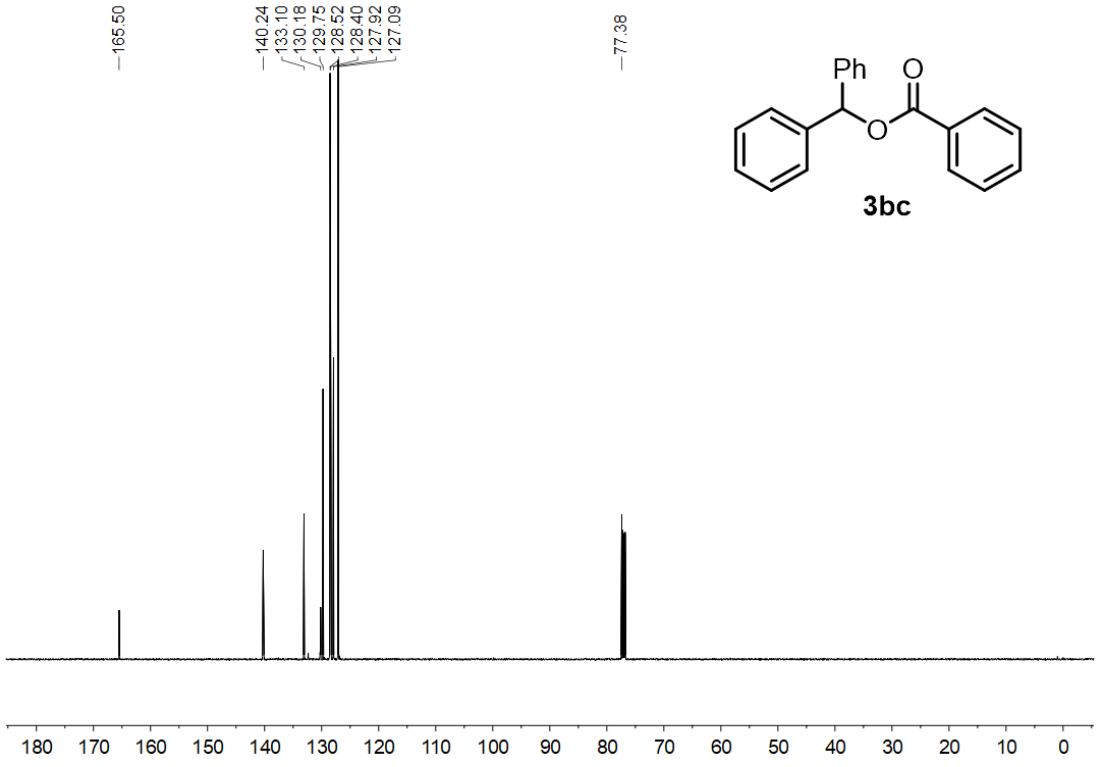

8.109
8.107
8.095
8.093
7.593
7.565
7.524
7.510
7.452
7.439
7.425
7.411
6.186
6.175
6.164
1.715
1.704
O
O
Ph
3az
2.00
5.19
2.00
4.12
1.00
1.01
3.10
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

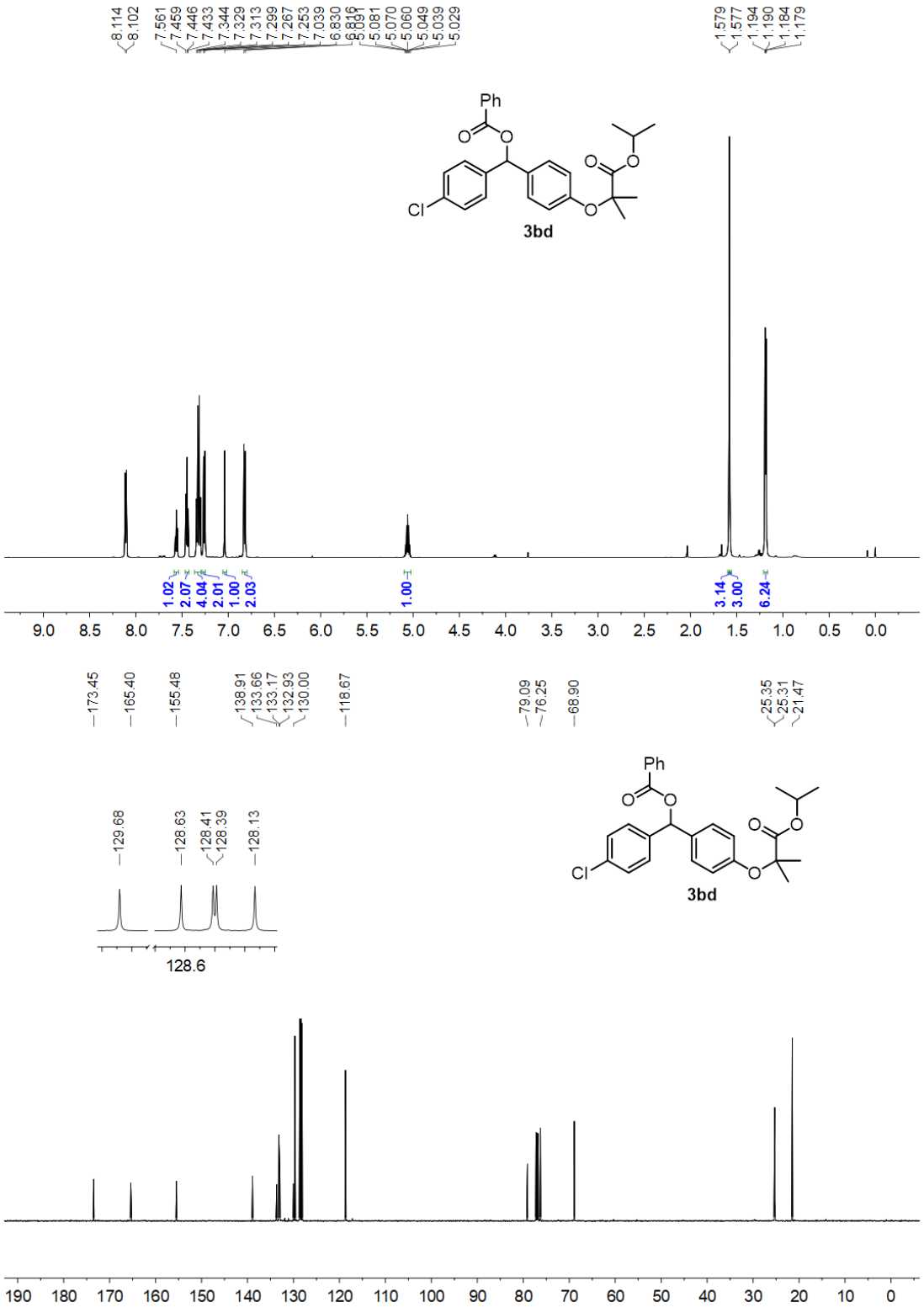

165.82
140.85
140.75
140.74
132.92
130.48
129.64
128.74
128.33
127.31
127.09
126.49
72.68
22.34
O
O
Ph
3az
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

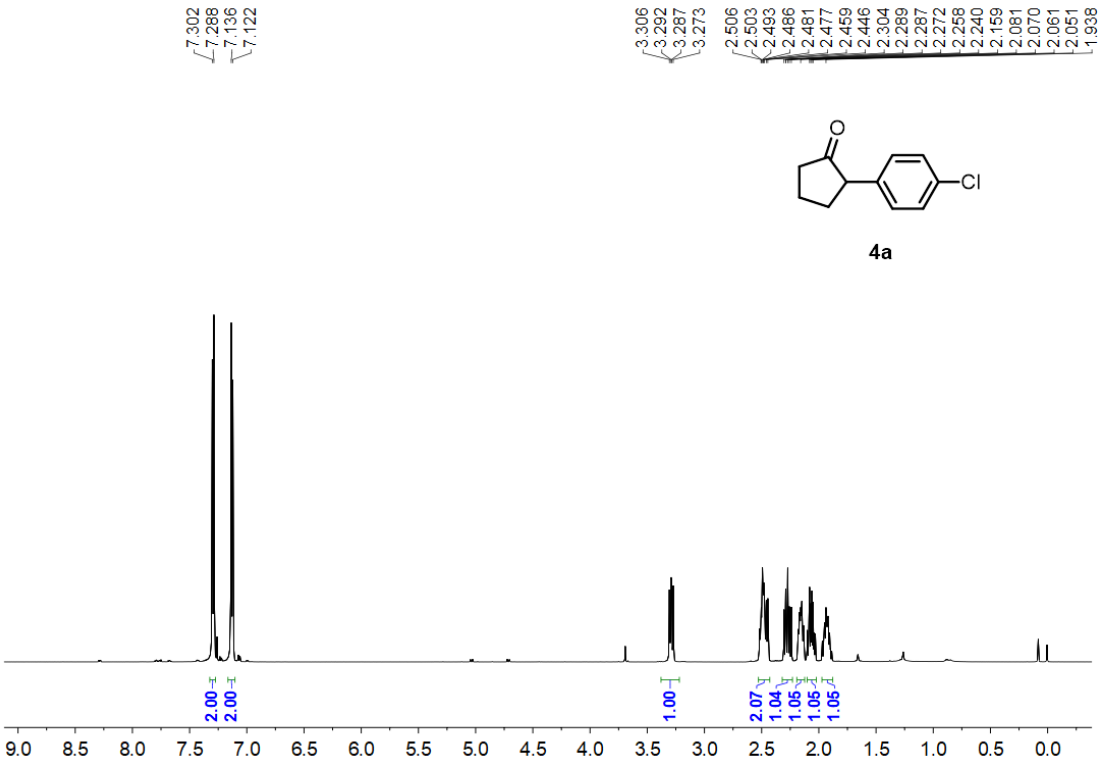

8.058
8.046
7.524
7.416
7.404
7.391
7.353
7.233
7.171
6.262
6.255
6.247
2.941
2.932
2.923
2.912
2.903
2.895
2.824
2.814
2.810
2.800
2.782
2.772
2.132
2.123
2.114
2.104
2.096
2.072
2.063
2.059
2.049
2.035
1.900
1.894
1.892
1.885
1.872
1.863
3bb
2.00
1.00
2.02
1.02
1.07
2.00
1.00
1.04
1.04
3.23
1.10
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


166.19
137.97
134.63
132.82
130.64
129.67
129.51
129.03
128.25
128.03
126.05
70.60
29.21
29.02
19.03
3bb
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

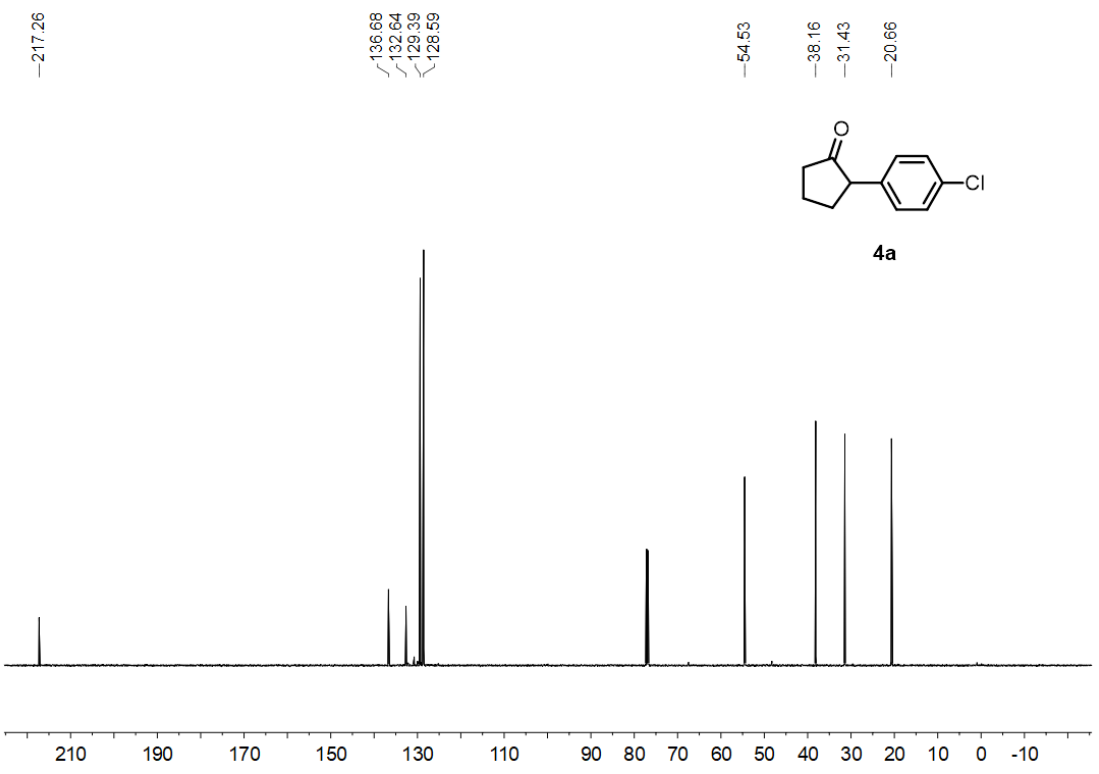

8.150
8.149
8.137
8.135
7.561
7.549
7.538
7.536
7.451
7.441
7.428
7.355
7.342
7.329
7.290
7.278
7.266
7.127
Ph
O
O
3bc
2.00
1.03
6.15
4.08
2.00
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


165.50
140.24
133.10
130.18
129.75
128.52
128.40
127.92
127.09
77.38
Ph
O
O
3bc
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

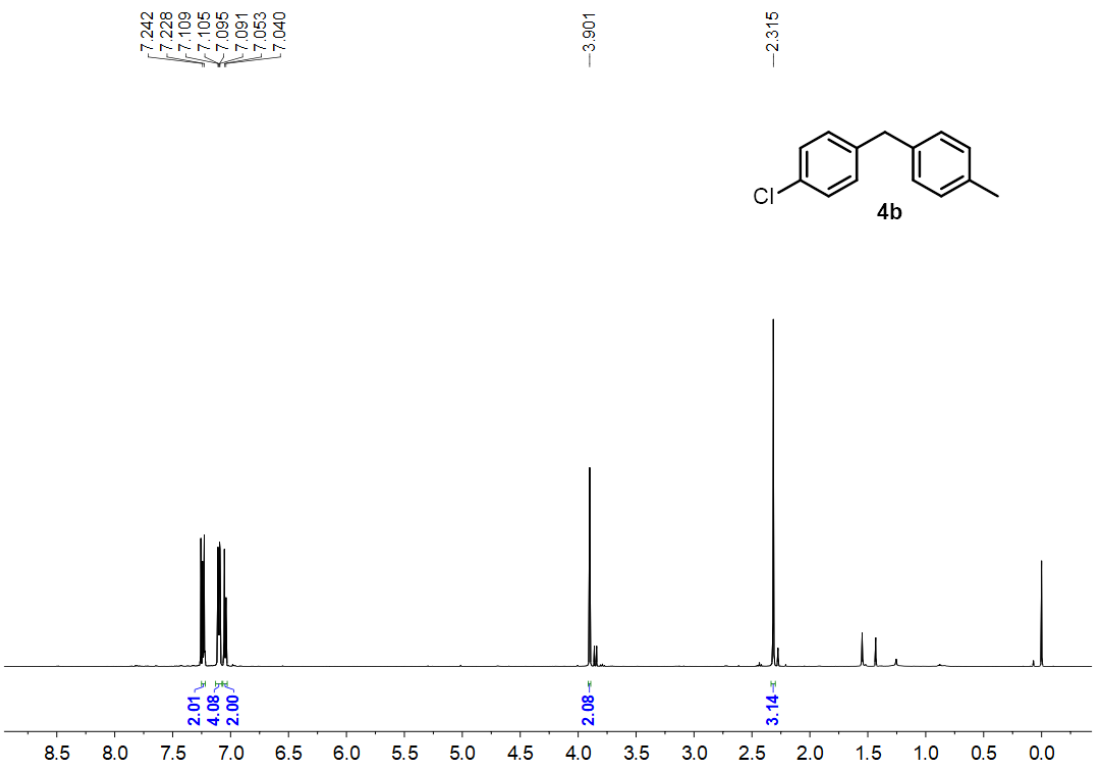

8.114
8.102
7.561
7.459
7.446
7.433
7.344
7.329
7.313
7.299
7.267
7.253
7.039
6.830
5.081
5.070
5.060
5.049
5.039
5.029
1.579
1.577
1.194
1.190
1.184
1.179
Ph
O
O
O
O
Cl
3bd
1.02
2.07
4.04
2.01
1.00
2.03
1.00
3.14
3.00
6.24
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
173.45
165.40
155.48
138.91
133.66
133.17
132.93
130.00
118.67
79.09
76.25
68.90
25.35
25.31
21.47
129.68
128.63
128.41
128.39
128.13
128.6
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


7.302
7.288
7.136
7.122
3.306
3.292
3.287
3.273
2.506
2.503
2.493
2.486
2.481
2.477
2.459
2.446
2.304
2.289
2.287
2.272
2.258
2.240
2.159
2.081
2.070
2.061
2.051
1.938
O
Cl
2.00
2.00
1.00
2.07
1.04
1.05
1.05
1.05
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

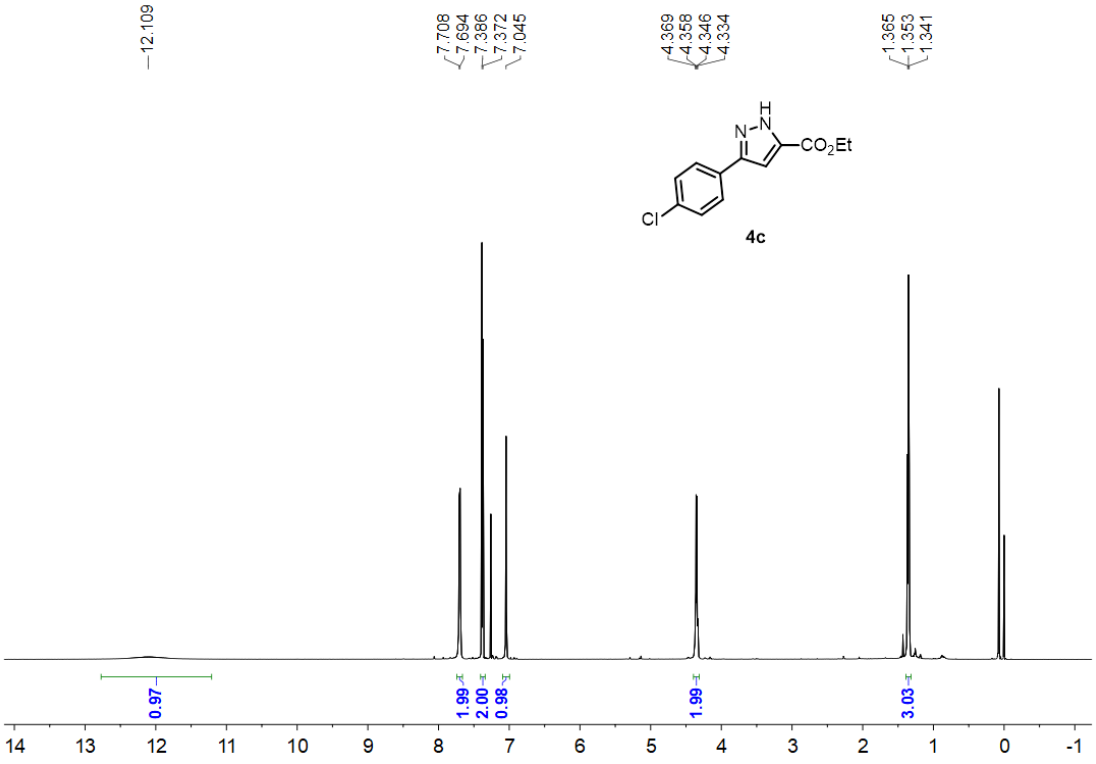
4a

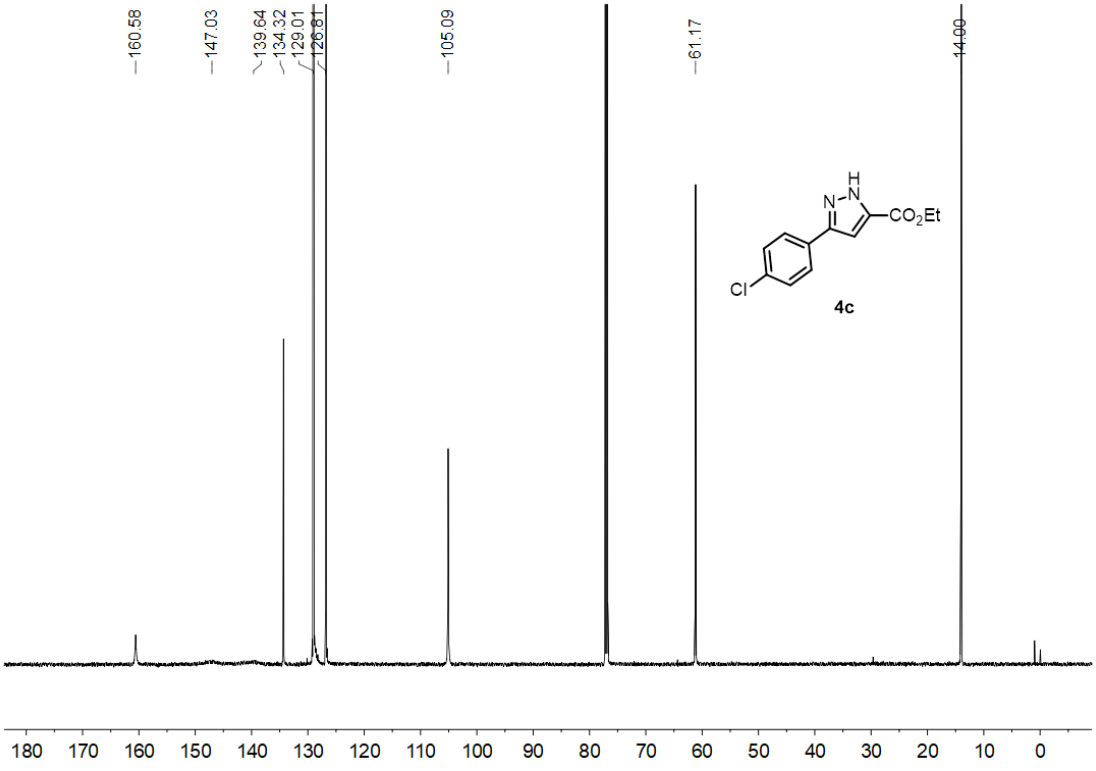

217.26
136.68
132.64
129.39
128.59
54.53
38.16
31.43
20.66
O
Cl
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10

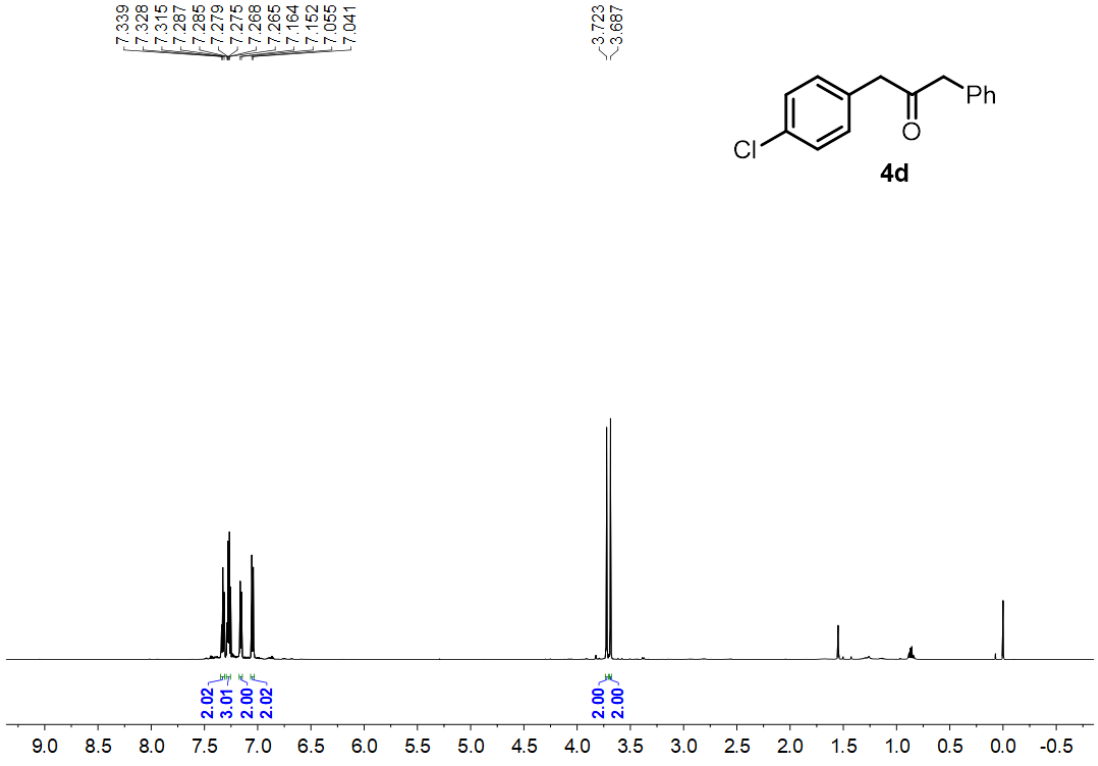
4a

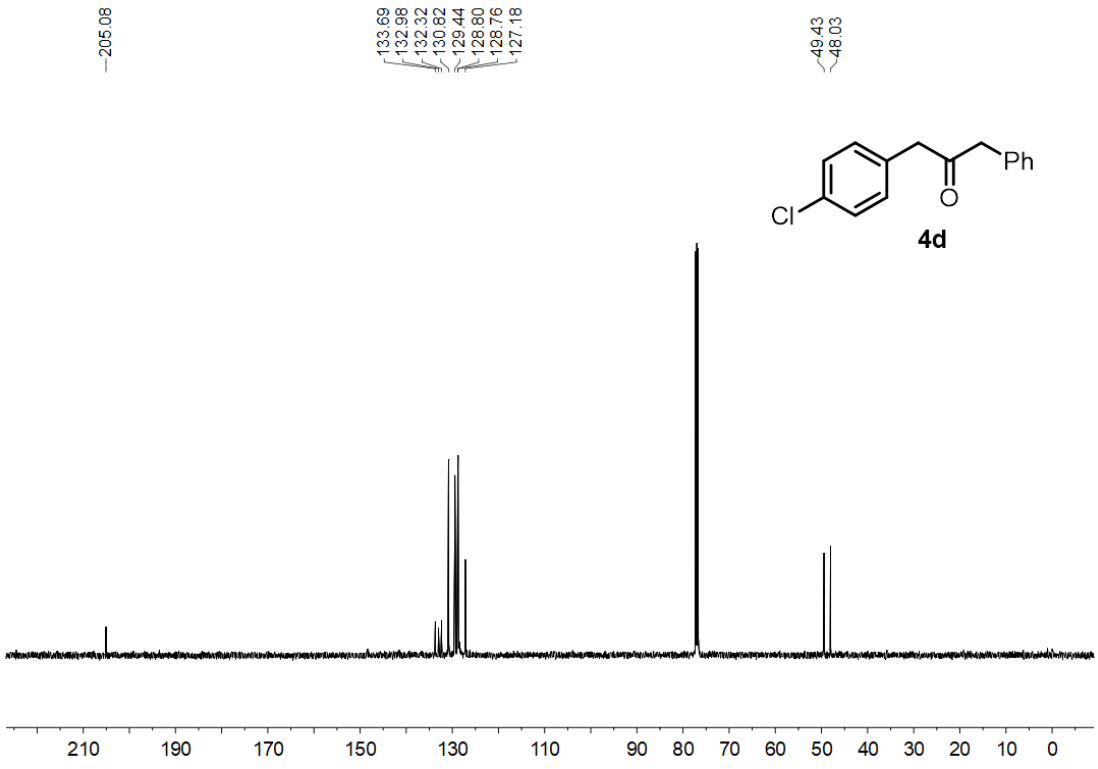

7.242
7.228
7.109
7.105
7.095
7.091
7.053
7.040
3.901
2.315
Cl
4b
2.01
4.08
2.00
2.08
3.14
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


139.87
137.49
135.80
131.76
130.17
129.23
128.71
128.50
40.80
20.99
Cl
4b
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


12.109
7.708
7.694
7.386
7.372
7.045
4.369
4.358
4.346
4.334
1.365
1.353
1.341
CO2Et
Cl
4c
0.97
1.99
2.00
0.98
1.99
3.03
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1


160.58
147.03
139.64
134.32
129.01
126.81
105.09
61.17
14.00
CO2Et
Cl
4c
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


7.339
7.328
7.315
7.287
7.285
7.279
7.275
7.268
7.265
7.164
7.152
7.055
7.041
3.723
3.687
Cl
Ph
O
4d
2.02
3.01
2.00
2.02
2.00
2.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


205.08
133.69
132.98
132.32
130.82
129.44
128.80
128.76
127.18
49.43
48.03
Cl
Ph
O
4d
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0