Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Electronic Supporting Information

Synthesis of pyridine *trans*-tetrafluoro-λ^6-sulfane derivatives via radical additions

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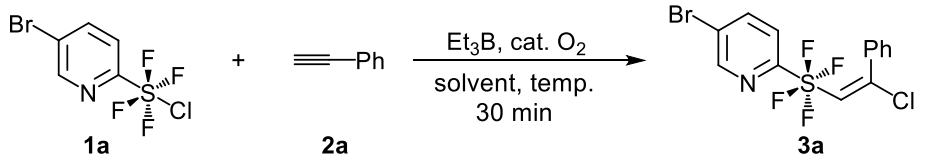
General information

All reactions were performed in oven-dried Nalgene® FEP bottles under positive pressure of nitrogen unless otherwise mentioned. Solvents were transferred via syringe and were introduced into the reaction vessels though a rubber septum. All of the reactions were monitored by thin-layer chromatography (TLC) carried out on 0.25 mm Merck silica gel (60-F254). The TLC plates were visualized with UV light. Products were purified by column chromatography carried out on columns packed with silica gel (60N spherical neutral size 63-210 μm). The ^{1}H NMR (300 MHz) and ^{19}F NMR (282 MHz) spectra were recorded for solution in $CDCl_3$ and $(CD_3)_2CO$ on a Varian Mercury 300. ^{13}C NMR (125 MHz) spectra for solution in $CDCl_3$ and $(CD_3)_2CO$ were recorded on a BRUKER 500 UltraShield^{TR}. Chemical shifts (δ) are expressed in ppm downfield from TMS (δ = 0.00) and C_6F_6 [δ = −162.2 ($CDCl_3$) or −163.5 ($(CD_3)_2CO$)] as an internal standard for ^{1}H and ^{19}F NMR respectively. For ^{13}C NMR, $CDCl_3$ (δ = 77.16) or $(CD_3)_2CO$ (δ = 29.84) is referred as residual standard. High resolution mass spectrometry was recorded on a SHIMADZU GCMS-QP5050A (EI-MS) and SHIMAZU LCMS-2020 (ESI-MS and APCI-MS). Infrared spectra were recorded on a JASCO FT/IR-4100 spectrometer. X-ray measurements were carried out on a Rigaku R-AXIS RAPID diffractometer with graphite monochromate Mo Kα radiation at –100 °C. Melting points were recorded on a BUCHI M-565. Chemicals were purchased and used without further purification unless otherwise noted. Solvents CH_3CN, CH_2Cl_2, toluene, DMF and NMP were dried and distilled before use.

Table S1 Optimization of reaction conditions.[a]



Entry	**2a** (equiv)	Et_3B (equiv)	solvent	temp.	yield (%)[b]
1	1.5	0.15	Et_2O	0 °C→ rt	54
2	3.0	0.15	Et_2O	0 °C→ rt	59
3	1.5	0.05	Et_2O	0 °C→ rt	33
4	1.5	0.50	Et_2O	0 °C→ rt	45
5	1.5	0.15	Et_2O	-30 °C→ rt	51
6	1.5	0.15	Hexane	0 °C→ rt	72
7	1.5	0.15	Pentane	0 °C→ rt	79
8	1.5	0.15	1,4-dioxane	0 °C→ rt	34
9	1.5	0.15	THF	0 °C→ rt	80
10	1.5	0.15	$ClCH_2CH_2Cl$	0 °C→ rt	64
11	1.5	0.15	$CHCl_3$	0 °C→ rt	81
12	1.5	0.15	CH_2Cl_2	0 °C→ rt	91

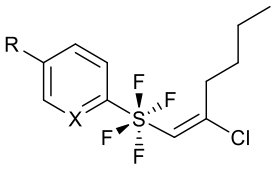
[a] Reactions were performed with **1a** (0.2 mmol) and **2a** in the presence of Et_3B in the respective solvent for 30 min. [b] ^{19}F NMR yields with PhF as an internal standard.

Evaluation of Chemical Hardness

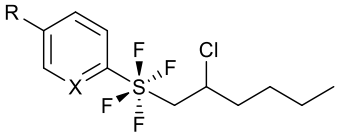
Chemical hardness is a parameter that measures a compound's resistance to change in electron distribution or charge transfer.[1] It can provide information about the stability and reactivity of a chemical system. On the basis of frontier molecular orbitals, chemical hardness corresponds to the gap between HOMO (highest occupied molecular orbital) and LUMO (lowest occupied molecular orbital), which relates to the kinetic stability of a molecule. It is calculated using equation 1[1c,d] where E_{LUMO} and E_{HOMO} are LUMO and HOMO energy, respectively. Thus, the higher the value of chemical hardness, the more stable the compound.

$$\eta = (E_{LUMO} - E_{HOMO})/2 \qquad (1)$$

Table S2 Chemical reactivity indices of tetrafluorosulfanyl pyridine and benzene derivatives



3ab, R = Br, X = N
3ab', R = Br, X = C
3ab'', R = NO_2, X = C



5aa, R = Br, X = N
5aa', R = Br, X = C
5aa'', R = NO_2, X = C

Entry	Compound	E (au)	E_{HOMO} (eV)	E_{LUMO} (eV)	η (eV)
1	**3ab**	–4313.81	–7.75	–2.13	2.81
2	**3ab'**	–4297.78	–7.42	–2.18	2.62
3	**5aa**	–4315.05	–7.72	–2.05	2.83
4	**5aa'**	–4299.02	–7.35	–2.13	2.61
5	**3ab''**	–1928.80	–8.00	–3.32	2.34
6	**5aa''**	–1930.04	–8.33	–3.27	2.53

We compared the aliphatic alkyne addition product **3ab** with its analogue **3ab'** (Table S2, Entries 1 and 2) and found that **3ab** had a higher value of chemical hardness than **3ab'**. Similar results were obtained for aliphatic alkene addition product **5aa** with its analogue **5aa'** (Entries 3 and 4). These findings could provide a plausible explanation for the kinetic stability of the pyridine-aliphatic addition products against their benzene analogues. However, on further evaluation of the chemical hardness value for the *p*-NO_2-benzene analogues **3ab''** and **5aa''** (Entries 5 and 6), the results seem to be contradictory. Although the *p*-NO_2-benzene analogues are reported to be stable, their chemical hardness value evaluated through theoretical calculations is found to be lower than **3ab'** and **5aa'**, which is a contradiction to the experimental results. Thus, the chemical hardness scale is not a universal scale to define and compare the kinetic stability of the compounds.

The pyridine chlrorotetrafluoro-λ^6-sulfane **1** were prepared according to the literature procedure[2,3] and stored in Nalgene® FEP bottles inside the glove box. The pyridine chlrorotetrafluoro-λ^6-sulfane **1** used for reaction are given in Figure S1.

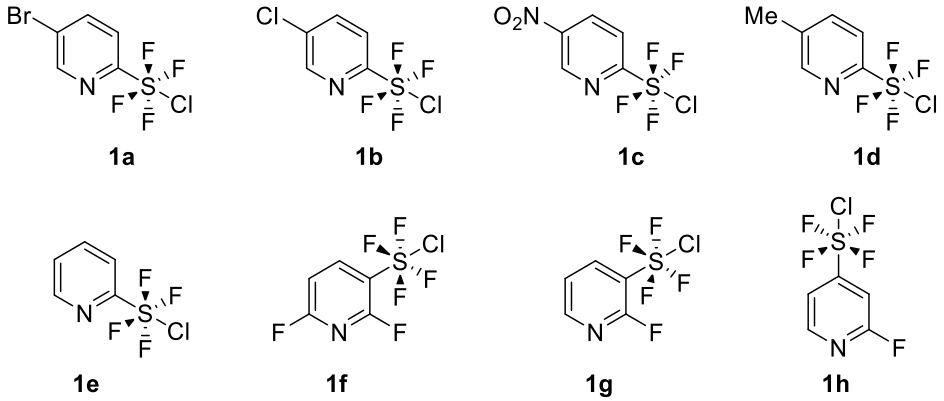
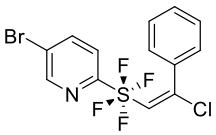


Figure S1 Pyridine chlrorotetrafluoro-λ^6-sulfane **1** used for radical addition.

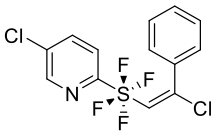
Synthesis and characterization of radical reaction adduct 3 and 5:
3 and **5** were prepared according to the general procedure.

(*E*)-5-Bromo-2-((2-chloro-2-phenylvinyl)tetrafluoro-λ^6-sulfaneyl)pyridine (**3aa**):



Prepared according to General Procedure, **3aa** was isolated as white solid (71 mg, 88%). mp: 91.8 °C; HRMS (ESI$^+$): *m/z* calcd. for $C_{13}H_9BrClF_4NNaS$ [M+Na]$^+$: 423.9161 found: 423.9144. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.20 (quint, *J* = 9.0 Hz, 1H), 7.36–7.39 (m, 3H), 7.42-7.45 (m, 2H), 7.49 (d, *J* = 9.0 Hz, 1H), 7.57 (d, *J* = 9 Hz, 1H), 8.49 (d, *J* = 3.0 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 61.04 (d, *J* = 8.2 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 122.88-122.73 (m), 128.15, 128.20, 129.45, 136.85, 139.57-139.32 (m), 140.79, 142.95 (quint, *J* = 29.0 Hz), 148.26, 168.65-168.15 (m). ATR-FTIR (KBr): *v* = 3437, 3099, 1638, 1567, 1492, 1369, 1093, 696, 594 cm^{-1}.

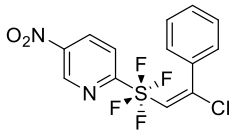
(*E*)-5-Chloro-2-((2-chloro-2-phenylvinyl)tetrafluoro-λ^6-sulfaneyl)pyridine (**3ba**):



Prepared according to General Procedure, **3ba** was isolated as white solid (71 mg, 88%). mp: 69.6 °C; HRMS (ESI$^+$): *m/z* calcd. for $C_{13}H_9NF_4NaSCl_2$ [M+Na]$^+$: 379.9667 found: 379.9667. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.12–7.23 (m, 1H), 7.36–7.39 (m, 3H), 7.41–7.44 (m, 2H), 7.55 (d, *J* = 9 Hz, 1H), 7.71–7.74 (m, 1H), 8.39 (d, *J* = 3 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 61.24 (d, *J* = 8.46 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 123.60, 127.91, 128.09, 128.15, 128.26, 128.96, 129.58, 131.06, 134.39, 136.37,

137.56, 149.30, 150.59, 155.70. ATR-FTIR (KBr): *v* = 3099, 3050, 1639, 1571, 1446, 1303, 1012, 636, 530 cm^{-1}.

(*E*)-5-Nitro-2-((2-chloro-2-phenylvinyl)tetrafluoro-λ^6-sulfaneyl)pyridine (**3ca**):

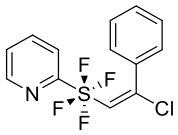


Prepared according to General Procedure, **3ca** was isolated as brown solid (25 mg, 34%). mp: 96.0 °C; HRMS (EI$^+$): *m/z* calcd. for $C_{13}H_9N_2O_2F_4SCl$ [M]$^+$: 368.0009 found: 368.0008. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.21 (quint, *J* = 9 Hz, 1H), 7.38–7.44 (m, 5H), 7.82 (d, *J* = 9 Hz, 1H), 8.55 (d, *J* = 9 Hz, 1H), 9.26 (d, *J* = 3 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 61.18 (d, *J* = 8.46 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 122.42 (quint, *J* = 5.04 Hz), 128.08, 128.27, 129.62, 133.65, 136.62, 140.23–140.35 (m), 142.25 (quint, *J* = 27.72 Hz), 143.21, 144.73, 172.47 (quint, *J* = 32.76 Hz). ATR-FTIR (KBr): *v* = 3139, 3060, 1631, 1527, 1355, 634 cm^{-1}.

(*E*)-5-Methyl-2-((2-chloro-2-phenylvinyl)tetrafluoro-λ^6-sulfaneyl)pyridine (**3da**):

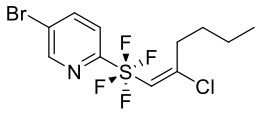
Prepared according to General Procedure, **3da** was isolated as yellow solid (71 mg, 88%). mp: 93.9 °C; HRMS (ESI$^+$): *m/z* calcd. for $C_{14}H_{12}NF_4NaSCl$ [M+Na]$^+$: 360.0213 found: 360.0205. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.31 (s, 3H), 7.21 (quint, *J* = 9 Hz, 1H), 7.34–7.40 (m, 3H), 7.42–7.51 (m, 4H), 8.23 (s, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 60.42 (d, *J* = 8.46 Hz, 4F). ^{13}C NMR (126 MHz, $CDCl_3$): δ = 18.06, 120.77 (quint, *J* = 3.78 Hz), 128.12, 128.20, 129.29, 136.17, 137.01. 138.61, 138.81 (quint, *J* = 7.56 Hz), 143.45 (quint, *J* = 30.24 Hz), 147.27, 168.09 (quint, *J* = 30.24 Hz). ATR-FTIR (KBr): *v* = 3052, 1606, 1589, 1446, 902, 717, 655 cm^{-1}.

(*E*)-2-((2-chloro-2-phenylvinyl)tetrafluoro- λ^6-sulfaneyl)pyridine (**3ea**):



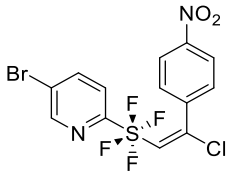
Prepared according to General Procedure, **3ea** was isolated as light-yellow solid (45 mg, 67%). mp: 78.0 °C; HRMS (ESI$^+$): *m/z* calcd. for $C_{13}H_{10}NNaSClF_4$ [M+Na]$^+$: 346.0056 found: 346.0060. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.22 (quint, *J* = 9 Hz, 1H), 7.29–7.38 (m, 4H), 7.40–7.46 (m, 2H), 7.58 (d, *J* = 6 Hz, 1H), 7.74 (t, *J* = 9 Hz, 1H), 8.44 (dd, *J* = 3 Hz, 1.5 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 59.81 (d, *J* = 8.46 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 121.41 (quint, *J* = 5.04 Hz), 125.94, 128.14, 128.17, 129.34, 136.96, 138.40, 139.03 (quint, *J* = 7.56 Hz), 143.26 (quint, *J* = 28.98 Hz), 147.35 (d, *J* = 2.52 Hz), 170.08 (quint, *J* = 30.24 Hz). ATR-FTIR (KBr): *v* = 3093, 1652, 1579, 1029, 904, 831, 694 cm^{-1}.

(*E*)-5-Bromo-2-((2-chlorohex-1-en-1-yl)tetrafluoro-λ^6-sulfaneyl)pyridine (**3ab**):



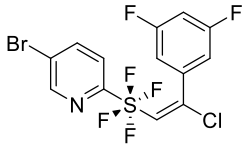
Prepared according to General Procedure, **3ab** was isolated as light-yellow oil (70 mg, 91%). HRMS (ESI$^+$): *m/z* calcd. for $C_{11}H_{13}BrClF_4NNaS$ [M+Na]$^+$: 403.9474 found: 403.9477. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.93 (t, *J* = 9.0 Hz, 3H), 1.45-1.33 (m, 2H), 1.65 (quint, *J* = 6.0 Hz, 2H), 2.78 (t, *J* = 9.0 Hz, 2H), 6.86 (quint, *J* = 9.0 Hz, 1H), 7.65 (d, *J* = 9.0 Hz, 1H), 7.98 (d, *J* = 9.0 Hz, 1H), 8.58 (d, *J* = 2.1 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 59.11 (d, *J* = 8.5 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 13.90, 22.28, 29.42, 35.96, 122.95-122.84 (m), 140.93, 141.91 (quint, *J* = 27.7 Hz), 144.76-144.53 (m), 148.31, 169.35-168.33 (m). ATR-FTIR (NaCl): *v* = 3095, 2959, 2934, 2872, 1447, 1093, 1005, 835, 757, 631 cm^{-1}.

(*E*)-5-Bromo-2-((2-chloro-2-(4-nitrophenyl)vinyl)tetrafluoro-λ^6-sulfaneyl)pyridine (**3ac**):



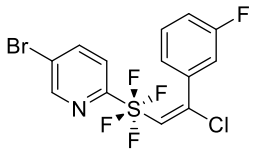
Prepared according to General Procedure, **3ac** was isolated as light-yellow solid (46 mg, 51%). mp: 100.9 °C; HRMS (ESI$^+$): *m/z* calcd. for $C_{13}H_8BrClF_4N_2NaO_2S$ [M+Na]$^+$: 468.9012 found: 468.8997. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.27 (quint, *J* = 6.0 Hz, 1H), 7.49 (d, *J* = 9.0 Hz, 1H), 7.61 (d, *J* = 6.0 Hz, 2H), 7.91 (d, *J* = 9.0 Hz, 1H), 8.26 (d, *J* = 9.0 Hz, 2H), 8.50 (d, *J* = 3.0 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 61.45 (d, *J* = 8.5 Hz, 4H), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 122.70-122.56 (m), 123.10, 123.63, 129.45, 136.55-136.31 (m), 140.97, 143.01, 144.39 (quint, *J* = 30.2 Hz), 148.21, 148.39, 168.46-167.48 (m). ATR-FTIR (KBr): *v* = 3423, 3107, 3084, 3054, 1602, 1568, 1288, 1092, 693, 608 cm^{-1}.

(*E*)-5-Bromo-2-((2-chloro-2-(3,5-difluorophenyl)vinyl)tetrafluoro-λ^6-sulfaneyl)pyridine (**3ad**):



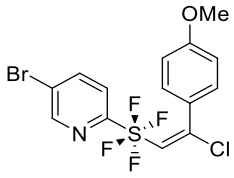
Prepared according to General Procedure, **3ad** was isolated as White solid (78 mg, 89%). mp: 84.4 °C; HRMS (ESI$^+$): *m/z* calcd. for $C_{13}H_7BrClF_6NNaS$ [M+Na]$^+$: 459.8973 found: 459.8956. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 6.86-6.79 (m, 1H), 6.97 (d, *J* = 6.0 Hz, 2H), 7.20 (quint, *J* = 9.0 Hz, 1H), 7.52 (d, *J* = 9.0 Hz, 1H), 7.92 (d, *J* = 6.0 Hz, 1H), 8.51 (d, *J* = 3.0 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): 61.12 (d, *J* = 8.5 Hz, 4F), −109.29 (s, 2F), ^{13}C NMR (126 MHz, $CDCl_3$): 105.14 (t, *J* = 25.2 Hz), 111.84-111.62 (m), 122.79-122.65 (m), 123.03, 139.37 (t, *J* = 10.1 Hz), 140.94, 143.95 (quint, *J* = 29.0 Hz), 148.38, 161.47 (d, *J* = 12.6 Hz), 163.46 (d, *J* = 12.6 Hz), 168.57-167.59 (m). ATR-FTIR (KBr): *v* = 3445, 3103, 2918, 2849, 1722, 1367, 1276, 1072, 880, 607 cm^{-1}.

(*E*)-5-Bromo-2-((2-chloro-2-(3-fluorophenyl)vinyl)tetrafluoro-λ^6-sulfaneyl)pyridine (**3ae**):



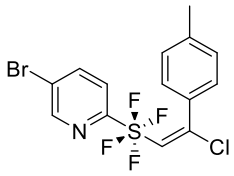
Prepared according to General Procedure, **3ae** was isolated as white solid (76 mg, 91%). mp: 89.6 °C; HRMS (ESI$^+$): *m/z* calcd. for $C_{13}H_8BrClF_5NNaS$ [M+Na]$^+$: 441.9067 found: 441.9068. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.08-7.03 (m, 1H), 7.23-7.14 (m, 3H), 7.35-7.30 (m, 1H), 7.48 (d, *J* = 9.0 Hz, 1H), 7.87 (d, *J* = 6.0 Hz, 1H), 8.49 (s, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 61.11 (d, *J* = 2.8 Hz, 4F), −112.87 (s, 1F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 115.48 (d, *J* = 23.9 Hz), 116.50 (d, *J* = 20.2 Hz), 122.76-122.62 (m), 122.85, 124.01, 129.90 (d, *J* = 8.8 Hz), 137.77-137.51 (m), 138.50 (d, *J* = 8.8 Hz), 140.81, 143.43 (quint, *J* = 29.0 Hz), 148.24, 162.05 (d, *J* = 245 Hz), 168.13 (quint, *J* = 31.5 Hz). ATR-FTIR (KBr): *v* = 3435, 3120, 3084, 3057, 1607, 1481, 1371, 968, 710, 596 cm^{-1}.

(*E*)-5-Bromo-2-((2-chloro-2-(4-methoxyphenyl)vinyl)tetrafluoro-λ^6-sulfaneyl)pyridine (**3af**):



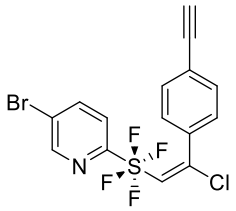
Prepared according to General Procedure, **3af** was isolated as white solid (61 mg, 71%). mp: 82.0 °C; HRMS (ESI$^+$): *m/z* calcd. for $C_{14}H_{11}BrClF_4NNaOS$ [M+Na]$^+$: 453.9267 found: 453.9266. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 3.81 (s, 3H), 6.89 (d, *J* = 9.0 Hz, 2H), 7.14 (quint, *J* = 9.0 Hz, 1H), 7.38 (d, *J* = 9.0 Hz, 2H), 7.50 (d, *J* = 9.0 Hz, 1H), 7.89 (d, *J* = 9.0 Hz, 1H), 8.50 (d, *J* = 2.1 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 60.92 (d, *J* = 8.5 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 55.35, 122.87-122.72 (m), 113.57, 128.89, 129.78, 139.67 (quint, *J* = 7.5 Hz), 140.76,168.48 (quint, *J* = 31.2 Hz), 142.66 (quint, *J* = 28.8 Hz), 148.21, 160.32. ATR-FTIR (KBr): *v* = 3053, 2917, 2848, 1636, 1457, 1174, 1116, 1006, 680, 545 cm^{-1}.

(*E*)-5-Bromo-2-((2-chloro-2-(*p*-tolyl)vinyl)tetrafluoro-λ^6-sulfaneyl)pyridine (**3ag**):



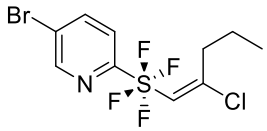
Prepared according to General Procedure, **3ag** was isolated as white solid (57 mg, 69%). mp: 100.5 °C; HRMS (ESI$^+$): *m/z* calcd. for $C_{14}H_{11}BrClF_4NNaS$ [M+Na]$^+$: 437.9318 found: 437.9311. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 3.27 (s, 3H), 7.24-7.12 (m, 3H), 7.32 (d, *J* = 9.0 Hz, 2H), 7.47 (d, *J* = 9.0 Hz, 1H), 7.83 (d, *J* = 9.0 Hz, 1H), 8.47 (d, *J* = 3.0 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 61.00 (d, *J* = 5.6 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 21.47, 122.85-122.68 (m), 128.04, 128.85, 133.90, 139.51, 139.86-139.61 (m), 140.72, 142.73 (quint, *J* = 29.0 Hz), 148.17, 168.92-167.92 (m). ATR-FTIR (KBr): *v* = 3083, 3054, 3029, 1637, 1507, 1446, 1368, 1005, 719, 531 cm^{-1}.

(*E*)-5-Bromo-2-((2-chloro-2-(4-ethynylphenyl)vinyl)tetrafluoro-λ^6-sulfaneyl)pyridine (**3ah**):



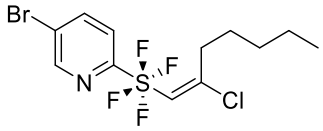
Prepared according to General Procedure, **3ah** was isolated as white solid (51 mg, 60%). mp: 125.5 °C; HRMS (ESI$^+$): *m/z* calcd. for $C_{15}H_9BrClF_4NNaS$ [M+Na]$^+$: 447.9161 found: 447.9157. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 3.12 (s, 1H), 7.20 (quint, *J* = 6.0 Hz, 1H), 7.39 (d, *J* = 6.0 Hz, 2H), 7.51-7.47 (m, 3H), 7.89 (d, *J* = 9.0 Hz, 1H), 8.49 (d, *J* = 3.0 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 61.16 (d, *J* = 8.5 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 78.75, 83.01, 122.87-122.71 (m), 123.41, 128.23, 131.97, 137.07, 138.51-138.39 (m), 140.84, 143.36 (quint, *J* = 29.0 Hz), 148.30, 168.76-167.77 (m). ATR-FTIR (KBr): *v* = 3228, 3098, 1497, 1444, 1363, 1092, 1007, 832, 741, 595 cm^{-1}.

(*E*)-5-Bromo-2-((2-chloropent-1-en-1-yl)tetrafluoro-λ^6-sulfaneyl)pyridine (**3ai**):



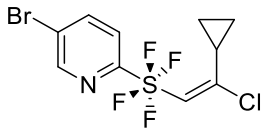
Prepared according to General Procedure, **3ai** was isolated as colorless oil (43 mg, 58%). HRMS (ESI$^+$): *m/z* calcd. for $C_{10}H_{11}BrClF_4NNaS$ [M+Na]$^+$: 389.9318 found: 389.9324. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.98 (t, *J* = 9.0 Hz, 3H), 1.77-1.65 (m, 2H), 2.77 (t, *J* = 9.0 Hz, 2H), 6.87 (quint, *J* = 9.0 Hz, 1H), 7.65 (d, *J* = 6.0 Hz, 1H), 7.98 (d, *J* = 9.0 Hz, 1H), 8.89 (d, *J* = 3.0 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 59.23 (d, *J* = 11.3 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 13.41, 20.61, 37.74, 122.96-122.84 (m), 140.93, 142.15 (quint, *J* = 27.7 Hz), 144.50-144.27 (m), 148.31, 169.34-168.32 (m). ATR-FTIR (NaCl): *v* = 3095, 2966, 2936, 2875, 1635, 1447, 1005, 834, 754, 631 cm^{-1}.

(*E*)-5-Bromo-2-((2-chlorohept-1-en-1-yl)tetrafluoro-λ^6-sulfaneyl)pyridine (**3aj**):



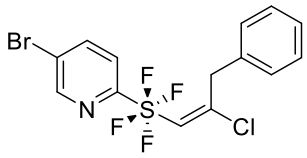
Prepared according to General Procedure, **3aj** was isolated as light-yellow oil. (71 mg, 90%). HRMS (ESI$^+$): *m/z* calcd. for $C_{12}H_{15}BrClF_4NNaS$ [M+Na]$^+$: 417.9631 found: 417.9614. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.90 (s, 3H), 1.34 (s, 4H), 2.78 (s, 4H), 6.85 (quint, *J* = 9.0 Hz, 1H), 7.65 (d, *J* = 9.0 Hz, 1H), 7.97 (d, *J* = 6.0 Hz, 1H), 8.58 (s, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 59.14 (d, *J* = 5.6 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 14.00, 22.50, 26.96, 31.16, 36.09, 122.89-122.80 (m), 140.89, 169.32-168.30 (m), 141.88 (quint, *J* = 27.7 Hz), 144.73-144.50 (m), 148.27. ATR-FTIR (NaCl): *v* = 3096, 2957, 2934, 2870, 1447, 1360, 1093, 1005, 758, 632 cm^{-1}.

(*E*)-5-Bromo-2-((2-chloro-2-cyclopropylvinyl)tetrafluoro-λ^6-sulfaneyl)pyridine (**3ak**):



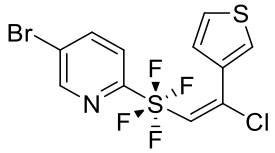
Prepared according to General Procedure, **3ak** was isolated as white solid (18 mg, 24%). mp: 88.7 °C; HRMS (ESI$^+$): *m/z* calcd. for $C_{10}H_9BrClF_4NNaS$ [M+Na]$^+$: 387.9161 found: 387.9143. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.96-0.89 (m, 2H), 1.10-1.05 (m, 2H), 2.70-2.61 (m, 1H), 6.96 (quint, *J* = 9.0 Hz, 1H), 7.67 (d, *J* = 9.0 Hz, 1H), 7.99 (d, *J* = 9.0 Hz, 1H), 8.59 (d, *J* = 3.0 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 59.60 (d, *J* = 8.5 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 7.60, 14.87-14.82 (m), 122.79, 122.99-122.84 (m), 140.94, 142.04 (quint, *J* = 27.7 Hz), 145.71-145.48 (m), 148.30, 169.56-168.53 (m). ATR-FTIR (KBr): *v* = 3436, 3118, 3099, 3057, 1621, 1444, 1368, 1094, 1006, 588 cm^{-1}.

(*E*)-5-Bromo-2-((2-chloro-3-phenylprop-1-en-1-yl)tetrafluoro-λ^6-sulfaneyl)pyridine (**3al**):



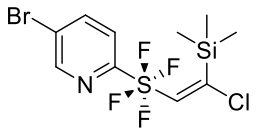
Prepared according to General Procedure, **3al** was isolated as light orange solid (17 mg, 20%). mp: 60.6 °C; HRMS (ESI$^+$): *m/z* calcd. for $C_{14}H_{11}BrClF_4NNaS$ [M+Na]$^+$: 437.9318 found: 437.9318. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 4.16 (s, 2H), 7.00 (quint, *J* = 6.0 Hz, 1H), 7.31-7.20 (m, 5H), 7.68 (d, *J* = 9.0 Hz, 1H), 7.99 (d, *J* = 9.0 Hz, 1H), 8.59 (s, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 59.89 (d, *J* = 8.5 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 41.70, 122.94-122.79 (m), 123.00, 127.34, 128.70, 129.19, 135.49, 141.02, 141.92-141.81 (m), 143.07 (quint, *J* = 27.7 Hz), 148.39, 168.95-168.45 (m). ATR-FTIR (KBr): *v* = 3280, 3088, 3060, 2924, 1601, 1554, 1284, 1224, 1116, 555 cm^{-1}.

(*E*)-5-Bromo-2-((2-chloro-2-(thiophen-3-yl)vinyl)tetrafluoro-λ^6-sulfaneyl)pyridine (**3am**):



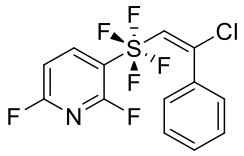
Prepared according to General Procedure, **3am** was isolated as light orange solid (58 mg, 71%). mp: 98.9 °C; HRMS (ESI$^+$): *m/z* calcd. for $C_{11}H_7BrClF_4NNaS_2$ [M+Na]$^+$: 429.8726 found: 429.8716. ^{1}H NMR (300 MHz, $CDCl_3$) : δ = 7.16 (quint, *J* = 6.0 Hz, 1H), 7.26-7.24 (m, 1H), 7.31-7.28 (m, 1H), 7.55 (d, *J* = 9.0 Hz, 1H), 7.60 (d, *J* = 3.0 Hz, 1H), 7.91 (d, *J* = 6.0 Hz, 1H), 8.53 (d, *J* = 3.0 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 60.59 (d, *J* = 8.5 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 122.88-122.74 (m), 125.45, 127.25-127.20 (m), 127.98, 134.63-134.39 (m), 135.50, 140.85, 142.60 (quint, *J* = 29.0 Hz), 148.30, 168.95-167.94 (m). ATR-FTIR (KBr): *v* = 3420, 3109, 3087, 3058, 1638, 1444, 1371, 1141, 878, 702 cm^{-1}.

(*E*)-5-Bromo-2-((2-chloro-2-(trimethylsilyl)vinyl)tetrafluoro-λ^6-sulfaneyl)pyridine (**3an**):



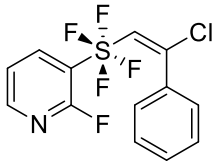
Prepared according to General Procedure, **3an** was isolated as white solid (26 mg, 33%). mp: 71.1 °C; HRMS (ESI$^+$): *m/z* calcd. for $C_{10}H_{13}BrClF_4NNaSSi$ [M+Na]$^+$: 419.9244 found: 419.9238. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.35 (s, 9H), 7.49 (quint, *J* = 9.0 Hz, 1H), 7.64 (d, *J* = 9.0 Hz, 1H), 7.98 (d, *J* = 9.0 Hz, 1H), 8.59 (d, *J* = 3.0 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 58.89 (d, *J* = 8.5 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 0.15, 0.28, 122.94-122.80 (m), 140.92, 147.17-147.03 (m), 148.43, 153.57 (quint, *J* = 27.5 Hz), 168.80-168.29 (m). ATR-FTIR (KBr): *v* = 3056, 2957, 2918, 2849, 1444, 1365, 1254, 1005, 715, 571 cm^{-1}.

(*E*)-3-((2-chloro-2-phenylvinyl)tetrafluoro-λ^6-sulfaneyl)-2,6-difluoropyridine (**3fa**):



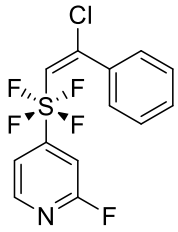
Prepared according to General Procedure, **3fa** was isolated as colorless oil (27 mg, 37%). HRMS (EI$^+$): *m/z* calcd. for $C_{13}H_8NF_6SCl$ [M]$^+$: 358.9970 found: 358.9998. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 6.78 (d, *J* = 9 Hz, 1H), 7.10–7.21 (m, 1H), 7.40 (brs, 5H), 8.08–8.16 (m, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = –63.10 (s, 1F), –58.45– –58.22 (m, 1F), 76.65 (dd, *J* = 5.64 Hz, 19.74 Hz), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 105.59–106.54 (m), 128.14 (d, *J* = 20.16 Hz), 129.59, 136.57, 139.69–140.10, 143.20 (quint, *J* = 46.62 Hz), 144.07–144.46 (m), 152.30 (d, *J* = 25.2 Hz), 155.68 (d, *J* = 26.46 Hz), 159.17 (d, *J* = 22.68 Hz), 162.50 (d, *J* = 23.94 Hz).

(*E*)-3-((2-chloro-2-phenylvinyl)tetrafluoro-λ^6-sulfaneyl)-2-fluoropyridine (**3ga**):



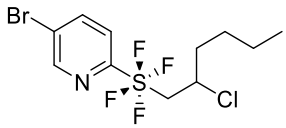
Prepared according to General Procedure, **3ga** was isolated as colorless oil (62 mg, 91%). HRMS (EI$^+$): *m/z* calcd. for $C_{13}H_9NF_5SCl$ [M]$^+$: 341.0064 found: 341.0077. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.15–7.20 (m, 2H), 7.33–7.44 (m, 5 H), 8.00–8.06 (m, 1H), 8.23 (d, *J* = 3 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = –60.30– –60.12 (m, 1F), 75.10 (dd, *J* = 8.46 Hz, 22.56 Hz), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 121.37 (d, *J* = 8.82 Hz), 128.08, 128.17, 129.51, 136.65, 139.53–139.66 (m), 140.53–141.65 (m), 142.61–144.13 (m), 149.34 (d, *J* = 25.2 Hz), 153.45, 156.71. ATR-FTIR (KBr): *v* = 3083, 1643, 1587, 1438, 902, 765, 671 cm^{-1}.

(*E*)-4-((2-chloro-2-phenylvinyl)tetrafluoro-λ^6-sulfaneyl)-2-fluoropyridine (**3ha**):



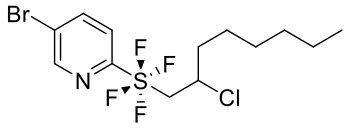
Prepared according to General Procedure, **3ha** was isolated as colorless oil (41 mg, 60%). HRMS (EI$^+$): *m/z* calcd. for $C_{13}H_9NF_5SCl$ [M]$^+$: 341.0064 found: 341.0090. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.10–7.21 (m, 2H), 7.35–7.42 (m, 6H), 8.23 (d, *J* = 3 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = –65.19 (s, 1F), 69.57 (d, *J* = 8.46 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 107.38–107.89 (m), 118.16–118.36 (m), 128.02, 128.25, 129.62, 126.57, 140.01 (quint, *J* = 7.56 Hz), 142.92 (quint, *J* = 27.72 Hz), 148.12 (d, *J* = 15.12 Hz), 162.57, 164.49, 168.94–169.91.

5-Bromo-2-((2-chlorohexyl)tetrafluoro-λ^6-sulfaneyl)pyridine (**5aa**):



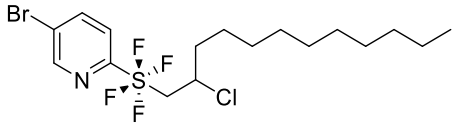
Prepared according to General Procedure, **5aa** was isolated as colorless oil (52 mg, 68%). HRMS (ESI$^+$): *m/z* calcd. for $C_{11}H_{15}BrClF_4NNaS$ [M+Na]$^+$: 405.9631 found: 451.9634. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.93 (t, *J* = 6.0 Hz, 3H), 1.62-1.29 (m, 4H), 1.84-1.73 (m, 1H), 2.16-2.04 (m, 1H), 4.41-4.11 (m, 2H), 4.60-4.52 (m, 1H), 7.62 (d, *J* = 9.0 Hz, 1H), 7.96 (d, *J* = 9.0 Hz, 1H), 8.56 (d, *J* = 3.0 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 57.47 (t, *J* = 8.5 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 11.97, 22.02, 28.28, 37.38, 57.28 (quint, *J* = 5.0 Hz), 81.99 (quint, *J* = 18.9 Hz), 122.64, 122.76 (quint, *J* = 3.8 Hz), 140.82, 148.11, 168.85 (quint, *J* = 31.5 Hz), ATR-FTIR (NaCl): *v* = 3055, 2959, 2931, 2872, 1563, 1447, 1360, 1005, 811, 740 cm^{-1}.

5-Bromo-2-((2-chlorooctyl)tetrafluoro-λ^6-sulfaneyl)pyridine (**5ab**):



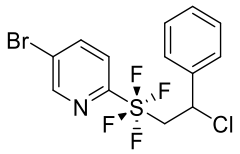
Prepared according to General Procedure, **5ab** was isolated as white solid (57 mg, 69%). mp: 29.4 °C; HRMS (ESI$^+$): *m/z* calcd. for $C_{13}H_{19}BrClF_4NNaS$ [M+Na]$^+$: 433.9944 found: 433.9942. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.89 (t, *J* = 6.0 Hz, 3H), 1.30 (brs, 6H), 1.62-1.35 (m, 2H), 1.84-1.73 (m, 1H), 2.17-2.03 (m, 1H), 4.41-4.11 (m, 2H), 4.60-4.52 (m, 1H), 7.63 (d, *J* = 9.0 Hz, 1H), 7.96 (d, *J* = 9.0 Hz, 1H), 8.56 (d, *J* = 3.0 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 57.60 (t, *J* = 8.5 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 14.05, 22.54, 26.08, 28.50, 31.62, 37.64, 57.26 (quint, *J* = 5.0 Hz), 81.96 (quint, *J* = 18.8 Hz), 122.60, 122.71 (quint, *J* = 3.8 Hz), 140.77, 148.08, 168.82 (quint, *J* = 32.5 Hz), ATR-FTIR (KBr): *v* = 3117, 3052, 2927, 2853, 1566, 1363, 1092, 919, 714, 583 cm^{-1}.

5-Bromo-2-((2-chlorododecyl)tetrafluoro-λ^6-sulfaneyl)pyridine (**5ac**):



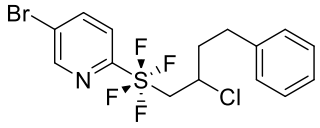
Prepared according to General Procedure, **5ac** was isolated as light-yellow oil (66 mg, 71%). HRMS (ESI$^+$): *m/z* calcd. for $C_{17}H_{27}BrClF_4NNaS$ [M+Na]$^+$: 490.0570 found: 490.0576. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.88 (t, *J* = 6.0 Hz, 3H), 1.27 (brs, 14H), 1.62-1.43 (m, 2H), 1.85-1.73 (m, 1H), 2.17-2.03 (m, 1H), 4.41-4.10 (m, 2H), 4.60-4.52 (m, 1H), 7.63 (d, *J* = 9.0 Hz, 1H), 7.96 (d, *J* = 9.0 Hz, 1H), 8.56 (d, *J* = 3.0 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 57.56 (t, *J* = 8.5 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 14.25, 22.81, 26.24, 28.96, 29.44, 29.56, 29.67 (d, *J* = 5.0 Hz), 32.01, 37.77, 57.42-57.30 (m), 82.08 (quint, *J* = 18.8 Hz), 122.79 (quint, *J* = 3.8 Hz), 140.88, 148.20, 168.94 (quint, *J* = 32.5 Hz). ATR-FTIR (NaCl): *v* = 2925, 2854, 1447, 1360, 1005, 831, 808, 742, 623, 603 cm^{-1}.

5-Bromo-2-((2-chloro-2-phenylethyl)tetrafluoro-λ^6-sulfaneyl)pyridine (**5ad**):



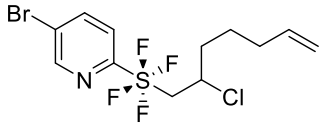
Prepared according to General Procedure, **5ad** was isolated as white solid (63 mg, 78%). mp: 88.5 °C; HRMS (ESI$^+$): *m/z* calcd. for $C_{13}H_{11}BrClF_4NNaS$ [M+Na]$^+$: 425.9318 found: 425.9305. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 4.68-4.55 (m, 2H), 5.57 (t, *J* = 6.0 Hz, 1H), 7.42-7.36 (m, 3H), 7.47-7.45 (m, 2H), 7.57 (d, *J* = 9.0 Hz, 1H), 7.92 (d, *J* = 9.0 Hz, 1H), 8.53 (d, *J* = 3.0 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 57.93 (t, *J* = 8.5 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 57.60 (quint, *J* = 5.0 Hz), 81.70 (quint, *J* = 18.8 Hz), 122.82 (quint, *J* = 5.0 Hz), 127.29, 129.05, 129.11, 139.52, 140.86, 148.21, 168.70 (quint, *J* = 32.5 Hz), ATR-FTIR (KBr): *v* = 3445, 3068, 3034, 2985, 1445, 1093, 1006, 942, 837, 623 cm^{-1}.

5-Bromo-2-((2-chloro-4-phenylbutyl)tetrafluoro-λ^6-sulfaneyl)pyridine (**5ae**):



Prepared according to General Procedure, **5ae** was isolated as white solid (51 mg, 59%). mp: 59.9 °C; HRMS (ESI$^+$): *m/z* calcd. for $C_{15}H_{15}BrClF_4NNaS$ [M+Na]$^+$: 453.9631 found: 453.9637. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.15-2.02 (m, 1H), 2.50-2.39 (m, 1H), 2.85-2.75 (m, 1H), 3.02-2.93 (m, 1H), 4.41-4.15 (m, 2H), 4.57-4.48 (m, 1H), 7.23-7.21 (m, 2H), 7.32-7.28 (m, 3H), 7.60 (d, *J* = 9.0 Hz, 1H), 7.95 (d, *J* = 9.0 Hz, 1H), 8.55 (d, *J* =3.0 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 57.78 (t, *J* = 8.5 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 32.51, 39.30, 56.66 (quint, *J* = 3.8 Hz), 81.79 (quint, *J* = 17.5 Hz), 122.90-122.78 (m), 126.42, 128.68 (d, *J* = 3.8 Hz), 140.36, 140.91, 148.22, 168.85 (quint, *J* = 31.2 Hz), ATR-FTIR (KBr): *v* = 3437, 3030, 2949, 2924, 1948, 1725, 1446, 1357, 1093, 913 cm^{-1}.

5-Bromo-2-((2-chlorohept-6-en-1-yl)tetrafluoro-λ^6-sulfaneyl)pyridine (**5af**):



Prepared according to General Procedure, **5af** was isolated as light-yellow oil (44 mg, 55%). HRMS (ESI$^+$): *m/z* calcd. for $C_{12}H_{15}BrClF_4NNaS$ $[M+Na]^+$: 417.9631 found: 417.9626. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.87-1.52 (m, 3H), 2.16-2.05 (m, 3H), 4.39-4.13 (m, 2H), 4.61-4.53 (m, 1H), 5.07-4.97 (m, 2H), 5.87-5.74 (m, 1H), 7.62 (d, *J* = 6.0 Hz, 1H), 7.96 (d, *J* = 9.0 Hz, 1H), 8.56 (d, *J* = 2.4 Hz, 1H), ^{19}F NMR (282 MHz, $CDCl_3$): δ = 57.57 (t, *J* = 8.5 Hz, 4F), ^{13}C NMR (126 MHz, $CDCl_3$): δ = 25.44, 32.99, 37.13, 57.18 (quint, *J* = 37.5 Hz), 81.96 (quint, *J* = 18.8 Hz), 115.31, 122.82 (quint, *J* = 5.0 Hz), 138.03, 140.90, 148.22, 168.90 (quint, *J* = 31.2 Hz), ATR-FTIR (NaCl): *v* = 3077, 2930, 2862, 1639, 1442, 1320, 1159, 1098, 1008, 914 cm^{-1}.

Reference:

1. (a) Z. Zhou, R. G. Parr and J. F. Garst, *Tetrahedron Lett.,* 1988, **29**, 4843–4846; (b) Z. Zhou and R. G. Parr, *J. Am. Chem. Soc*., 1989, **111**, 7371–7379; (c) R. G. Parr and Z. Zhou, Acc. *Chem. Res.,* 1993, **26**, 256–258; (d) R. G. Pearson, *Acc. Chem. Res*., 1993, **26**, 250-255; (e) S. Š.-Halilović, M. Salihović, E. Veljović, A. Osmanović, S. Trifunović and D. Završnik, *Bulletin of the Chemists and Technologists of Bosnia and Herzegovina*, 2014, **43**, 57-60; (f) S. Armaković, S. J. Armaković and B. F. Abramović, *J Mol. Model*., 2016, **22**, 240–254.
2. O. S. Kanishchev and W. R. Dolbier, Jr *Angew. Chem. Int. Ed.,* 2015, **54**, 280–284.
3. M. Kosobokov, B. Cui, A. Balia, K. Matsuzaki, E. Tokunaga, N. Saito and N. Shibata, *Angew. Chem. Int. Ed.,* 2016, **55**, 10781–10785.

Crystal Data:

Bond precision:	C-C = 0.0032 Å		Wavelength=0.71075
Cell:	a = 6.18585(12)	b = 19.0140(5)	c = 13.0299(3)
	alpha = 90	beta = 104.0863(7)	gamma = 90
Temperature:	173 K		

	Calculated	Reported
Volume	1486.46(6)	1486.46(6)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C13 H9 Br Cl F4 N S	C13 H9 Br Cl F4 N S
Sum formula	C13 H9 Br Cl F4 N S	C13 H9 Br Cl F4 N S
Mr	402.62	402.63
Dx,g cm^{-3}	1.799	1.799
Z	4	4
Mu (mm-1)	3.119	3.127
F000	792.0	792.0
F000’	792.38	
h,k,lmax	8,24,16	8,24,16
Nref	3380	3375
Tmin, Tmax	0.694,0.791	0.607,0.791
Tmin’	0.242	

Correction method = # Reported T Limits: Tmin = 0.607 Tmax = 0.791

AbsCorr = MULTI-SCAN

Data completeness = 0.999 Theta (max) = 27.450

R(reflections) = 0.0243 (3039) wR2(reflections) = 0.0607 (3375)

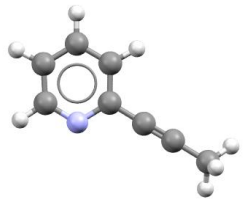
S = 1.095 Npar = 190

Computational Details

The calculations were performed in Spartan'14 software using B3LYP/6-311+G** level of theory for all the compounds.

The optimized geometry coordinates of the compounds are given below:

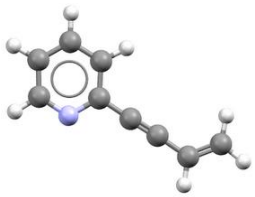
1. Pyridine–C≡C–Me



	Coordinates (Angstroms)		
ATOM	X	Y	Z
1 H	2.714269	-2.110467	0.001140
2 C	2.151493	-1.183572	0.000530
3 N	0.692389	1.203972	-0.000845
4 C	0.763273	-1.206063	-0.000661
5 C	2.803984	0.046476	0.001165
6 C	2.025296	1.203070	0.000377
7 C	0.063603	0.012505	-0.001249
8 H	0.214214	-2.139332	-0.000929
9 H	3.885325	0.113521	0.002344
10 H	2.497795	2.181926	0.000806
11 C	-1.367973	0.018619	-0.001858
12 C	-2.573983	0.002179	-0.001391
13 C	-4.029568	0.003044	0.001110
14 H	-4.418057	-0.009738	1.024106
15 H	-4.426493	-0.873502	-0.519056
16 H	-4.420052	0.896786	-0.493977

Point Group: c1 Number of degrees of freedom: 42

2. Pyridine–C≡C–CH=CH_2

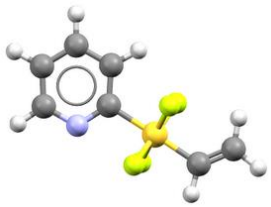


	Coordinates (Angstroms)		
ATOM	X	Y	Z
1 H	2.975310	-2.251387	0.000000

2 C	2.492221	-1.280800	0.000000
3 N	1.239528	1.222552	0.000000
4 C	1.106900	-1.187271	0.000000
5 C	3.244935	-0.109570	0.000000
6 C	2.566780	1.109743	0.000000
7 C	0.512829	0.086810	0.000000
8 H	0.481464	-2.070971	0.000000
9 H	4.327998	-0.133881	0.000000
10 H	3.120488	2.044726	0.000000
11 C	-0.908678	0.216001	0.000000
12 C	-2.116299	0.296627	0.000000
13 C	-3.524676	0.454241	0.000000
14 H	-3.886694	1.480018	0.000000
15 C	-4.406127	-0.556130	0.000000
16 H	-5.471945	-0.361972	0.000000
17 H	-4.084795	-1.591200	0.000000

Point Group: cs Number of degrees of freedom: 31

3. Pyridine–SF_4–$CH=CH_2$



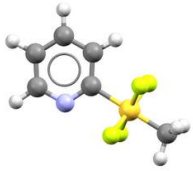
Coordinates (Angstroms)

ATOM	X	Y	Z
1 H	3.429841	-2.275940	0.000000
2 C	2.923499	-1.317681	0.000000
3 N	1.617212	1.127150	0.000000
4 C	1.533040	-1.271294	0.000000
5 C	3.650606	-0.128174	0.000000
6 C	2.955620	1.075933	0.000000
7 C	0.970261	0.000099	0.000000
8 H	0.926941	-2.163609	0.000000
9 H	4.733709	-0.133215	0.000000
10 H	3.472486	2.029561	0.000000
11 S	-0.916213	0.152963	0.000000
12 F	-0.992170	-1.064368	-1.192513
13 F	-0.839177	1.329375	1.203855
14 F	-0.992170	-1.064368	1.192513
15 F	-0.839177	1.329375	-1.203855

16 C	-2.735945	0.346398	0.000000
17 H	-2.982393	1.397612	0.000000
18 C	-3.568527	-0.673769	0.000000
19 H	-4.635937	-0.481863	0.000000
20 H	-3.235489	-1.702296	0.000000

Point Group: cs Number of degrees of freedom: 35

4. Py-SF_4-Me (**6a**)

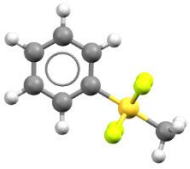


Coordinates (Angstroms)

ATOM	X	Y	Z
1 H	3.368072	-2.078240	0.000000
2 C	2.791514	-1.160610	0.000000
3 N	1.306232	1.180505	0.000000
4 C	1.401500	-1.218381	0.000000
5 C	3.427941	0.080226	0.000000
6 C	2.645057	1.229317	0.000000
7 C	0.745902	0.008045	0.000000
8 H	0.863507	-2.153278	0.000000
9 H	4.508398	0.156195	0.000000
10 H	3.089115	2.218978	0.000000
11 S	-1.146020	0.017350	0.000000
12 C	-2.988271	0.020244	0.000000
13 H	-3.303231	-0.493466	0.902031
14 H	-3.303231	-0.493466	-0.902031
15 H	-3.281784	1.065043	0.000000
16 F	-1.124382	-1.206799	-1.195584
17 F	-1.160048	1.191039	1.208825
18 F	-1.124382	-1.206799	1.195584
19 F	-1.160048	1.191039	-1.208825

Point Group: cs Number of degrees of freedom: 32

5. Ph-SF_4-Me (**6b**)

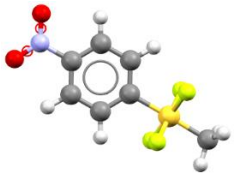


Coordinates (Angstroms)

ATOM	X	Y	Z
1 H	3.313556	-2.137495	0.000000
2 C	2.773554	-1.197957	0.000000
3 C	1.370073	1.220175	0.000000
4 C	1.379827	-1.214779	0.000000
5 C	3.465004	0.011338	0.000000
6 C	2.763772	1.214999	0.000000
7 C	0.708325	-0.000011	0.000000
8 H	0.838625	-2.148964	0.000000
9 H	4.548895	0.015777	0.000000
10 H	3.295996	2.158957	0.000000
11 H	0.821298	2.149956	0.000000
12 S	-1.144817	-0.006917	0.000000
13 C	-2.991236	0.035155	0.000000
14 H	-3.314690	-0.472923	0.902100
15 H	-3.314690	-0.472923	-0.902100
16 H	-3.264275	1.084747	0.000000
17 F	-1.152515	-1.214469	-1.194567
18 F	-1.156879	1.190735	1.208040
19 F	-1.152515	-1.214469	1.194567
20 F	-1.156879	1.190735	-1.208040

Point Group: cs Number of degrees of freedom: 34

6. NO_2-SF_4-Ph-Me (**6c**)



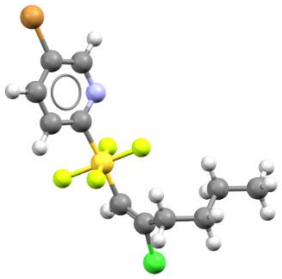
Coordinates (Angstroms)

ATOM	X	Y	Z
1 H	2.379268	-2.140197	0.000000
2 C	1.818063	-1.216216	0.000000
3 C	0.422751	1.216791	0.000000
4 C	0.427106	-1.220467	0.000000
5 C	2.486251	0.002079	0.000000
6 C	1.813603	1.217920	0.000000
7 C	-0.241960	-0.003043	0.000000
8 H	-0.115009	-2.153864	0.000000
9 H	2.371337	2.143982	0.000000
10 H	-0.122633	2.148294	0.000000
11 S	-2.096864	-0.005731	0.000000

12 C	-3.941407	0.039950	0.000000
13 H	-4.265616	-0.467514	0.902346
14 H	-4.265616	-0.467514	-0.902346
15 H	-4.212122	1.090271	0.000000
16 F	-2.094075	-1.209083	-1.191837
17 F	-2.093395	1.187922	1.204833
18 F	-2.094075	-1.209083	1.191837
19 F	-2.093395	1.187922	-1.204833
20 N	3.969445	0.004957	0.000000
21 O	4.532146	1.090922	0.000000
22 O	4.536370	-1.078787	0.000000

Point Group: cs Number of degrees of freedom: 38

7. Compound **3ab**



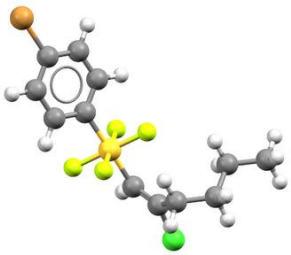
Coordinates (Angstroms)

ATOM	X	Y	Z
1 H	3.347610	-1.664357	-1.333369
2 C	2.982092	-0.837031	-0.736704
3 C	1.960583	1.246087	0.740452
4 N	1.676820	-0.561564	-0.806783
5 C	3.834064	-0.087329	0.069577
6 C	3.320409	0.967430	0.820870
7 C	1.214333	0.429565	-0.101949
8 H	3.965471	1.561505	1.455667
9 H	1.513843	2.052308	1.301718
10 S	-0.637135	0.755313	-0.276211
11 C	-2.398059	1.182043	-0.476540
12 C	-3.428102	0.717181	0.221404
13 H	-2.482284	1.913370	-1.264349
14 F	-0.957893	-0.880345	-0.072802
15 F	-0.721378	0.976709	1.416289
16 F	-0.534604	0.558917	-1.937458
17 F	-0.286521	2.413907	-0.457907
18 Cl	-4.989678	1.417408	-0.251109
19 C	-3.523390	-0.264892	1.348508
20 H	-3.925948	0.276359	2.212101

21 H	-2.521668	-0.594473	1.613596
22 C	-4.425380	-1.483261	1.056701
23 H	-4.429166	-2.101258	1.961400
24 H	-5.456731	-1.146646	0.910793
25 C	-3.987820	-2.333191	-0.141696
26 H	-2.949415	-2.651628	-0.005255
27 H	-3.998193	-1.720658	-1.049636
28 C	-4.885636	-3.556509	-0.346667
29 H	-4.866312	-4.214663	0.527608
30 H	-4.563881	-4.143864	-1.210882
31 H	-5.926046	-3.260801	-0.515258
32 Br	5.690818	-0.508278	0.133036

Point Group: c1 Number of degrees of freedom: 90

8. Compound **3ab'**



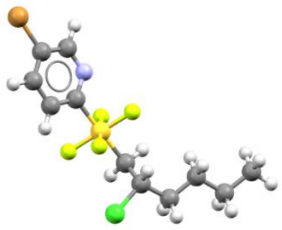
Coordinates (Angstroms)

ATOM	X	Y	Z
1 H	3.491557	-1.701226	-1.372877
2 C	3.058693	-0.896188	-0.794035
3 C	1.946918	1.191815	0.700869
4 C	1.695778	-0.626069	-0.891374
5 C	3.851778	-0.123146	0.048239
6 C	3.309361	0.917539	0.795851
7 C	1.164700	0.414238	-0.141729
8 H	1.070870	-1.219168	-1.542432
9 H	3.935491	1.512845	1.447300
10 H	1.515598	1.996452	1.277820
11 S	-0.646478	0.777144	-0.271738
12 C	-2.413299	1.199618	-0.468106
13 C	-3.440189	0.729643	0.230867
14 H	-2.499514	1.933165	-1.253628
15 F	-0.988864	-0.873823	-0.101083
16 F	-0.733026	0.973356	1.409831
17 F	-0.569453	0.584519	-1.951667
18 F	-0.303922	2.424902	-0.447340
19 Cl	-5.003670	1.430139	-0.235404
20 C	-3.530905	-0.254203	1.357136

21 H	-3.923770	0.288231	2.224531
22 H	-2.528609	-0.588653	1.613838
23 C	-4.440111	-1.468893	1.073408
24 H	-4.441483	-2.084377	1.979824
25 H	-5.470701	-1.128410	0.932232
26 C	-4.012937	-2.324658	-0.124355
27 H	-2.972684	-2.640670	0.004615
28 H	-4.033565	-1.717064	-1.035736
29 C	-4.910051	-3.551490	-0.312313
30 H	-4.878676	-4.204037	0.565952
31 H	-4.597012	-4.143726	-1.176458
32 H	-5.953198	-3.259728	-0.470725
33 Br	5.721538	-0.497796	0.177607

Point Group: c1 Number of degrees of freedom: 93

9. Compound **5aa**



Coordinates (Angstroms)

ATOM	X	Y	Z
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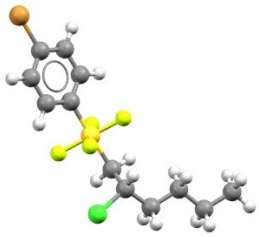
3 F	-0.576295	1.153775	0.975973
4 F	-0.765308	-1.155025	0.412165
5 F	-0.397982	-0.601259	-1.916447
6 F	-0.237666	1.715326	-1.322956
7 C	-2.353640	0.384926	-0.781391
8 H	-2.433790	1.032198	-1.650581
9 H	-2.582450	-0.641323	-1.054997
10 C	-3.239375	0.836272	0.365275
11 H	-2.851180	0.500136	1.323457
12 C	-4.679232	0.338236	0.167388
13 H	-5.310317	0.883505	0.874114
14 H	-5.024439	0.619930	-0.834048
15 C	-4.864783	-1.170355	0.390995
16 H	-4.512297	-1.438202	1.394593
17 H	-4.251935	-1.747910	-0.310176
18 C	-6.328403	-1.598992	0.232776

19 H	-6.945643	-1.045272	0.949859
20 H	-6.681920	-1.305910	-0.763185
21 C	-6.540755	-3.102818	0.425695
22 H	-5.955351	-3.681459	-0.295682
23 H	-7.591496	-3.374151	0.292815
24 H	-6.240422	-3.423375	1.428098
25 C	1.357685	0.097007	-0.229264
26 C	3.996044	-0.221456	0.083936
27 N	1.848899	-1.087404	-0.451681
28 C	2.082917	1.218053	0.159786
29 C	3.452290	1.038749	0.320549
30 C	3.163768	-1.268550	-0.301955
31 H	1.614468	2.175752	0.327762
32 H	4.081434	1.865726	0.623189
33 H	3.552653	-2.261529	-0.494214
34 Br	5.868268	-0.522787	0.280758

Point Group: c1 Number of degrees of freedom: 96

10. Compound **5aa'**



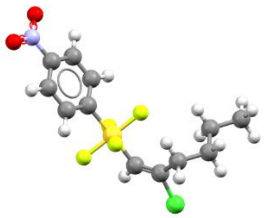
Coordinates (Angstroms)

ATOM	X	Y	Z
1 Cl	-3.221727	2.704652	0.391069
2 S	-0.518791	0.236558	-0.460667
3 F	-0.595309	1.120678	0.973337
4 F	-0.806557	-1.196058	0.426919
5 F	-0.436096	-0.668745	-1.905267
6 F	-0.254839	1.662387	-1.329611
7 C	-2.373647	0.358746	-0.778793
8 H	-2.442159	0.967218	-1.676465
9 H	-2.614887	-0.675821	-1.004813
10 C	-3.252902	0.876031	0.343858
11 H	-2.882789	0.560399	1.316178
12 C	-4.706393	0.416808	0.150986
13 H	-5.321139	0.998021	0.843426
14 H	-5.039875	0.687022	-0.857480
15 C	-4.941739	-1.079651	0.407573
16 H	-4.586226	-1.340432	1.412011

17 H	-4.359163	-1.691809	-0.290366
18 C	-6.422159	-1.457871	0.276841
19 H	-7.007739	-0.873788	0.996359
20 H	-6.780737	-1.164504	-0.717159
21 C	-6.684520	-2.950605	0.491956
22 H	-6.133082	-3.557942	-0.232769
23 H	-7.746588	-3.185473	0.380787
24 H	-6.377998	-3.270217	1.492860
25 C	1.303571	0.020534	-0.232348
26 C	4.011857	-0.287226	0.112058
27 C	1.867914	-1.231818	-0.429941
28 C	2.063731	1.123015	0.133795
29 C	3.436173	0.963876	0.308859
30 C	3.241476	-1.386129	-0.255486
31 H	1.260576	-2.077954	-0.714492
32 H	1.609186	2.091434	0.281780
33 H	4.044510	1.811331	0.594954
34 H	3.699055	-2.354927	-0.406877
35 Br	5.898043	-0.497497	0.350640

Point Group: c1 Number of degrees of freedom: 99

11. **3ab''**



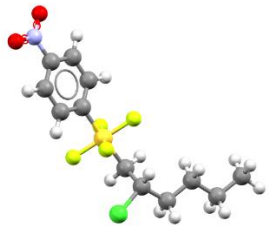
Coordinates (Angstroms)

ATOM	X	Y	Z
1 H	3.853543	-1.878098	-1.292050
2 C	3.418173	-1.053702	-0.744752
3 C	2.354301	1.105186	0.695639
4 C	2.065554	-0.750280	-0.857854
5 C	4.213667	-0.275368	0.086841
6 C	3.706251	0.797924	0.808595
7 C	1.561169	0.323954	-0.135391
8 H	1.426495	-1.339606	-1.497820
9 H	4.360521	1.378746	1.443671
10 H	1.936491	1.934305	1.246533
11 N	5.655924	-0.600617	0.206850
12 O	6.329970	0.089873	0.958751
13 O	6.079709	-1.539127	-0.453330

14 S	-0.243837	0.733067	-0.290032
15 C	-1.994900	1.194686	-0.516366
16 C	-3.039512	0.776560	0.190327
17 H	-2.055227	1.897540	-1.331960
18 F	-0.622173	-0.900348	-0.066786
19 F	-0.327629	0.981954	1.381731
20 F	-0.150389	0.485334	-1.959678
21 F	0.154093	2.359617	-0.514599
22 Cl	-4.579034	1.493019	-0.321666
23 C	-3.164401	-0.156753	1.355935
24 H	-3.555488	0.432092	2.193379
25 H	-2.173218	-0.501932	1.640527
26 C	-4.096954	-1.363197	1.113834
27 H	-4.134383	-1.929392	2.050811
28 H	-5.115129	-1.006578	0.929921
29 C	-3.661918	-2.291023	-0.025413
30 H	-2.631663	-2.620305	0.144166
31 H	-3.650503	-1.734995	-0.969186
32 C	-4.578981	-3.509798	-0.165450
33 H	-4.575897	-4.114918	0.746556
34 H	-4.261679	-4.153076	-0.990598
35 H	-5.613216	-3.208258	-0.359113

Point Group: c1 Number of degrees of freedom: 99

12. **5aa''**

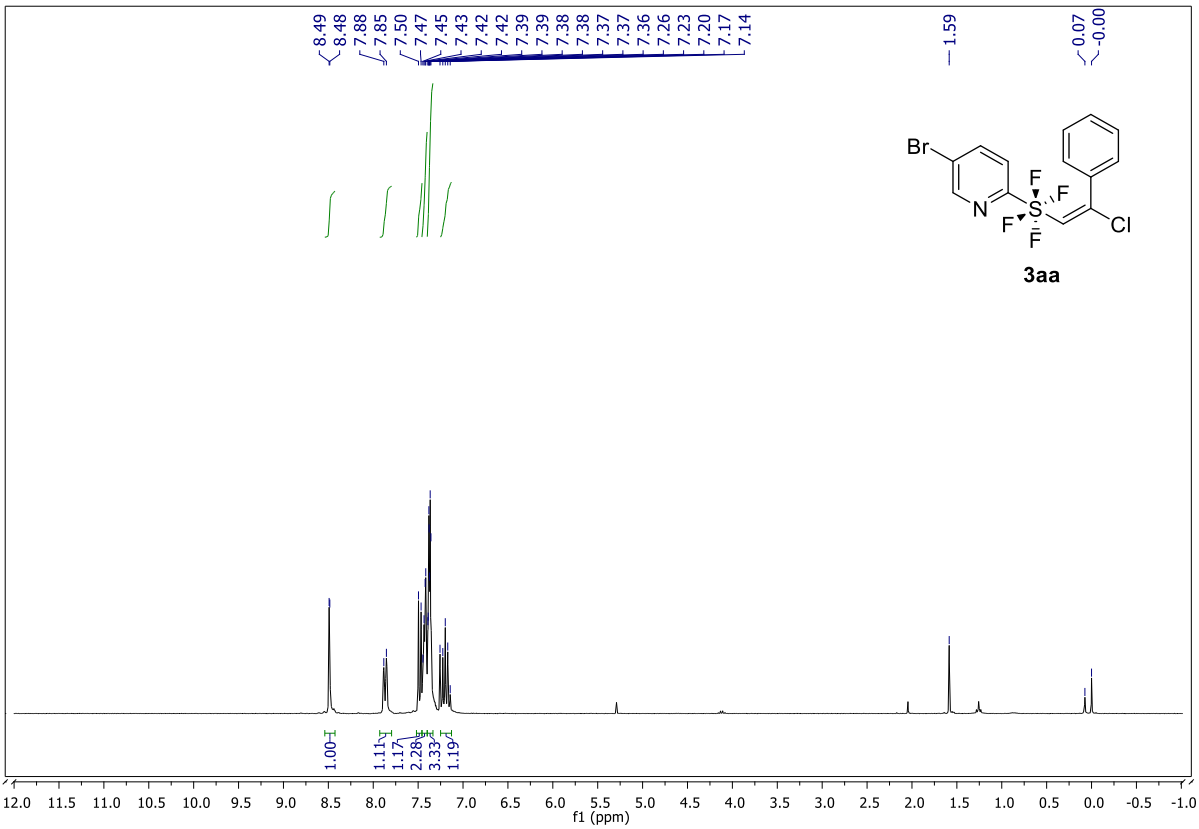


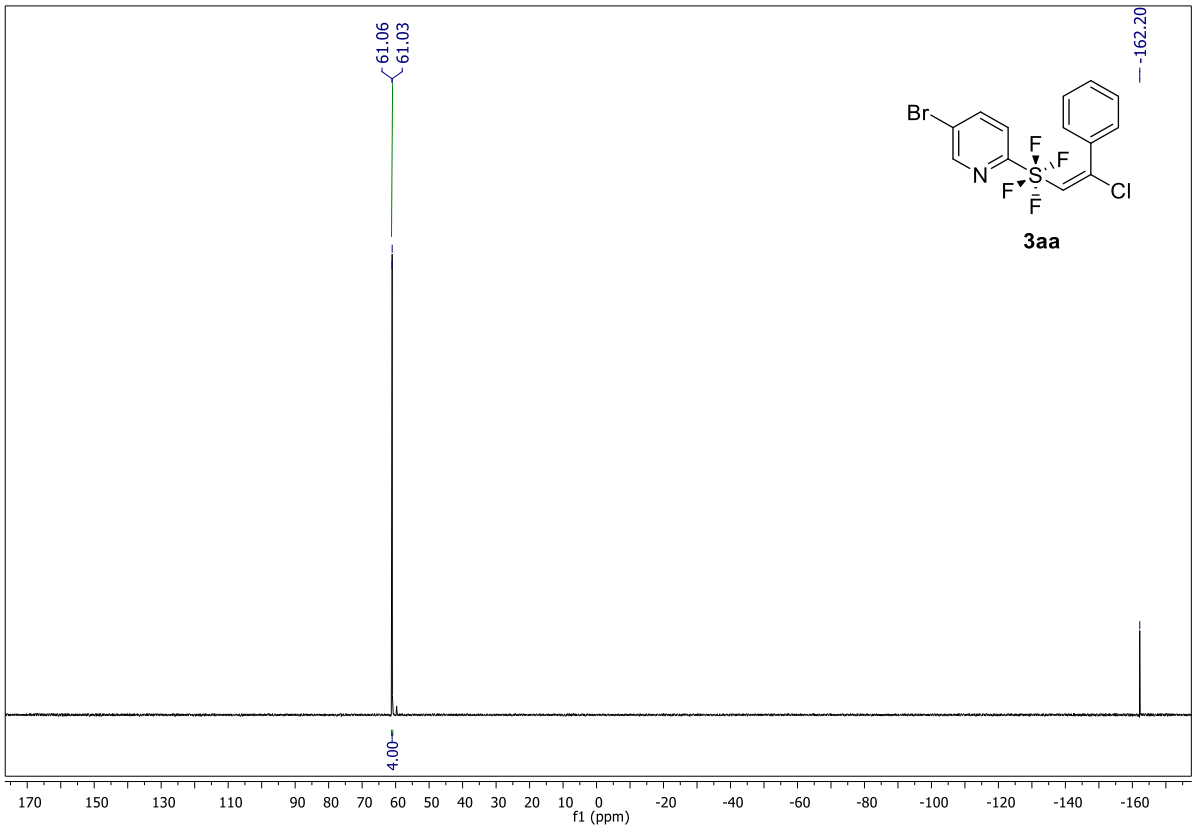
Coordinates (Angstroms)

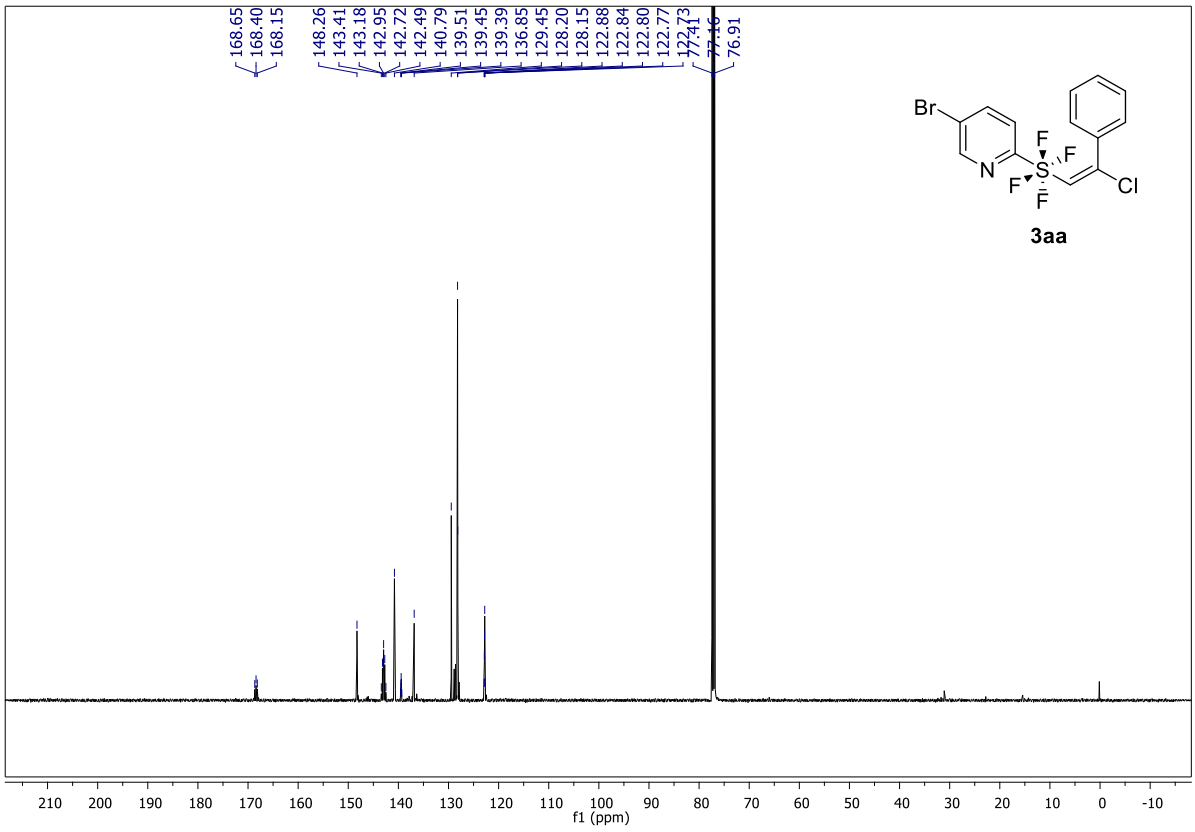
ATOM	X	Y	Z
1 Cl	2.811514	2.737701	-0.327113
2 S	0.116080	0.227158	0.455953
3 F	0.192329	1.116091	-0.972289
4 F	0.435046	-1.195079	-0.432855
5 F	0.015367	-0.683149	1.893218
6 F	-0.197172	1.640145	1.322942
7 C	1.962170	0.377133	0.804997
8 H	2.006780	0.985662	1.704363
9 H	2.214866	-0.654216	1.034322
10 C	2.848326	0.909628	-0.305640

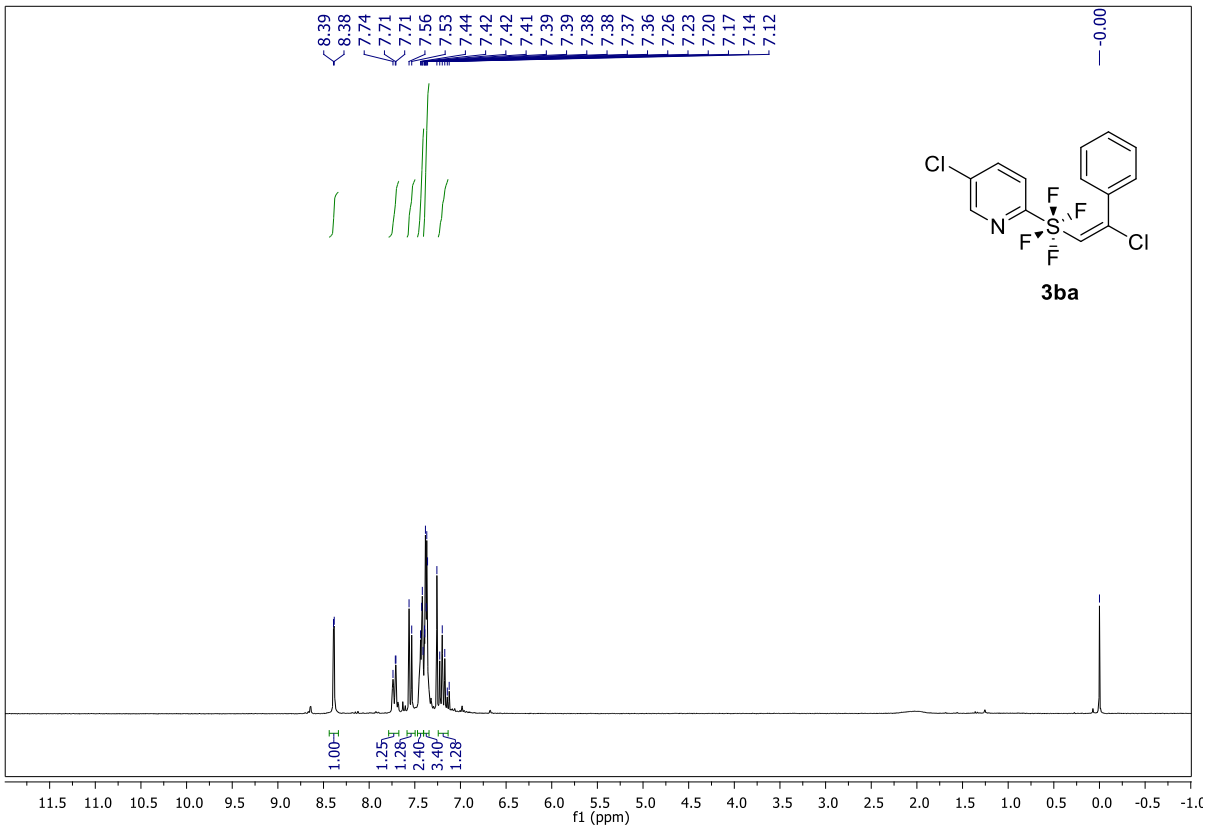
11 H	2.484992	0.606469	-1.284354
12 C	4.299069	0.442518	-0.112014
13 H	4.922940	1.044270	-0.778052
14 H	4.623917	0.675224	0.908385
15 C	4.526522	-1.045791	-0.419556
16 H	4.191811	-1.263125	-1.441137
17 H	3.920295	-1.677372	0.240067
18 C	5.998870	-1.446612	-0.268287
19 H	6.608879	-0.840274	-0.948015
20 H	6.335447	-1.199518	0.745699
21 C	6.248865	-2.932384	-0.540229
22 H	5.672537	-3.562617	0.144332
23 H	7.304735	-3.185617	-0.413412
24 H	5.963401	-3.205159	-1.560829
25 C	-1.702084	-0.024844	0.193655
26 C	-4.376805	-0.391851	-0.203937
27 C	-2.236997	-1.293428	0.379084
28 C	-2.476141	1.065226	-0.185313
29 C	-3.838959	0.875497	-0.389451
30 C	-3.600570	-1.479122	0.177919
31 H	-1.612142	-2.122857	0.673308
32 H	-2.036633	2.041961	-0.321018
33 H	-4.478555	1.694404	-0.687544
34 H	-4.058103	-2.449056	0.313091
35 N	-5.830368	-0.591189	-0.421188
36 O	-6.282811	-1.710380	-0.223227
37 O	-6.484925	0.376055	-0.784925

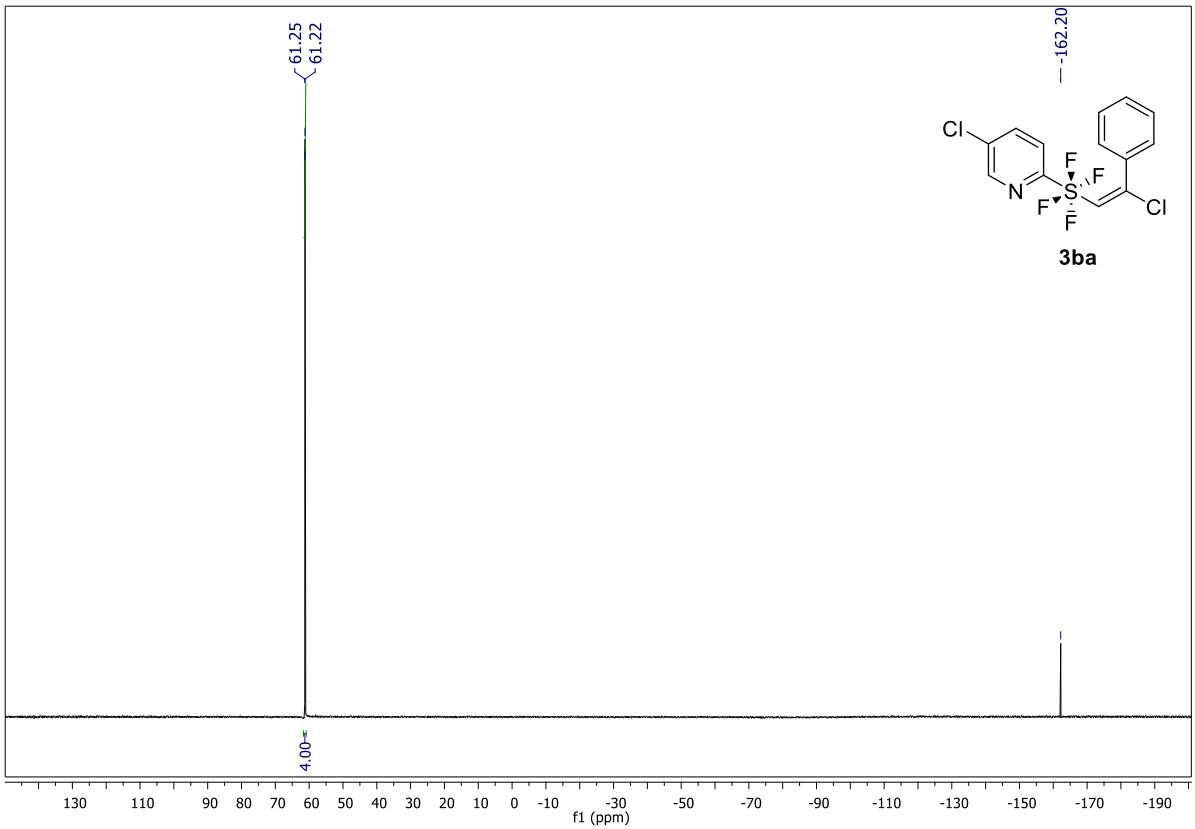
Point Group: c1 Number of degrees of freedom: 105

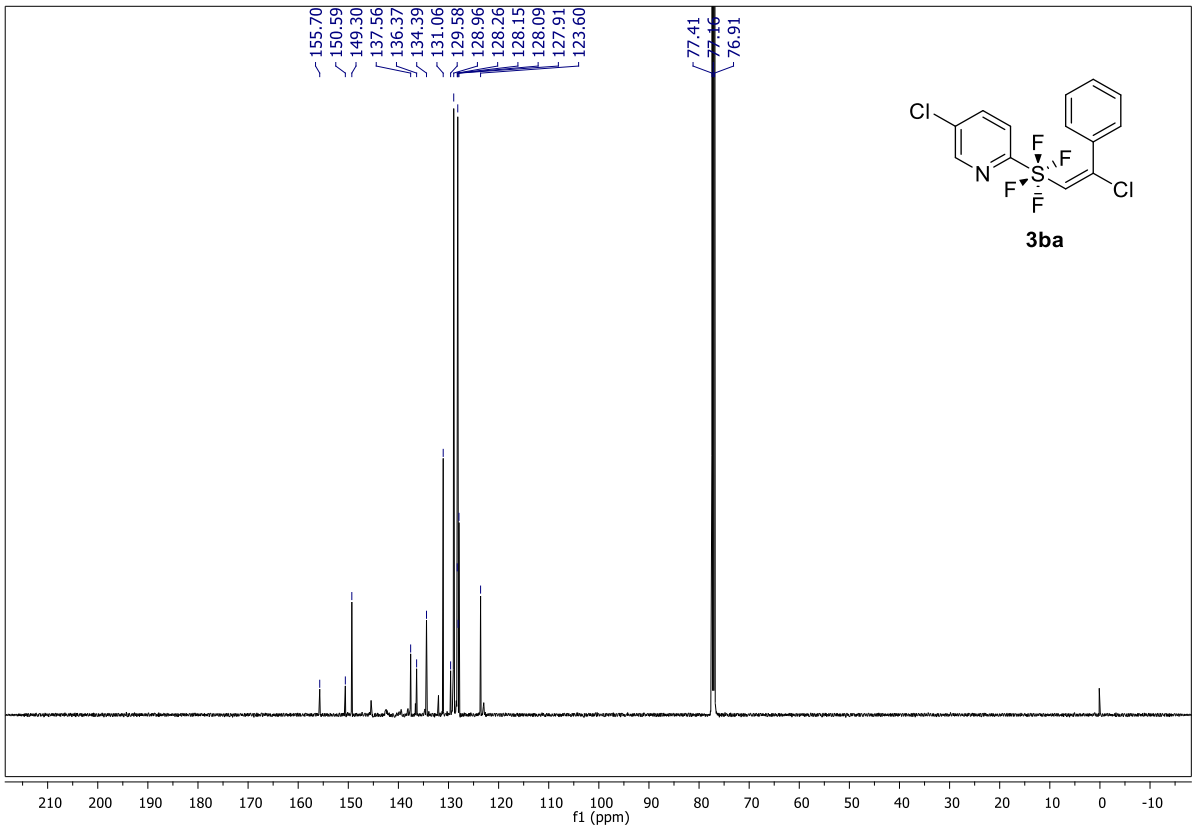

8.49
8.48
7.88
7.85
7.50
7.47
7.45
7.43
7.42
7.42
7.39
7.39
7.38
7.38
7.37
7.37
7.36
7.26
7.23
7.20
7.17
7.14
1.59
0.07
-0.00
Br
N
F
F
S
F
F
Cl
3aa
1.00
1.11
1.17
2.28
3.33
1.19
f1 (ppm)

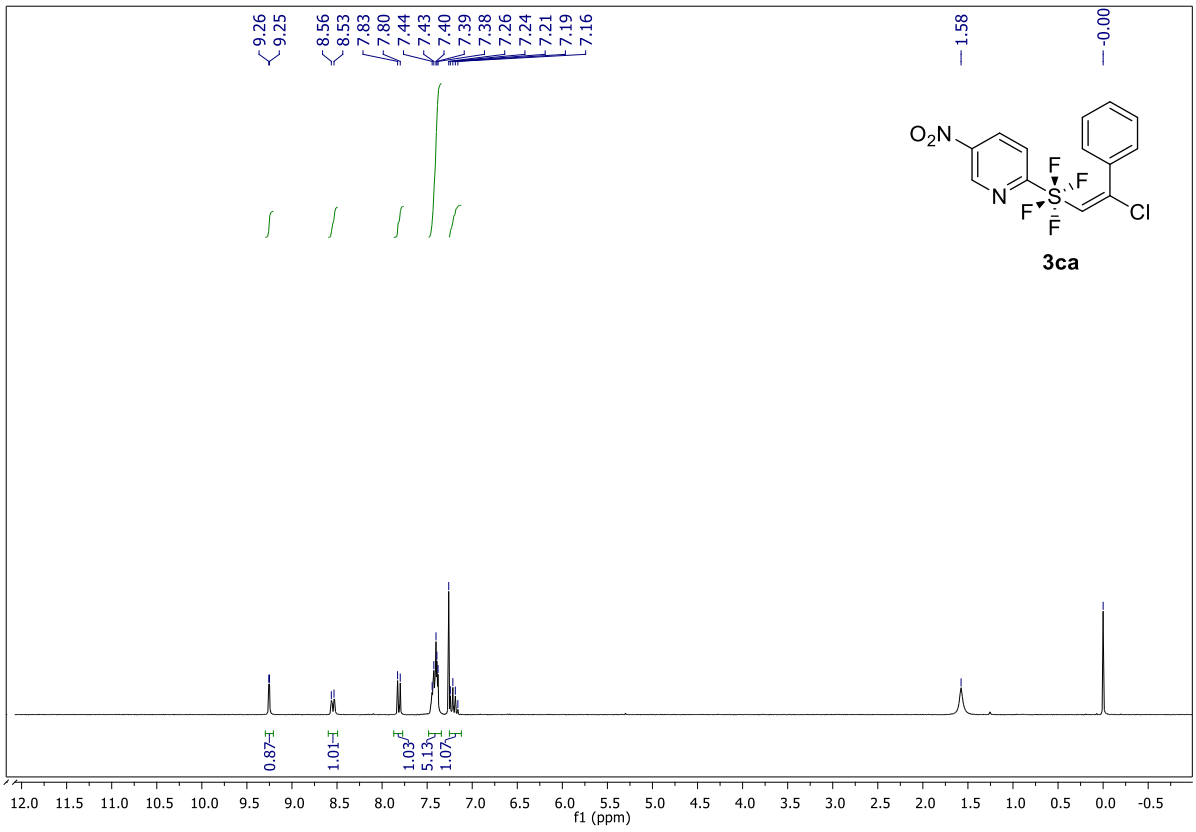

61.06
61.03
-162.20
Br
N
F
F
S
F
F
Cl
3aa
4.00
f1 (ppm)

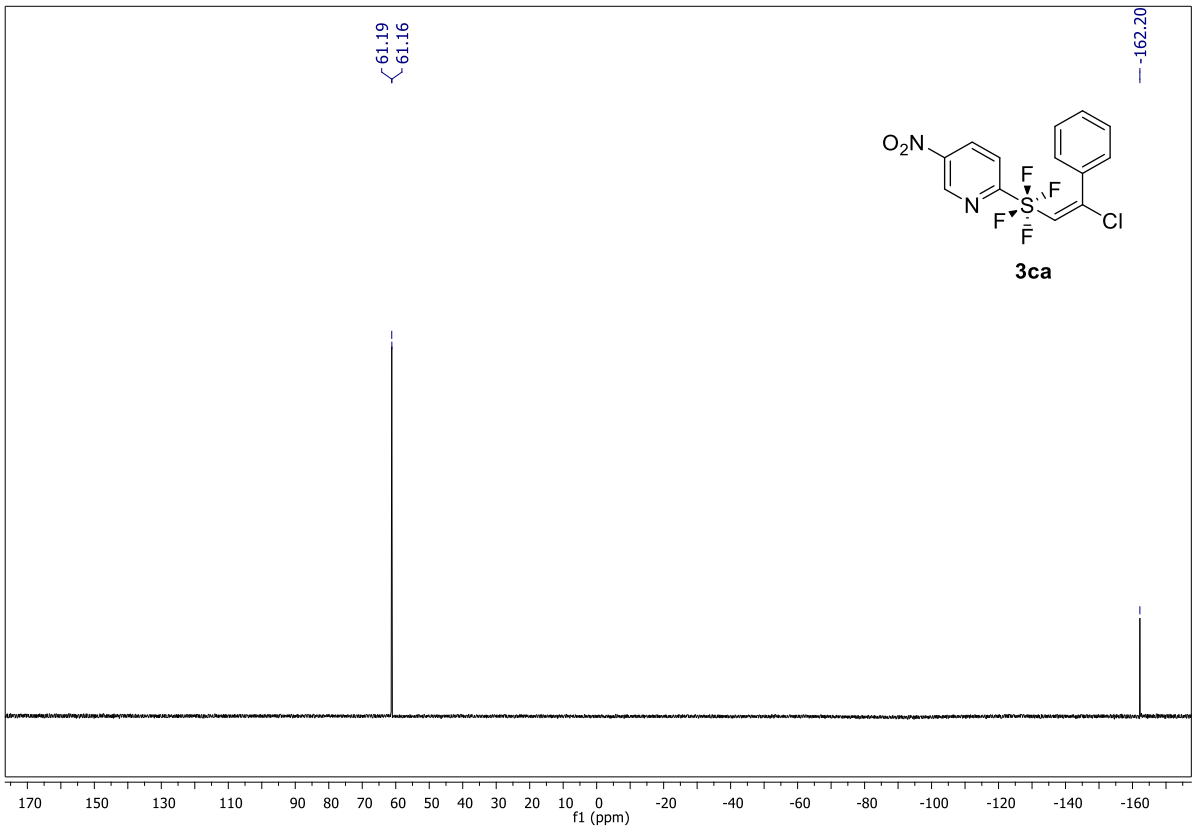

168.65
168.40
168.15
148.26
143.41
143.18
142.95
142.72
142.49
140.79
139.51
139.45
139.39
136.85
129.45
128.20
128.15
122.88
122.84
122.80
122.77
122.73
77.41
77.16
76.91
Br
N
F
F
F
S
F
Cl
3aa
f1 (ppm)

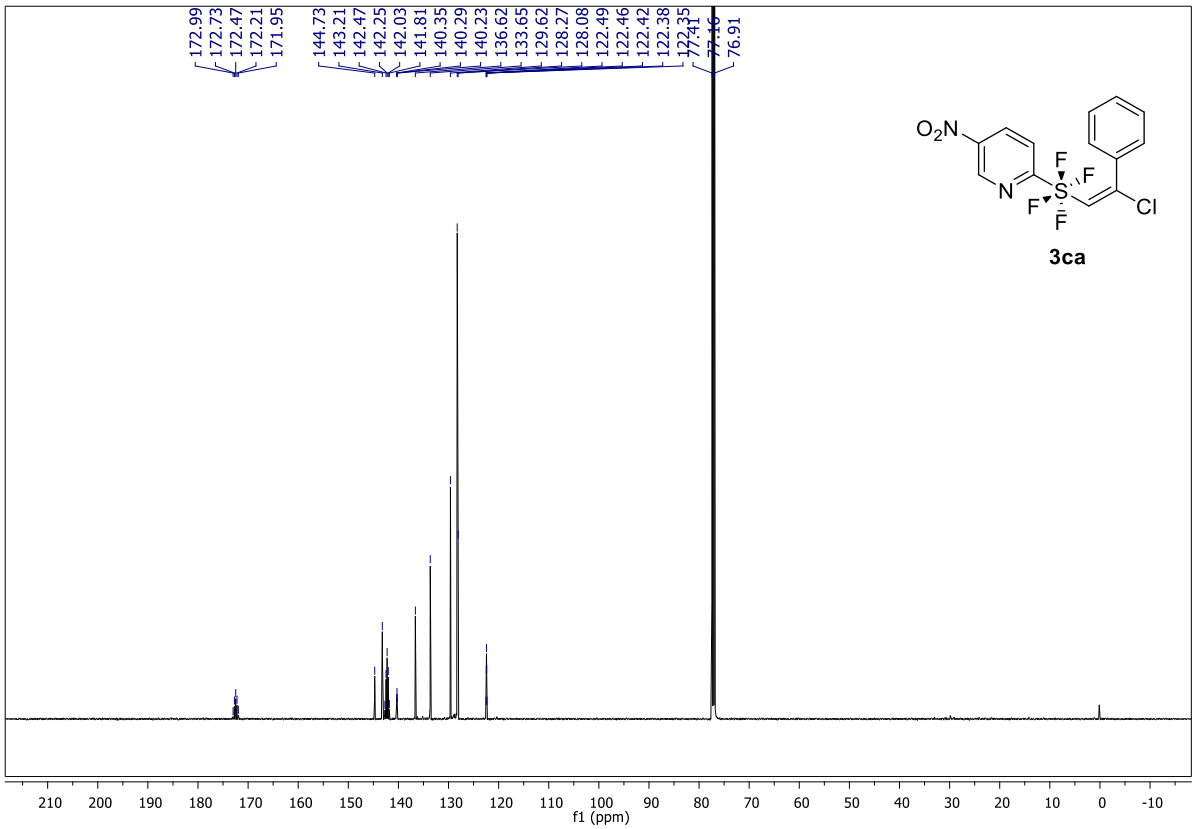

8.39
8.38
7.74
7.71
7.71
7.56
7.53
7.44
7.42
7.42
7.41
7.39
7.39
7.38
7.38
7.37
7.36
7.26
7.23
7.20
7.17
7.14
7.12
-0.00
Cl
N
F
F
F
S
F
Cl
3ba
1.00
1.25
1.28
2.40
3.40
1.28
f1 (ppm)

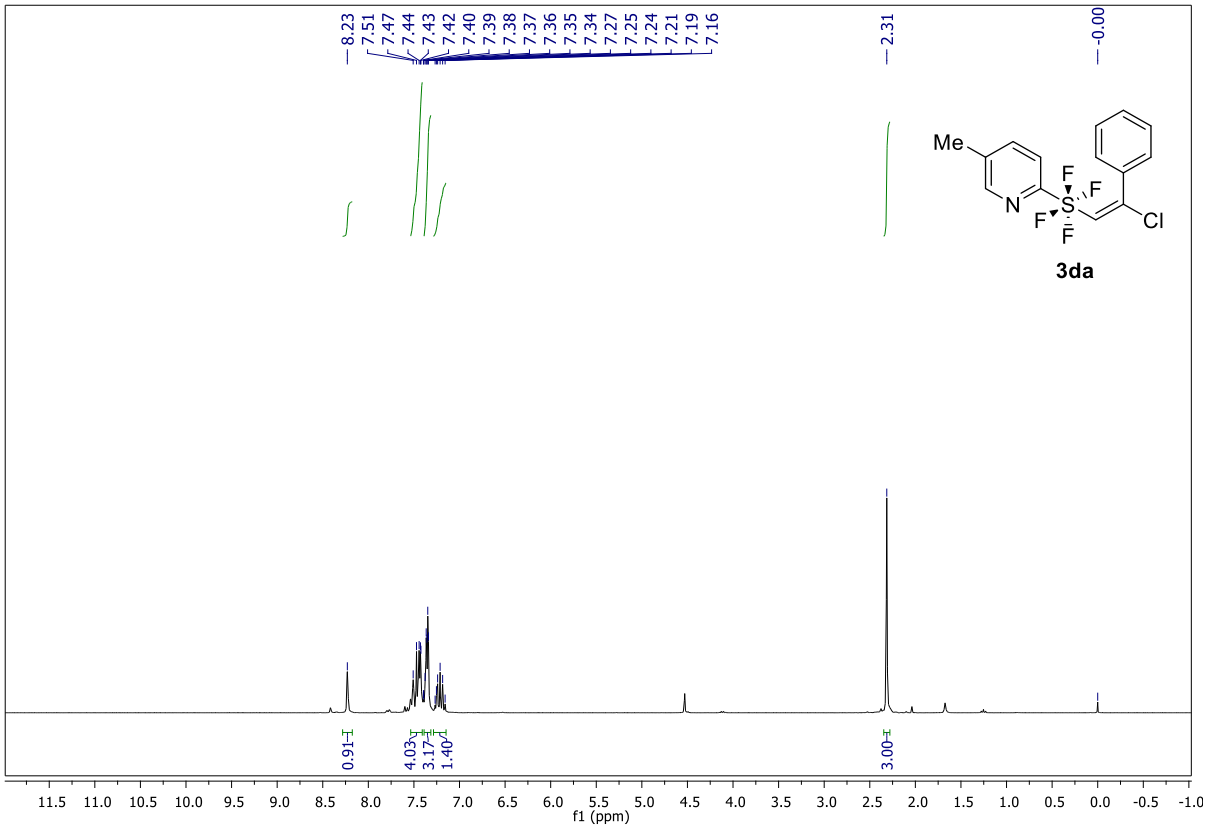

61.25
61.22
-162.20
Cl
F
F
N
S
F
F
Cl
3ba
4.00
130 110 90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190
f1 (ppm)

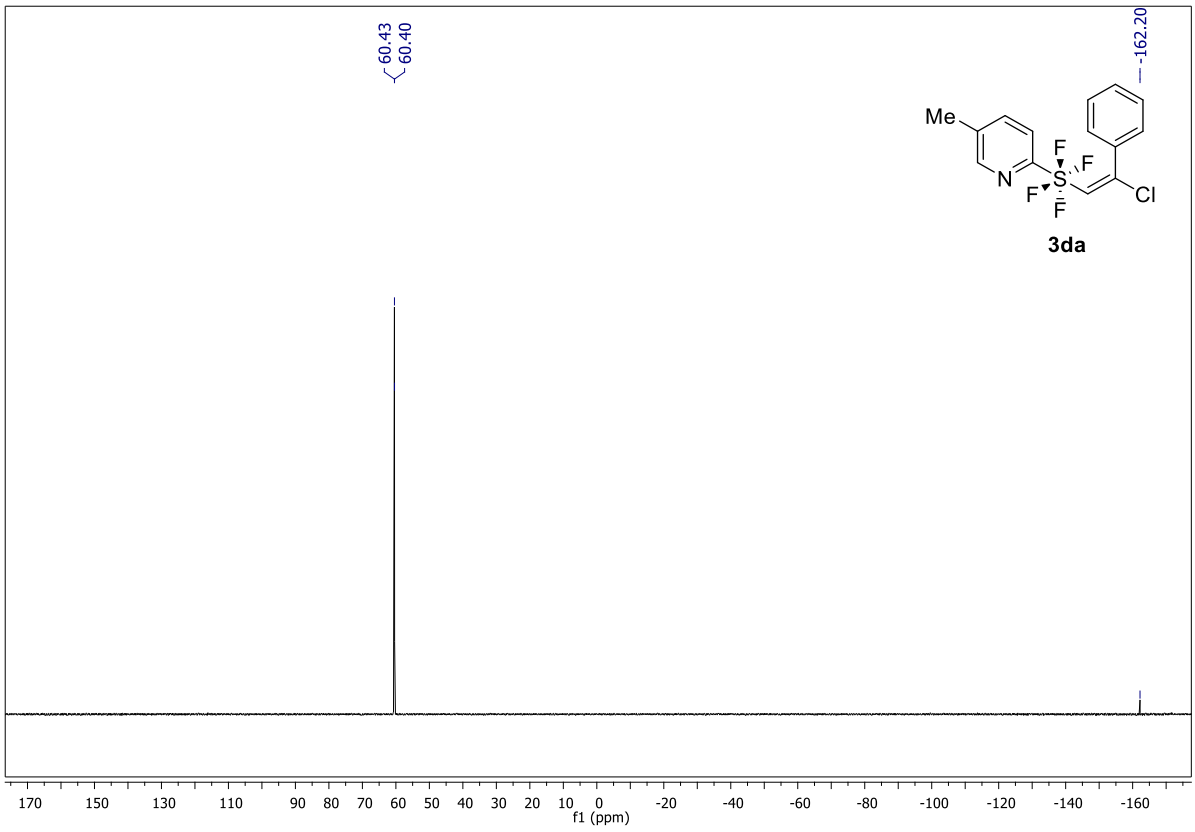

155.70
150.59
149.30
137.56
136.37
134.39
131.06
129.58
128.96
128.26
128.15
128.09
127.91
123.60
77.41
77.16
76.91
Cl
F
F
N
S
F
F
Cl
3ba
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

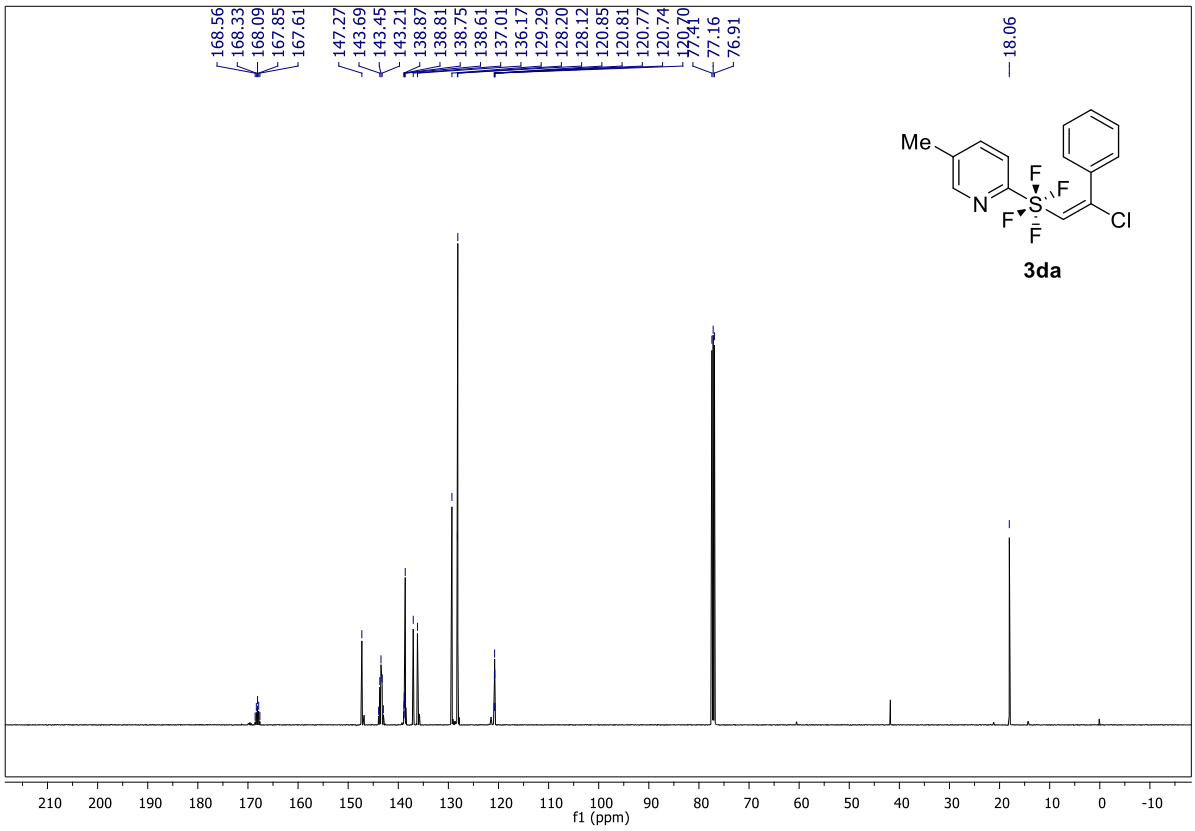

9.26
9.25
8.56
8.53
7.83
7.80
7.44
7.43
7.40
7.39
7.38
7.26
7.24
7.21
7.19
7.16
1.58
-0.00
0.87
1.01
1.03
5.13
1.07
f1 (ppm)
3ca

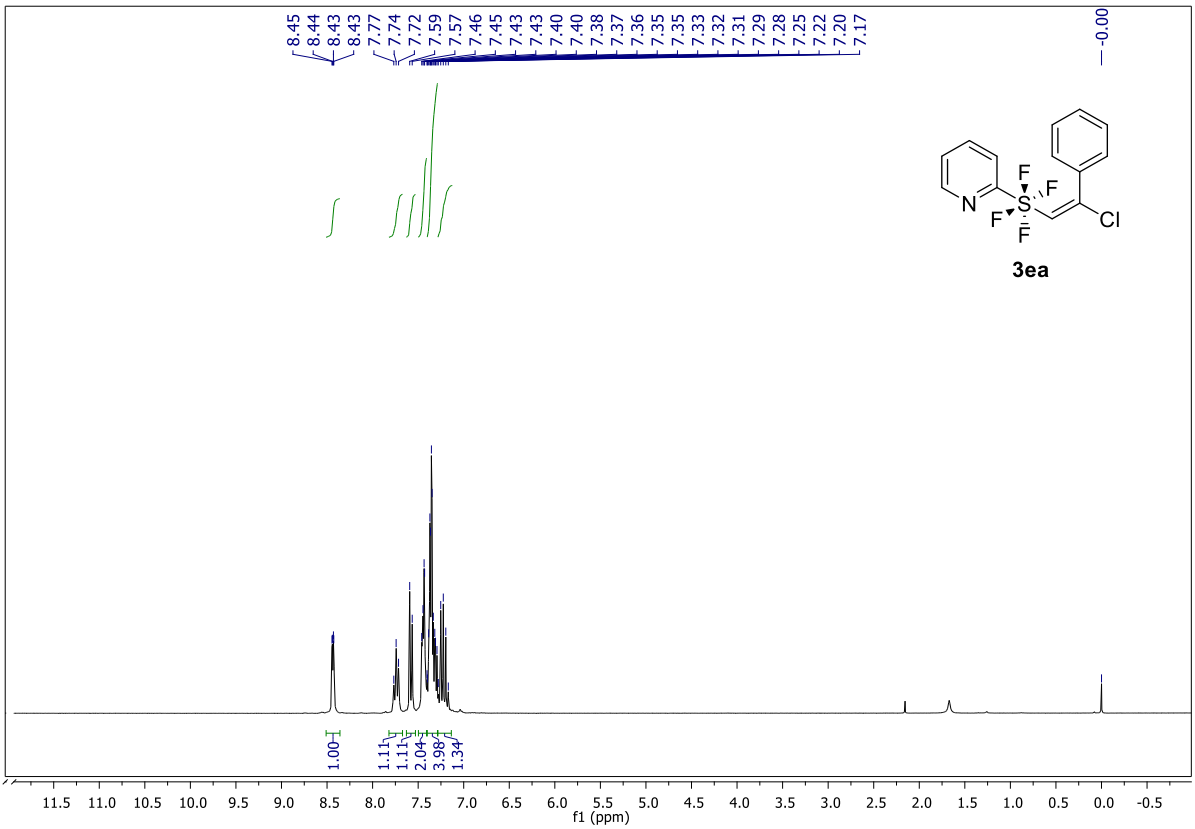

61.19
61.16
-162.20
f1 (ppm)
3ca


172.99
172.73
172.47
172.21
171.95
144.73
143.21
142.47
142.25
142.03
141.81
140.35
140.29
140.23
136.62
133.65
129.62
128.27
128.08
122.49
122.46
122.42
122.38
122.35
77.41
77.16
76.91
O2N
N
F
F
S
F
F
Cl
3ca
f1 (ppm)


8.23
7.51
7.47
7.44
7.43
7.42
7.40
7.39
7.38
7.37
7.36
7.35
7.34
7.27
7.25
7.24
7.21
7.19
7.16
2.31
-0.00
Me
N
F
F
S
F
F
Cl
3da
0.91
4.03
3.17
1.40
3.00
f1 (ppm)


60.43
60.40
-162.20
Me
F
F
N
S
F
F
Cl
3da
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)


168.56
168.33
168.09
167.85
167.61
147.27
143.69
143.45
143.21
138.87
138.81
138.75
138.61
137.01
136.17
129.29
128.20
128.12
120.85
120.81
120.77
120.74
120.70
77.41
77.16
76.91
18.06
Me
F
F
N
S
F
F
Cl
3da
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.45
8.44
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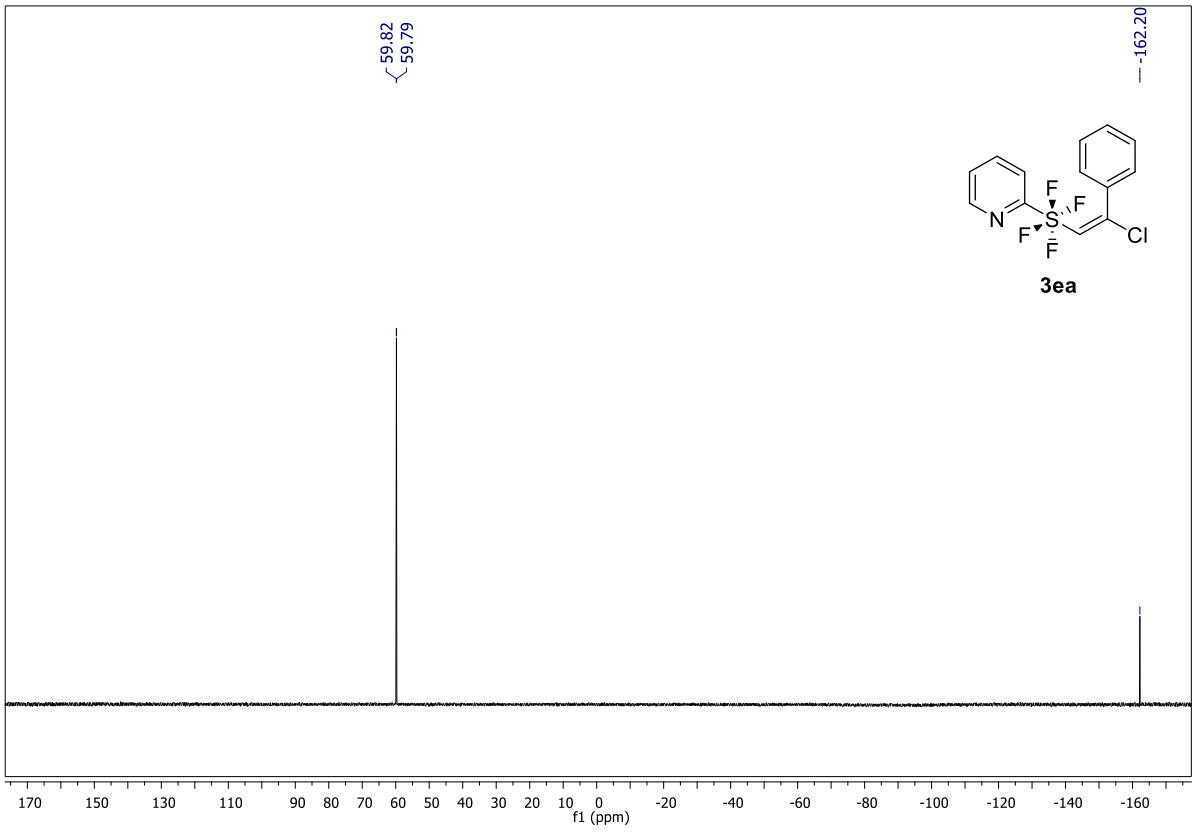
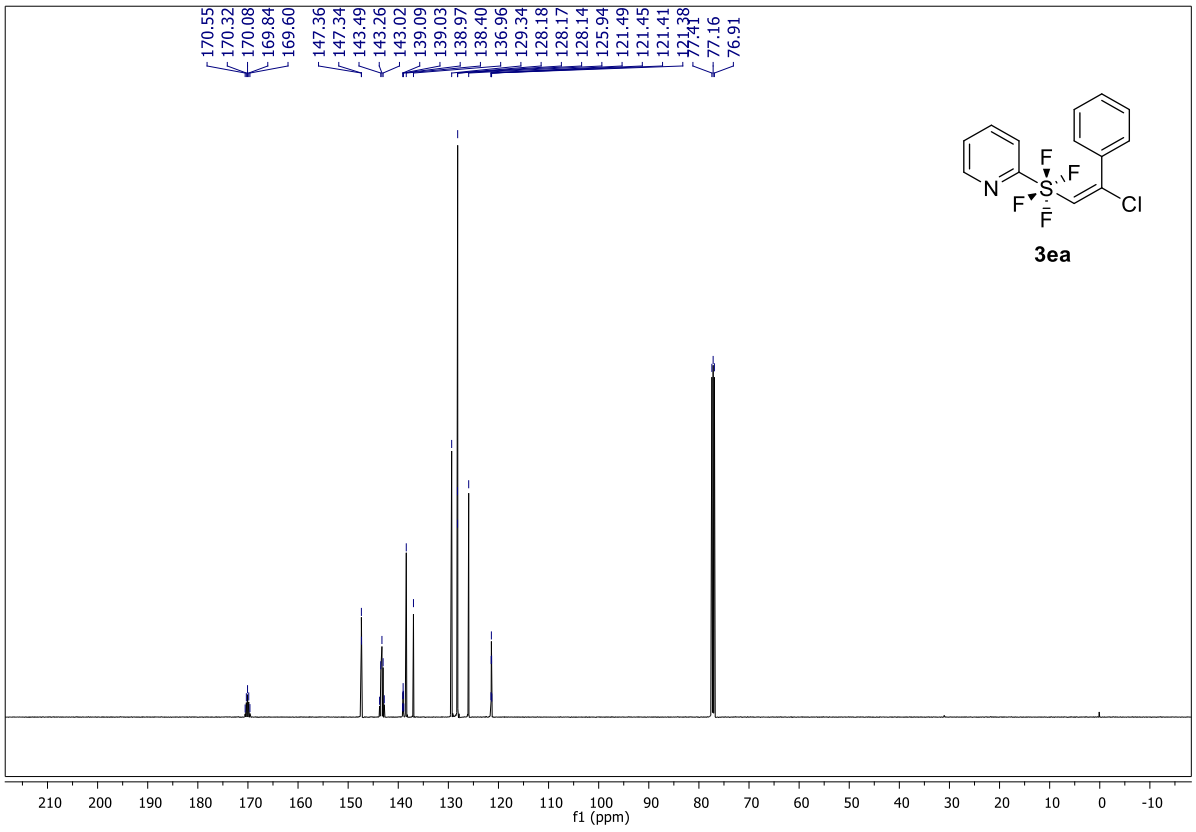
8.43
7.77
7.74
7.72
7.59
7.57
7.46
7.45
7.43
7.43
7.40
7.40
7.38
7.37
7.36
7.35
7.35
7.33
7.32
7.31
7.29
7.28
7.25
7.22
7.20
7.17
-0.00
1.00
1.11
1.11
2.04
3.98
1.34
f1 (ppm)
3ea


59.82
59.79
-162.20
f1 (ppm)
3ea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170.32
170.08
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147.34
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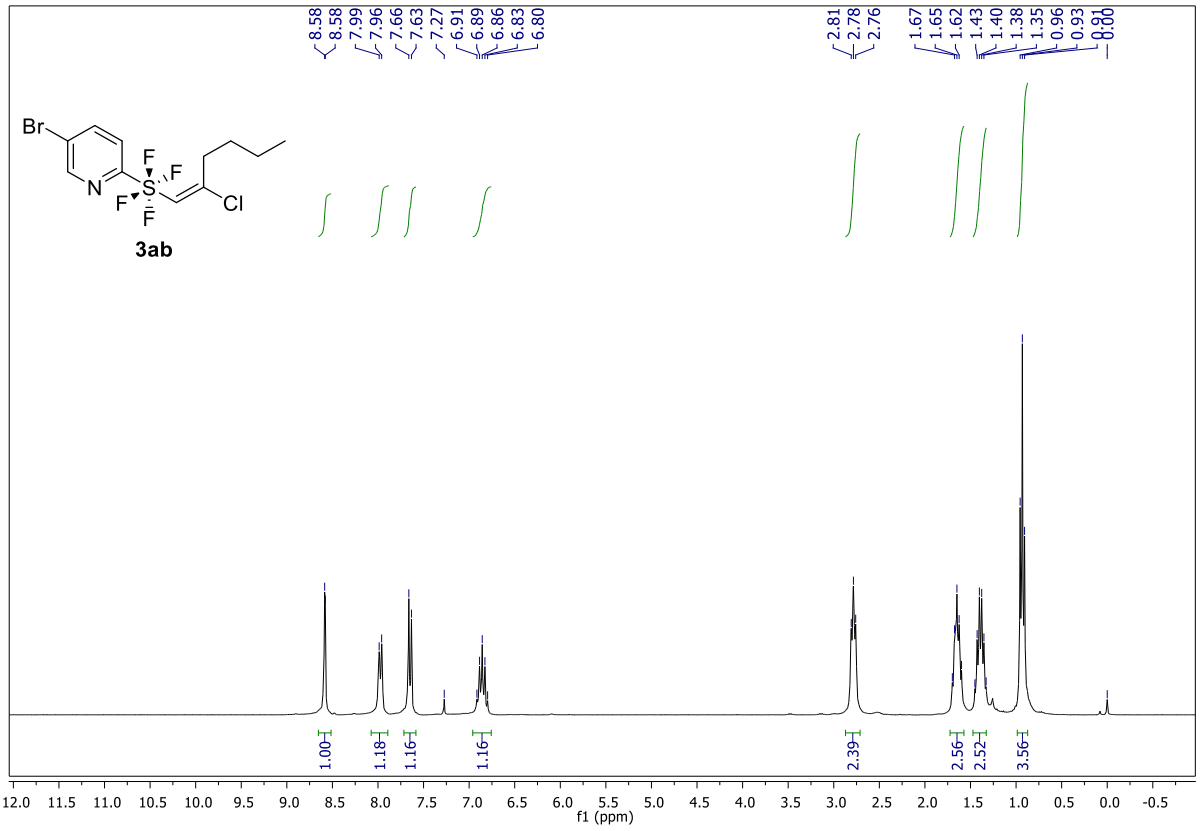
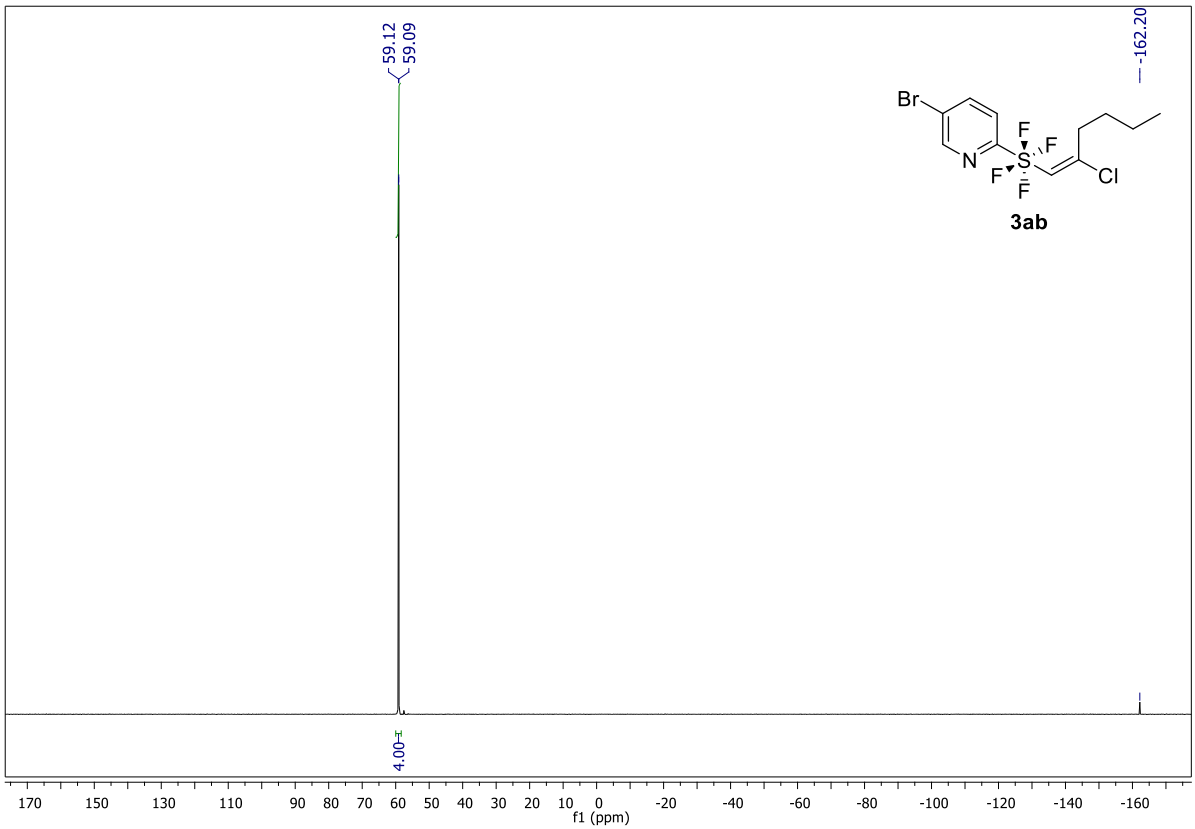
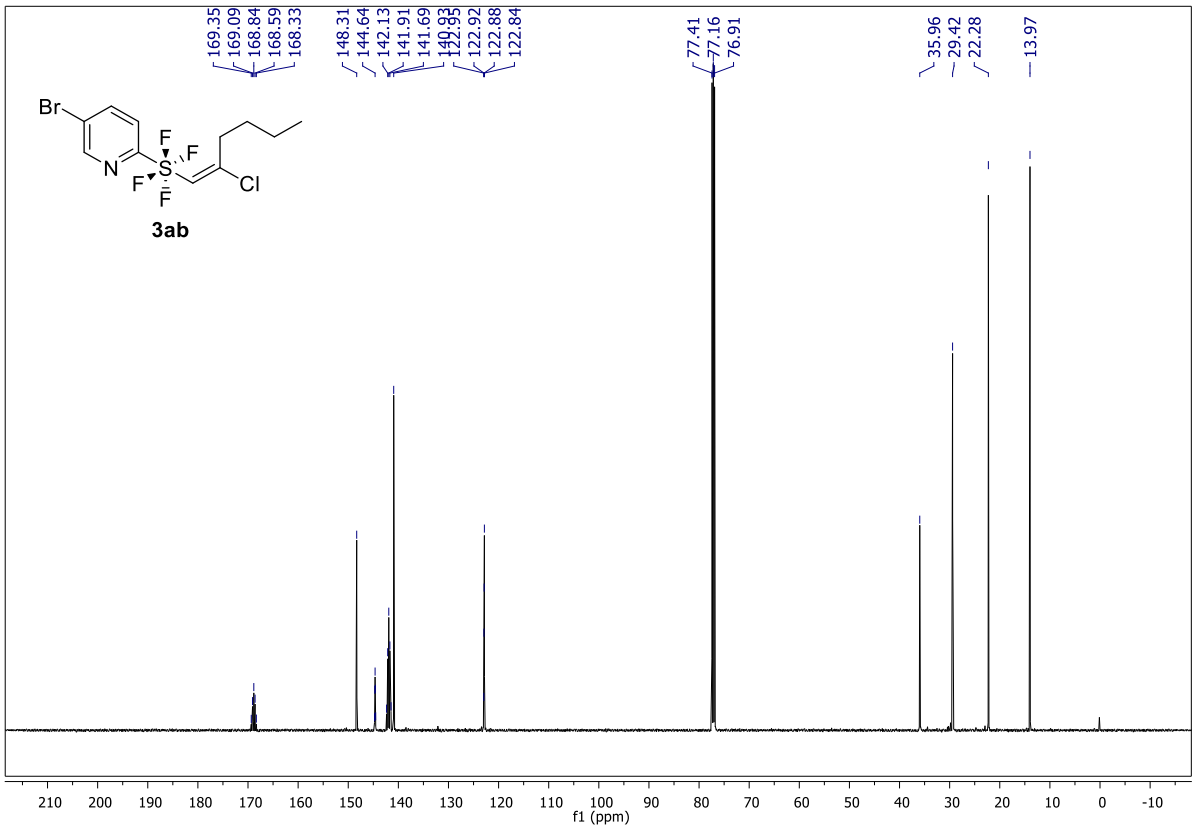
143.26
143.02
139.09
139.03
138.97
138.40
136.96
129.34
128.18
128.17
128.14
125.94
121.49
121.45
121.41
121.38
77.41
77.16
76.91
F
F
F
F
N
S
Cl
3ea
f1 (ppm)


8.58
8.58
7.99
7.96
7.66
7.63
7.27
6.91
6.89
6.86
6.83
6.80
2.81
2.78
2.76
1.67
1.65
1.62
1.43
1.40
1.38
1.35
0.96
0.93
0.91
0.00
Br
F
F
F
F
N
S
Cl
3ab
1.00
1.18
1.16
1.16
2.39
2.56
2.52
3.56
f1 (ppm)


59.12
59.09
-162.20
Br
N
F
F
S
F
F
Cl
3ab
4.00
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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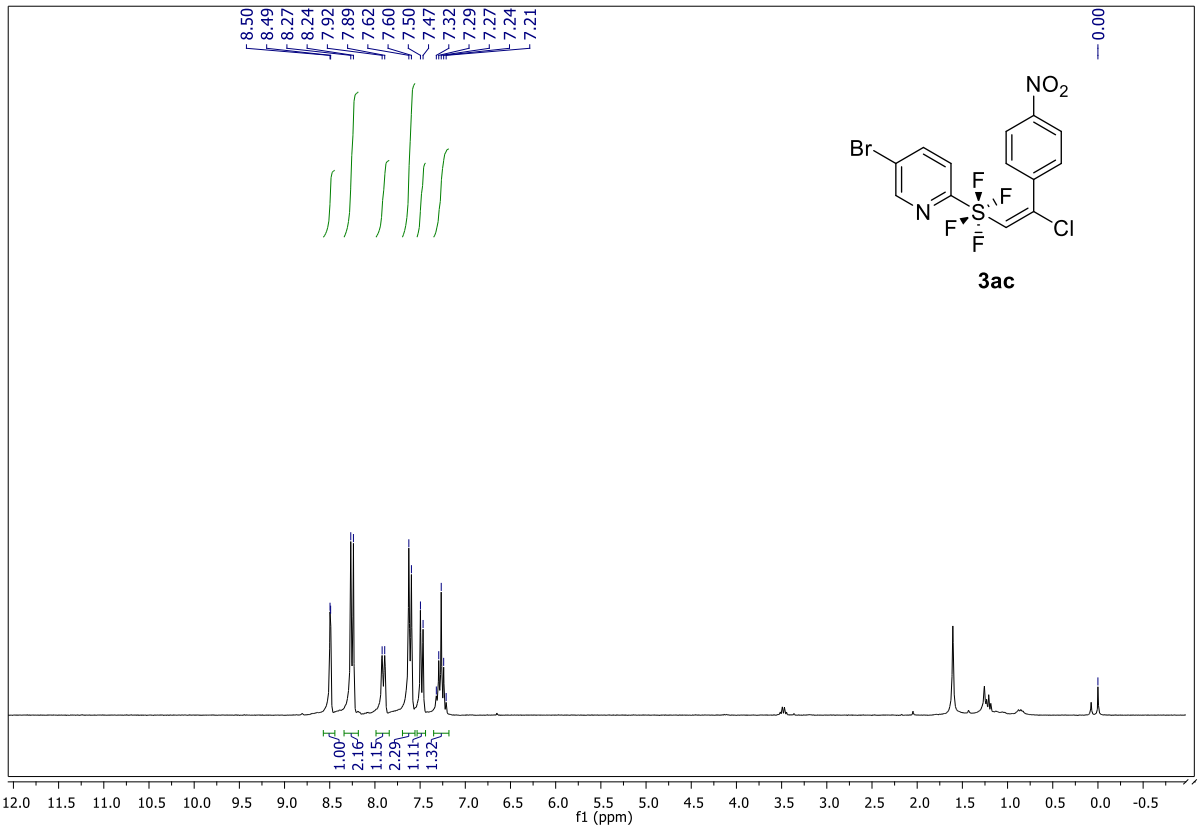
169.09
168.84
168.59
168.33
148.31
144.64
142.13
141.91
141.69
122.92
122.88
122.84
77.41
77.16
76.91
35.96
29.42
22.28
13.97
Br
N
F
F
S
F
F
Cl
3ab
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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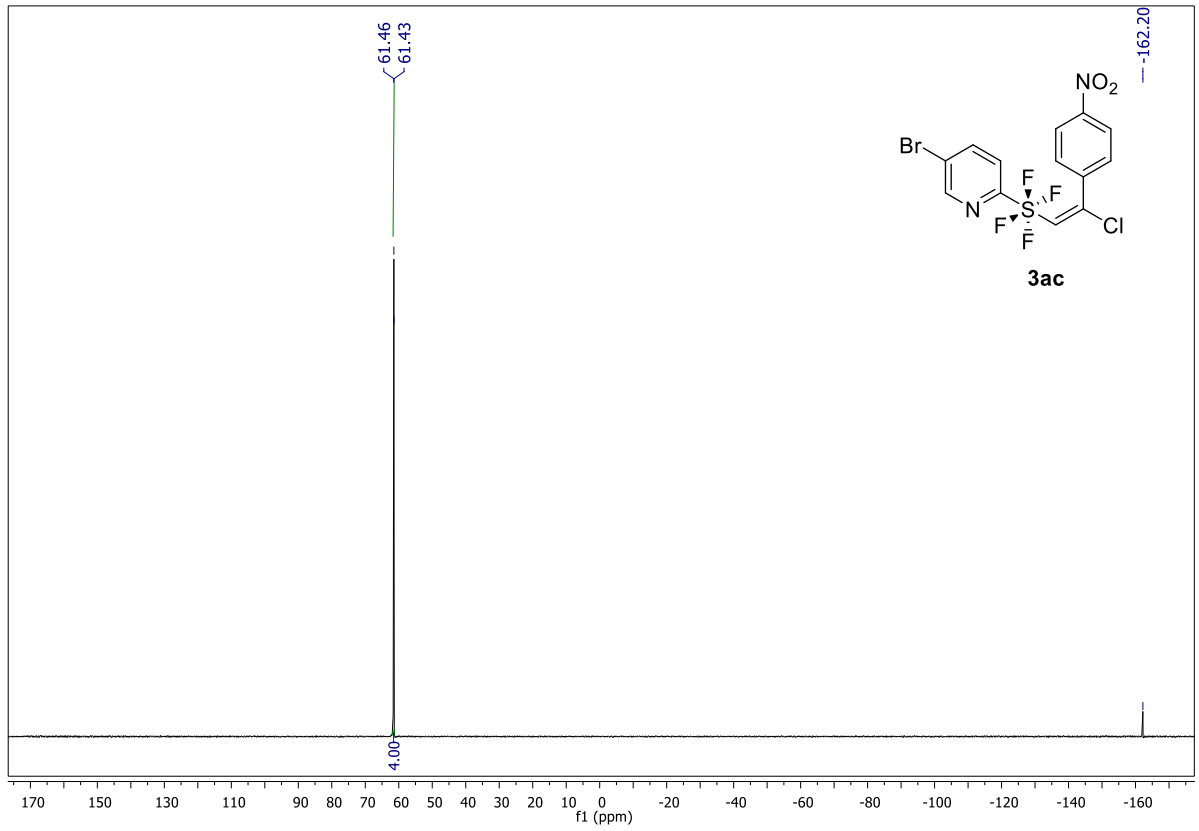
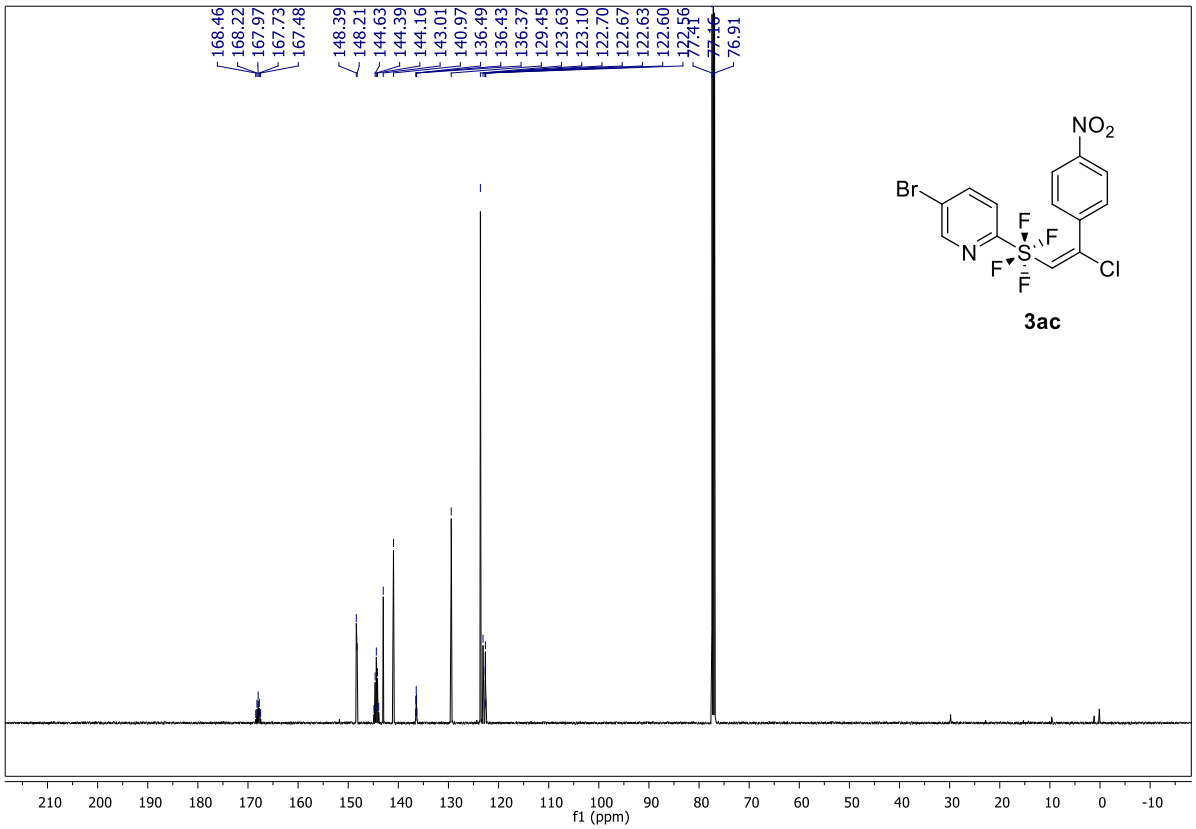
8.27
8.24
7.92
7.89
7.62
7.60
7.50
7.47
7.32
7.29
7.27
7.24
7.21
0.00
NO2
Br
N
F
S
F
F
F
Cl
3ac
1.00
2.16
1.15
2.29
1.11
1.32
f1 (ppm)


61.46
61.43
-162.20
NO2
Br
N
F
S
F
F
F
Cl
3ac
4.00
f1 (ppm)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167.97
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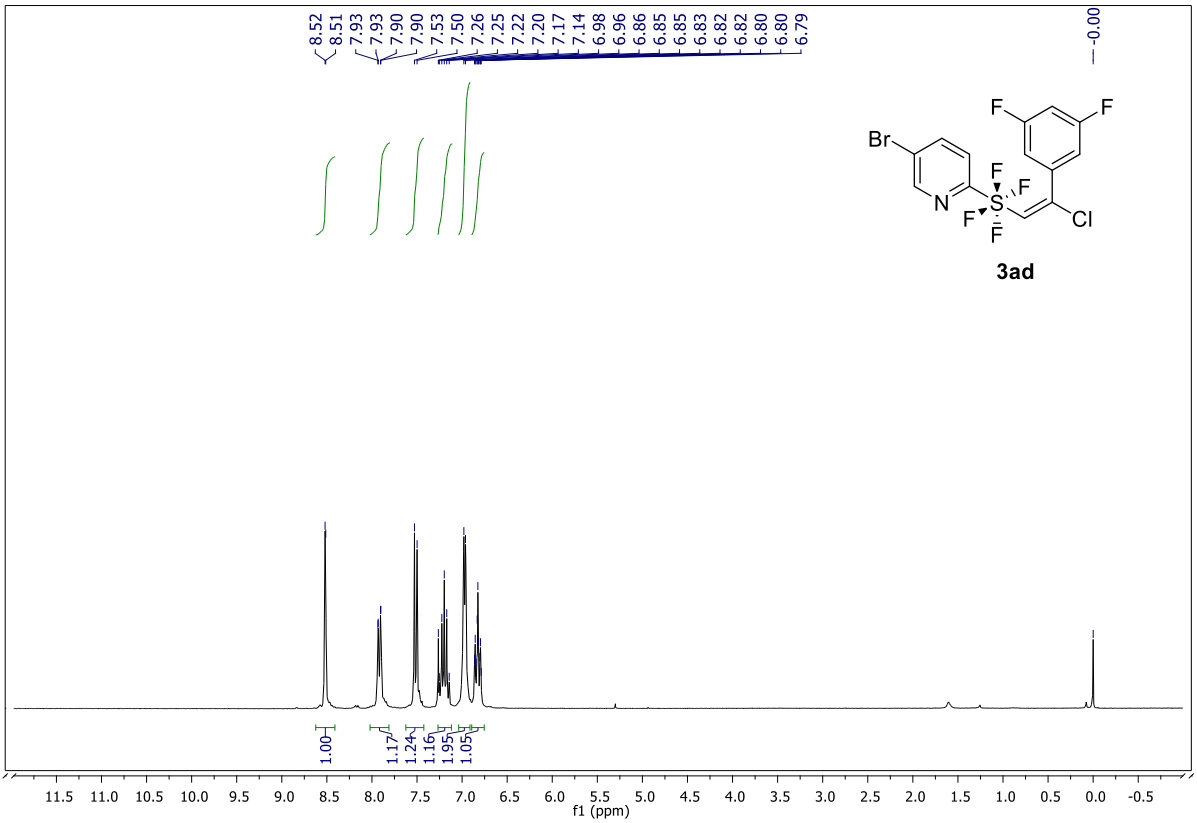
167.48
148.39
148.21
144.63
144.39
144.16
143.01
140.97
136.49
136.43
136.37
129.45
123.63
123.10
122.70
122.67
122.63
122.60
122.56
77.41
77.16
76.91
NO2
Br
N
F
F
S
F
F
Cl
3ac
f1 (ppm)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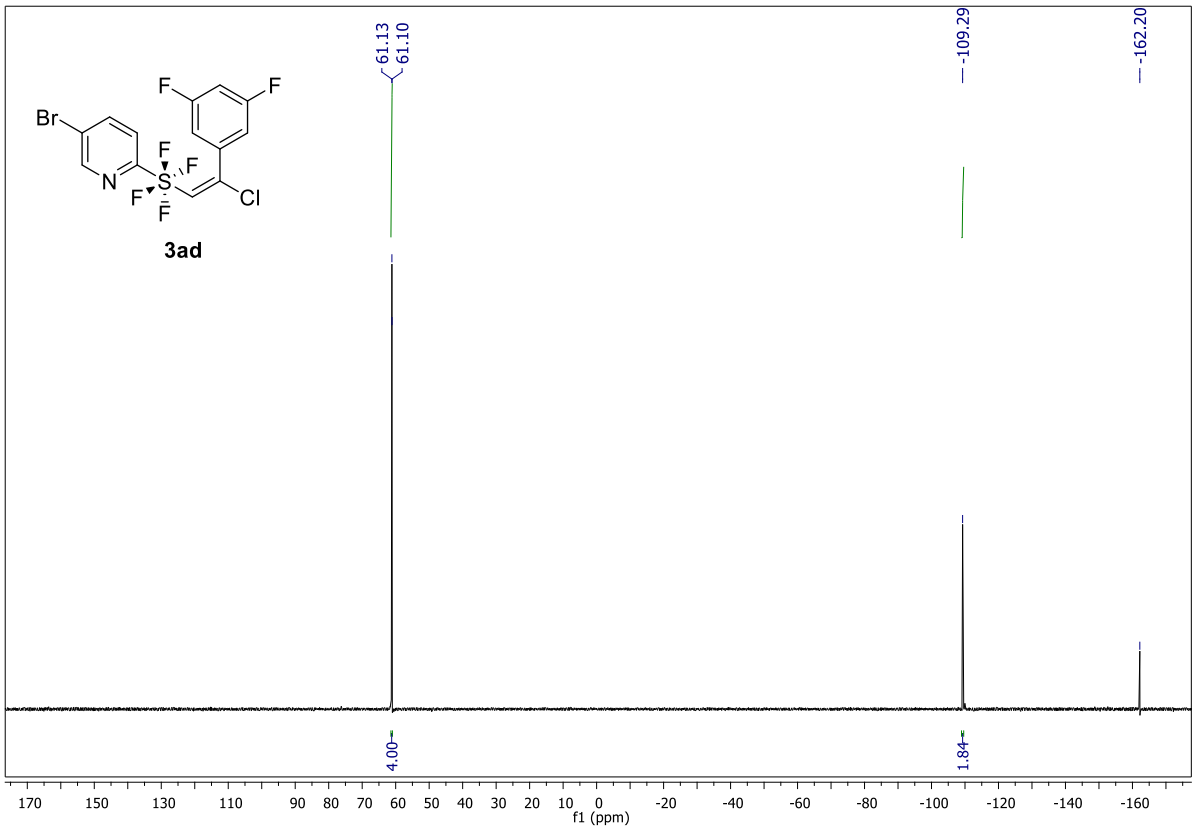
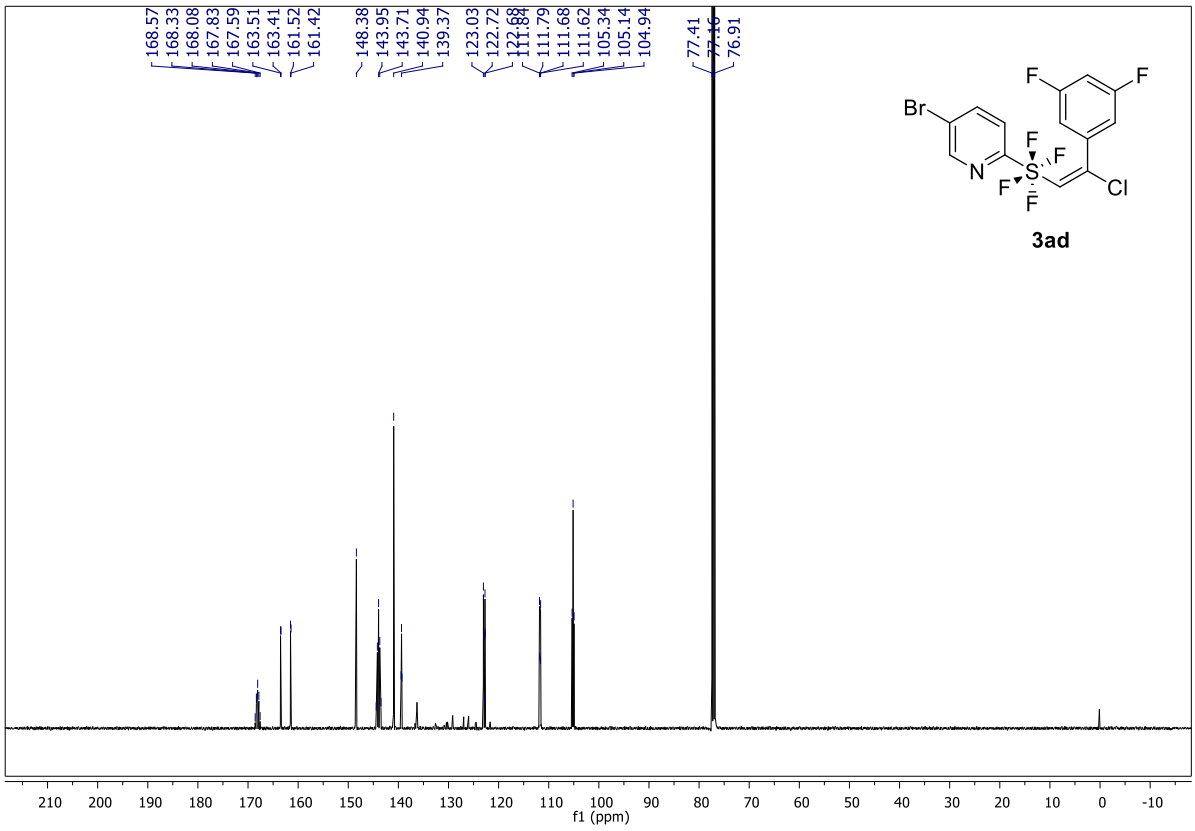
8.51
7.93
7.93
7.90
7.90
7.53
7.50
7.26
7.25
7.22
7.20
7.17
7.14
6.98
6.96
6.86
6.85
6.85
6.83
6.82
6.82
6.80
6.80
6.79
-0.00
F
F
Br
N
F
F
S
F
F
Cl
3ad
1.00
1.17
1.24
1.16
1.95
1.05
f1 (ppm)


61.13
61.10
-109.29
-162.20
3ad
4.00
1.84
f1 (ppm)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168.33
168.08
167.83
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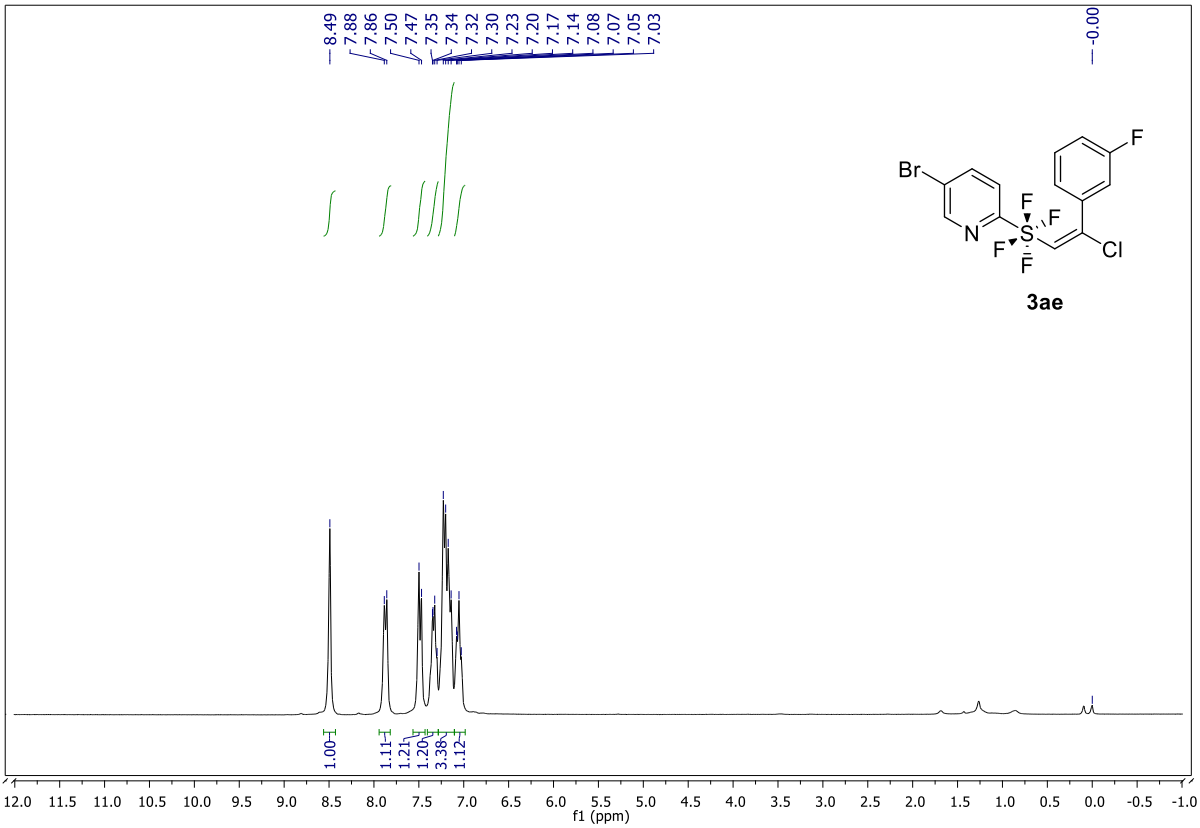
163.51
163.41
161.52
161.42
148.38
143.95
143.71
140.94
139.37
123.03
122.72
111.79
111.68
111.62
105.34
105.14
104.94
77.41
77.16
76.91
3ad
f1 (ppm)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7.34
7.32
7.30
7.23
7.20
7.17
7.14
7.08
7.07
7.05
7.03
-0.00
Br
F
F
F
F
N
S
Cl
3ae
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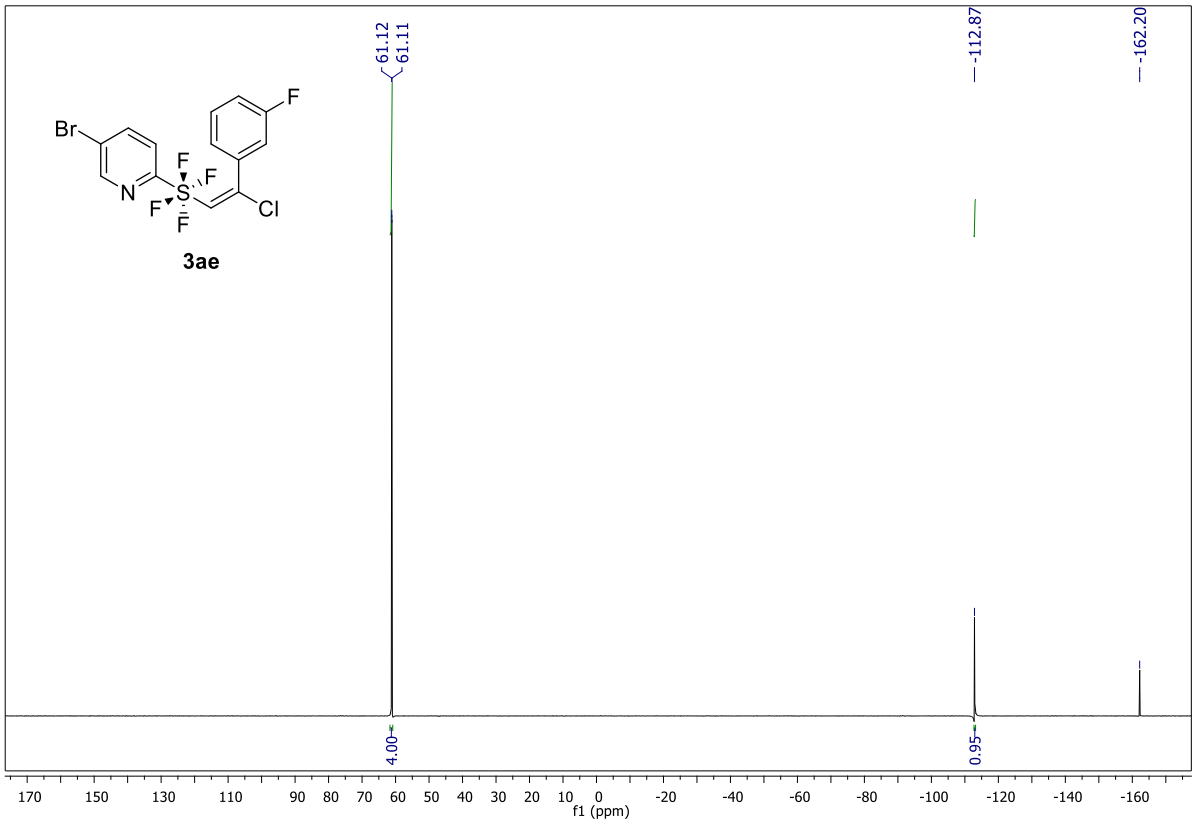
1.21
1.20
3.38
1.12
f1 (ppm)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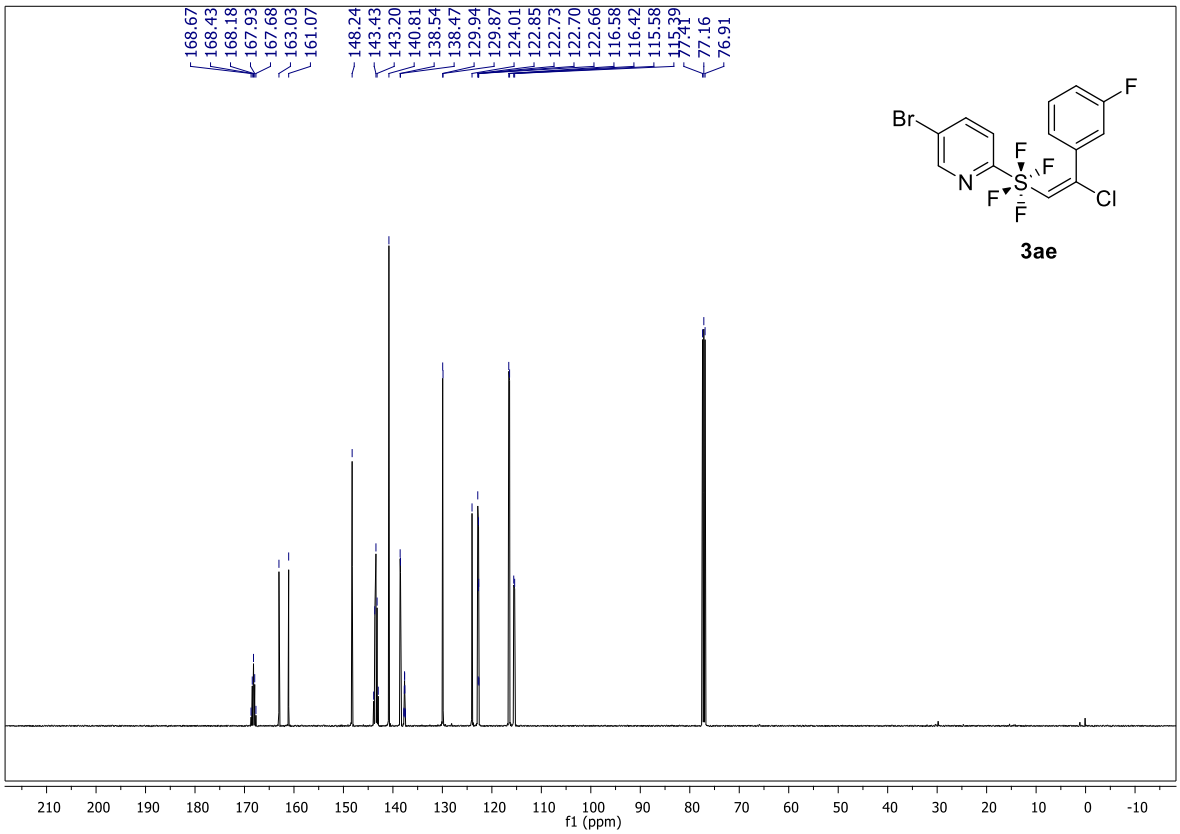
61.11
-112.87
-162.20
Br
F
F
F
F
N
S
Cl
3ae
4.00
0.95
f1 (ppm)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168.43
168.18
167.93
167.68
163.03
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148.24
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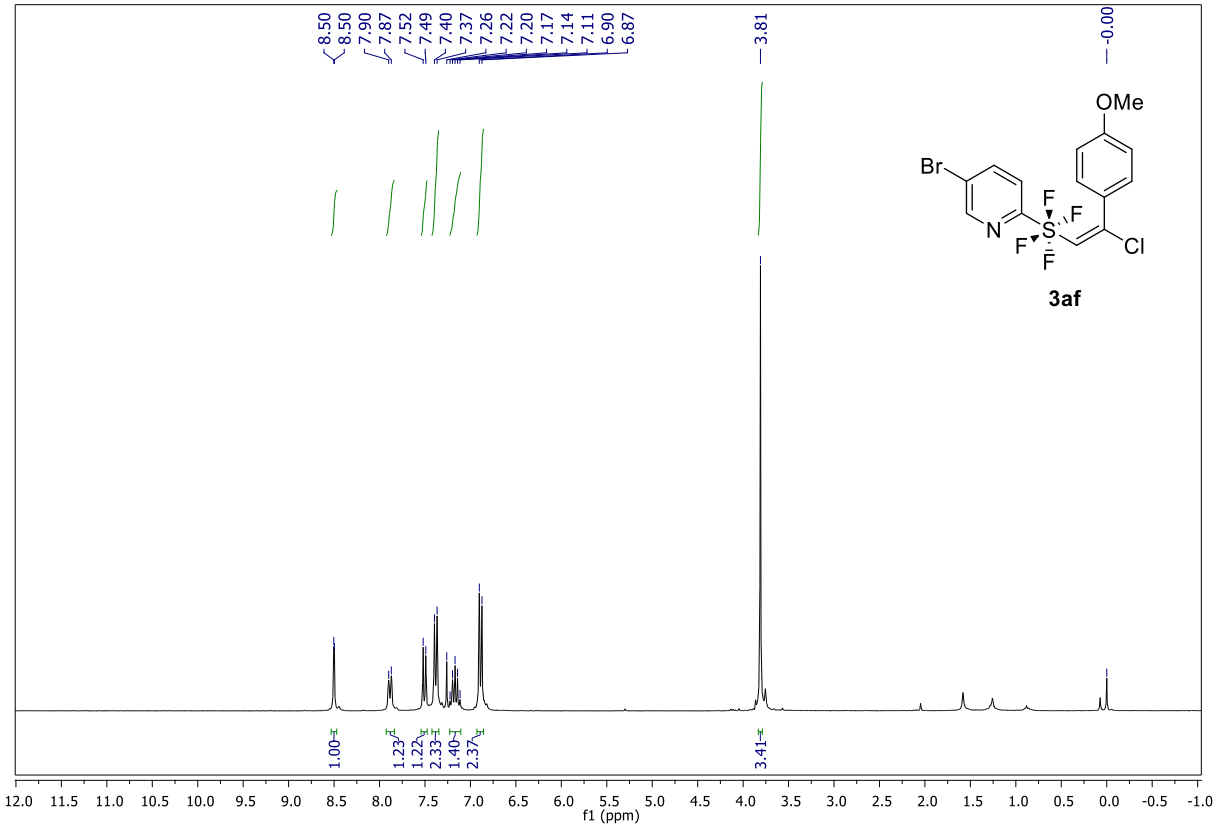
143.20
140.81
138.54
138.47
129.94
129.87
124.01
122.85
122.73
122.70
122.66
116.58
116.42
115.58
115.39
77.41
77.16
76.91
Br
N
F
F
F
S
F
F
Cl
3ae
f1 (ppm)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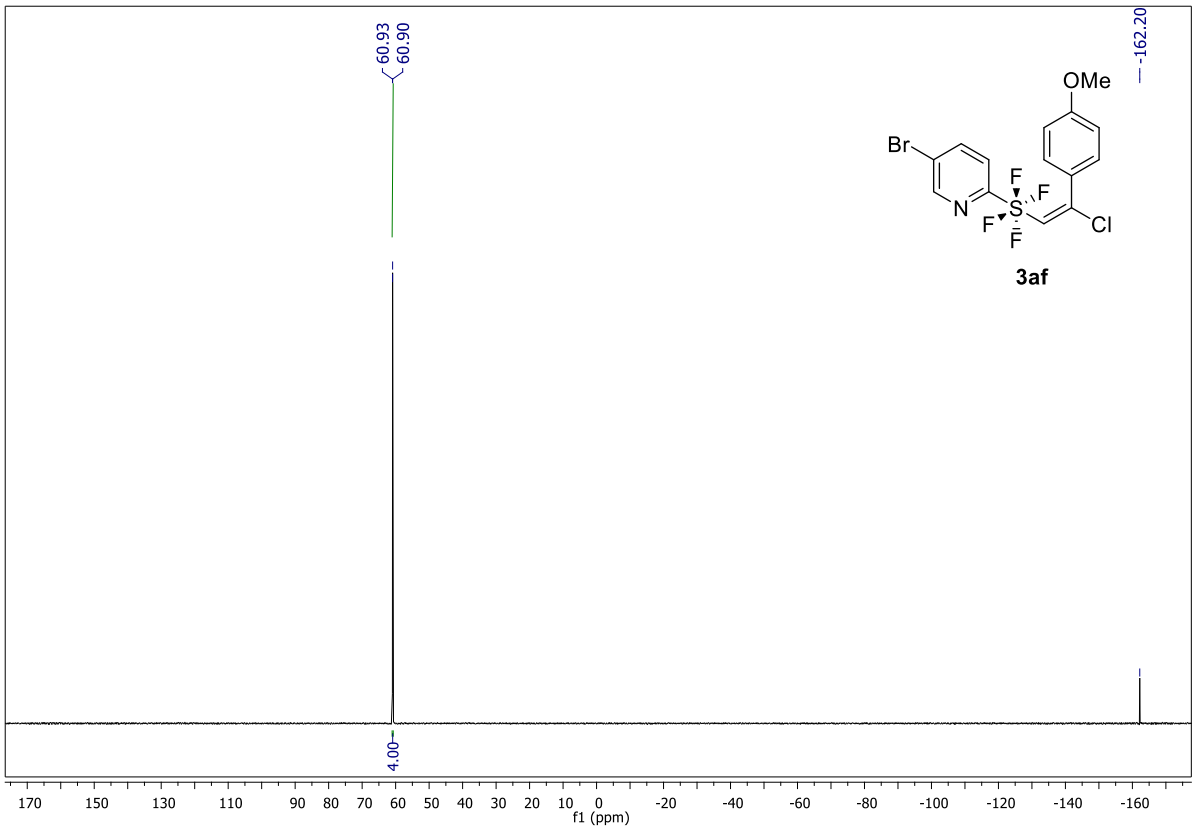
7.49
7.40
7.37
7.26
7.22
7.20
7.17
7.14
7.11
6.90
6.87
3.81
-0.00
OMe
Br
N
F
F
F
S
F
F
Cl
3af
1.00
1.23
1.22
2.33
1.40
2.37
3.41
f1 (ppm)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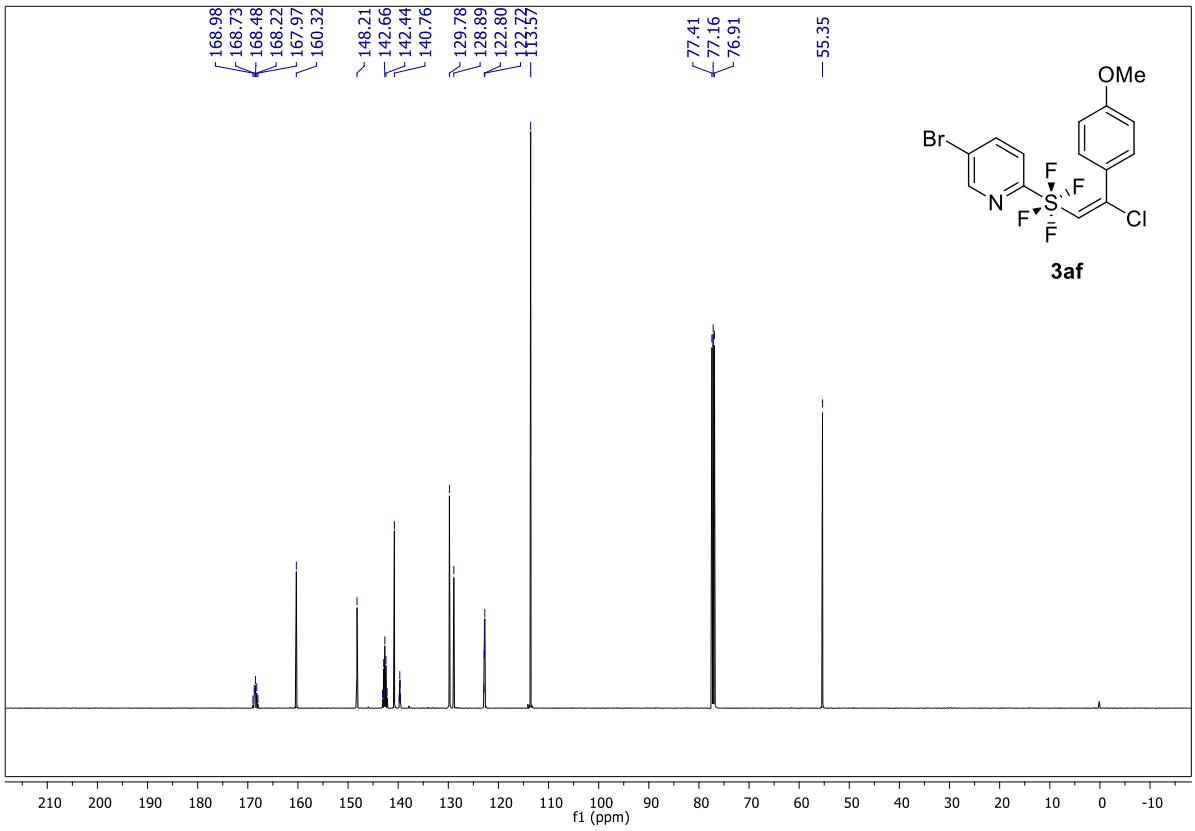
60.90
-162.20
OMe
Br
F
F
N
S
F
F
Cl
3af
4.00
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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168.48
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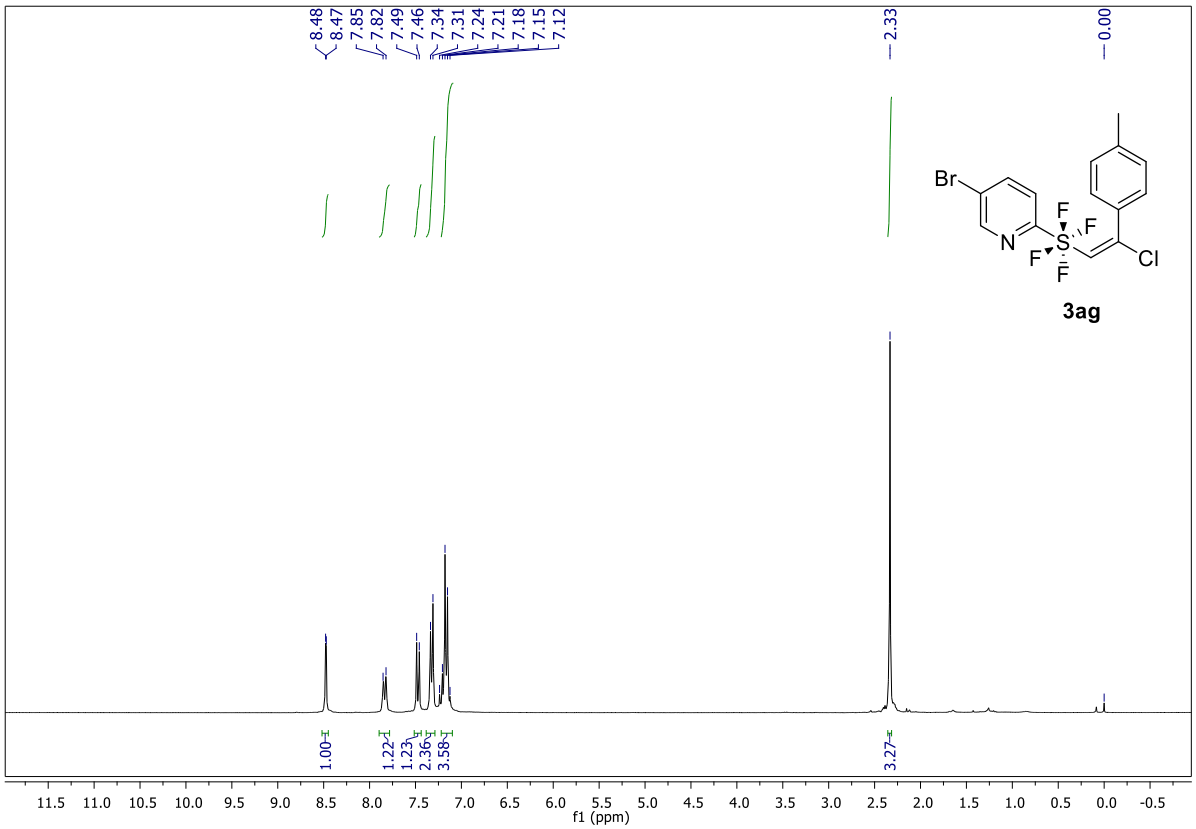
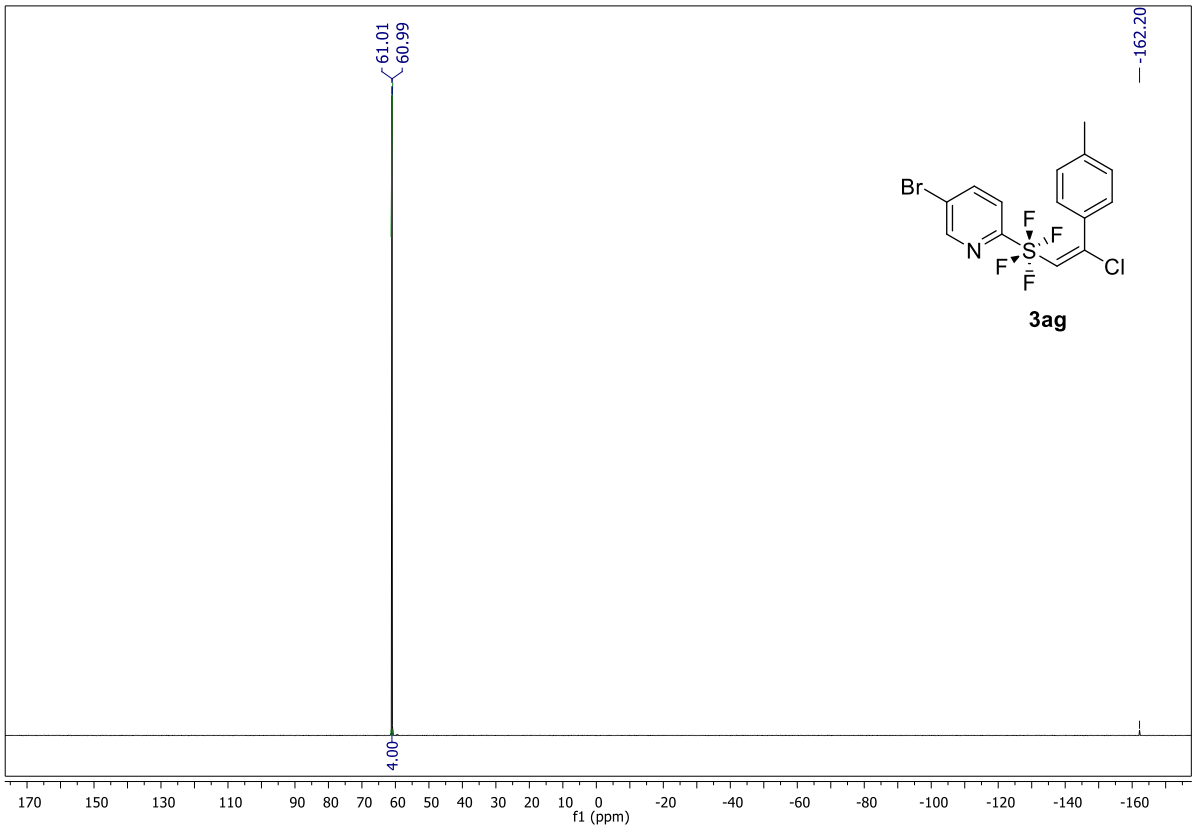
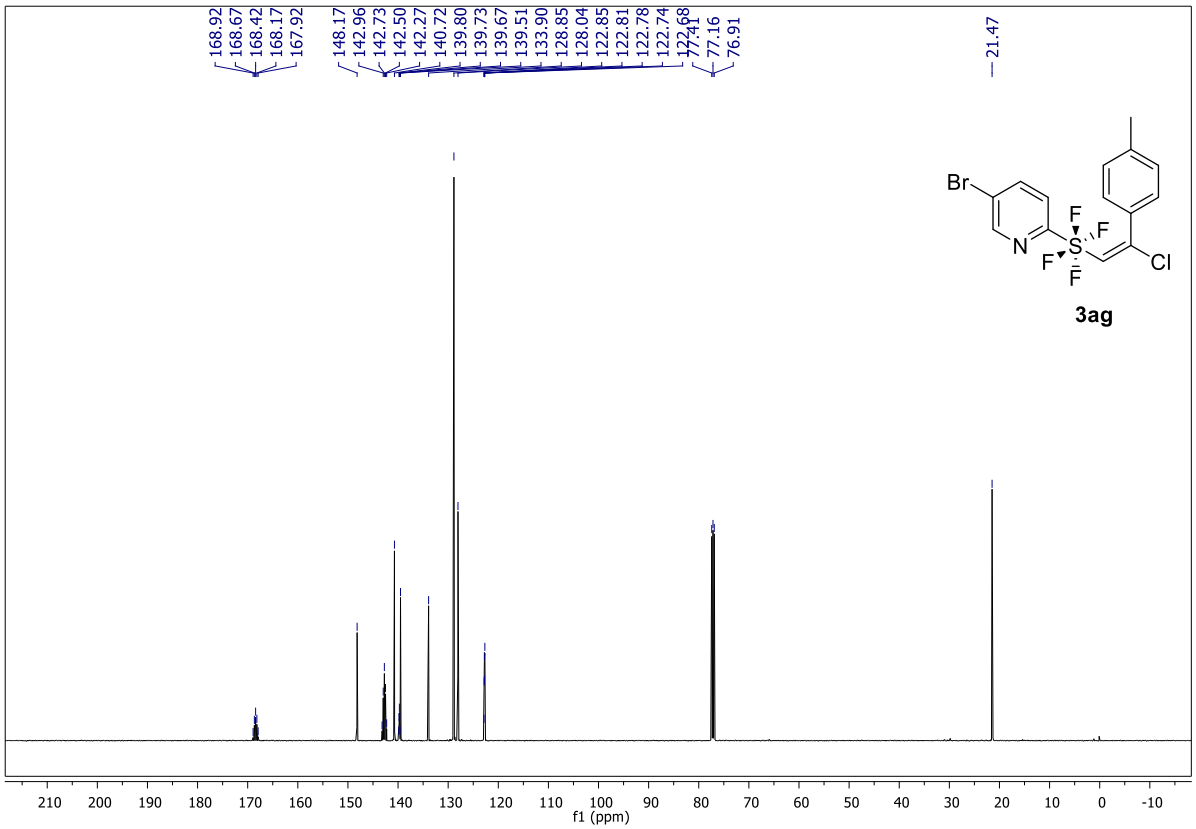
167.97
160.32
148.21
142.66
142.44
140.76
129.78
128.89
122.80
113.57
77.41
77.16
76.91
55.35
OMe
Br
F
F
N
S
F
F
Cl
3af
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.48
8.47
7.85
7.82
7.49
7.46
7.34
7.31
7.24
7.21
7.18
7.15
7.12
2.33
0.00
Br
N
F
F
S
F
F
Cl
3ag
1.00
1.22
1.23
2.36
3.58
3.27
11.5 11.0 10.5 10.0 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
f1 (ppm)


61.01
60.99
-162.20
Br
N
F
F
S
F
F
Cl
3ag
4.00
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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142.27
140.72
139.80
139.73
139.67
139.51
133.90
128.85
128.04
122.85
122.81
122.78
122.74
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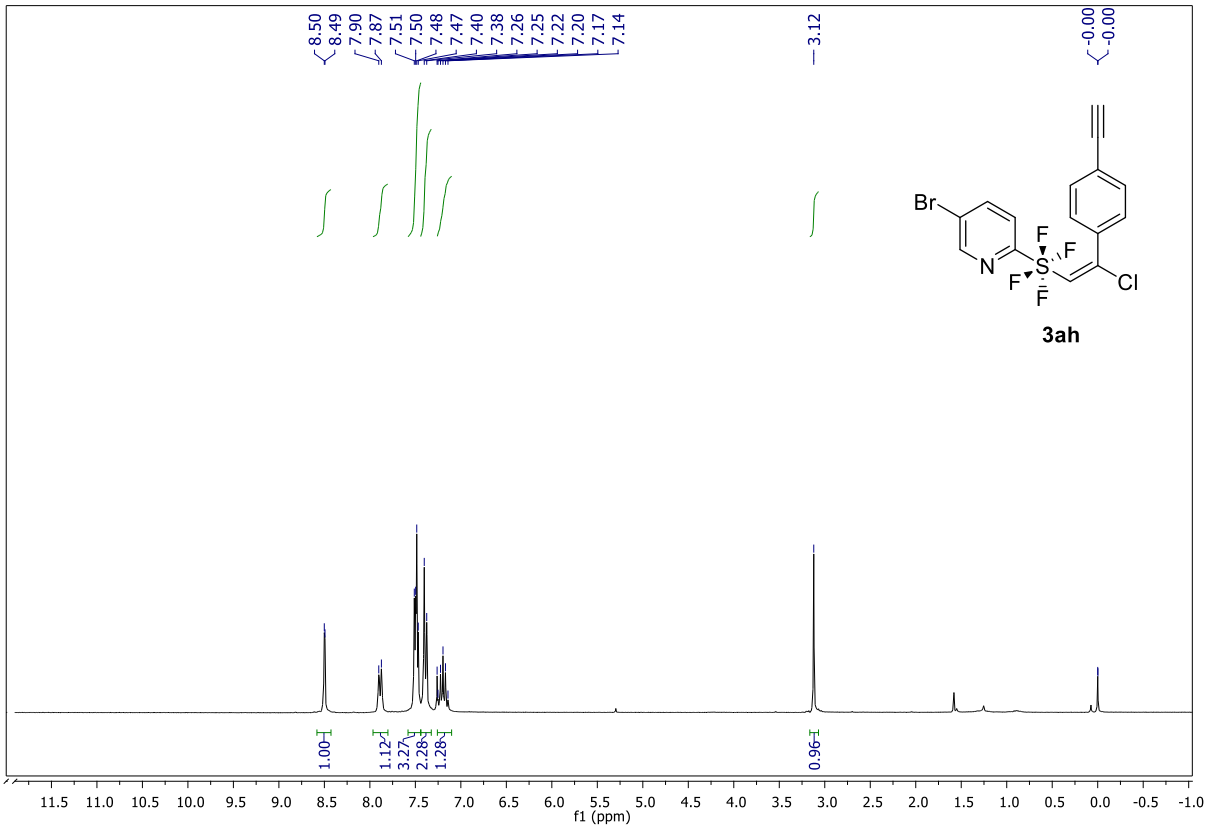
77.41
77.16
76.91
21.47
Br
N
F
S
F
F
F
Cl
3ag
f1 (ppm)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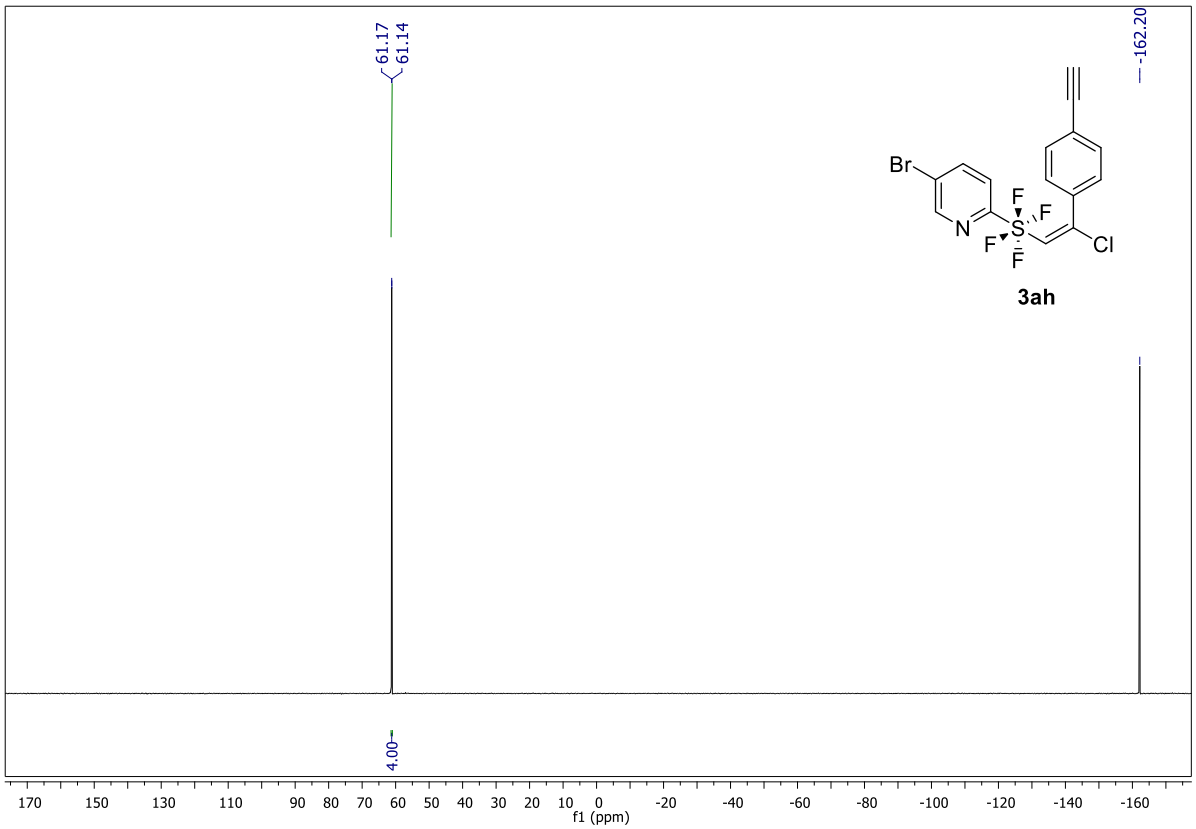
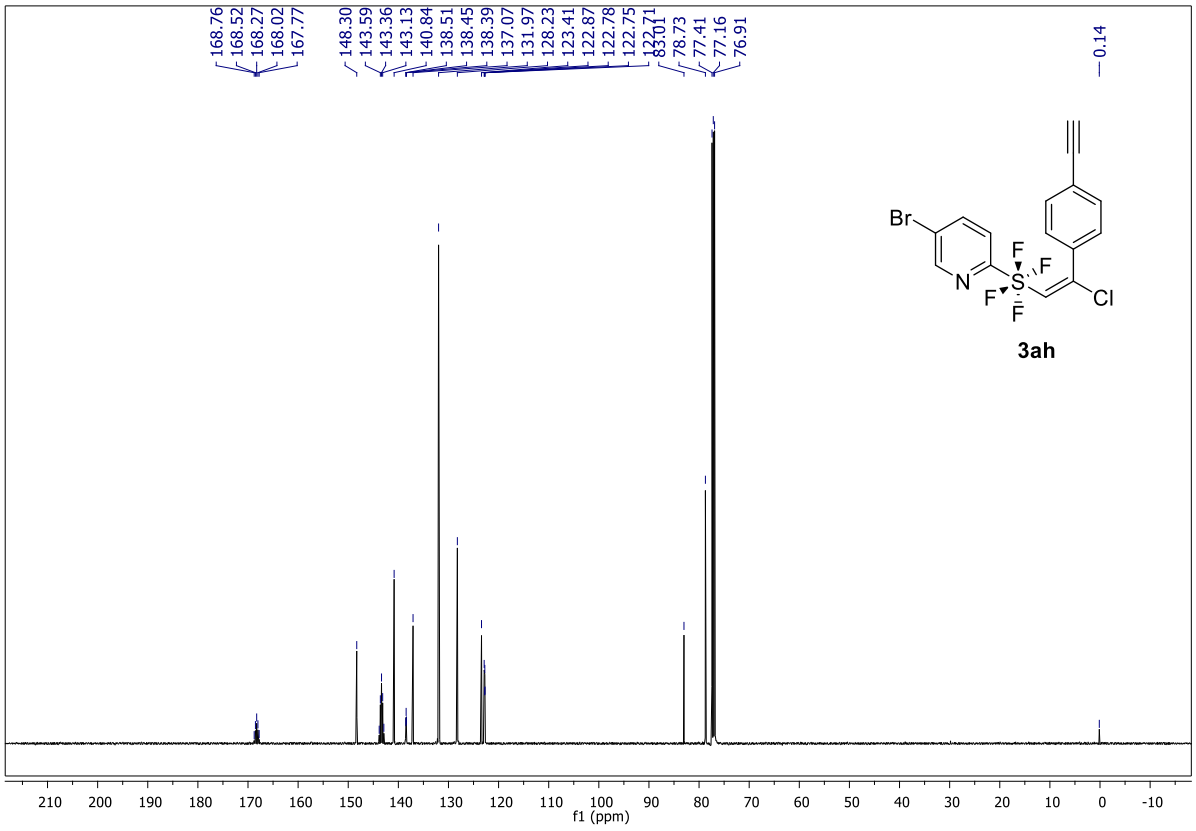
7.50
7.48
7.47
7.40
7.38
7.26
7.25
7.22
7.20
7.17
7.14
3.12
-0.00
-0.00
Br
N
F
S
F
F
F
Cl
3ah
1.00
1.12
3.27
2.28
1.28
0.96
f1 (ppm)


61.17
61.14
-162.20
Br
F
F
F
F
S
N
Cl
3ah
4.00
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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168.52
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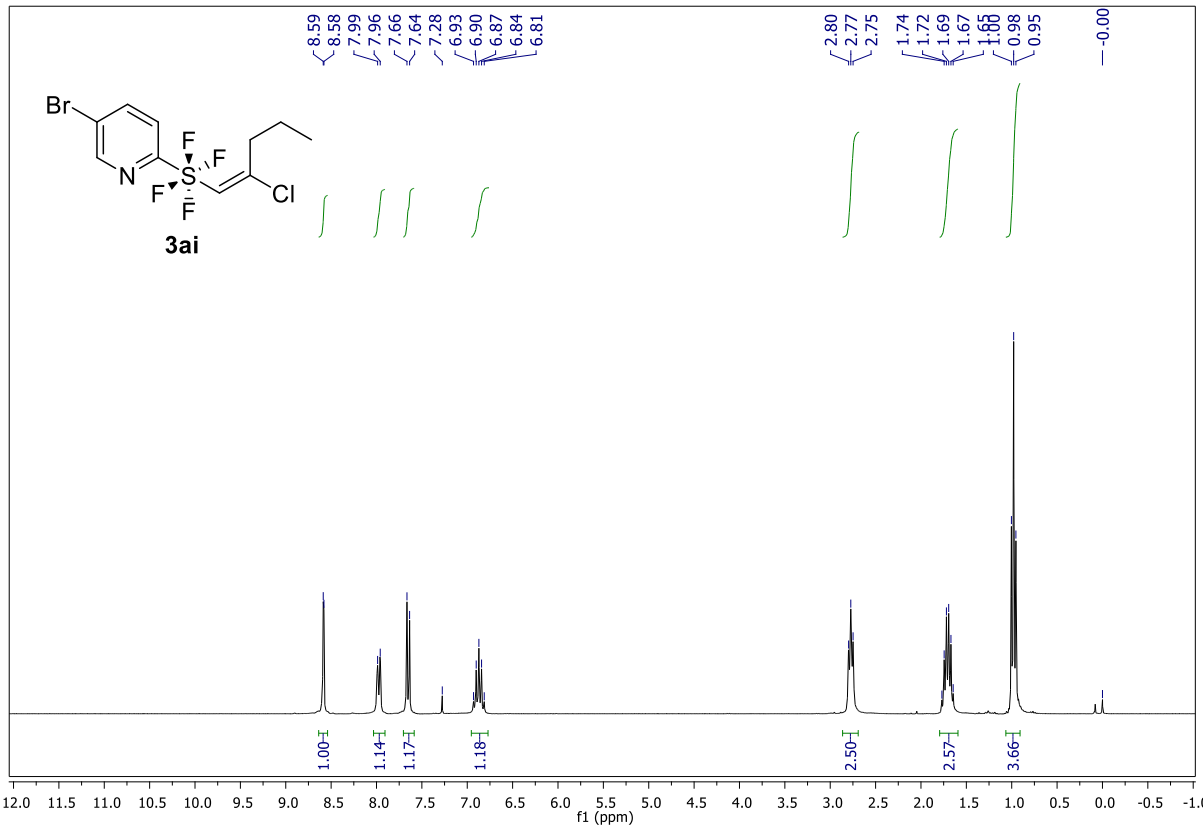
168.02
167.77
148.30
143.59
143.36
143.13
140.84
138.51
138.45
138.39
137.07
131.97
128.23
123.41
122.87
122.78
122.75
122.71
83.01
78.73
77.41
77.16
76.91
0.14
Br
F
F
F
F
S
N
Cl
3ah
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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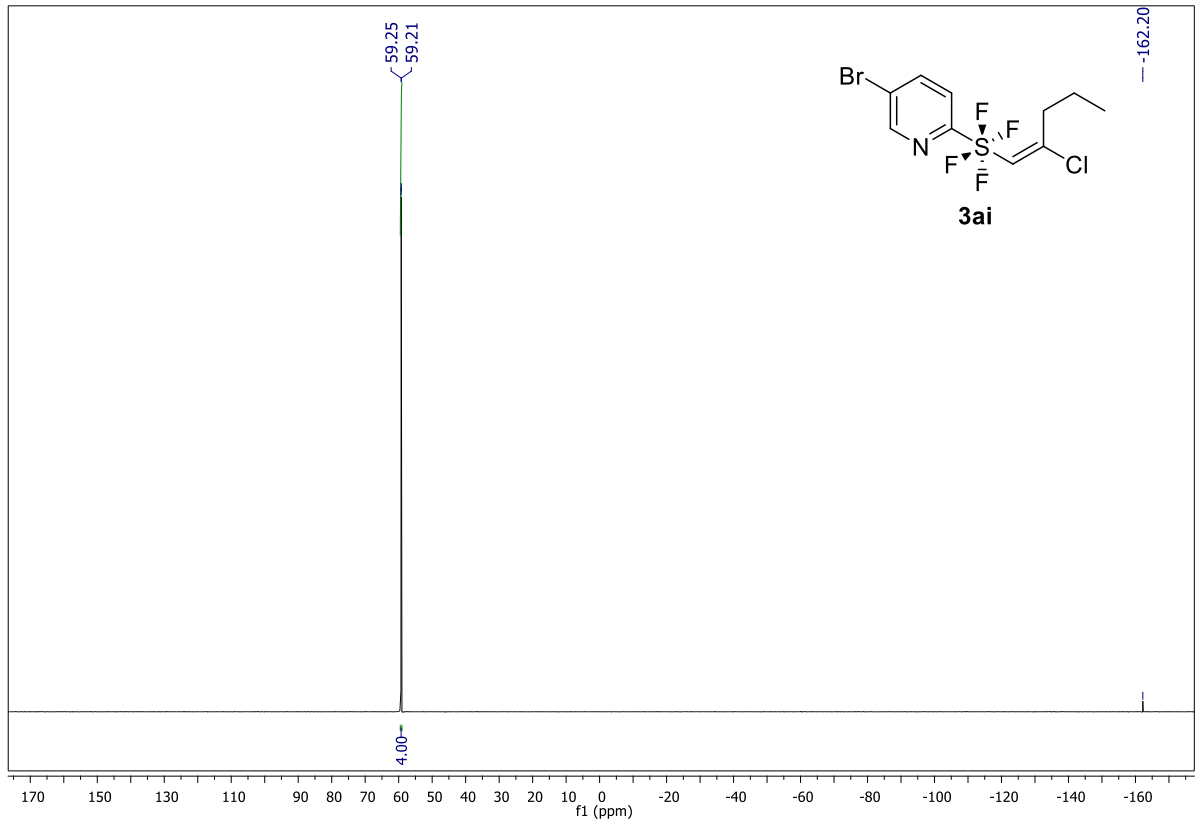
7.64
7.28
6.93
6.90
6.87
6.84
6.81
2.80
2.77
2.75
1.74
1.72
1.69
1.67
0.98
0.95
-0.00
Br
N
F
F
F
F
S
Cl
3ai
1.00
1.14
1.17
1.18
2.50
2.57
3.66
f1 (ppm)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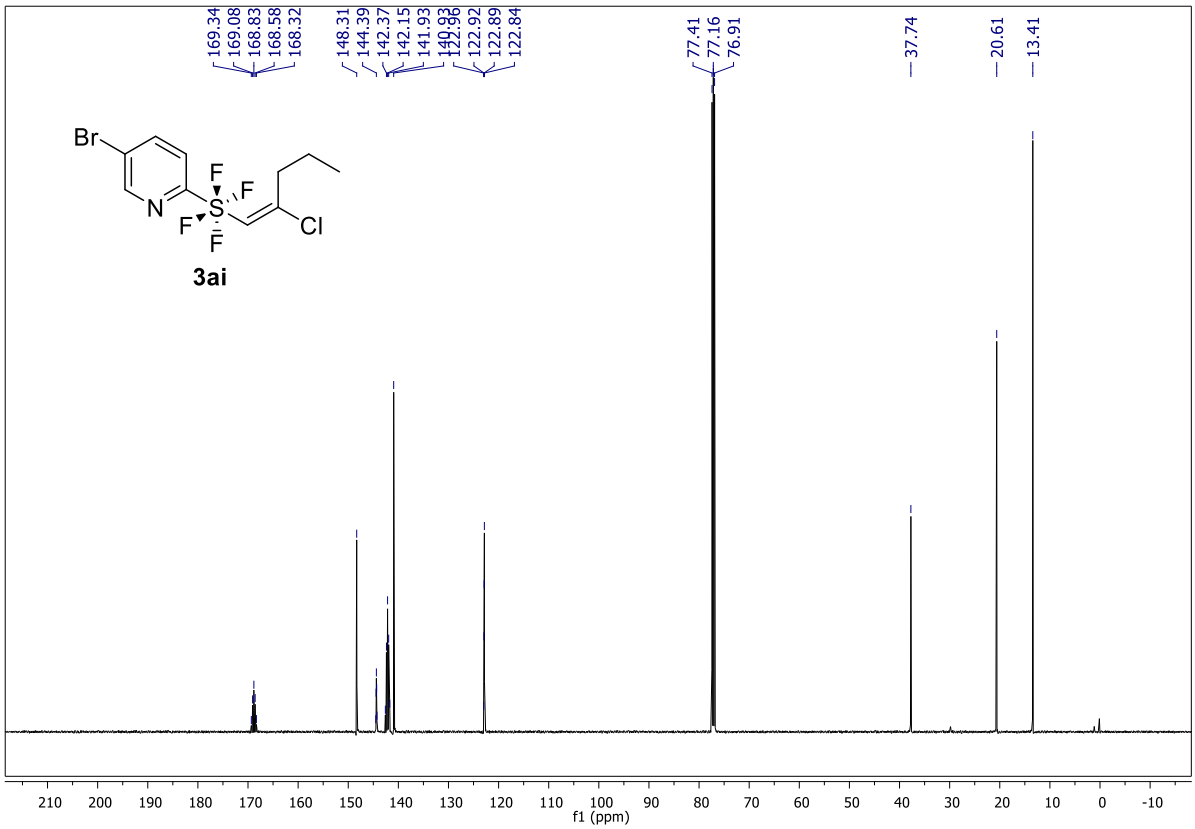
N
F
F
F
F
S
Cl
3ai
4.00
f1 (ppm)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168.58
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144.39
142.37
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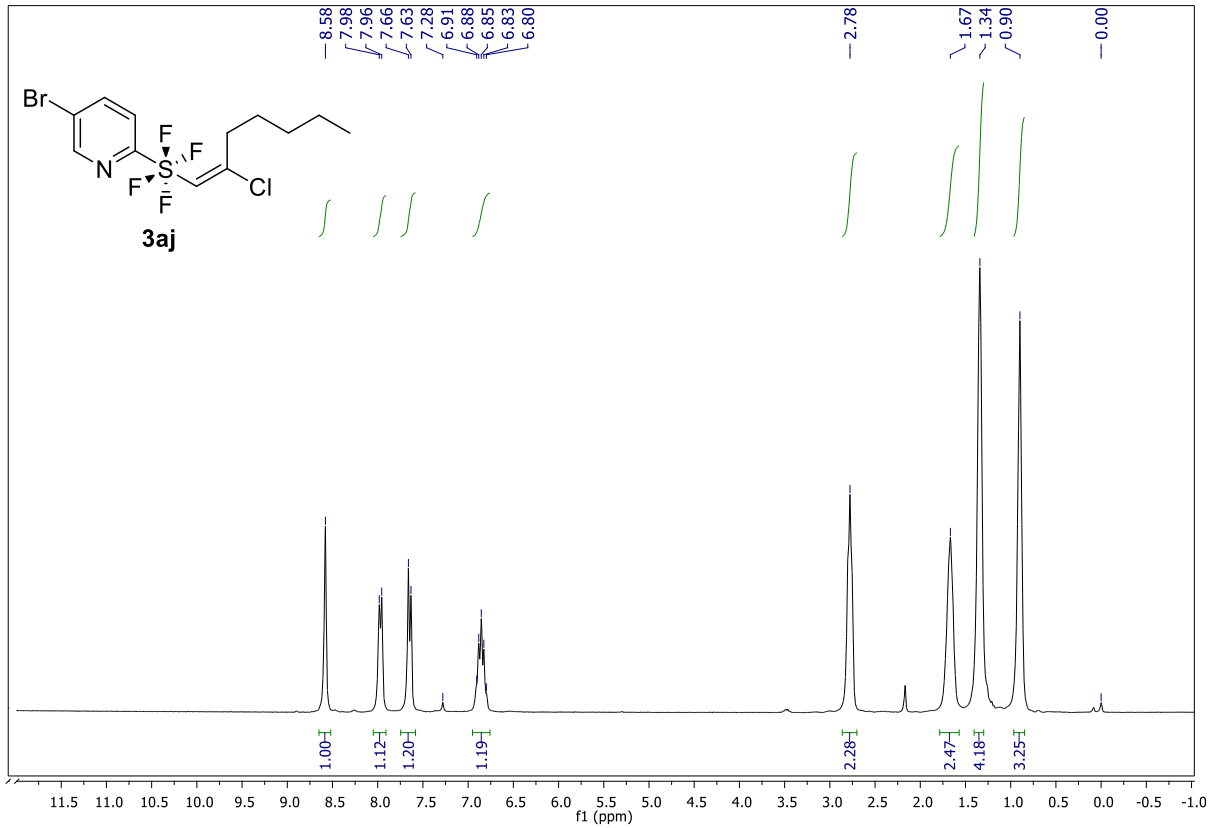
141.93
140.93
122.98
122.92
122.89
122.84
77.41
77.16
76.91
37.74
20.61
13.41
Br
N
S
F
F
F
F
Cl
3ai
f1 (ppm)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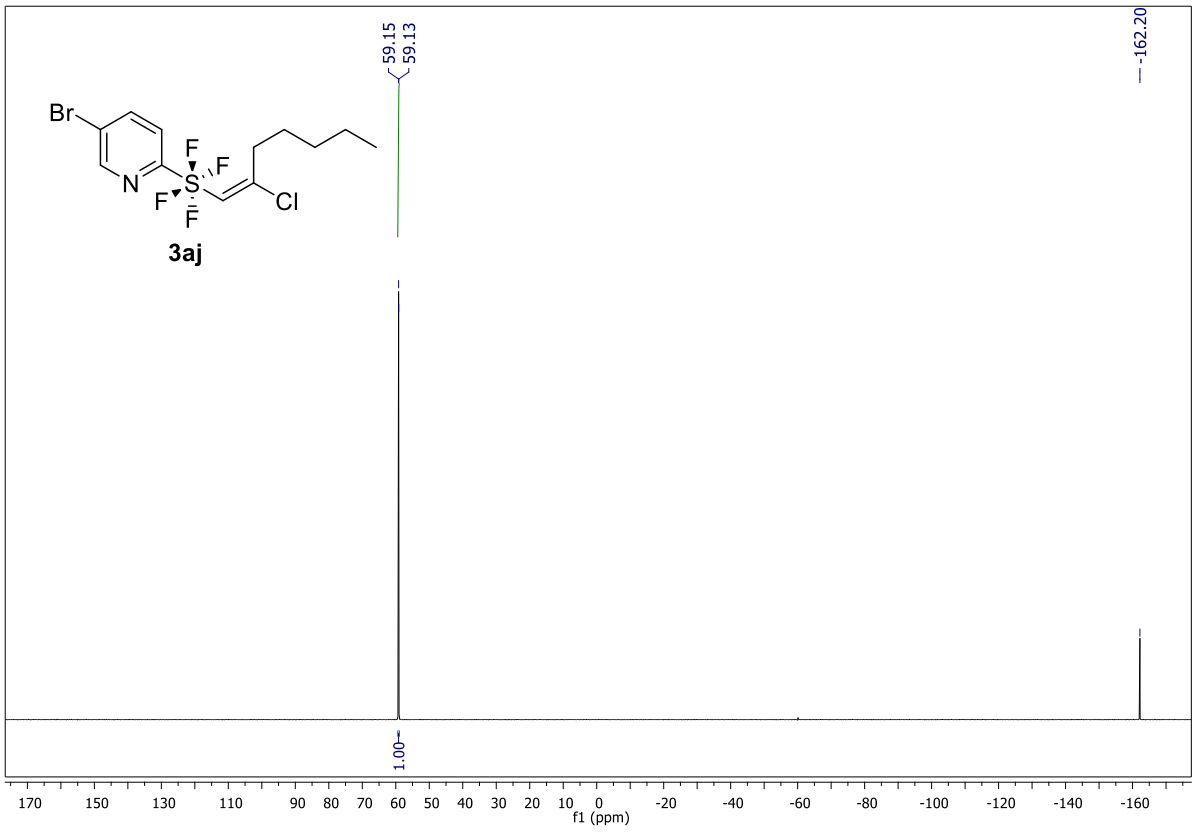
7.98
7.96
7.66
7.63
7.28
6.91
6.88
6.85
6.83
6.80
2.78
1.67
1.34
0.90
0.00
Br
N
S
F
F
F
F
Cl
3aj
1.00
1.12
1.20
1.19
2.28
2.47
4.18
3.25
f1 (ppm)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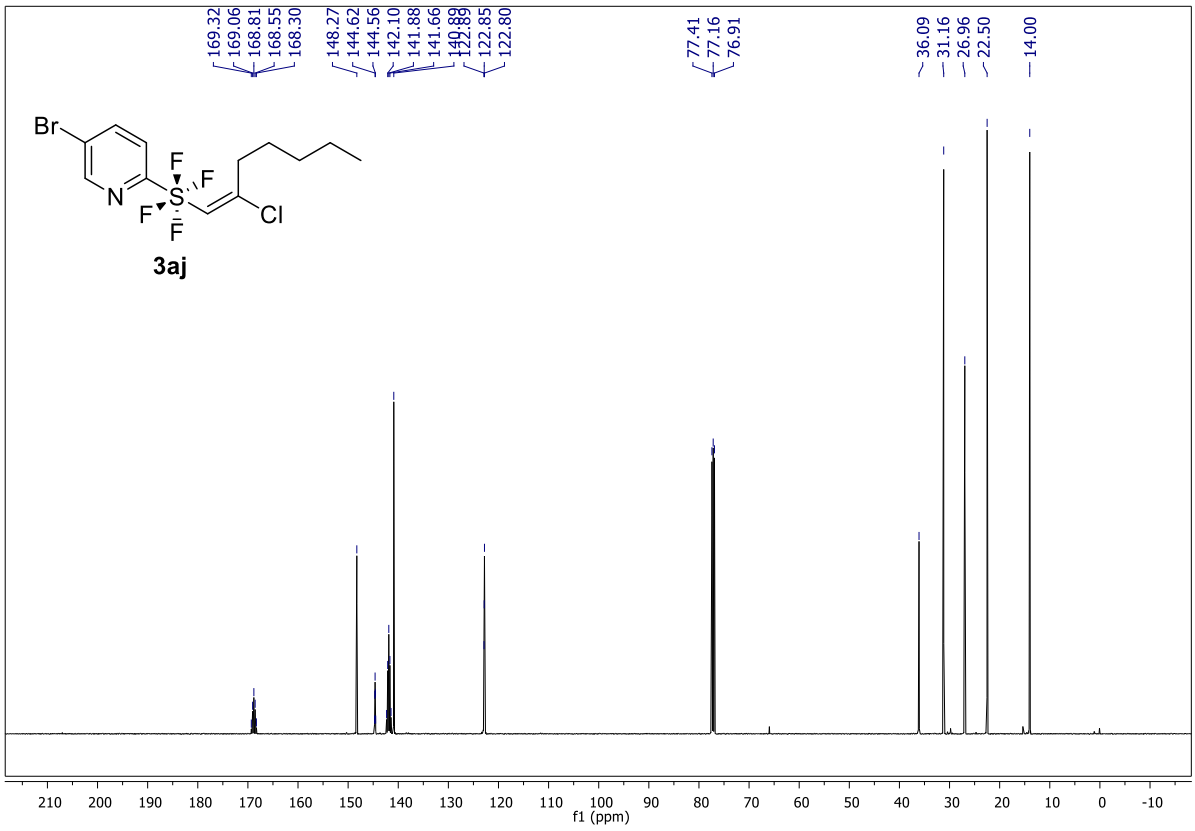
-162.20
Br
F
F
N
S
F
F
Cl
3aj
1.00
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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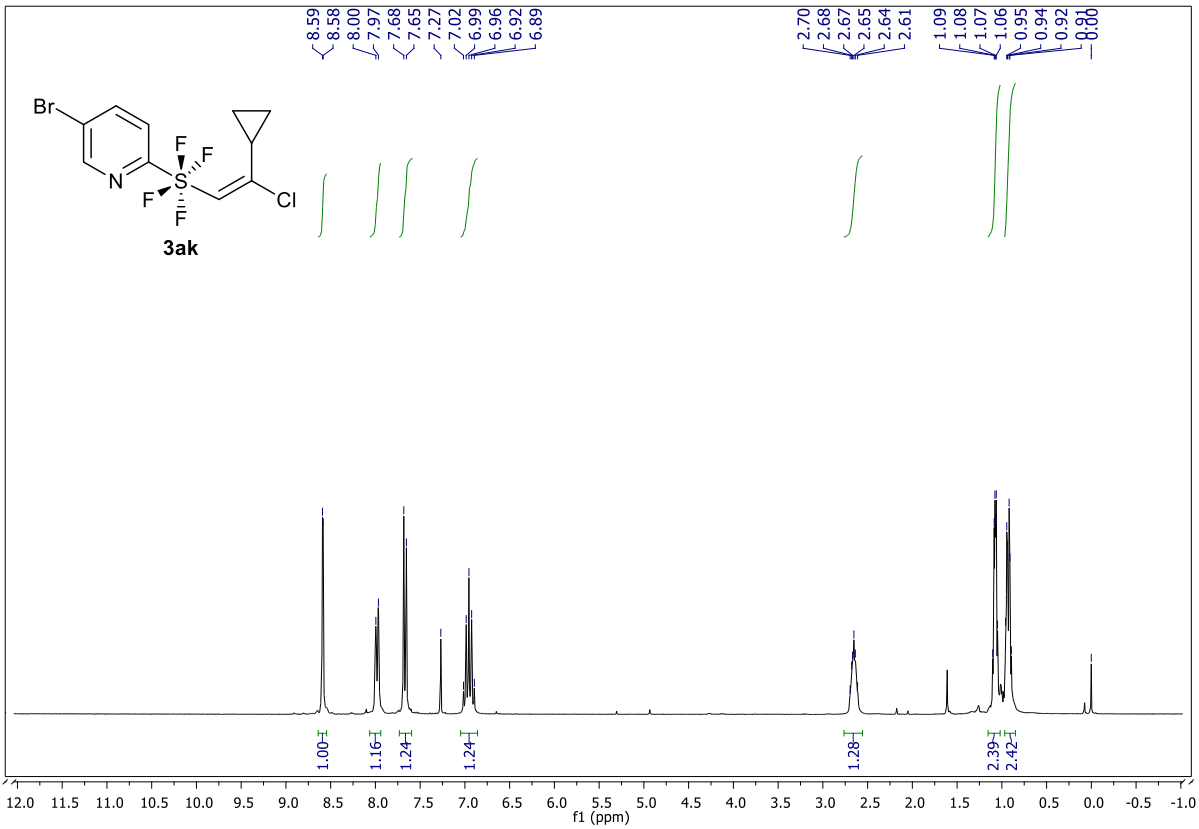
148.27
144.62
144.56
142.10
141.88
141.66
122.85
122.80
77.41
77.16
76.91
36.09
31.16
26.96
22.50
14.00
Br
F
F
N
S
F
F
Cl
3aj
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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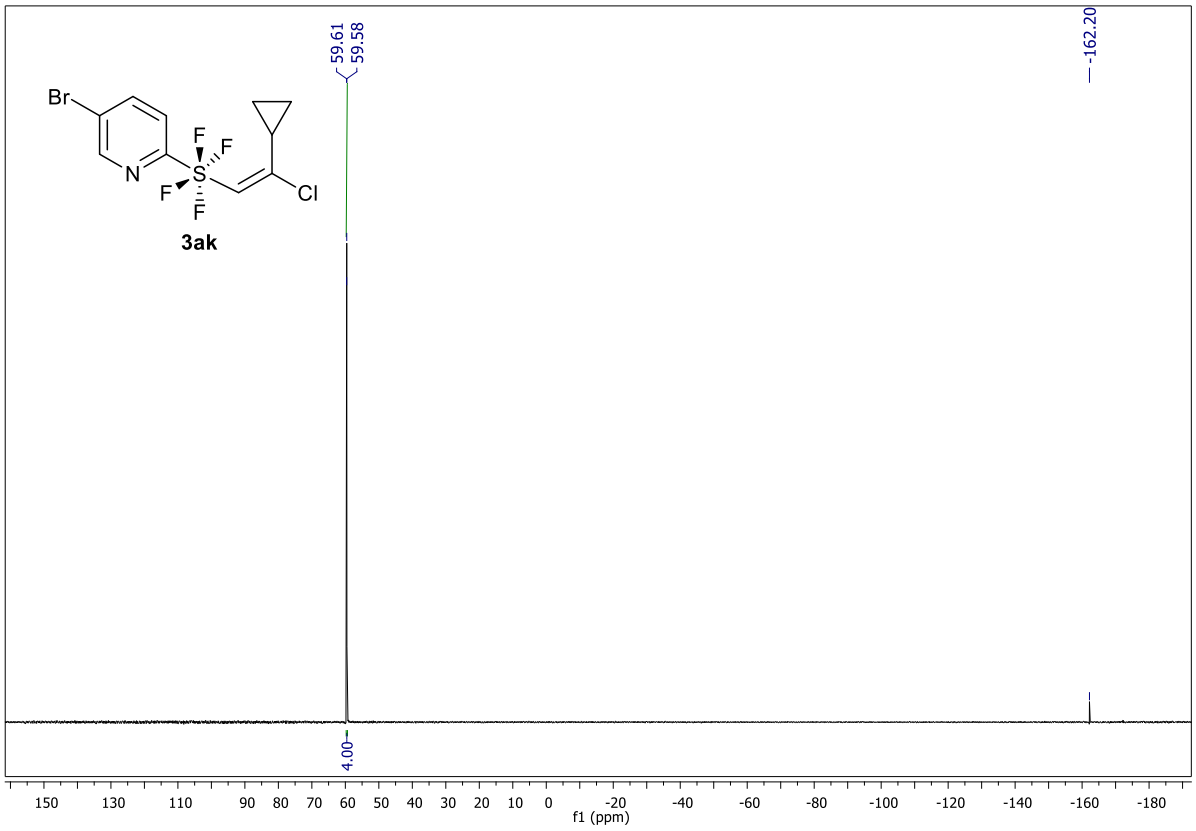
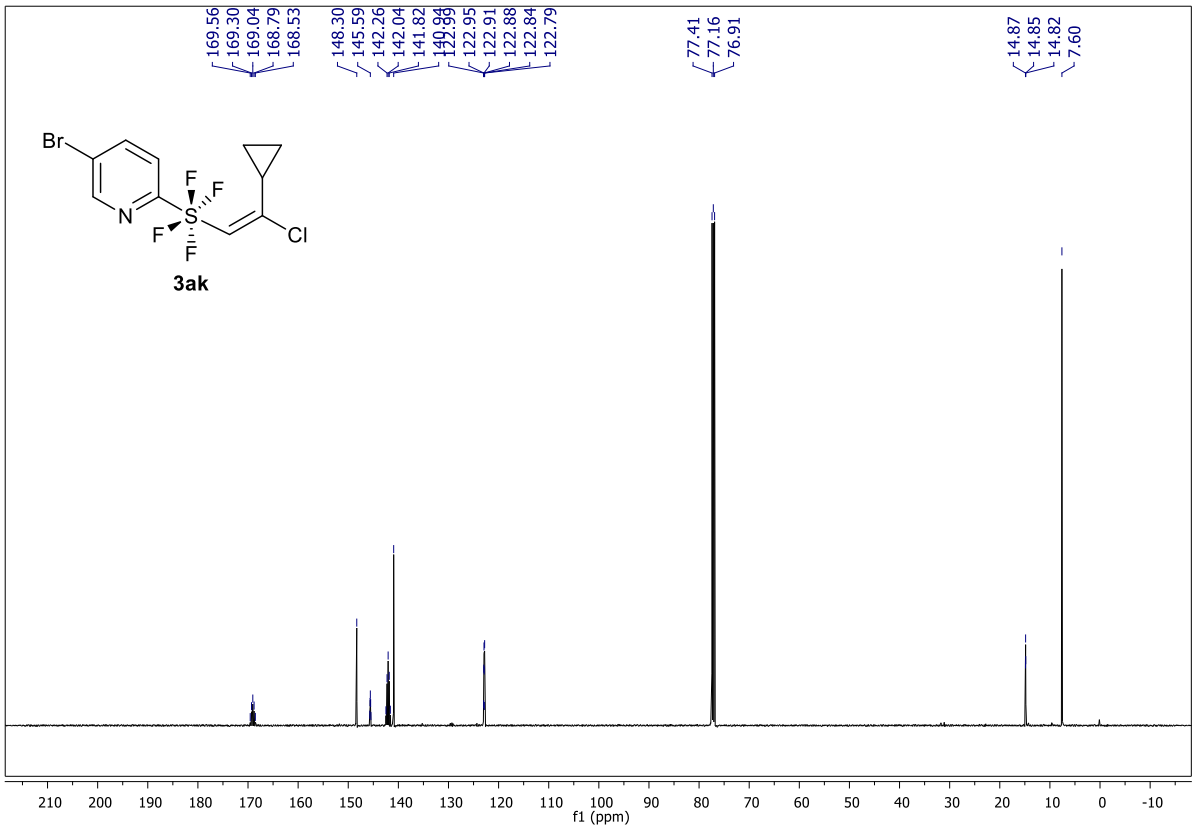
7.68
7.65
7.27
7.02
6.99
6.96
6.92
6.89
2.70
2.68
2.67
2.65
2.64
2.61
1.09
1.08
1.07
1.06
0.95
0.94
0.92
0.91
0.00
Br
F
F
N
S
F
F
Cl
3ak
1.00
1.16
1.24
1.24
1.28
2.39
2.42
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


59.61
59.58
-162.20
Br
F
F
N
S
F
F
Cl
3ak
4.00
150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180
f1 (ppm)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169.04
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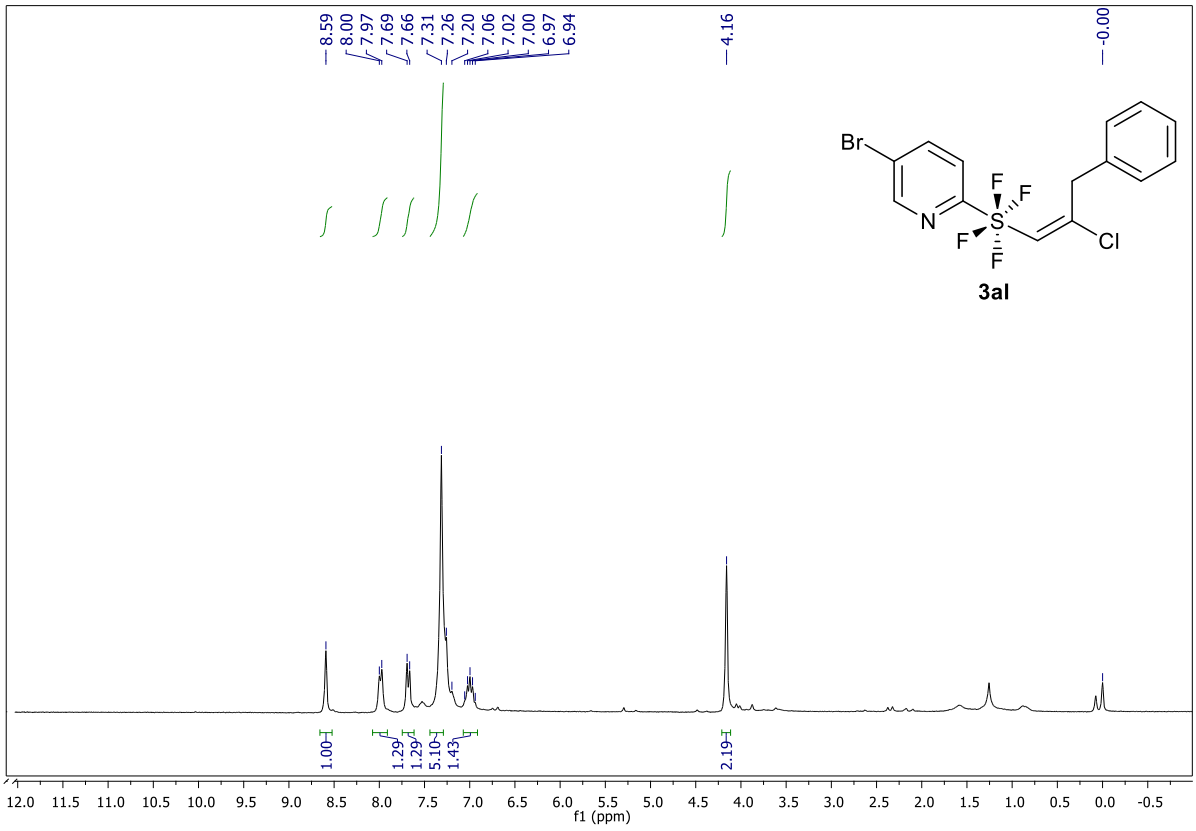
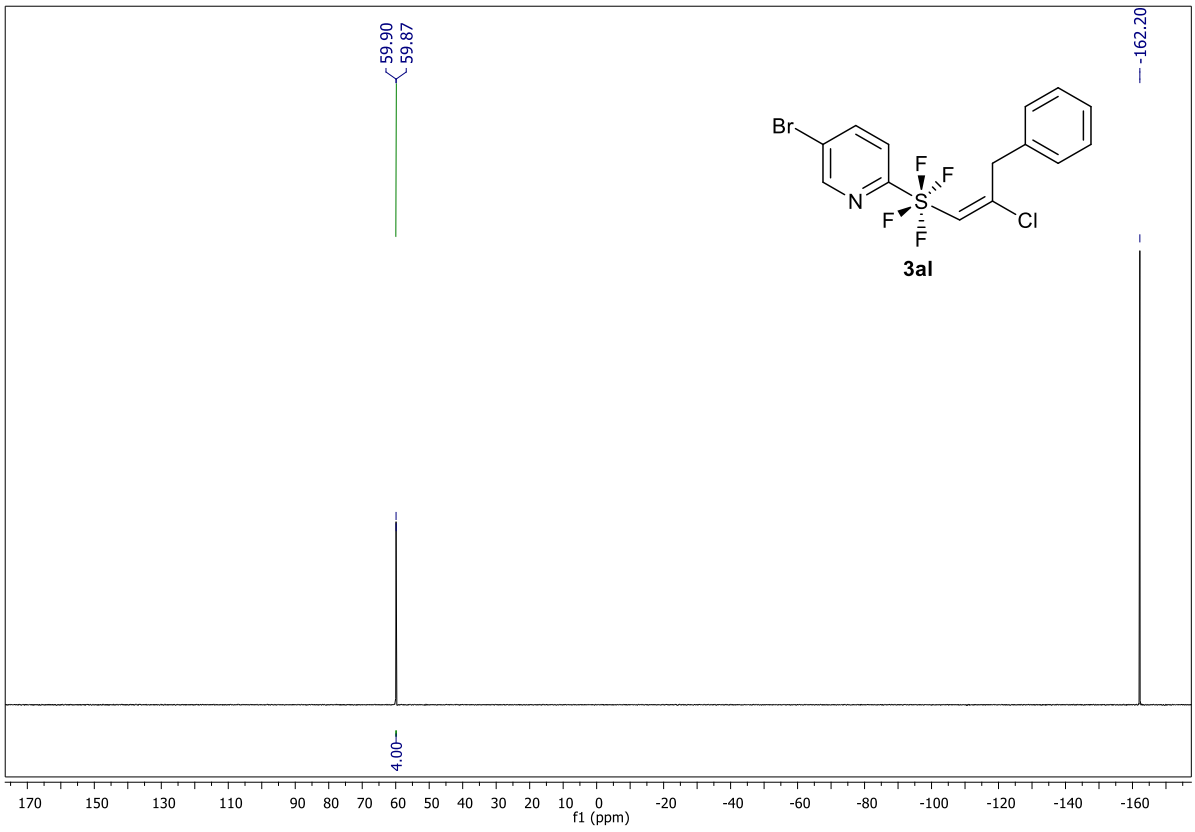
168.53
148.30
145.59
142.26
142.04
141.82
122.95
122.91
122.88
122.84
122.79
77.41
77.16
76.91
14.87
14.85
14.82
7.60
Br
F
F
N
S
F
F
Cl
3ak
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.59
8.00
7.97
7.69
7.66
7.31
7.26
7.20
7.06
7.02
7.00
6.97
6.94
4.16
-0.00
Br
F
F
N
S
F
F
Cl
3al
1.00
1.29
1.29
5.10
1.43
2.19
12.0 11.5 11.0 10.5 10.0 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
f1 (ppm)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59.87
-162.20
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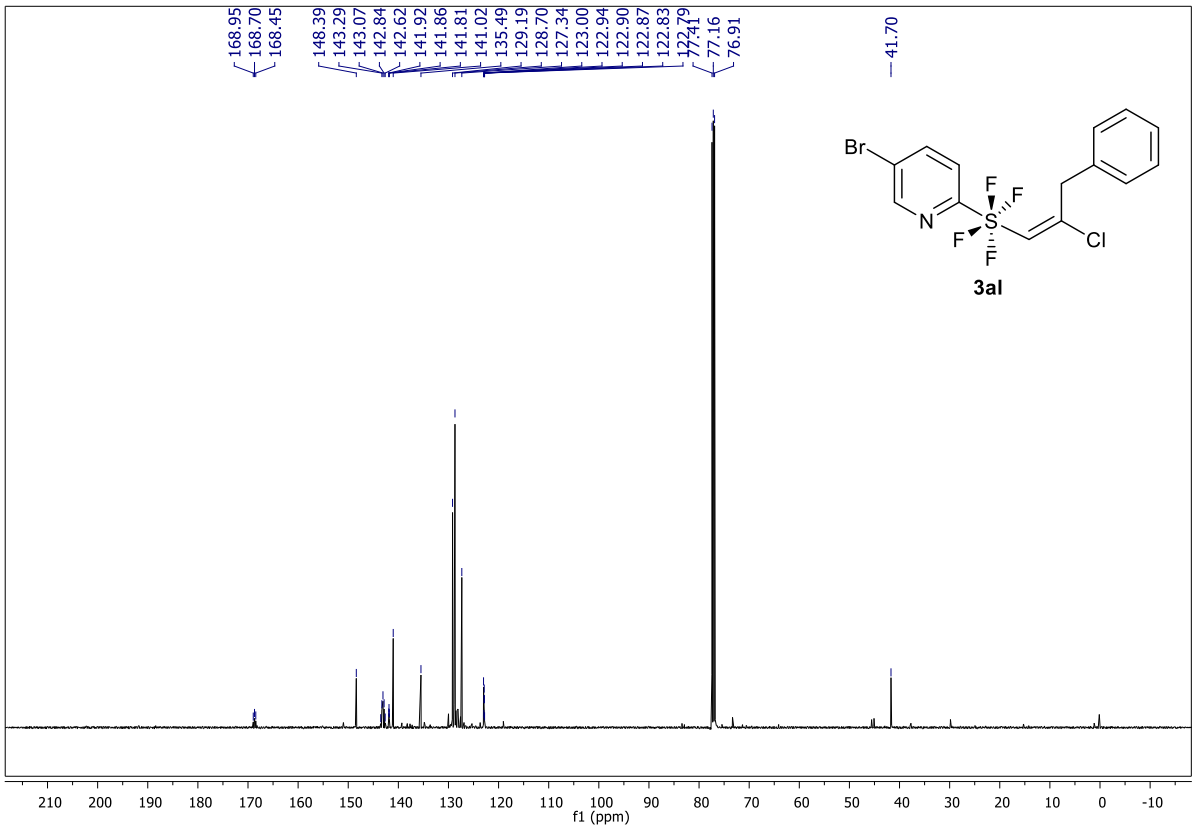
N
F
F
S
F
F
Cl
3al
4.00
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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168.70
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143.07
142.84
142.62
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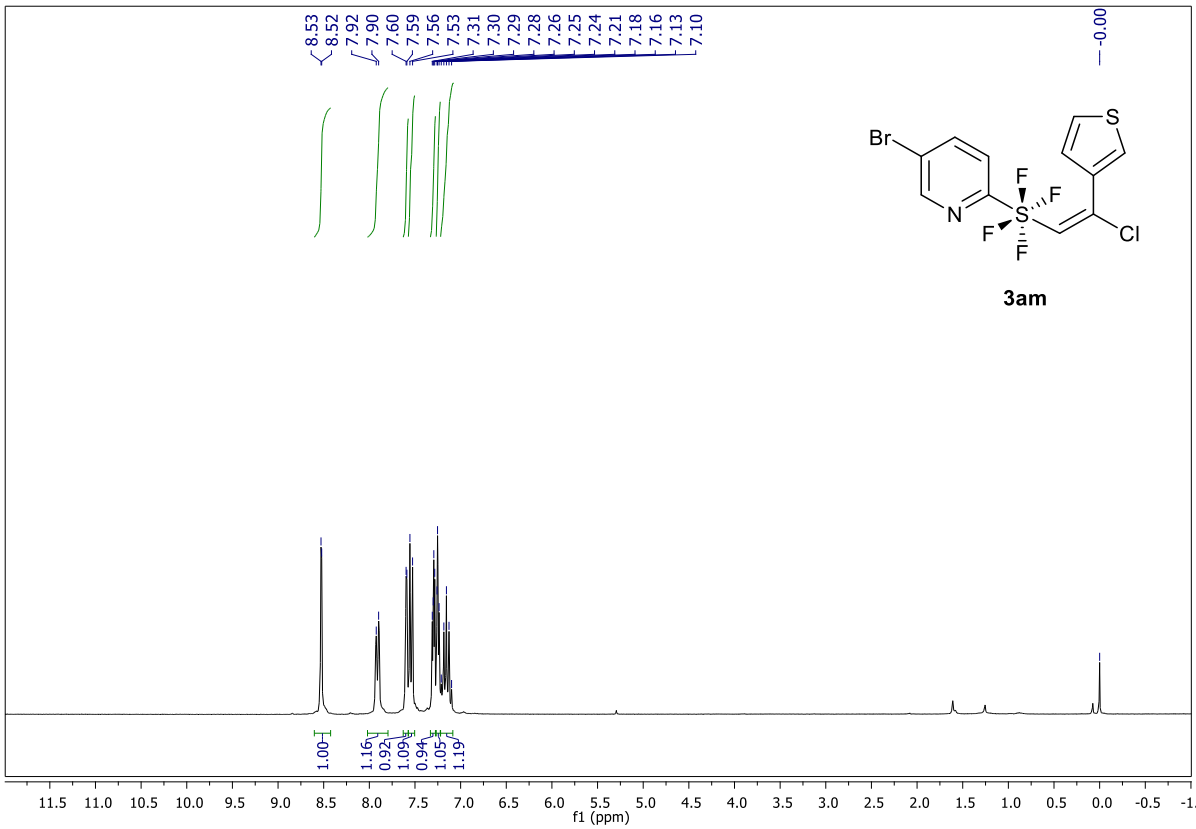
141.81
141.02
135.49
129.19
128.70
127.34
123.00
122.94
122.90
122.87
122.83
122.79
77.41
77.16
76.91
41.70
Br
N
F
F
S
F
F
Cl
3al
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.52
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7.90
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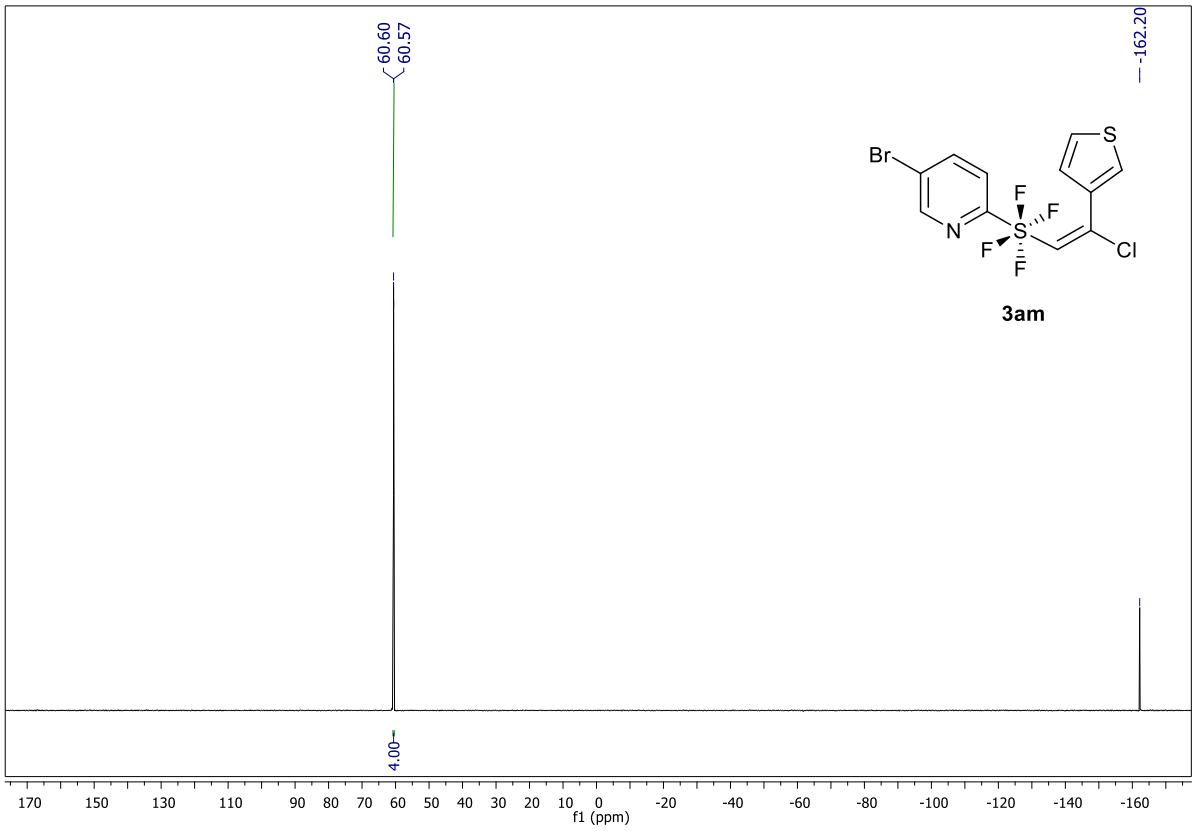
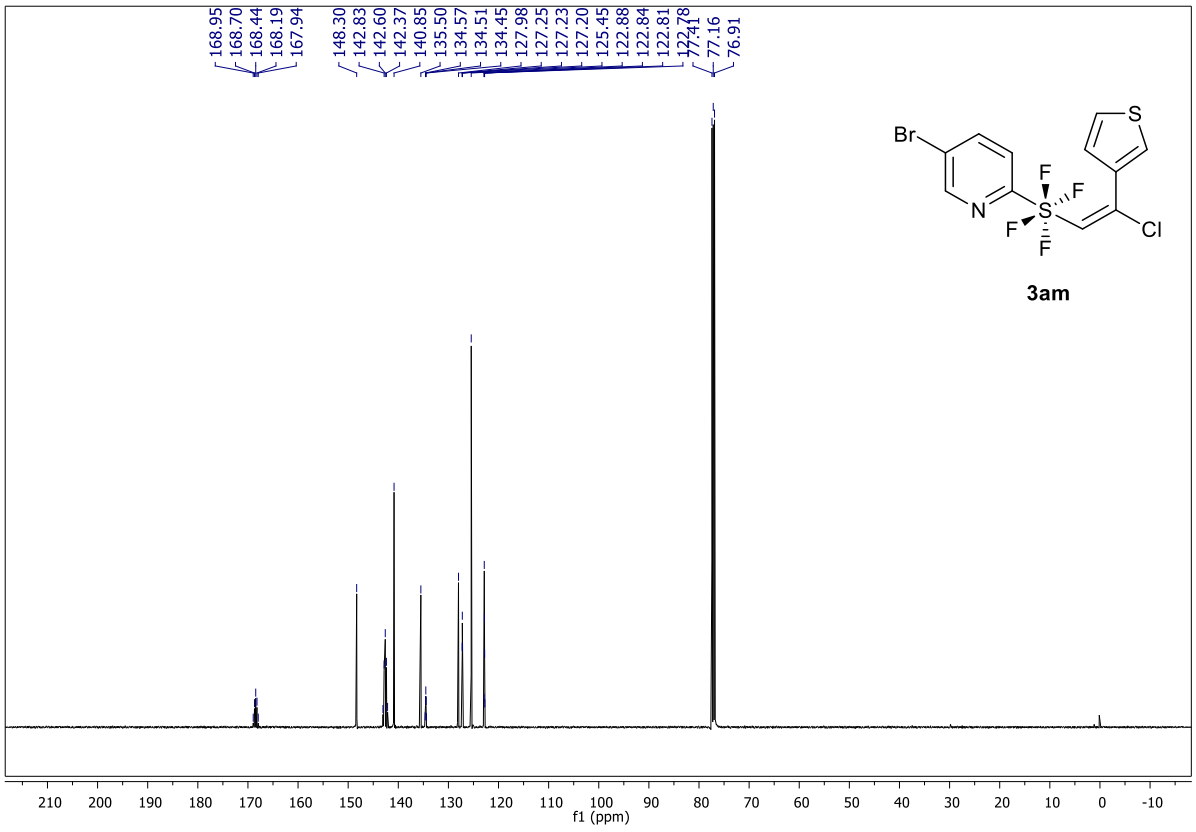
7.59
7.56
7.53
7.31
7.30
7.29
7.28
7.26
7.25
7.24
7.21
7.18
7.16
7.13
7.10
-0.00
Br
N
S
F
F
F
F
S
Cl
3am
1.00
1.16
0.92
1.09
0.94
1.05
1.19
f1 (ppm)


60.60
60.57
-162.20
Br
N
S
F
F
F
F
S
Cl
3am
4.00
f1 (ppm)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168.44
168.19
167.94
148.30
142.83
142.60
142.37
140.85
135.50
134.57
134.51
134.45
127.98
127.25
127.23
127.20
125.45
122.88
122.84
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122.78
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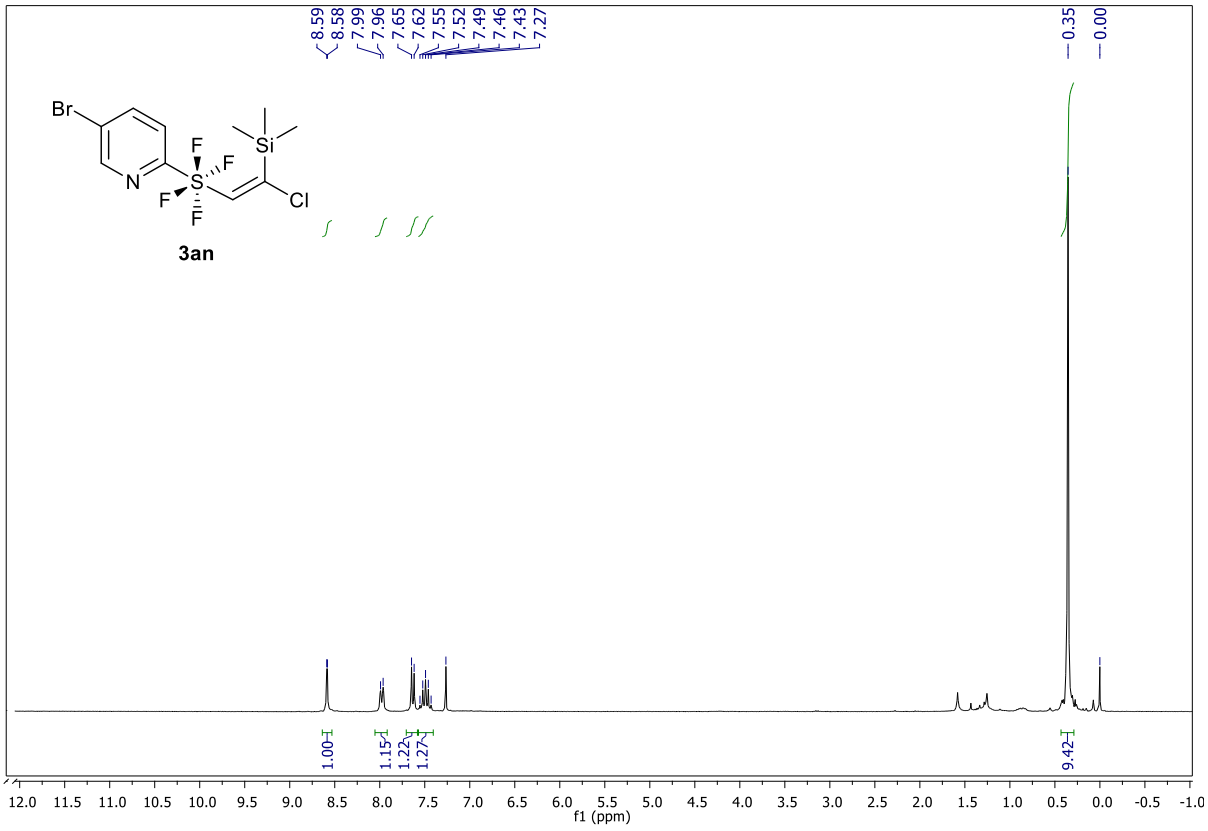
77.16
76.91
Br
N
S
F
F
F
F
S
Cl
3am
f1 (ppm)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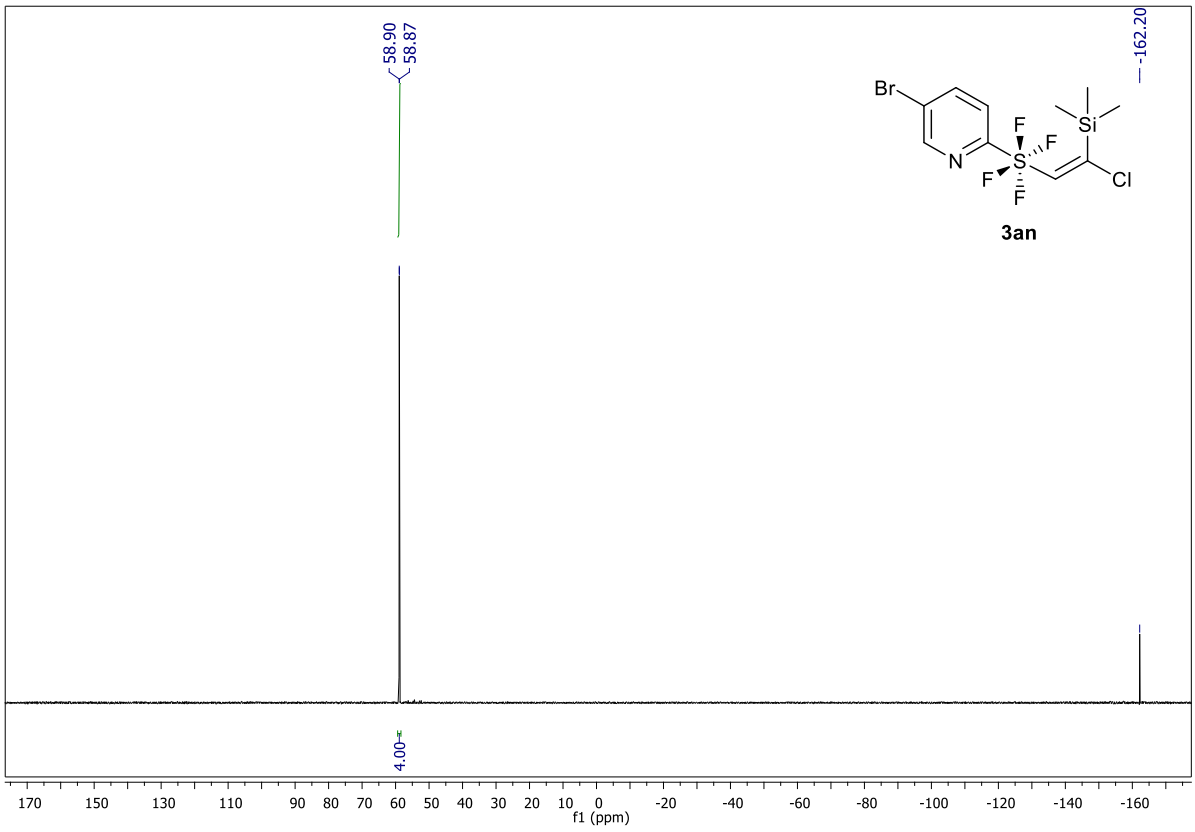
8.58
7.99
7.96
7.65
7.62
7.55
7.52
7.49
7.46
7.43
7.27
0.35
0.00
Br
N
F
F
F
F
Si
Cl
3an
1.00
1.15
1.22
1.27
9.42
f1 (ppm)


58.90
58.87
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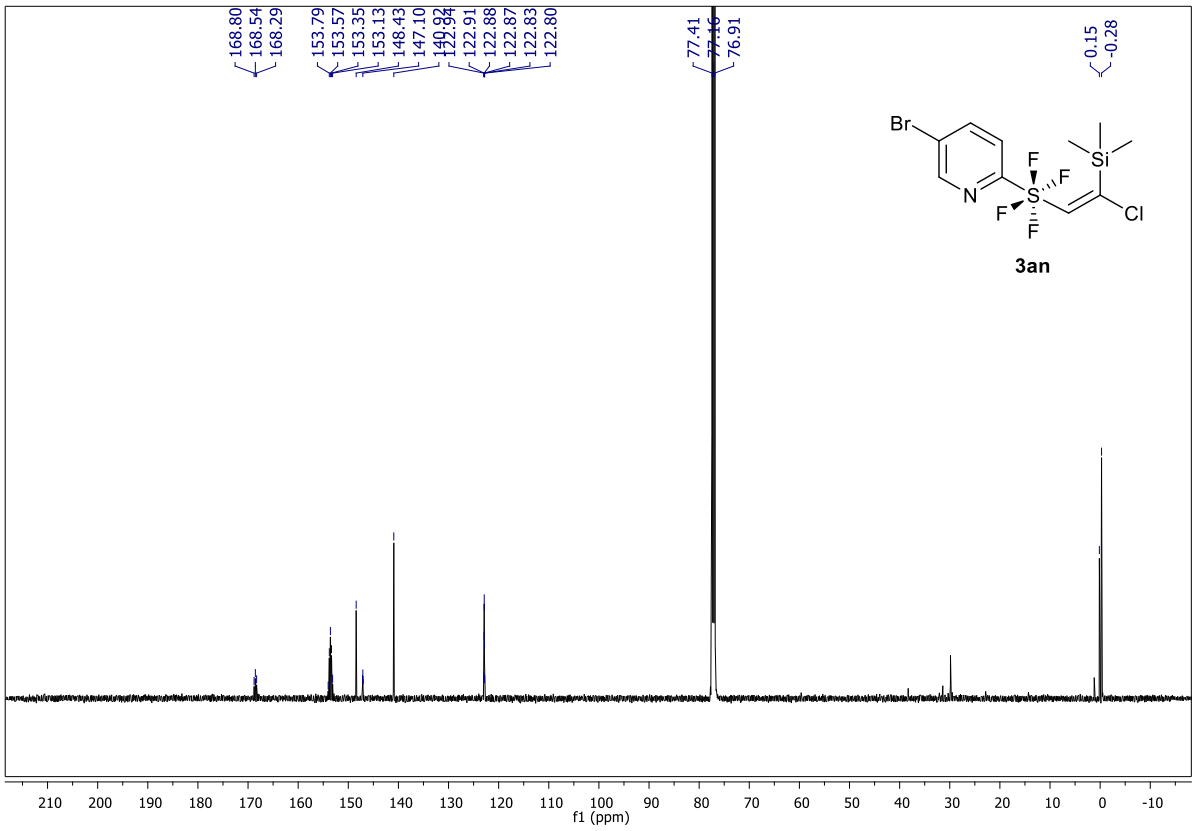
Br
N
S
F
F
F
F
Si
Cl
3an
4.00
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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153.35
153.13
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147.10
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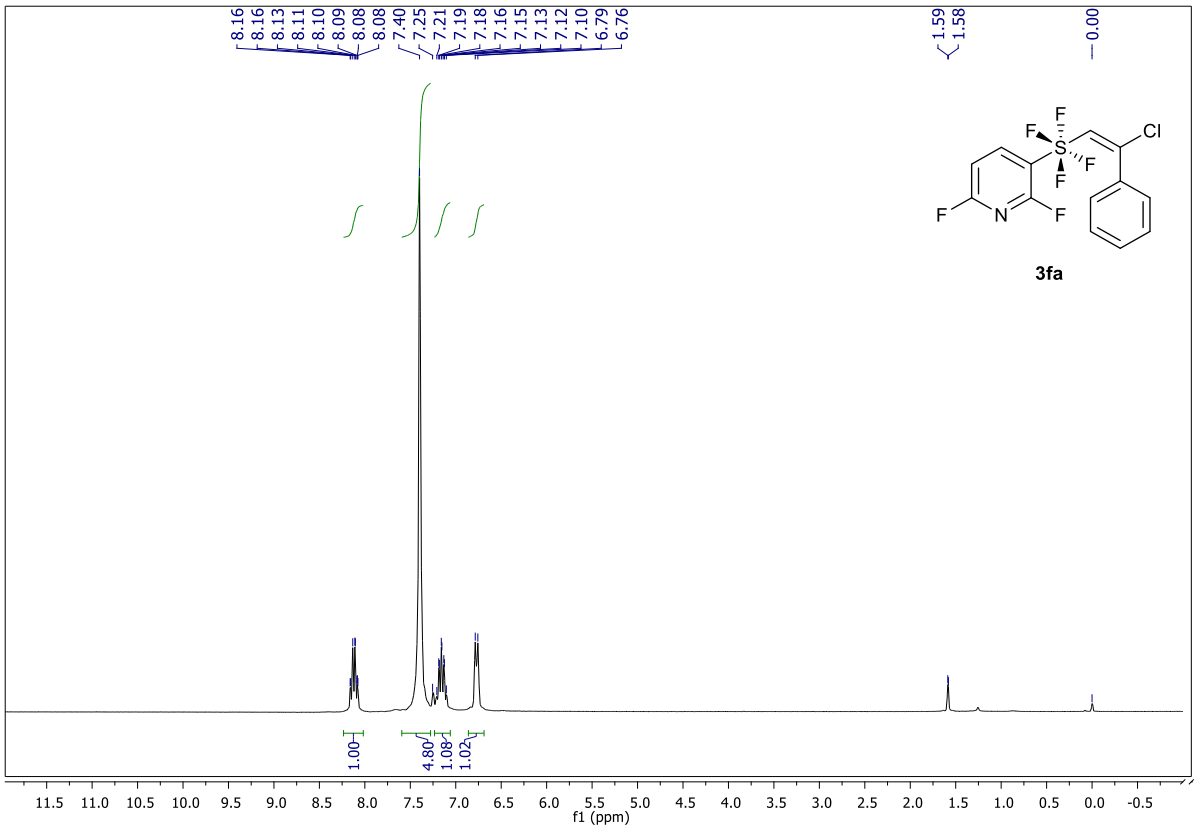
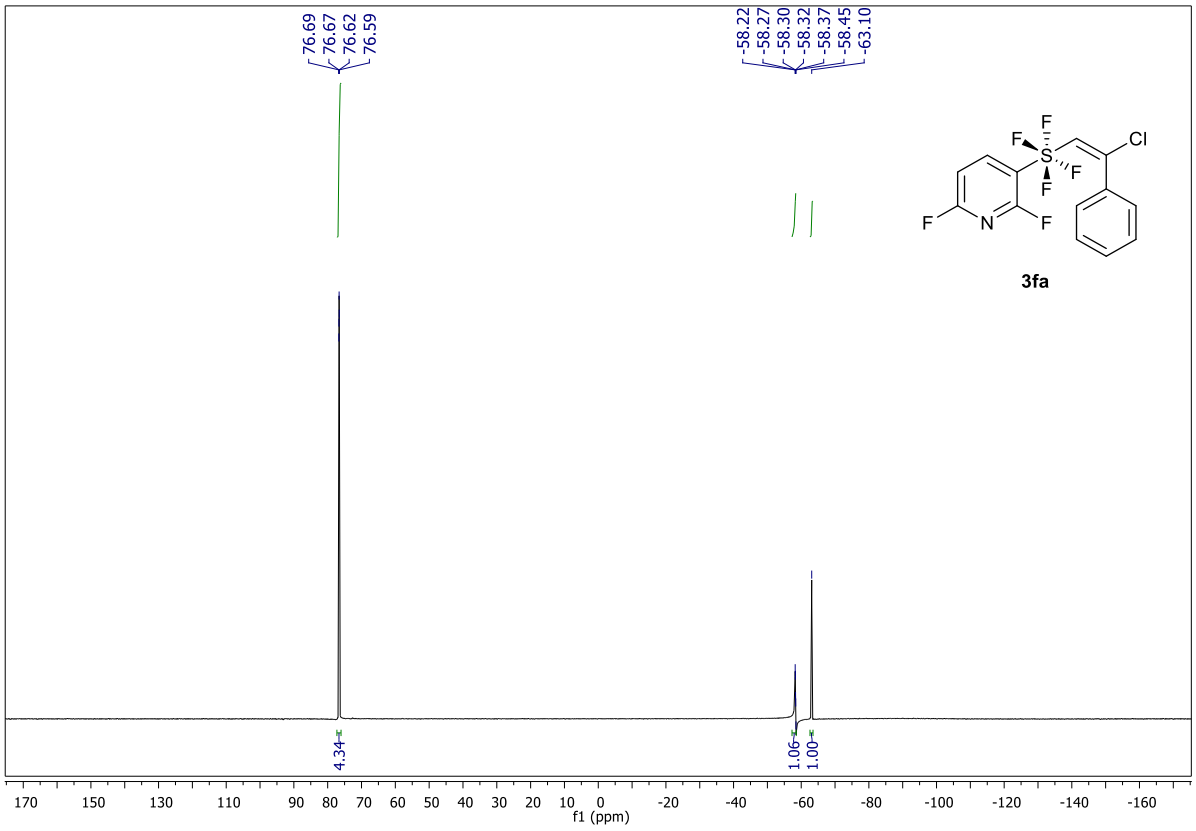
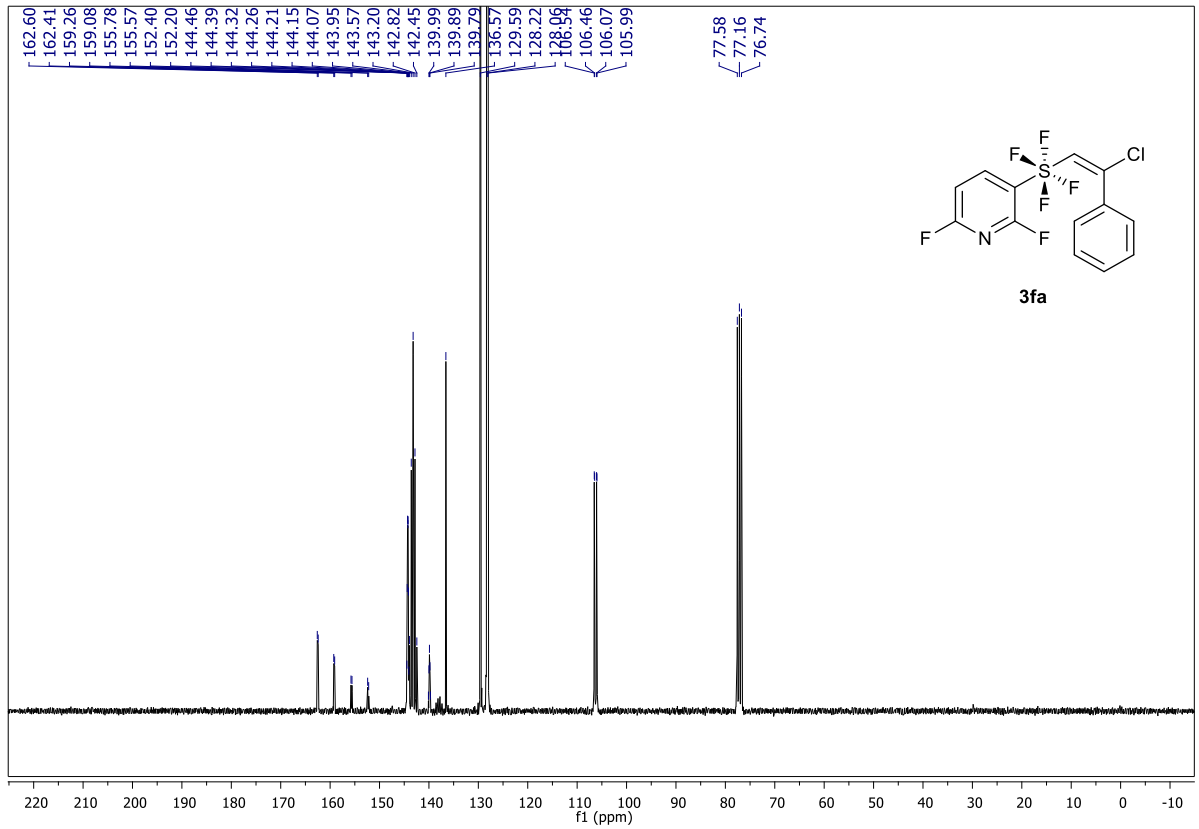
122.88
122.87
122.83
122.80
77.41
77.16
76.91
0.15
-0.28
Br
N
S
F
F
F
F
Si
Cl
3an
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.16
8.16
8.13
8.11
8.10
8.09
8.08
8.08
7.40
7.25
7.21
7.19
7.18
7.16
7.15
7.13
7.12
7.10
6.79
6.76
1.59
1.58
0.00
1.00
4.80
1.08
1.02
11.5 11.0 10.5 10.0 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
f1 (ppm)
F
F
S
F
F
Cl
F
N
F
3fa


76.69
76.67
76.62
76.59
-58.22
-58.27
-58.30
-58.32
-58.37
-58.45
-63.10
4.34
1.06
1.00
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)
F
F
S
F
F
Cl
F
N
F
3fa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162.41
159.26
159.08
155.78
155.57
152.40
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144.46
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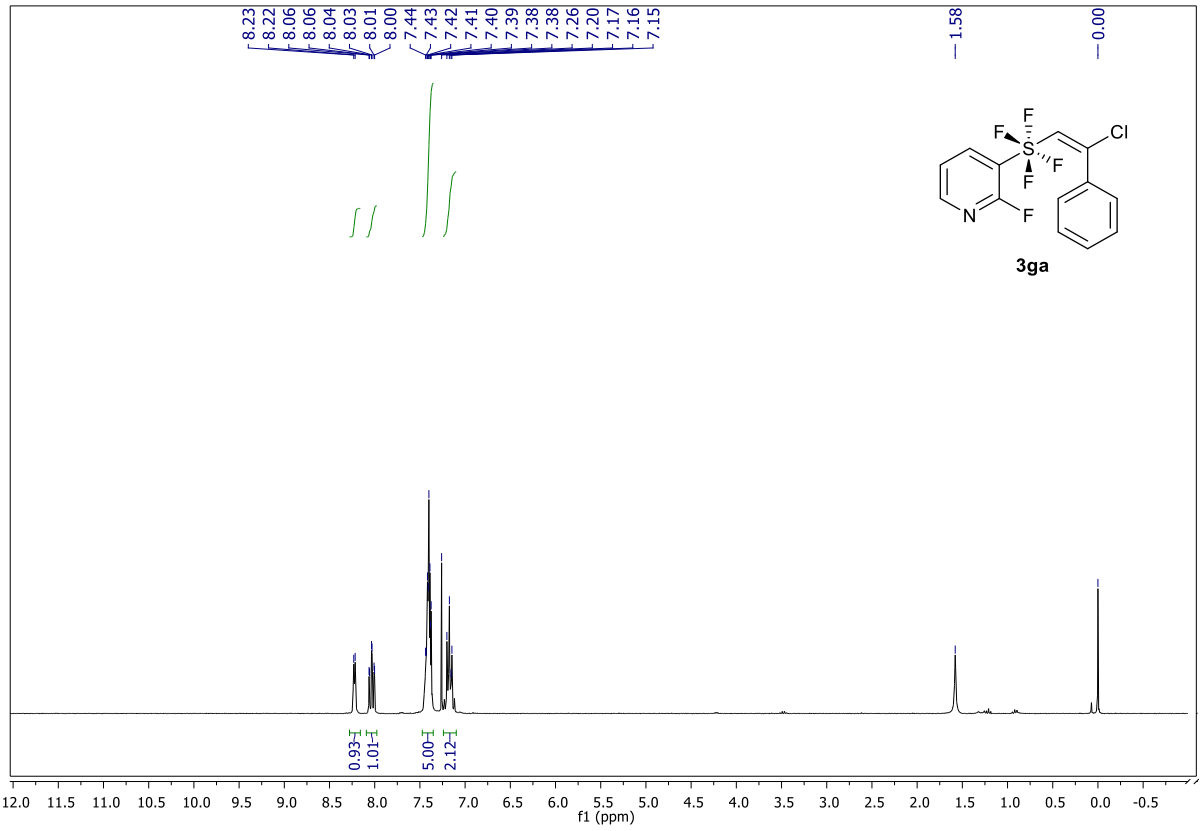
144.32
144.26
144.21
144.15
144.07
143.95
143.57
143.20
142.82
142.45
139.99
139.89
139.79
136.57
129.59
128.22
128.06
106.54
106.46
106.07
105.99
77.58
77.16
76.74
F
F
S
F
F
Cl
F
N
F
3fa
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.23
8.22
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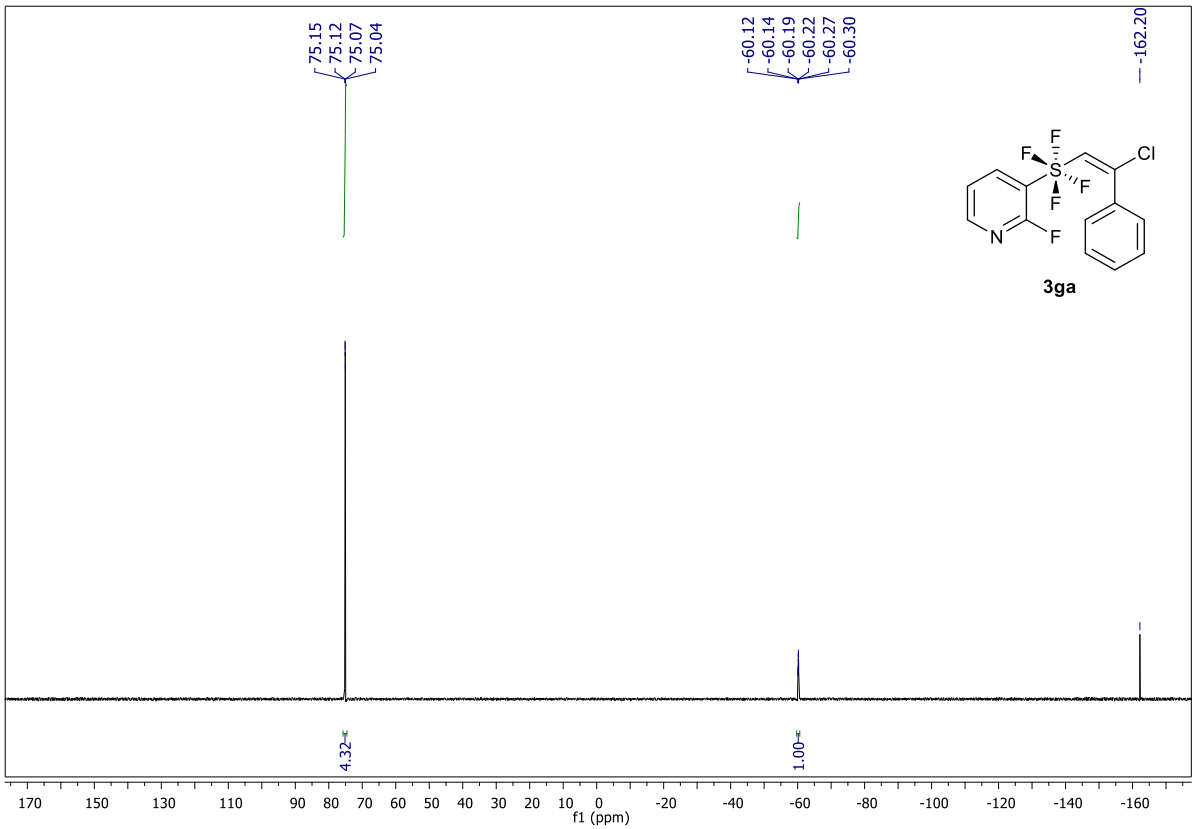
8.06
8.04
8.03
8.01
8.00
7.44
7.43
7.42
7.41
7.40
7.39
7.38
7.38
7.26
7.20
7.17
7.16
7.15
1.58
0.00
F
F
S
F
F
Cl
N
F
3ga
0.93
1.01
5.00
2.12
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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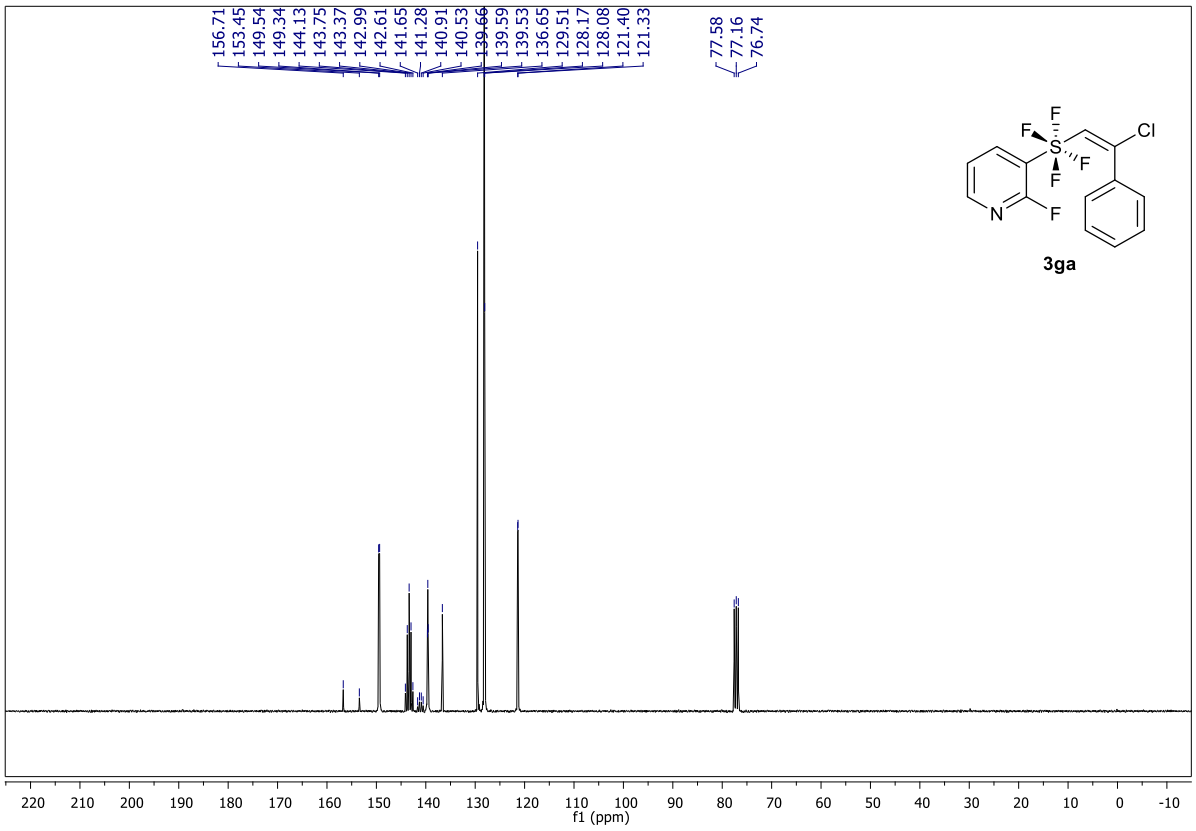
75.12
75.07
75.04
-60.12
-60.14
-60.19
-60.22
-60.27
-60.30
-162.20
F
F
S
F
F
Cl
N
F
3ga
4.32
1.00
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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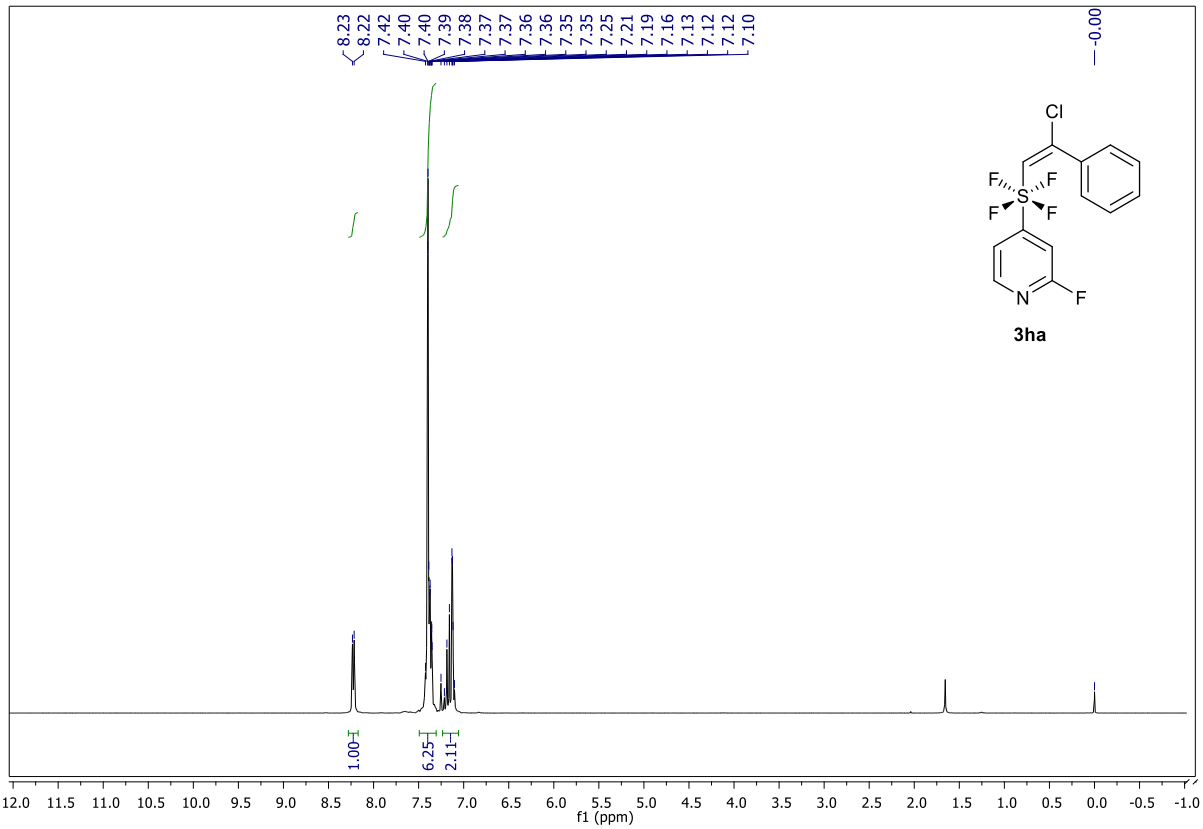
140.53
139.66
139.59
139.53
136.65
129.51
128.17
128.08
121.40
121.33
77.58
77.16
76.74
F
F
S
F
F
Cl
N
F
3ga
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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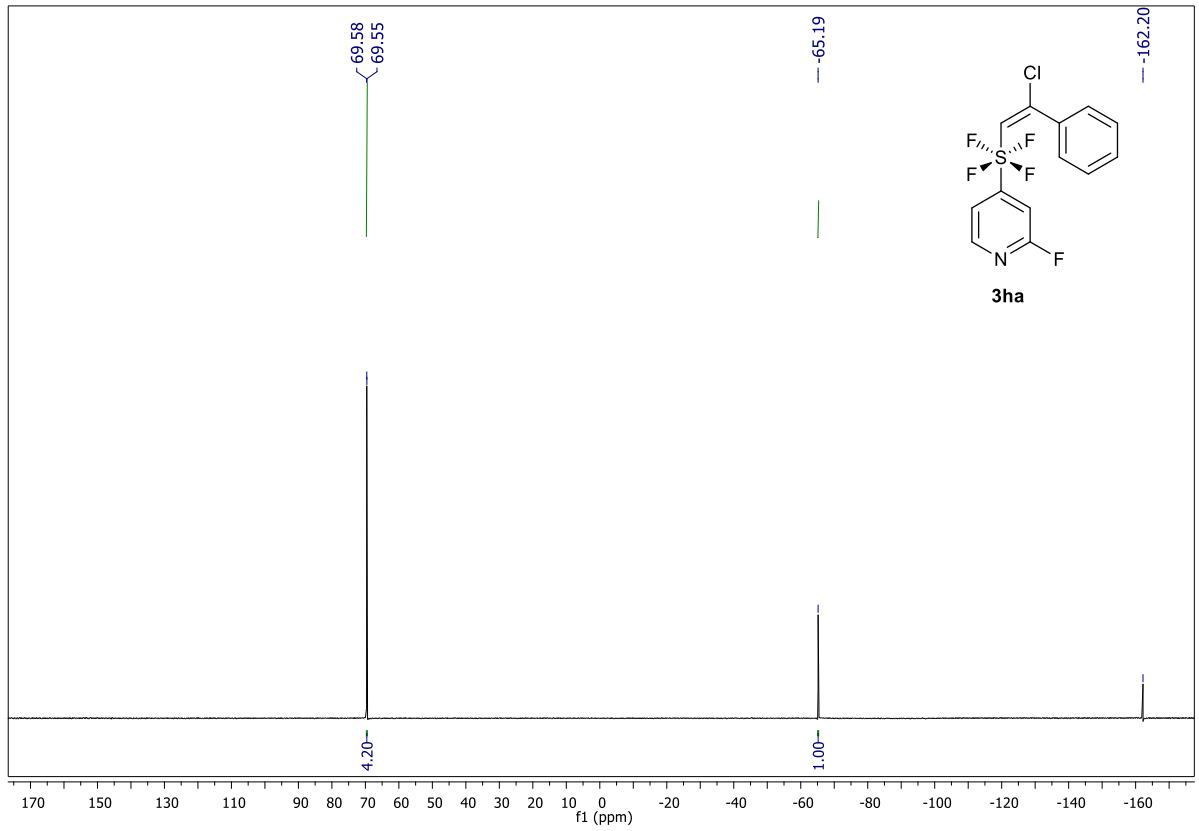
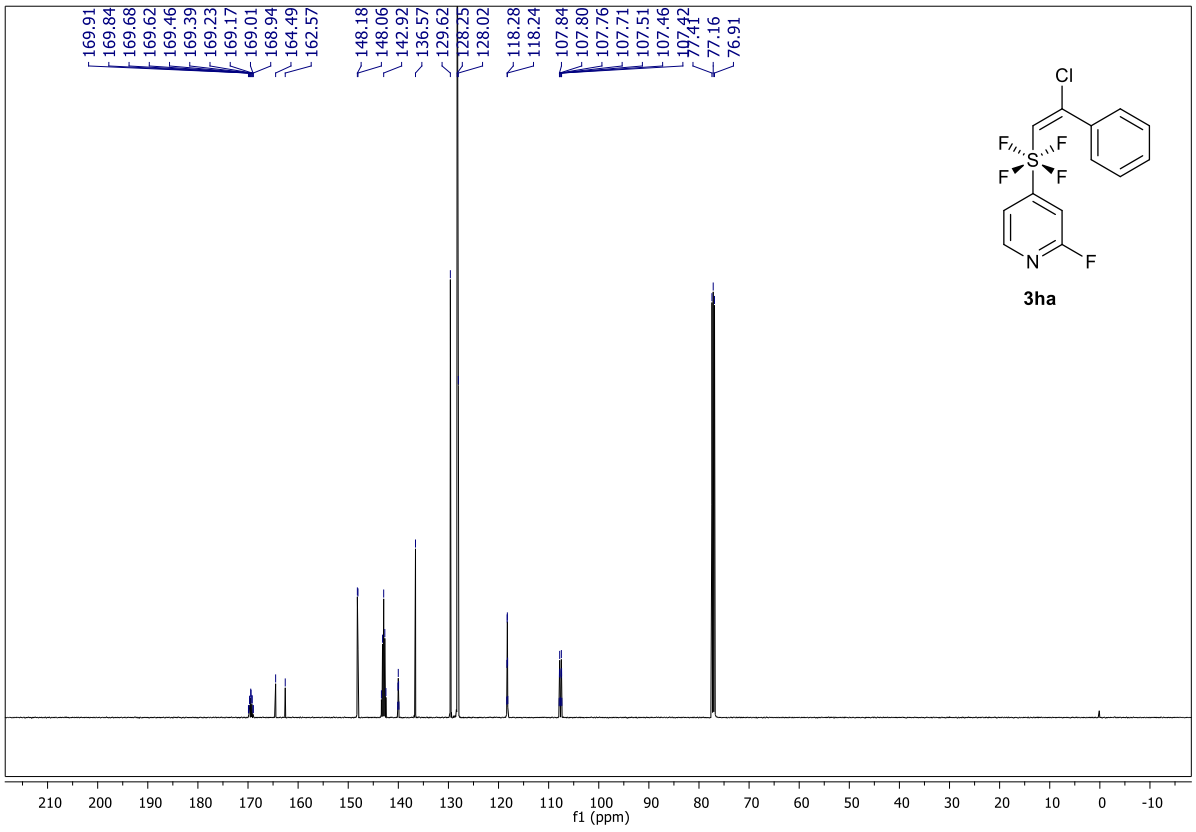
7.39
7.38
7.37
7.37
7.36
7.36
7.35
7.35
7.25
7.21
7.19
7.16
7.13
7.12
7.12
7.10
-0.00
Cl
F
F
S
F
F
N
F
3ha
1.00
6.25
2.11
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


69.58
69.55
-65.19
-162.20
Cl
F
F
S
F
F
N
F
3ha
4.20
1.00
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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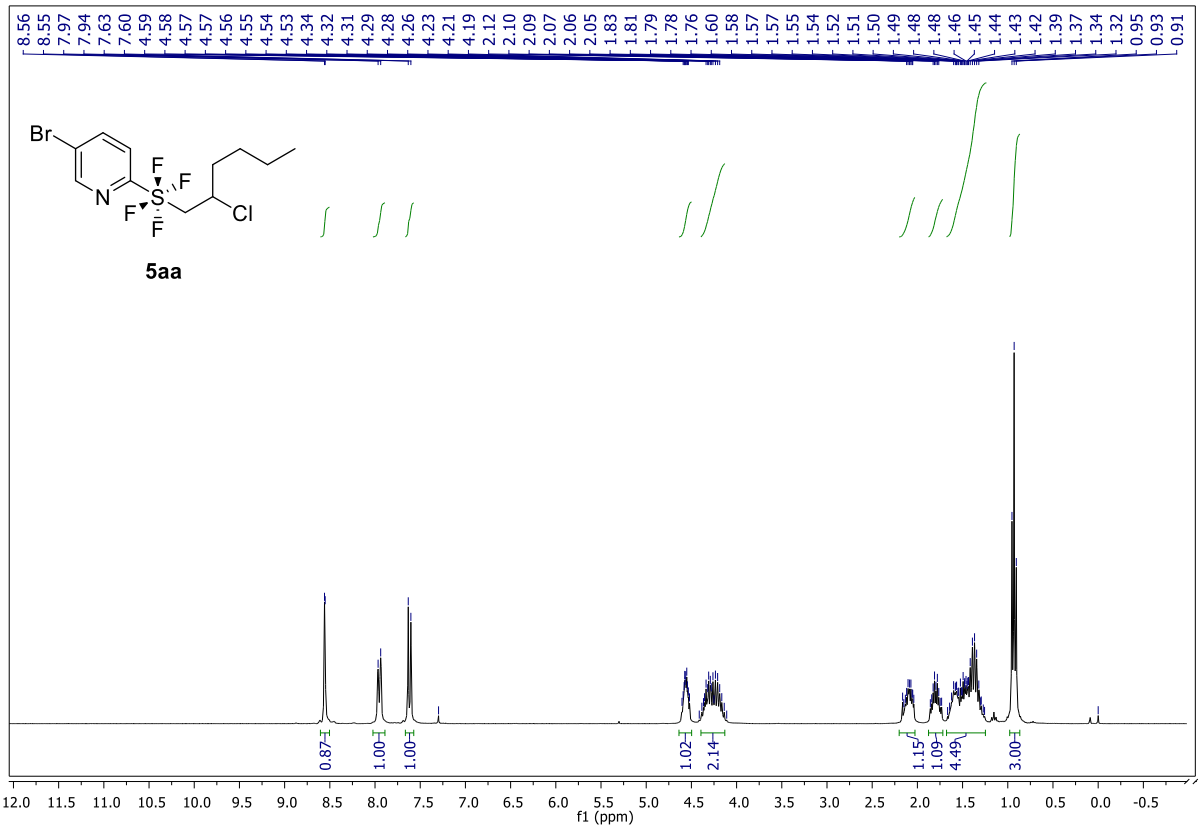
148.18
148.06
142.92
136.57
129.62
128.25
128.02
118.28
118.24
107.84
107.80
107.76
107.71
107.51
107.46
107.42
77.41
77.16
76.91
Cl
F
F
S
F
F
N
F
3ha
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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4.57
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4.56
4.55
4.54
4.53
4.34
4.32
4.31
4.29
4.28
4.26
4.23
4.21
4.19
2.12
2.10
2.09
2.07
2.06
2.05
1.83
1.81
1.79
1.78
1.76
1.60
1.58
1.57
1.57
1.55
1.54
1.52
1.51
1.50
1.49
1.48
1.48
1.46
1.45
1.44
1.43
1.42
1.39
1.37
1.34
1.32
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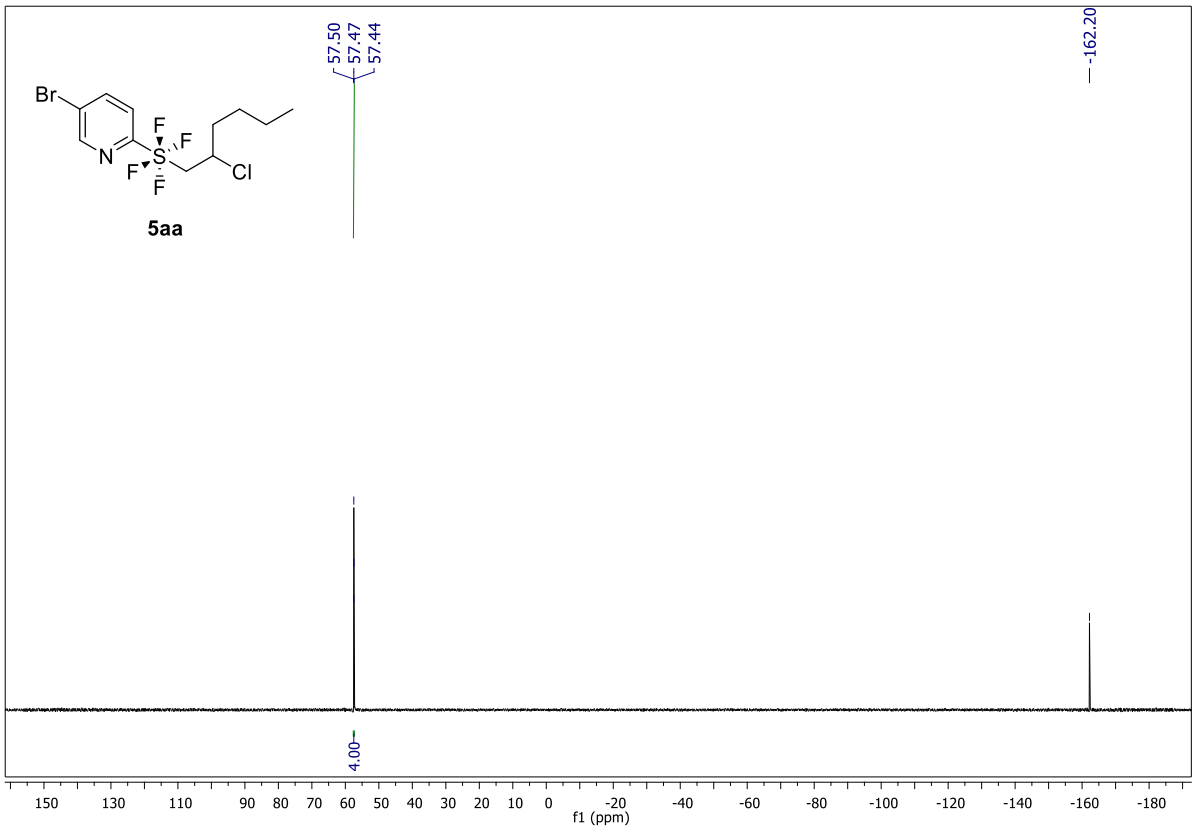
0.93
0.91
Br
N
F
F
S
F
F
Cl
5aa
0.87
1.00
1.00
1.02
2.14
1.15
1.09
4.49
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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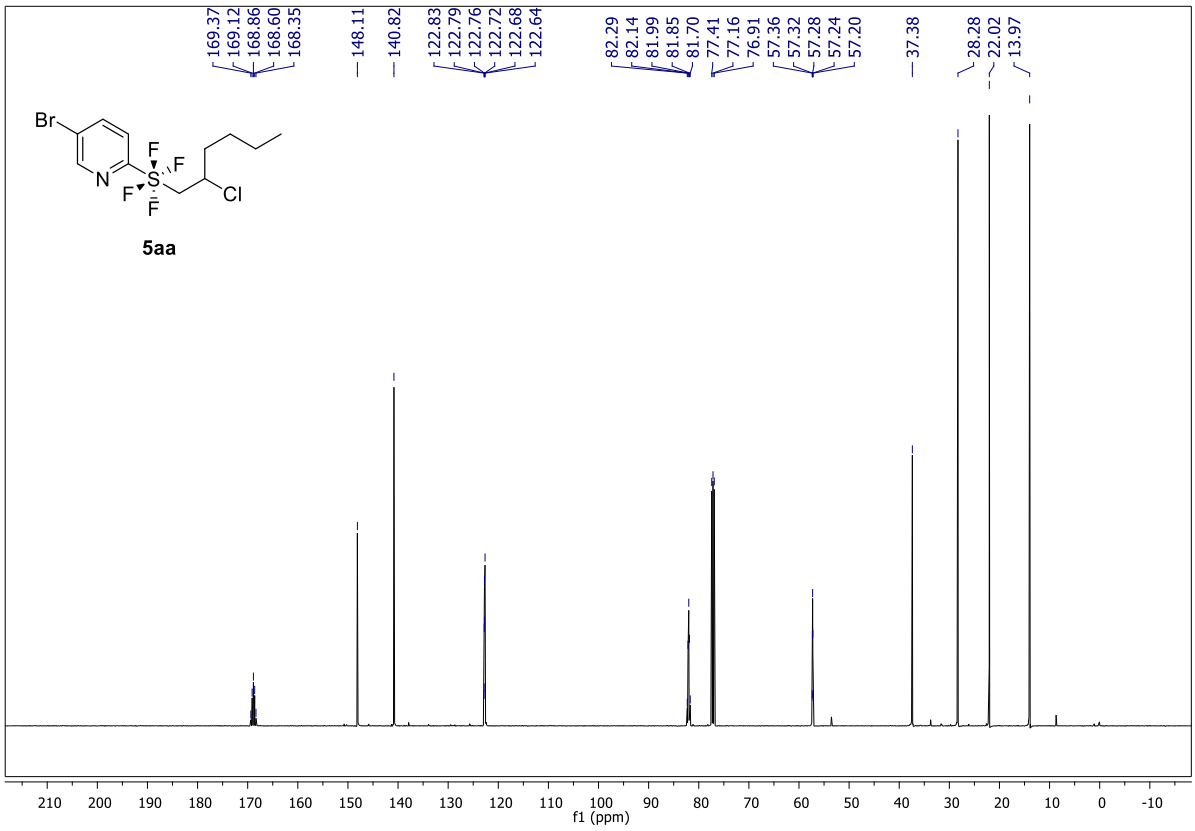
Br
F
F
F
F
S
N
Cl
5aa
4.00
150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180
f1 (ppm)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140.82
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122.76
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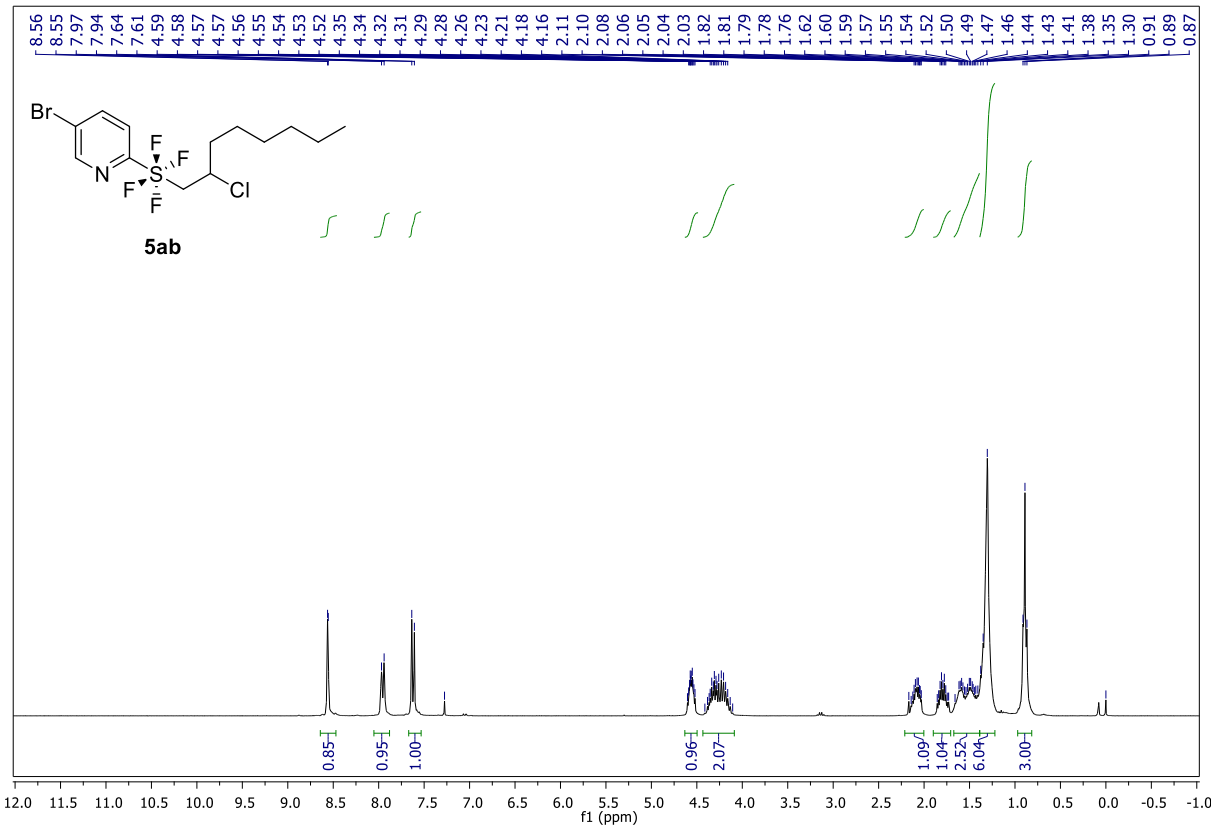
122.64
82.29
82.14
81.99
81.85
81.70
77.41
77.16
76.91
57.36
57.32
57.28
57.24
57.20
37.38
28.28
22.02
13.97
Br
F
F
F
F
S
N
Cl
5aa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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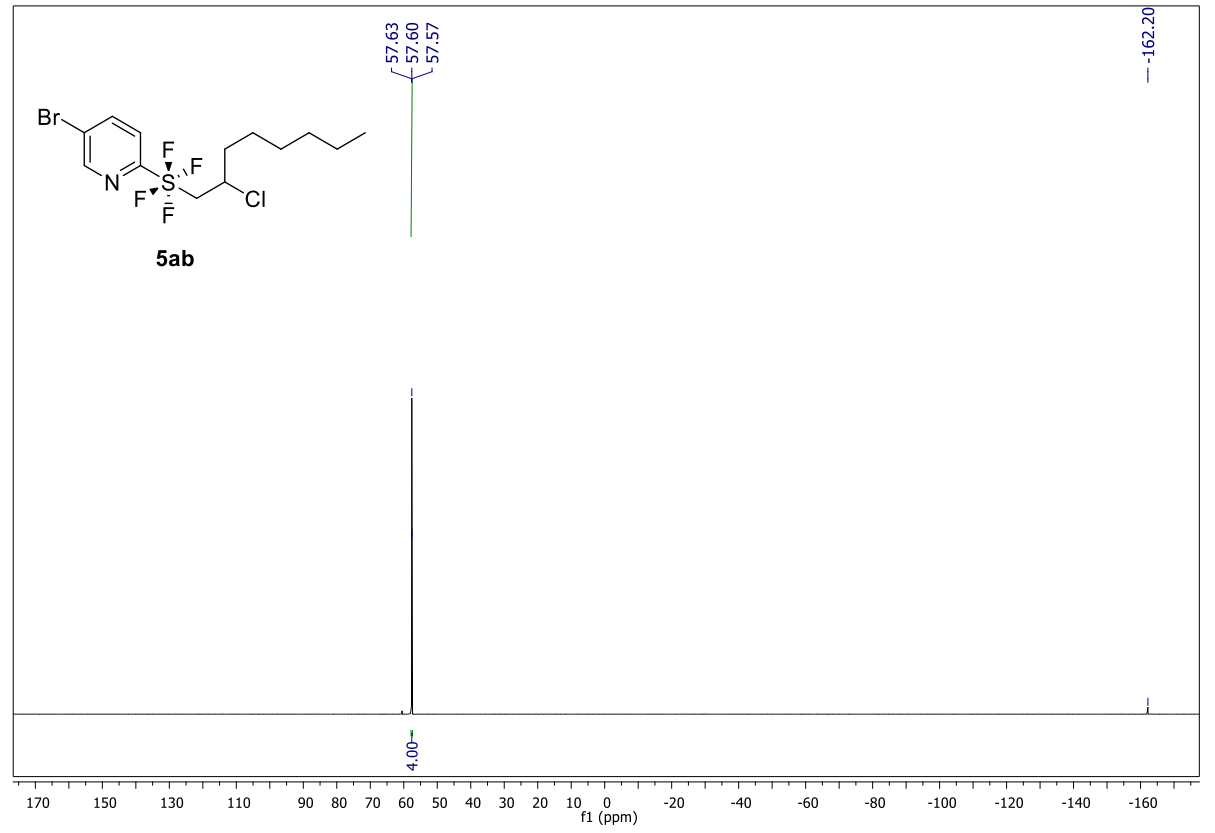
Br
N
S
F
F
F
F
Cl
5ab
0.85
0.95
1.00
0.96
2.07
1.09
1.04
2.52
6.04
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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57.57
-162.20
Br
N
S
F
F
F
F
Cl
5ab
4.00
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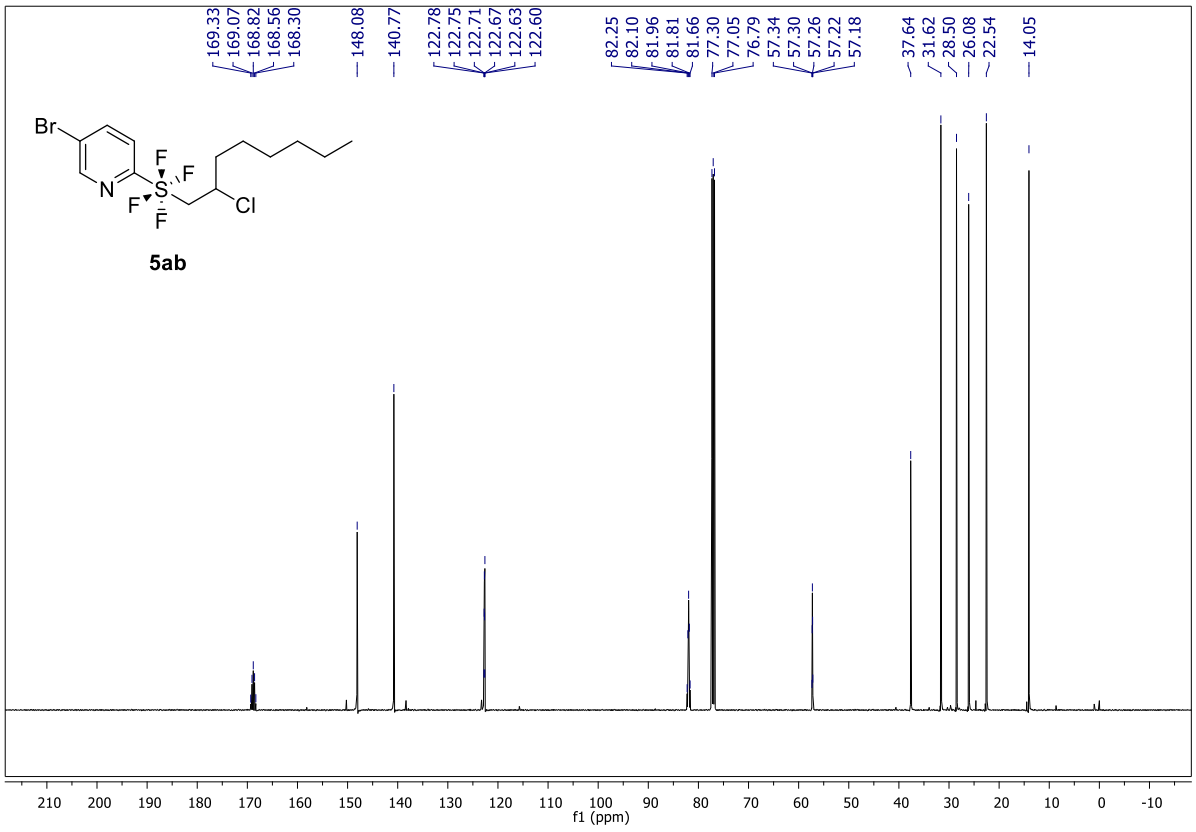
f1 (ppm)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168.30
148.08
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122.71
122.67
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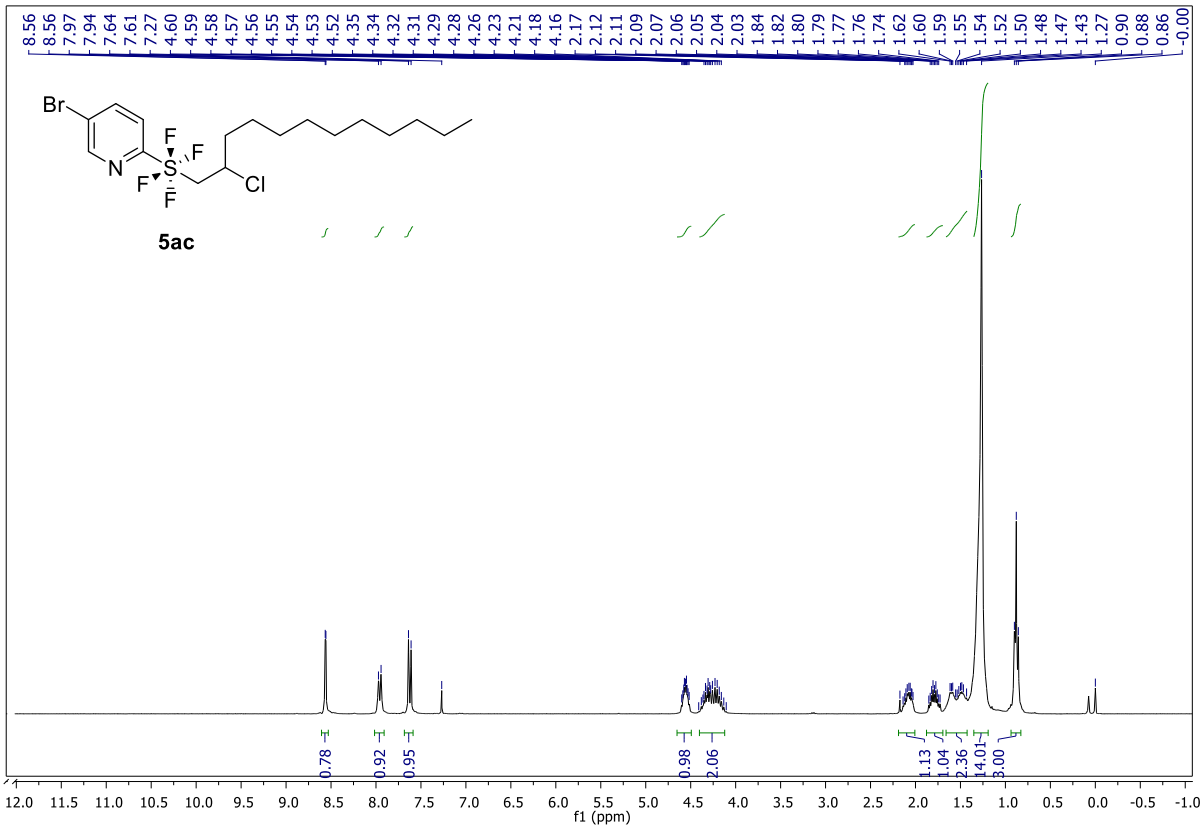
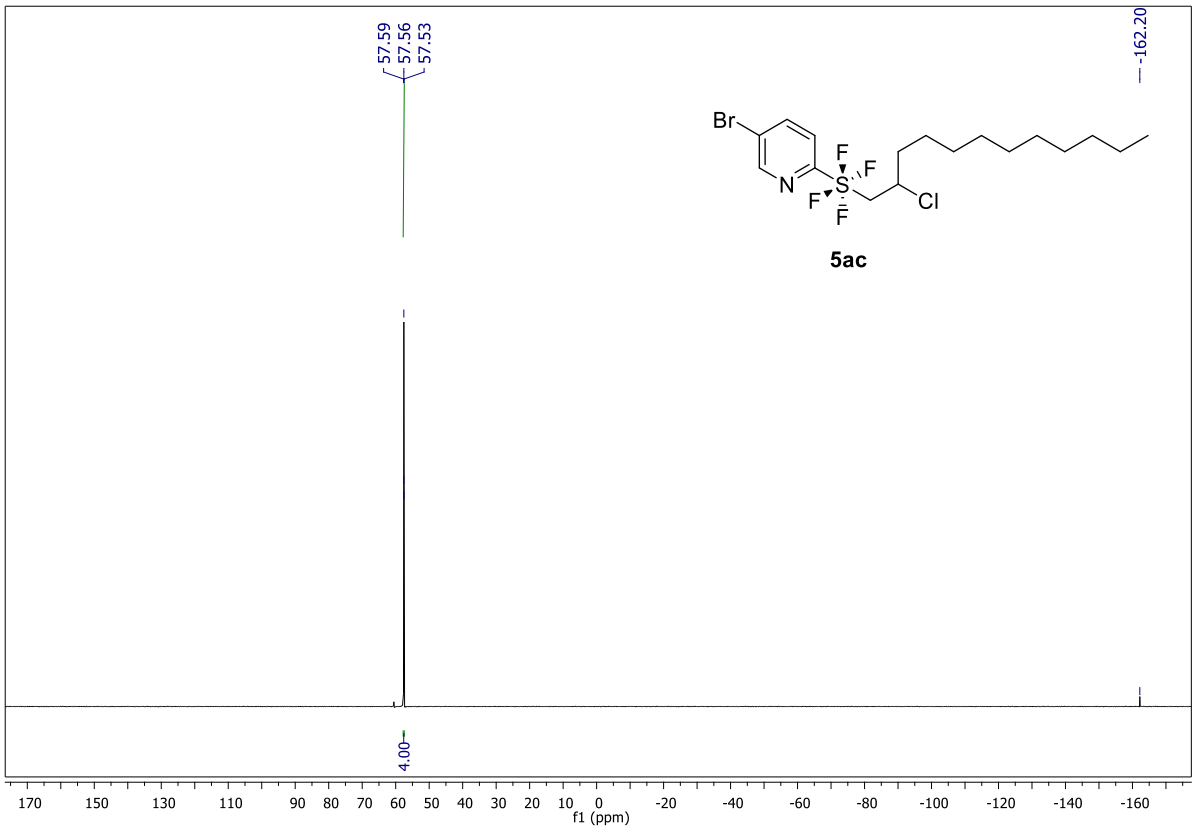
122.60
82.25
82.10
81.96
81.81
81.66
77.30
77.05
76.79
57.34
57.30
57.26
57.22
57.18
37.64
31.62
28.50
26.08
22.54
14.05
Br
N
S
F
F
F
F
Cl
5ab
f1 (ppm)


Br
N
S
F
F
F
F
Cl
5ac
0.78
0.92
0.95
0.98
2.06
1.13
1.04
2.36
14.01
3.00
f1 (ppm)


57.59
57.56
57.53
-162.20
Br
N
F
F
S
F
F
Cl
5ac
4.00
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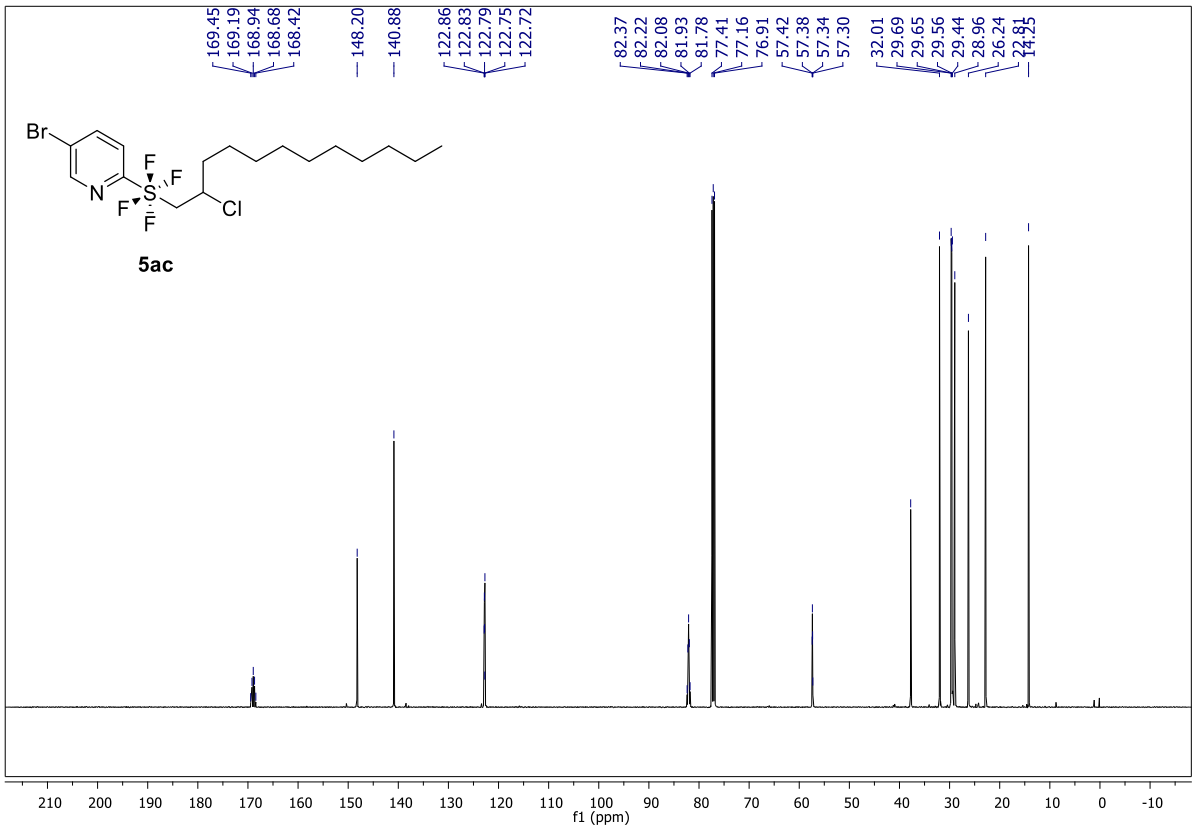
f1 (ppm)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122.79
122.75
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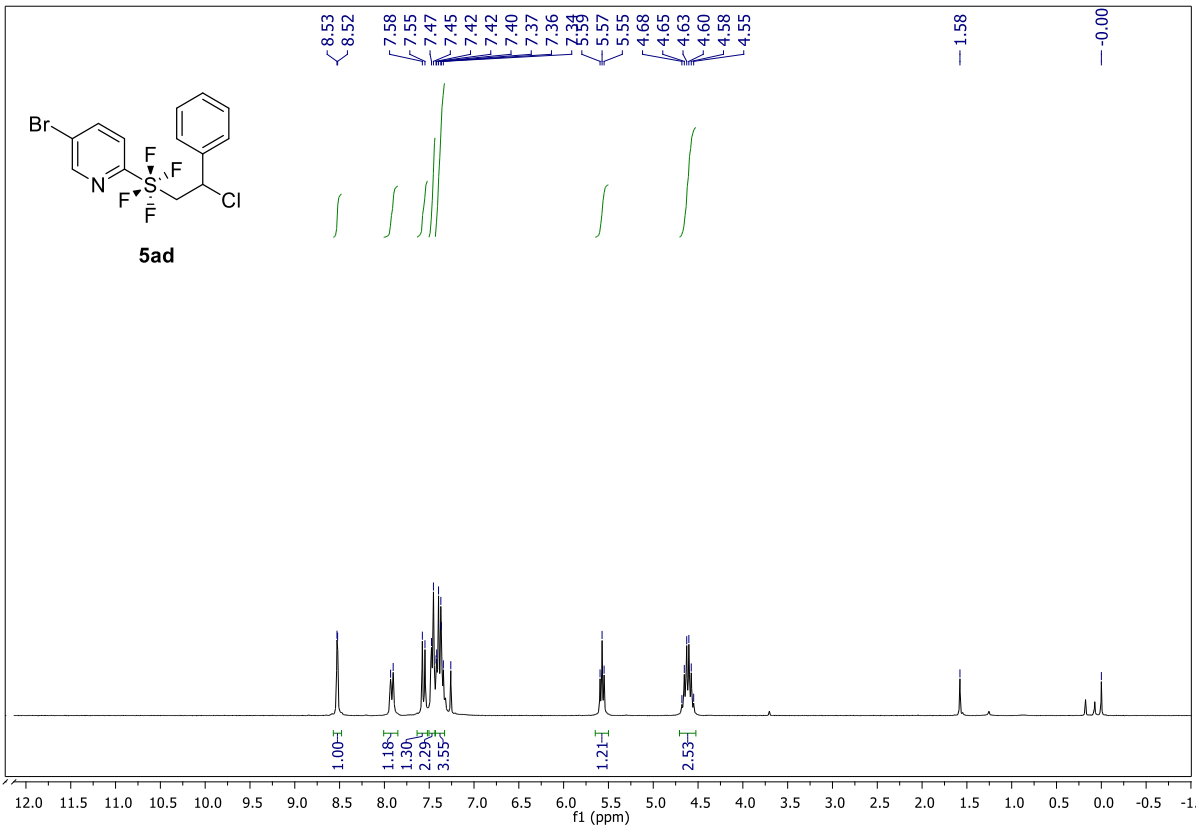
82.37
82.22
82.08
81.93
81.78
77.41
77.16
76.91
57.42
57.38
57.34
57.30
32.01
29.69
29.65
29.56
29.44
28.96
26.24
22.81
14.25
Br
N
F
F
S
F
F
Cl
5ac
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.53
8.52
7.58
7.55
7.47
7.45
7.42
7.42
7.40
7.37
7.36
7.34
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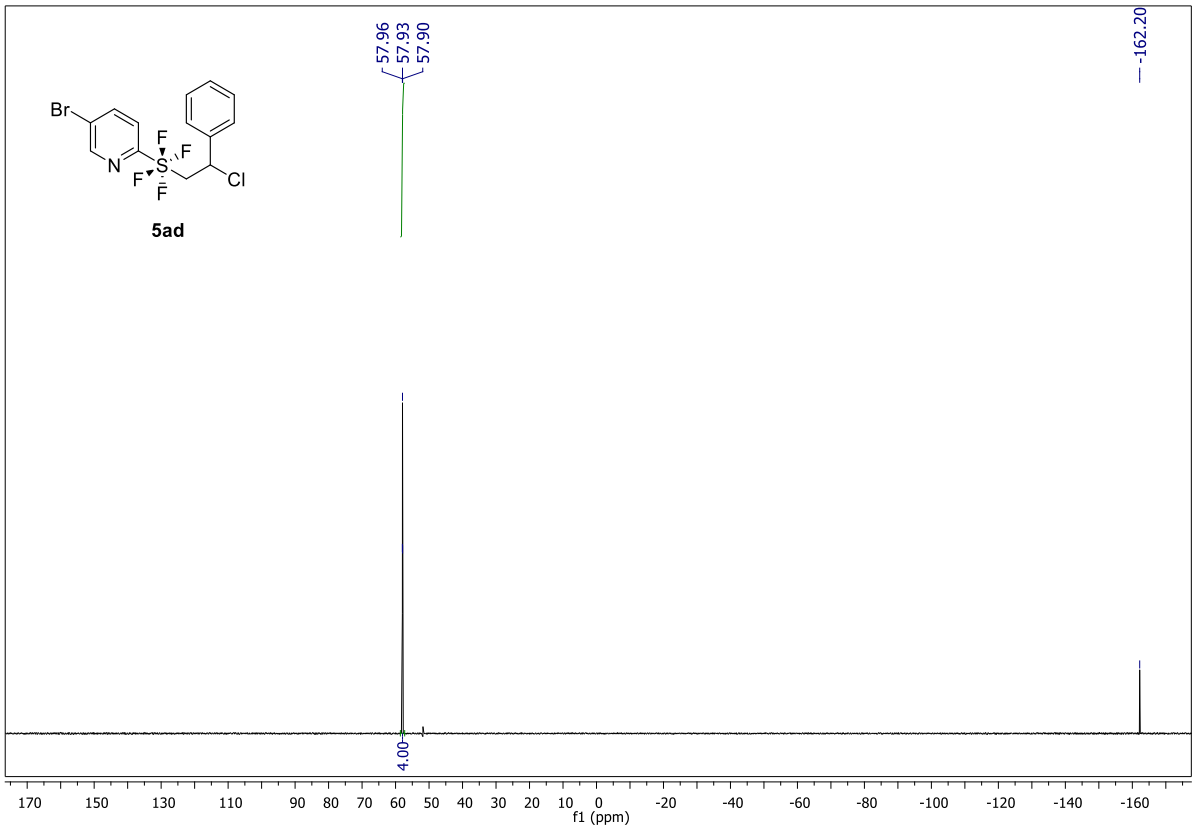
5.57
5.55
4.68
4.65
4.63
4.60
4.58
4.55
1.58
-0.00
Br
N
F
F
S
F
F
Cl
5ad
1.00
1.18
1.30
2.29
3.55
1.21
2.53
f1 (ppm)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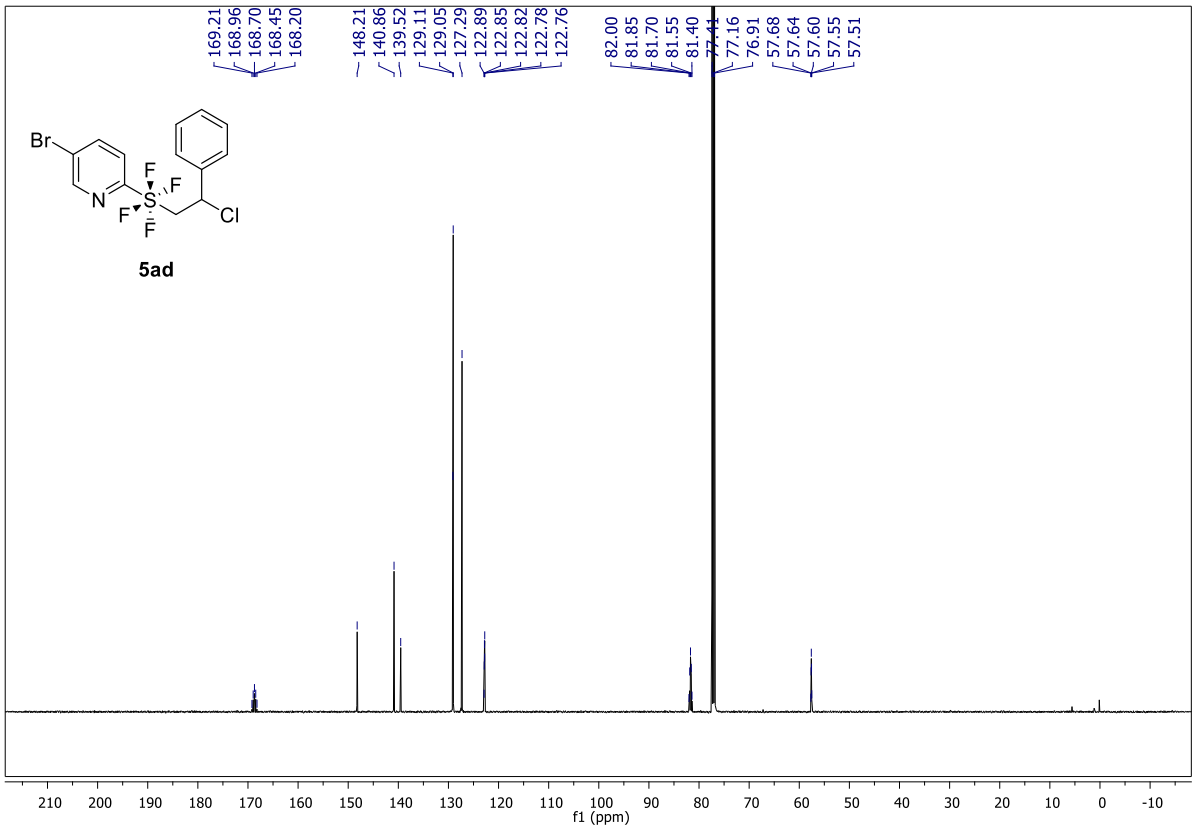
57.93
57.90
-162.20
Br
N
F
F
S
F
F
Cl
5ad
4.00
f1 (ppm)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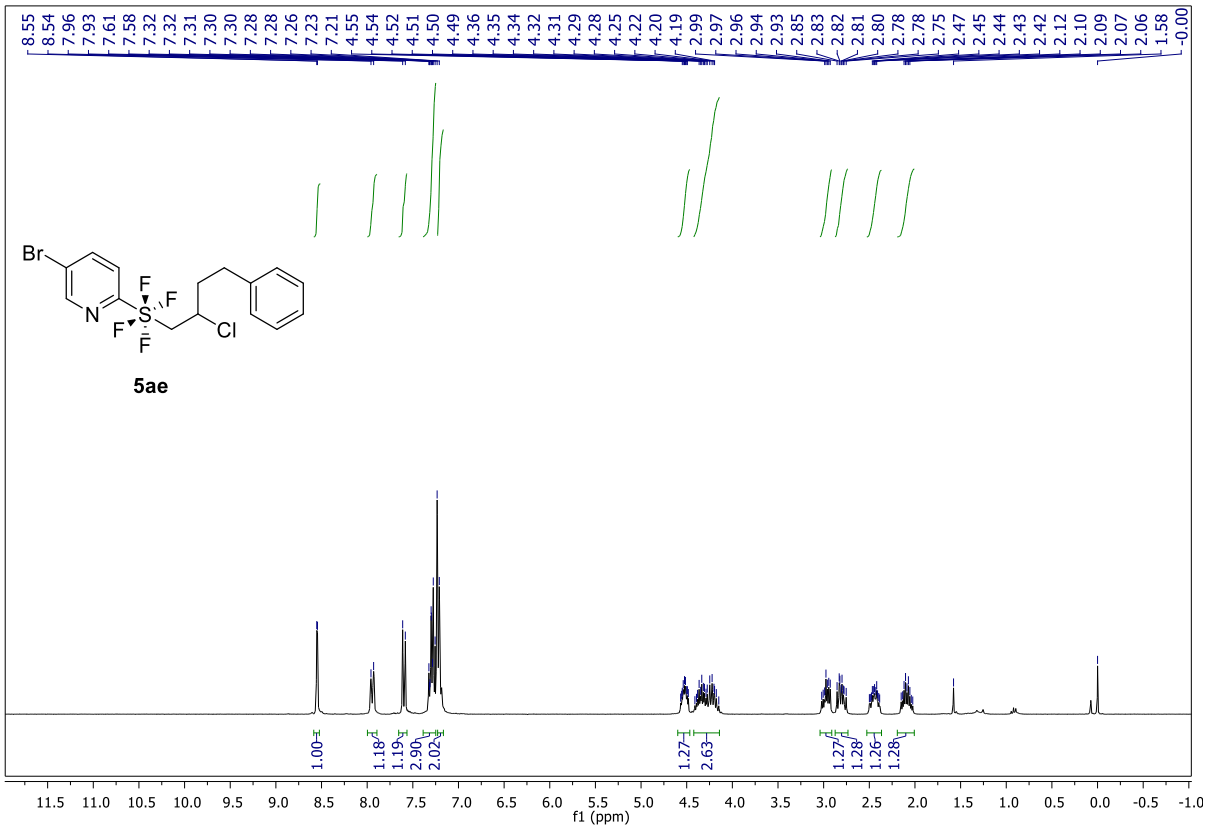
168.70
168.45
168.20
148.21
140.86
139.52
129.11
129.05
127.29
122.89
122.85
122.82
122.78
122.76
82.00
81.85
81.70
81.55
81.40
77.41
77.16
76.91
57.68
57.64
57.60
57.55
57.51
Br
F
F
F
F
S
N
Cl
5ad
f1 (ppm)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8.54
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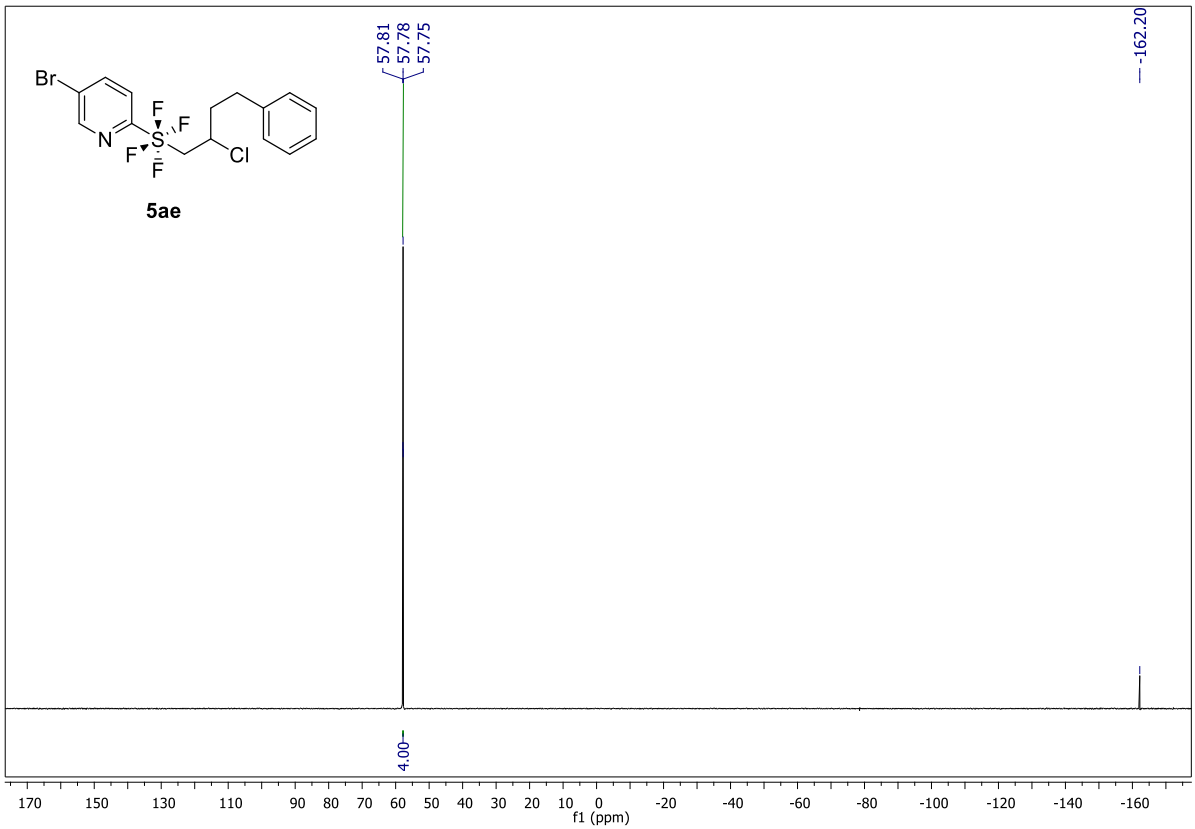
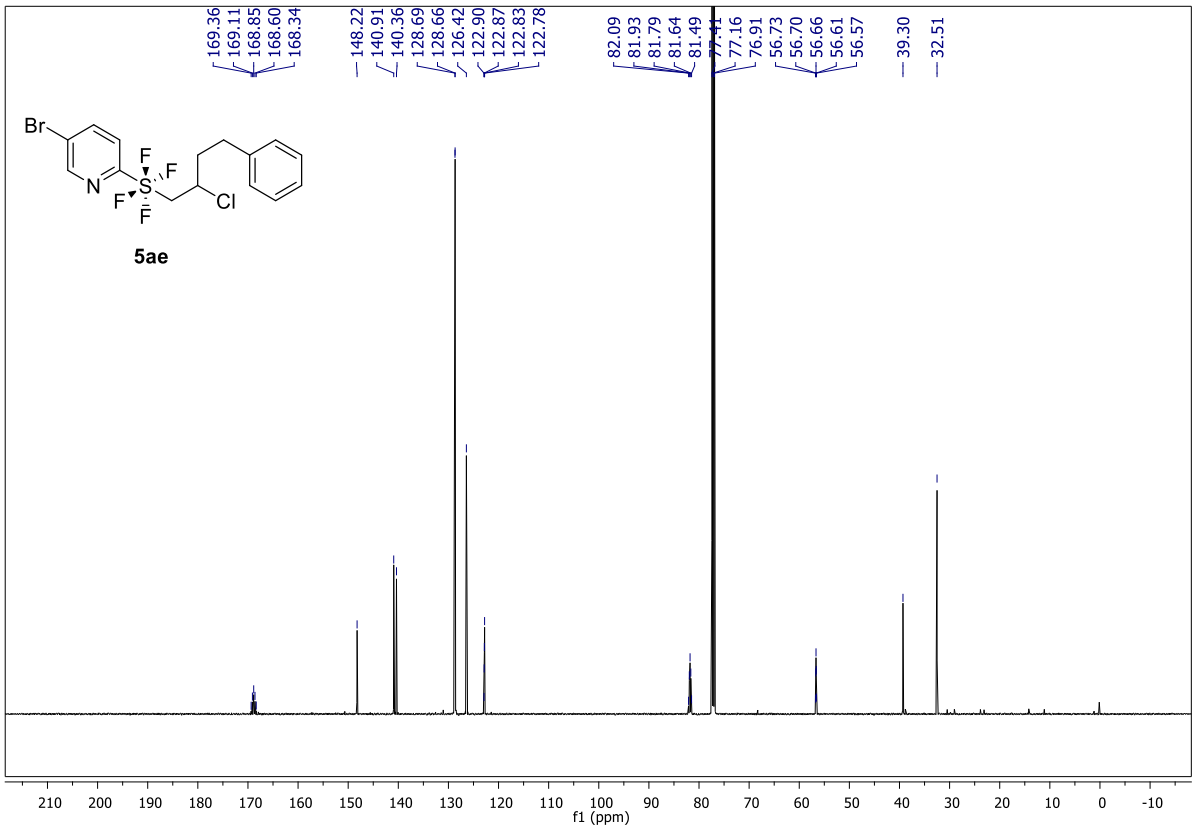
7.93
7.61
7.58
7.32
7.32
7.31
7.30
7.30
7.28
7.28
7.26
7.23
7.21
4.55
4.54
4.52
4.51
4.50
4.49
4.36
4.35
4.34
4.32
4.31
4.29
4.28
4.25
4.22
4.20
4.19
2.99
2.97
2.96
2.94
2.93
2.85
2.83
2.82
2.81
2.80
2.78
2.78
2.75
2.47
2.45
2.44
2.43
2.42
2.12
2.10
2.09
2.07
2.06
1.58
-0.00
Br
F
F
F
F
S
N
Cl
5ae
1.00
1.18
1.19
2.90
2.02
1.27
2.63
1.27
1.28
1.26
1.28
f1 (ppm)


Br
F
F
F
F
S
N
Cl
5ae
57.81
57.78
57.75
-162.20
4.00
f1 (ppm)


169.36
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168.85
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148.22
140.91
140.36
128.69
128.66
126.42
122.90
122.87
122.83
122.78
82.09
81.93
81.79
81.64
81.49
77.41
77.16
76.91
56.73
56.70
56.66
56.61
56.57
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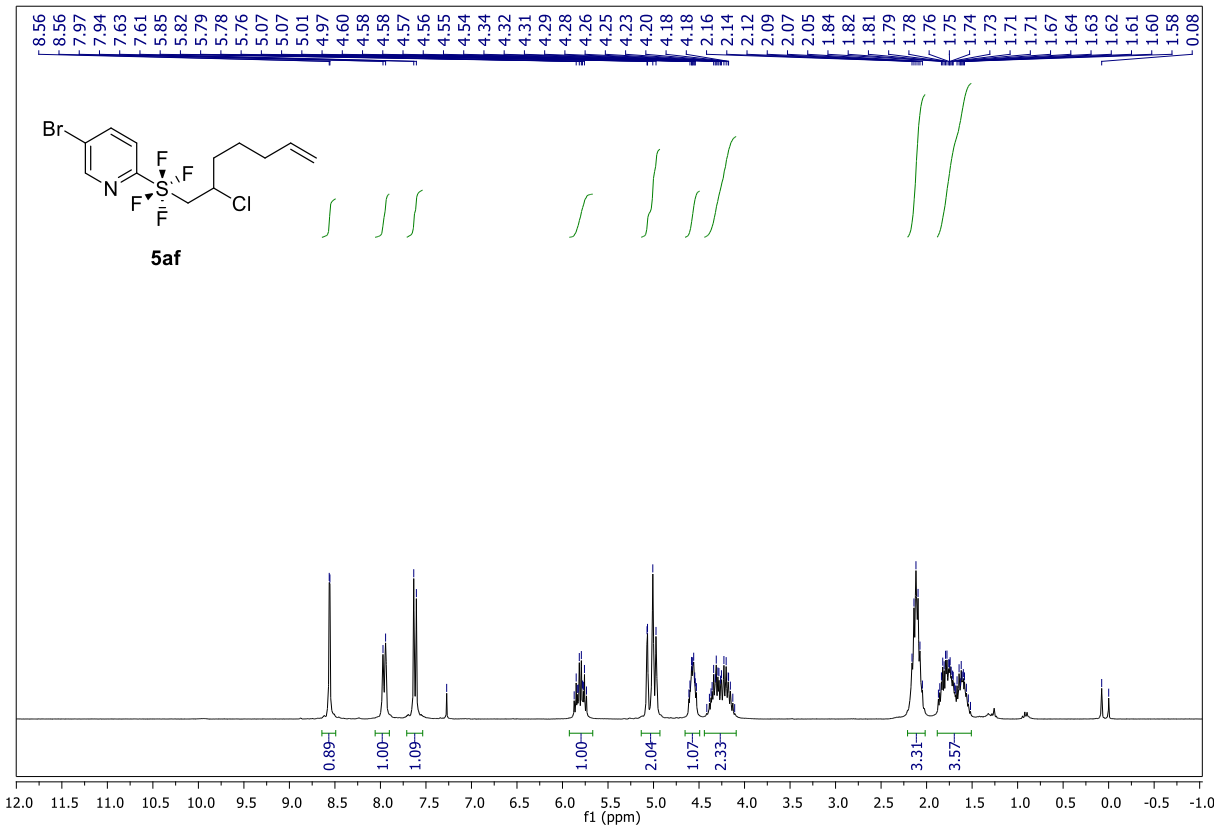
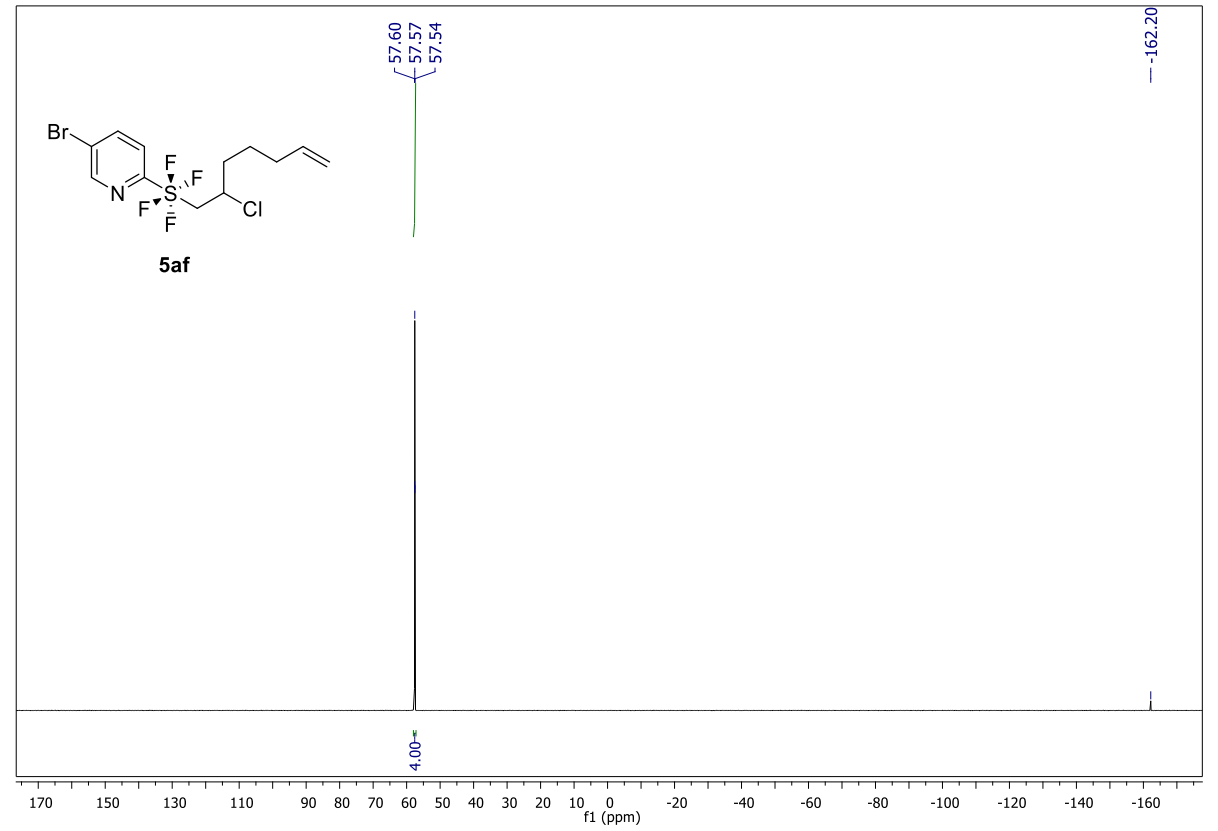
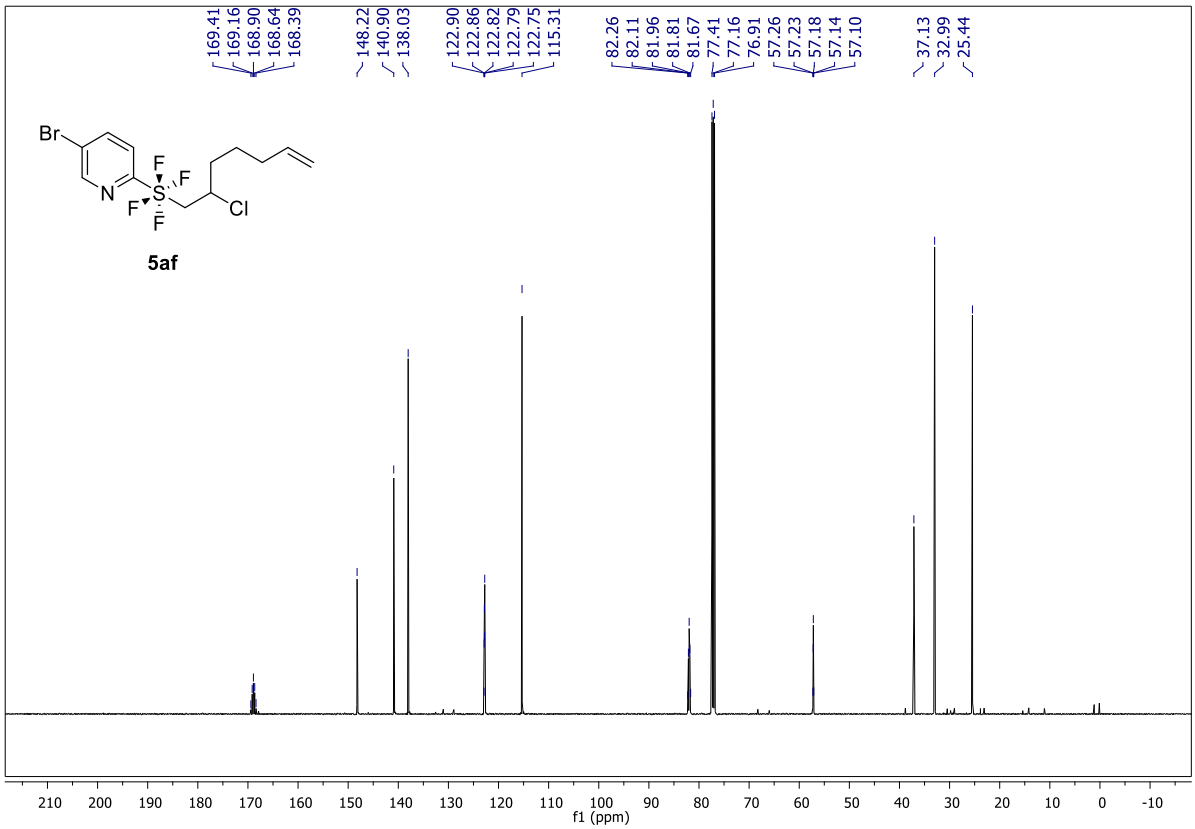
F
F
F
S
N
Cl
5ae
f1 (ppm)


8.56 8.56 7.97 7.94 7.63 7.61 5.85 5.82 5.79 5.78 5.76 5.07 5.07 5.01 4.97 4.60 4.58 4.58 4.57 4.56 4.55 4.54 4.34 4.32 4.31 4.29 4.28 4.26 4.25 4.23 4.20 4.18 4.18 2.16 2.14 2.12 2.09 2.07 2.05 1.84 1.82 1.81 1.79 1.78 1.76 1.75 1.74 1.73 1.71 1.71 1.67 1.64 1.63 1.62 1.61 1.60 1.58 0.08
Br
N
F
S
F
F
F
Cl
5af
0.89 1.00 1.09 1.00 2.04 1.07 2.33 3.31 3.57
12.0 11.5 11.0 10.5 10.0 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 -1.0
f1 (ppm)


57.60
57.57
57.54
-162.20
Br
N
F
S
F
F
F
Cl
5af
4.00
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)


169.41
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168.90
168.64
168.39
148.22
140.90
138.03
122.90
122.86
122.82
122.79
122.75
115.31
82.26
82.11
81.96
81.81
81.67
77.41
77.16
76.91
57.26
57.23
57.18
57.14
57.10
37.13
32.99
25.44
Br
N
F
F
S
F
F
Cl
5af
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)