Electronic Supporting Information

SF_5-pyridylaryl-λ^3-iodonium salts and their utility as electrophilic reagents to access SF_5-pyridine derivatives in the late-stage of synthesis

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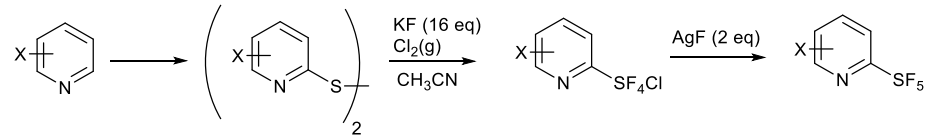
Contents

General information

All reactions were performed in oven-dried glassware 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 and $KMnO_4$ in water/heat. Products were purified by preparative thin-layer plates (PLC) carried out on 2.0 mm Merck silica gel (60-F254) or Column chromatography. Column chromatography was carried out on columns packed with silica gel (60N spherical neutral size 63-210 µm). The ^1H 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 ^1H 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 Waters Synapt G2 HDMS (ESI-MS). Infrared spectra were recorded on a JASCO FT/IR-4100 spectrometer. Melting point 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.

Scheme S1: Synthesis of the SF_5-pyridines from commercial reagents:



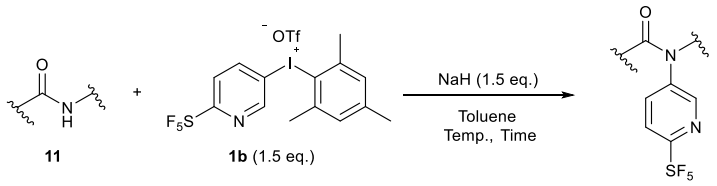
a) X = 2,6-Br
b) X = 5-Br, 2-OH
c) X = 3-Br, 2-Cl
d) X = 2-Br, 4-F

a) **i**: X = 6-Br
b) **ii**: X = 5-Br
c) **iii**:X = 3-Br
d) **iv**: X = 4-F

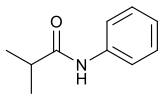
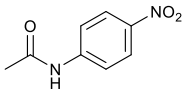
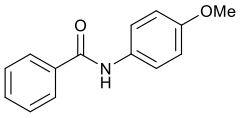
a) **8a'**: X = 6-Br
b) **8b'**: X = 5-Br
c) **8c'**: X = 3-Br
d) **8d'**: X = 4-F

a) **8a**: X = 6-Br
b) **8b**: X = 5-Br
c) **8c**: X = 3-Br
d) **8d**: X = 4-F

Table S1: Optimization of Temperature for Reagent **1b** with amides **11**[a]



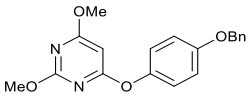
11 **1b** (1.5 eq.)

Entry	Substrate **11**	Temp. (°C)	Time (h)	Yield (%)[b]
1		rt	24	60
2		65	5	68
3		rt	24	7
4		55	5	50
6		rt	19	25
7		55	5	30

[a]Reaction conditions: **11** (0.10 mmol), reagent **1b** (0.15 mmol), NaH (0.15 mmol), Toluene, Temperature, Time. [b]Isolated yield

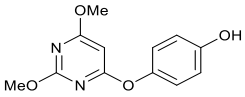
Synthesis of starting material for 6al:

4-(4-(benzyloxy)phenoxy)-2,6-dimethoxypyrimidine (13l'):



It was prepared following a literature condition.[1] In a flame dried round bottomed flask, Cs_2CO_3 (652mg, 2 mmol) was added to 4-chloro-2,6-dimethoxypyrimidine (350 mg, 2mmol) in DMF (15 mL) and the mixture was stirred at rt for 10 minutes. 4-(benzyloxy)phenol (400 mg, 2mmol) was added to the reaction mixture and the reaction vessel was transferred to a preheated oil bath at 85 °C and stirred at that temperature for 4 hours. The reaction was quenched with water and extracted with ethyl acetate 3 times. The combined organic phase was washed with brine and then dried over Na_2SO_4. The solvent was evaporated under reduced pressure to give the crude product which was purified under column chromatography on silica gel (n-hexane/EtOAc, 4/1) to give the desired product **13l'** as a white solid (576.7 mg) in 85% yield.
m.p.: (110.8 °C); HRMS (ESI) calcd. for $C_{19}H_{18}N_2O_4Na$ [(M+Na)$^+$]: 361.1164 found 361.1165; ^{1}H NMR ($CDCl_3$, 300 MHz): δ =7.45-7.34 (m, 5H), 7.05 (d, *J* = 9 Hz, 2H), 6.98 (d, *J* = 9 Hz, 2H) 5.63 (s, 1H), 5.06 (s, 2H), 3.92 (s, 3H), 3.93 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz): δ = 54.36, 55.01, 70.59, 83.98, 115.88, 122.57, 127.65, 128.23, 128.78, 136.88, 146.43, 156.54, 165.35, 173.12, 173.56. ATR-FTIR (KBr): *v* = 3656, 3017, 2947, 2553, 2001, 1815, 1540, 1296, 1118, 933 cm^{-1}.

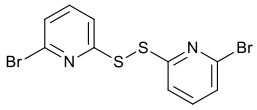
4-((2,6-dimethoxypyrimidin-4-yl)oxy)phenol (13l):



It was prepared from modified procedure from the literature.[2] In a dry round bottomed flask $NiCl_2$·6H2O (535 mg, 2.25 mmol) was added to solution of **13l'** (507 mg, 1.5 mmol) in methanol/ethyl acetate (1:1, 5 mL) and it was stirred at rt till a homogenous solution was formed. The reaction mixture was cooled to 0 °C and $NaBH_4$ (170 mg, 4.5 mmol) was added in portions. The reaction was stirred at 0 °C for 30 minutes and then warmed to rt. It was then transferred to a preheated oil bath at 65 °C and allowed to stir at that temperature for 5 days. The reaction mixture was filtered through a pad of celite and washed with ethyl acetate. The organic phase was washed with water and then dried over Na_2SO_4. The solvent was evaporated under reduced pressure to give the crude product which was purified under column chromatography on silica gel (n-hexane/EtOAc, 7/3) to give the desired product **13l** as a white solid (153 mg) in 41% yield.
m.p.: (120.5 °C); HRMS (ESI) calcd. for $C_{12}H_{12}N_2O_4Na$ [(M+Na)$^+$]: 270.0695 found 271.0701; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 6.98 (d, *J* = 9 Hz, 2H), 6.83 (d, *J* = 9 Hz, 2H), 5.65 (s, 1H), 5.40 (s, 1H), 3.93 (s, 3H), 3.94 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz): δ = 54.40, 55.04, 84.00, 116.46, 122.66, 146.15, 153.56, 165.33, 173.17, 173.56. ATR-FTIR (KBr): *v* = 3676, 3112, 2950, 2898, 2679, 2572, 1870, 1592, 1114, 806 cm^{-1}.

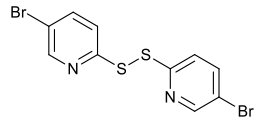
Synthesis of disulfide:

1,2-bis(6-bromopyridin-2-yl)disulfane (i):



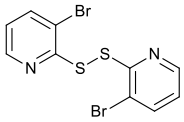
Prepared according to literature procedure.[3] In a 500 ml round bottom flask, under Ar atmosphere, a mixture of 2,6-dibromopyridine (18.95 g, 80.0 mmol) and THF (114 ml) at 0 °C was stirred for 30 min. At 0 °C, isopropylmagnesium chloride lithium chloride (^{i}PrMgCl.LiCl) complex solution (70.2 mL, 80.0 mmol) was added slowly to the reaction mixture and was stirred at room temperature for 2 h.[4] After cooling to -78 °C, a solution of sulfur (2.57 g, 80.0 mmol) in toluene (258 ml) was added to the mixture and was stirred at room temperature for 1 h. The reaction mixture was then transferred to another round bottom flask containing a mixture of aqueous solution of NaOH (3.84 g in 155 mL of H_2O) and $K_3[Fe(CN)_6]$ (31.6 g in 20 mL of H_2O) and was stirred at room temperature for 12 h. The reaction mixture was extracted by CH_2Cl_2, and the combined organic phase was washed with aq. NH_4Cl (200 ml X 2) and brine and then dried over $MgSO_4$. The solvent was removed *in vacuo* to give a crude product which was purified by column chromatography on silica gel (n-hexane/EtOAc, 4/1) to give the target product as a yellow solid (17 mg) in 56% yield.
m.p.: (96.8 °C); HRMS (ESI) calcd. for $C_{10}H_6N_2NaS_2Br_2$ [(M+Na)$^+$]: 398.8237 found 398.8237; ^{1}H NMR ($CDCl_3$l, 300 MHz): δ = 7.3 (d, *J* = 7.1 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 1H), 7.59 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR ($CDCl_3$l, 126 MHz): δ = 118.47, 125.59, 139.54, 141.58, 159.79. ATR-FTIR (KBr): *v* = 3102, 3030, 2924, 1543, 1409, 1143, 1131, 1106, 784, 760 cm^{-1}.

1,2-bis(5-bromopyridin-2-yl)disulfane (ii):



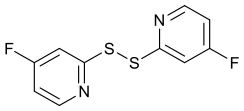
A dry 500 mL flask was charged with 2-hydroxy-5-bromopyridine (5.0 g; 28.7 mmol), Lawesson's reagent (10.9 g; 27 mmol) and toluene (250 mL). The reaction mixture was stirred at reflux for 24 h. After cooling it was transferred into the separatory funnel which contained a solution of NaOH (25 g) in water (250 mL). After shaking, the aqueous layer was separated and washed with Et_2O (100 mL). The organic phases were discarded, and the aqueous phase was acidified with AcOH (200 mL) and extracted with CH_2Cl_2 (3×100 mL). The combined CH_2Cl_2 extracts were washed with brine (100 mL) and dried with $MgSO_4$. The crude residue that was obtained after filtration and CH_2Cl_2 evaporation was further coevaporated *in vacuo* with toluene (2×100 mL) to remove residual AcOH and to give pure 5-bromopyridine-2-thiol as a yellow solid (4.95 g; 88%). In a 250 mL flask containing the obtained 5-bromopyridine-2-thiol (4.9 g; 39 mmol) was added a solution of NaOH (1.8 g; 45 mmol) in water (75 mL), and the mixture was stirred for 30 minutes and then a solution of $K_3[Fe(CN)_6]$ (14.82 g; 45 mmol) in water (100 mL) was added to it. The resulting reaction mixture was stirred for 14 h, and the formed precipitate was filtered, thoroughly washed with water and dried, first in air then *in vacuo* to give 4.02 g (83%) of pure 1,2-bis(5-bromopyridin-2-yl)disulfane as a beige solid. The ^{1}H NMR spectrum matched the one reported by Dolbier *et al*.[5]

1,2-bis(3-bromopyridin-2-yl)disulfane (iii):



A dry 250 mL flask was charged with 2-chloro-3-bromopyridine (5.00 g; 38 mmol), thiourea (2.9 g; 38 mmol) and anhydrous ethanol (50 mL). The reaction mixture was then stirred at reflux for 48 h. After cooling, the solvent was evaporated *in vacuo*. To the obtained residue, a solution of NaOH (3.6 g; 90 mmol) in water (75 mL) was added, and the mixture was stirred at reflux for 2 h. After cooling, it was extracted with CH_2Cl_2 (2×50 mL), and the organic extracts were discarded. The aqueous phase was transferred into 250 mL flask, and a solution of $K_3[Fe(CN)_6]$ (14.8 g; 45 mmol) in water (75 mL) was added to it. The resulting reaction mixture was stirred for 14 h, and the formed precipitate was filtered, thoroughly washed with water and dried, first in air then *in vacuo* to give 1.34 g (18%) of pure 1,2-bis(3-bromopyridin-2-yl)disulfane as a brown solid. The ^{1}H NMR spectrum matched the one reported by Dolbier *et al*.[5]

1,2-bis(4-fluoropyridin-2-yl)disulfane (iv):



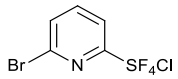
Prepared according to literature procedure.[3] In a 500 ml round bottom flask, under Ar atmosphere, a mixture of 2-bromo-4-fluoropyridine (4 g, 22.7 mmol) and THF (58 ml) at 0 °C was stirred for 30 min. At 0 °C, isopropylmagnesium chloride lithium chloride (^{i}PrMgCl.LiCl) complex solution (23.1 mL, 25.0 mmol) was added slowly to the reaction mixture and was stirred at room temperature for 2 h.[3] After cooling to -78 °C, a solution of sulfur (802 mg, 25.0 mmol) in toluene (81 ml) was added to the mixture and was stirred at room temperature for 1 h. The reaction mixture was then transferred to another round bottom flask containing a mixture of aqueous solution of KOH (2.55 g) and $K_3[Fe(CN)_6]$ (11.19 g) in 220 mL of H_2O and was stirred at room temperature for 12 h. The reaction mixture was extracted by CH_2Cl_2, and the combined organic phase was washed with aq. NH_4Cl (50 ml X 2) and brine and then dried over $MgSO_4$. The solvent was removed *in vacuo* to give a crude product which was purified by column chromatography on silica gel (n-hexane/EtOAc, 9/1) to give the target product as a yellow solid (1.68 g) in 58% yield.
m.p.: 57.4 °C; HRMS (ESI) calcd. for $C_{10}H_7N_2F_2S_2$ [$(M+H)^+$]:257.0019 found 257.0023; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 6.87–6.93 (m, 1H), 7.38 (dd, *J* = 3 Hz, 6 Hz, 1H), 8.44–8.49 (m, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz): δ = 100.38 (q, *J* = 9 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz): δ = 107.43 (d, *J* = 21.25 Hz), 109.89 (d, *J* = 17.5 Hz), 152.13 (d, *J* = 6.25 Hz), 161.63 (d, *J* = 6.25 Hz), 168.59, 170.71. ATR-FTIR (KBr): *v* = 3090, 3057, 1283, 1068, 1611, 1556, 1100, 835, 826, 715, 595 cm^{-1}.

Synthesis of 2-pyridylsulfur chlorotetrafluoride 8':

The 2-pyridylsulfur chlorotetrafluorides were prepared by modified procedure as given in the literature.[5] An oven-dried 60 mL narrow mouth FEP bottle (Nalgene®) equipped with magnetic stirring bar was charged with anhydrous spray dried KF (4.65 g, 80 mmol) and anhydrous MeCN (30 mL) inside the glove box. It was sealed with the closure and taken out of the glove box. The closure was replaced by a rubber septum connected by teflon tubes to the chlorine gas cylinder. The tube's

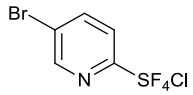
free edge was immersed into the solvent and chlorine gas was bubbled through it as the bottle was being cooled by ice bath. The chlorine gas was bubbled for approximately 10 minutes. The septum was removed and the disulfide was added in one portion (1.89 g, 5 mmol) and then sealed with the closure. The FEP bottle was placed inside an ice bath and the reaction mixture was stirred for 2 h and then at room temperature for 20-72 h. The reaction mixture was transferred to another FEP bottle using a PP/ETFE suction filter (Flom Cat. # 8800) under nitrogen environment and the solvent was evaporated *in vacuo* to give crude 2-pyridylsulfur chlorotetrafluorides.
(*The purity of crude 2-pyridylsulfur chlorotetrafluorides was usually in the range of 80-95% according to ^{1}H, ^{19}F NMR data.*)

6-bromo-2-pyridylsulfur chlorotetrafluoride (8a'):



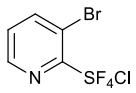
Prepared according to the general procedure from 1,2-bis(6-bromopyridin-2-yl)disulfane (**i**) by stirring at rt for 48 h and obtained the crude product as white solid in 90% yield (2.75 g).
^{1}H NMR ($CDCl_3$, 300 MHz) δ = 8.63 (d, *J* = 1.9 Hz, 1H), 8.04 (d, *J* = 8.8 Hz, 1H), 7.65 (d, *J* = 8.7 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 124.77 (s, 4F).

5-bromo-2-pyridylsulfur chlorotetrafluoride (8b'):



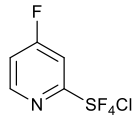
Prepared according to the general procedure from 1,2-bis(5-bromopyridin-2-yl)disulfane (**ii**) by stirring at rt for 20 h and obtained the crude product as white solid in 94% yield (2.85 g). The ^{19}F NMR spectrum matched the one reported by Dolbier *et al*.[5]
^{19}F NMR ($CDCl_3$, 282 MHz) δ = 124.82 (s, 4F)

3-bromo-2-pyridylsulfur chlorotetrafluoride (8c'):



Prepared according to the general procedure from 1,2-bis(3-bromopyridin-2-yl)disulfane (**iii**) (1.25g, 3.3 mmol) by stirring at rt for 72 h and obtained the crude product as an oil in 75% yield (1.5 g) which was a crude mixture of the required product and the SF_3 derivative. The ^{19}F NMR spectrum matched the one reported by Dolbier *et al*.[5]
^{19}F NMR ($CDCl_3$, 282 MHz) δ = 124. 87 (s, 4F)

4-fluoro-2-pyridylsulfur chlorotetrafluoride (8d'):



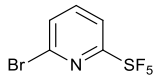
Prepared according to the general procedure from 1,2-bis(6-bromopyridin-2-yl)disulfane (**iv**) by stirring at rt for 48 h and obtained the crude product as white solid in 48% yield (1.4 g).
^{1}H NMR ($CDCl_3$, 300 MHz) δ = 7.25–7.30 (m, 1H), 7.51 (d, *J* = 9 Hz, 1H), 8.58 (t, *J* = 6 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ= 96.42 (s, 1F), 123.80 (s, 4F).

Synthesis of 2-pyridylsulfur pentafluorides 8:

The 2-pyridylsulfur pentafluorides were prepared according to the literature procedure.[5] The crude 2-pyridylsulfur chlorotetrafluorides was transferred into FEP bottles (Nalgene®) in the glove box and their exact amount was measured. Solid AgF (2 equiv) was then added in one portion and the bottle was sealed with closure. It was taken out of the glove box, covered with tin foil, placed in a preheated oil bath at 60-70 °C and then left for 16 - 72 h. The content of the vial was washed out into a beaker first with CH_2Cl_2 (30 mL) and then with water (30 mL), the contents of the beaker stirred for 1h and then filtered from solids. The organic phase was separated and the aqueous phase extracted with CH_2Cl_2 (20 X 3 mL). The

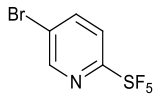
combined CH_2Cl_2 extracts were dried with Na_2SO_4. The residue obtained after filtration and evaporation of solvent *in vacuo* was purified by column chromatography, eluting with pentane/CH_2Cl_2 to give title 2-pyridylsulfur pentafluorides.

6-bromo-2-pyridylsulfur pentafluoride (8a):



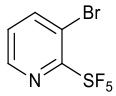
Prepared according to the general procedure from 6-bromo-2-pyridylsulfur chlorotetrafluoride **8a'** (2.75 g, 9.15 mmol) and AgF (2.32 g, 18.3 mmol), by stirring at 60 °C for 40 h. It was isolated by column chromatography on silica gel (pentane/CH_2Cl_2 : 9/1) to give 6-bromo-2-pyridylsulfur pentafluoride as a white solid in 69% yield (1.95 g).
m.p.: 65.3 °C; HRMS (EI) calcd. for $C_5H_3NF_5SBr$ [$(M)^+$]:282.9090 found 282.9109; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 7.70–7.83 (m, 3H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.42 (d, *J* = 146.64 Hz, 4F), 76.45 (quintet, *J* = 152.28 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 120.34 (quintet, *J* = 5 Hz), 131.83, 139.91, 140.64, 164.50–164.88 (m). ATR-FTIR (KBr): *v* = 3118, 3096, 3051, 2011, 1567, 1553, 1426, 1126, 811, 739 cm^{-1}.

5-bromo-2-pyridylsulfur pentafluoride (8b):



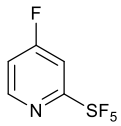
Prepared according to the general procedure from 5-bromo-2-pyridylsulfur chlorotetrafluoride **8b'** (2.85 g, 9.5 mmol) and AgF (2.4 g, 19 mmol), by stirring at 60 °C for 20 h. It was isolated by column chromatography on silica gel (pentane/CH_2Cl_2 : 9/1) to give 5-bromo-2-pyridylsulfur pentafluoride as a white solid in 70% yield (1.98 g). The ^{1}H NMR and ^{19}F NMR spectrum matched the one reported by Dolbier *et al*.[5]
^{1}H NMR ($CDCl_3$, 300 MHz) δ = 7.66 (d, *J* = 9 Hz, 1H), 8.05 (d, *J* = 9 Hz, 1H), 8.65 (s, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.68 (d, *J* = 149.45 Hz, 4F), 77.12 (quintet, *J* = 149.46 Hz, 1F)

3-bromo-2-pyridylsulfur pentafluoride (8c)



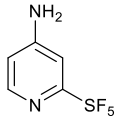
Prepared according to the general procedure from 3-bromo-2-pyridylsulfur chlorotetrafluoride **8c'** (1.5 g, 4.8 mmol) and AgF (1.2 g, 9.6 mmol), by stirring at 70 °C for 72 h. It was isolated by column chromatography on silica gel (pentane/CH_2Cl_2 : 4/1) to give 3-bromo-2-pyridylsulfur pentafluoride as a white solid in 20% yield (275.8 mg). The ^{1}H NMR and ^{19}F NMR spectrum matched the one reported by Dolbier *et al*.[5]
^{1}H NMR ($CDCl_3$, 300 MHz) δ = 7.37 (q, *J* = 3 Hz, 1H), 8.18 (d, *J* = 9 Hz, 1H), 8.56 (d, *J* = 3 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 53.97 (d, *J* = 152.28, 4F), 76.55 (quintet, *J* = 152.28, 1F).

4-fluoro-2-pyridylsulfur pentafluoride (8d):



Prepared according to the general procedure from 4-fluoro-2-pyridylsulfur chlorotetrafluoride (1.4 g, 5.8 mmol) and AgF (1.5 g, 11.6 mmol), by stirring at 80 °C for 72 h. After workup, CH_2Cl_2 was removed by distillation and crude was purified by column chromatography on silica gel (pentane/CH_2Cl_2 : 5/5). The solvent was removed by distillation to give 4-fluoro-2-pyridylsulfur pentafluoride as a volatile liquid. The solvent could not be removed completely fearing loss of the compound and it was used as such for the next step.
HRMS (EI) calcd. for $C_5H_3NF_6Sr$ [$(M)^+$]:222.9890 found 222.9882; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 7.25–7.30 (m, 1H), 7.52 (dd, *J* = 3 Hz, 6 Hz, 1H), 8.58–8.63 (m, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = -96.94 (q, *J* = 8.46 Hz, 1F), 51.91 (d, *J* = 149.46 Hz, 4F), 76.57 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ =100.34–110.64 (m), 115.12 (d, *J* = 15 Hz), 150.37–150.46 (m), 166.77-167.22 (m), 168.27, 170.39.

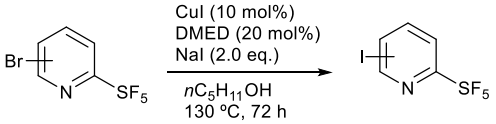
Synthesis of 4-amino-2-pyridylsulfur pentafluoride (8e):



8d (1.6 g including CH_2Cl_2) and excess of NH_3 (6 ml, 28% aqueous solution) was placed in the tight-cap vial.[12] The reaction mixture was stirred for 72 h at 120 °C. After cooling, the mixture was diluted with water and extracted with ether (3×20 mL). Combined organic layer were dried over anhydrous Na_2SO_4, filtered, and solvent was evaporated under reduced pressure to give practically pure 4-amino-2-pyridylsulfur pentafluoride **8e** as a brown solid (566 mg) in 44% yield with respect to 4-fluoro-2-pyridylsulfur chlorotetrafluoride **10d**.
m.p.: 93.4 °C; HRMS (EI) calcd. for $C_5H_6N_2F_5S$ [$(M+H)^+$]:221.0172 found 221.0172; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 4.58 (brs, 1H), 6.65 (dd, *J* = 1.5 Hz, 6 Hz 1H), 6.94 (d, *J* = 1.5 Hz, 1H), 8.15 (d, *J* = 6 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 51.41 (d, *J* = 149.46 Hz, 4F), 79.18 (quintet, *J* = 146.64 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 106.46 (quintet, *J* = 5 Hz), 112.06, 148.30 (t, *J* = 1.25 Hz), 154.84, 167.02 (quintet, *J* = 22.5 Hz). ATR-FTIR (KBr): *v* = 3508, 3190, 3343, 2709, 1642, 1605, 1310, 1269, 988, 797, 656 cm^{-1}.

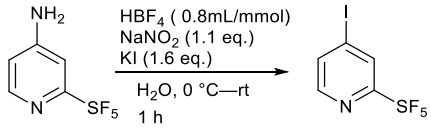
Synthesis of Iodo-2-pyridylsulfur pentafluorides 7:

General method A: Iodo-2-pyridylsulfur pentafluorides **7a–c** were prepared from the corresponding Bromo-2-pyridylsulfur pentafluorides **8a–c** by aromatic Finkelstein reaction[6] (Scheme S2). Although the resulting aryl iodides contained traces of the aryl bromide starting material due to the difficulties in separation, these products were used in next step without further purification.



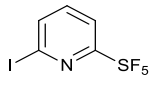
To a flame dried Schlenk-tube, CuI (10 mol %), NaI (2.0 eq.) and Bromo-2-pyridylsulfur pentafluorides (1.0 eq.) were added and evacuated and backfilled with argon. *n*-Pentyl alcohol and *N*,*N*′-dimethylethylenediamine (20 mol %) were then added and the mixture was stirred at room temperature for 5 min then at 130 °C for 48 - 96 h. The resulting suspension was cooled to room temperature, diluted with aqueous NH_3 solution (28 wt%) and H_2O, extracted with CH_2Cl_2 for three times. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (pentane/CH_2Cl_2) to give the desired product.

General method B: Iodo-2-pyridylsulfur pentafluoride **7d** was prepared from amino-2-pyridylsulfur pentafluoride by sandmayer reaction.[13]



To a cooled (0 °C) solution of amino-2-pyridylsulfur pentafluoride (1.0 eq.) in 50 % aqueous tetrafluoroboric acid (1 mL/mmol) was added aqueous $NaNO_2$ solution (1.1 eq.) dropwise. The resultant slurry was stirred at 0 °C for 30 min. The reaction mixture was then quickly transferred portion-wise to a stirring saturated solution of KI (1.6 eq.) in water. The resultant brown slurry was allowed to stir at room temperature for 30 min and then extracted with Et_2O (3 x 15 mL). The combined organic layer was washed with $Na_2S_2O_8$ (20 mL), $NaHCO_3$ (20 mL) and brine. It was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (*n*-hexane/EtOAc,) to give the desired product.

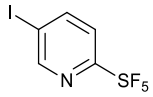
6-iodo-2-pyridylsulfur pentafluoride (7a):



Following the **General method A**, CuI (123.7 mg, 0.65 mmol), NaI (1.92 g, 13 mmol), 6-bromo-2-pyridylsulfur pentafluorides **8a** (1.85 g, 6.5 mmol) and *N,N*′-dimethylethylenediamine (139 µL, 1.3 mmol) were used in *n*-Pentyl alcohol (6.5 mL) at 130

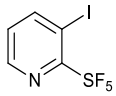
°C for 48 h. The crude product was purified by column chromatography on silica gel (pentane/CH_2Cl_2 9/1) to give the desired product (1.55 g, 72% yield) as white solid.
m.p.: 50.3 °C; HRMS (EI) calcd. for $C_5H_3NF_5SI$ [$(M)^+$]: 330.8951 found 330.8965; ^1H NMR ($CDCl_3$, 300 MHz) δ = 7.55 (t, *J* = 6 Hz, 1H), 7.73 (d, *J* = 6 Hz, 1H), 7.93 (d, *J* = 6 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.27 (d, *J* = 152.28 Hz, 4F), 76.67 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 114.37, 120.62 (quintet, *J* = 3.78 Hz), 138.48, 139.68, 164.80 (quintet, *J* = 23.94 Hz). ATR-FTIR (KBr): *v* = 3108, 3086, 3042, 2005, 1565, 1420, 1109, 798, 723, 665 cm^{-1}.

5-iodo-2-pyridylsulfur pentafluoride (7b):

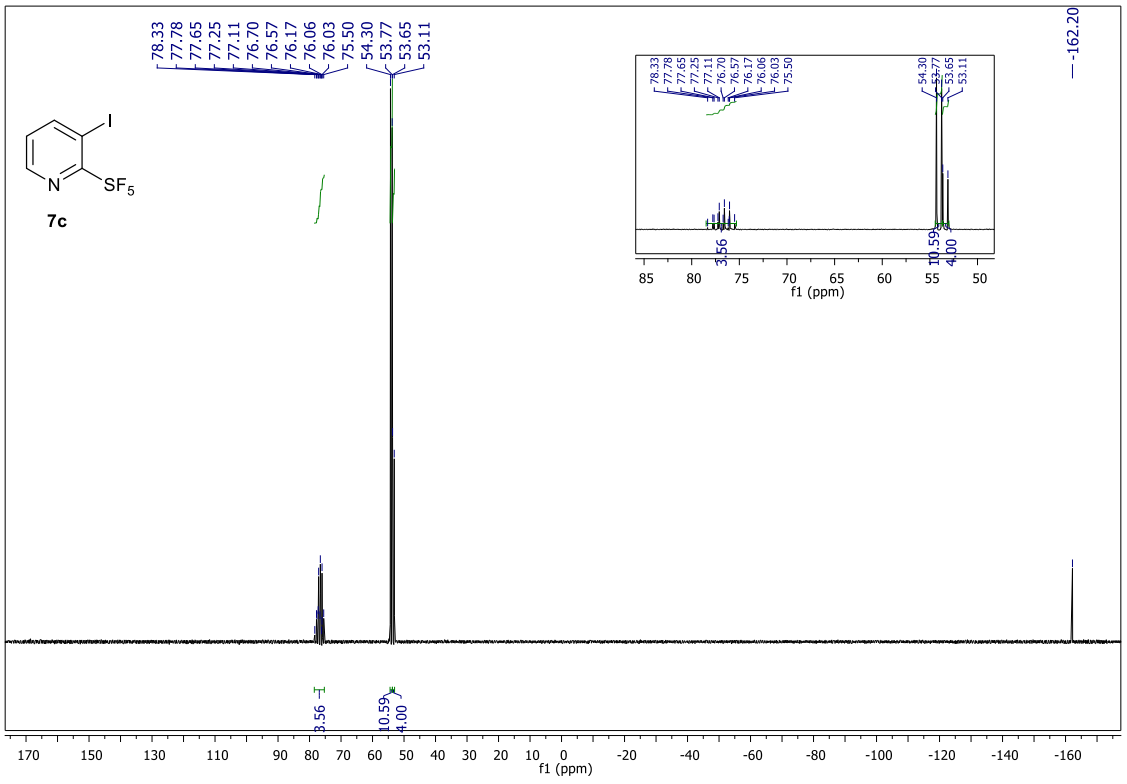


Following the **General method A**, CuI (110.5 mg, 0.58 mmol), NaI (1.72 g, 11.6 mmol), 5-bromo-2-pyridylsulfur pentafluorides **8b** (1.65 g, 5.8 mmol) and *N,N'*-dimethylethylenediamine (124 µL, 1.16 mmol) were used in *n*-Pentyl alcohol (6.0 mL) at 130 °C for 72 h. The crude product was purified by column chromatography on silica gel (pentane/CH_2Cl_2 9/1) to give the desired product (1.82 g, 95% yield) as light yellow oil.
HRMS (EI) calcd. for $C_5H_3NF_5SI$ [$(M)^+$]: 330.8951 found 330.8974; ^1H NMR ($CDCl_3$, 300 MHz) δ = 7.54 (d, *J* = 9 Hz, 1H), 8.24 (d, *J* = 6 Hz, 1H), 8.80 (d, *J* = 2.1 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.38 (d, *J* = 149.46 Hz, 4F), 77.07, (quintet, *J* = 152.28 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 97.03, 123.01 (quintet, *J* = 3.78 Hz), 147.06, 154.30, 164.82 (quintet, *J* = 23.94 Hz). ATR-FTIR (NaCl): *v* = 3186, 3044, 2926, 1557, 1445, 1002, 844, 662, 600 cm^{-1}.

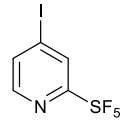
3-iodo-2-pyridylsulfur pentafluoride (7c):



Following the **General method A**, CuI (23.4 mg, 0.123 mmol), NaI (364 mg, 2.46 mmol), 3-bromo-2-pyridylsulfur pentafluorides **8c** (350 mg, 1.23 mmol) and *N,N'*-dimethylethylenediamine (25.6 µL, 0.246 mmol) were used in *n*-Pentyl alcohol (2 mL) at 130 °C for 96 h. Only a minor portion was converted to the iodide (as determined from GC MS). Isolation by column chromatography on silica gel (pentane/CH_2Cl_2 9/1) provided with an inseparable mixture of the starting material **8c** (from ^{19}F NMR). This mixture of compounds was used for the next step without any further purification.
^{19}F NMR ($CDCl_3$, 282 MHz) δ = 53.38 (d, 4F), 77.25 (quintet, 1F).



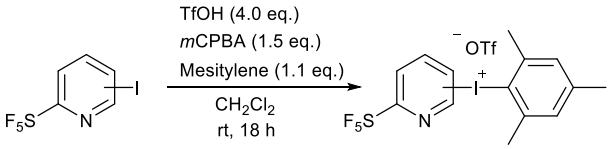
4-iodo-2-pyridylsulfur pentafluoride (7d):



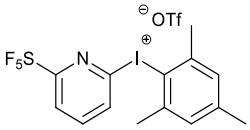
Following the **General method B**, 4-amino-2-pyridylsulfur pentafluoride (550 mg, 2.5 mmol), tetrafluoroboric acid (2 mL), $NaNO_2$ (190 mg, 2.75 mmol in 1.5 mL H_2O) and KI (664 mg, 4 mmol in 6 mL H_2O) were used at 0 °C—rt for 1h. The crude product was purified by column chromatography on silica gel (*n*-hexane/EtOAc, 9/1) to give the desired product (633 mg, 76% yield) as white solid.
m.p.: 77.8 °C; HRMS (EI) calcd. for $C_5H_3NF_5SI$ [$(M)^+$]:330.8951 found 330.8973; ^1H NMR ($CDCl_3$, 300 MHz) δ = 7.88 (d, *J* = 3 Hz, 1H), 8.12 (s, 1H), 8.27 (d, *J* = 6 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.26 (d, *J* = 149.46 Hz, 4F), 76.83, (quintet, *J* = 152.28 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 106.60, 130.53 (quintet, *J* = 5Hz), 136.24, 148.47, 165.38 (quintet, *J* = 22.5 Hz). ATR-FTIR (NaCl): *v* = 3119, 3051, 2466, 1558, 1457, 1376, 1140, 1086, 823, 655 cm^{-1}.

Synthesis of pyridine aryliodonium salts 1:

Pyridine aryliodonium salts **1** were prepared by modified procedure as given in the literature.[7]

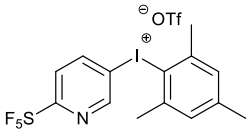


*m*CPBA (assume 70-77 wt%, 1.5 eq.) was dried *in vacuo* at room temperature for 1 h before addition of iodo-2-pyridylsulfur pentafluoride 2 (1.0 eq.) and CH_2Cl_2 (6.0 mL/mmol ArI) in a round bottomed flask. The solution was cooled to 0 °C followed by dropwise addition of TfOH (4.0 eq.), resulting mixture was stirred at room temperature for 2 h. It was then cooled to 0 °C and mesitylene (1.1 eq.) was added dropwise. The mixture was warmed to room temperature and stirred for 18 h. The solvent was then removed under reduced pressure. The resulting crude product was precipitated by the addition of Et_2O and storing at -20 °C for several hours. The precipitate was filtered and dried *in vacuo* to give **1** as white to brown solid.
Mesityl(2-(pentafluoro-λ⁶-sulfaneyl)pyridyl)-6-iodonium trifluoromethanesulfonate 1a:



Following the general procedure, *m*CPBA (assume 70 wt%, 1.85 g, 7.5 mmol), 6-iodo-2-pyridylsulfur pentafluoride **7a** (1.8 g, 5.0 mmol), TfOH (2.3 mL, 20 mmol) and mesitylene (0.76 mL, 5.5 mmol) were used in CH_2Cl_2 (30 mL) at room temperature for 18 h to give **1a** (1.8 g, 61% yield) as white solid.
m.p.: 124.0 °C; HRMS (ESI) calcd. for $C_{14}H_{14}NF_5SI$ [$(M\text{-}OTf)^+$]:449.9812 found 449.9807; ^1H NMR ($CDCl_3$, 300 MHz) δ = 2.36 (s, 3H), 2.64 (s, 6H), 7.11 (s, 2H) 7.85 (d, *J* = 9 Hz, 1H), 8.03 (t, *J* = 6 Hz, 1H), 8.55 (d, *J* = 9 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = -78.95 (s, 3F), 52.66 (d, *J* = 152.28 Hz, 4F), 74.78 (quintet, *J* = 152.28 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 21.31, 27.13, 121.99, 124.10, 130.06, 130.66, 134.70, 143.06 (d, *J* = 12.6 Hz), 144.73, 164.86–165.26 (m). ATR-FTIR (KBr): *v* = 3024, 2928, 1550, 1420, 1407, 1260, 1177, 1098, 1035, 799 cm^{-1}.

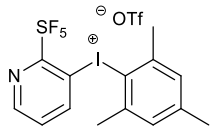
Mesityl(2-(pentafluoro-λ⁶-sulfaneyl)pyridyl)-5-iodonium trifluoromethanesulfonate 1b:



Following the general procedure, *m*CPBA (assume 77 wt%, 1.8 g, 8.1 mmol), 5-iodo-2-pyridylsulfur pentafluoride **7b** (1.8 g, 5.4 mmol), TfOH (2.5 mL, 21.7 mmol) and mesitylene (0.80 mL, 5.94 mmol) were used in CH_2Cl_2 (30 mL) at room temperature for 18 h to give **1b** (1.97 g, 61% yield) as white solid.
m.p.: 175.1 °C; HRMS (ESI) calcd. for $C_{14}H_{14}NF_5SI$ [$(M\text{-}OTf)^+$]:449.9812 found 449.9825; ^1H NMR ($(CD_3)_2CO$, 300 MHz) δ = 2.38 (s, 3H), 2.76 (s, 6H), 7.33 (s, 2H), 8.15 (d, *J* = 9 Hz, 1H), 8.82 (d, *J* = 9 Hz, 1H), 9.15 (s, 1H); ^{19}F NMR ($(CD_3)_2CO$, 282 MHz) δ = -

77.89 (s, 3F), 53.28 (d, *J* = 146.64 Hz, 4F), 77.34 (quintet, *J* = 146.64 Hz, 1F); ^{13}C NMR ($(CD_3)_2CO$, 126 MHz) δ = 20.01, 26.19, 114.43, 121.01, 124.61-124.77 (m), 130.36, 142.76, 144.87, 145.23, 151.37, 165.56-166.31. ATR-FTIR (KBr): *v* = 3060, 2992, 1451, 1275, 1231, 1170, 1029, 995, 879, 844 cm^{-1}.

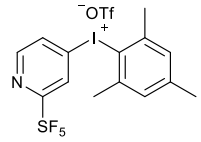
Mesityl(2-(pentafluoro-λ^6-sulfaneyl)pyridyl)-3-iodonium trifluoromethanesulfonate 1c:



Following the general procedure, *m*CPBA (assume 70 wt%, 347.6 mg, 1.41 mmol), 3-iodo-2-pyridylsulfur pentafluoride **7c** (310 mg, 0.94 mmol), TfOH (0.4 mL, 3.76 mmol) and mesitylene (0.14 mL, 1.034 mmol) were used in CH_2Cl_2 (6 mL) at room temperature for 18 h to give **1c** (40 mg, 5% yield in overall two steps starting from the 3-bromo-2-pyridylsulfur pentafluoride **8c**) as brown solid.

m.p.: 129.4 °C; HRMS (ESI) calcd. for $C_{14}H_{14}NF_5SI$ [(M-OTf)$^+$]:449.9812 found 449.9812; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 2.44 (s, 3H), 2.60 (s, 6H), 7.25 (s, 2H), 7.52 (t, *J* = 6 Hz, 2H), 8.71 (s, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = -78.98 (s, 3F), 53.63 (d, *J* = 149.46 Hz, 4F), 75.86 (quintet, *J* = 152.28 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 21.45, 27.25, 104.29, 121.61, 130.44, 131.36, 142.09, 143.41, 146.87, 149.66, 163.16-163.58 (m). ATR-FTIR (KBr): 3061, 2925, 1550, 1456, 1394, 1283, 1241, 1172, 1025, 848 cm^{-1}.

Mesityl(2-(pentafluoro-λ^6-sulfaneyl)pyridyl)-4-iodonium trifluoromethanesulfonate 1d:

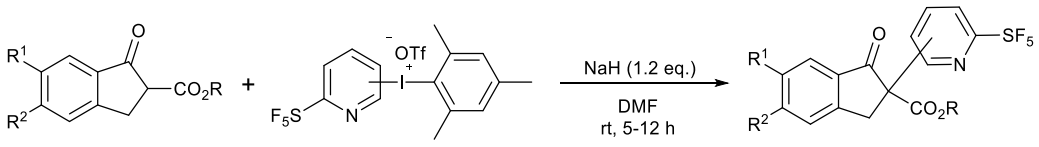


Following the general procedure, *m*CPBA (assume 70 wt%, 554 mg, 2.25 mmol), 4-iodo-2-pyridylsulfur pentafluoride (496 mg, 1.5 mmol), TfOH (0.68 mL, 6.0 mmol) and mesitylene (0.23 mL, 1.65 mmol) were used in CH_2Cl_2 (9 mL) at room temperature for 18 h to give **1d** (500 mg, 56% yield) as beige solid.

m.p.: 156.9 °C; HRMS (ESI) calcd. for $C_{14}H_{14}NF_5SI$ [(M-OTf)$^+$]:449.9812 found 449.9808; ^{1}H NMR ($(CD_3)_2CO$, 300 MHz) δ = 2.41 (s, 3H), 2.72 (s, 6H), 7.37 (s, 2H), 8.01 (d, *J* = 6 Hz, 1H), 8.65 (s, 1H), 8.71 (d, *J* = 3 Hz, 1H); ^{19}F NMR ($(CD_3)_2CO$, 282 MHz) δ = -76.78 (s, 3F), 54.61 (d, *J* = 152.28 Hz, 4F), 78.62 (quintet, *J* = 152.28 Hz, 1F); ^{13}C NMR ($(CD_3)_2CO$, 126 MHz) δ = 20.07, 26.12, 120.46, 124.19, 125.57 (quintet, *J* = 3.75 Hz), 130.46, 130.72, 143.07, 145.30, 150.92, 164.78–165.53, 209.11. ATR-FTIR (KBr): *v* = 3038, 2972, 2250, 1700, 1551, 1538, 1166, 1024, 827, 712 cm^{-1}.

SF_5-heteroarylation of β-ketoesters:

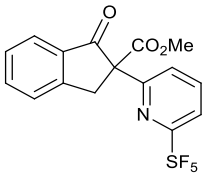
The β-ketoesters were prepared according to the literature procedure.[8]



9a: R = Me, R^1 = R^2 = H
9b: R = Et, R^1 = R^2 = H
9c: R = ^{t}Bu, R^1 = R^2 = H
9d: R = Me, R^1 = Me, R^2 = H
9e: R = Me, R^1 = R^2 = OMe

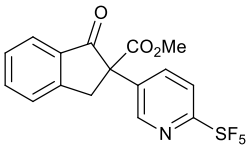
A flame dried test tube was charged with the β-ketoester **9** (0.1 mmol), NaH (60% suspension in oil, 0.12 mmol) in DMF (10 mL/mmol β-ketoester) and stirred for 10 min at room temperature. The reagent **1** (0.11 mmol) was then added to the mixture in one portion at room temperature. After completion of the reaction, H_2O was slowly added to the reaction mixture and extracted with Et_2O three times. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel to give (2-pyridyl-SF_5)-β-ketoester **2**.

Methyl 1-oxo-2-(6-(pentafluoro-λ⁶-sulfaneyl)pyridin-2-yl)-2,3-dihydro-1H-indene-2-carboxylate (2aa):



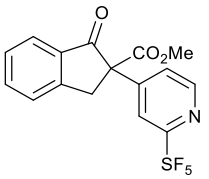
Following general procedure β-ketoester **9a**, (19 mg, 0.1 mmol), NaH (60% suspension in oil, 4.8 mg, 0.12 mmol) and reagent **1a** (66 mg, 0.11mmol) in DMF (1 mL) were used at room temperature for 5 h. Isolated by column chromatography on silica gel (*n*-hexane/EtOAc, 7/3) to give the desired product **2aa** as white solid (30 mg) in 76% yield.
m.p.: 124.7 °C; HRMS (EI) calcd. for $C_{16}H_{12}NO_3F_5S$ [$(M)^+$]:393.0458 found 393.0464; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 3.22 (d, *J* = 18 Hz, 1H), 3.71 (s, 3H), 4.58 (d, *J* = 18 Hz, 1H) 7.31 (d, *J* = 6 Hz, 1H), 7.45 (t, *J* = 9 Hz, 1H), 7.52 (d, *J* = 9 Hz, 2H), 7.70 (t, *J* = 9 Hz, 1H), 7.86 (t, *J* = 9 Hz, 2H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 62.70 (d, *J* = 155.1 Hz, 4F), 76.74 (quintet, *J* -= 155.1 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 37.77, 53.77, 64.31, 123.56, 125.35, 126.41, 126.83, 127.05, 128.26, 134.61, 136.80, 153.68, 157.03-157.35 (m), 166.72, 198.52. ATR-FTIR (KBr): *v* = 2958, 1709, 1392, 1281, 1247, 1214, 1159, 910, 877, 853 cm^{-1}

Methyl 1-oxo-2-(6-(pentafluoro-λ⁶-sulfaneyl)pyridin-3-yl)-2,3-dihydro-1H-indene-2-carboxylate (2ba):



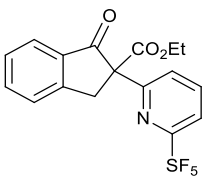
Following general procedure β-ketoester **9a**, (19 mg, 0.1 mmol), NaH (60% suspension in oil, 4.8 mg, 0.12 mmol) and reagent **1b** (66 mg, 0.11mmol) in DMF (1 mL) were used at room temperature for 5 h. Isolated by column chromatography on silica gel (*n*-hexane/EtOAc, 7/3) to give the desired product **2ba** as white solid (20 mg) in 51% yield.
m.p.: 150.4 °C; HRMS (ESI) calcd. for $C_{16}H_{12}NO_3F_5NaS$ [$(M+Na)^+$]:416.0356 found 416.0353; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 3.63 (d, *J* = 18 Hz, 1H), 3.76 (s, 3H), 4.27 (d, *J* = 18 Hz, 1H), 7.48 (t, *J* = 6 Hz, 1H), 7.55 (d, *J* = 6 Hz, 1H), 7.69–7.67 (m, 2H) 7.85 (d, *J* = 9 Hz, 1H), 8.16 (d, *J* = 9 Hz, 1H), 8.63 (d, *J* = 6 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.14 (d, *J* = 149.46 Hz, 4F), 77.70 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 39.72, 53.97, 63.00, 121.15 (t, *J* = 3.78 Hz), 125.65, 126.47, 128.74, 134.31, 136.55, 137.60, 138.45, 147.47, 151.77, 164.55 (t, *J* = 22.68 Hz), 169.78, 198.60. ATR-FTIR (KBr): *v* = 2961, 1724, 1468, 1434, 1285, 1228, 1208, 1177, 846, 761 cm^{-1}.

Methyl 1-oxo-2-(6-(pentafluoro-λ⁶-sulfaneyl)pyridin-4-yl)-2,3-dihydro-1H-indene-2-carboxylate (2da):



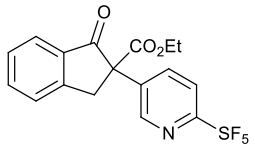
Following general procedure β-ketoester **2a**, (19 mg, 0.1 mmol), NaH (60% suspension in oil, 4.8 mg, 0.12 mmol) and reagent **1d** (66 mg, 0.11mmol) in DMF (1 mL) were used at room temperature for 5 h. Isolated by column chromatography on silica gel (*n*-hexane/EtOAc, 6/4) to give the desired product **2da** as yellow oil (30.3 mg) in 77% yield.
HRMS (ESI) calcd. for $C_{16}H_{13}NO_3F_5S$ [$(M+H)^+$]:394.0536 found 394.0539; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 3.59 (d, *J* = 18 Hz, 1H), 3.76 (s, 3H), 4.24 (d, *J* = 18 Hz, 1H), 7.49 (t, *J* = 9 Hz, 1H), 7.56 (d, *J* = 6 Hz, 1H), 7.66–7.75 (m, 2H) 7.85–7.90 (m, 2H), 8.57 (d, *J* = 6 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.06 (d, *J* = 149.46 Hz, 4F), 77.78 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 39.67, 54.02, 64.41, 120.70 (t, *J* = 3.75 Hz), 125.69, 126.19, 126.46, 128.76, 134.32, 136.59, 148.32, 150.17, 151.65, 166.03 (quintet, *J* = 22.5 Hz), 169.31, 197.98. ATR-FTIR (KBr): *v* = 3421, 2957, 2847, 1744, 1594, 1217, 1039, 844 cm^{-1}.

Ethyl 1-oxo-2-(6-(pentafluoro-λ⁶-sulfaneyl)pyridin-2-yl)-2,3-dihydro-1H-indene-2-carboxylate (2ab):



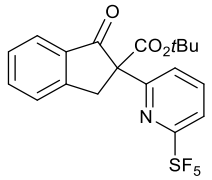
Following general procedure β-ketoester **9b**, (20 mg, 0.1 mmol), NaH (60% suspension in oil, 4.8 mg, 0.12 mmol) and reagent **1a** (66 mg, 0.11mmol) in DMF (1 mL) were used at room temperature for 5 h. Isolated by column chromatography on silica gel (*n*-hexane/EtOAc, 8/2) to give the desired product **2ab** as yellow solid (28.5 mg) in 70% yield.
m.p.: 89.0 °C HRMS (EI) calcd. for $C_{17}H_{14}NO_3F_5S$ [$(M)^+$]:407.0615 found 407.0611 ; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 1.15 (t, *J* = 9 Hz, 3H), 3.22 (d, *J* = 18 Hz, 1H), 4.03–4.14 (m, 1H), 4.24–4.34 (m, 1H), 4.58 (d, *J* = 18 Hz, 1H), 7.30 (d, *J* = 9 Hz, 1H), 7.45 (t, *J* = 9 Hz, 1H), 7.50–7.54 (m, 2H), 7.67–7.72 (m, 1H), 7.83–7.88 (m, 2H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 63.24 (d, *J* = 155.1 Hz, 4F), 77.32, (quintet, *J* = 152.28 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 13.93, 37.74, 62.81, 64.41, 123.46, 125.29, 126.32, 126.81, 127.04, 128.20, 134.67, 136.73, 153.75, 153.82, 166.12, 198.70. IR (KBr): *v* = 3118, 1736, 1393, 1288, 1272, 1242, 1208, 909, 833, 785 cm^{-1}.

Ethyl 1-oxo-2-(6-(pentafluoro-λ^6-sulfaneyl)pyridin-3-yl)-2,3-dihydro-1H-indene-2-carboxylate (2bb):



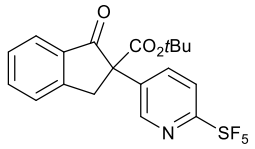
Following general procedure β-ketoester **9b**, (20 mg, 0.1 mmol), NaH (60% suspension in oil, 4.8 mg, 0.12 mmol) and reagent **1b** (66 mg, 0.11mmol) in DMF (1 mL) were used at room temperature for 3 h. Isolated by column chromatography on silica gel (*n*-hexane/EtOAc, 8/2) to give the desired product **2bb** as white solid (23.6 mg) in 58% yield.
m.p.: 80.1 °C; HRMS (ESI) calcd. for $C_{17}H_{14}NO_3F_5NaS$ [$(M+Na)^+$]:430.0512 found 430.0515; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 1.21 (t, *J* = 9 Hz, 3H), 3.63 (d, *J* = 18 Hz, 1H), 4.19–4.26 (m, 3H), 7.48 (t, *J* = 6 Hz, 1H), 7.56 (d, *J* = 6 Hz, 1H), 7.69–7.76 (m, 2H), 7.86 (d, *J* = 6 Hz, 1H), 8.16 (d, *J* = 9 Hz, 1H), 8.64 (s, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.12 (d, *J* = 152.28 Hz, 4F), 77.74 (quintet, *J* = 152.28 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 14.06, 39.64, 63.14, 121.10 (t, *J* = 3.78 Hz), 125.60, 126.44, 128.69, 134.36, 136.46, 137.69, 138.49, 147.46, 151.79, 164.51 (t, *J* = 22.68 Hz), 169.23, 198.68. ATR-FTIR (KBr): *v* = 2971, 1715, 1466, 1370, 1288, 1224, 1187, 1006, 759, 747 cm^{-1}.

Tert-butyl 1-oxo-2-(6-(pentafluoro-λ^6-sulfaneyl)pyridin-2-yl)-2,3-dihydro-1H-indene-2-carboxylate (2ac):



Following general procedure β-ketoester **9c**, (23 mg, 0.1 mmol), NaH (60% suspension in oil, 4.8 mg, 0.12 mmol) and reagent **1a** (66 mg, 0.11mmol) in DMF (1 mL) were used at room temperature for 5 h. Isolated by column chromatography on silica gel (*n*-hexane/EtOAc, 8/2) to give the desired product **2ac** as white solid (26.1 mg) in 60% yield.
m.p.: 146.3 °C; The compound was unstable for both ESI and EI conditions while analysing HRMS. Hence, it was characterized by ^{1}H, ^{19}F and ^{13}C NMR for purity. ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 1.34 (s, 9H), 3.20 (d, *J* = 18 Hz, 1H), 4.51 (d, *J* = 18 Hz, 1H), 7.27 (t, *J* = 6 Hz, 1H), 7.43, (t, *J* = 9 Hz, 1H), 7.49–7.53 (m, 2H), 7.65–7.70 (m, 1H), 7.81–7.87 (m, 2H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 62.79 (d, *J* = 155.1 Hz, 4F), 77.11 (quintet, *J* = 152.28 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 27.56, 37.62, 65.10, 83.05, 123.13, 125.17, 125.97, 126.72, 126.85, 128.05, 134.86, 136.55, 153.87, 154.28, 157.07 (t, *J* = 18.9 Hz), 164.93, 199.11. ATR-FTIR (KBr): *v* = 3112, 2978, 1714, 1606, 1389, 1287, 1243, 1149, 900, 870 cm^{-1}. ATR-FTIR (KBr): *v* = 2954, 1714, 1498, 1468, 1430, 1234, 1156, 836, 770, 597 cm^{-1}.

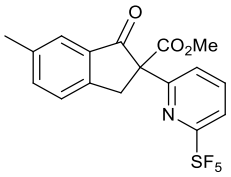
Tert-butyl 1-oxo-2-(6-(pentafluoro-λ^6-sulfaneyl)pyridin-3-yl)-2,3-dihydro-1H-indene-2-carboxylate (2bc):



Following general procedure β-ketoester **9c**, (23 mg, 0.1 mmol), NaH (60% suspension in oil, 4.8 mg, 0.12 mmol) and reagent **1b** (66 mg, 0.11mmol) in DMF (1 mL) were used at room temperature for 12 h. Isolated by column chromatography on silica gel (*n*-hexane/EtOAc, 8/2) to give the desired product **2bc** as yellow oil (31.3 mg) in 72% yield.
HRMS (ESI) calcd. for $C_{19}H_{18}NO_3F_5NaS$ [$(M+Na)^+$]:458.0825 found 458.0825; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 1.38 (s, 9H), 3.61 (d, *J* = 18 Hz, 1H), 4.15 (d, *J* = 18 Hz, 1H), 7.46 (t, *J* = 9 Hz, 1F), 7.54 (d, *J* = 9 Hz, 1H), 7.71 (q, *J* = 9 Hz, 2H), 7.84 (d, *J* = 9 Hz, 1H),

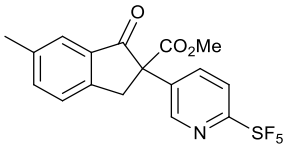
8.18 (d, *J* = 9 Hz, 1H), 8.65 (s, 1H) ; ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.14 (d, *J* = 149.46 Hz, 4F), 77.86 (quintet, *J* = 152.28 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 27.78, 39.49, 63.91, 84.05, 120.93 (t, J = 7.56 Hz), 125.43, 126.35, 128.55, 134.55, 136.23, 137.88, 138.53, 147.48, 151.80, 164.39 (t, *J* = 23.94 Hz), 168.15, 198.99. ATR-FTIR (NaCl): *v* = 2980, 1715, 1606, 1592, 1466, 1395, 1371, 1252, 1148, 847 cm^{-1}.

Methyl 6-methyl-1-oxo-2-(6-(pentafluoro-λ^6-sulfaneyl)pyridin-2-yl)-2,3-dihydro-1H-indene-2-carboxylate (2ad):



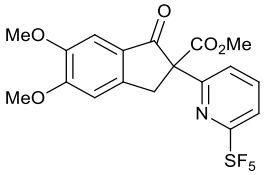
Following general procedure β-ketoester **9d**, (20 mg, 0.1 mmol), NaH (60% suspension in oil, 4.8 mg, 0.12 mmol) and reagent **1a** (66 mg, 0.11mmol) in DMF (1 mL) were used at room temperature for 5 h. Isolated by column chromatography on silica gel (*n*-hexane/EtOAc, 8/2) to give the desired product **2ad** as white solid (16 mg) in 40% yield.
m.p.: 150.2 °C; HRMS (EI) calcd. for $C_{17}H_{14}NO_3F_5S$ [(M)$^+$]:407.0615 found 407.0627; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 2.43 (s, 3H), 3.16 (d, *J* = 18 Hz, 1H), 3.70 (s, 3H), 4.52 (d, *J* = 18 Hz, 1H), 7.29 (d, *J* = 9 Hz, 1H), 7.39 (d, *J* = 9 Hz, 1H), 7.51 (d, *J* = 6 Hz, 2H), 7.66 (s, 1H), 7.84 (dd, *J* = 9 Hz, 3 Hz, 1H) ; ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 62.68 (d, *J* = 155.1 Hz, 4F), 76.77 (quintet, *J* = 155.1 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 21.22, 37.44, 53.73, 64.64, 123.50, 125.12, 126.36, 126.49, 127.01, 134.79, 138.16, 138.38, 151.15, 153.85, 157.18, 166.80, 198.56. ATR-FTIR (KBr): *v* = 2955, 1746, 1718, 1391, 1291, 1234, 886, 855, 835, 819 cm^{-1}.

Methyl 6-methyl-1-oxo-2-(6-(pentafluoro-λ^6-sulfaneyl)pyridin-3-yl)-2,3-dihydro-1H-indene-2-carboxylate (2bd):



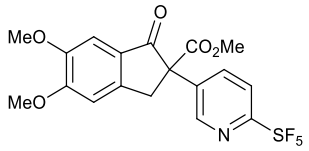
Following general procedure β-ketoester **9d**, (20 mg, 0.1 mmol), NaH (60% suspension in oil, 4.8 mg, 0.12 mmol) and reagent **1b** (66 mg, 0.11mmol) in DMF (1 mL) were used at room temperature for 5 h. Isolated by column chromatography on silica gel (*n*-hexane/EtOAc, 8/2) to give the desired product **2bd** as white solid (21.3 mg) in 56% yield.
m.p.: 112.9 °C; HRMS (ESI) calcd. for $C_{17}H_{14}NO_3F_5NaS$ [(M+Na)$^+$]:430.0512 found 430.0517; ^{1}H NMR ($CDCl_3$, 300 MHz) δ =2.43 (s, 3H), 3.57 (d, *J* = 18 Hz, 1H), 3.75 (s, 3H), 4.17 (d, *J* = 15 Hz, 1H), 7.43 (d, *J* = 6 Hz, 1H), 7.52 (d, *J* = 6 Hz, 1H), 7.65 (s, 1H), 7.73 (d, *J* = 9 Hz, 1H), 8.14 (d, *J* = 9 Hz, 1H), 8.62 (s, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.15 (d, *J* = 149.46 Hz, 4F), 77.76 (quintet, *J* = 152.28 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 21.24, 39.45, 53.90, 63.33, 121.11 (t, *J* = 3.78 Hz), 125.46, 126.12, 134.47, 137.74, 137.84, 138.44, 138.90, 147.48, 149.19, 164.49 (t, *J* = 23.94 Hz), 169.92, 198.65. ATR-FTIR (KBr): *v* = 2954, 1714, 1498, 1468, 1430, 1234, 1156, 836, 770, 597 cm^{-1}.

Methyl 5,6-dimethoxy-1-oxo-2-(6-(pentafluoro-λ^6-sulfaneyl)pyridin-2-yl)-2,3-dihydro-1H-indene-2-carboxylate (2ae):



Following general procedure β-ketoester **9e**, (25 mg, 0.1 mmol), NaH (60% suspension in oil, 4.8 mg, 0.12 mmol) and reagent **1a** (66 mg, 0.11mmol) in DMF (1 mL) were used at room temperature for 5 h. Isolated by column chromatography on silica gel (*n*-hexane/EtOAc, 8/2) to give the desired product **2ae** as white solid (41.6 mg) in 92% yield.
m.p.: 163.7 °C; HRMS (ESI) calcd. for $C_{18}H_{16}NO_5F_5NaS$ [(M+Na)$^+$]:476.0567 found 476.0577; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 3.75–3.82 (m, 4H), 3.90 (s, 3H), 4.01 (s, 3H), 4.47 (d, *J* = 18 Hz, 1H), 7.00 (s, 1H), 7.16 (s, 1H), 7.67 (d, *J* = 6 Hz, 1H), 7.94 (t, *J* = 6 Hz, 1H), 8.10 (d, *J* = 9 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.26 (d, *J* = 149.46 Hz, 4F), 77.98 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 36.19, 53.50, 56.24, 56.55, 67.39, 105.24, 107.34, 120.37 (t, *J* = 5.04 Hz), 126.67, 127.80, 139.04, 149.71, 150.04, 154.65, 156.77, 163.96 (t, *J* = 22.68 Hz), 170.69, 197.50. ATR-FTIR (KBr): *v* = 2945, 1726, 1682, 1590, 1507, 1439, 1278, 1260, 1237, 1127, 850, 610 cm^{-1}.

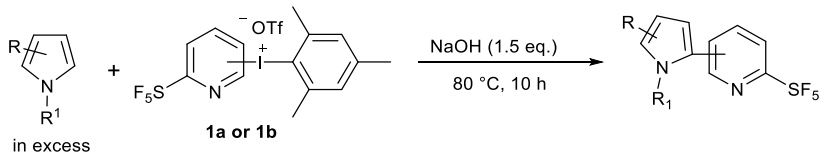
Methyl 5,6-dimethoxy-1-oxo-2-(6-(pentafluoro-λ⁶-sulfaneyl)pyridin-3-yl)-2,3-dihydro-1H-indene-2-carboxylate (2be):



Following general procedure β-ketoester **9e**, (25 mg, 0.1 mmol), NaH (60% suspension in oil, 4.8 mg, 0.12 mmol) and reagent **1b** (66 mg, 0.11mmol) in DMF (1 mL) were used at room temperature for 5 h. Isolated by column chromatography on silica gel (*n*-hexane/EtOAc, 7/3) to give the desired product **2be** as white solid (30.3 mg) in 67% yield.
m.p.: 165.4 °C; HRMS (ESI) calcd. for $C_{18}H_{16}NO_5F_5NaS$ [(M+Na)$^+$]:476.0567 found 476.0566; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 3.49 (d, *J* = 18 Hz, 1H), 3.76 (s, 3H), 3.93 (s, 3H), 4.01 (s, 3H), 4.14 (d, *J* = 15 Hz, 1H), 6.94 (s, 1H), 7.23 (s, 1H), 7.73 (d, *J* = 9 Hz, 1H), 8.14, (*J* = 9 Hz, 1H), 8.60 (d, *J* = 3 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.15, (d, *J* = 149.46 Hz, 4F), 77.81 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 53.89, 56.37, 56.64, 63.35, 105.41, 107.11, 121.11 (t, *J* = 3.78 Hz), 127.02, 138.20, 138.39, 147.51, 147.66, 150.46, 157.08, 164.43 (t, *J* = 23.94 Hz), 170.05, 196.95. ATR-FTIR (KBr): *v* = 2959, 1732, 1700, 1594, 1505, 1468, 1316, 1284, 1120, 874, 833, 769 cm^{-1}.

SF_5-heteroarylation of pyrroles:

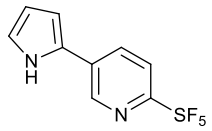
The heteroarylation of pyrroles were performed according to literature procedure.[9]



10a: R = R^1 = H
10b: R = 2,4-Me, R^1 = H
10c: R = H, R^1 = Me

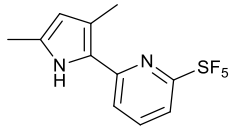
A reflux tube equipped with a magnetic stir bar was charged with reagent **1a** or **1b** (1.0 eq.), NaOH (1.5 eq.), pyrrole **10** (0.5 mL/mmol), and the reaction vessel was placed in an 80 °C oil bath. After stirring at this temperature for 10 h, the mixture was distilled *in vacuo* to recover the redundant pyrrole. The residue was cooled to room temperature, diluted with of ethyl acetate, and washed with brine (15 mL) and water (15 mL), and then the organic layer was dried over Na_2SO_4. After being concentrated *in vacuo*, the crude product was purified by column chromatography on silica gel (*n*-hexane/EtOAc).

5-(1H-pyrrol-2-yl)-2-(pentafluoro-λ⁶-sulfaneyl)pyridine (3ba):



Following general procedure reagent **1b** (60 mg, 0.1 mmol), NaOH (6 mg, 0.15 mmol) in pyrrole **10a** (0.5 mL) were used at 80 °C for 10 h. Isolated by column chromatography on silica gel (*n*-hexane/EtOAc, 4/1) to give the desired product **3ba** as white solid (18 mg) in 66% yield.
m.p.: 158.3 °C; HRMS (ESI) calcd. for $C_9H_8N_2F_5S$ [(M)$^+$]:271.0328 found 271.0320; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 6.375 (q, *J* = 3 Hz, 1H), 6.71 (s, 1H), 7.005 (d, *J* = 3 Hz, 1H), 7.72 (d, *J* = 9 Hz, 1H), 7.89 (d, *J* = 9 Hz, 1H), 8.65 (s, 1H), 8.66 (s, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.49 (d, *J* = 149.46 Hz, 4F), 78.76 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 109.74, 111.34, 121.75 (quintet, *J* = 3.78 Hz), 121.90, 126.84, 131.85, 132.56, 142.57, 162.75 (t, *J* = 23.94 Hz). ATR-FTIR (KBr): *v* = 3253, 2996, 1594, 1479, 1456, 114, 1120, 870, 780, 680 cm^{-1}.

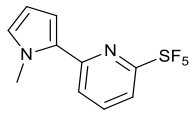
2-(3,5-dimethyl-1H-pyrrol-2-yl)-6-(pentafluoro-λ⁶-sulfaneyl)pyridine (3ab):



Following general procedure reagent **1a** (60 mg, 0.1 mmol), NaOH (6 mg, 0.15 mmol) in pyrrole **10b** (0.5 mL) were used at 80 °C for 10 h. Isolated by column chromatography on silica gel (*n*-hexane/EtOAc, 4/1) to give the desired product **3ab** as light yellow solid (29 mg) in 97% yield.

m.p.: 66.9 °C; HRMS (ESI) calcd. for $C_{11}H_{12}N_2F_5S$ [$(M)^+$]:299.0641 found 299.0644; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 2.31 (s, 3H), 2.35 (s, 3H), 5.80 (s, 1H), 7.33 (d, *J* = 6 Hz, 1H), 7.52 (d, *J* = 9 Hz, 1H), 7.77 (t, *J* = 9 Hz, 1H), 9.04 (brs, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 51.03 (d, *J* = 149.46 Hz, 4F), 78.77 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 13.22, 14.15, 112.37, 115.48 (quintet, *J* = 8.46 Hz), 120.39, 121.95, 124.32, 130.69, 138.96, 150.17, 164.97 (t, *J* = 21.42 Hz). ATR-FTIR (KBr): *v* = 3453, 2924, 1600, 1508, 1464, 850, 820, 790, 760, 720 cm^{-1}.

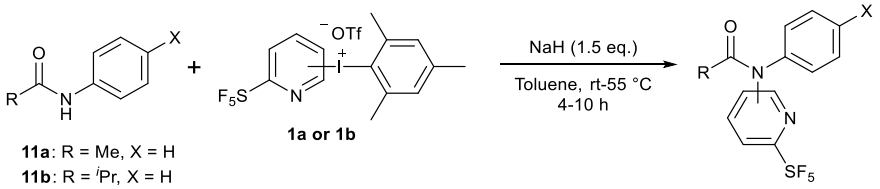
2-(1-methyl-1H-pyrrol-2-yl)-6-(pentafluoro-λ^6-sulfaneyl)pyridine (3ac):



Following general procedure reagent **1a** (60 mg, 0.1 mmol), NaOH (6 mg, 0.15 mmol) in pyrrole **10c** (0.5 mL) were used at 80 °C for 10 h. Isolated by column chromatography on silica gel (*n*-hexane/EtOAc, 4/1) to give the desired product **3ac** as white solid (12.6 mg) in 44% yield.
m.p.: 56.6 °C; HRMS (ESI) calcd. for $C_{10}H_{10}N_2F_5S$ [$(M)^+$]:285.0485 found 285.0492; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 4.03 (s, 3H), 6.19 (s, 1H), 6.76 (d, *J* = 12 Hz, 2H), 7.43 (d, *J* = 9 Hz, 1H), 7.68 (d, *J* = 9 Hz, 1H), 7.80 (t, *J* = 9 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 51.21 (d, *J* = 149.46 Hz, 4F), 78.53 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 37.74, 108.04, 112.34, 116.54 (quintet, *J* = 3.78 Hz), 122.91, 128.30, 129.61, 138.61, 151.10, 163.96 (t, *J* = 21.42 Hz). ATR-FTIR (KBr): *v* = 3111, 2958, 1595, 1542, 1486, 1451, 1181, 1090, 910, 855, 733, 680, 611 cm^{-1}.

SF_5-heteroarylation of secondary amides:

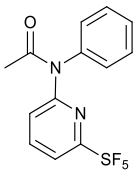
The heteroarylation of secondary amides were performed according to literature procedure.[10]



11a: R = Me, X = H
11b: R = ^{i}Pr, X = H
11c: R = Me, X = NO_2
11d: R = Ph, X = H
11e: R = Ph, X = OMe

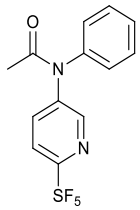
The secondary amide **11** (1.0 eq.), reagent **1a** or **1b** (1.5 eq.) and NaH (60%, 1.5 eq.) were added to a flame dried schlenk tube. The tube was evacuated and backfilled with nitrogen three times. The stirring was started and anhydrous toluene (2 mL/mmol) was added. The solution was stirred at rt–65 °C for 4–10 h. The crude reaction mixture was then transferred to a round flask using ethyl acetate. The solvent was evaporated and then the crude reaction mixture was purified using column chromatography on silica gel or preparative thin-layer plates (PLC) to yield the product **4**.

***N*-phenyl-*N*-(6-(pentafluoro-λ^6-sulfaneyl)pyridin-2-yl)acetamide (4aa):**



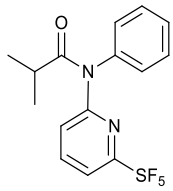
Prepared according to general procedure using amide **11a** (14 mg, 0.1 mmol), reagent **1a** (90 mg, 0.15 mmol), NaH (60%, 6.1 mg, 0.15 mmol) in toluene (2 mL) at rt for 10 h. Isolated by column chromatograaohy on silica gel (*n*-hexane/EtOAc, 7/3) to give the desired product **4aa** as yellow solid (14 mg) in 43% yield.
m.p.: 108.2 °C; HRMS (ESI) calcd. for $C_{13}H_{11}N_2OF_5NaS$ [$(M+Na)^+$]:361.0410 found 361.0414; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 2.17 (s, 3H), 7.27 (d, *J* = 9 Hz, 2H), 7.37–7.49 (m, 4H), 7.79–7.90 (m, 2H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 51.63 (d, *J* = 152.28 Hz, 4F), 77.47 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 25.14, 117.53 (quintet, J = 3.78 Hz), 122.36, 128.53, 129.15, 129.75, 140.07, 141.09, 153.00, 163.00 (t, *J* = 22.68 Hz), 171.62. ATR-FTIR (NaCl): *v* = 3067, 1694, 1589, 1441, 1371, 1295, 848, 738, 698, 595 cm^{-1}.

***N*-phenyl-*N*-(6-(pentafluoro-λ^6-sulfaneyl)pyridin-3-yl)acetamide (4ba):**



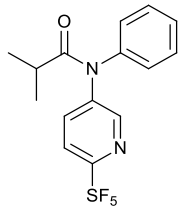
Prepared according to general procedure using amide **11a** (14 mg, 0.1 mmol), reagent **1b** (90 mg, 0.15 mmol), NaH (60%, 6.1 mg, 0.15 mmol) in toluene (2 mL) at 55 °C for 4 h. Isolated by column chromatograohy on silica gel (*n*-hexane/EtOAc, 7/3) to give the desired product **4ba** as yellow solid (15 mg) in 44% yield.
m.p.: 129.8 °C; HRMS (ESI) calcd. for $C_{13}H_{11}N_2OF_5NaS$ [(M+Na)$^+$]:361.0410 found 361.0410; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 2.09 (s, 3H), 7.26–7.31 (m, 2H), 7.44–7.56 (m, 3H), 7.69 (d, *J* = 9 Hz, 1H), 7.64 (d, *J* = 9 Hz, 1H), 8.395 (d, *J* = 3 Hz, 1H) ; ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.63 (d, *J* = 149.46 Hz, 4F), 78.20 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 24.34, 121.41, 128.87, 129.31, 130.72, 134.00, 141.29, 141.67, 143.97, 170.98. ATR-FTIR (KBr): *v* = 3120, 3071, 1440, 1380, 1299, 1255, 1190, 1151, 792, 709 cm^{-1}.

***N*-phenyl-*N*-(6-(pentafluoro-λ^6-sulfaneyl)pyridin-2-yl)isobutyramide (4ab):**



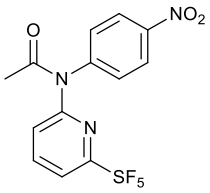
Prepared according to general procedure using amide **11b** (16 mg, 0.1 mmol), reagent **1a** (90 mg, 0.15 mmol), NaH (60%, 6.1 mg, 0.15 mmol) in toluene (2 mL) at rt for 7.5 h. Isolated by column chromatograohy on silica gel (*n*-hexane/EtOAc, 4/1) to give the desired product **4ab** as colourless oil (30 mg) in 82% yield.
HRMS (ESI) calcd. for $C_{15}H_{15}N_2OF_5NaS$ [(M+Na)$^+$]:389.0723 found 389.0730; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 1.16 (d, *J* = 6 Hz, 6H), 2.78 (quintet, *J* = 9 Hz, 1H), 7.27 (d, *J* = 6 Hz, 2H), 7.38–7.48 (m, 4H), 7.77–7.86(m, 2H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ =51.65 (d, *J* = 149.46 Hz, 4F), 77.55 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 19.71, 33.33, 117.48 (quintet, *J* = 8.46 Hz), 122.80, 128.37, 129.22, 129.64, 139.90, 140.88, 153.29, 163.07 (t, *J* = 53.58 Hz), 178.91. ATR-FTIR (NaCl): *v* = 2978, 2936, 2876, 1683, 1588, 1442, 1252, 851, 801, 597 cm^{-1}.

***N*-phenyl-*N*-(6-(pentafluoro-λ^6-sulfaneyl)pyridin-3-yl)isobutyramide (4bb):**



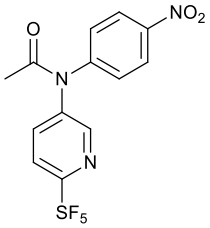
Prepared according to general procedure using amide **11b** (16.3 mg, 0.1 mmol), reagent **1b** (90 mg, 0.15 mmol), NaH (60%, 6.1 mg, 0.15 mmol) in toluene (2 mL) at 65 °C for 5 h. Isolated by using preparative thin-layer plates (PLC) (*n*-hexane/EtOAc, 4/1) to give the desired product **4bb** as yellow oil (23 mg) in 63% yield.
HRMS (ESI) calcd. for $C_{15}H_{15}N_2OF_5NaS$ [(M+Na)$^+$]:389.0723 found 389.0719; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 1.14 (t, *J* = 3 Hz, 6H), 2.61 – 2.74 (m, 1H) 7.26–7.30 (m, 2H), 7.43–7.54 (m, 3H), 7.68 (d, *J* = 9 Hz, 1H), 7.90 (d, *J* = 9 Hz, 1H), 8.32 (d, *J* = 2.7 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.63 (d, *J* =152.28 Hz, 4F), 78.26 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 19.65, 32.53, 121.29 (t, *J* = 3.78 Hz), 128.91, 129.16, 130.66, 134.36, 140.96, 142.04, 144.24, 161.08 (t, *J* = 21.42 Hz), 178.20. ATR-FTIR (NaCl): *v* = 2979, 2935, 2876, 1682, 1595, 1492, 1386, 1299, 1242, 858, 702, 598 cm^{-1}.

***N*-(4-nitrophenyl)-*N*-(6-(pentafluoro-λ^6-sulfaneyl)pyridin-2-yl)acetamide (4ac):**



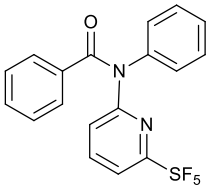
Prepared according to general procedure using amide **11c** (18 mg, 0.1 mmol), reagent **1a** (90 mg, 0.15 mmol), NaH (60%, 6.1 mg, 0.15 mmol) in toluene (2 mL) at rt for 10 h. Isolated by column chromatograohy on silica gel (*n*-hexane/EtOAc, 7/3) to give the desired product **4ac** as yellow solid (37.5 mg) in 98% yield.
m.p.: 108.2 °C; HRMS (ESI) calcd. for $C_{13}H_{10}N_3O_3F_5NaS$ [(M+Na)$^+$]:406.0261 found 406.0258; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 2.21 (s, 3H), 7.45 (d, *J* = 9 Hz, 2H), 7.59 (d, *J* = 9 Hz, 1H), 7.74 (d, *J* = 6 Hz, 1H), 7.96 (t, *J* = 9 Hz, 1H), 8.32 (d, *J* = 9 Hz, 2H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 51.86 (d, *J* = 149.46 Hz, 4F), 76.92 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 25.12, 118.61 (t, *J* = 3.78 Hz), 122.71, 125.06, 129.61, 140.85, 146.73, 147.07, 152.40, 163.22 (t, *J* = 23.94 Hz), 170.60. ATR-FTIR (KBr): *v* = 3116, 3086, 1697, 1523, 1447, 1370, 1348, 1296, 883, 807, 741 cm^{-1}.

***N*-(4-nitrophenyl)-*N*-(6-(pentafluoro-λ^6-sulfaneyl)pyridin-3-yl)acetamide (4bc):**



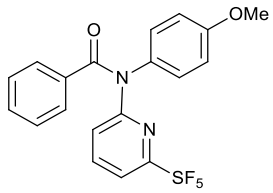
Prepared according to general procedure using amide **11c** (18 mg, 0.1 mmol), reagent **1b** (90 mg, 0.15 mmol), NaH (60%, 6.1 mg, 0.15 mmol) in toluene (2 mL) at 55 °C for 5.5 h. Isolated by using preparative thin-layer plates (PLC) (*n*-hexane/EtOAc, 7/3) to give the desired product **4bc** as yellow oil (22 mg) in 50% yield.
HRMS (ESI) calcd. for $C_{13}H_{11}N_3O_3F_5S$ [(M)$^+$]:384.0441 found 384.0438; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 2.21 (s, 3H), 7.45 (d, *J* = 9 Hz, 2H), 7.59 (d, *J* = 9 Hz, 1H), 7.74 (d, *J* = 6 Hz, 1H), 7.96 (t, *J* = 9 Hz, 1H), 8.32 (d, *J* = 9 Hz, 2H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 51.88 (d, *J* = 152.28 Hz, 4F), 76.94 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 24.18, 122.17, 125.68, 128.94, 131.04, 141.07, 146.91, 169.76. IR (NaCl): *v* = 2357, 1652, 1507, 1456, 1260, 900, 820, 513 cm^{-1}.

***N*-phenyl-*N*-(6-(pentafluoro-λ^6-sulfaneyl)pyridin-2-yl)benzamide (4ad):**



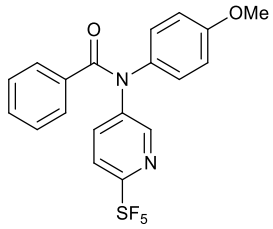
Prepared according to general procedure using amide **11d** (20 mg, 0.1 mmol), reagent **1a** (90 mg, 0.15 mmol), NaH (60%, 6.1 mg, 0.15 mmol) in toluene (2 mL) at rt for 10 h. Isolated by column chromatograohy on silica gel (*n*-hexane/EtOAc, 7/3) to give the desired product **4ad** as white solid (28 mg) in 70% yield.
m.p.: 119.5 °C; HRMS (ESI) calcd. for $C_{18}H_{13}N_2OF_5NaS$ [(M+Na)$^+$]: 423.0566 found 423.0556; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 7.18–7.38 (m, 8H), 7.44–7.50 (m, 4H), 7.85 (t, *J* = 6 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 51.74 (d, *J* = 160.74 Hz, 4F), 77.18 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 117.77 (t, *J* = 3.78 Hz), 122.82, 127.64, 128.18, 128.37, 129.56, 130.84, 135.77, 140.07, 141.80, 154.50, 163.28 (t, *J* = 23.94 Hz), 171.62. ATR-FTIR (KBr): *v* = 3102, 3074, 1682, 1655, 1586, 1445, 1306, 1269, 867, 835 cm^{-1}.

***N*-(4-methoxyphenyl)-*N*-(6-(pentafluoro-λ^6-sulfaneyl)pyridin-2-yl)benzamide (4ae):**



Prepared according to general procedure using amide **11e** (23 mg, 0.1 mmol), reagent **1a** (90 mg, 0.15 mmol), NaH (60%, 6.1 mg, 0.15 mmol) in toluene (2 mL) at rt for 10 h. Isolated by column chromatograohy on silica gel (*n*-hexane/EtOAc, 7/3) to give the desired product **4ae** as yellow solid (22.3 mg) in 52% yield.
m.p.: 121.5 °C; HRMS (ESI) calcd. for $C_{19}H_{16}N_2O_2F_5NaS$ [(M+Na)$^+$]: 454.0750 found 453.0672; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 3.80 (s, 3H), 6.86 (d, *J* = 9 Hz, 2H), 7.12 (d, *J* = 9 Hz, 2H), 7.22–7.32 (m, 4H), 7.44–7.50 (m, 4H), 7.84 (t, *J* = 6 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 51.72 (d, *J* = 149.46 Hz, 4F), 77.26 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 54.57, 113.79, 116.57 (t, *J* = 3.78 Hz), 121.57, 127.17, 127.88, 128.63, 129.69, 133.47, 134.93, 138.98, 153.63, 157.86, 162.24 (t, *J* = 23.94 Hz), 170.71. ATR-FTIR (KBr): *v* = 2962, 1410, 1377, 1311, 1266, 1140, 1106, 1004, 953, 781 cm^{-1}.

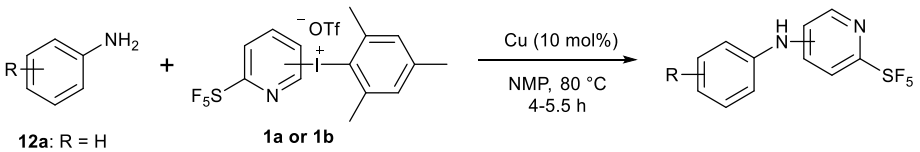
***N*-(4-methoxyphenyl)-*N*-(6-(pentafluoro-λ^6-sulfaneyl)pyridin-3-yl)benzamide (4be):**



Prepared according to general procedure using amide **11e** (23 mg, 0.1 mmol), reagent **1b** (90 mg, 0.15 mmol), NaH (60%, 6.1 mg, 0.15 mmol) in toluene (2 mL) at 55 °C for 5.5 h. Isolated by column chromatograohy on silica gel (*n*-hexane/EtOAc, 7/3) to give the desired product **4be** as yellow oil (11.8 mg) in 30% yield.
HRMS (ESI) calcd. for $C_{19}H_{15}N_2O_2F_5NaS$ [(M+Na)$^+$]: 453.0672 found 453.0672; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 3.78 (s, 3H), 6.83 (d, *J* = 9 Hz, 2H), 7.01 (d, *J* = 9 Hz, 2H), 7.23–7.37 (m, 3H), 7.44 (d, *J* = 6 Hz, 2H), 7.69–7.78 (m, 2H), 8.385 (d, *J* = 3 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.72 (d, *J* = 149.46 Hz, 4F), 78.24 (quintet, *J* = 152.28 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 55.57, 114.79, 117.57 (t, *J* = 3.78 Hz), 122.57, 128.17, 128.88, 129.63, 130.69, 134.47, 135.93, 139.98, 154.63, 158.86, 163.24 (t, *J* = 23.94 Hz), 171.72. ATR-FTIR (NaCl): *v* = 3063, 2936, 2841, 1681, 1578, 1506, 1470, 1287, 1031, 874 cm^{-1}.

SF_5-heteroarylation of amines:

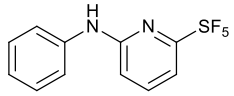
The heteroarylation of amines were performed according to literature procedure.[11]



12a: R = H
12b: R = 4-Br
12c: R = 3,5-OMe
12d: R = 2-Br

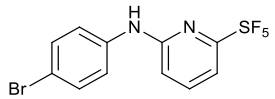
To a flame dried test tube, Cu (0) powder (10 mol %), NMP (2.0 mL/mmol aniline) and aniline **12** (1.0 eq.) were added and the resulting mixture was stirred at room temperature for 10 min under nitrogen. To the mixture, reagent **1a** or **1b** (1.1 eq.) was added in one portion and the mixture was then stirred at 80 °C. After completion of the reaction, the mixture was cooled to room temperature, filtered through a pad of silica and the residue was rinsed with Et_2O. The filtrate was concentrated *in vacuo*. The crude product was purified by column chromatography on silica gel to give the desired product **5**.

***N*-phenyl-6-(pentafluoro-λ^6-sulfaneyl)pyridin-2-amine (5aa):**



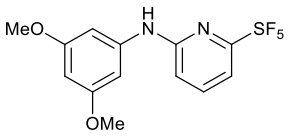
Prepared according to the general procedure using aniline **12a** (18.2 μL, 0.2 mmol), Cu (0) powder (1.2 mg, 0.02 mmol) and reagent **1a** (132mg, 0.22 mmol) in NMP (0.4 mL) at 80 °C for 5.5 h. Isolated by column chromatography (*n*-hexane/EtOAc, 7/3) to give the desired product **5aa** as green solid (44 mg) in 74% yield.
m.p.: 58.0 °C; HRMS (ESI) calcd. for $C_{11}H_{10}N_2F_5S$ [$(M)^+$]: 297.0485 found 297.0485; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 6.68 (brs, 1H), 6.92 (d, *J* = 9 Hz, 1H), 7.12 (d, *J* = 6 Hz, 2H), 7.36–7.38 (m, 4H), 7.64 (t, *J* = 9 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 51.40 (d, *J* = 149.46 Hz, 4F), 79.01 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 111.05, 111.27 (quintet, *J* = 3.78 Hz), 120.70, 124.01, 129.60, 139.29, 139.78, 154.38, 164.14 (t, *J* = 22.68 Hz). ATR-FTIR (KBr): *v* = 3116, 3086, 1697, 1586, 1523, 1434, 1296, 883, 807, 741 cm^{-1}.

***N*-(4-bromophenyl)-6-(pentafluoro-λ^6-sulfaneyl)pyridin-2-amine (5ab):**



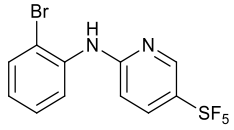
Prepared according to the general procedure using aniline **12b** (34 mg, 0.2 mmol), Cu (0) powder (1.2 mg, 0.02 mmol) and reagent **1a** (132mg, 0.22 mmol) in NMP (0.4 mL) at 80 °C for 4 h. Isolated by column chromatography (*n*-hexane/EtOAc, 7/3) to give the desired product **5ab** as white solid (42 mg) in 56% yield.
m.p.: 127.6 °C; HRMS (ESI) calcd. for $C_{11}H_9N_2F_5SBr$ [$(M)^+$]: 374.9590 found 374.9592; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 6.63 (brs, 1H), 6.87 (d, *J* = 9 Hz, 1H), 7.15 (d, *J* = 9 Hz, 1H), 7.35 (d, *J* = 9 Hz, 2H), 7.46 (d, *J* = 9 Hz, 2H), 7.67 (t, *J* = 9 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 51.43 (d, *J* = 149.46 Hz, 4F), 78.75 (quintet, *J* = 152.28 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 111.74 (quintet, *J* = 3.78 Hz), 116.05, 121.63, 132.45, 138.49, 139.87, 153.66, 163.95 (t, *J* = 21.42 Hz). ATR-FTIR (KBr): *v* = 3454, 1611, 1517, 1491, 1473, 845, 825, 810, 795, 781 cm^{-1}.

***N*-(3,5-dimethoxyphenyl)-6-(pentafluoro-λ^6-sulfaneyl)pyridin-2-amine (5ac):**



Prepared according to the general procedure using aniline **12c** (30 mg, 0.2 mmol), Cu (0) powder (1.2 mg, 0.02 mmol) and reagent **1a** (132mg, 0.22 mmol) in NMP (0.4 mL) at 80 °C for 4 h. Isolated by column chromatography (*n*-hexane/EtOAc, 3/2) to give the desired product **5ac** as white solid (40 mg) in 56% yield.
m.p.: 90.9 °C; HRMS (ESI) calcd. for $C_{13}H_{14}N_2O_2F_5S$ [$(M)^+$]: 357.0696 found 357.0699; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 3.80 (s, 6H), 6.23 (t, *J* = 3 Hz, 1H), 6.65 (brs, 1H), 6.73 (d, *J* = 2.1 Hz, 2H), 6.91 (d, *J* = 8.1 Hz, 1H), 7.14 (d, *J* = 7.8 Hz, 1H), 7.66 (t, *J* = 8.1 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 51.42 (d, *J* = 149.46 Hz, 4F), 79.00 (quintet, *J* = 146.64 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 55.51, 95.95, 97.96, 111.42 (t, *J* = 3.78 Hz), 112.24, 139.67, 141.27, 153.86, 161.49, 163.91 (t, *J* = 22.68 Hz). ATR-FTIR (KBr): *v* = 3359, 3000, 2968, 2918, 2848, 1621, 1593, 1484, 1457, 1208, 1148, 1062, 855, 835, 787 cm^{-1}.

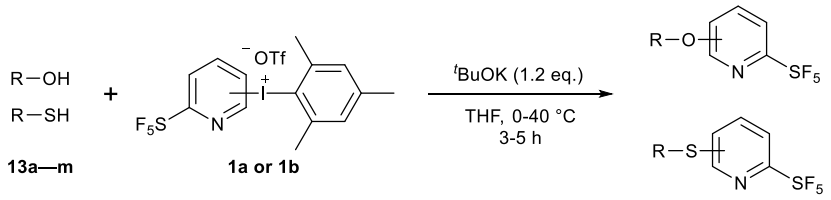
***N*-(2-bromophenyl)-6-(pentafluoro-λ^6-sulfaneyl)pyridin-2-amine (5bd):**



Prepared according to the general procedure using aniline **12d** (34.4 mg, 0.2 mmol), Cu (0) powder (1.2 mg, 0.02 mmol) and reagent **1b** (132mg, 0.22 mmol) in NMP (0.4 mL) at 80 °C for 5 h. Isolated by column chromatography (*n*-hexane/EtOAc, 9/1) to give the desired product **5bd** as white solid (21.3 mg) in 57% yield.
m.p.: 72.8 °C; HRMS (ESI) calcd. for $C_{11}H_9N_2F_5SBr$ [$(M)^+$]: 374.9590 found 374.9590; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 6.26 (brs, 1H), 6.95–7.01 (m, 1H), 7.26–7.40 (m, 2H), 7.48 (d, *J* = 6 Hz, 1H), 7.64 (t, *J* = 9 Hz, 2H), 8.27 (d, *J* = 6 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 51.39 (d, *J* = 149.46 Hz, 4F), 79.35 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 115.92, 119.89, 122.23 (quintet, *J* = 5.04 Hz), 123.74, 125.03, 128.64, 130.80, 136.24 (t, *J* = 1.26 Hz), 138.11, 141.95, 198.06 (quintet, *J* = 22.68 Hz). ATR-FTIR (KBr): *v* = 3394, 1586, 1576, 1507, 1461, 1323, 1121, 1026, 760, 741 cm^{-1}.

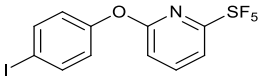
SF_5-heteroarylation of phenols, alcohols and thiol:

The heteroarylation of phenols, alcohols and thiol were performed according to literature procedure.[7a]



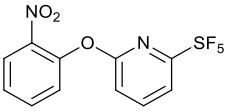
To a suspension of ^{t}BuOK (1.2 eq.) in THF (0.3 mL/mmol), was added the phenol/alcohol/thiol **13** (1.0 eq.) at 0 °C and the reaction mixture was stirred at this temperature for 10 minutes. The reagent **1a** or **1b** (1.2 eq.) was added in one portion and the reaction was stirred in a preheated oil bath at 40 °C till completion. The reaction was quenched by water at 0 °C. The organic phase was separated and the aqueous phase was extracted with dichloromethane (10 mL X 3). The combined organic phases were dried over anhydrous Na_2SO_4, filtered and the solvent was concentrated under reduced pressure. The crude product was isolated by column chromatography over silica gel (*n*-hexane/EtOAc) to give the desired product **6**.

2-(4-iodophenoxy)-6-(pentafluoro-λ^6-sulfaneyl)pyridine (6aa):



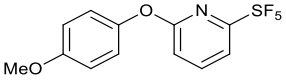
Prepared according to the general procedure using ^{t}BuOK (13.5 mg, 0.12 mmol), phenol **13a** (22 mg, 0.1 mmol) and reagent **1a** (72 mg, 0.12 mmol) in THF (0.3 mL) at 80 °C for 4 h. Isolated using column chromatography over silica gel (*n*-hexane/EtOAc, 9/1) to give the desired product **6aa** as white solid (39.2 mg) in 92% yield.
m.p.: 46.3 °C; HRMS (EI) calcd. for $C_{11}H_7NOF_5SI$ [$(M)^+$]:422.9213 found 422.9240; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 6.98 (d, *J* = 9 Hz, 2H), 7.07 (d, *J* = 9 Hz, 1H), 7.45 (d, *J* = 9 Hz, 1H), 7.70 (d, *J* = 9 Hz, 2H), 7.89 (t, *J* = 9 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.22 (d, *J* = 152.28 Hz, 4F), 77.53 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 89.02, 114.79, 115.80 (quintet, *J* = 3.78 Hz), 123.20, 138.75, 141.75, 153.12, 160.75, 162.81 (quintet, *J* = 22.68 Hz). ATR-FTIR (KBr): *v* = 3519, 3164, 2953, 1381, 1260, 1244, 1146, 1110, 1060, 922, 778 cm^{-1}.

2-(2-nitrophenoxy)-6-(pentafluoro-λ^6-sulfaneyl)pyridine (6ab):



Prepared according to the general procedure using ^{t}BuOK (13.5 mg, 0.12 mmol), phenol **13b** (14 mg, 0.1 mmol) and reagent **1a** (72 mg, 0.12 mmol) in THF (0.3 mL) at 80 °C for 5 h. Isolated using column chromatography over silica gel (*n*-hexane/EtOAc, 9/1) to give the desired product **6ab** as a white solid (28.4 mg) in 83% yield.
m.p.: 76.6 °C; HRMS (ESI) calcd. for $C_{11}H_7N_2O_3F_5NaS$ [$(M+Na)^+$]:364.9995 found 364.9998; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 7.25 (d, *J* = 6 Hz, 1H), 7.37–7.47 (m, 3H), 7.66–7.72 (m, 1H), 7.95 (t, *J* = 9 Hz, 1H) 8.12 (dd, *J* = 6 Hz, 3 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.29 (d, *J* = 149.46 Hz, 4F), 77.23 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 114.85, 116.15 (quintet, *J* = 3.78 Hz), 125.26, 125.93, 126.35, 134.84, 142.02, 142.39, 145.93, 160.20, 162.47 (quintet, *J* = 22.68 Hz). ATR-FTIR (KBr): *v* = 3442, 3110, 2865, 1979, 1713, 1594, 1446, 1349, 1264, 809 cm^{-1}.

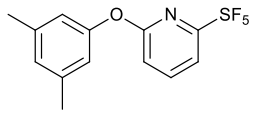
2-(4-methoxyphenoxy)-6-(pentafluoro-λ^6-sulfaneyl)pyridine (6ac):



Prepared according to the general procedure using ^{t}BuOK (13.5 mg, 0.12 mmol), phenol **13c** (9.4 mg, 0.1 mmol) and reagent **1a** (72 mg, 0.12 mmol) in THF (0.3 mL) at 80 °C for 4.5 h. Isolated using column chromatography over silica gel (*n*-hexane/EtOAc, 9/1) to give the desired product **6ac** as a colorless oil (20.8 mg) in 82% yield.
HRMS (ESI) calcd. for $C_{12}H_{10}NO_2F_5S$ [$(M)^+$]:350.0250 found 350.0236; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 3.83 (s, 3H), 6.91–6.99 (m, 3H), 7.11 (d, *J* = 9 Hz, 2H), 7.40 (d, *J* = 9 Hz, 1H), 7.83 (t, *J* = 9 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.11 (d, *J* = 149.46 Hz, 4F), 77.81 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 55.72, 113.85, 114.83, 115.11 (quintet, *J* = 3.78 Hz),

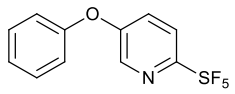
122.14, 141.48, 146.69, 157.09, 162.03, 163.07 (quintet, *J* = 22.68 Hz). ATR-FTIR (NaCl): *v* = 3711, 2975, 1505, 1439, 1246, 1207, 1173, 1029, 834, 795 cm^{-1}.

2-(3,5-dimethylphenoxy)-6-(pentafluoro-λ⁶-sulfaneyl)pyridine (6ad):



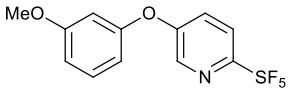
Prepared according to the general procedure using ^{t}BuOK (13.5 mg, 0.12 mmol), phenol **11d** (12 mg, 0.1 mmol) and reagent **1a** (72 mg, 0.12 mmol) in THF (0.3 mL) at 80 °C for 4 h. Isolated using column chromatography over silica gel (*n*-hexane/EtOAc, 9/1) to give the desired product **6ad** as a white solid (20 mg) in 62% yield.
m.p.: 44.7 °C; HRMS (ESI) calcd. for $C_{13}H_{12}NOF_5NaS$ [$(M+Na)^+$]:348.0457 found 348.0459; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 2.32 (s, 6H), 6.80 (s, 2H), 6.87 (s, 1H), 6.95 (d, *J* = 9 Hz, 1H), 7.41 (d, *J* = 9 Hz, 1H), 7.83 (t, *J* = 9, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.14 (d, *J* = 152.28 Hz, 4F), 77.78 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 21.26, 113.58, 115.08 (quintet, *J* = 3.78 Hz), 118.35, 127.03, 139.66, 141.33, 153.16, 161.67, 162.98 (quintet, *J* = 23.94 Hz). FTIR (KBr): *v* = 3668, 3018, 2920, 1982, 1742, 1587, 1445, 1274, 1026, 777 cm^{-1}.

5-phenoxy-2-(pentafluoro-λ⁶-sulfaneyl)pyridine (6be):



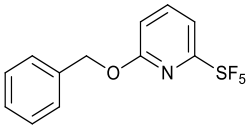
Prepared according to the general procedure using ^{t}BuOK (13.5 mg, 0.12 mmol), phenol **13e** (9.4 mg, 0.1 mmol) and reagent **1b** (72 mg, 0.12 mmol) in THF (0.3 mL) at 80 °C for 4.5 h. Isolated using column chromatography over silica gel (*n*-hexane/EtOAc, 9/1) to give the desired product **6be** as a colourless oil (20.8 mg) in 70% yield.
HRMS (ESI) calcd. for $C_{11}H_9NOF_5S$ [$(M)^+$]:298.0325 found 298.0322; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 7.09 (d, *J* = 9 Hz, 2H), 7.26 (t, *J* = 6 Hz, 1H), 7.40 (d, *J* = 9 Hz, 1H), 7.44 (t, *J* = 9 Hz, 2H), 7.69 (d, *J* = 9 Hz, 1H), 8.27 (d, *J* = 3 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 53.35 (d, *J* = 149.46 Hz, 4F), 78.90 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 120.17, 122.59 (quintet, *J* = 3.78 Hz), 125.66, 125.77, 130.62, 137.89, 154.70, 156.57, 159.28 (t, *J* = 23.94 Hz). ATR-FTIR (NaCl): *v* = 3665, 3067, 1574, 1491, 1464, 1286, 1262, 1241, 840, 758 cm^{-1}.

5-(3-methoxyphenoxy)-2-(pentafluoro-λ⁶-sulfaneyl)pyridine (6bf):



Prepared according to the general procedure using ^{t}BuOK (13.5 mg, 0.12 mmol), phenol **13f** (11 μL, 0.1 mmol) and reagent **1b** (72 mg, 0.12 mmol) in THF (0.3 mL) at 80 °C for 3 h. Isolated using column chromatography over silica gel (*n*-hexane/EtOAc, 9/1) to give the desired product **6bf** as a yellow solid (11.4 mg) in 31% yield.
m.p.: 31.6 °C; HRMS (ESI) calcd. for $C_{12}H_{11}NO_2F_5S$ [$(M)^+$]:328.0431 found 328.0436; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 3.81 (s, 3H), 6.65 (d, *J* = 3 Hz, 2H), 6.80 (d, *J* = 9 Hz, 1H), 7.30–7.39 (m, 2H), 7.69 (d, *J* = 9 Hz, 1H), 8.28 (s, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 53.35 (d, *J* = 149.46 Hz, 4F), 78.89 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 55.67, 106.23, 111.32, 112.03, 122.58 (t, *J* = 3.78 Hz), 125.82, 131.03, 137.99, 155.79, 156.41, 159.35 (t, *J* = 23.94 Hz), 161.51. ATR-FTIR (KBr): *v* = 3649, 3057, 2946, 2844, 1609, 1573, 1490, 1464, 1283, 1238, 1141, 846 cm^{-1}.

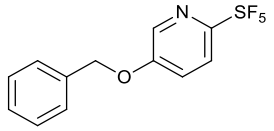
2-(benzyloxy)-6-(pentafluoro-λ⁶-sulfaneyl)pyridine (6ag):



Prepared according to the general procedure using ^{t}BuOK (13.5 mg, 0.12 mmol), alcohol **13g** (10 μL, 0.1 mmol) and reagent **1a** (72 mg, 0.12 mmol) in THF (0.3 mL) at 80 °C for 3 h. Isolated using column chromatography over silica gel (*n*-hexane/EtOAc, 9/1) to give the desired product **6ag** as white solid (22.5 mg) in 72% yield.
m.p.: 82.8 °C; HRMS (ESI) calcd. for $C_{12}H_{10}NOF_5NaS$ [$(M+Na)^+$]:334.0301 found 334.0308; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 5.39 (s, 2H), 6.94 (d, *J* = 9 Hz, 1H), 7.29–7.40 (m, 4H), 7.49 (d, *J* = 6 Hz, 2H), 7.74 (t, *J* = 9 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.12 (d, *J* = 149.46 Hz, 4F), 78.60 (quintet, *J* = 152.28 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 68.81, 113.84 (quintet, *J* = 3.78

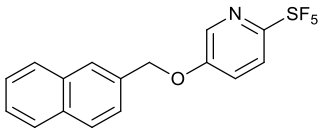
Hz), 114.86, 128.40, 128.62, 128.94, 136.36, 140.54, 161.61, 162.75 (quintet, *J* = 21.42 Hz). ATR-FTIR (KBr): *v* = 3645, 3031, 2946, 2589, 1982, 1600, 1447, 1277, 998, 845 cm^{-1}.

5-(benzyloxy)-2-(pentafluoro-λ⁶-sulfaneyl)pyridine (6bg):



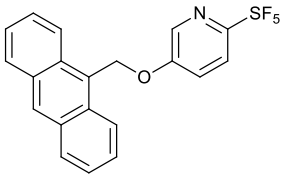
Prepared according to the general procedure using ^{t}BuOK (13.5 mg, 0.12 mmol), alcohol **13g** (10 μL, 0.1 mmol) and reagent **1b** (72 mg, 0.12 mmol) in THF (0.3 mL) at 80 °C for 3 h. Isolated using column chromatography over silica gel (*n*-hexane/EtOAc, 9/1) to give the desired product **6bg** as white solid (22 mg) in 70% yield.
m.p.: 76.9 °C; HRMS (ESI) calcd. for $C_{12}H_{11}NOF_5S$ [$(M)^+$]:312.0482 found 312.0482; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 5.18 (s, 2H), 7.37–7.43 (m, 6H), 7.68 (d, *J* = 9 Hz, 1H), 8.265 (d, *J* = 3 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 53.49 (d, *J* = 149.46 Hz, 4F), 79.43 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 71.08, 122.45 (quintet, *J* = 3.78 Hz), 123.14, 127.69, 128.90, 129.07, 135.12, 135.69, 156.72, 158.28 (t, *J* = 22.68 Hz). ATR-FTIR (KBr): *v* = 3649, 2748, 2558, 1574, 1467, 1393, 1278, 1120, 1016, 838 cm^{-1}.

5-(naphthalen-2-ylmethoxy)-2-(pentafluoro-λ⁶-sulfaneyl)pyridine (6bh):



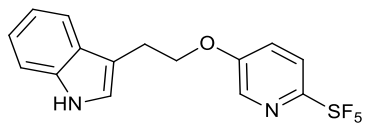
Prepared according to the general procedure using ^{t}BuOK (13.5 mg, 0.12 mmol), alcohol **13h** (16 mg, 0.1 mmol) and reagent **1b** (72 mg, 0.12 mmol) in THF (0.3 mL) at 80 °C for 3 h. Isolated using column chromatography over silica gel (*n*-hexane/EtOAc, 9/1) to give the desired product **6bh** as white solid (14.6 mg) in 40% yield.
m.p.: 92.8 °C; HRMS (ESI) calcd. for $C_{16}H_{13}NOF_5S$ [$(M)^+$]:362.0638 found 362.0635; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 5.34 (s, 2H), 7.41 (d, *J* = 6 Hz, 1H), 7.52 (d, *J* = 3 Hz, 3H), 7.68 (d, *J* = 9 Hz, 1H), 7.89 (d, *J* = 9 Hz, 4H), 8.31 (s, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 53.52 (d, *J* = 149.46 Hz, 4F), 79.43 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 71.25, 112.48 (quintet, *J* = 3.78 Hz), 123.23, 125.01, 126.75, 126.78, 126.91, 127.96, 128.11, 129.06, 132.52, 133.32, 133.43, 135.75, 156.73, 158.32 (t, *J* = 23.94 Hz). ATR-FTIR (KBr): *v* = 3755, 3649, 2937, 2311, 1576, 1465, 1306, 875, 835, 820 cm^{-1}.

5-(anthracen-9-ylmethoxy)-2-(pentafluoro-λ⁶-sulfaneyl)pyridine (6bi):



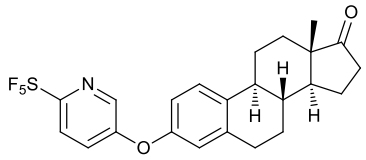
Prepared according to the general procedure using ^{t}BuOK (13.5 mg, 0.12 mmol), alcohol **13i** (21 mg, 0.1 mmol) and reagent **1b** (72 mg, 0.12 mmol) in THF (0.3 mL) at 80 °C for 3 h. Isolated using column chromatography over silica gel (*n*-hexane/EtOAc, 9/1) to give the desired product **6bi** as yellow solid (15 mg) in 36% yield.
m.p.: 144.1 °C; HRMS (ESI) calcd. for $C_{20}H_{14}NOF_5NaS$ [$(M + Na)^+$]:434.0614 found 434.0616; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 6.10 (s, 2H), 7.52–7.60 (m, 5H), 7.75 (d, *J* = 9 Hz, 1H), 8.05 (d, *J* = 9 Hz, 2H), 8.21 (d, *J* = 9 Hz, 2H), 8.40 (s, 1H), 8.57 (s, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 53.55 (d, *J* = 141 Hz, 4F), 79.43 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 63.96, 122.61 (t, *J* = 3.78 Hz), 123.22, 123.42, 124.88, 125.40, 127.29, 129.54, 130.04, 131.09, 131.52, 135.51, 157.12, 158.47 (t, *J* = 22.68 Hz). ATR-FTIR (KBr): *v* = 3648, 3045, 2966, 2311, 1573, 1462, 1291, 1242, 837, 822 cm^{-1}.

3-(2-((6-(pentafluoro-λ⁶-sulfaneyl)pyridin-3-yl)oxy)ethyl)-1*H*-indole (6bj):



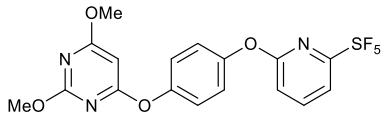
Prepared according to the general procedure using ^{t}BuOK (13.5 mg, 0.12 mmol), alcohol **13j** (16 mg, 0.1 mmol) and reagent **1b** (72 mg, 0.12 mmol) in THF (0.3 mL) at 80 °C for 5 h. Isolated using column chromatography over silica gel (*n*-hexane/EtOAc, 4/1) to give the desired product **6bj** as yellow oil (20 mg) in 56% yield.
HRMS (ESI) calcd. for $C_{15}H_{14}N_2OF_5S$ [$(M)^+$]:365.0747 found 365.0754; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 3.28 (t, *J* = 6 Hz, 2H), 4.29 (t, *J* = 6 Hz, 2H), 7.08 (s, 1H), 7.12–7.19 (m, 1H), 7.22–7.25 (m, 1H), 7.35 (d, d, *J* = 9 Hz, 1H), 7.61 (d, *J* = 3 Hz, 1H), 7.64 (s, 1H), 8.12 (brs, 1H), 8.16 (d, *J* = 2.7 Hz); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 53.68 (d, *J* = 149.46 Hz, 4F), 79.82 (quintet, *J* = 146.64 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 25.28, 69.36, 111.47, 111.50, 118.68, 119.72, 122.31–122.40 (m), 122.49, 122.57, 127.36, 135.39, 136.31, 157.01, 157.94 (quintet, *J* = 23.75 Hz). ATR-FTIR (NaCl): *v* = 3687, 3414, 3298, 3058, 2928, 1577, 1459, 1249, 862, 743 cm^{-1}.

(8*R*,9*S*,13*S*,14*S*)-13-methyl-3-((6-(pentafluoro-λ^6-sulfaneyl)pyridin-3-yl)oxy)-7,8,9,11,12,13,15,16-octahydro-6*H*-cyclopenta[*a*]phenanthren-17(14*H*)-one (6bk):



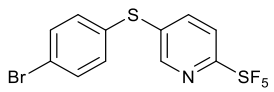
Prepared according to the general procedure using ^{t}BuOK (13.5 mg, 0.12 mmol), phenol **13k** (27 mg, 0.1 mmol) and reagent **1b** (72 mg, 0.12 mmol) in THF (0.3 mL) at 80 °C for 5 h. Isolated using column chromatography over silica gel (*n*-hexane/EtOAc, 4/1) to give the desired product **6bk** as white solid (33 mg) in 70% yield.
m.p.: 158.0 – 164.3 °C; HRMS (ESI) calcd. for $C_{23}H_{24}NO_2F_5S$ [$(M)^+$]:496.1346 found 496.1345; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 0.94 (s, 3H), 1.55–1.65 (m, 6H), 1.98–2.11 (m, 3H), 2.17–2.22 (m, 1H), 2.32 (s, 1H), 2.41–2.57 (m, 2H), 2.915 (d, *J* = 3 Hz, 2H), 6.83 (s, 1H), 6.87 (d, *J* = 6 Hz, 1H), 7.34 (d, *J* = 6 Hz, 2H), 7.67 (d, *J* = 9 Hz, 1H), 8.26 (s, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 53.39 (d, *J* = 149.46 Hz, 4F), 79.09 (quintet, *J* = 149.46 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 13.96, 21.71, 25.94, 26.40, 29.99, 31.65, 35.96, 38.16, 44.24, 48.06, 50.51, 117.41, 120.16, 122.43–122.52 (m), 125.45, 127.48, 137.40, 137.73, 139.34, 152.51, 156.77, 159.07 (quintet, *J* = 23.94 Hz). ATR-FTIR (KBr): *v* = 3649, 2933, 2881, 2372, 2311, 1736, 1492, 1462, 1288, 1246, 846, 823 cm^{-1}.

2,4-dimethoxy-6-(4-((6-(pentafluoro- λ^6-sulfaneyl)pyridin-2-yl)oxy)phenoxy)pyrimidine (6al):



Prepared according to the general procedure using ^{t}BuOK (67.3 mg, 0.6 mmol), phenol **13l** (124 mg, 0.5 mmol) and reagent **1b** (360 mg, 0.6 mmol) in THF (45 mL) at 65 °C for 5 h. Isolated using column chromatography over silica gel (*n*-hexane/EtOAc, 3/2) to give the desired product **6al** as white solid (226 mg) in 70% yield.
m.p.: 40.5 °C; HRMS (EI) calcd. for $C_{17}H_{14}N_3O_4F_5S$ [$(M)^+$]: 451.0625 found 451.0622; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 3.36 (s, 3H), 3.90 (s, 3H), 5.78 (s, 1H), 7.09–7.13 (m, 3H), 7.18–7.23 (m, 2H), 7.26–7.28 (m, 1H), 7.67 (dd, *J* = 9 Hz, 3 Hz, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 63.37 (d, *J* = 155.1 Hz, 4F), 76.56(quintet, *J* = 152.28 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 54.44, 55.02, 84.61, 115.57, 119.93, 121.59, 123.48, 123.63, 150.10, 151.16, 157.95 (quintet, *J* = 18.9 Hz), 159.65, 165.19, 172.12, 173.60. ATR-FTIR (KBr): *v* = 3699, 3150, 1725, 1581, 1476, 1450, 984, 845, 803 cm^{-1}.

5-((4-bromophenyl)thio)-2-(pentafluoro- λ^6-sulfaneyl)pyridine (6bm)



Prepared according to the general procedure using ^{t}BuOK (13.5 mg, 0.12 mmol), thiol **13m** (27 mg, 0.1 mmol) and reagent **1b** (72 mg, 0.12 mmol) in THF (0.3 mL) at 40 °C for 5 h. Isolated using column chromatography over silica gel (*n*-hexane/EtOAc, 3/2) to give the desired product **6bm** as pale yellow solid (23 mg) in 74% yield.
m.p.: 63.3 °C; HRMS (EI) calcd. for $C_{11}H_7NF_5S_2Br$ [$(M)^+$]: 390.9123 found 390.9128; ^{1}H NMR ($CDCl_3$, 300 MHz) δ = 7.36–7.40 (m, 2H), 7.55–7.59 (m, 4H), 8.31 (s, 1H); ^{19}F NMR ($CDCl_3$, 282 MHz) δ = 52.61 (d, *J* = 152.28 Hz, 4F), 78.03 (quintet, *J* = 146.64 Hz, 1F); ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 121.56–121.68, 124.33, 129.60, 133.47, 135.63, 137.17, 139.70, 146.21, 162.84–163.57. ATR-FTIR (KBr): *v* = 2963, 1558, 1471, 1452, 1354, 1261, 1085, 1008, 811, 745, 598 cm^{-1}.

Reference:

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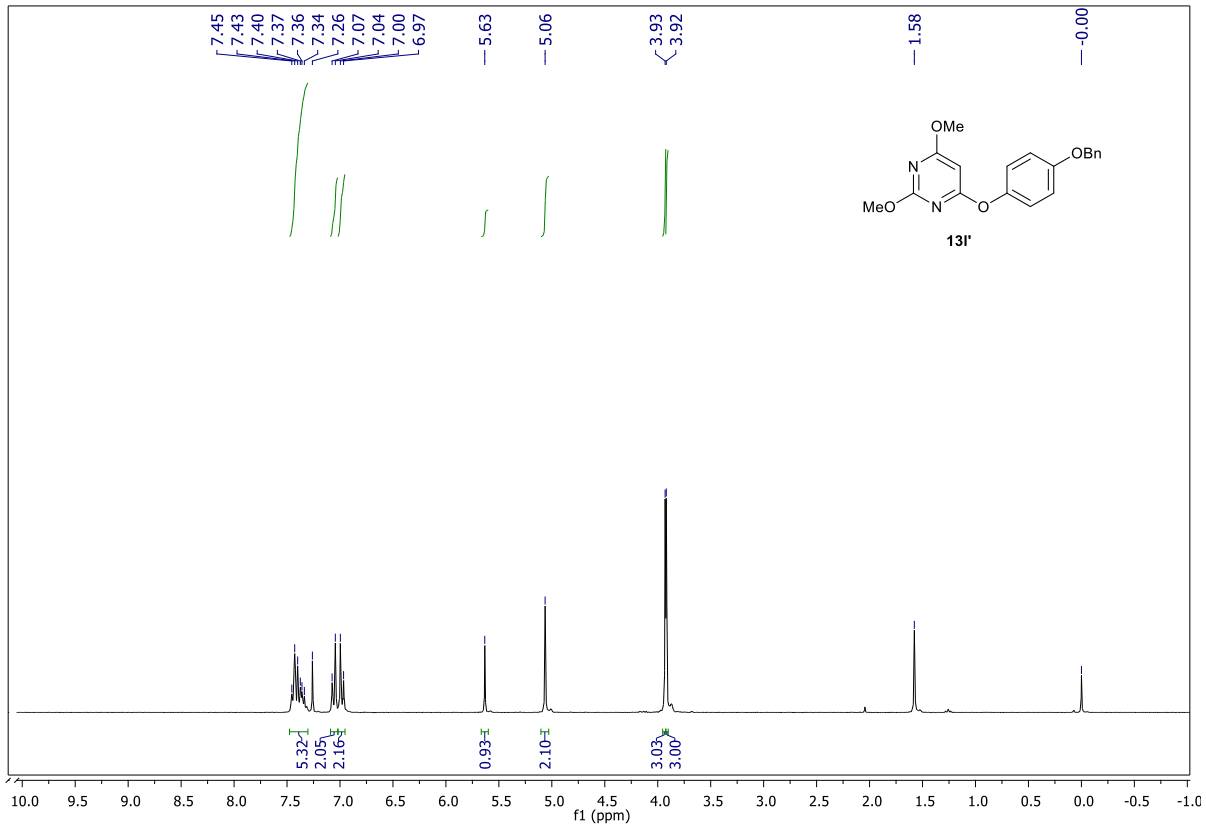
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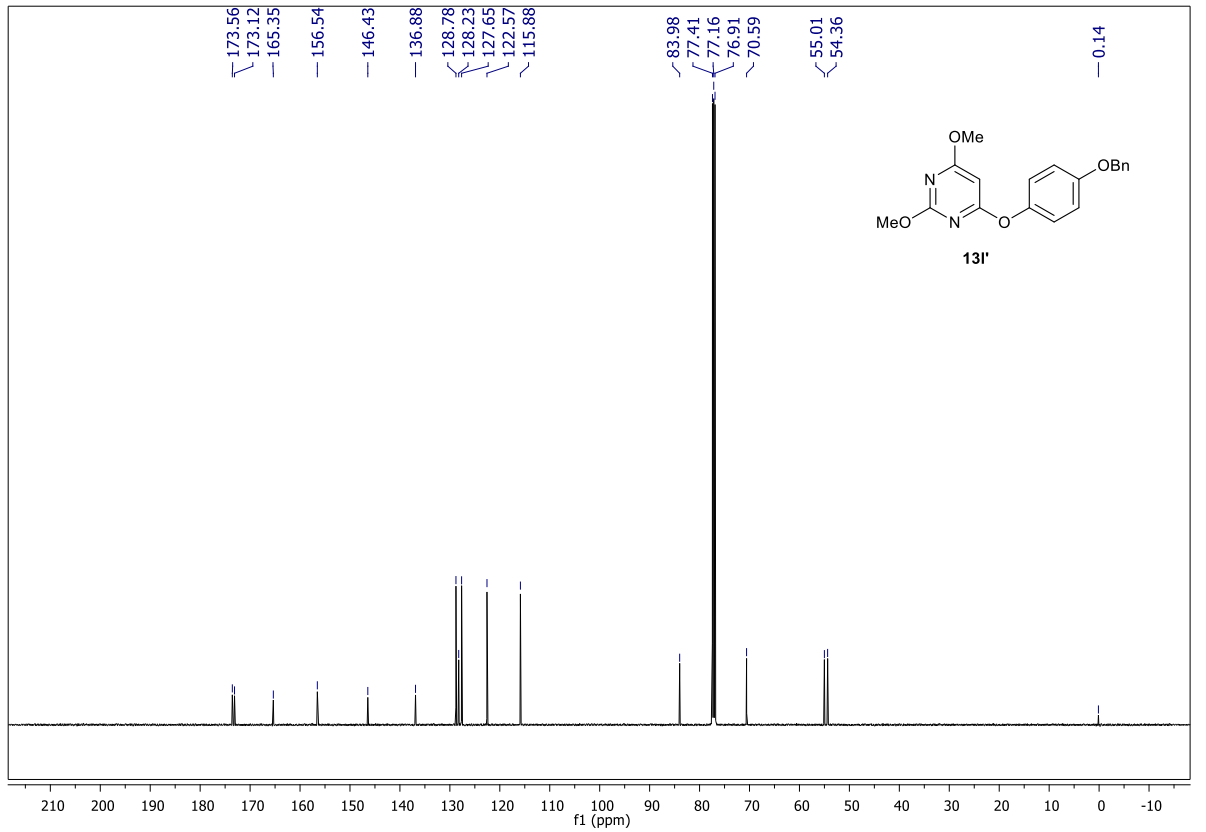
7.43
7.40
7.37
7.36
7.34
7.26
7.07
7.04
7.00
6.97
5.63
5.06
3.93
3.92
1.58
-0.00
OMe
OBn
N
MeO
N
O
13l'
5.32
2.05
2.16
0.93
2.10
3.03
3.00
f1 (ppm)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122.57
115.88
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77.41
77.16
76.91
70.59
55.01
54.36
0.14
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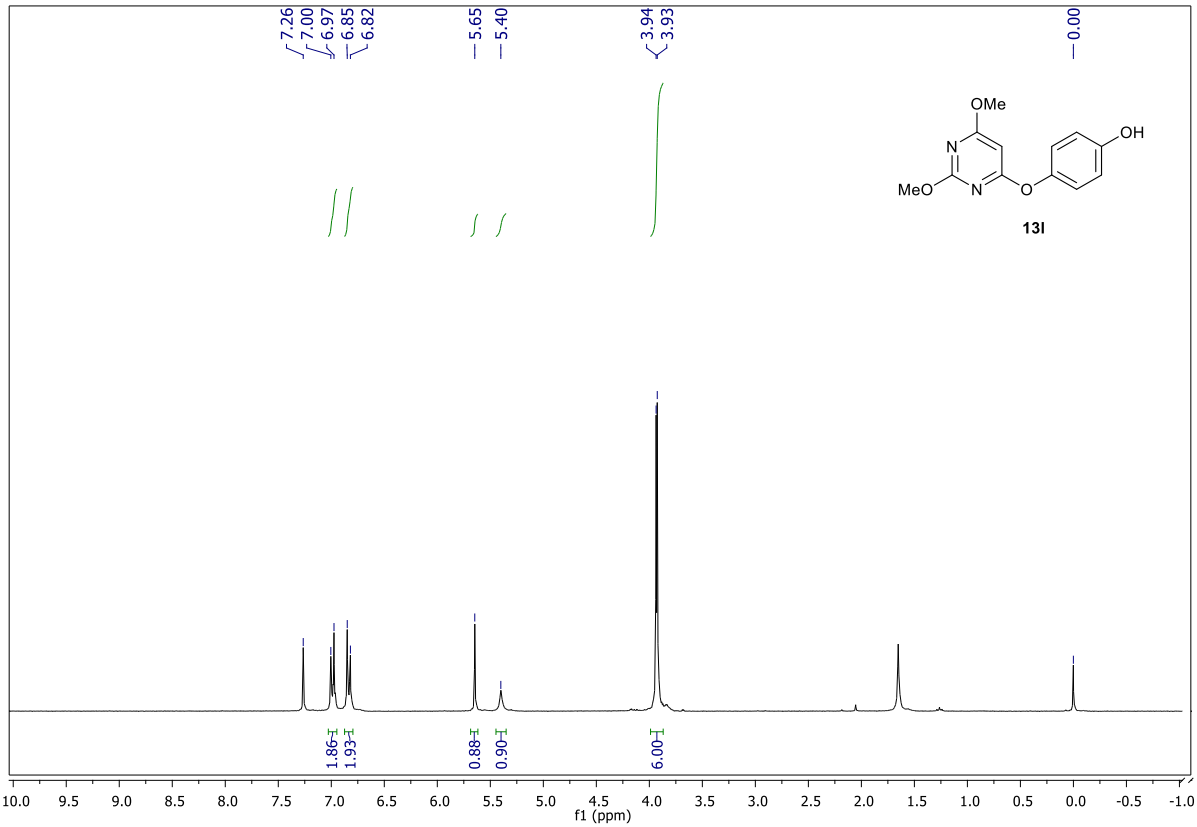
OBn
N
MeO
N
O
13l'
f1 (ppm)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O
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13l
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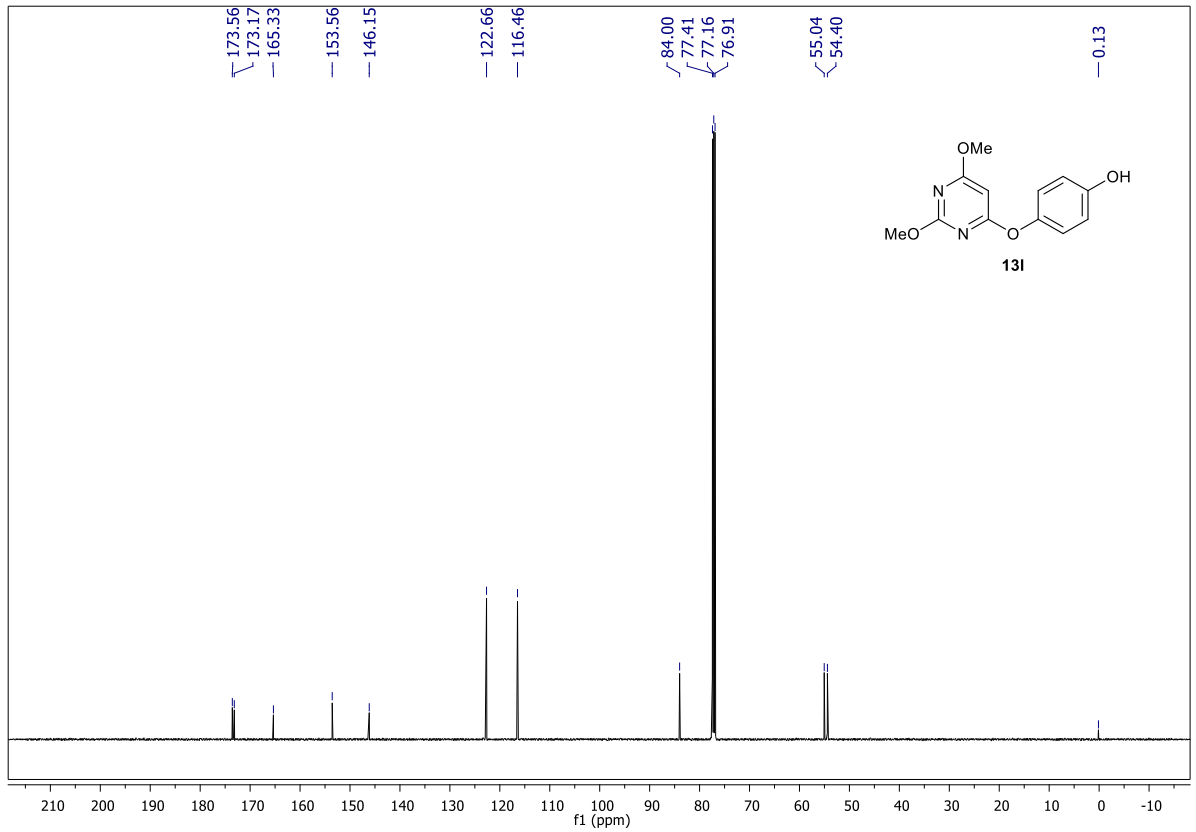
f1 (ppm)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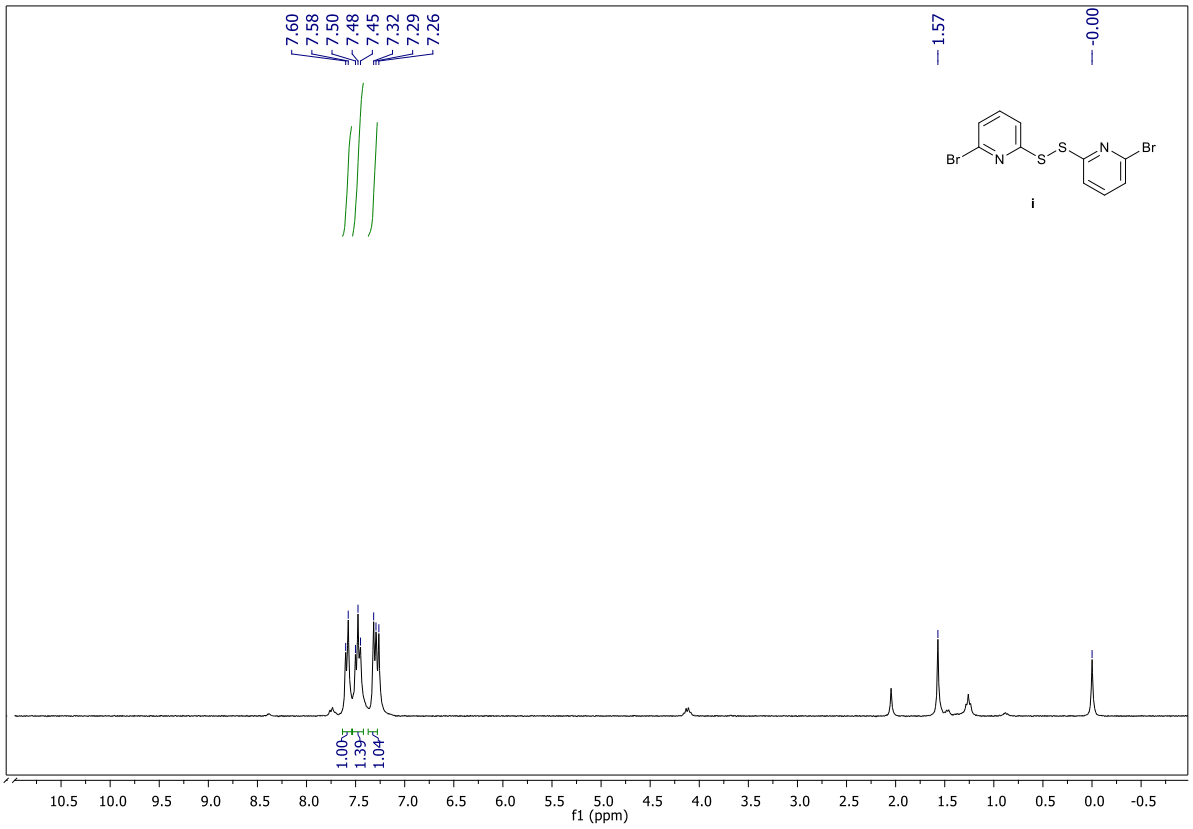
N
O
OH
13l
f1 (ppm)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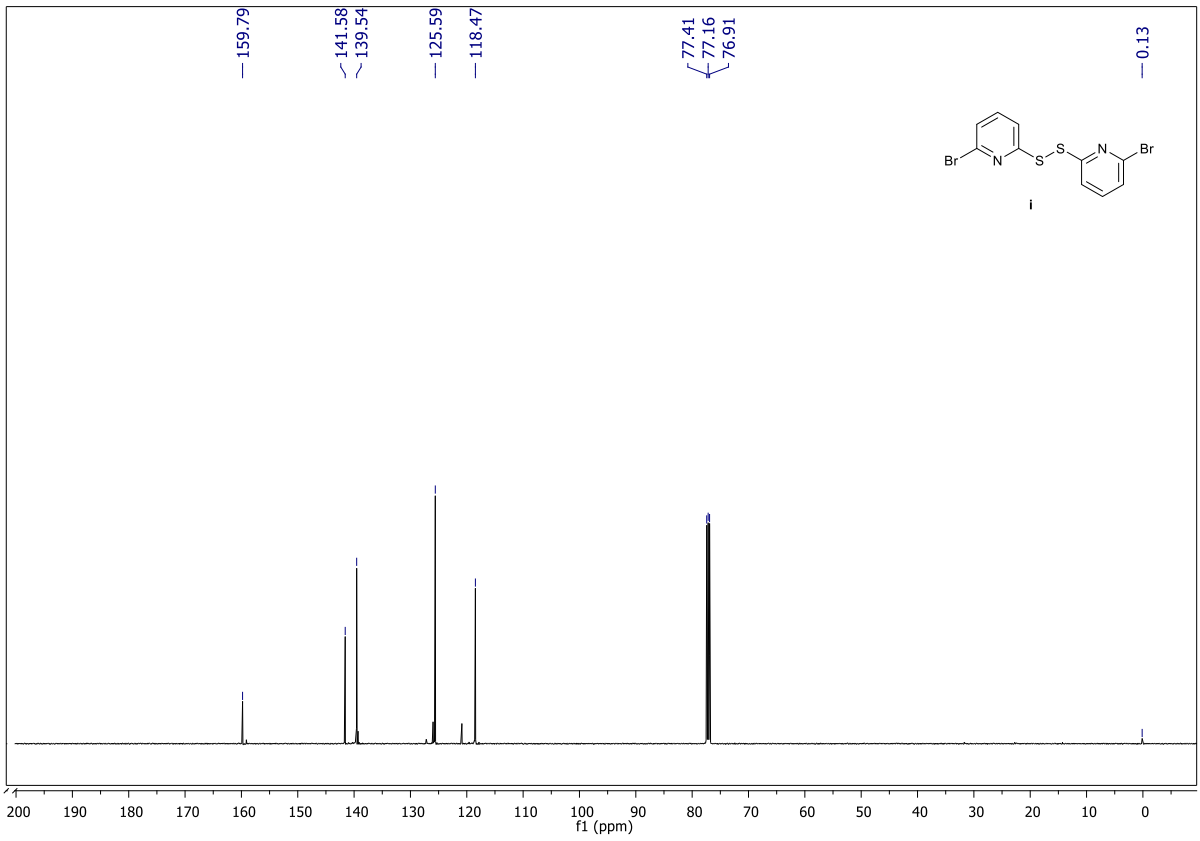
N
S
S
N
Br
i
1.00
1.39
1.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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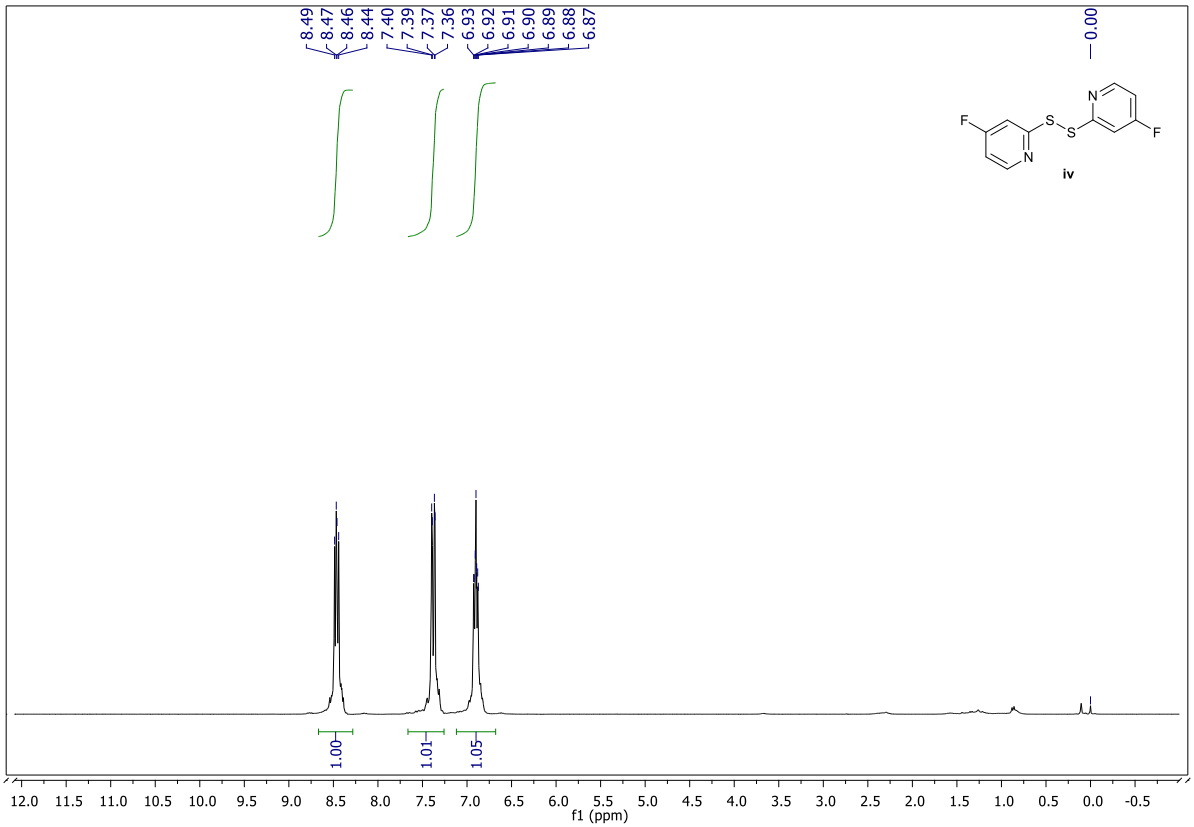
f1 (ppm)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6.92
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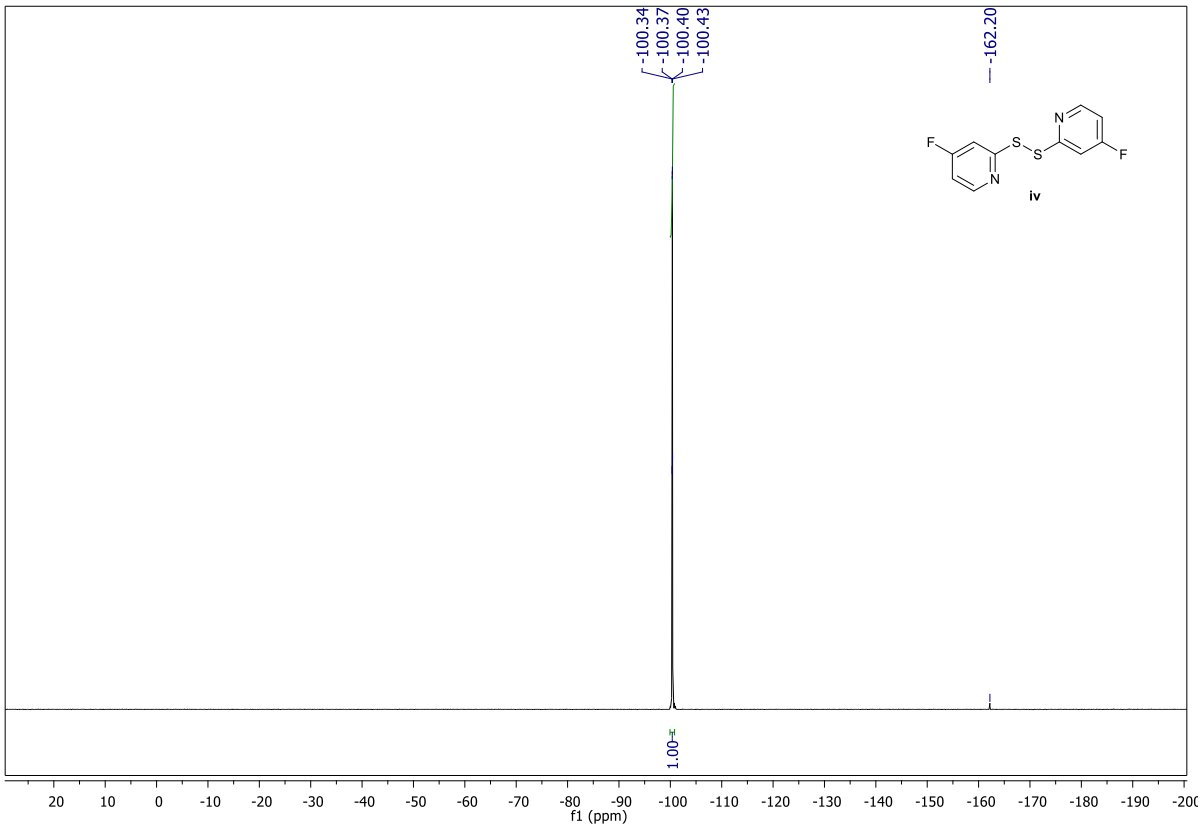
6.89
6.88
6.87
0.00
F
S
S
N
N
F
iv
1.00
1.01
1.05
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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-100.40
-100.43
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F
S
S
N
N
F
iv
1.00
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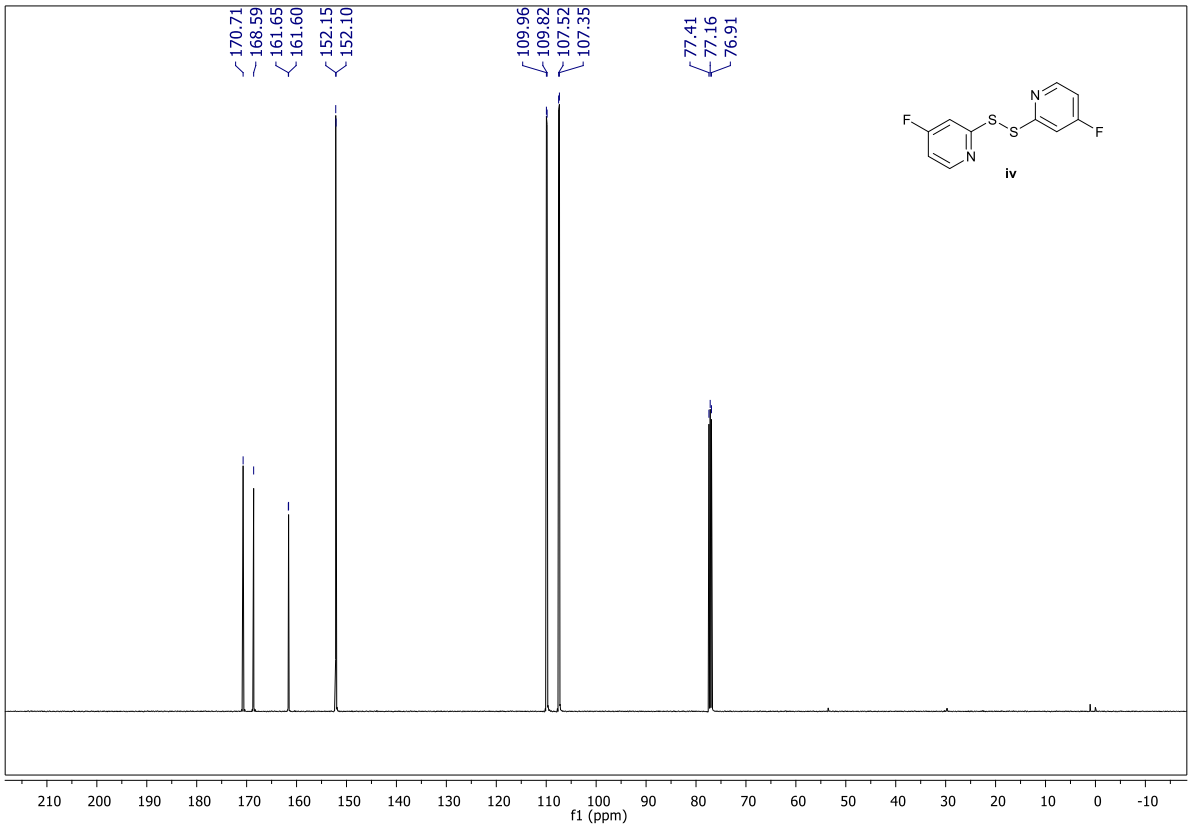
f1 (ppm)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152.10
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109.82
107.52
107.35
77.41
77.16
76.91
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S
S
N
N
F
iv
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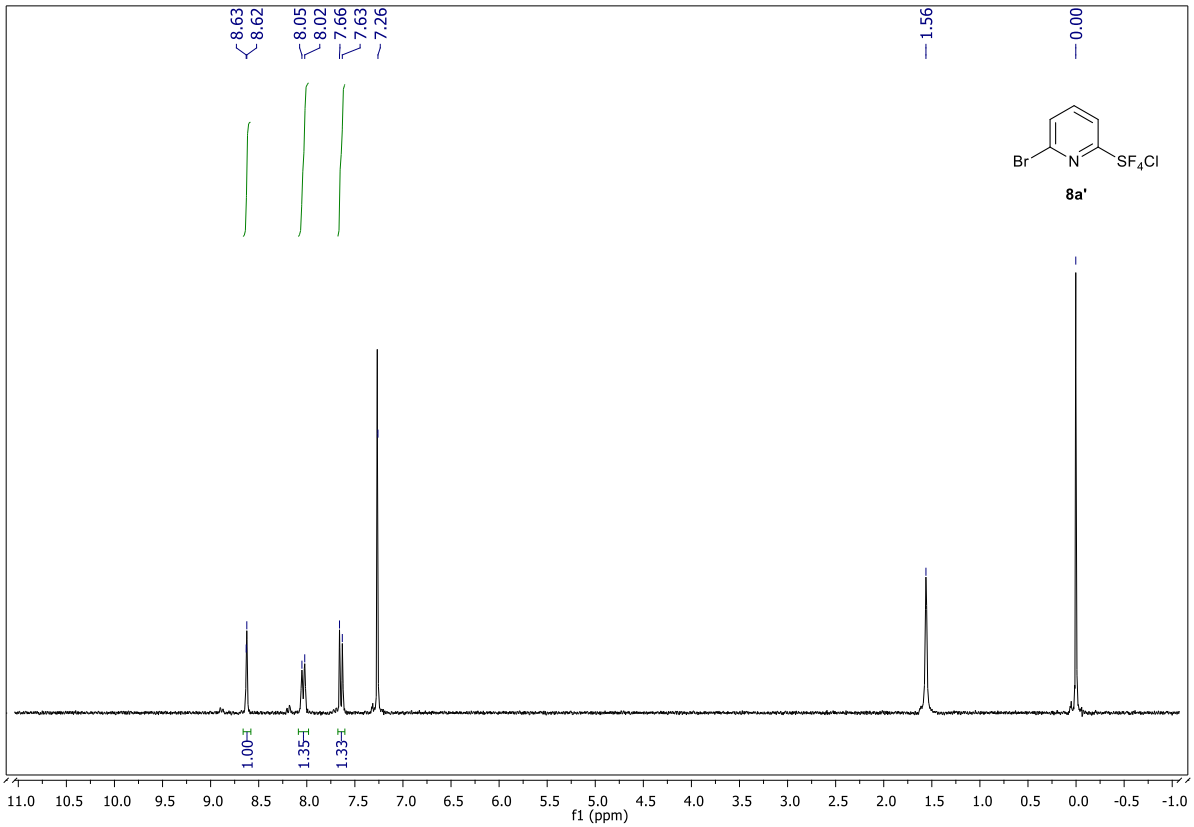
f1 (ppm)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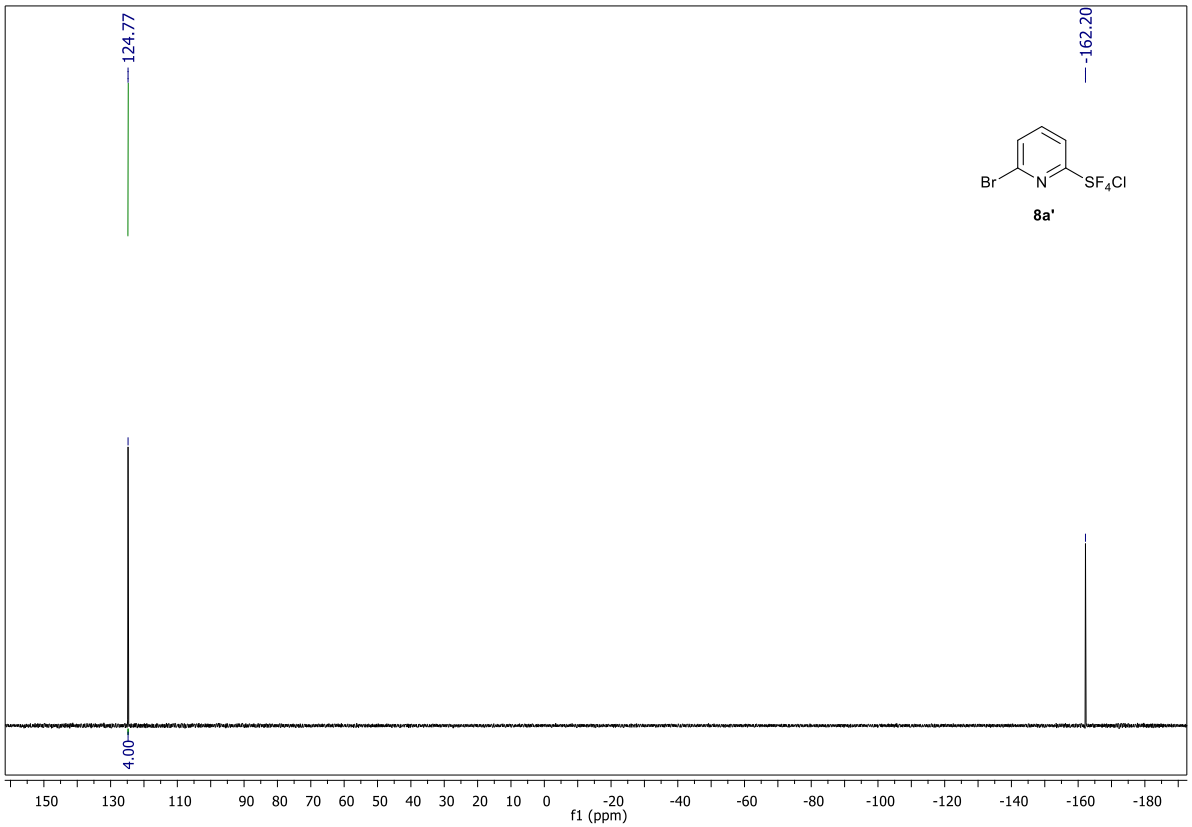
Br
N
SF4Cl
8a'
1.00
1.35
1.33
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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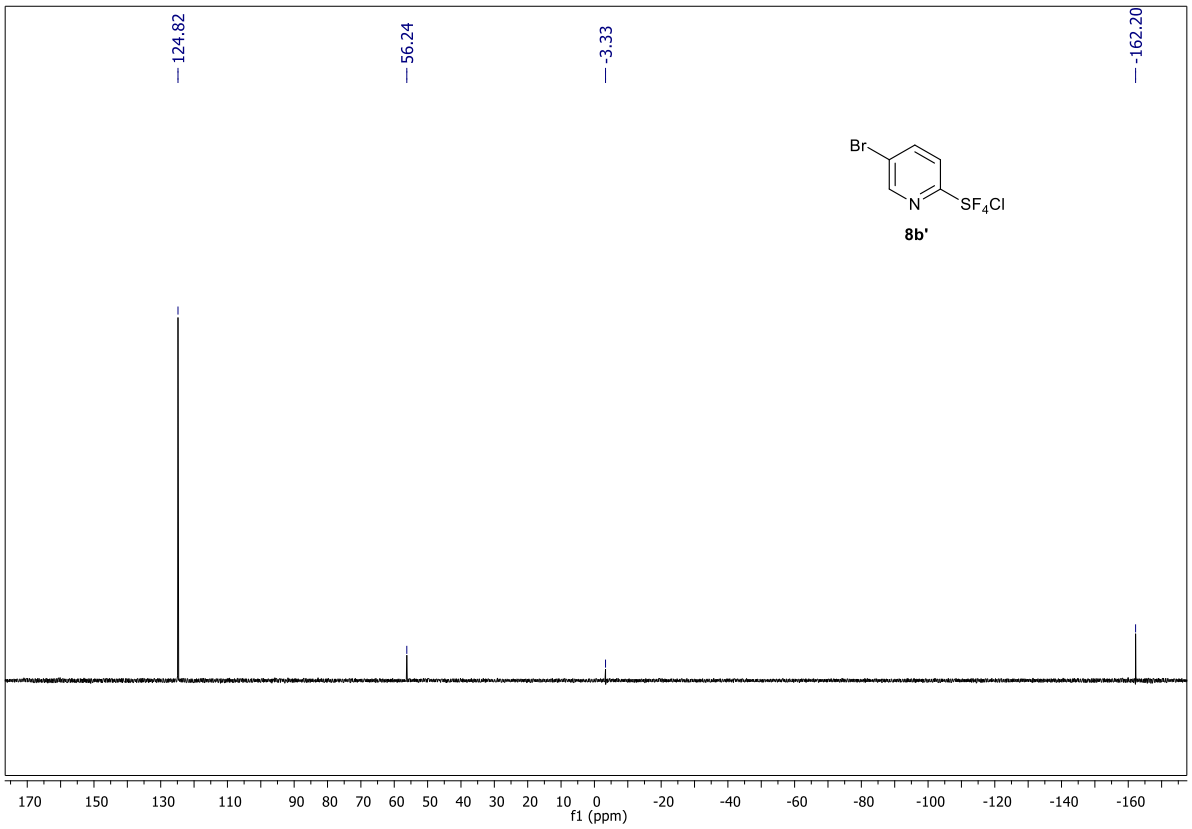
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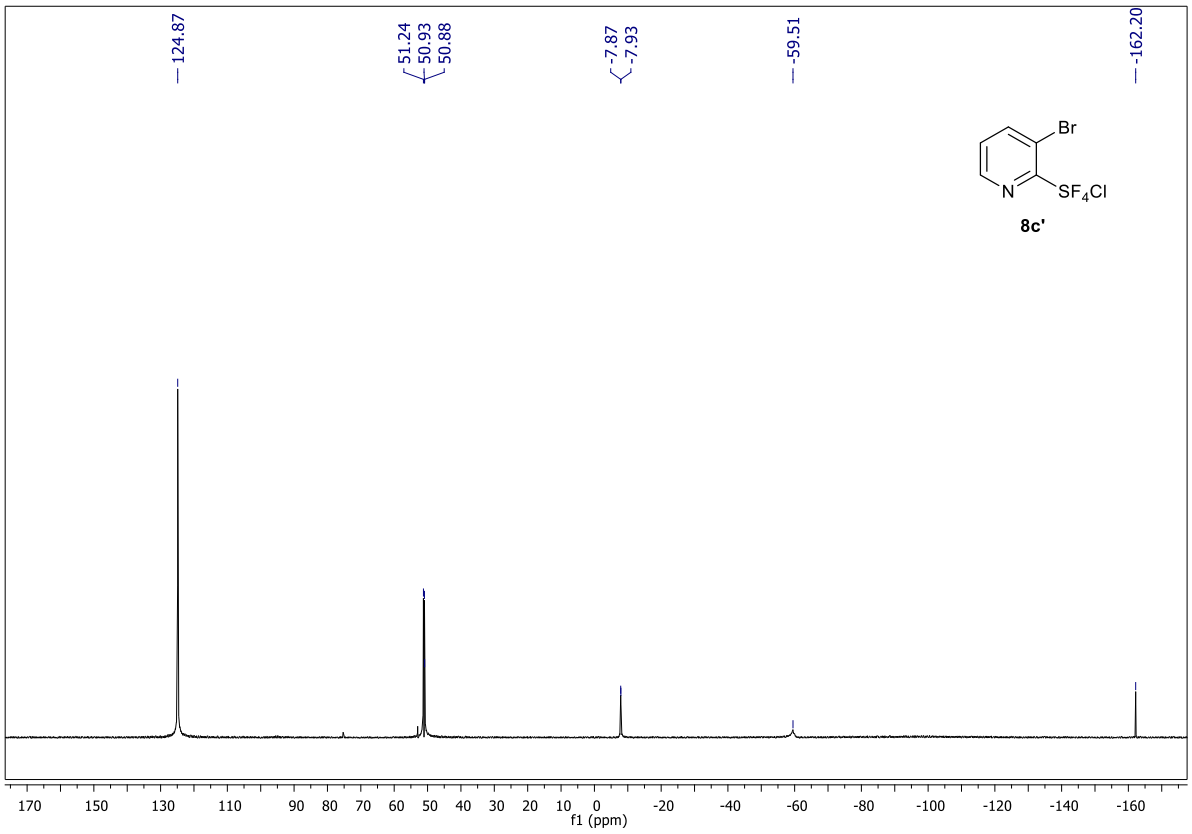
f1 (ppm)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SF4Cl
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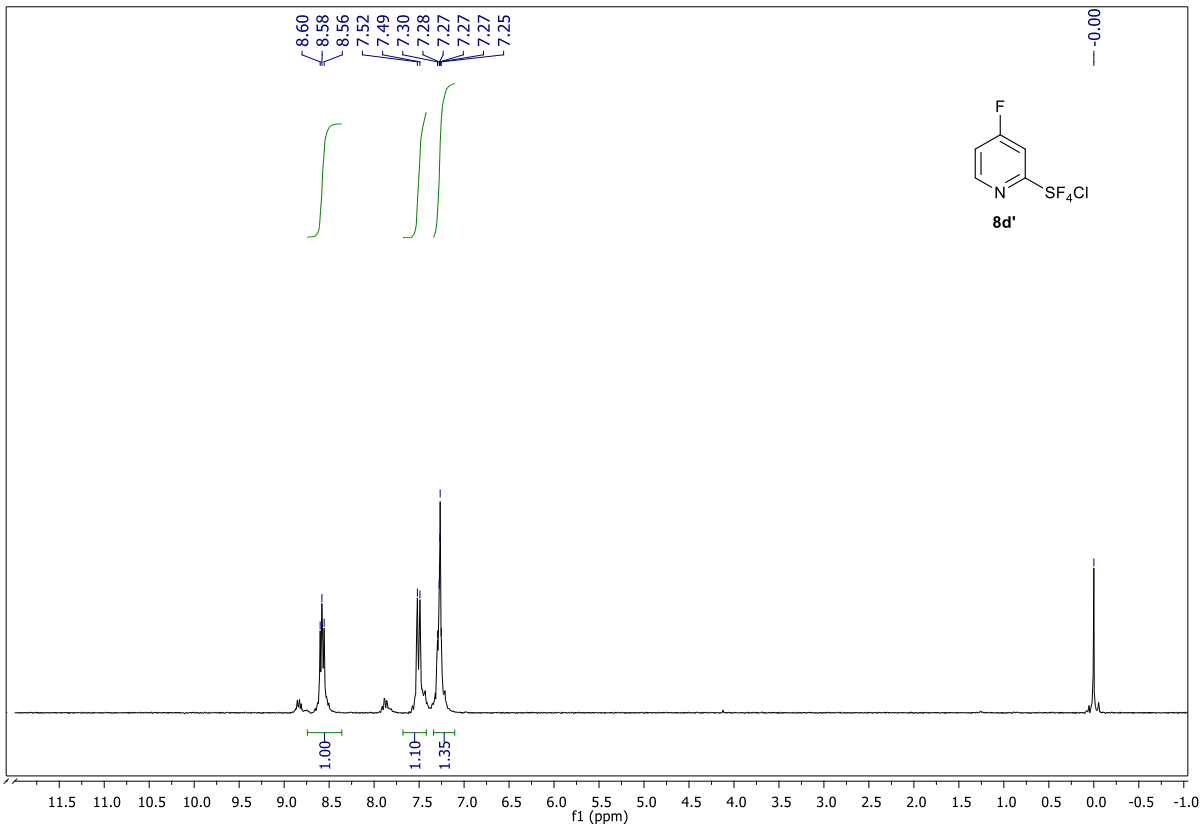
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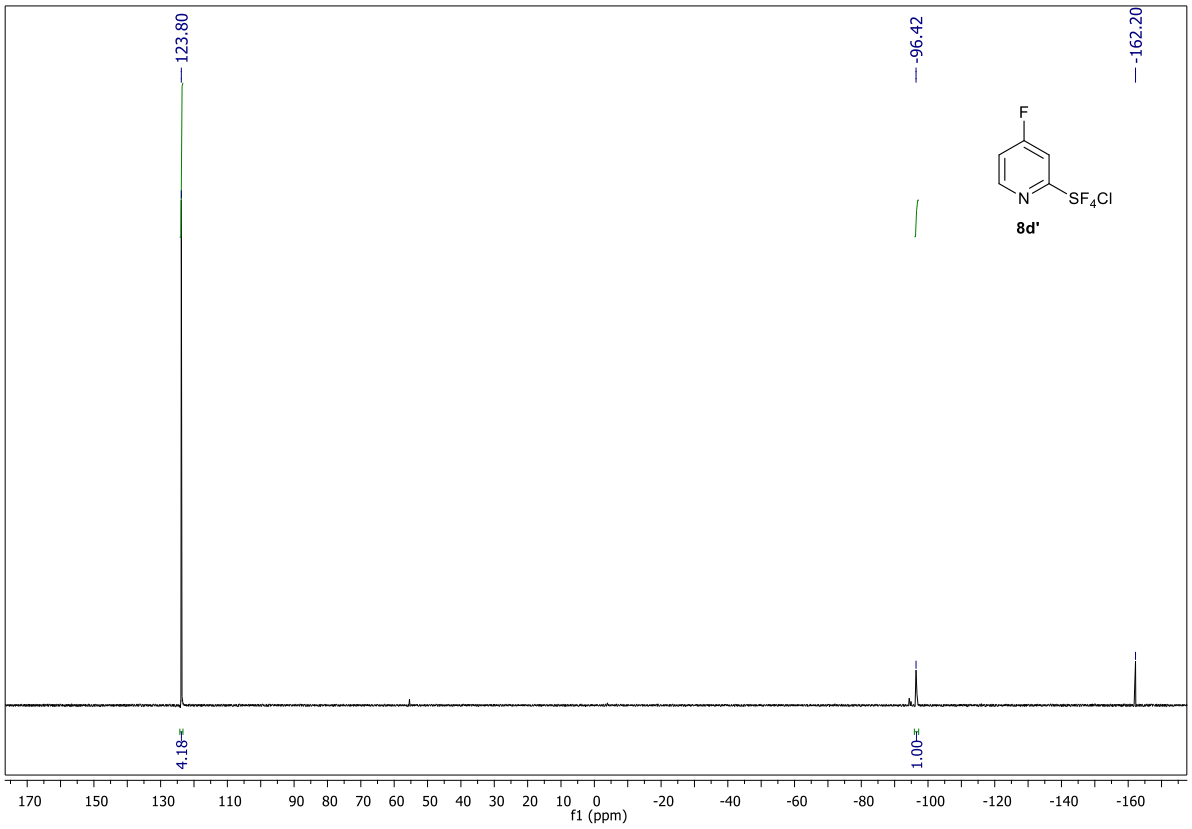
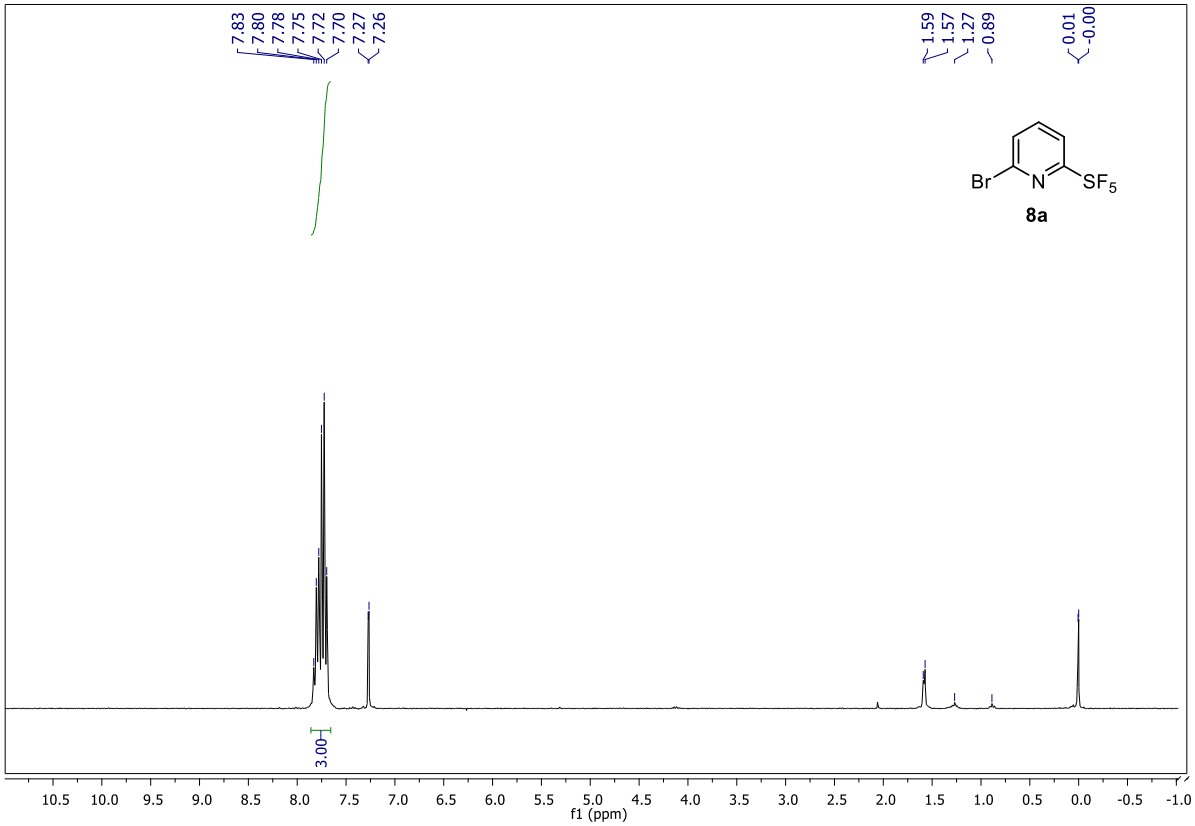
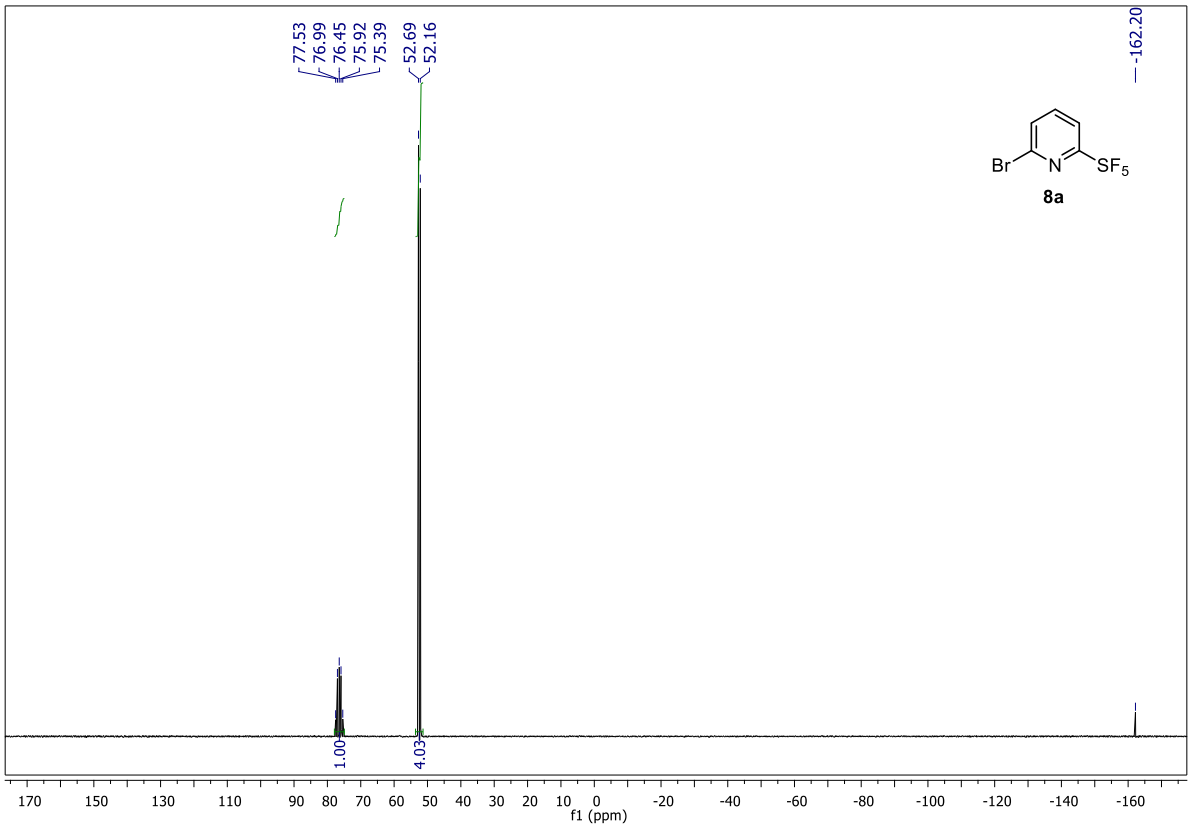
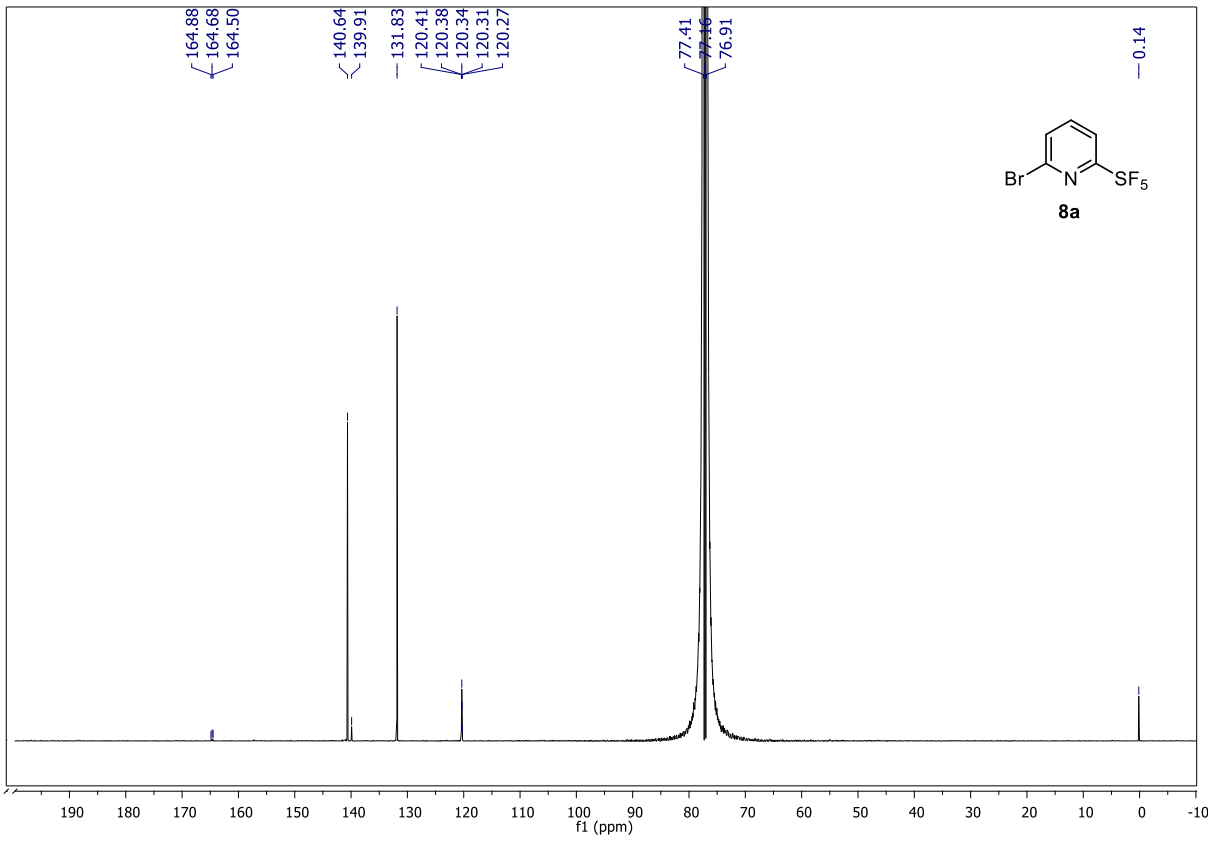
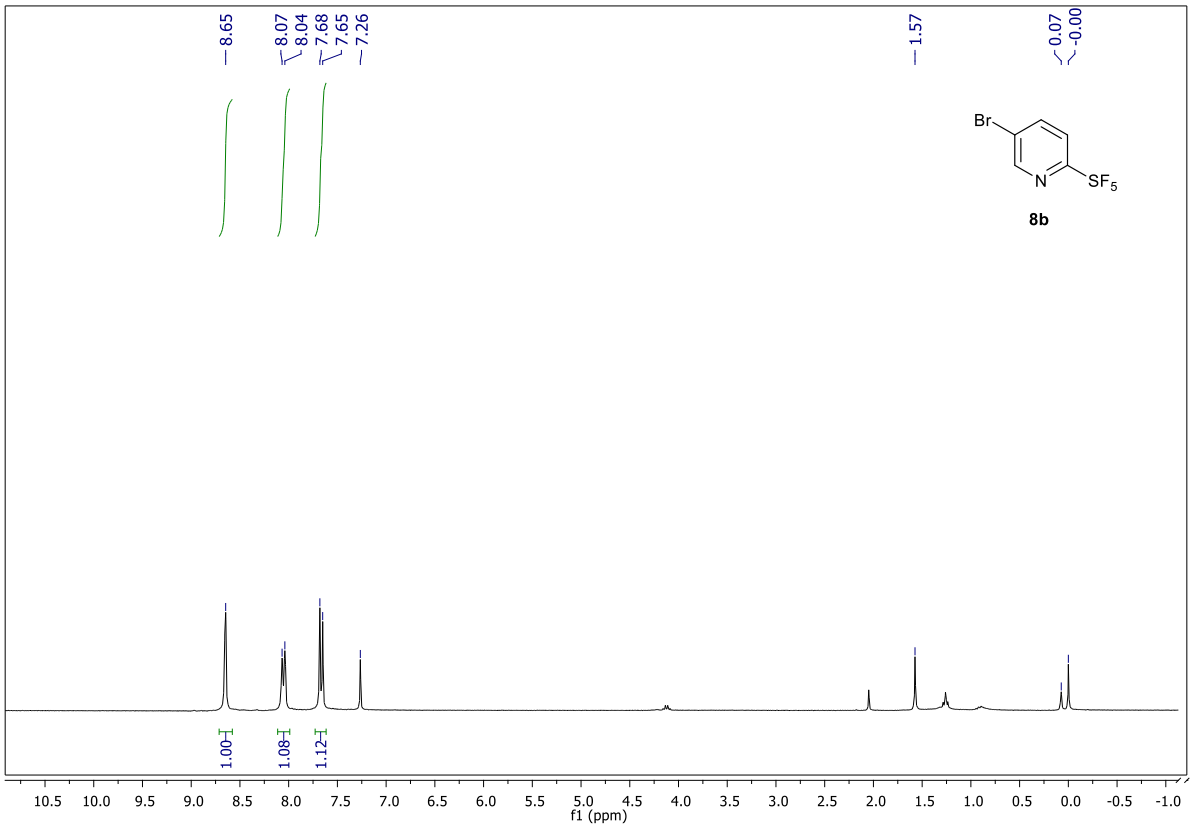
SF4Cl
8d'
1.00
1.10
1.35
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

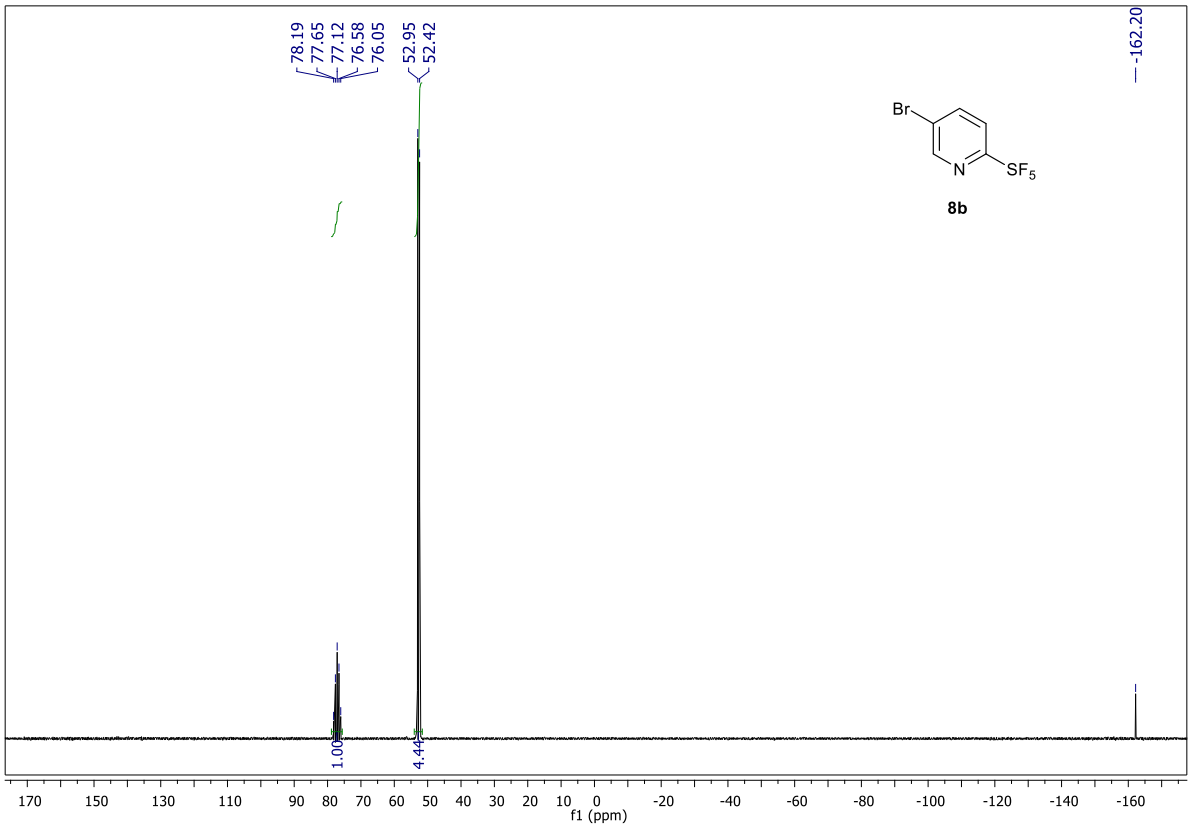

123.80
-96.42
-162.20
F
N
SF4Cl
8d'
4.18
1.00
f1 (ppm)


7.83
7.80
7.78
7.75
7.72
7.70
7.27
7.26
1.59
1.57
1.27
0.89
0.01
-0.00
Br
N
SF5
8a
3.00
f1 (ppm)


77.53
76.99
76.45
75.92
75.39
52.69
52.16
-162.20
Br
N
SF5
8a
1.00
4.03
f1 (ppm)


164.88
164.68
164.50
140.64
139.91
131.83
120.41
120.38
120.34
120.31
120.27
77.41
77.16
76.91
0.14
Br
N
SF5
8a
f1 (ppm)


8.65
8.07
8.04
7.68
7.65
7.26
1.57
0.07
-0.00
Br
N
SF5
8b
1.00
1.08
1.12
f1 (ppm)


78.19
77.65
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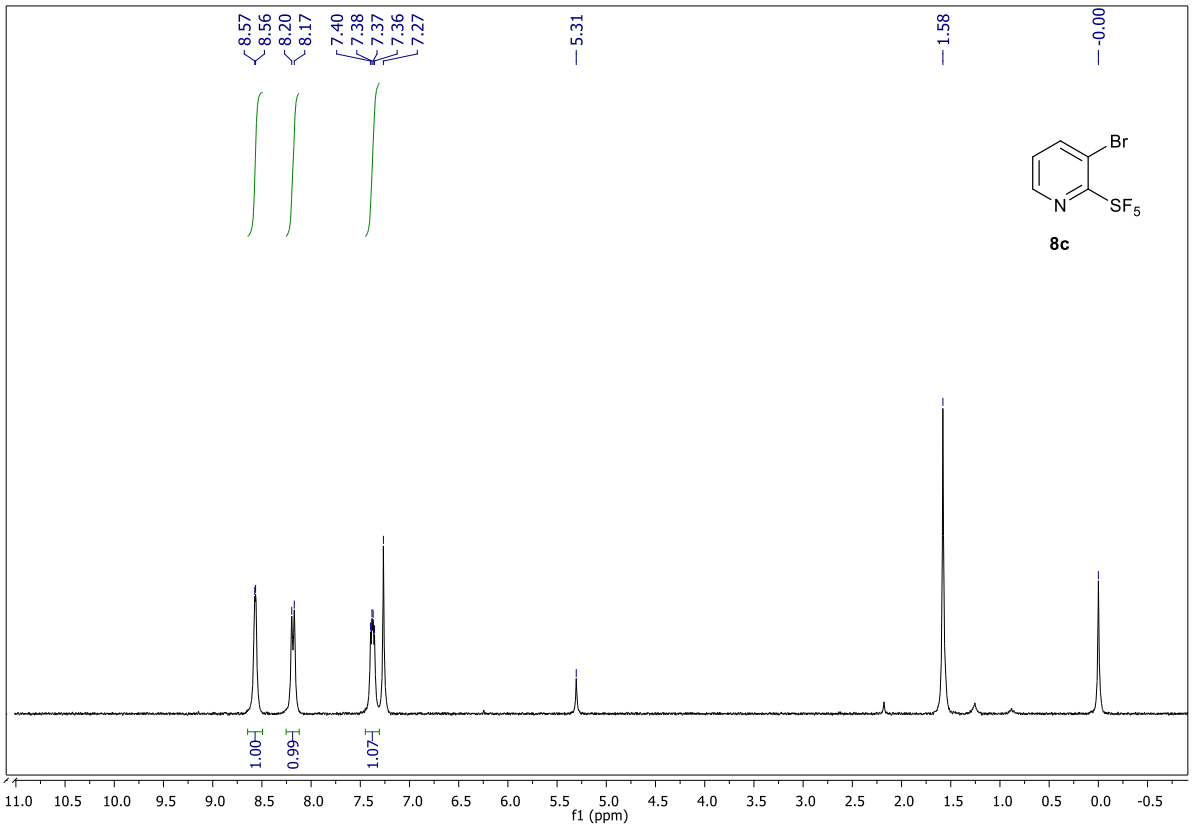
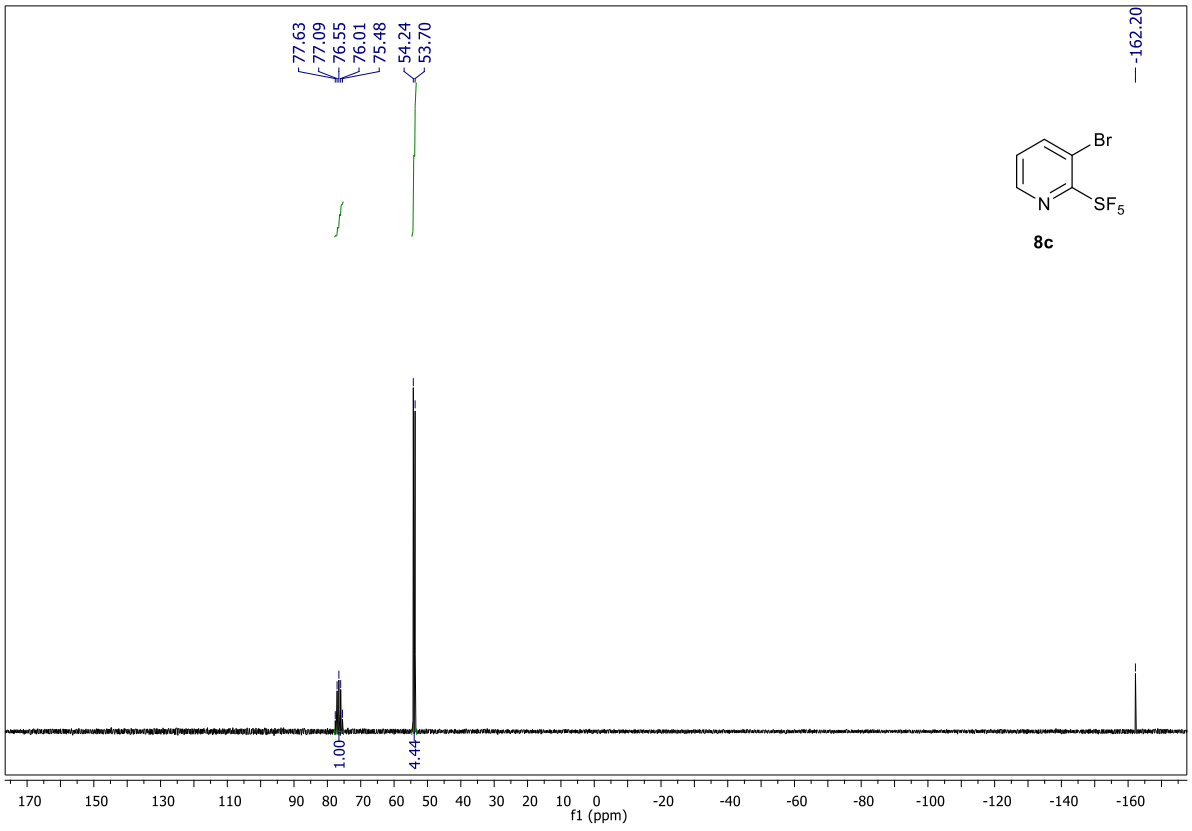
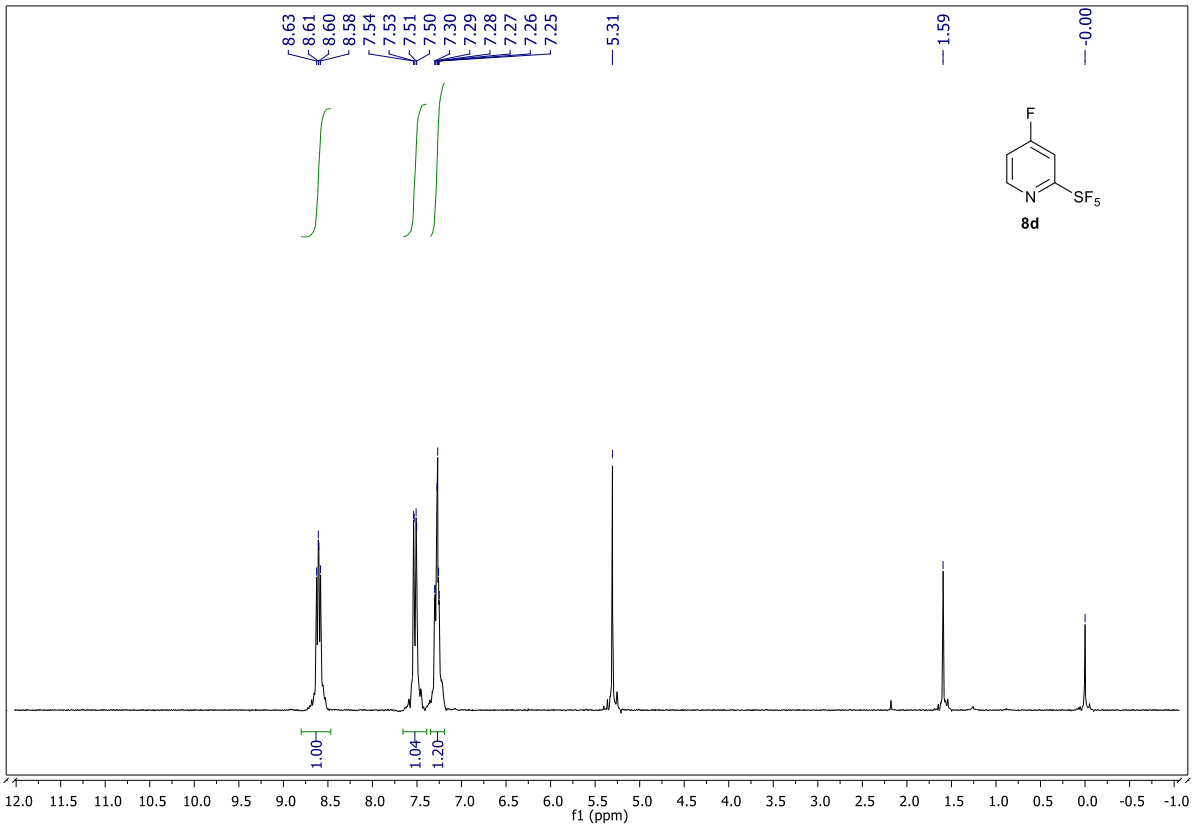
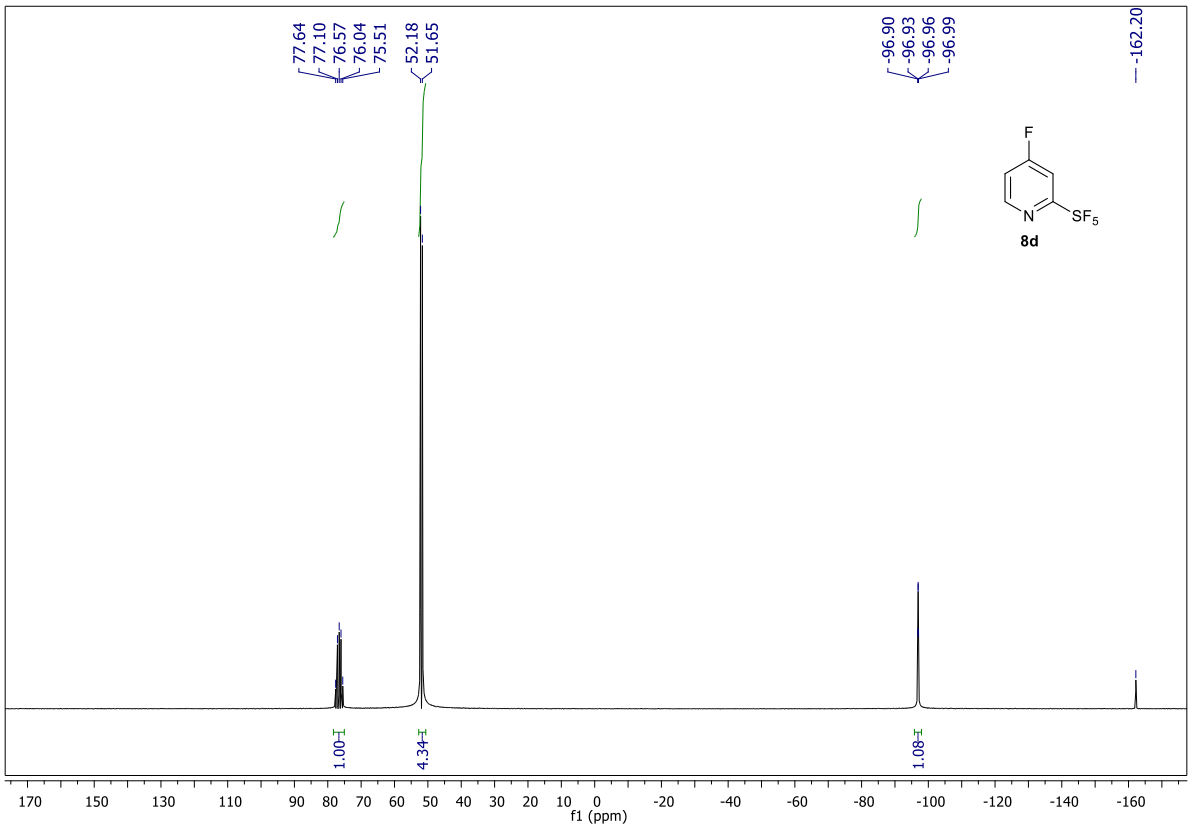
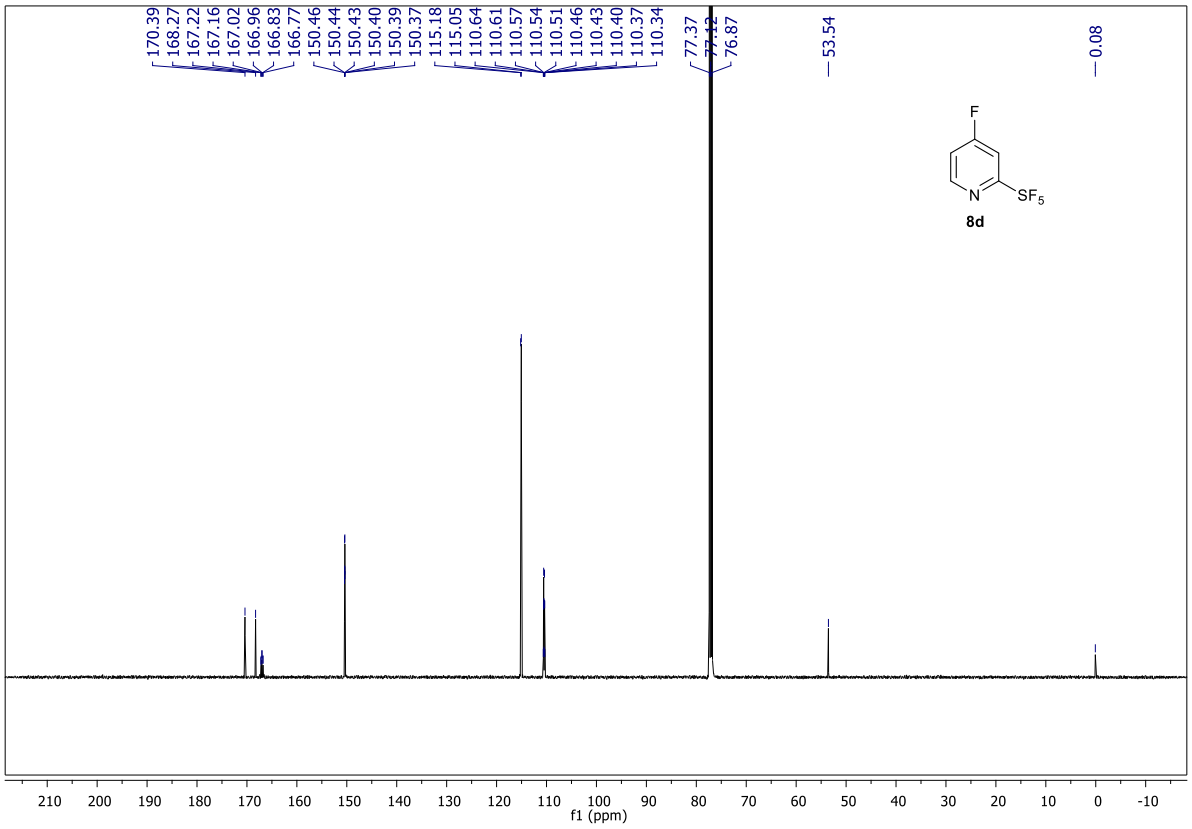
76.58
76.05
52.95
52.42
-162.20
Br
N
SF5
8b
1.00
4.44
f1 (ppm)

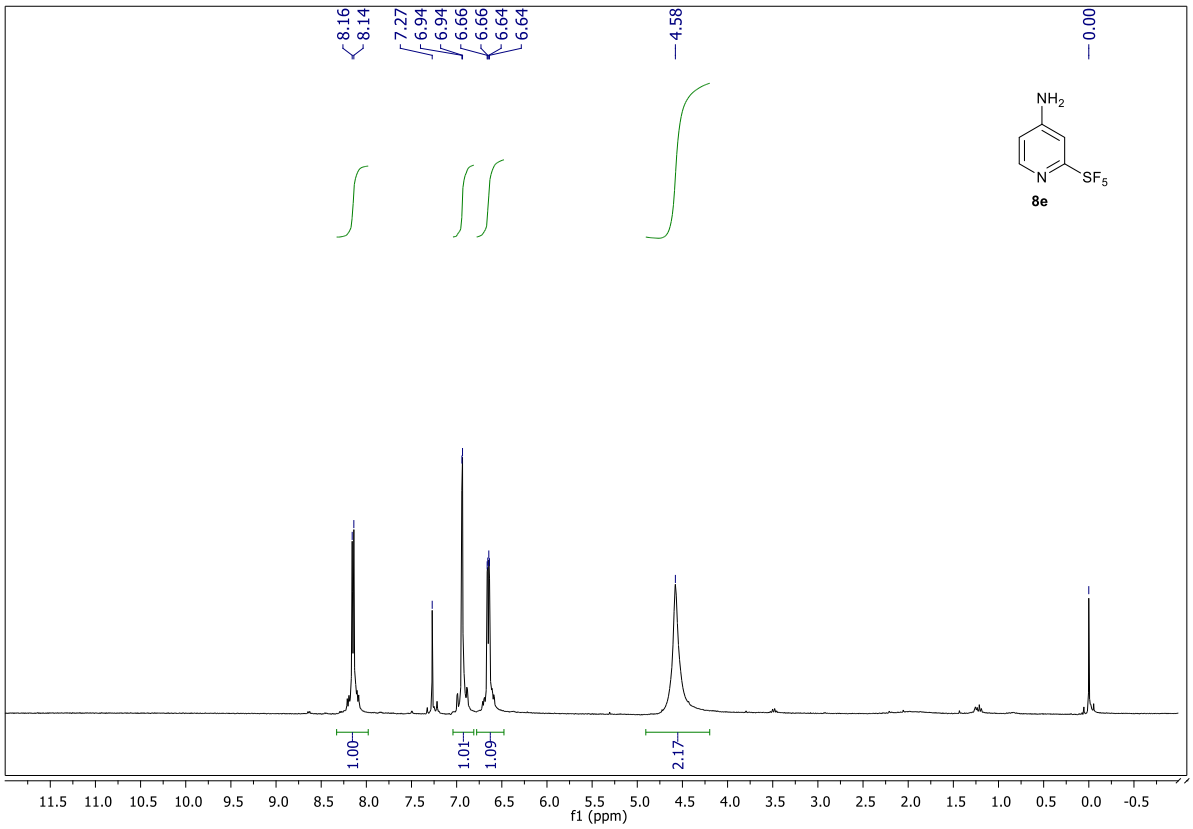

8.57
8.56
8.20
8.17
7.40
7.38
7.37
7.36
7.27
5.31
1.58
0.00
Br
N
SF5
8c
1.00
0.99
1.07
f1 (ppm)

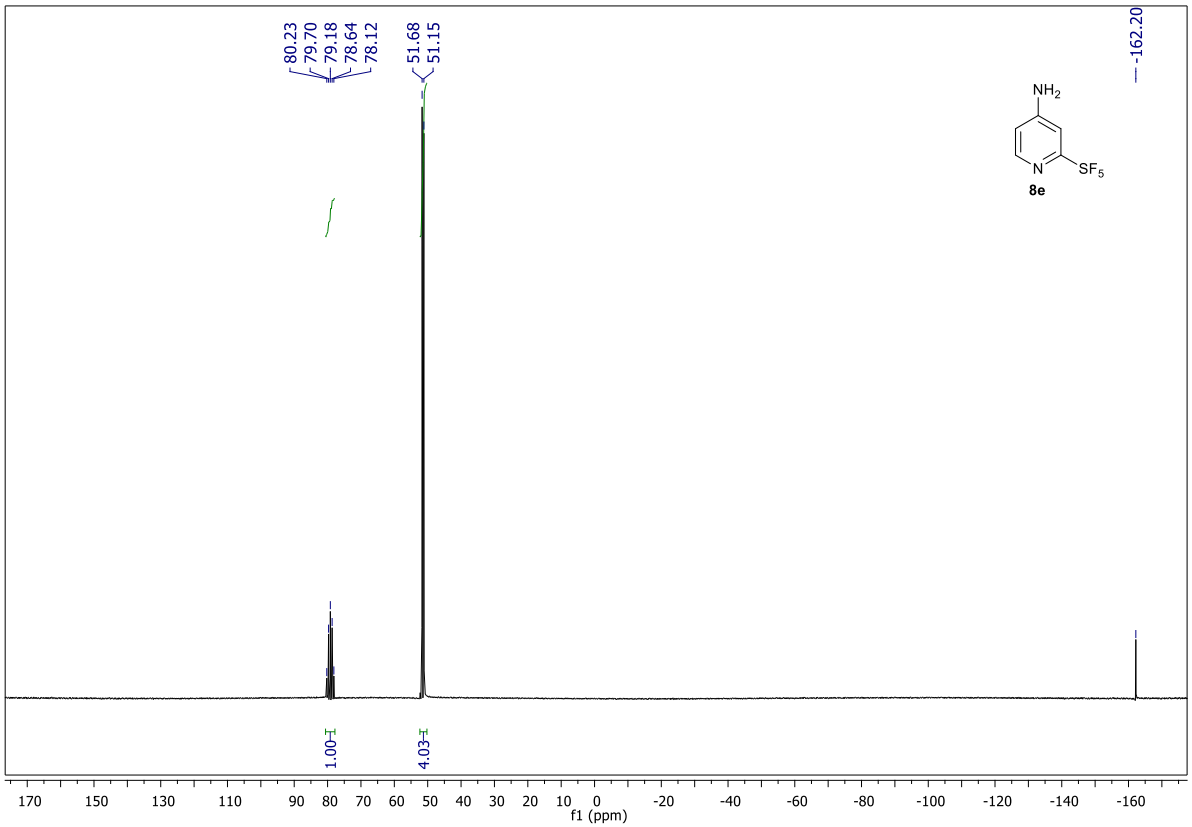

77.63
77.09
76.55
76.01
75.48
54.24
53.70
-162.20
Br
N
SF5
8c
1.00
4.44
f1 (ppm)

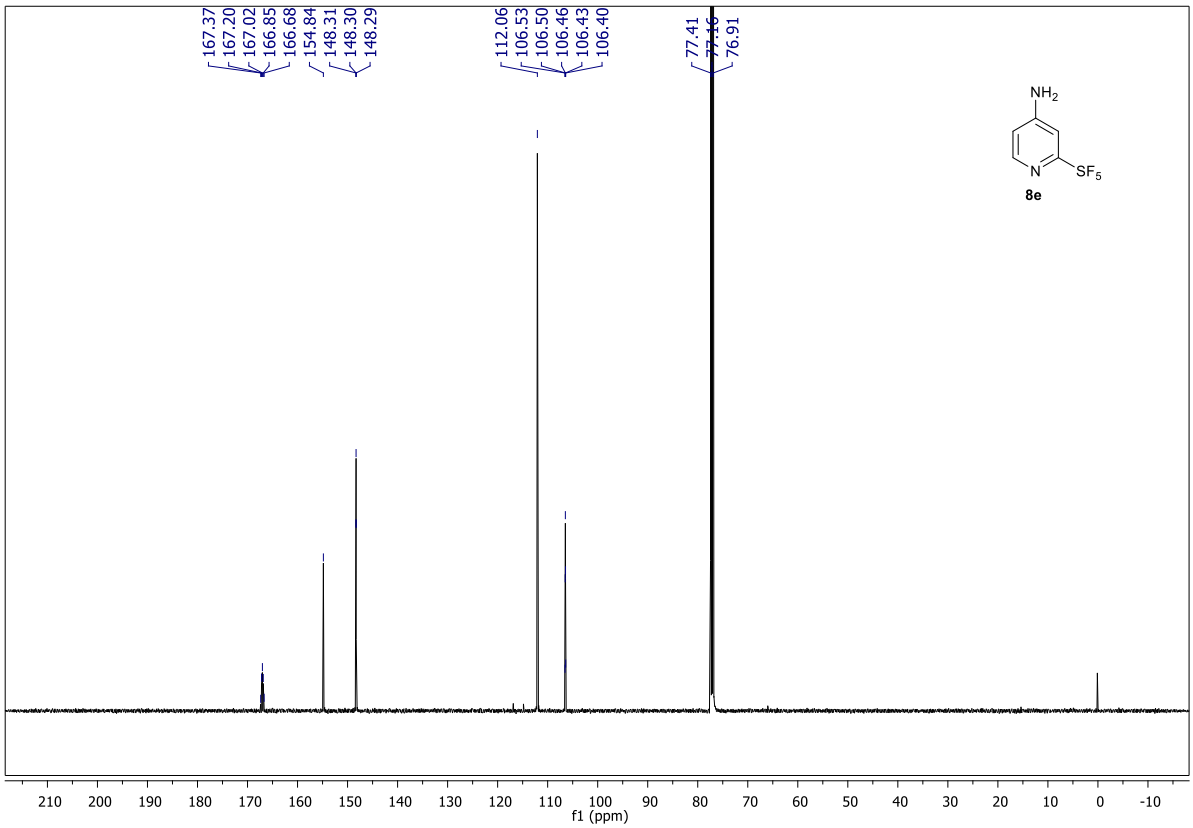

8.63
8.61
8.60
8.58
7.54
7.53
7.51
7.50
7.30
7.29
7.28
7.27
7.26
7.25
5.31
1.59
-0.00
F
N
SF5
8d
1.00
1.04
1.20
f1 (ppm)

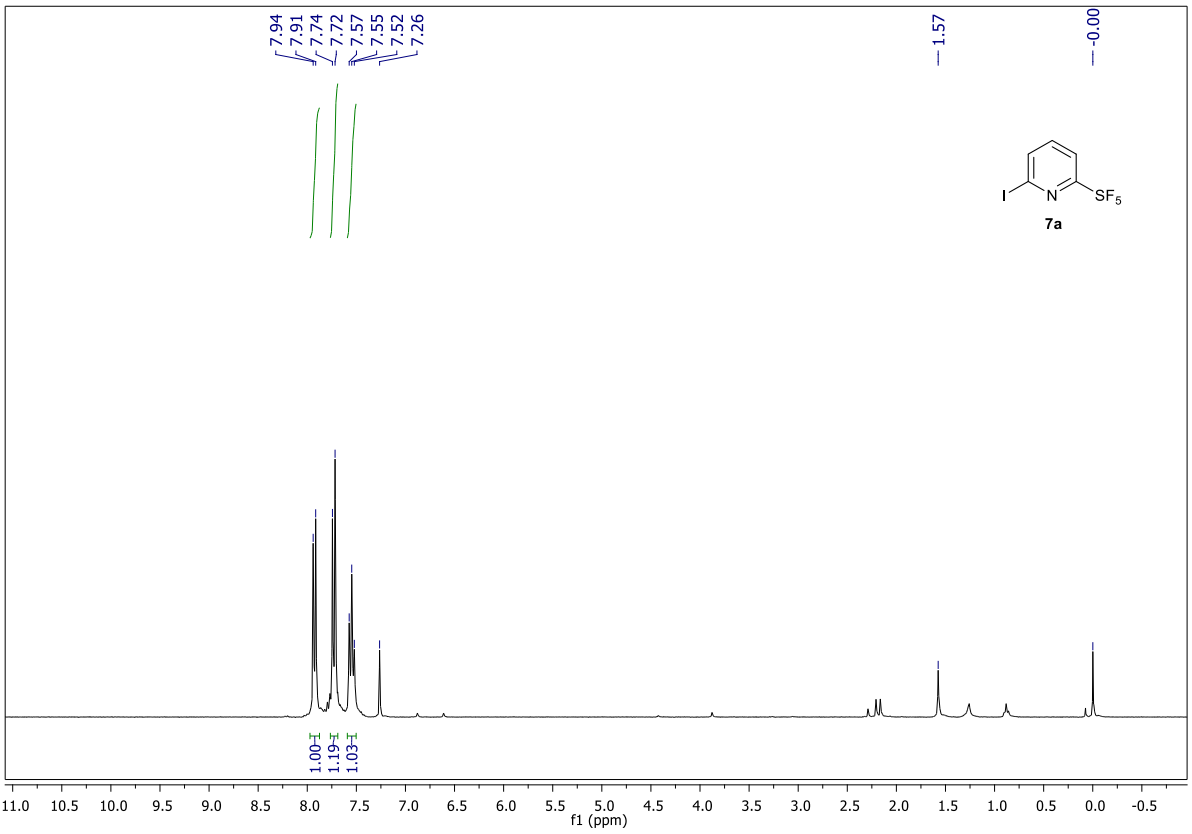

77.64
77.10
76.57
76.04
75.51
52.18
51.65
-96.90
-96.93
-96.96
-96.99
-162.20
F
N
SF5
8d
1.00
4.34
1.08
f1 (ppm)

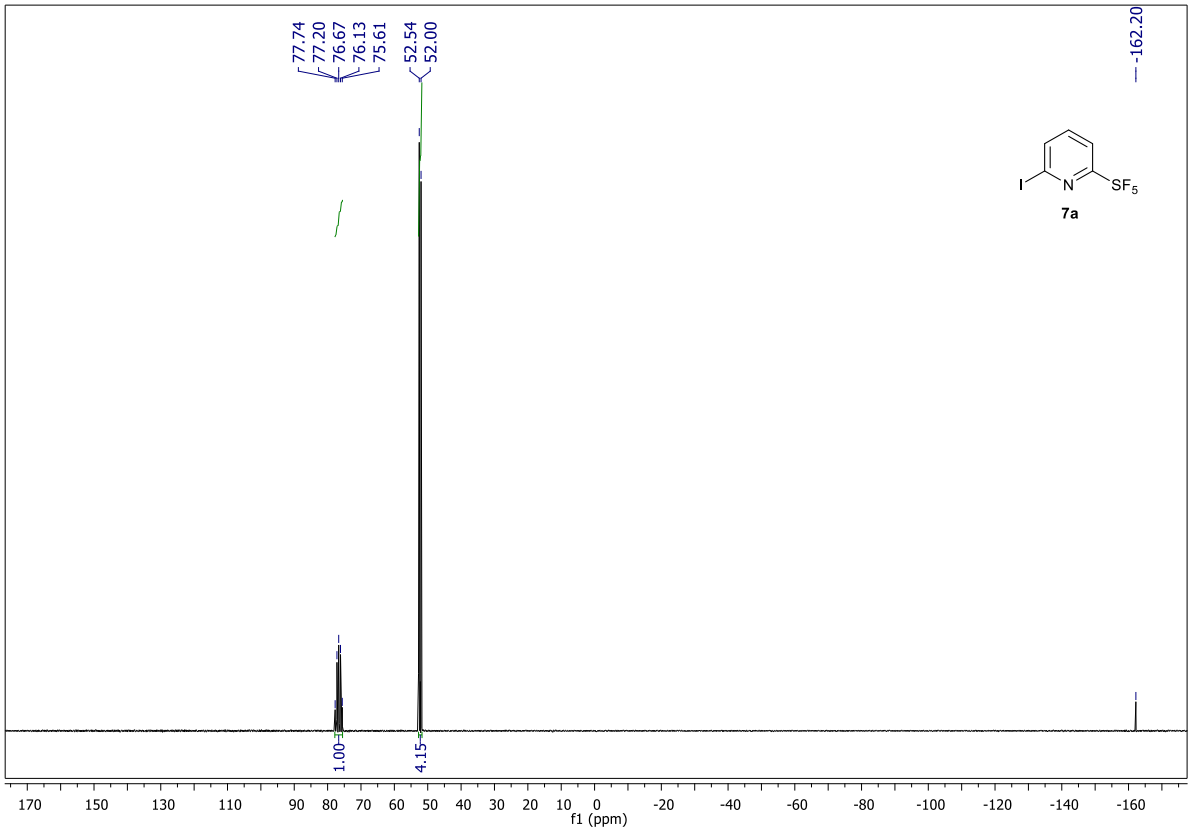

170.39
168.27
167.22
167.16
167.02
166.96
166.83
166.77
150.46
150.44
150.43
150.40
150.39
150.37
115.18
115.05
110.64
110.61
110.57
110.54
110.51
110.46
110.43
110.40
110.37
110.34
77.37
77.12
76.87
53.54
0.08
F
N
SF5
8d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

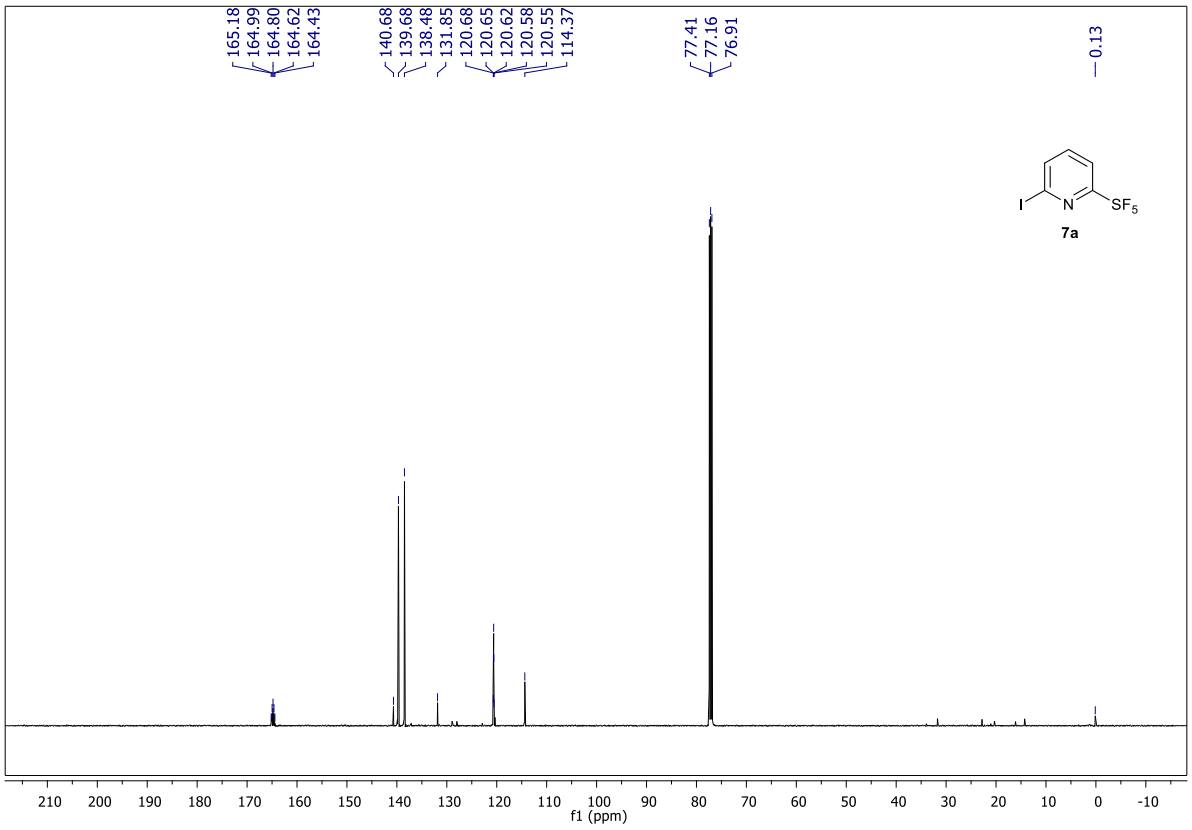

8.16
8.14
7.27
6.94
6.94
6.66
6.66
6.64
6.64
4.58
0.00
NH2
N
SF5
8e
1.00
1.01
1.09
2.17
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

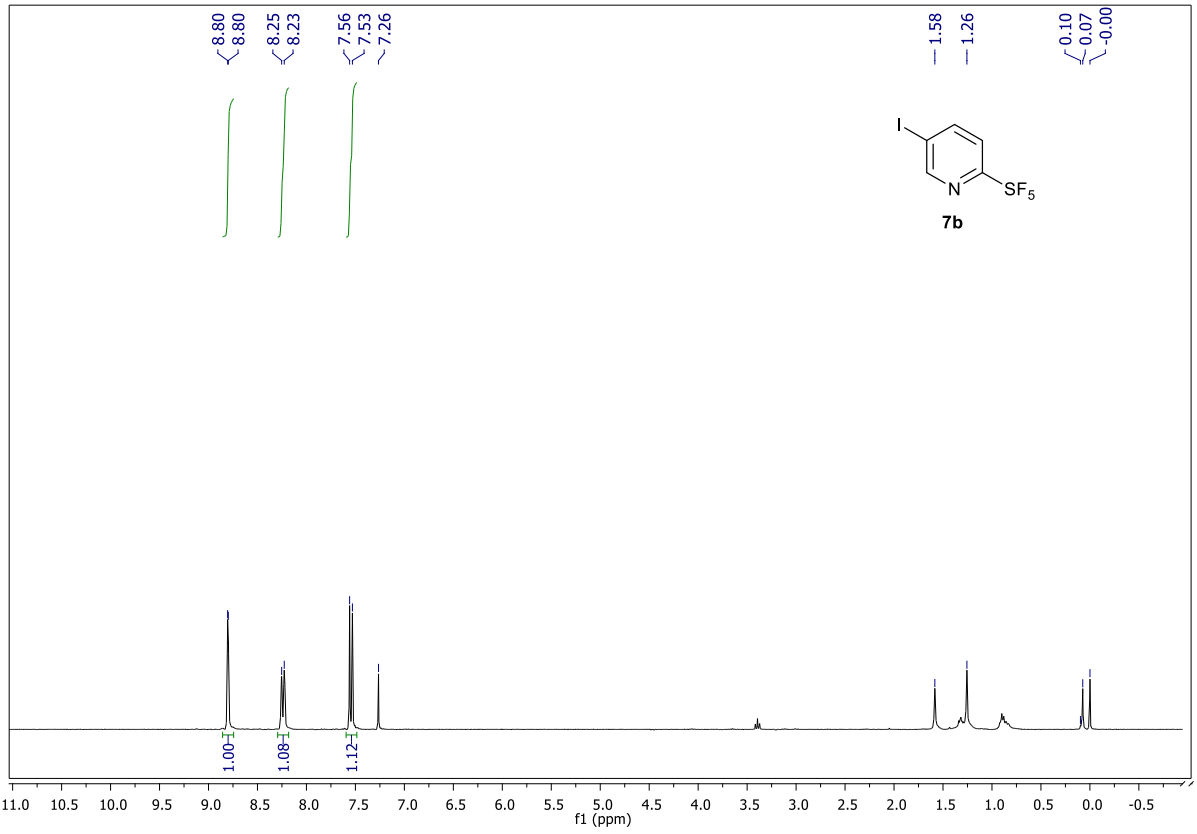

80.23
79.70
79.18
78.64
78.12
51.68
51.15
-162.20
NH2
N
SF5
8e
1.00
4.03
f1 (ppm)

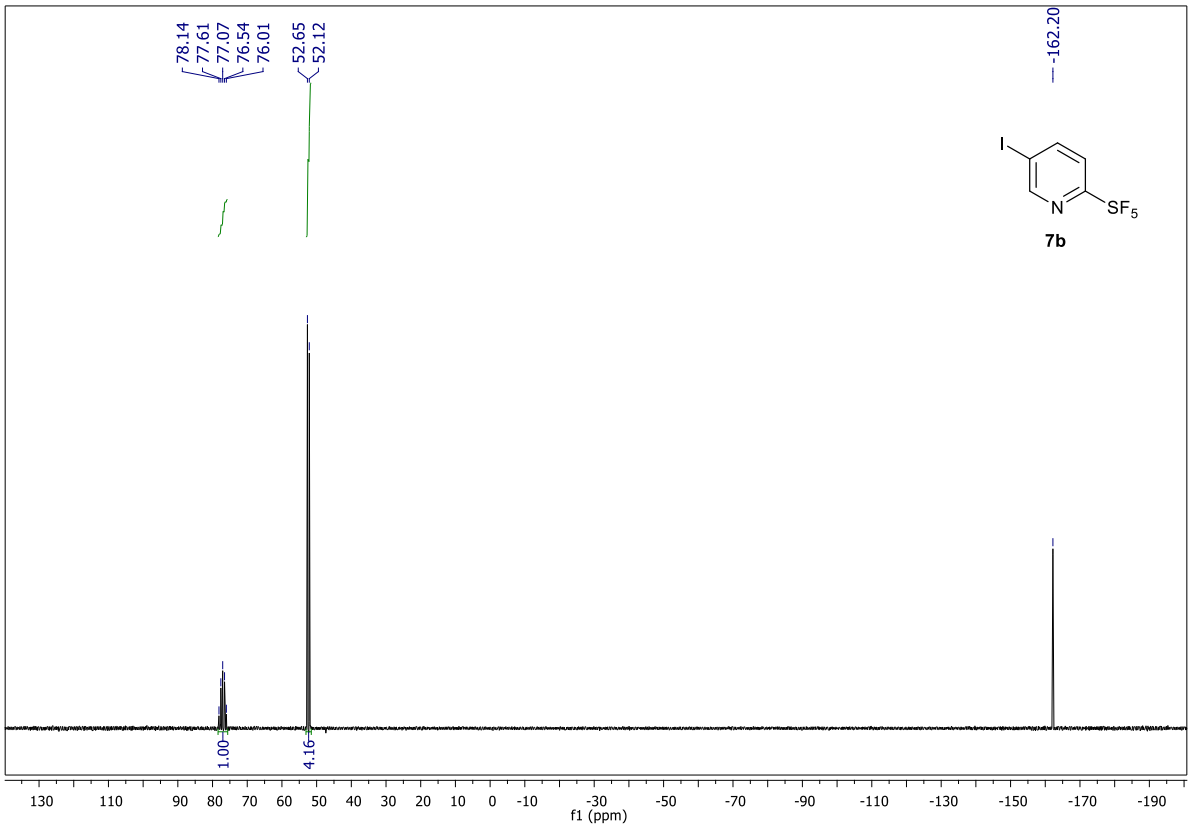

167.37
167.20
167.02
166.85
166.68
154.84
148.31
148.30
148.29
112.06
106.53
106.50
106.46
106.43
106.40
77.41
77.16
76.91
NH2
N
SF5
8e
f1 (ppm)

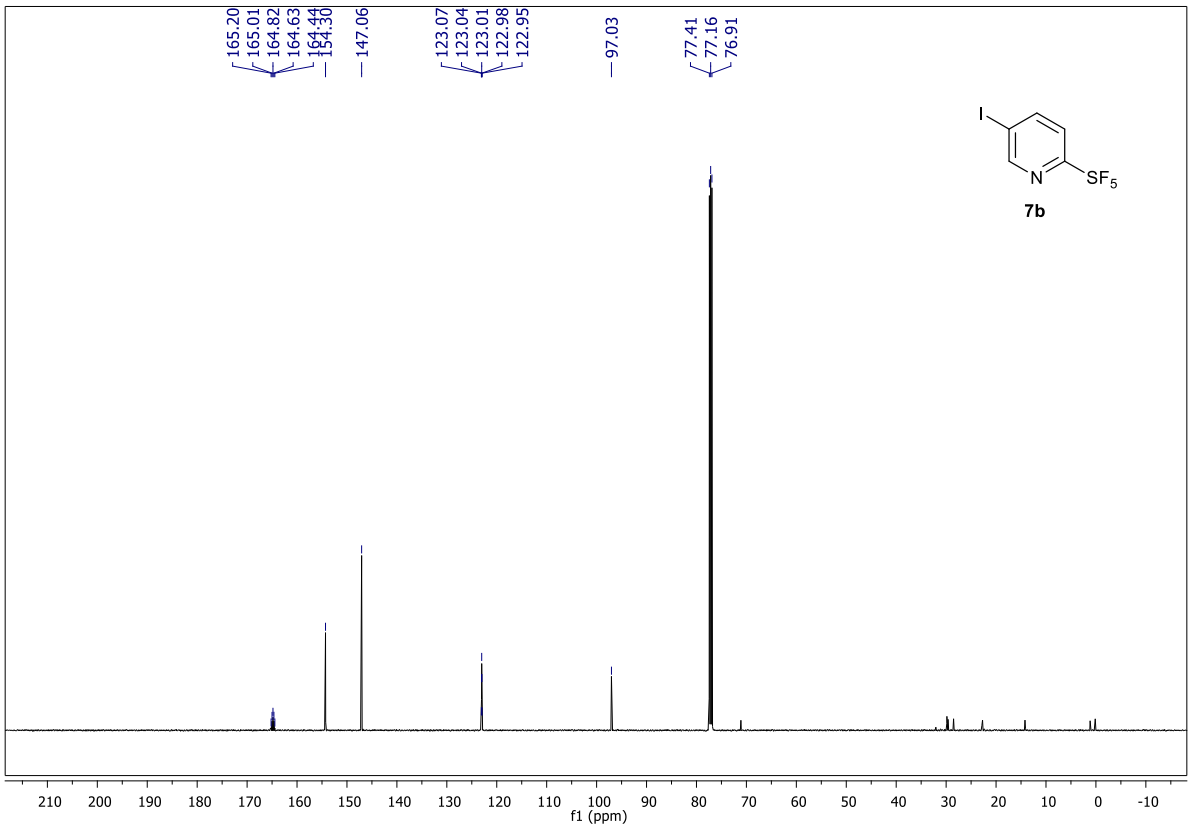

7.94
7.91
7.74
7.72
7.57
7.55
7.52
7.26
1.57
-0.00
I
N
SF5
7a
1.00
1.19
1.03
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


77.74
77.20
76.67
76.13
75.61
52.54
52.00
-162.20
I
N
SF5
7a
1.00
4.15
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)


165.18
164.99
164.80
164.62
164.43
140.68
139.68
138.48
131.85
120.68
120.65
120.62
120.58
120.55
114.37
77.41
77.16
76.91
0.13
I
N
SF5
7a
f1 (ppm)


8.80
8.80
8.25
8.23
7.56
7.53
7.26
1.58
1.26
0.10
0.07
-0.00
I
N
SF5
7b
1.00
1.08
1.12
f1 (ppm)


78.14
77.61
77.07
76.54
76.01
52.65
52.12
-162.20
I
N
SF5
7b
1.00
4.16
130 110 90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190
f1 (ppm)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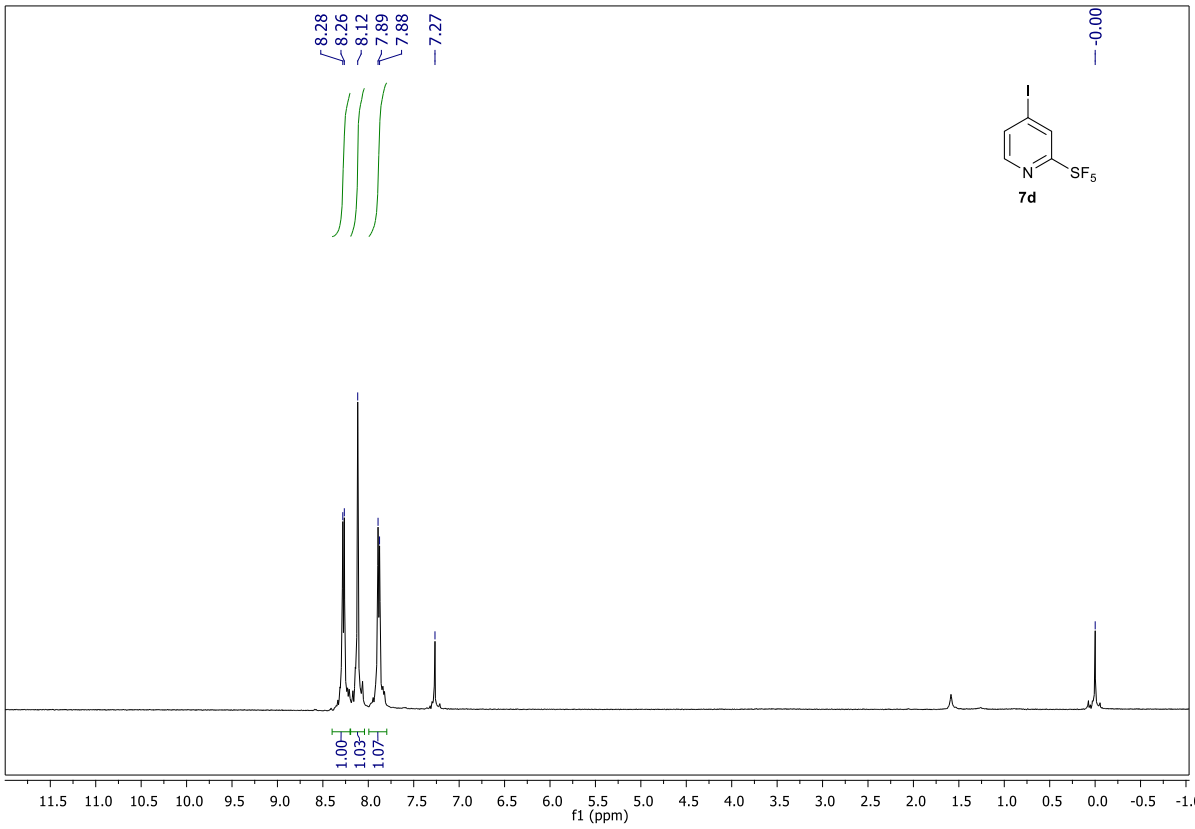
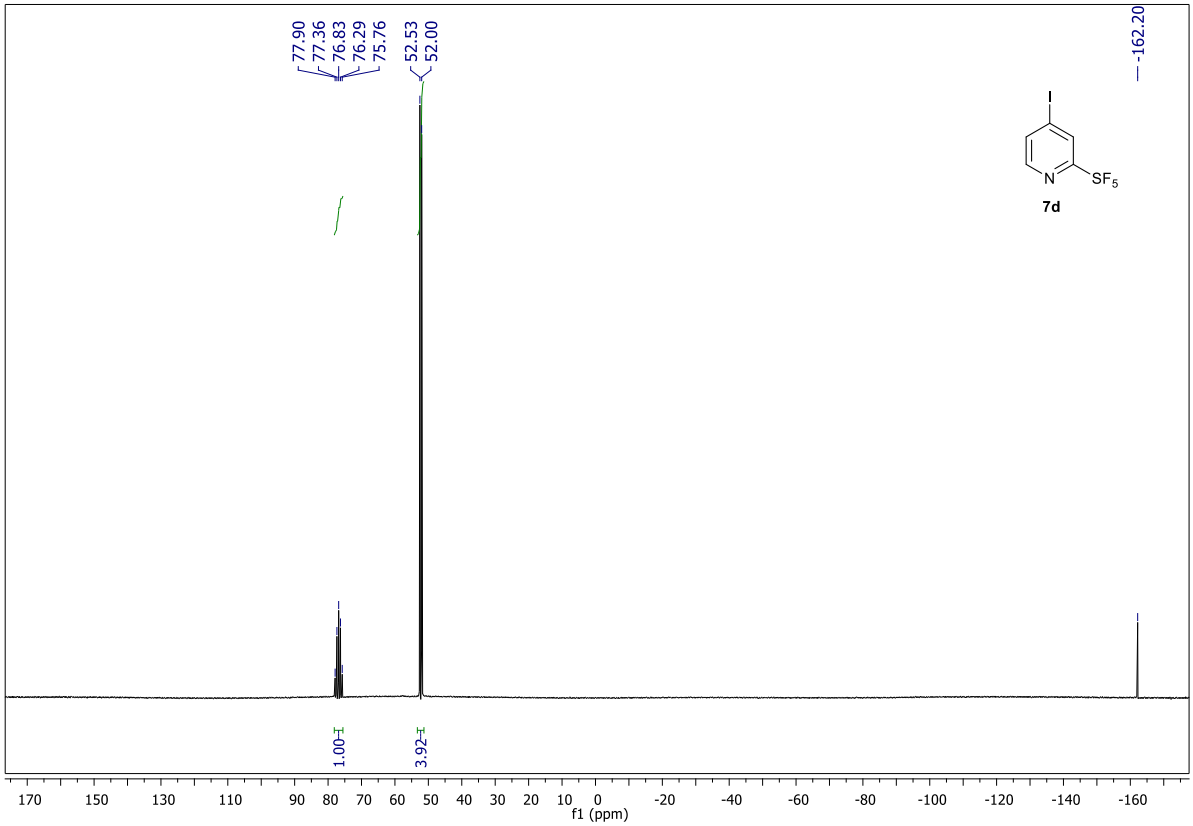
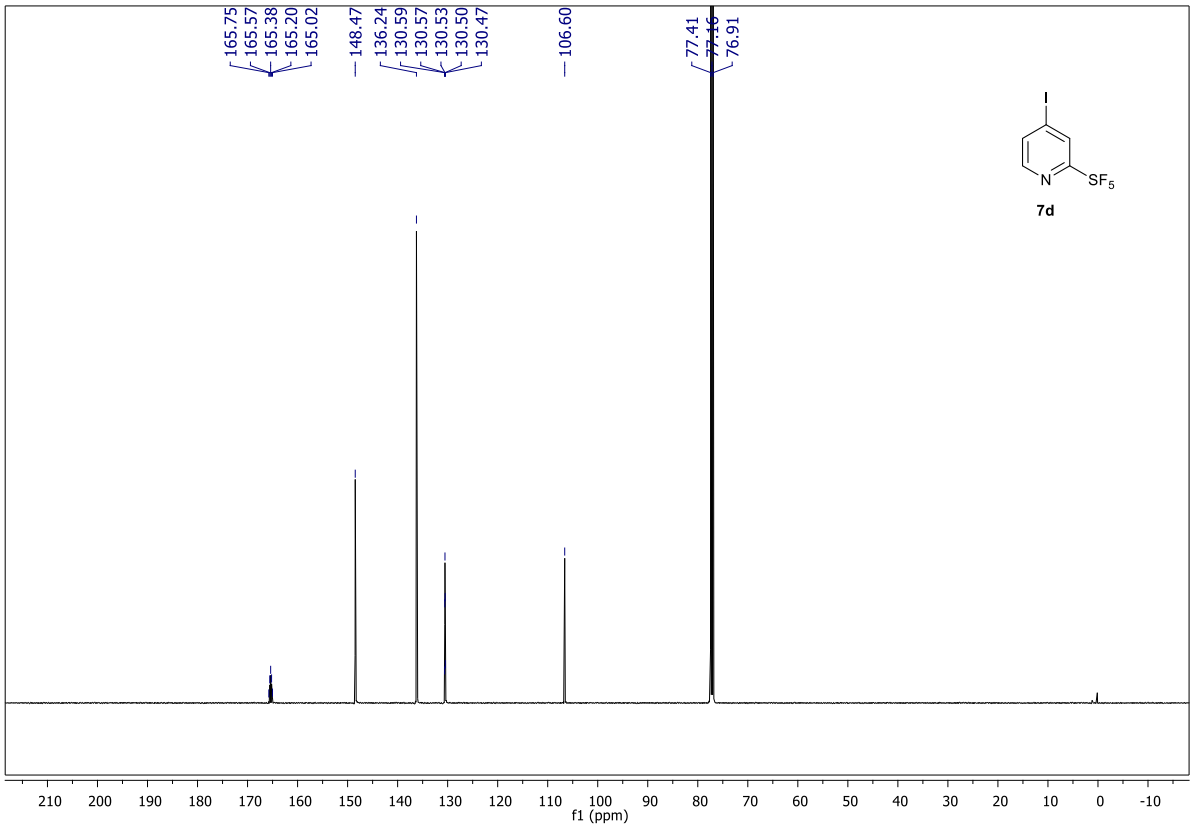
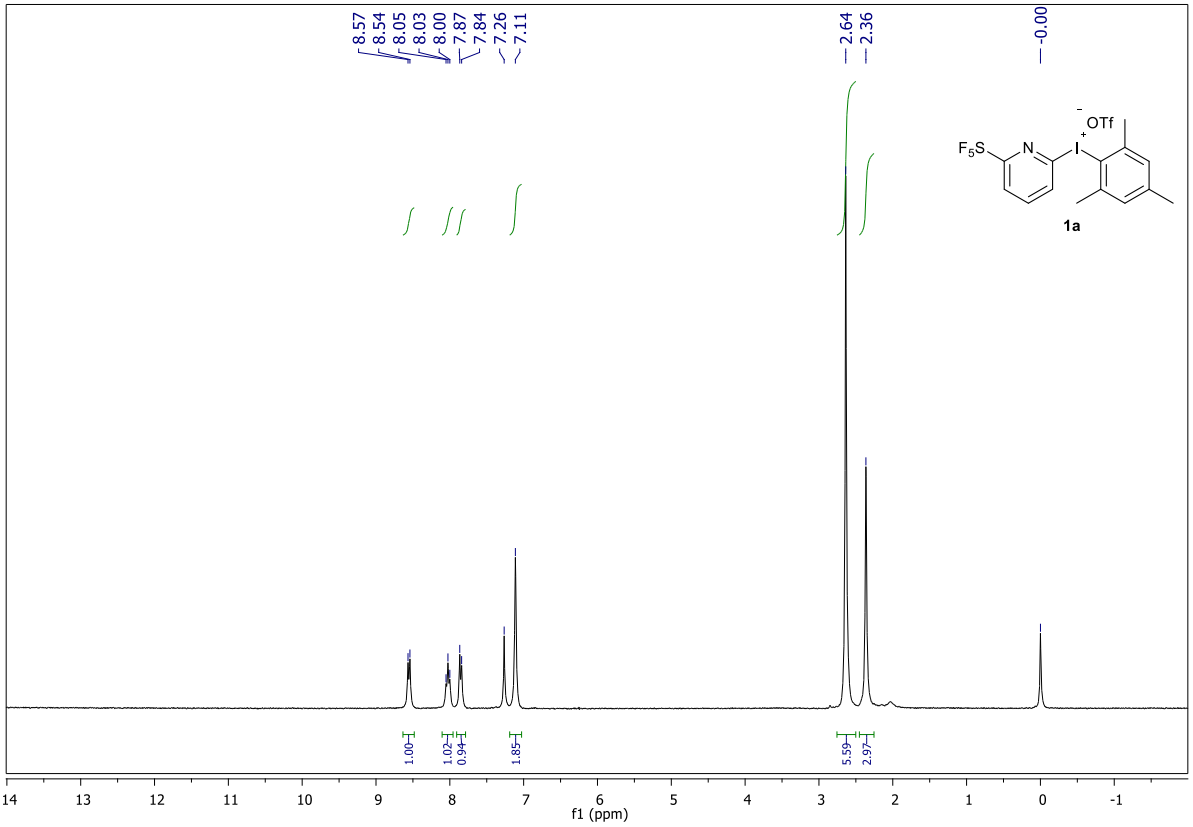
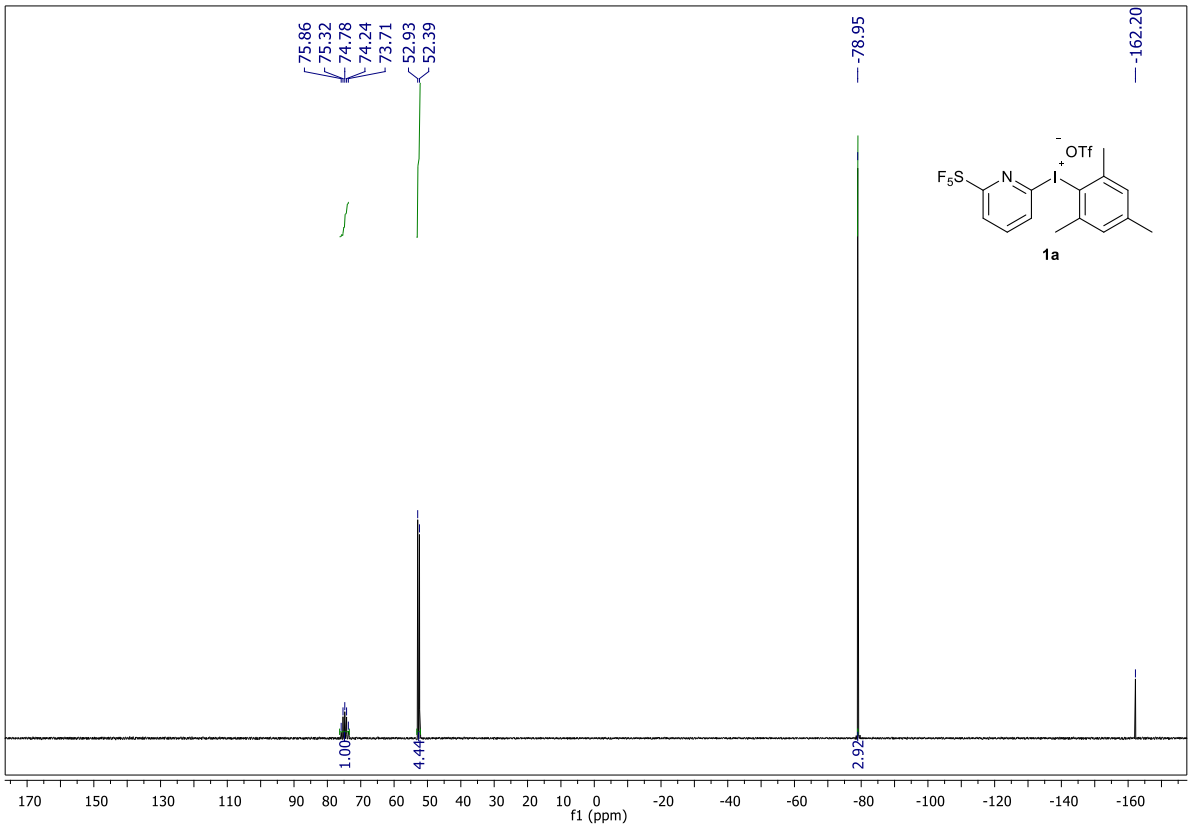
165.01
164.82
164.63
164.44
154.30
147.06
123.07
123.04
123.01
122.98
122.95
97.03
77.41
77.16
76.91
I
N
SF5
7b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

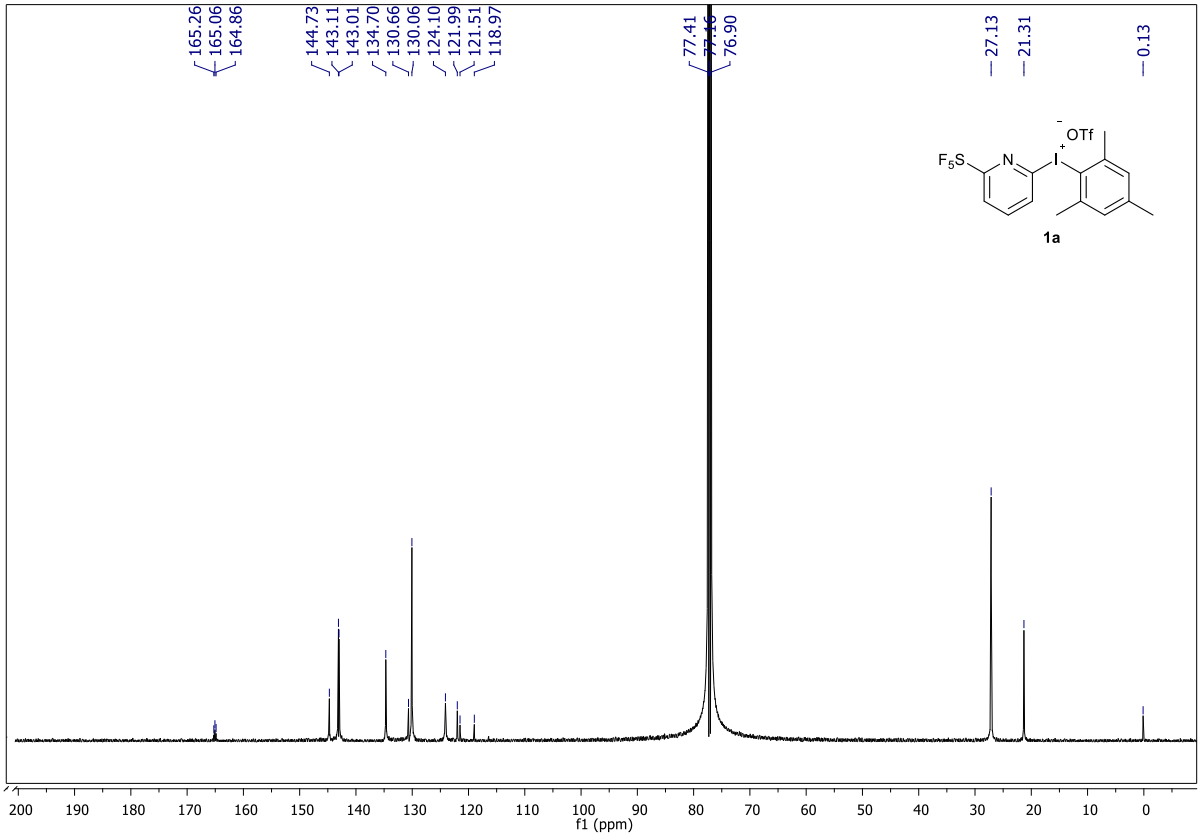

8.28
8.26
8.12
7.89
7.88
7.27
-0.00
I
N
SF5
7d
1.00
1.03
1.07
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

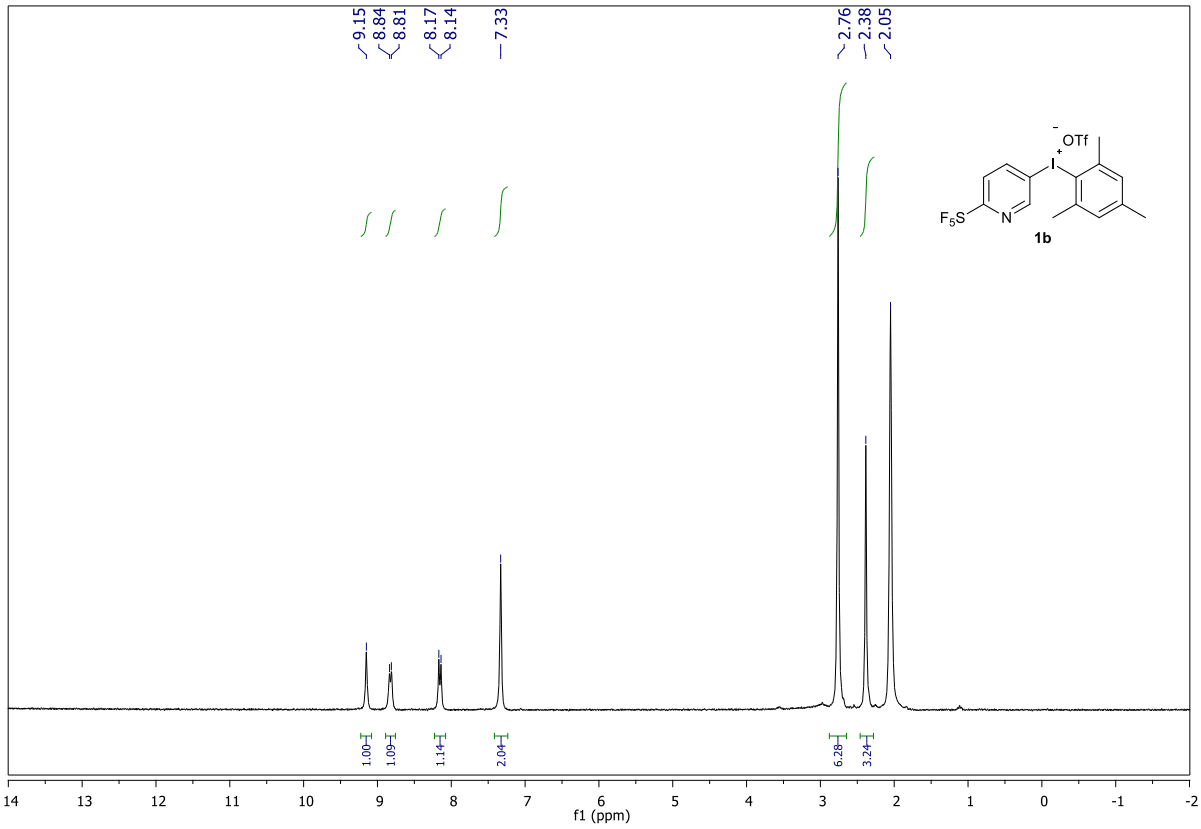

77.90
77.36
76.83
76.29
75.76
52.53
52.00
-162.20
I
N
SF5
7d
1.00
3.92
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)

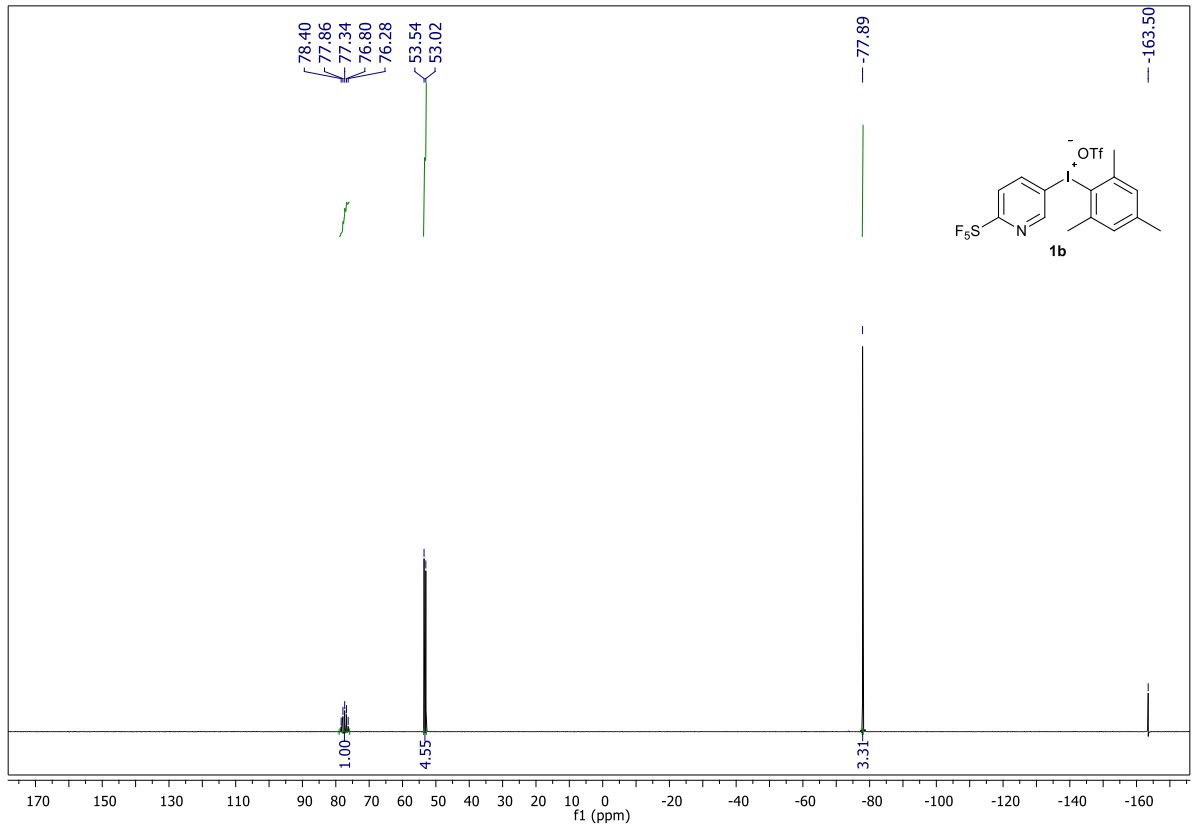

165.75
165.57
165.38
165.20
165.02
148.47
136.24
130.59
130.57
130.53
130.50
130.47
106.60
77.41
77.16
76.91
I
N
SF5
7d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

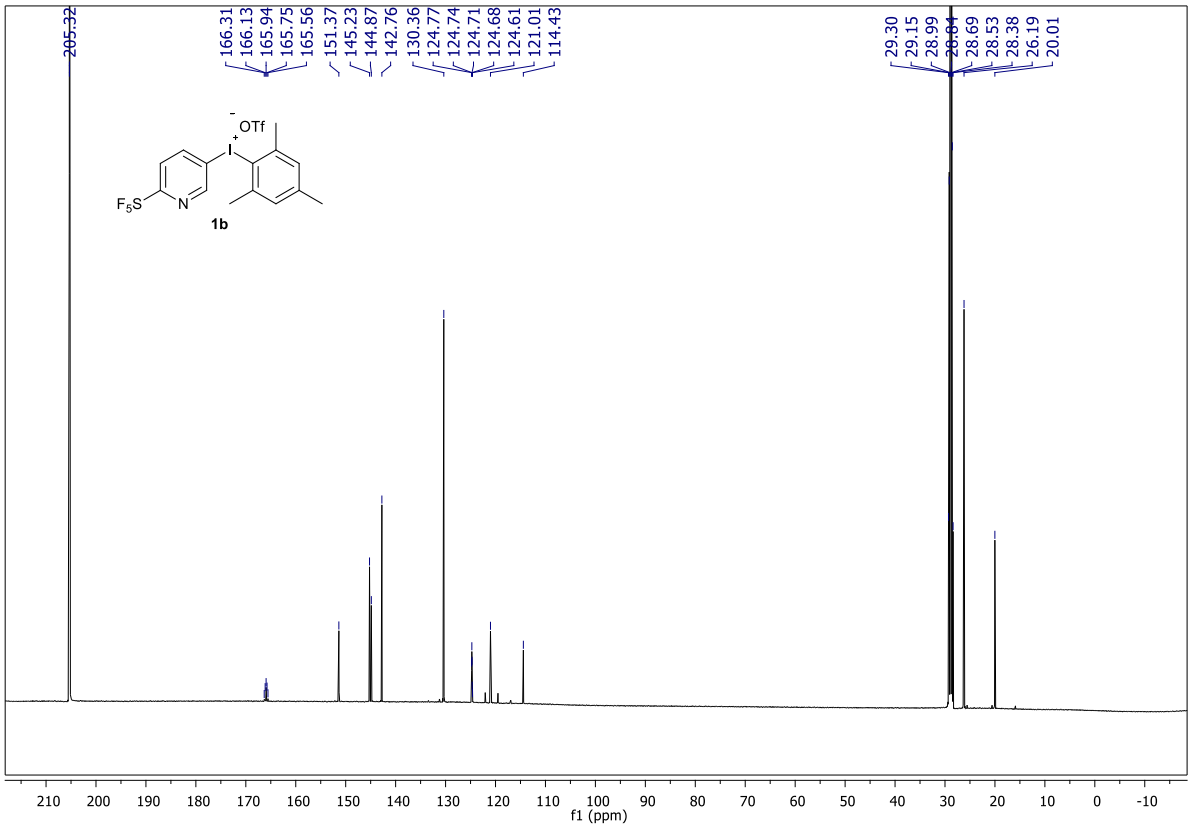

8.57
8.54
8.05
8.03
8.00
7.87
7.84
7.26
7.11
2.64
2.36
-0.00
OTf
F5S
N
I
1a
1.00
1.02
0.94
1.85
5.59
2.97
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


75.86
75.32
74.78
74.24
73.71
52.93
52.39
-78.95
-162.20
OTf
F5S
N
I
1a
1.00
4.44
2.92
f1 (ppm)


165.26
165.06
164.86
144.73
143.11
143.01
134.70
130.66
130.06
124.10
121.99
121.51
118.97
77.41
77.16
76.90
27.13
21.31
0.13
OTf
F5S
N
I
1a
f1 (ppm)


9.15
8.84
8.81
8.17
8.14
7.33
2.76
2.38
2.05
OTf
I
F5S
N
1b
1.00
1.09
1.14
2.04
6.28
3.24
f1 (ppm)


78.40
77.86
77.34
76.80
76.28
53.54
53.02
-77.89
-163.50
OTf
I
F5S
N
1b
1.00
4.55
3.31
f1 (ppm)


205.32
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166.13
165.94
165.75
165.56
151.37
145.23
144.87
142.76
130.36
124.77
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124.71
124.68
124.61
121.01
114.43
29.30
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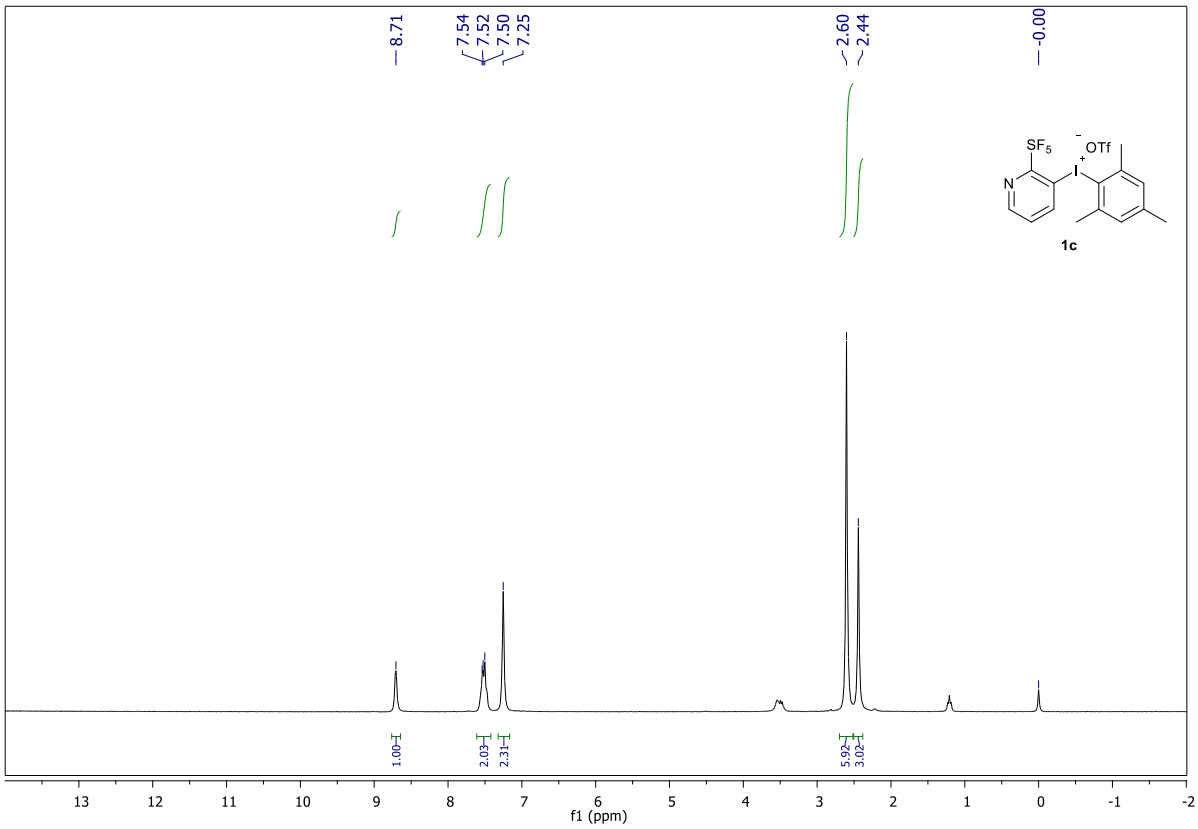
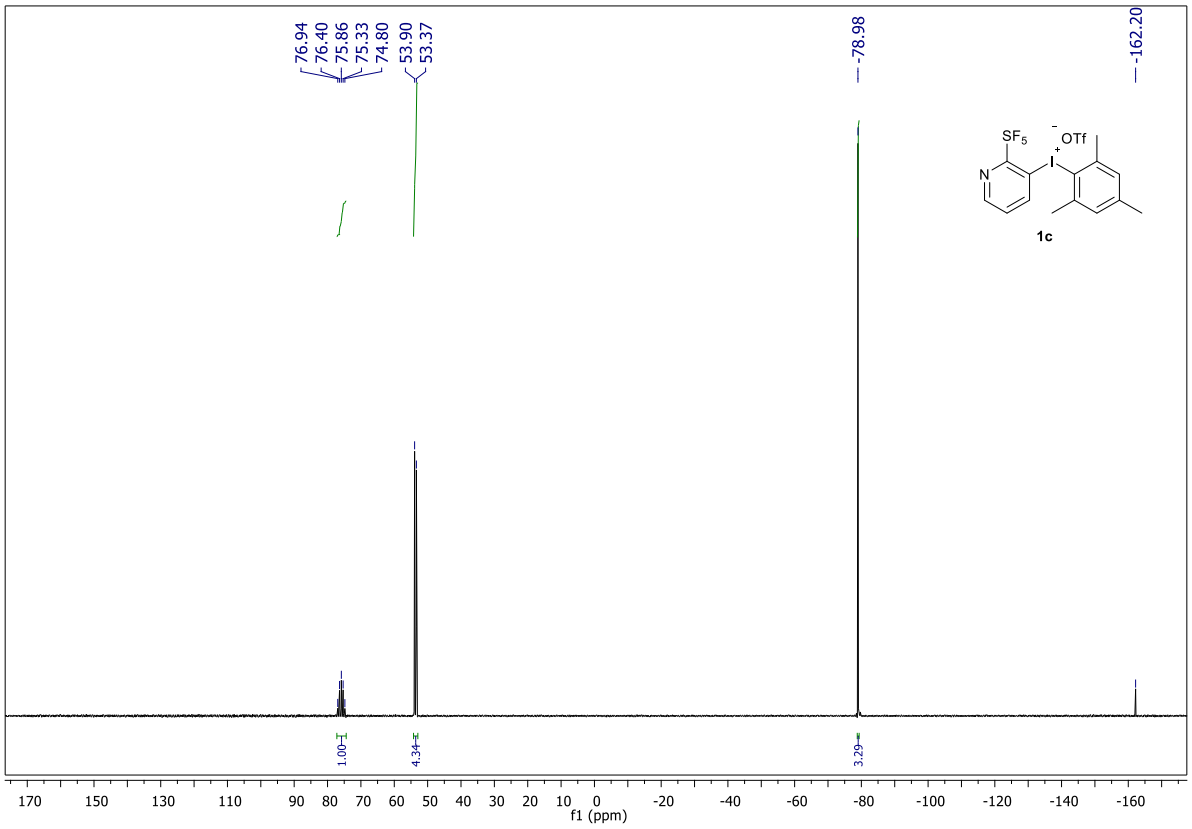
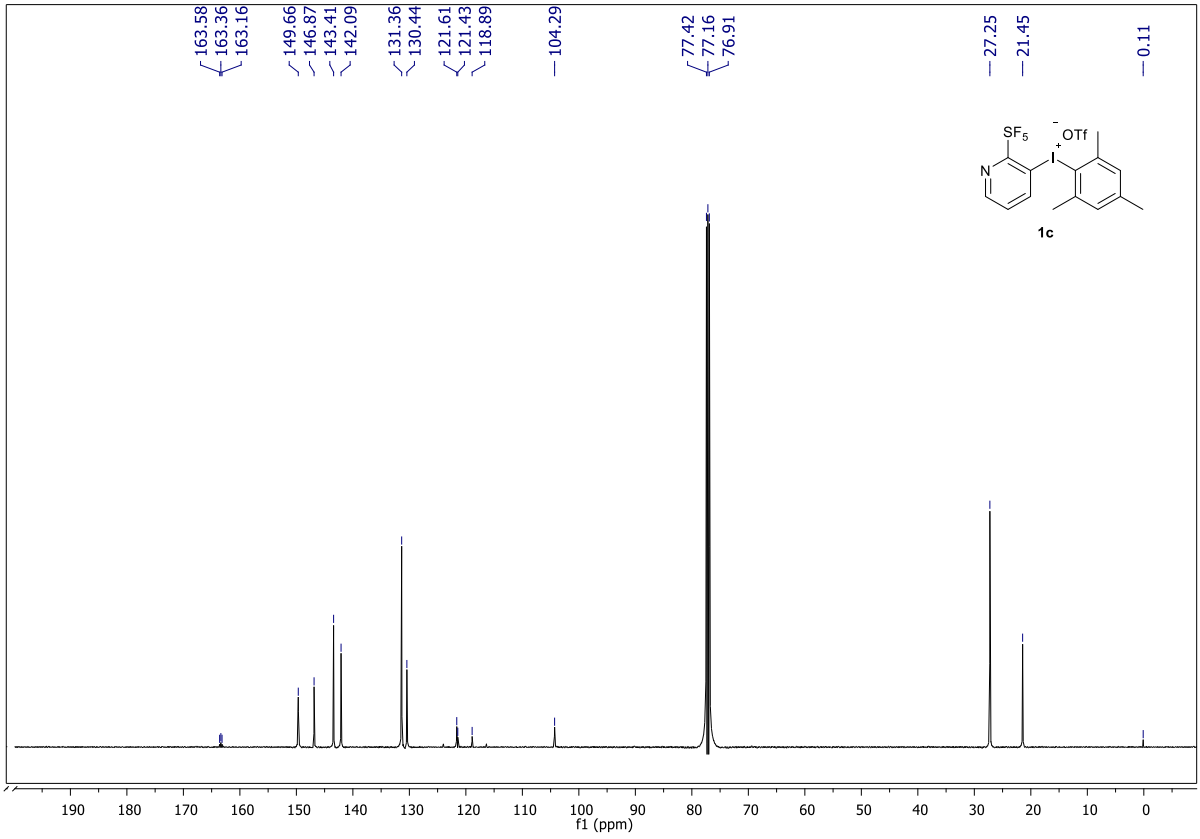
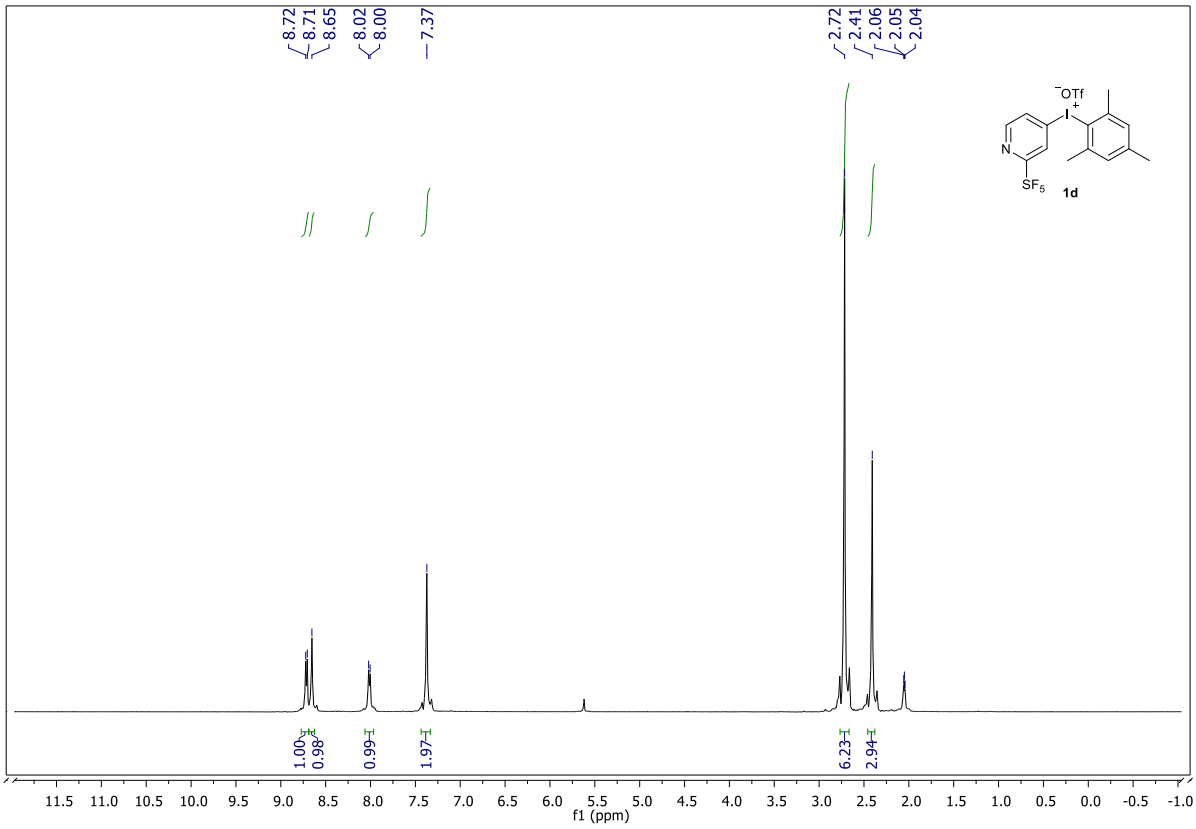
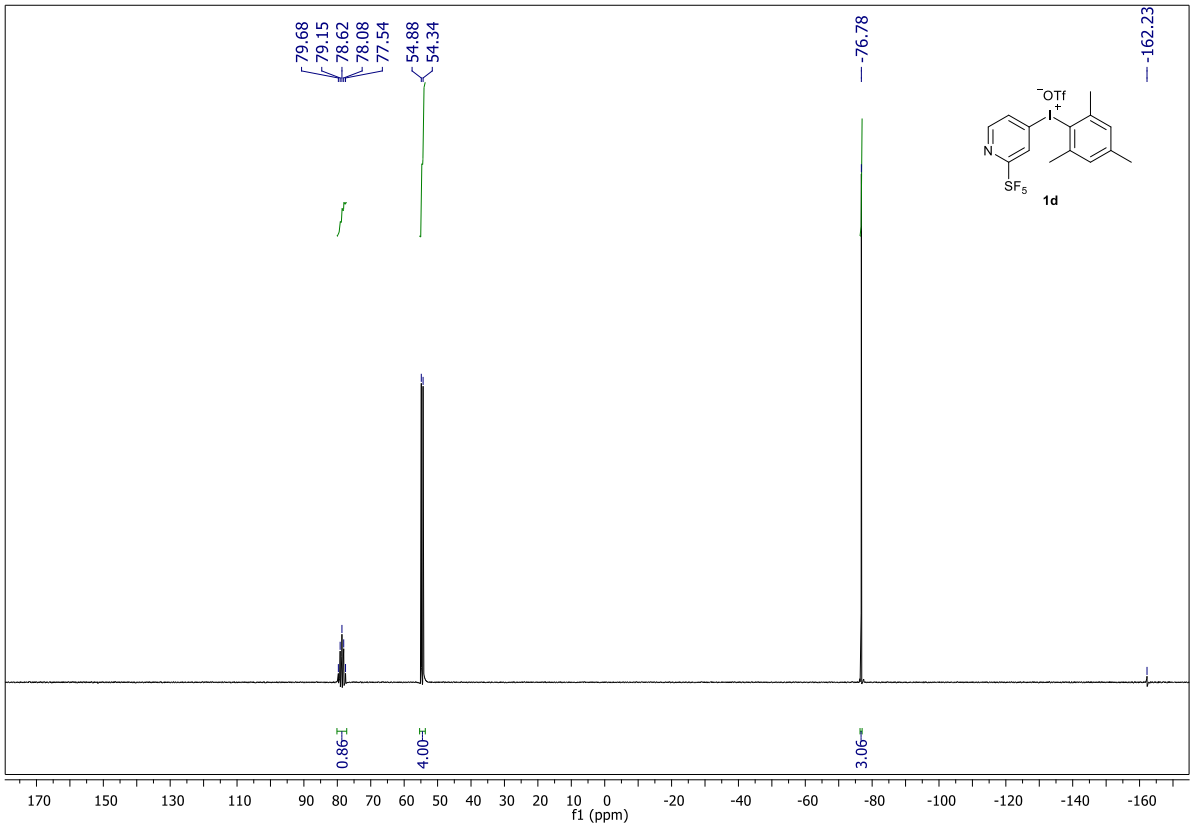
20.01
OTf
F5S
N
1b
f1 (ppm)


8.71
7.54
7.52
7.50
7.25
2.60
2.44
-0.00
SF5
OTf
N
1c
1.00
2.03
2.31
5.92
3.02
f1 (ppm)


76.94
76.40
75.86
75.33
74.80
53.90
53.37
-78.98
-162.20
SF5
OTf
N
I
1c
1.00
4.34
3.29
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)


163.58
163.36
163.16
149.66
146.87
143.41
142.09
131.36
130.44
121.61
121.43
118.89
104.29
77.42
77.16
76.91
27.25
21.45
0.11
SF5
OTf
N
I
1c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.72
8.71
8.65
8.02
8.00
7.37
2.72
2.41
2.06
2.05
2.04
1.00
0.98
0.99
1.97
6.23
2.94
f1 (ppm)
1d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54.34
-76.78
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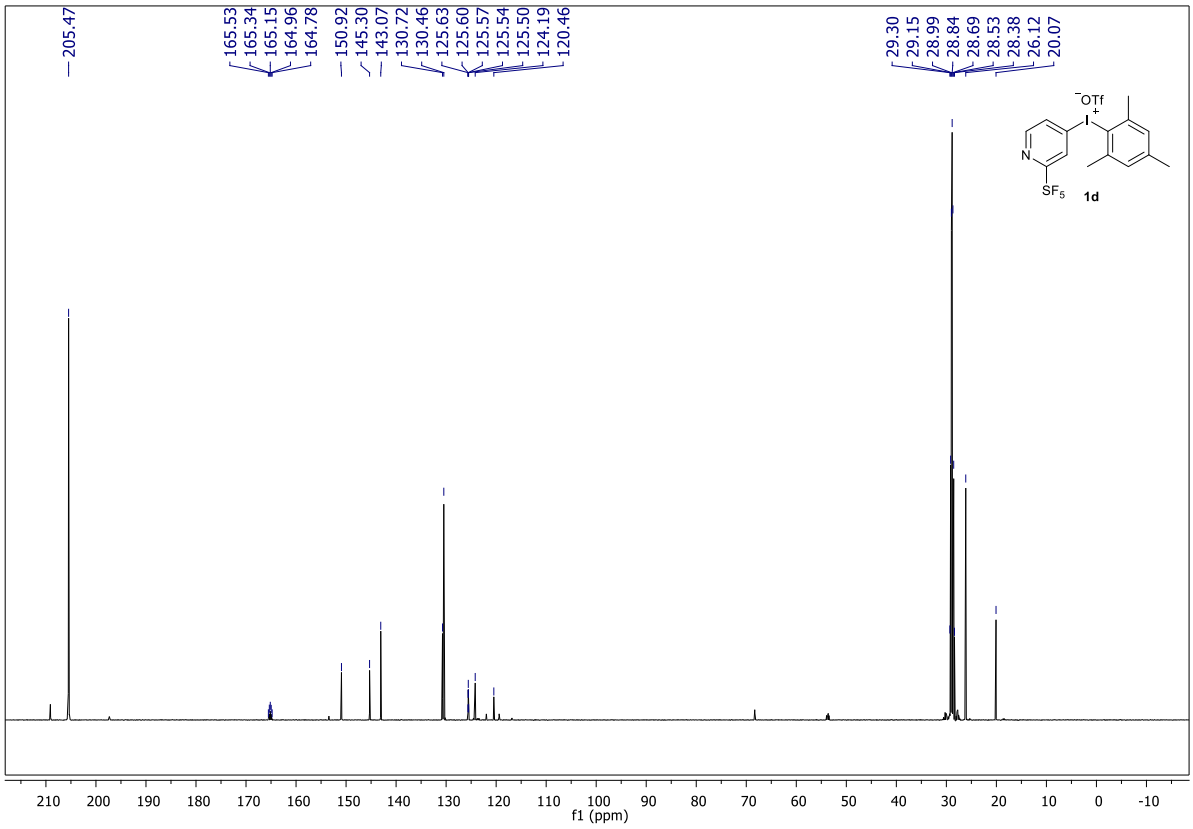
0.86
4.00
3.06
f1 (ppm)
1d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165.34
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164.78
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145.30
143.07
130.72
130.46
125.63
125.60
125.57
125.54
125.50
124.19
120.46
29.30
29.15
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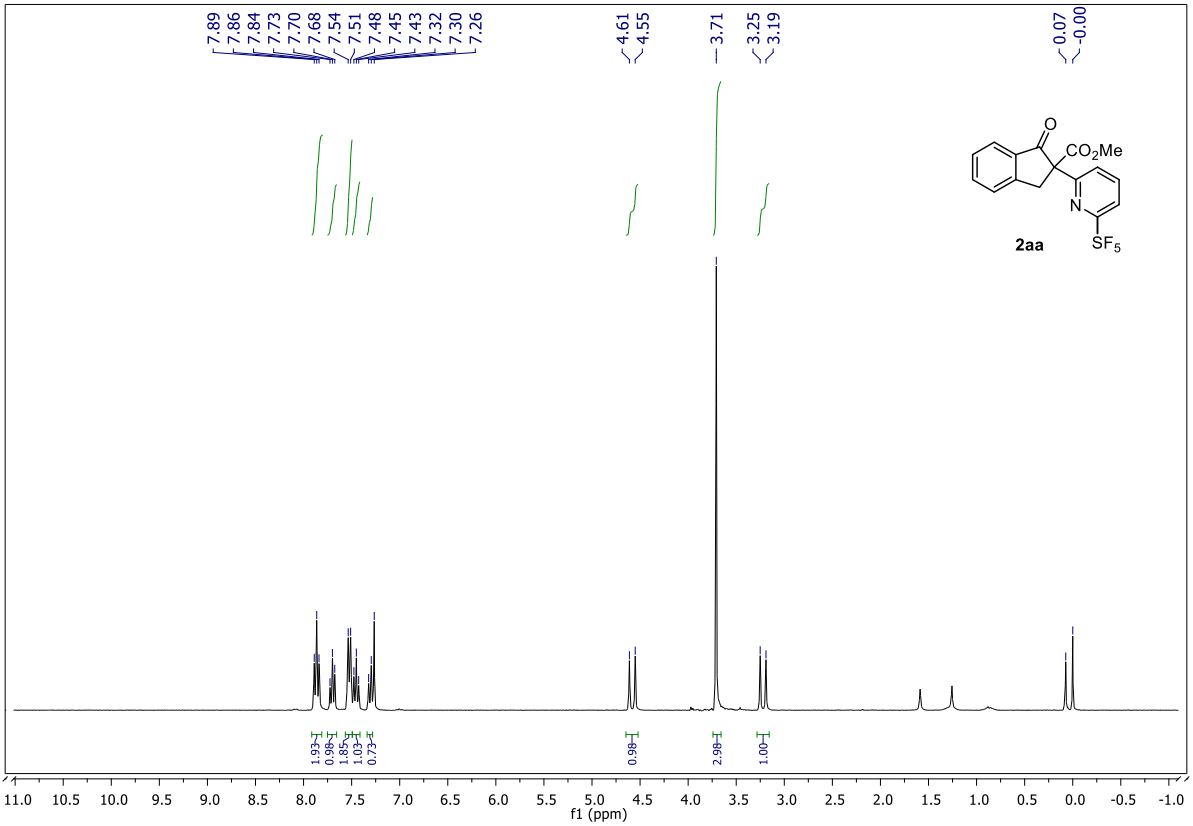
28.69
28.53
28.38
26.12
20.07
OTf
N
SF5
1d
f1 (ppm)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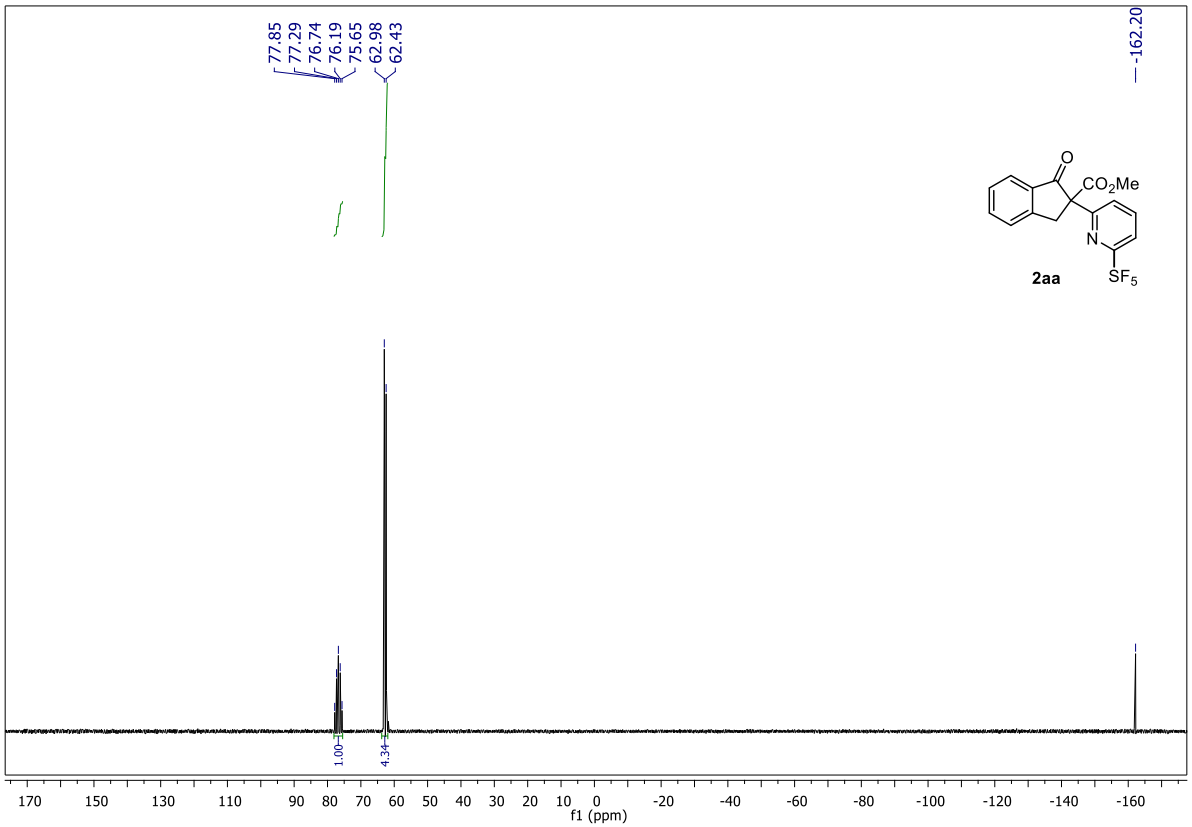
7.51
7.48
7.45
7.43
7.32
7.30
7.26
4.61
4.55
3.71
3.25
3.19
0.07
-0.00
O
CO2Me
N
SF5
2aa
1.93
0.98
1.85
1.03
0.73
0.98
2.98
1.00
f1 (ppm)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-162.20
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CO2Me
N
SF5
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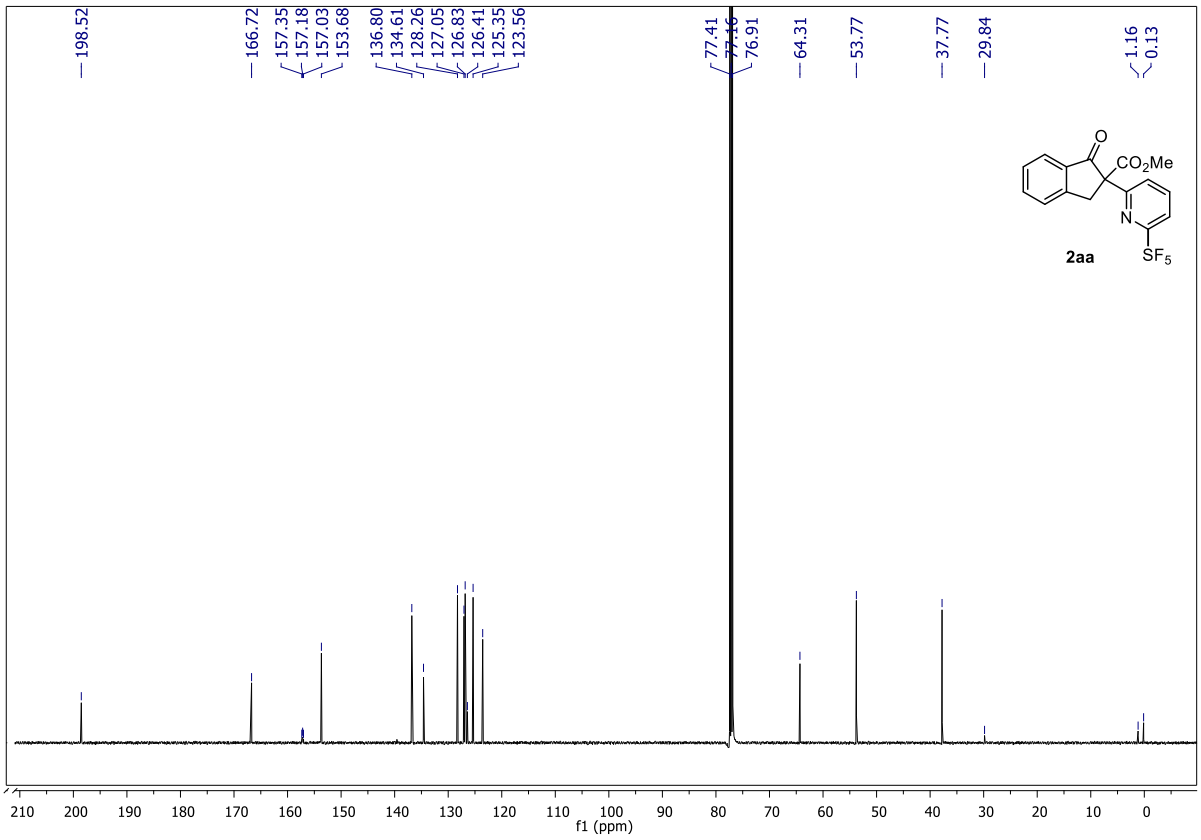
1.00
4.34
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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134.61
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126.83
126.41
125.35
123.56
77.41
77.16
76.91
64.31
53.77
37.77
29.84
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CO2Me
N
SF5
2aa
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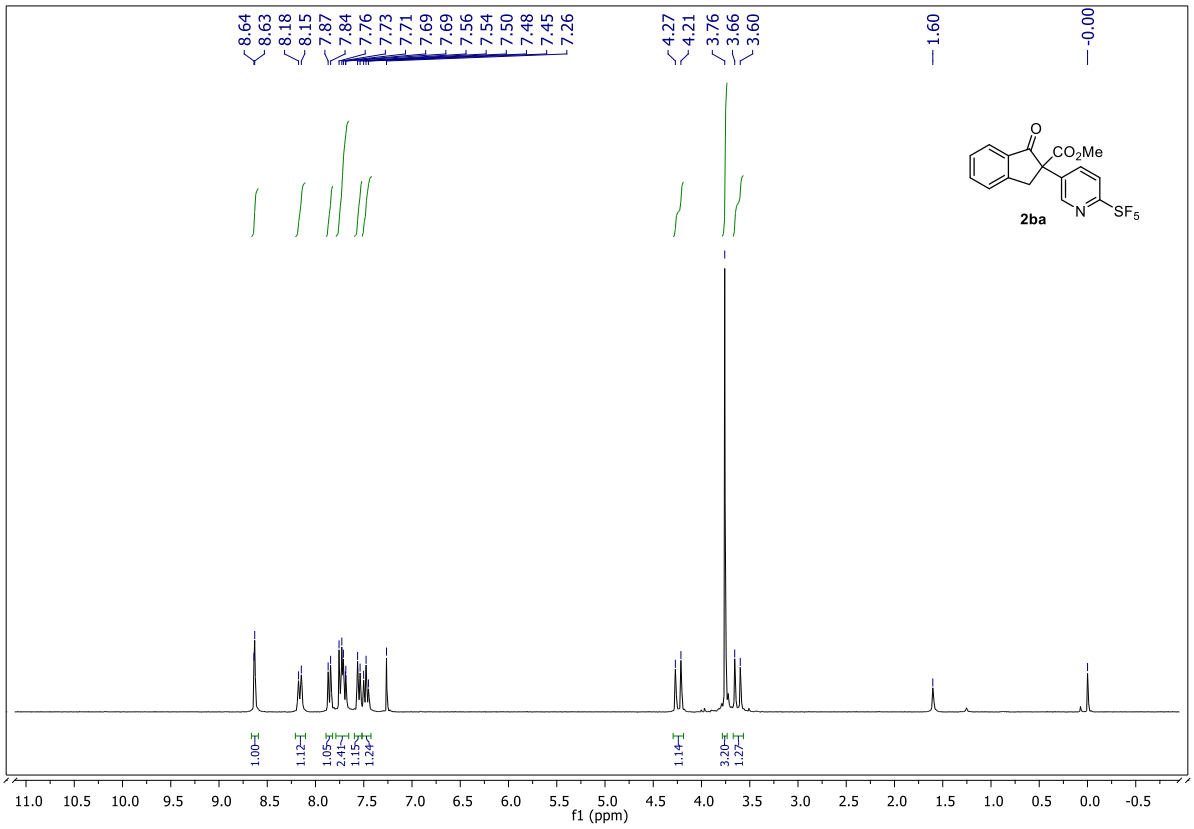
f1 (ppm)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7.73
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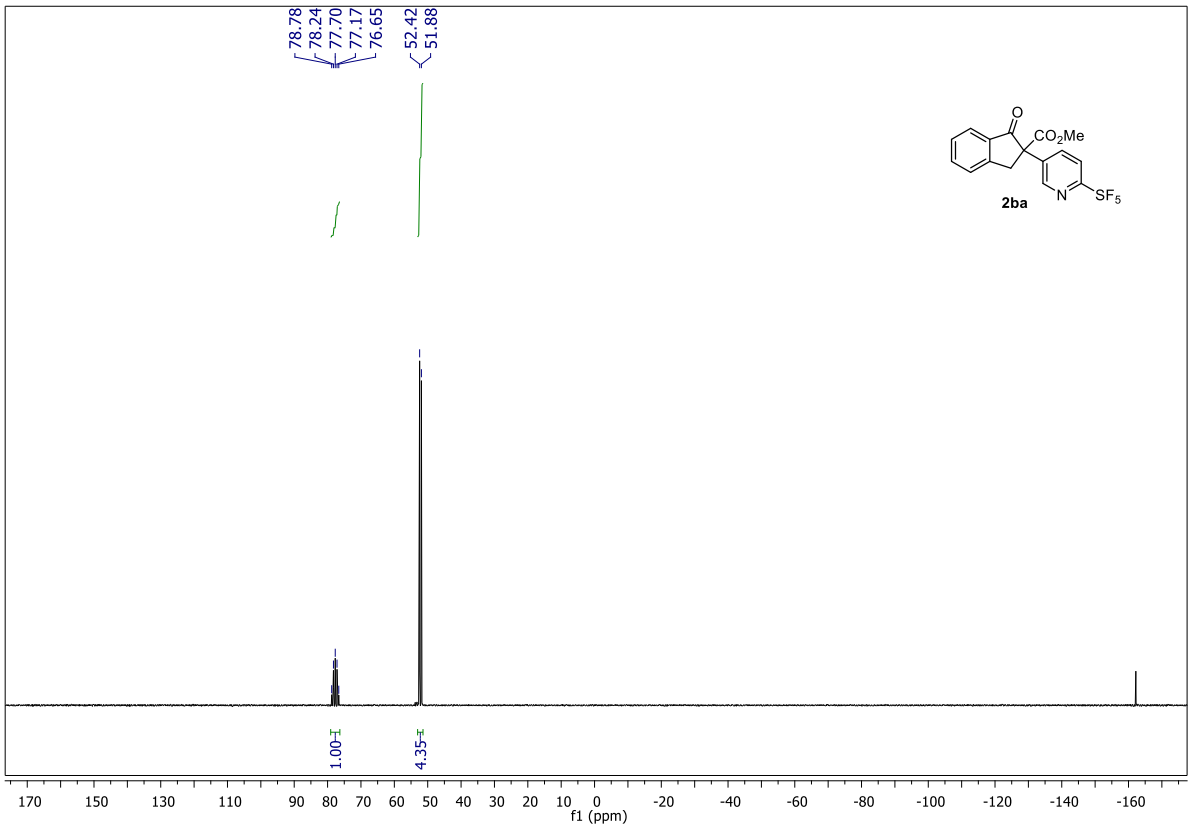
7.69
7.69
7.56
7.54
7.50
7.48
7.45
7.26
4.27
4.21
3.76
3.66
3.60
1.60
-0.00
O
CO2Me
N
SF5
2ba
1.00
1.12
1.05
2.41
1.15
1.24
1.14
3.20
1.27
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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51.88
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SF5
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4.35
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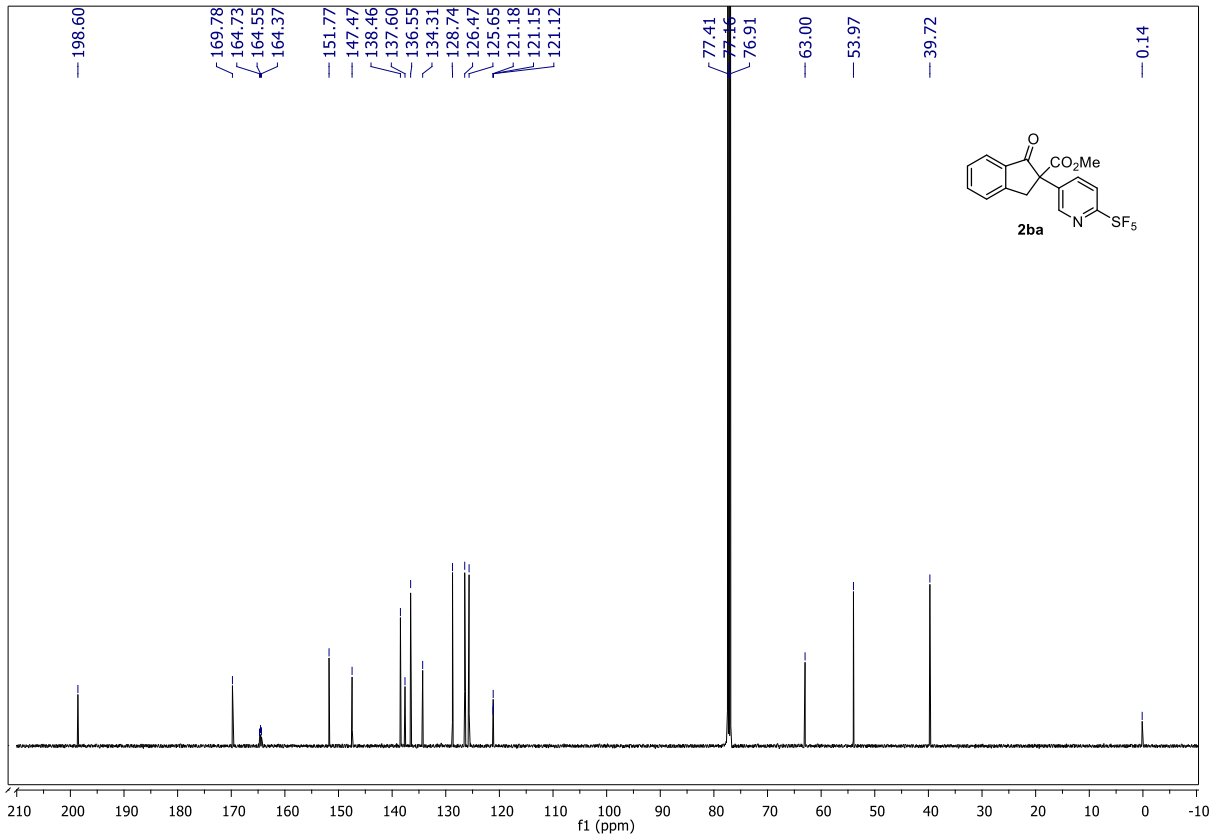
f1 (ppm)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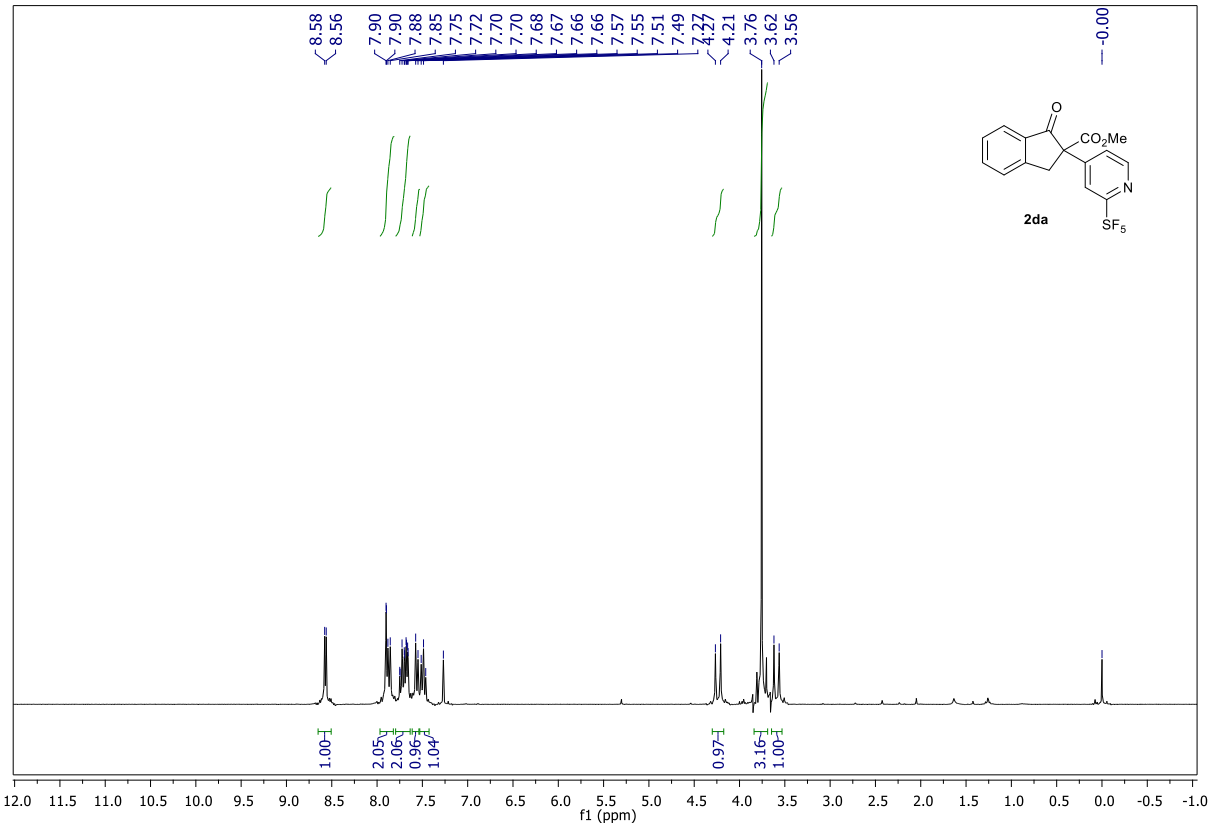
138.46
137.60
136.55
134.31
128.74
126.47
125.65
121.18
121.15
121.12
77.41
77.16
76.91
63.00
53.97
39.72
0.14
O
CO2Me
N
SF5
2ba
f1 (ppm)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8.56
7.90
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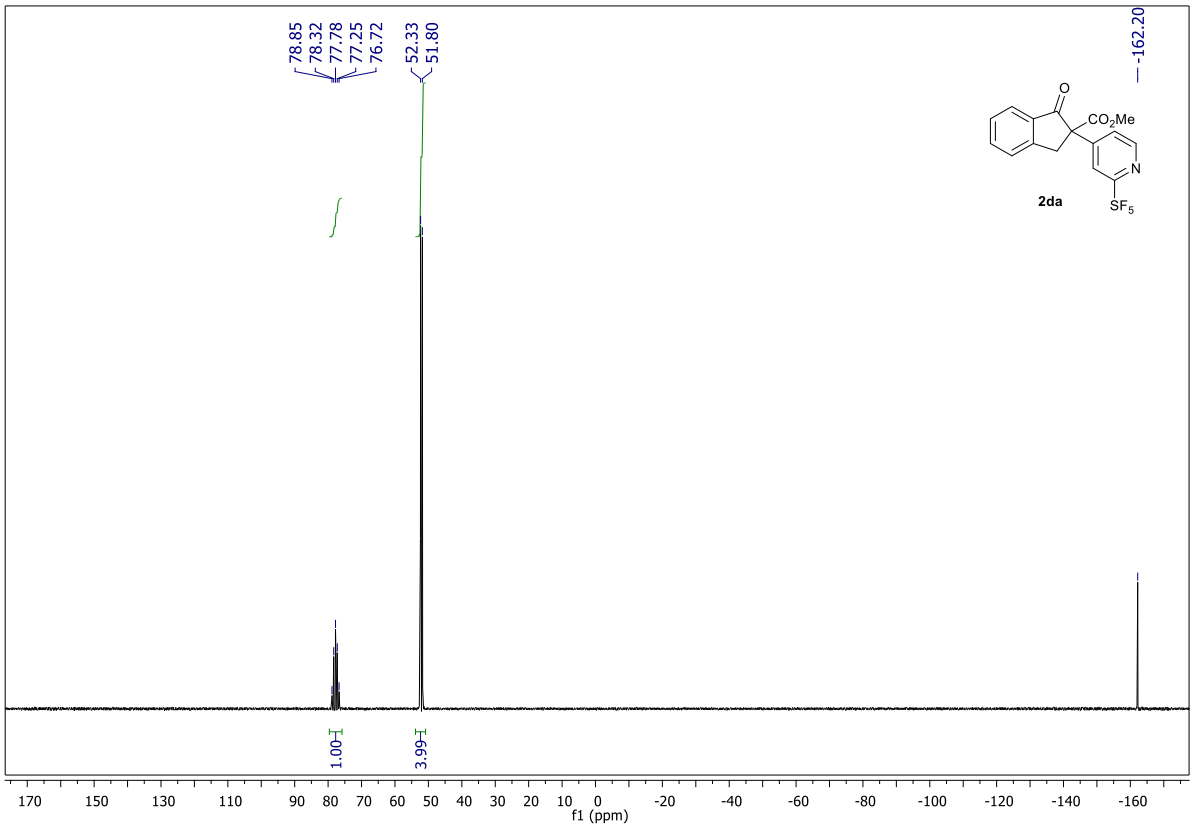
7.85
7.75
7.72
7.70
7.70
7.68
7.67
7.66
7.66
7.57
7.55
7.51
7.49
4.27
4.21
3.76
3.62
3.56
-0.00
1.00
2.05
2.06
0.96
1.04
0.97
3.16
1.00
O
CO2Me
N
SF5
2da
f1 (ppm)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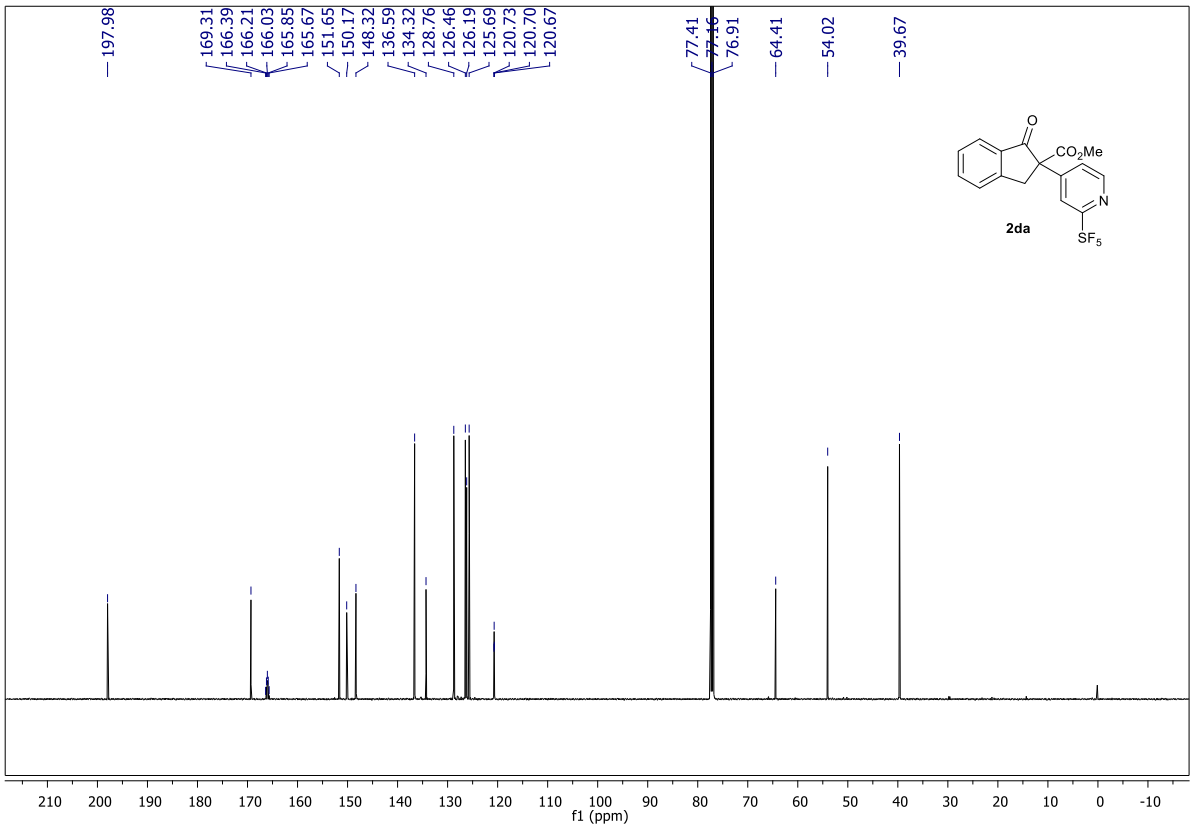
77.25
76.72
52.33
51.80
-162.20
O
CO2Me
N
SF5
2da
1.00
3.99
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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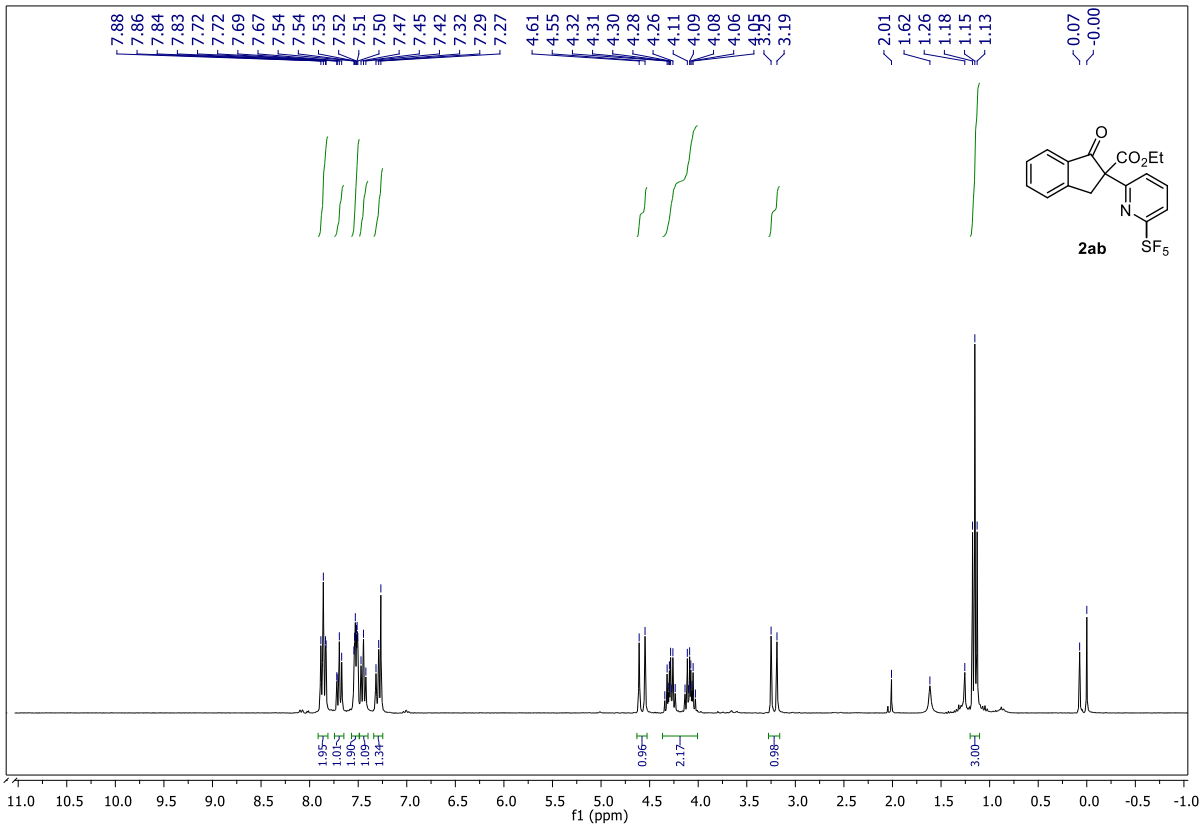
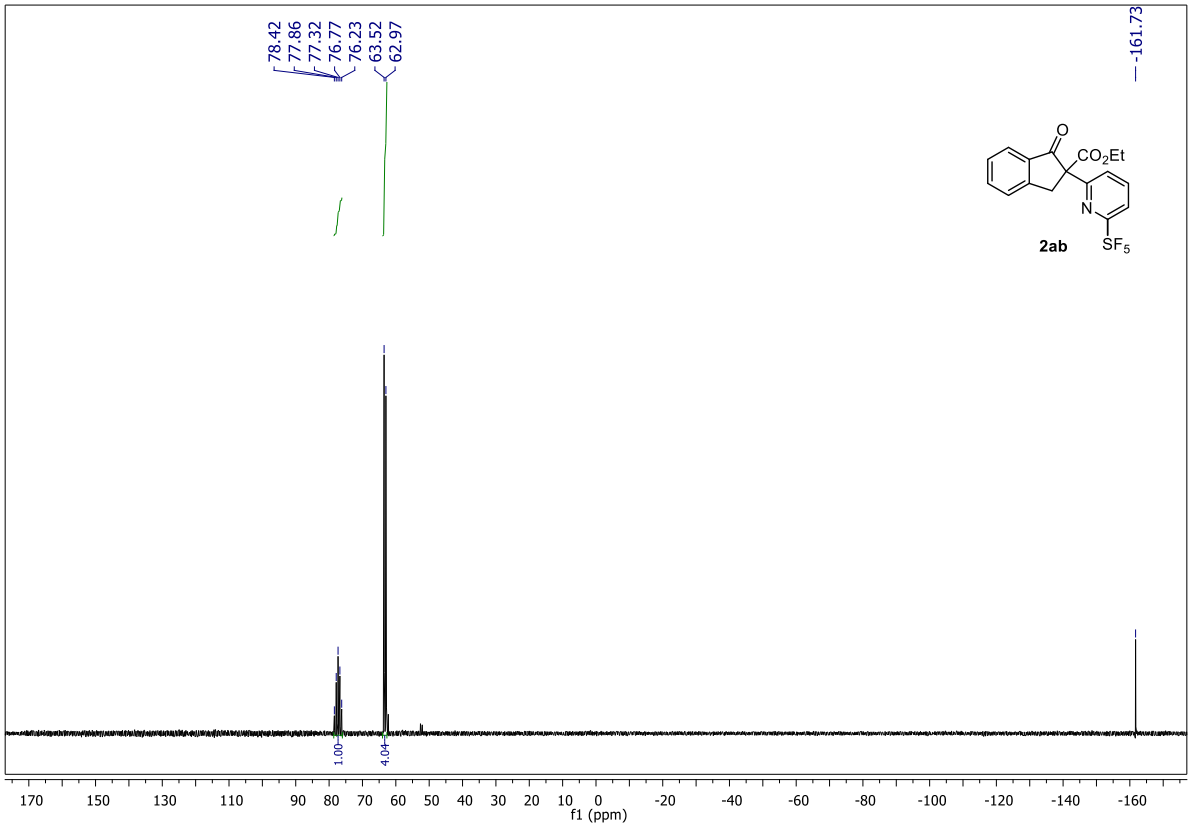
166.21
166.03
165.85
165.67
151.65
150.17
148.32
136.59
134.32
128.76
126.46
126.19
125.69
120.73
120.70
120.67
77.41
77.16
76.91
64.41
54.02
39.67
O
CO2Me
N
SF5
2da
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.88 7.86 7.84 7.83 7.72 7.72 7.69 7.67 7.54 7.54 7.53 7.52 7.51 7.50 7.47 7.45 7.42 7.32 7.29 7.27
4.61 4.55 4.32 4.31 4.30 4.28 4.26 4.11 4.09 4.08 4.06 4.05 3.25 3.19
2.01 1.62 1.26 1.18 1.15 1.13
0.07 -0.00
O
CO2Et
N
SF5
2ab
1.95 1.01 1.90 1.09 1.34
0.96 2.17 0.98 3.00
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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-161.73
O
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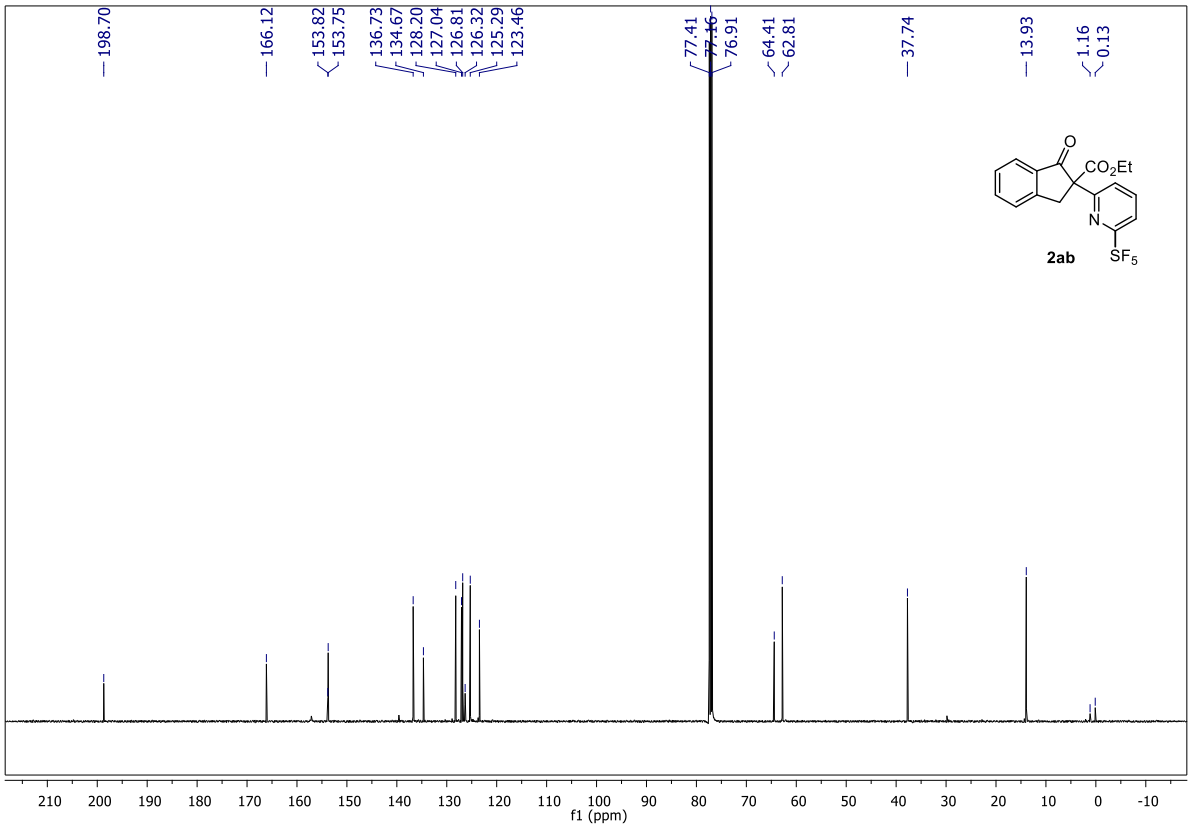
N
SF5
2ab
1.00 4.04
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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126.32
125.29
123.46
77.41
77.16
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37.74
13.93
1.16
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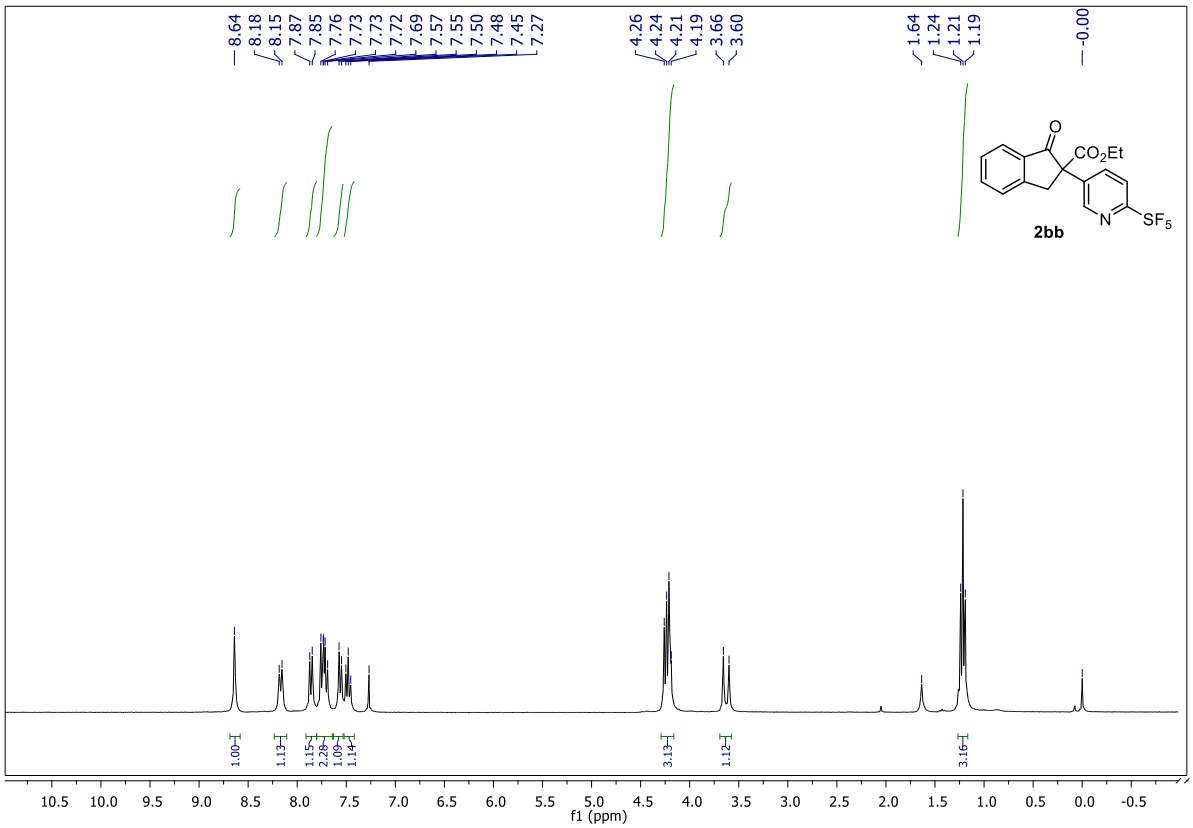
O
CO2Et
N
SF5
2ab
f1 (ppm)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7.73
7.73
7.72
7.69
7.57
7.55
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7.48
7.45
7.27
4.26
4.24
4.21
4.19
3.66
3.60
1.64
1.24
1.21
1.19
-0.00
O
CO2Et
N
SF5
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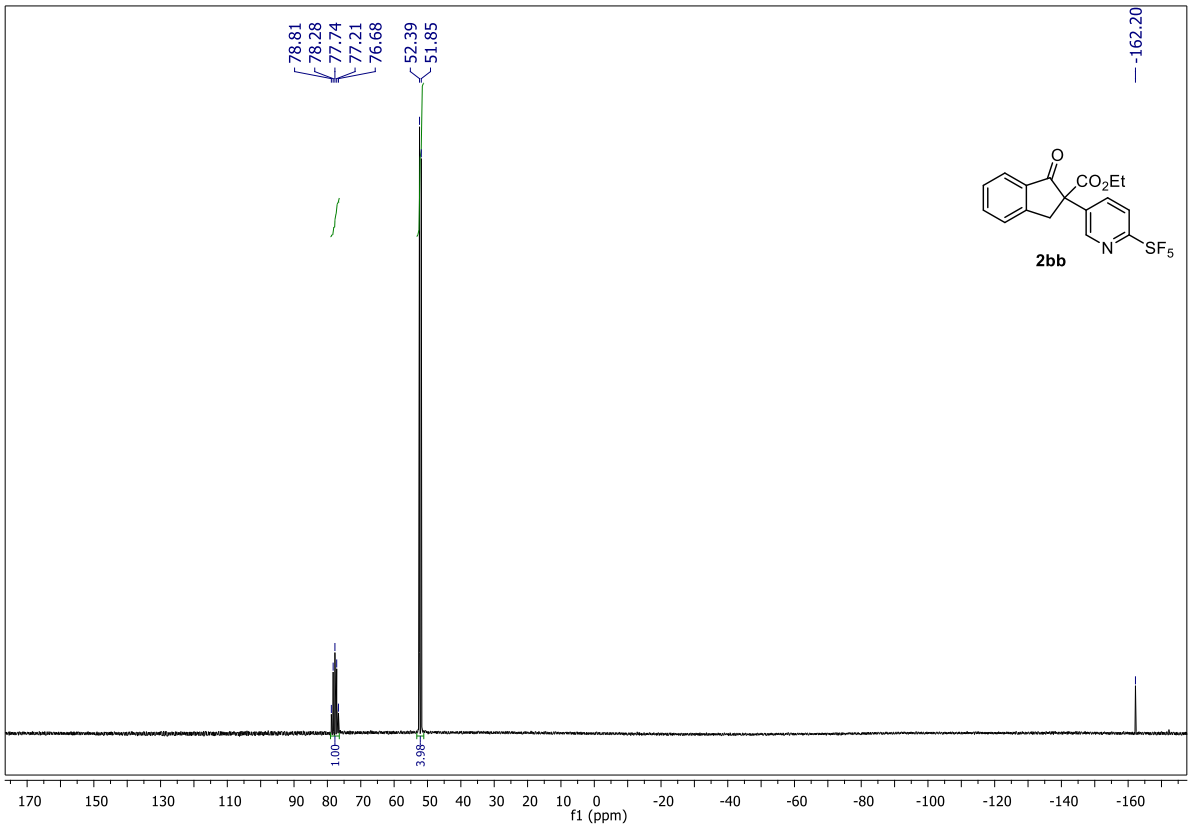
1.13
1.15
2.28
1.09
1.14
3.13
1.12
3.16
f1 (ppm)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77.21
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52.39
51.85
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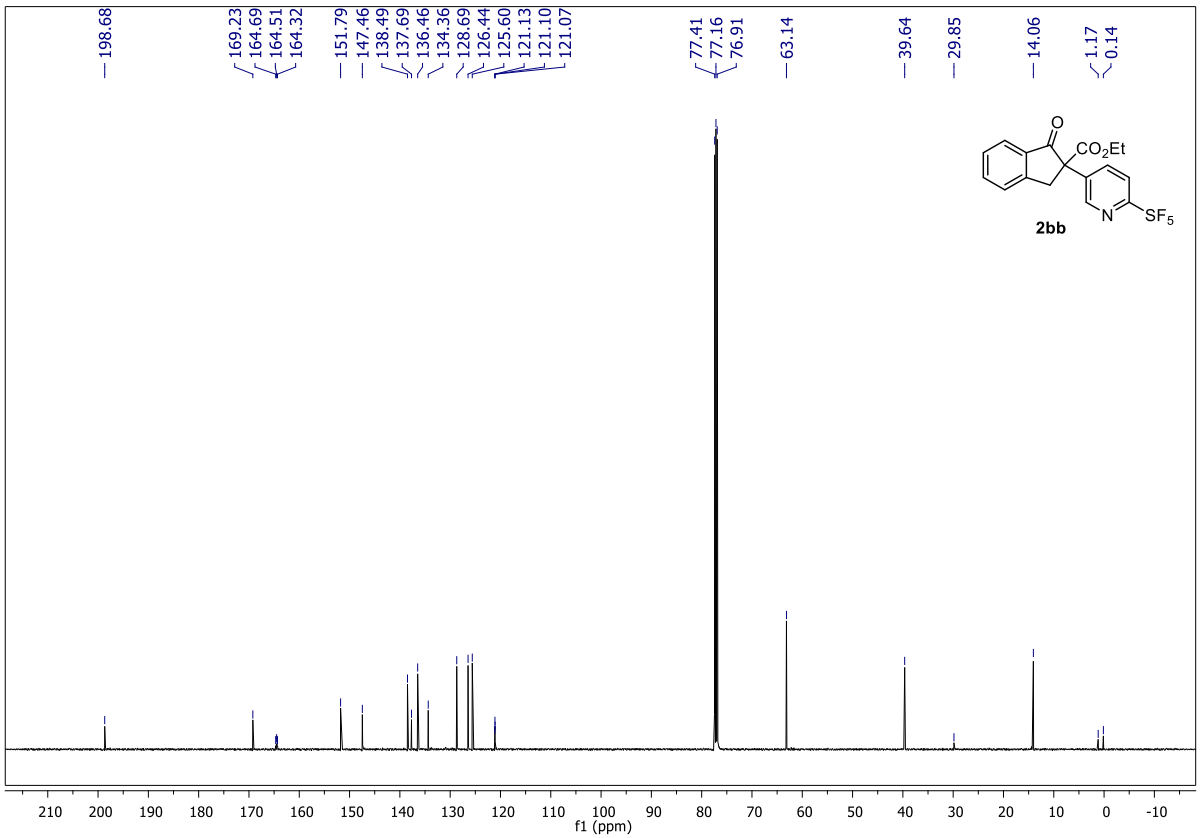
O
CO2Et
N
SF5
2bb
1.00
3.98
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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128.69
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125.60
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121.07
77.41
77.16
76.91
63.14
39.64
29.85
14.06
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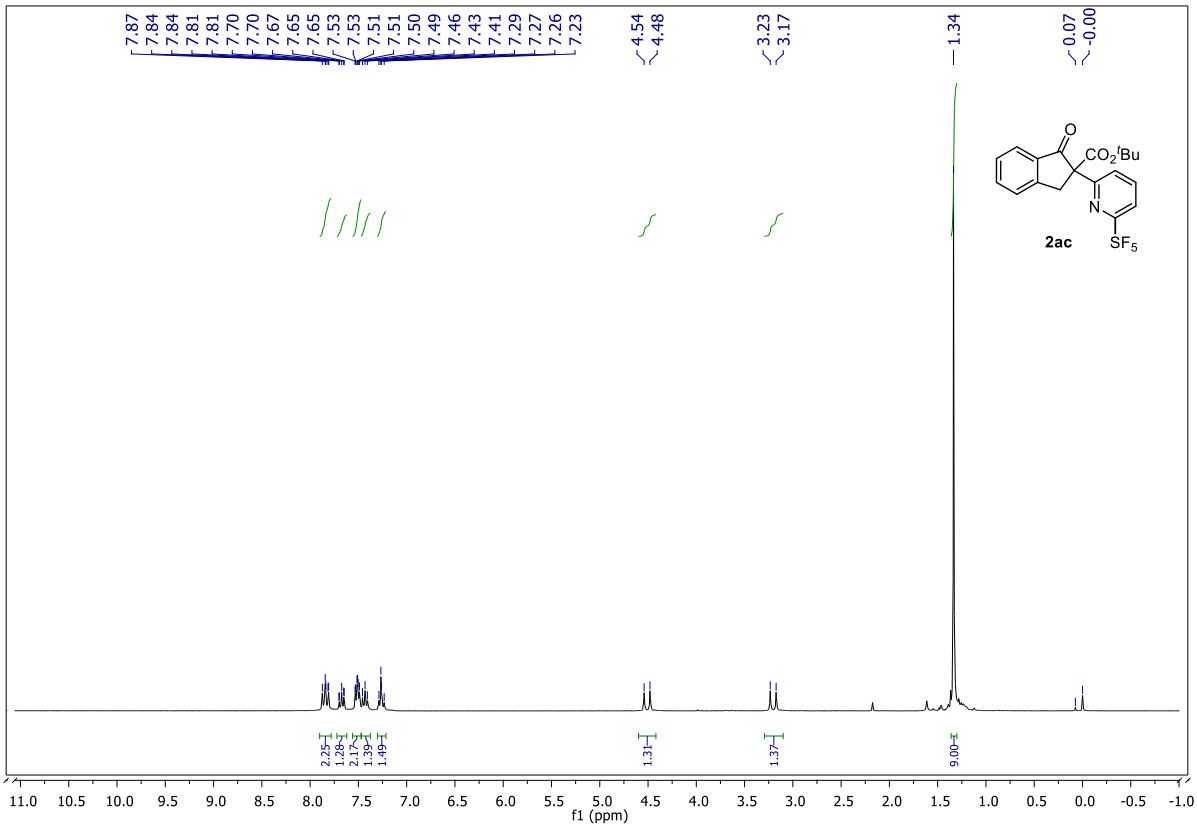
N
SF5
2bb
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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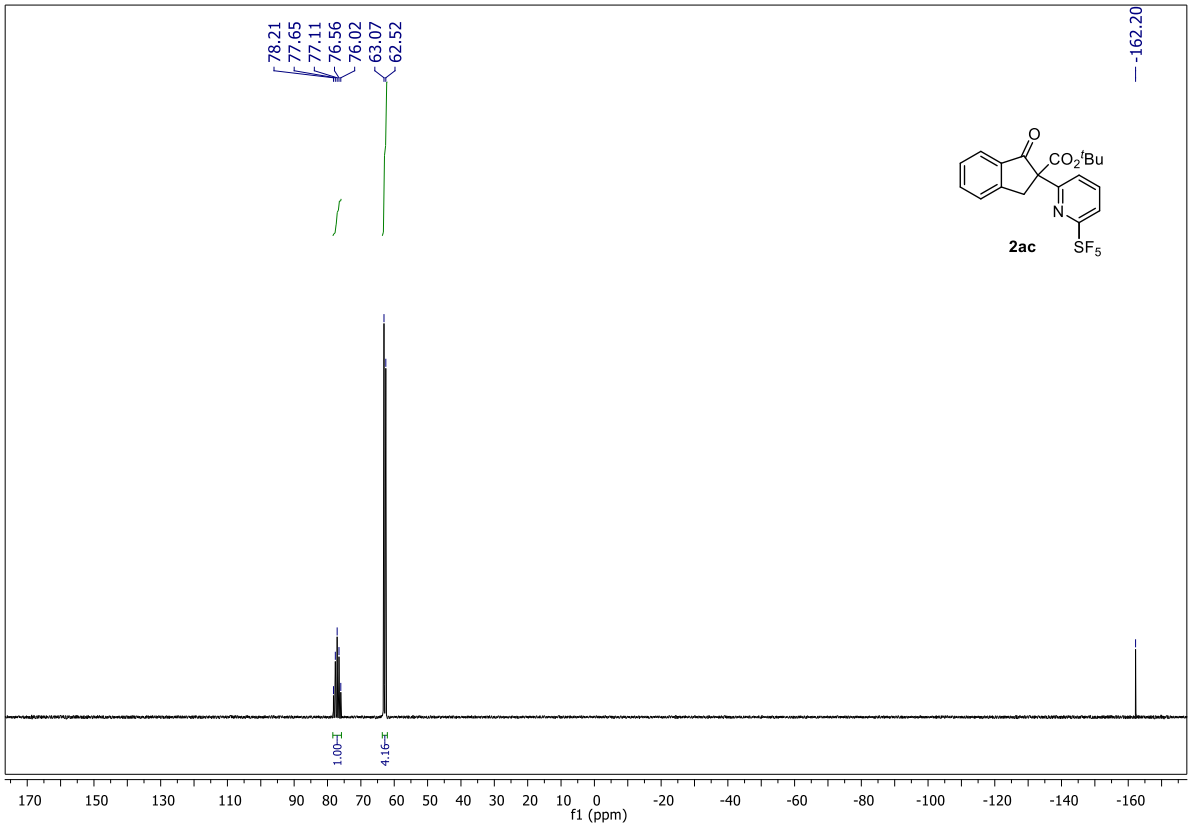
7.46
7.43
7.41
7.29
7.27
7.26
7.23
4.54
4.48
3.23
3.17
1.34
0.07
-0.00
O
CO2tBu
N
SF5
2ac
2.25
1.28
2.17
1.39
1.49
1.31
1.37
9.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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CO2tBu
N
SF5
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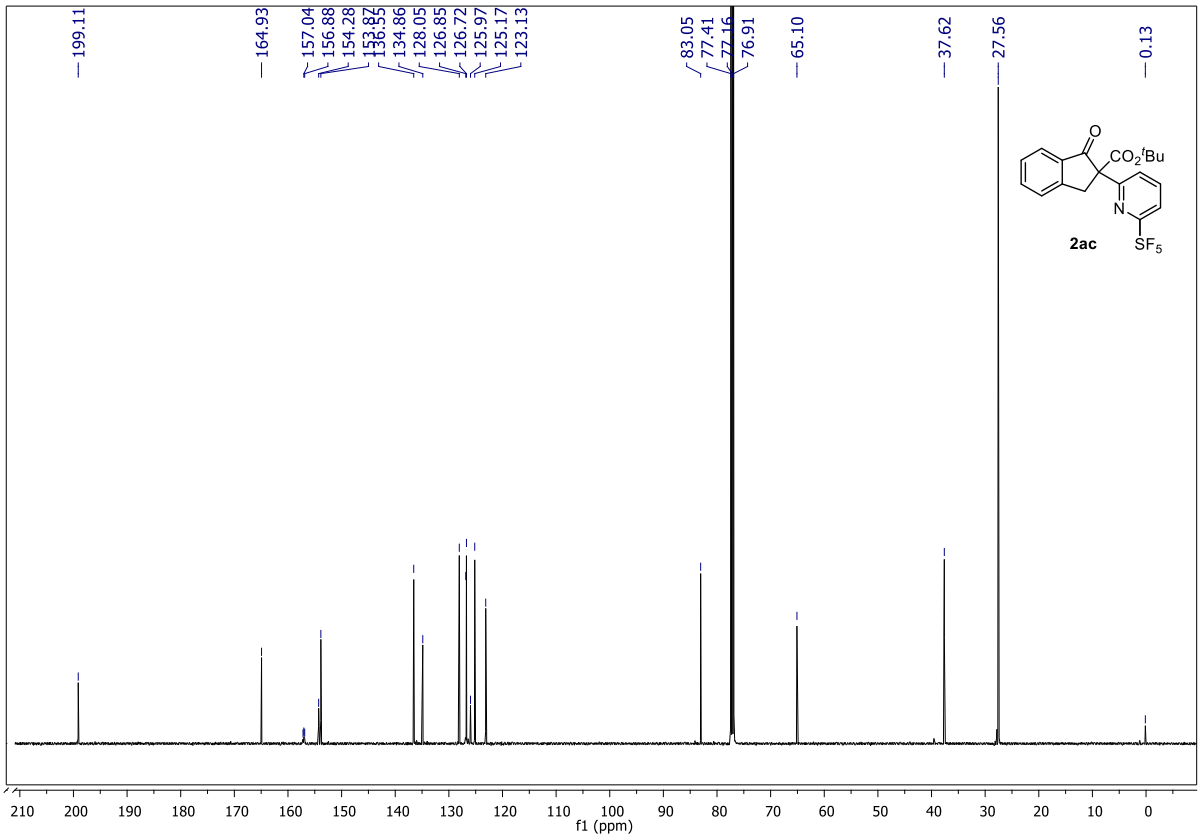
1.00
4.16
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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126.85
126.72
125.97
125.17
123.13
83.05
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77.16
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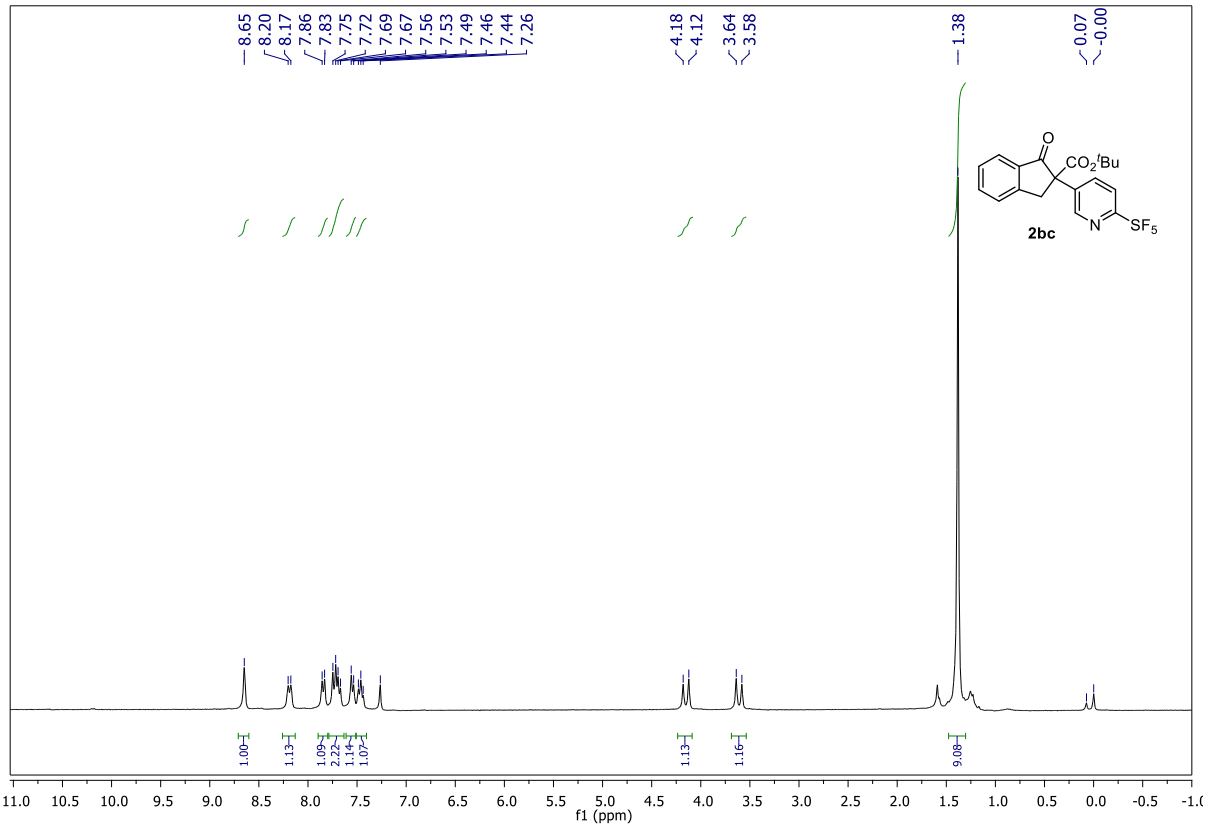
65.10
37.62
27.56
0.13
O
CO2tBu
N
2ac
SF5
f1 (ppm)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7.67
7.56
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7.49
7.46
7.44
7.26
4.18
4.12
3.64
3.58
1.38
0.07
-0.00
O
CO2tBu
N
SF5
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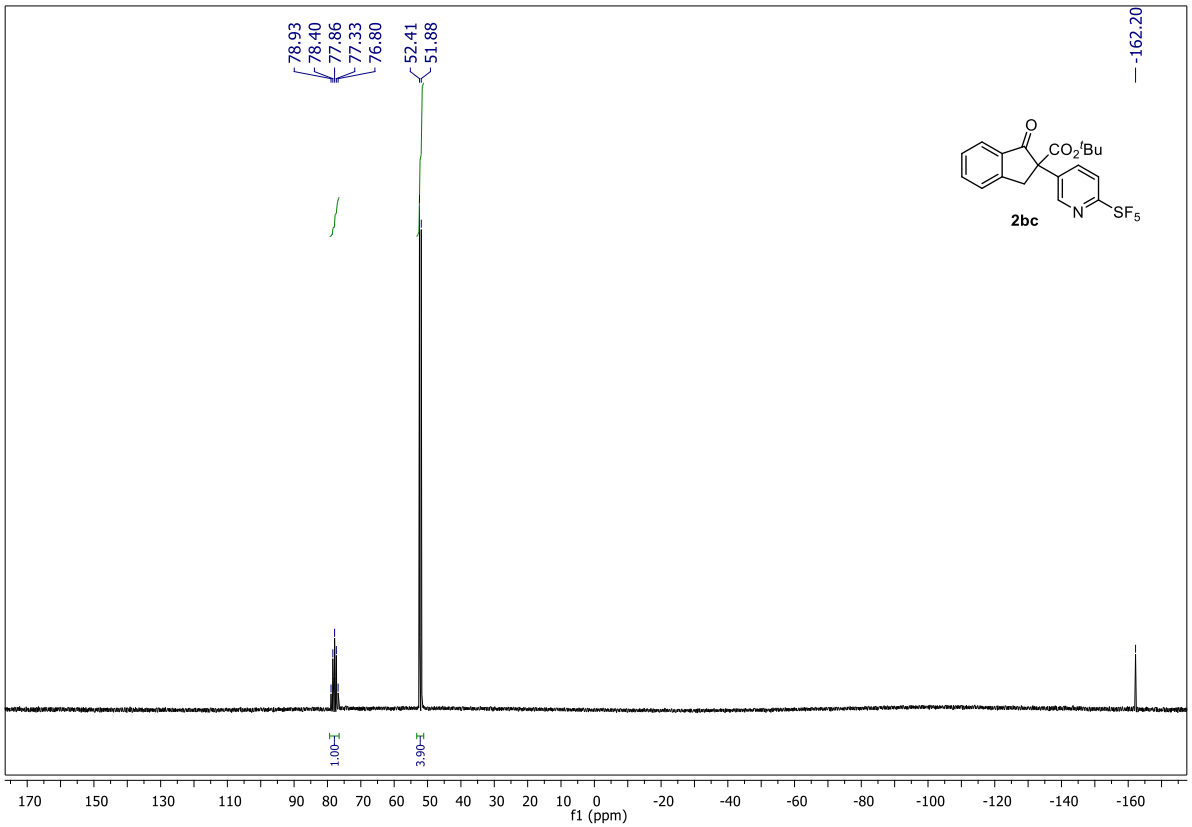
1.09
2.22
1.14
1.07
1.13
1.16
9.08
f1 (ppm)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CO2tBu
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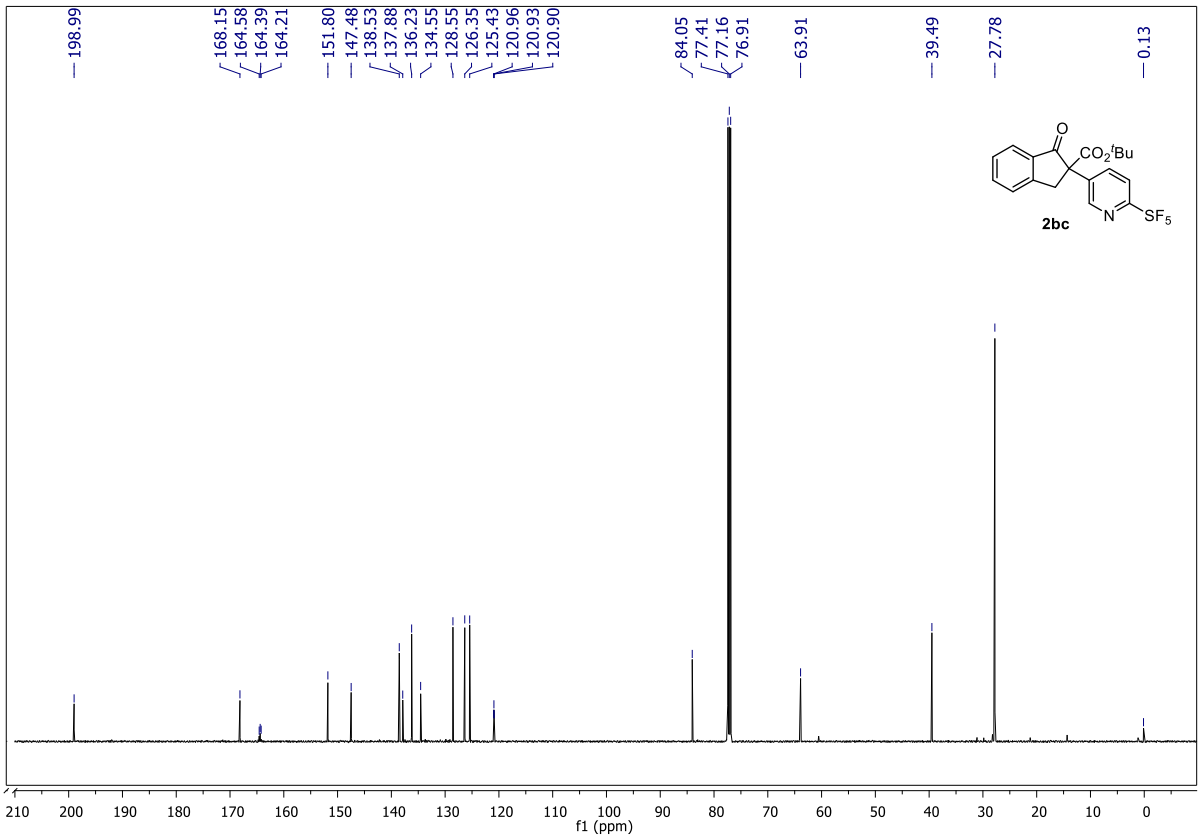
3.90
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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125.43
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84.05
77.41
77.16
76.91
63.91
39.49
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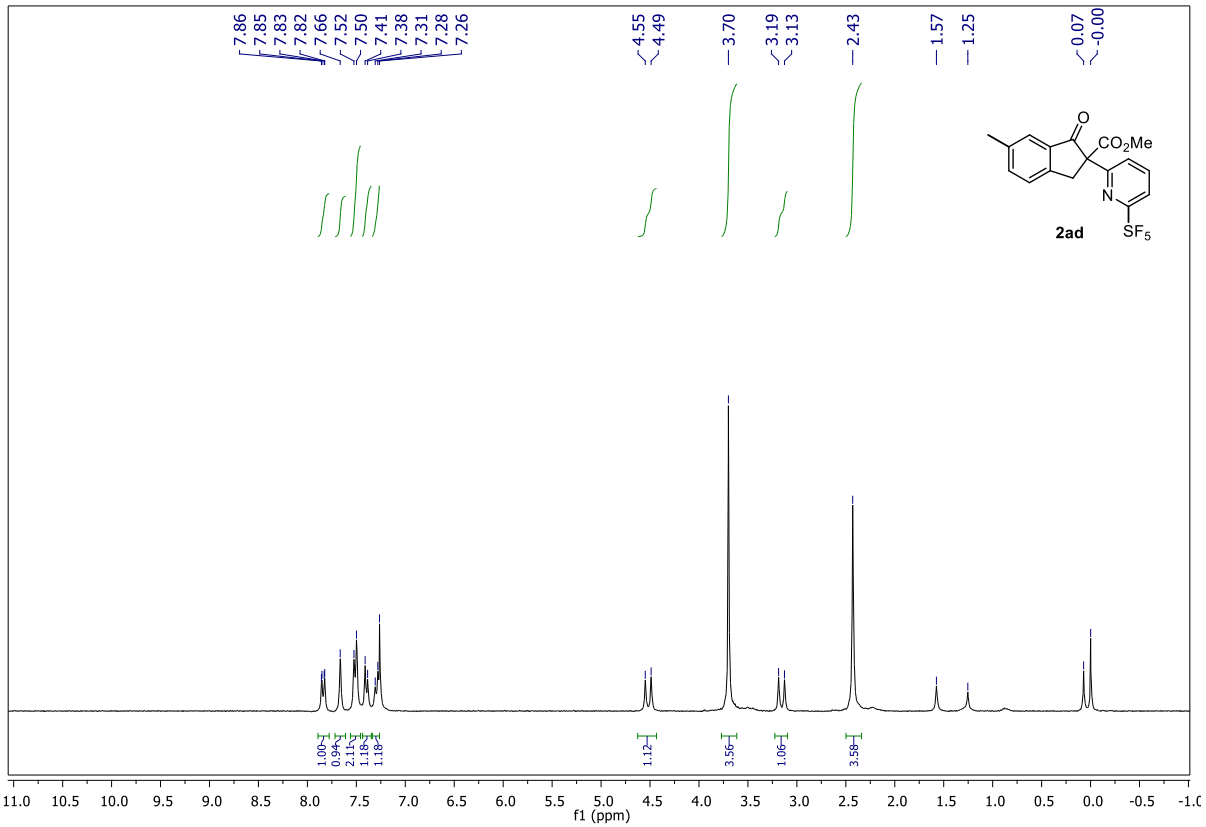
CO2tBu
N
SF5
2bc
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.26
4.55
4.49
3.70
3.19
3.13
2.43
1.57
1.25
0.07
-0.00
O
CO2Me
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2.11
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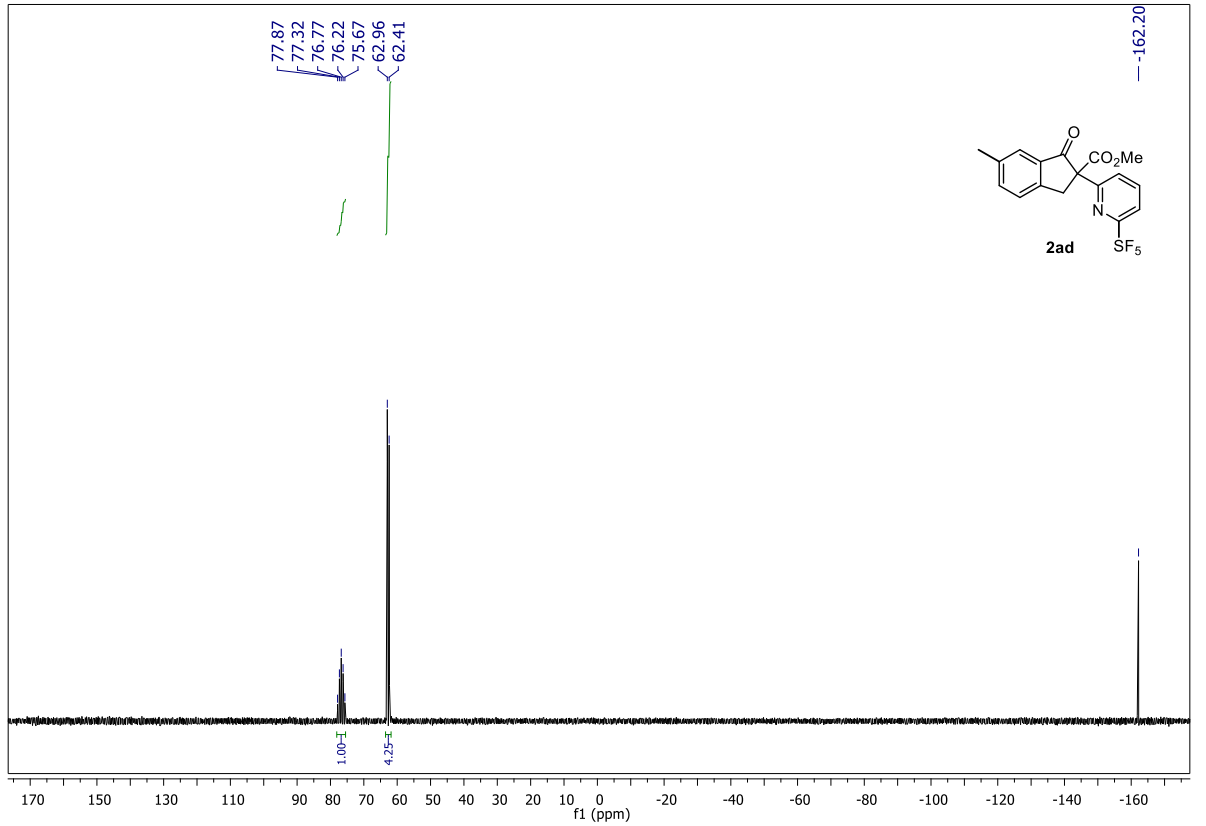
1.18
1.12
3.56
1.06
3.58
f1 (ppm)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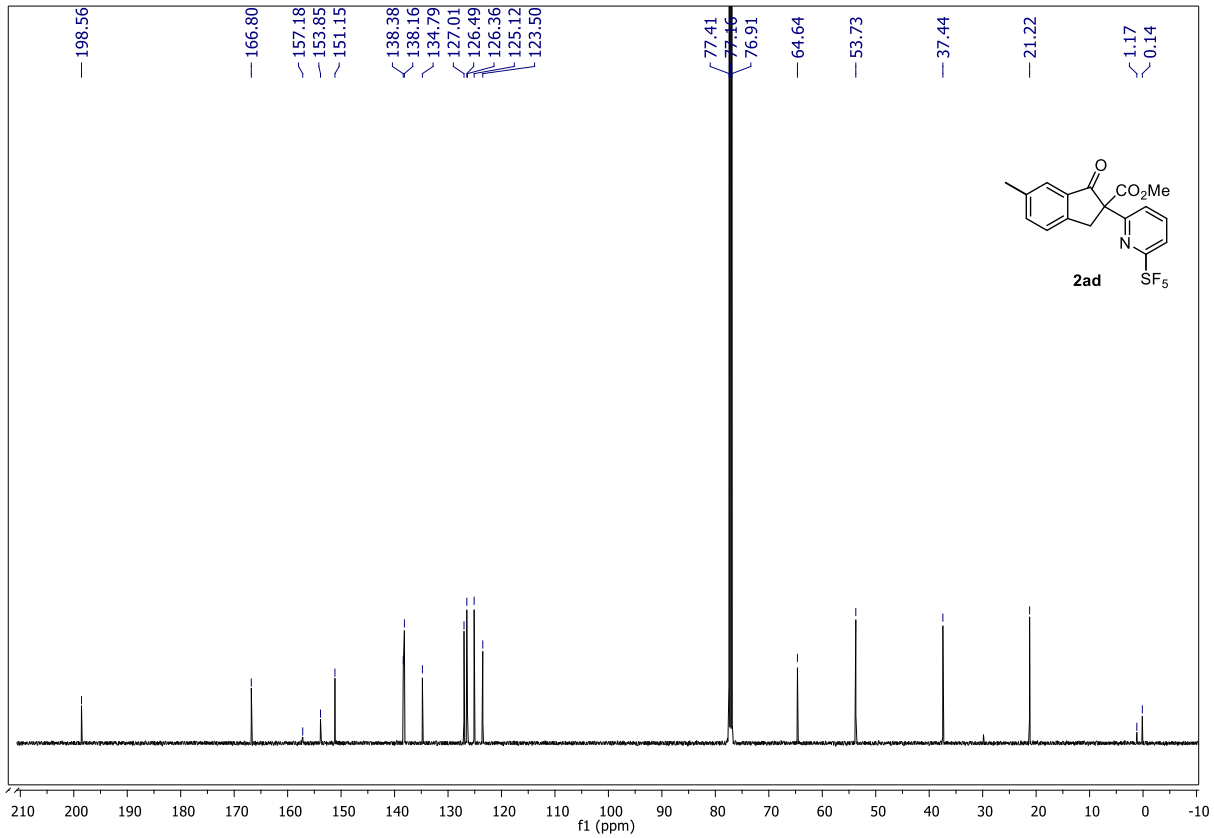
-162.20
O
CO2Me
N
SF5
2ad
1.00
4.25
f1 (ppm)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123.50
77.41
77.16
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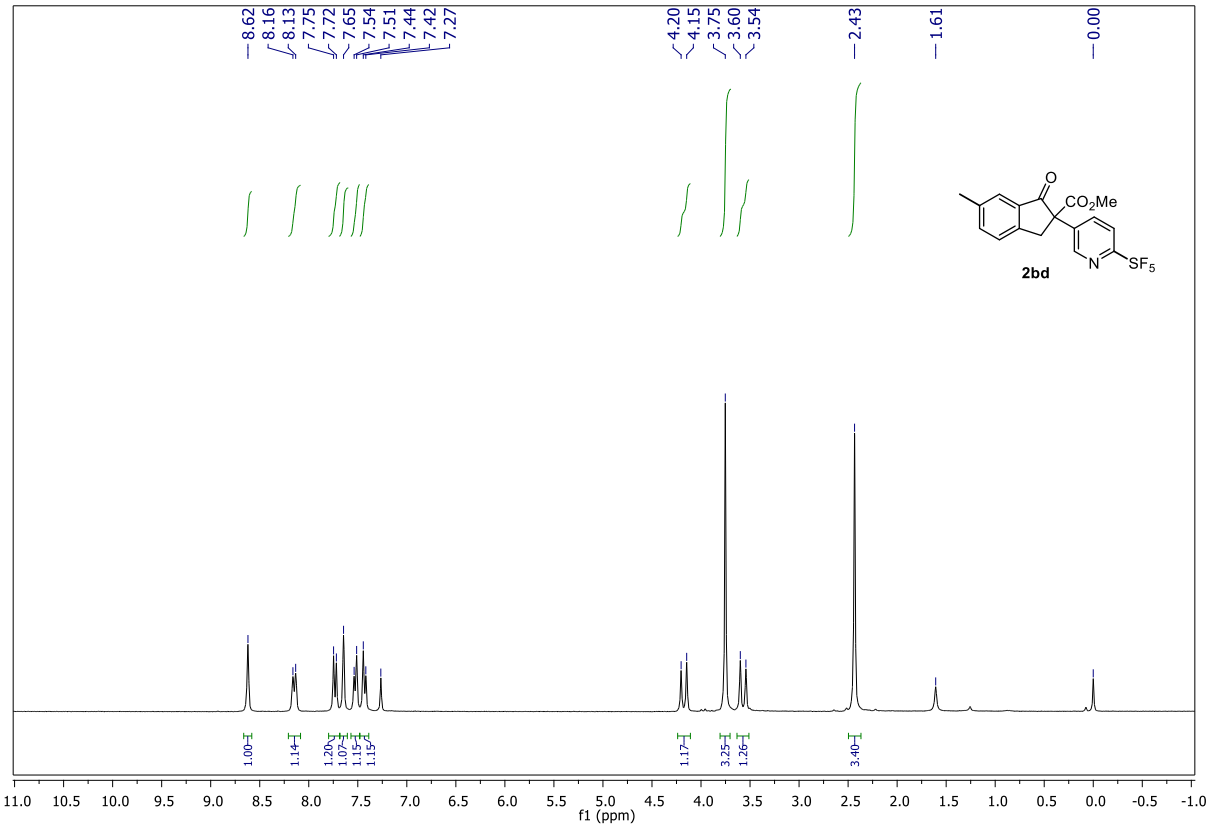
CO2Me
N
SF5
2ad
f1 (ppm)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4.15
3.75
3.60
3.54
2.43
1.61
0.00
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CO2Me
N
SF5
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1.07
1.15
1.15
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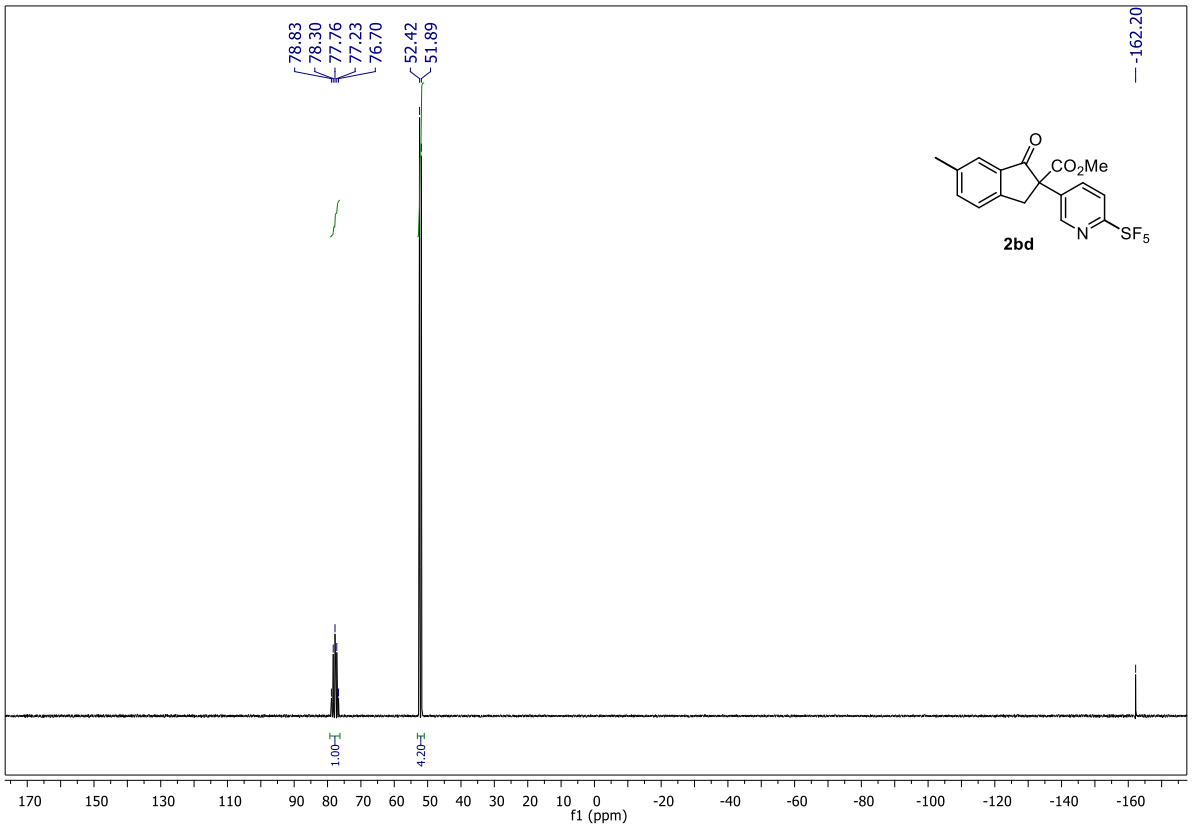
3.25
1.26
3.40
f1 (ppm)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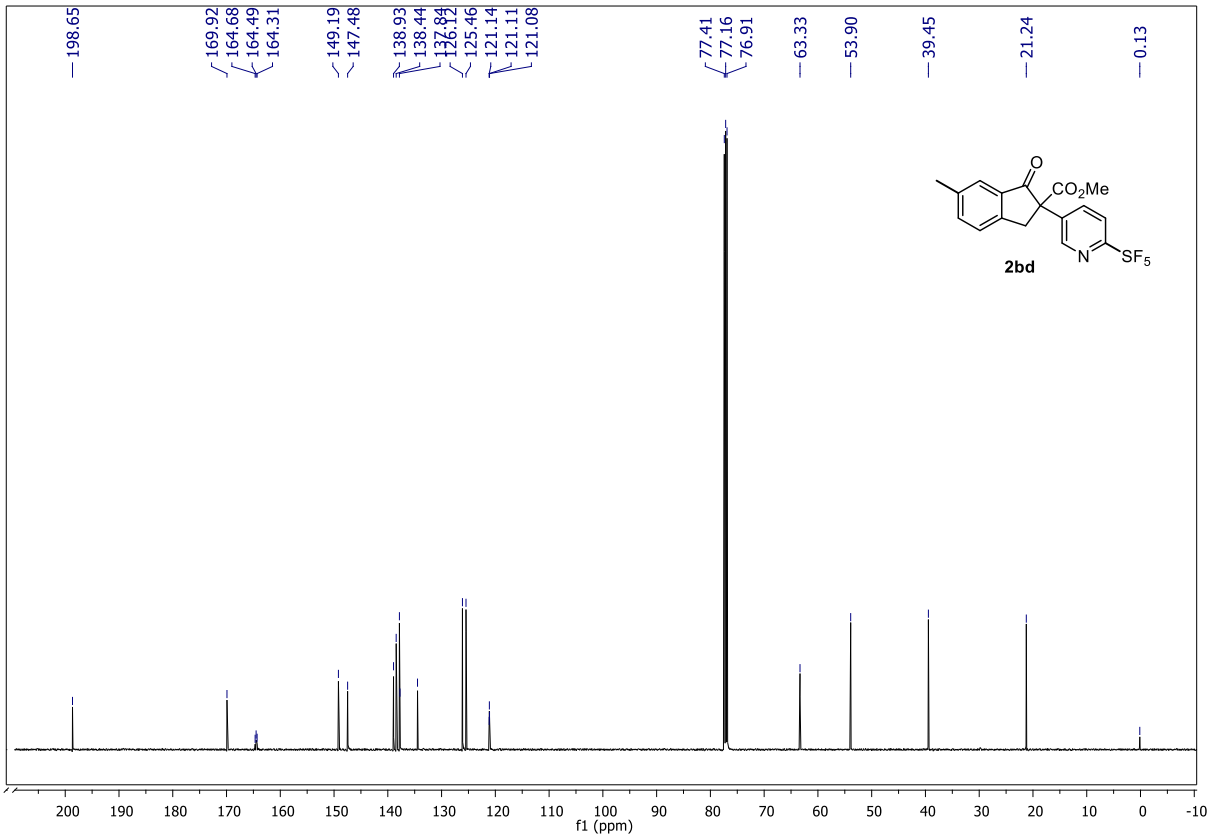
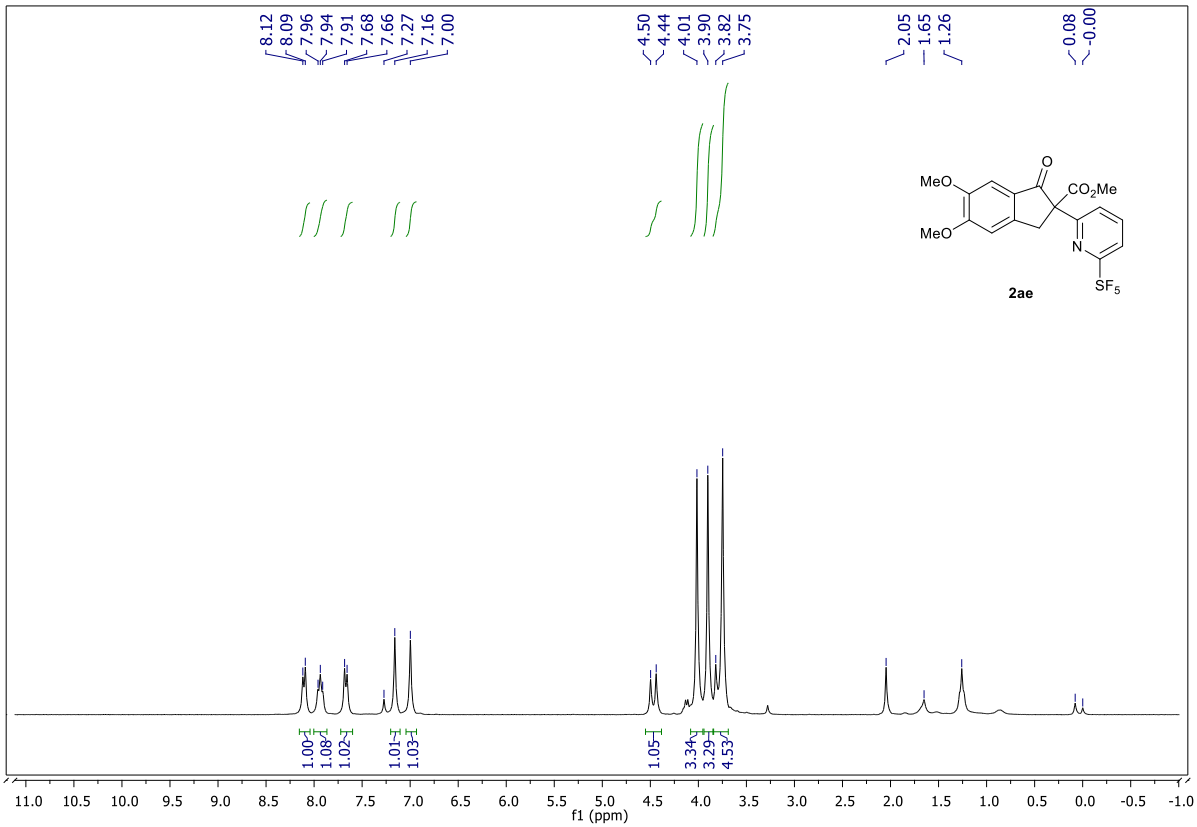
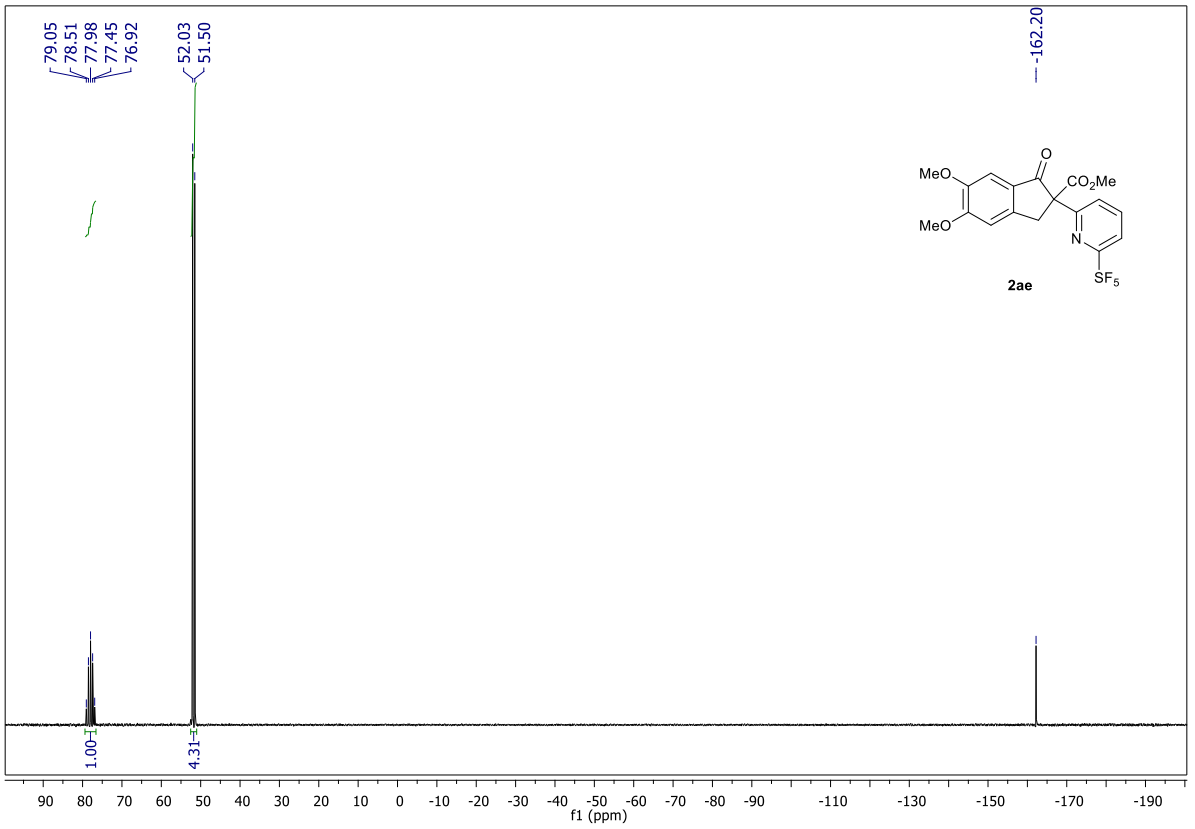
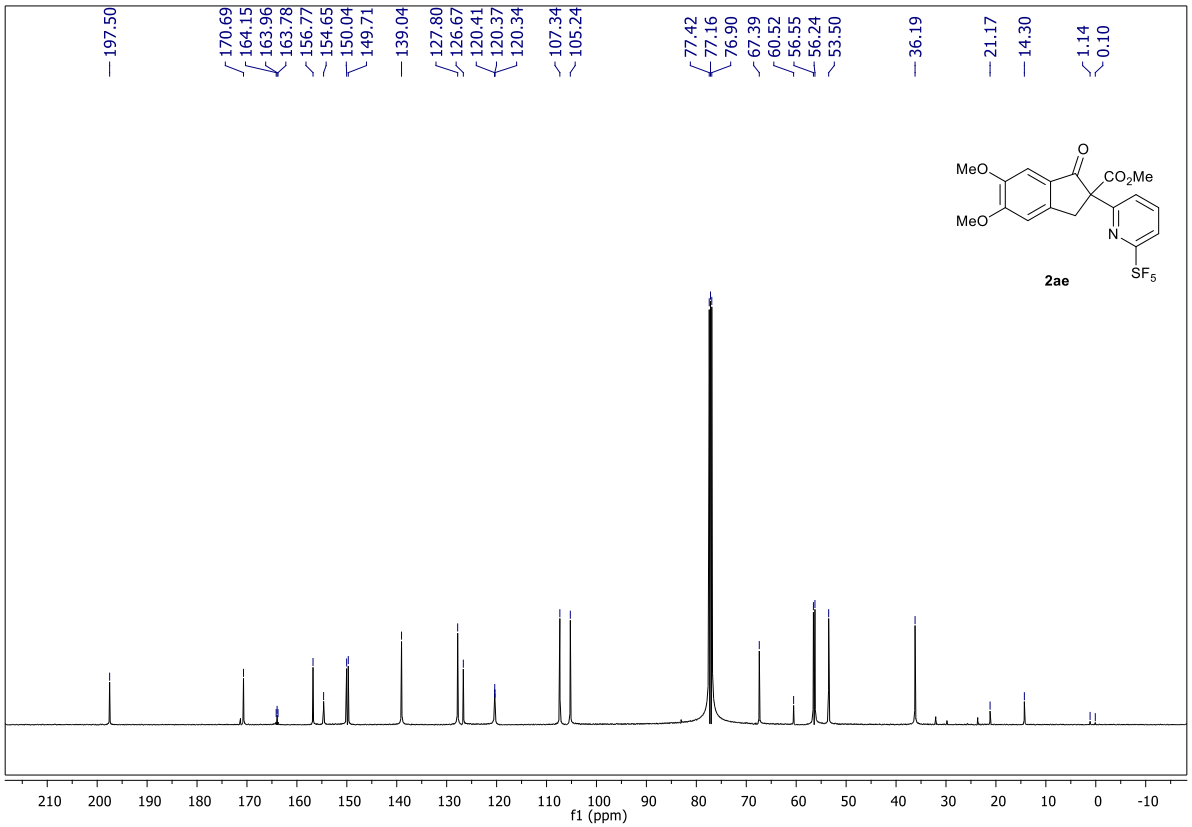
76.70
52.42
51.89
-162.20
1.00
4.20
O
CO2Me
N
SF5
2bd
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)


198.65
169.92
164.68
164.49
164.31
149.19
147.48
138.93
138.44
137.84
126.12
125.46
121.14
121.11
121.08
77.41
77.16
76.91
63.33
53.90
39.45
21.24
0.13
O
CO2Me
N
SF5
2bd
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.12
8.09
7.96
7.94
7.91
7.68
7.66
7.27
7.16
7.00
4.50
4.44
4.01
3.90
3.82
3.75
2.05
1.65
1.26
0.08
-0.00
MeO
MeO
O
CO2Me
N
SF5
2ae
1.00
1.08
1.02
1.01
1.03
1.05
3.34
3.29
4.53
f1 (ppm)


79.05
78.51
77.98
77.45
76.92
52.03
51.50
-162.20
MeO
MeO
O
CO2Me
N
SF5
2ae
1.00
4.31
f1 (ppm)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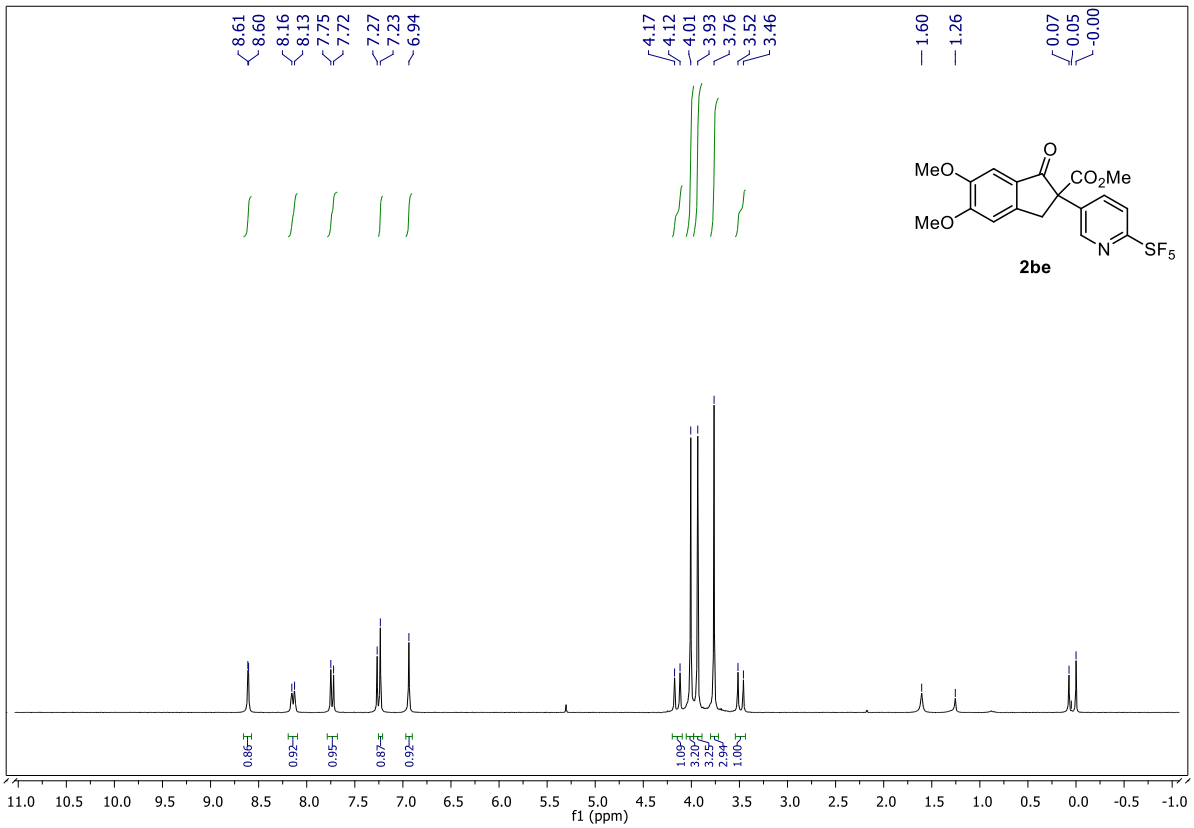
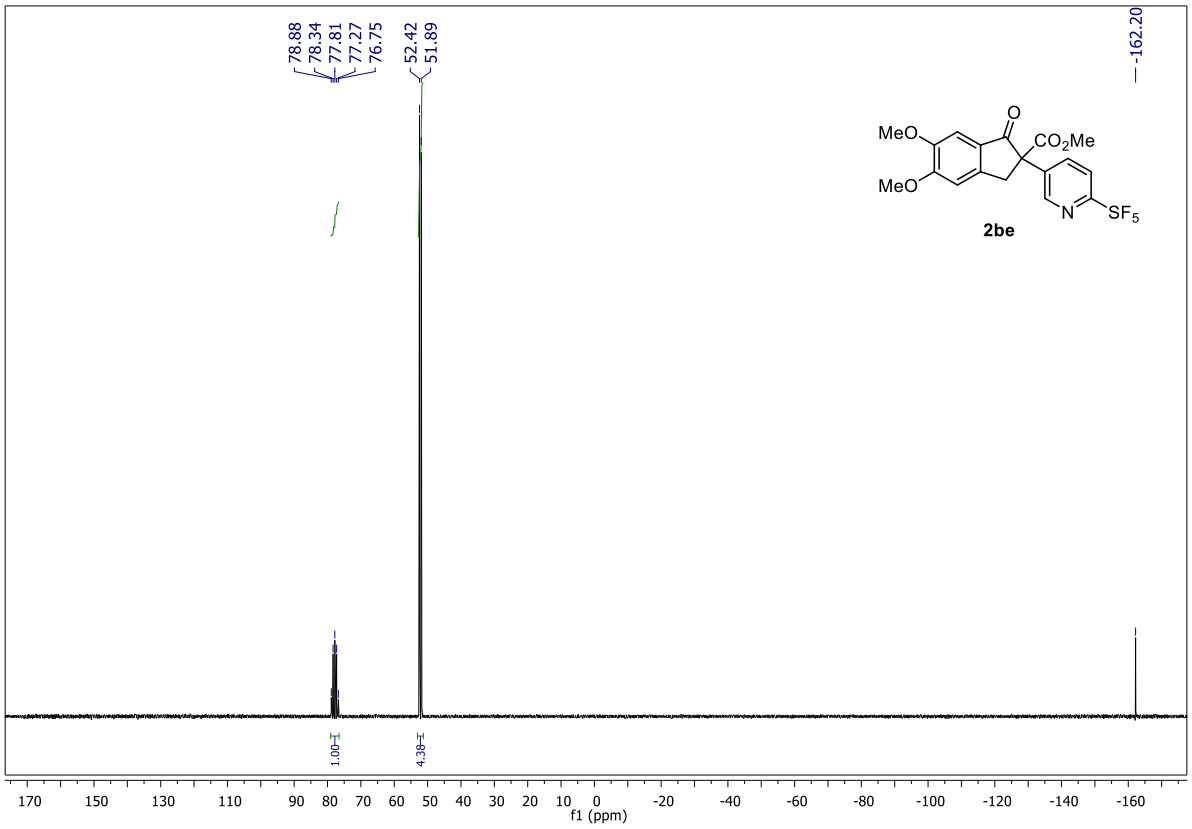
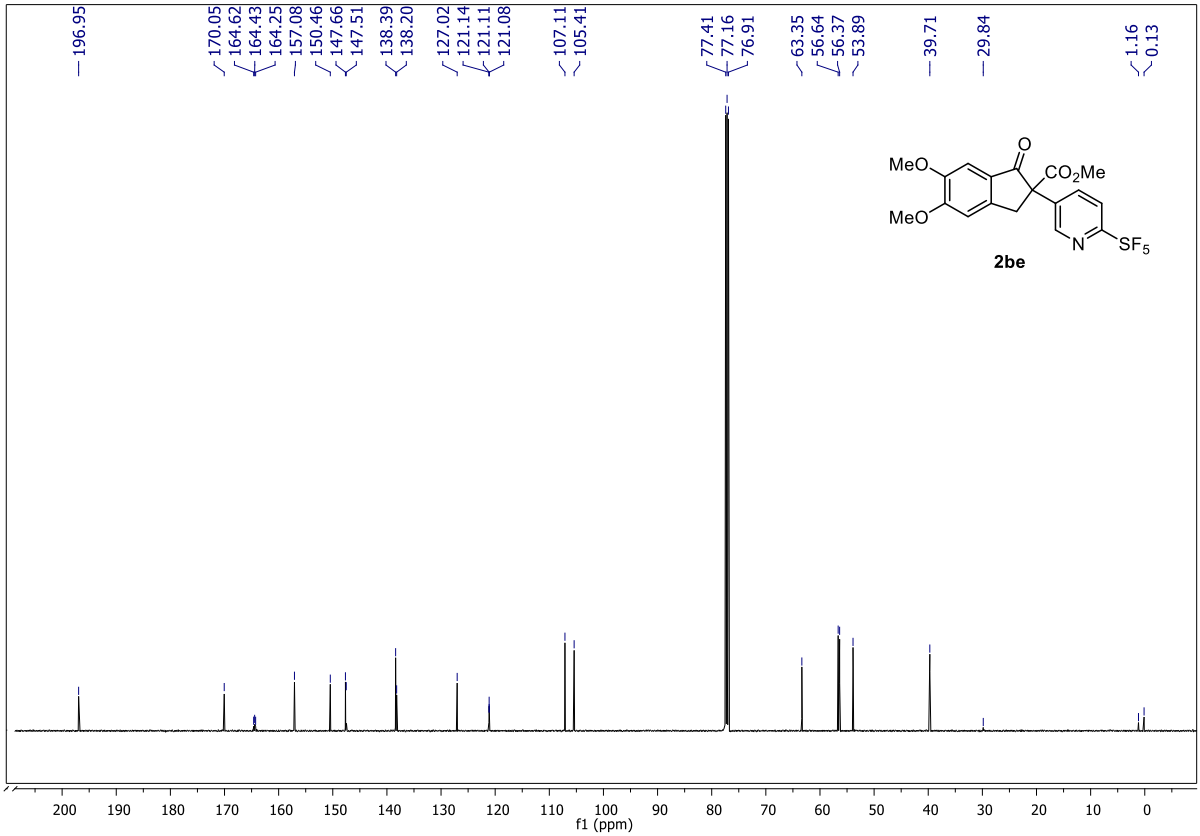
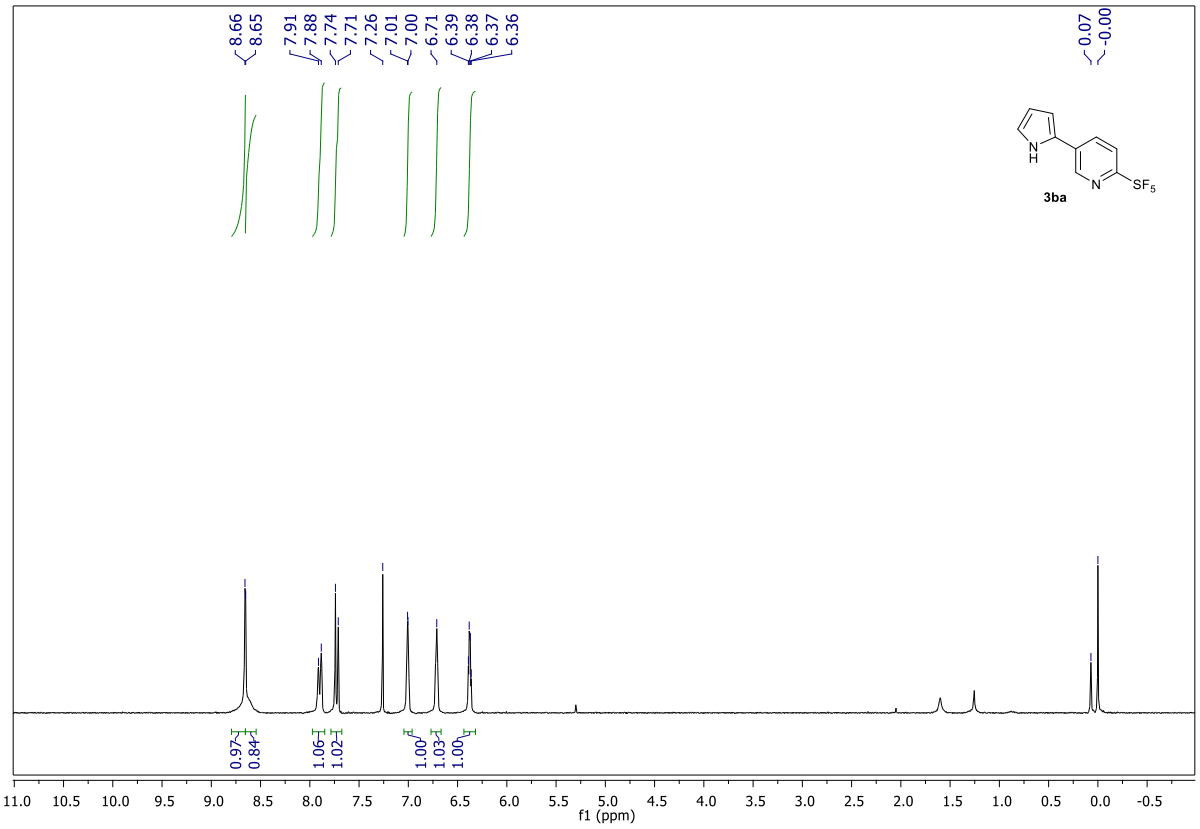
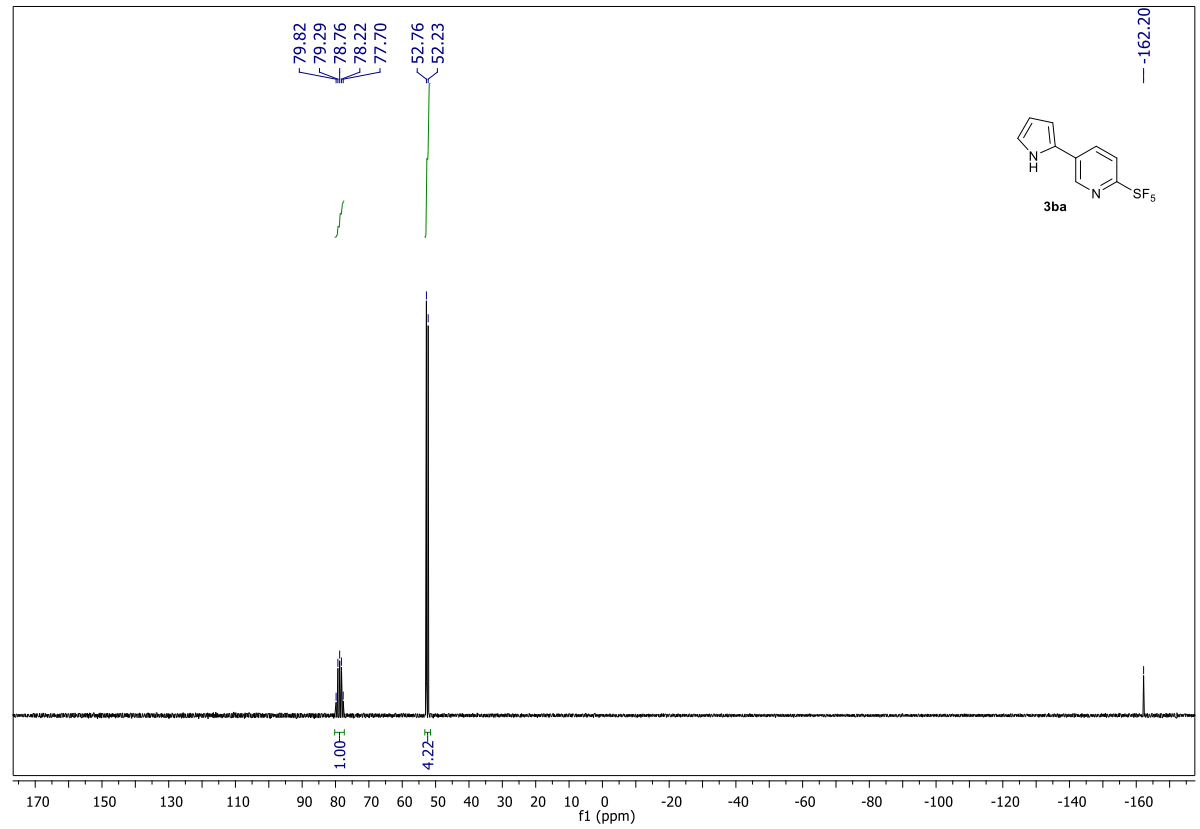
164.15
163.96
163.78
156.77
154.65
150.04
149.71
139.04
127.80
126.67
120.41
120.37
120.34
107.34
105.24
77.42
77.16
76.90
67.39
60.52
56.55
56.24
53.50
36.19
21.17
14.30
1.14
0.10
MeO
MeO
O
CO2Me
N
SF5
2ae
f1 (ppm)

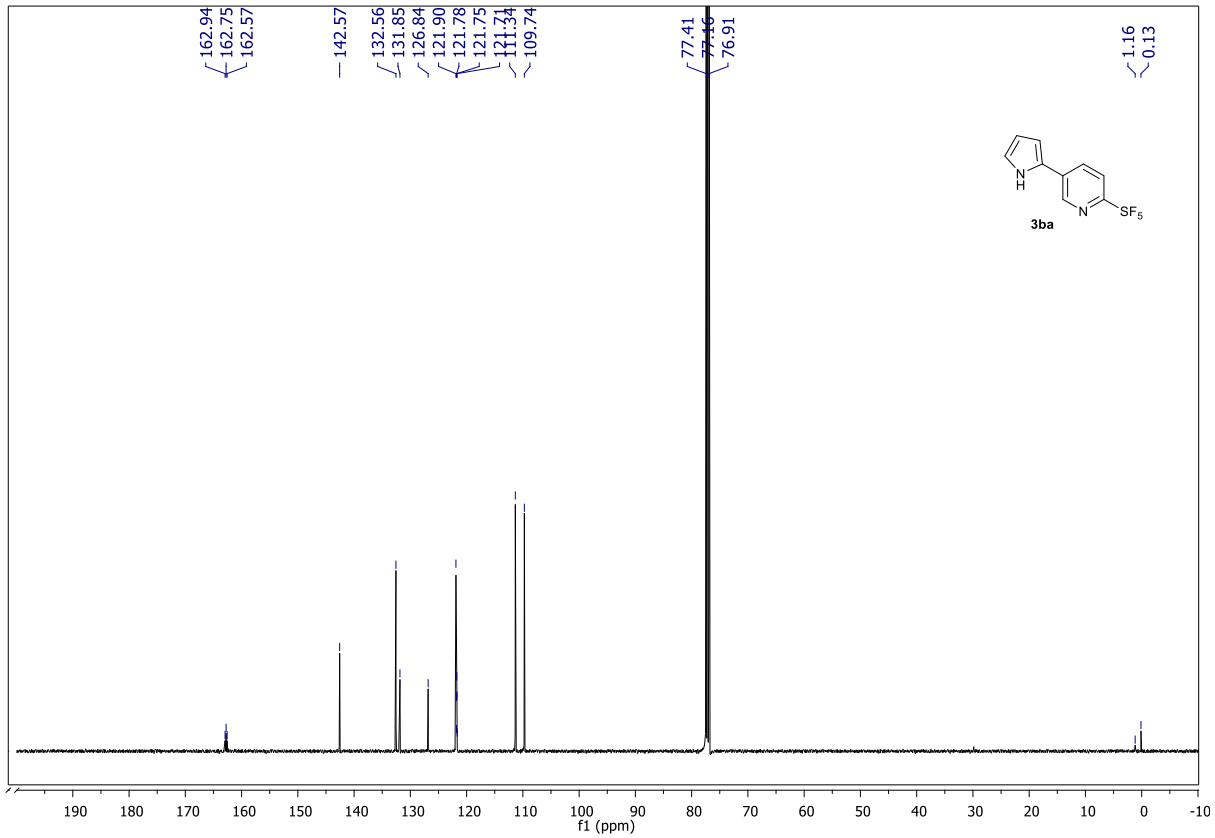

8.61
8.60
8.16
8.13
7.75
7.72
7.27
7.23
6.94
4.17
4.12
4.01
3.93
3.76
3.52
3.46
1.60
1.26
0.07
0.05
-0.00
0.86
0.92
0.95
0.87
0.92
1.09
3.20
3.25
2.94
1.00
MeO
MeO
O
CO2Me
N
SF5
2be
f1 (ppm)

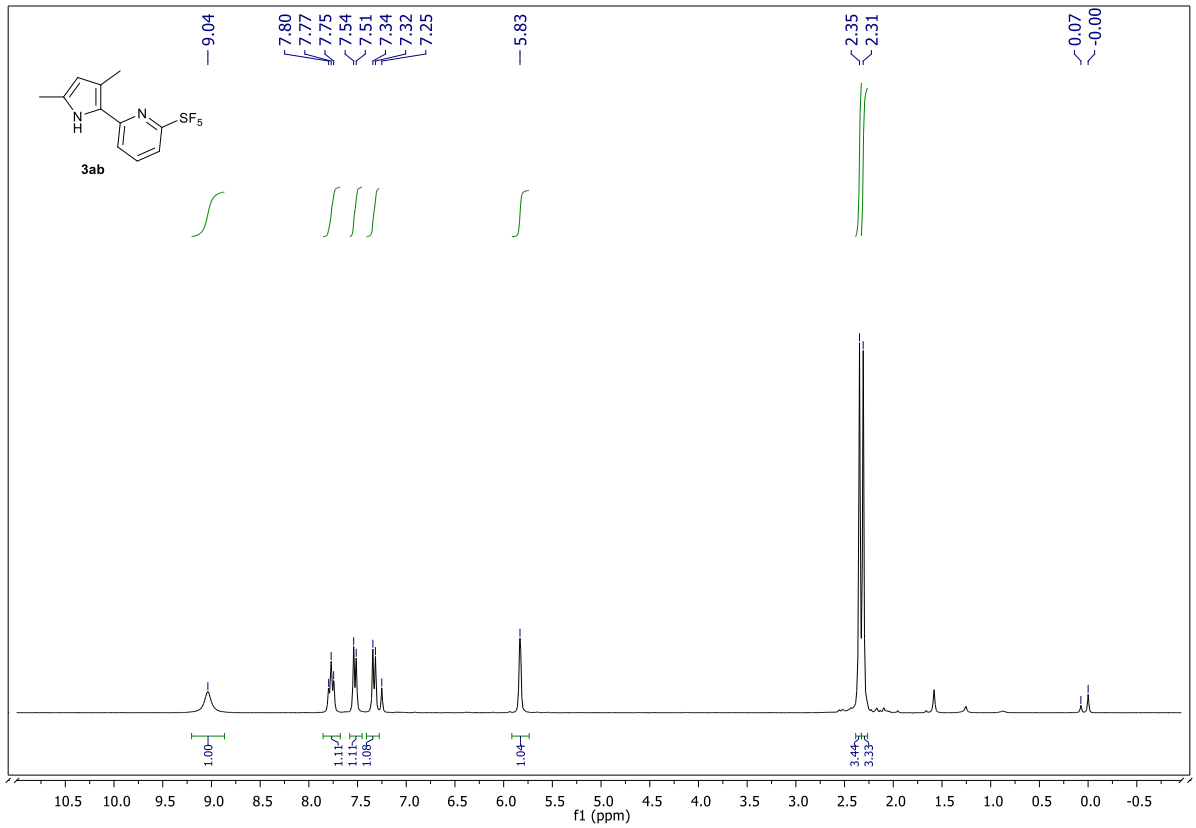

78.88
78.34
77.81
77.27
76.75
52.42
51.89
-162.20
MeO
MeO
O
CO2Me
N
SF5
2be
1.00
4.38
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-20
-40
-60
-80
-100
-120
-140
-160
f1 (ppm)

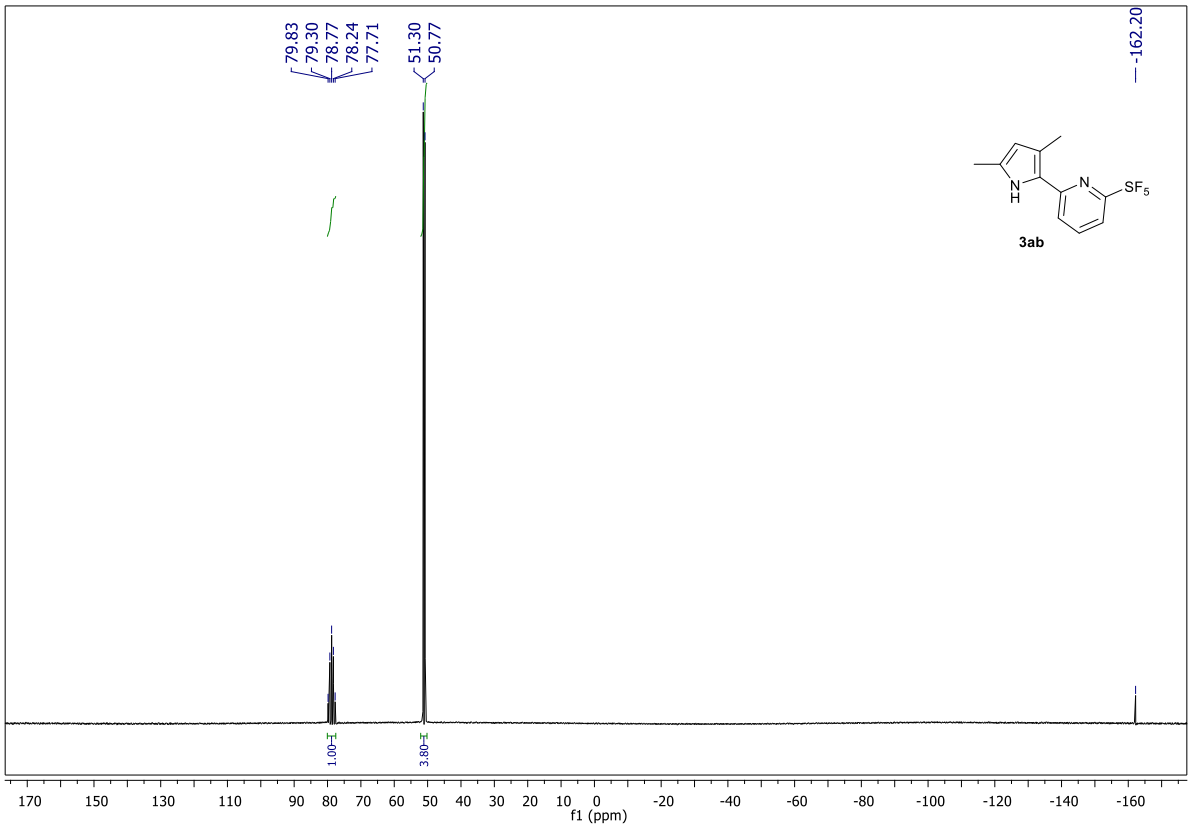

196.95
170.05
164.62
164.43
164.25
157.08
150.46
147.66
147.51
138.39
138.20
127.02
121.14
121.11
121.08
107.11
105.41
77.41
77.16
76.91
63.35
56.64
56.37
53.89
39.71
29.84
1.16
0.13
MeO
MeO
O
CO2Me
N
SF5
2be
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

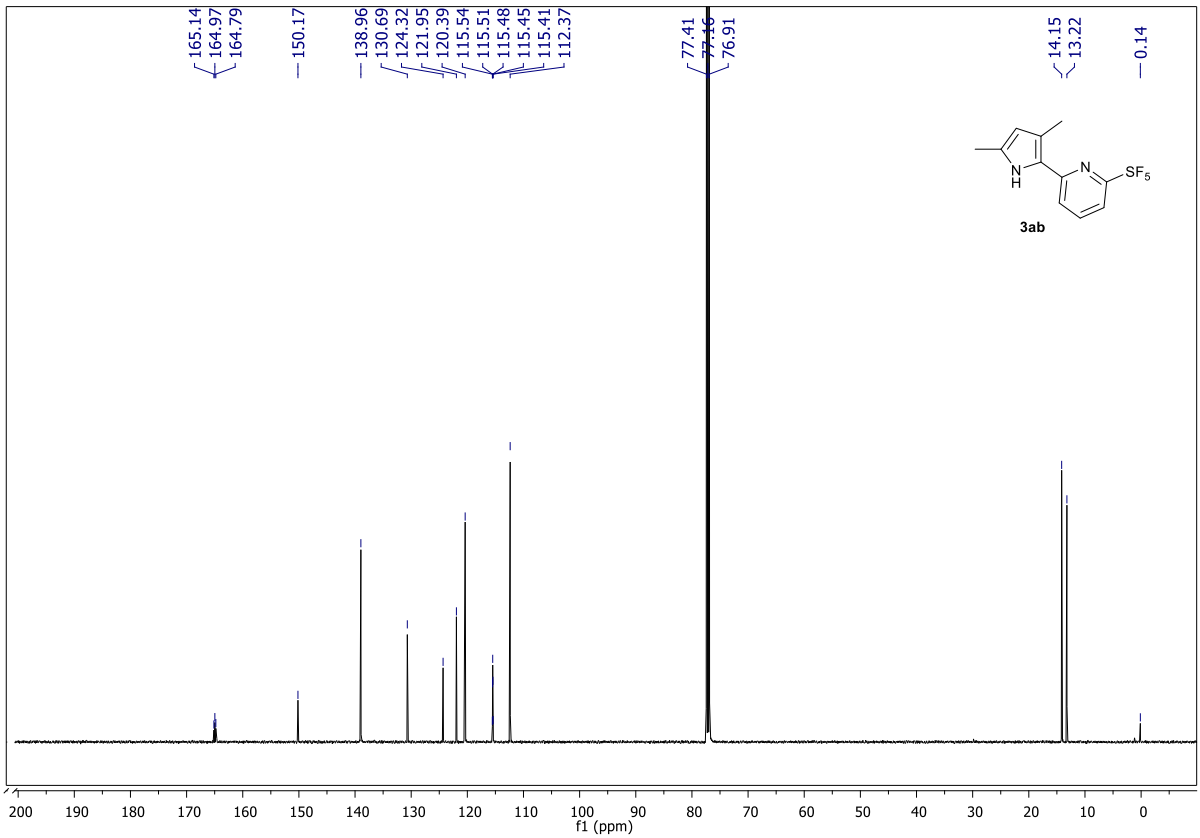

8.66
8.65
7.91
7.88
7.74
7.71
7.26
7.01
7.00
6.71
6.39
6.38
6.37
6.36
0.07
-0.00
3ba
0.97
0.84
1.06
1.02
1.00
1.03
1.00
f1 (ppm)

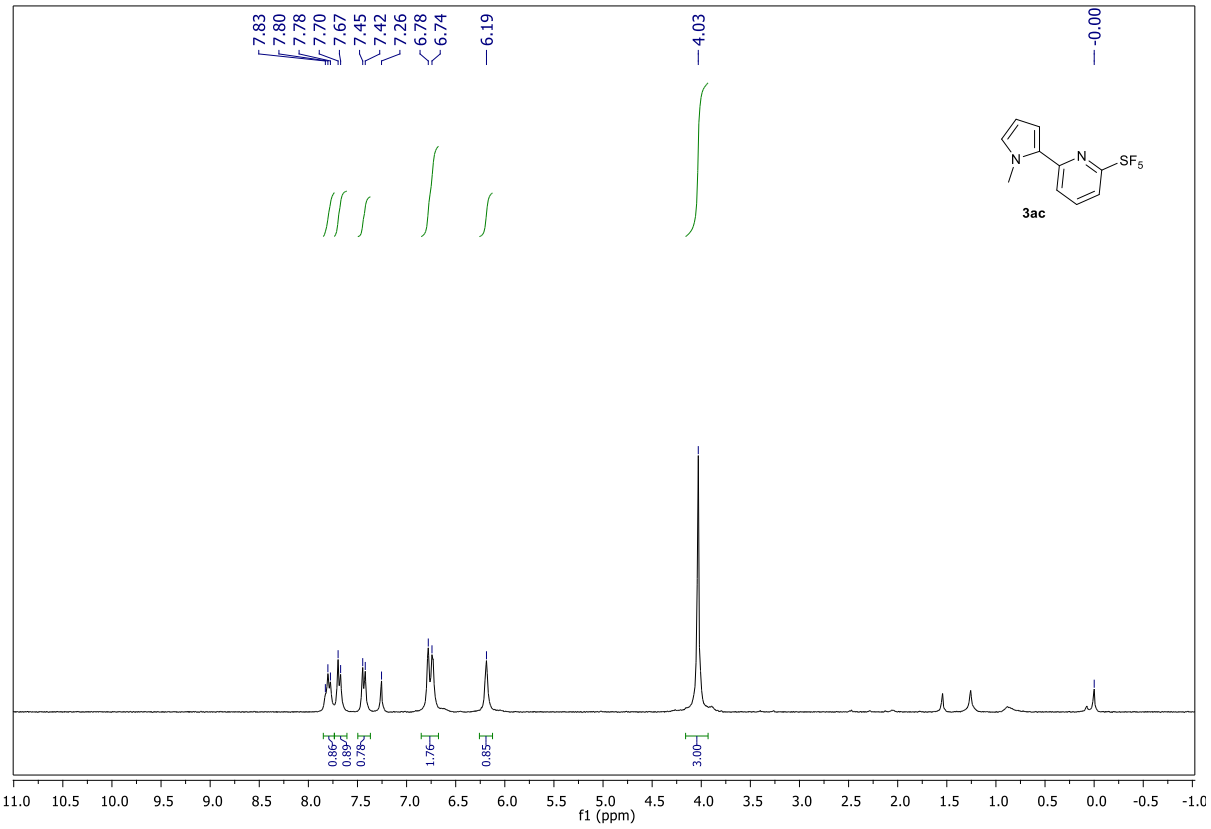

79.82
79.29
78.76
78.22
77.70
52.76
52.23
-162.20
3ba
1.00
4.22
f1 (ppm)

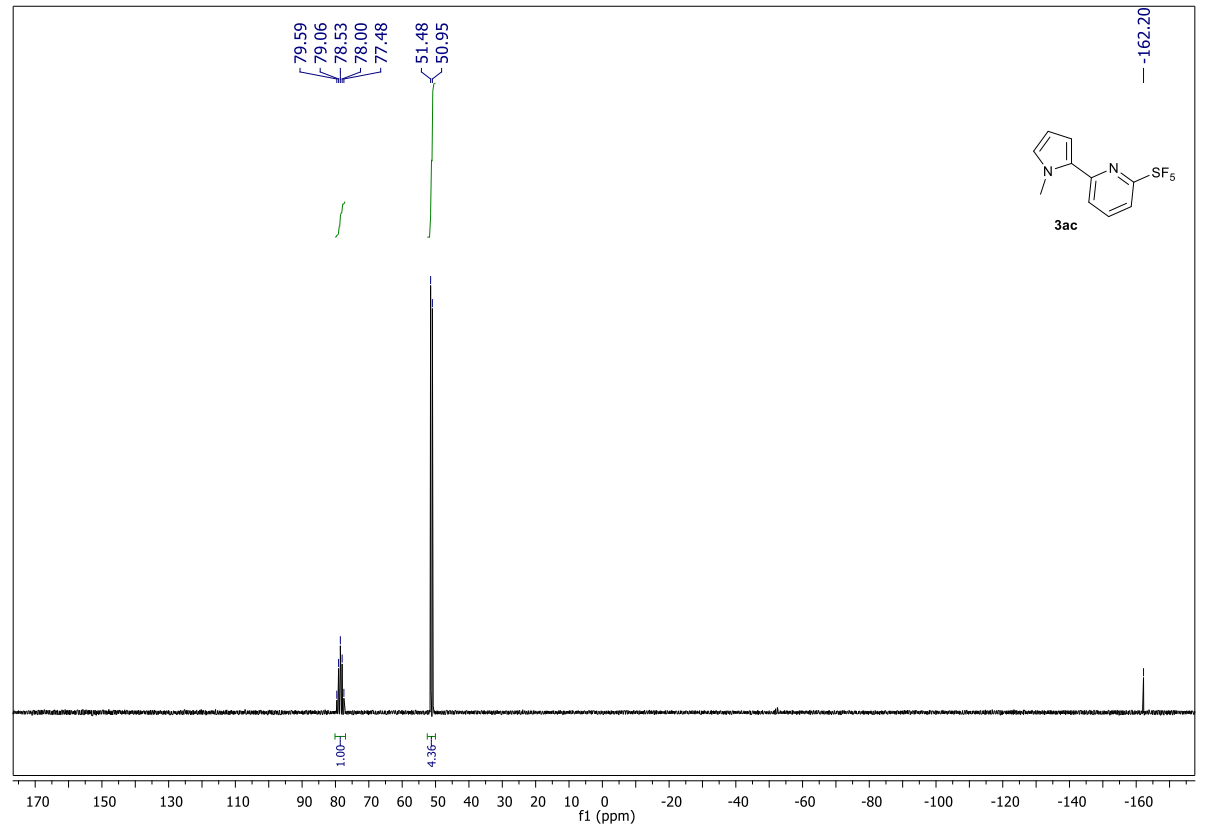

162.94
162.75
162.57
142.57
132.56
131.85
126.84
121.90
121.78
121.75
121.71
111.34
109.74
77.41
77.16
76.91
1.16
0.13
N
H
N
SF5
3ba
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

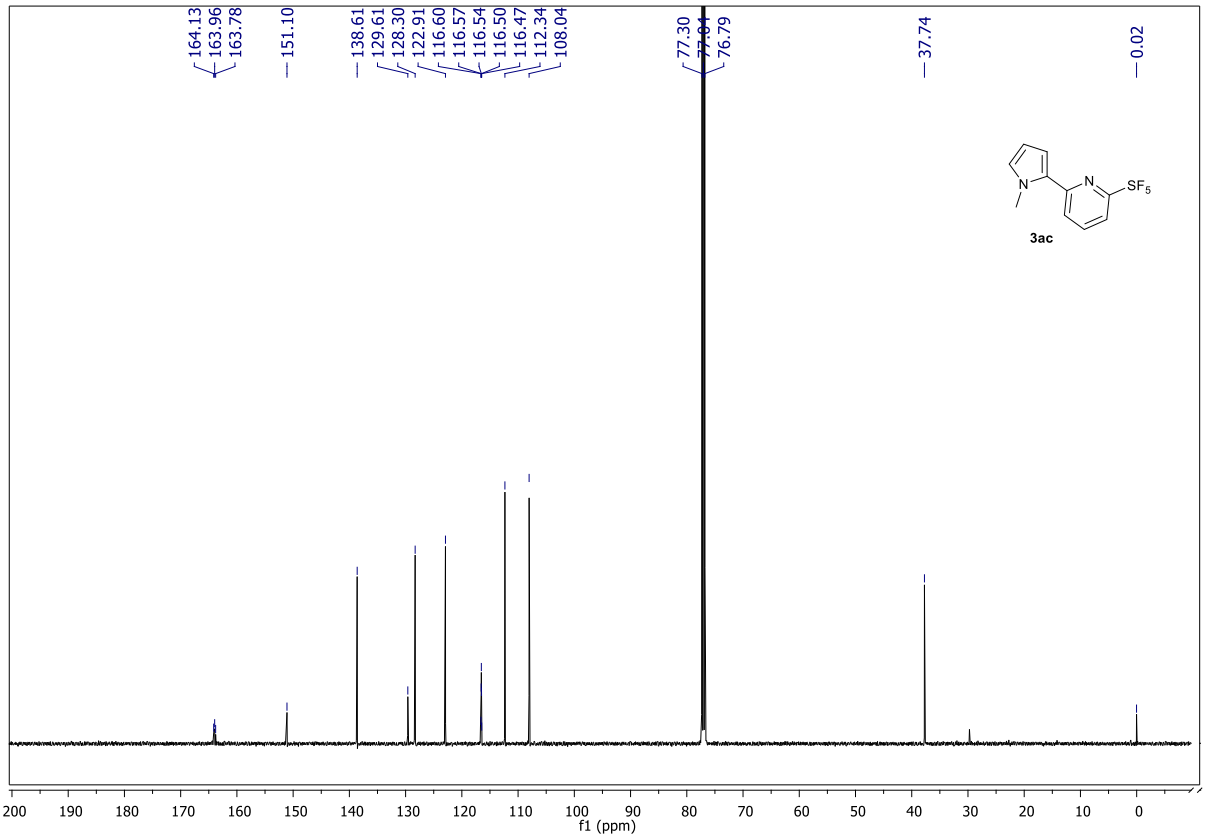

9.04
7.80
7.77
7.75
7.54
7.51
7.34
7.32
7.25
5.83
2.35
2.31
0.07
-0.00
N
H
N
SF5
3ab
1.00
1.11
1.11
1.08
1.04
3.44
3.33
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

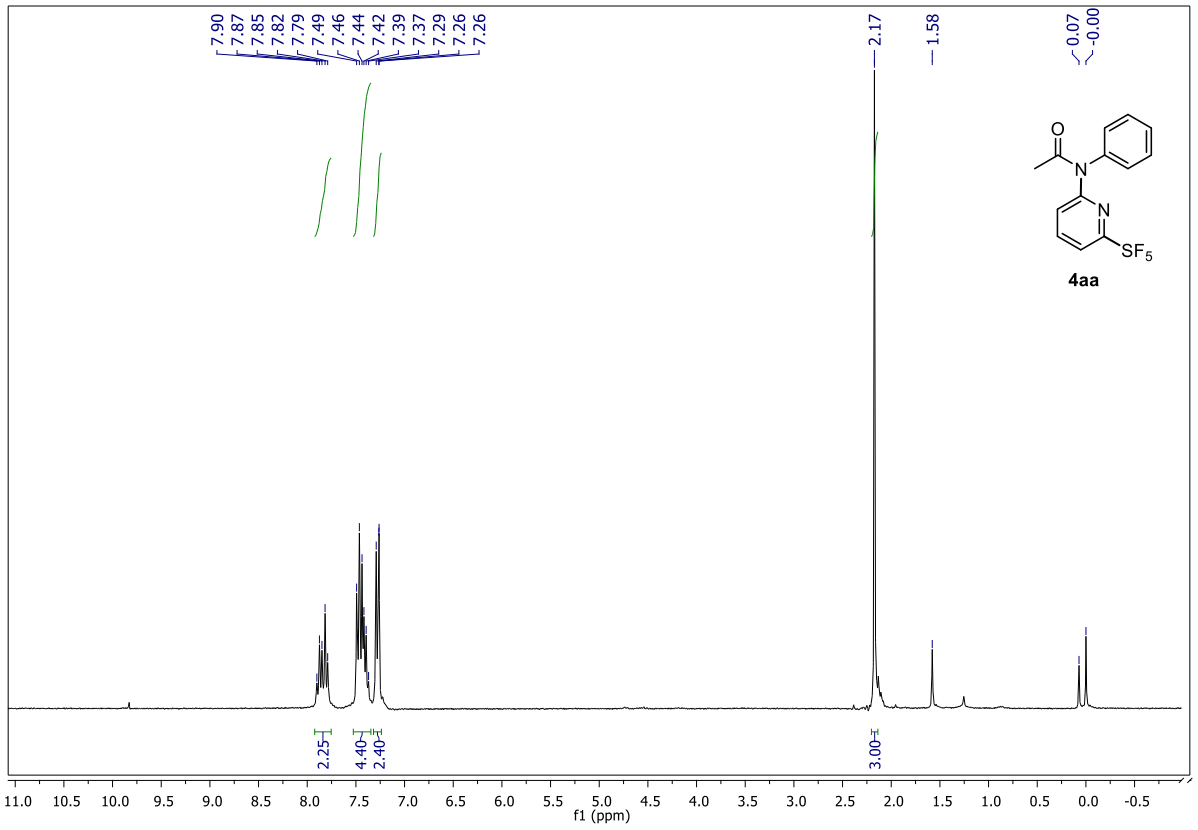

79.83
79.30
78.77
78.24
77.71
51.30
50.77
-162.20
1.00
3.80
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)
3ab


165.14
164.97
164.79
150.17
138.96
130.69
124.32
121.95
120.39
115.54
115.51
115.48
115.45
115.41
112.37
77.41
77.16
76.91
14.15
13.22
0.14
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
3ab


7.83
7.80
7.78
7.70
7.67
7.45
7.42
7.26
6.78
6.74
6.19
4.03
-0.00
N
N
SF5
3ac
0.86
0.89
0.78
1.76
0.85
3.00
f1 (ppm)


79.59
79.06
78.53
78.00
77.48
51.48
50.95
-162.20
N
N
SF5
3ac
1.00
4.36
f1 (ppm)


164.13
163.96
163.78
151.10
138.61
129.61
128.30
122.91
116.60
116.57
116.54
116.50
116.47
112.34
108.04
77.30
77.04
76.79
37.74
0.02
N
N
SF5
3ac
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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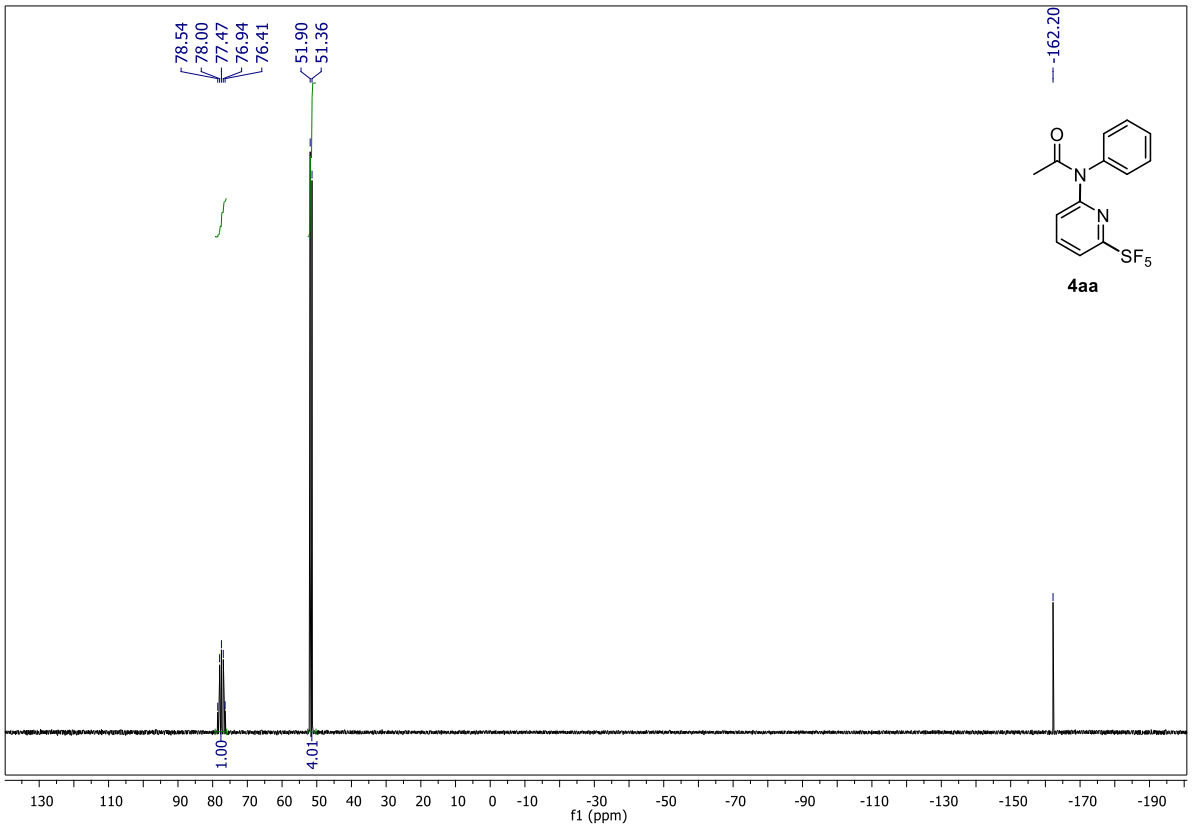
7.87
7.85
7.82
7.79
7.49
7.46
7.44
7.42
7.39
7.37
7.29
7.26
7.26
2.17
1.58
0.07
-0.00
O
N
N
SF5
4aa
2.25
4.40
2.40
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


78.54
78.00
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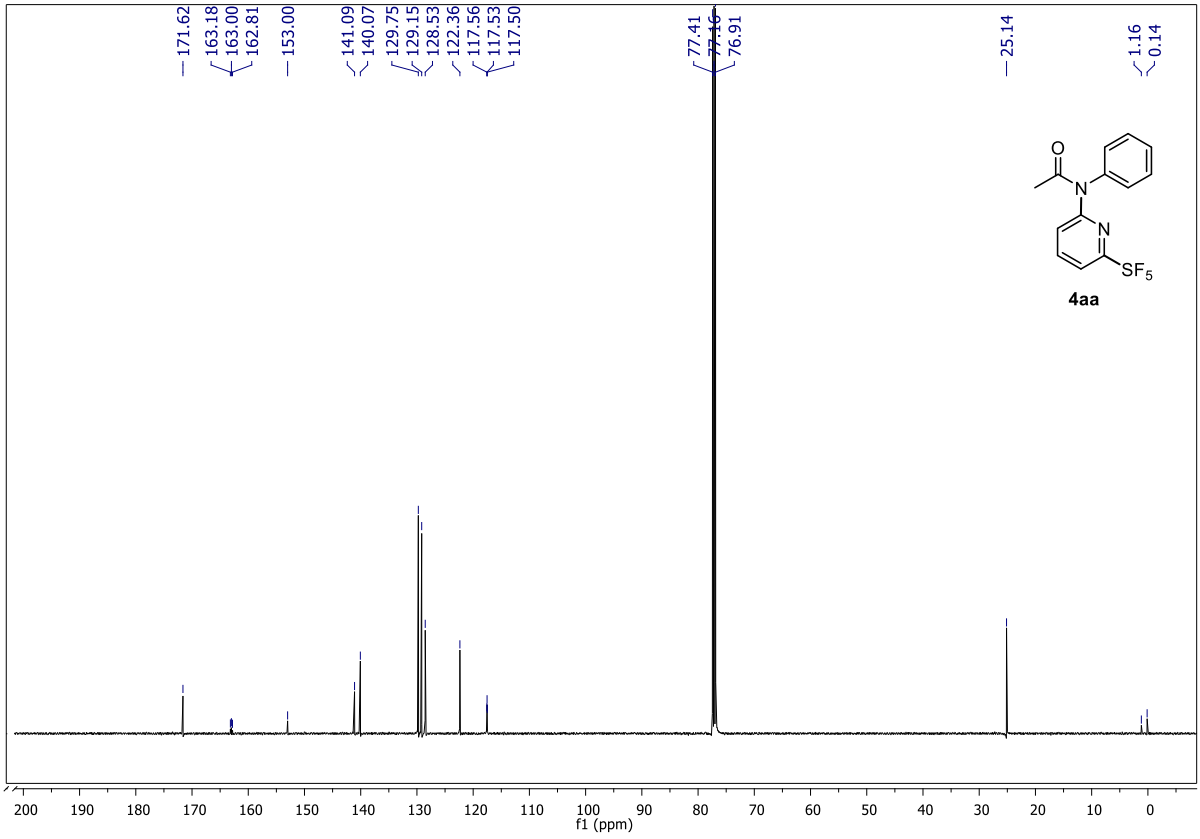
76.94
76.41
51.90
51.36
-162.20
1.00
4.01
f1 (ppm)
4aa


171.62
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163.00
162.81
153.00
141.09
140.07
129.75
129.15
128.53
122.36
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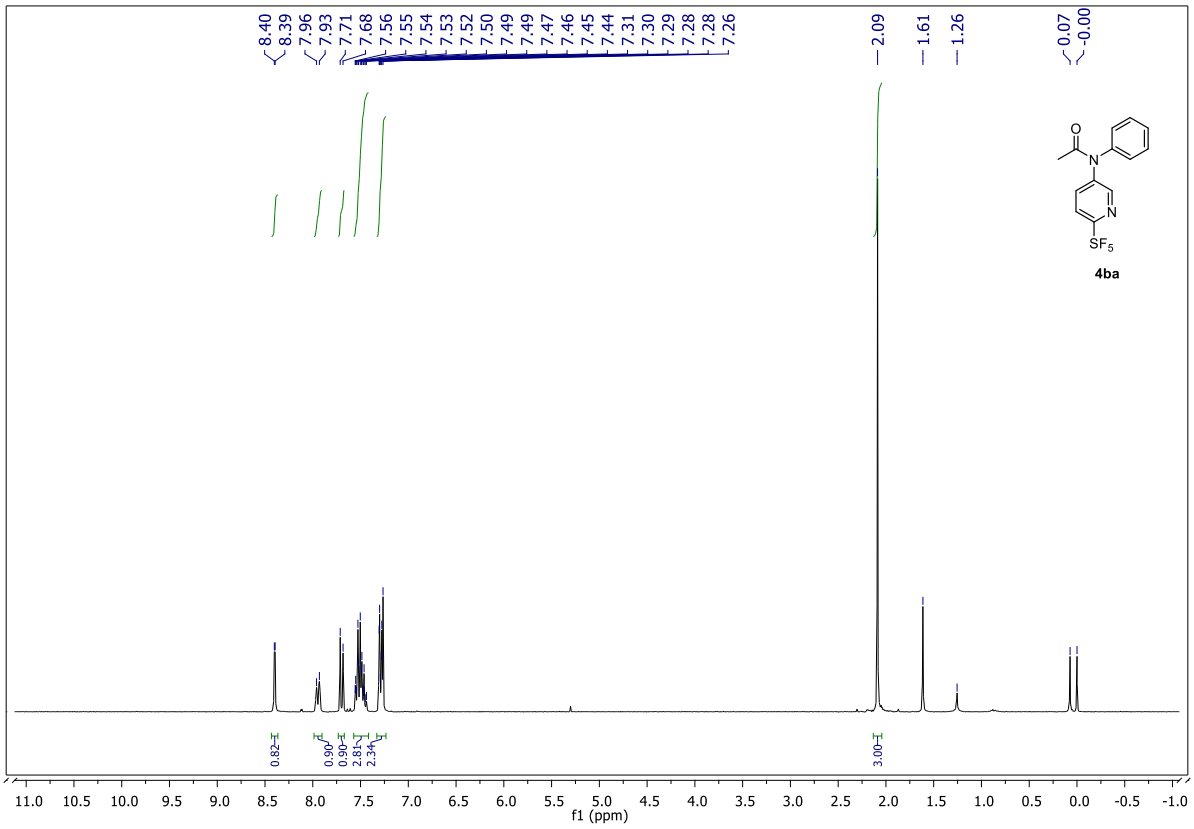
117.50
77.41
77.16
76.91
25.14
1.16
0.14
f1 (ppm)
4aa


8.40
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7.68
7.56
7.55
7.54
7.53
7.52
7.50
7.49
7.49
7.47
7.46
7.45
7.44
7.31
7.30
7.29
7.28
7.28
7.26
2.09
1.61
1.26
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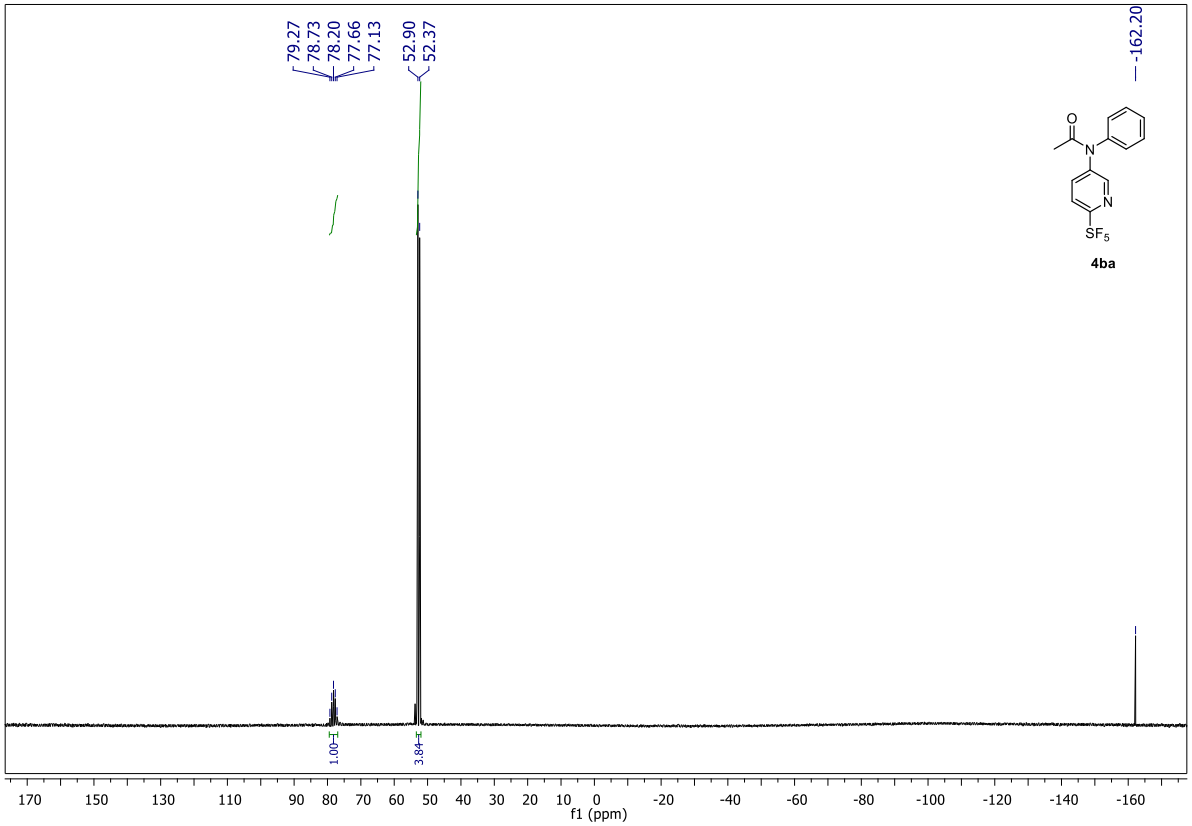
-0.00
0.82
0.90
0.90
2.81
2.34
3.00
f1 (ppm)
4ba


79.27
78.73
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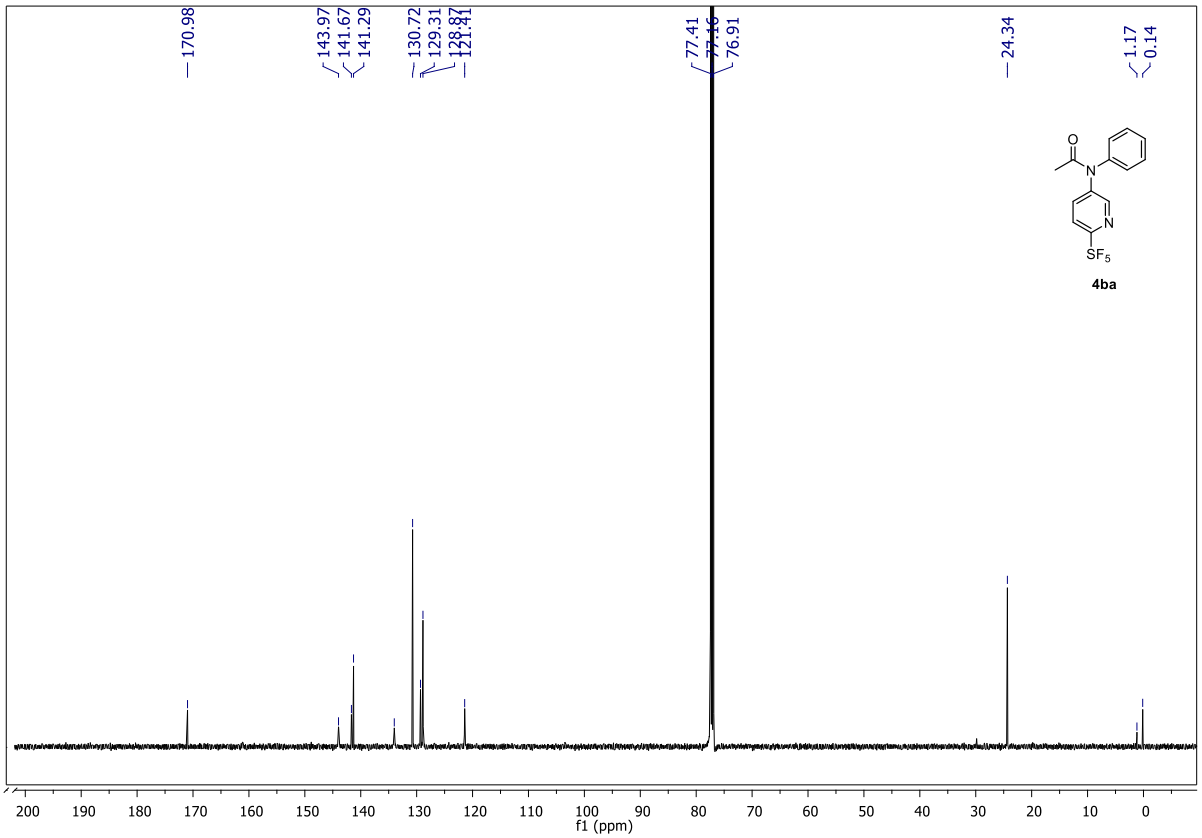
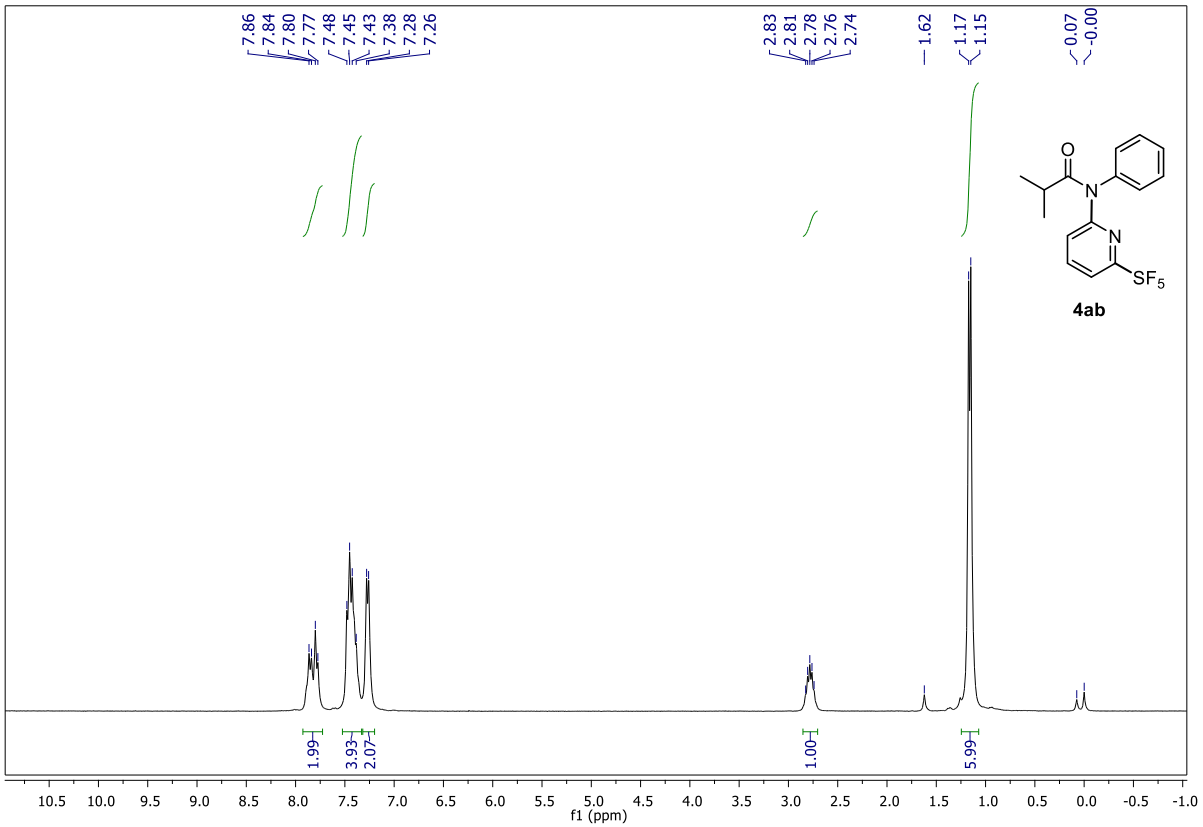
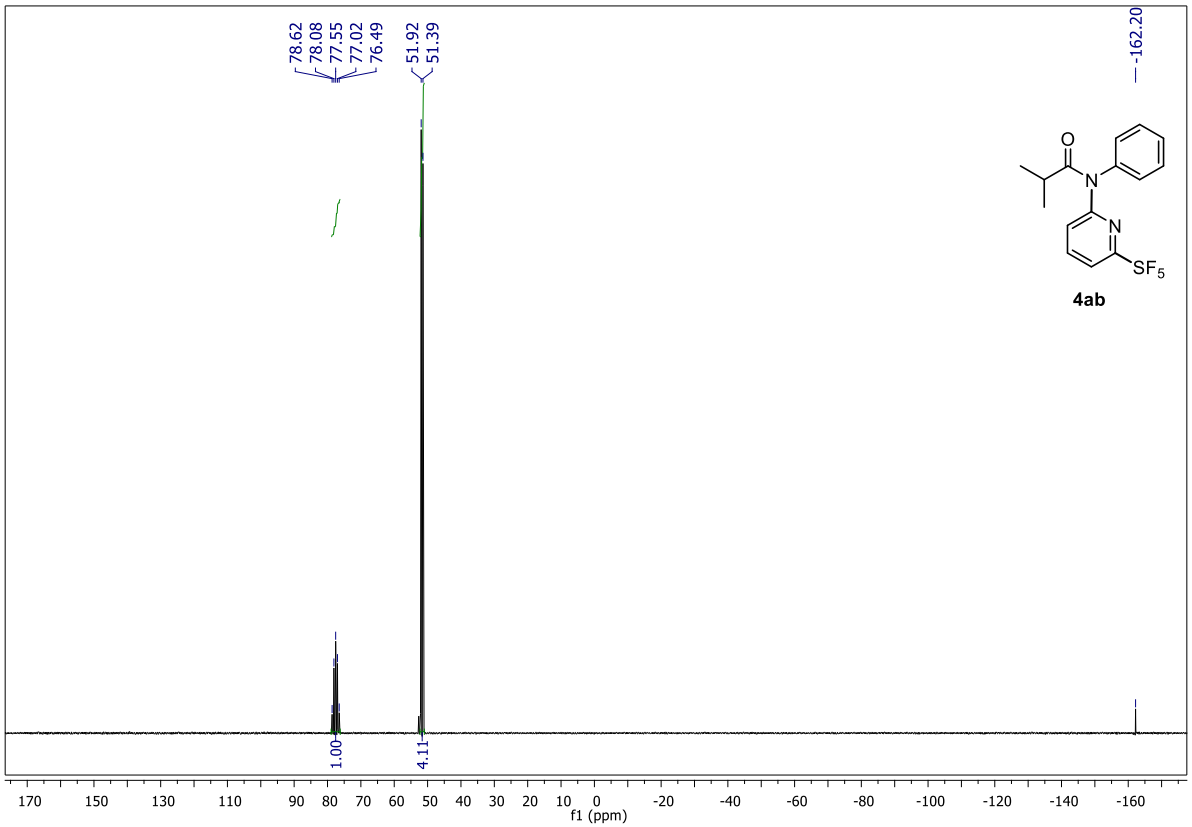
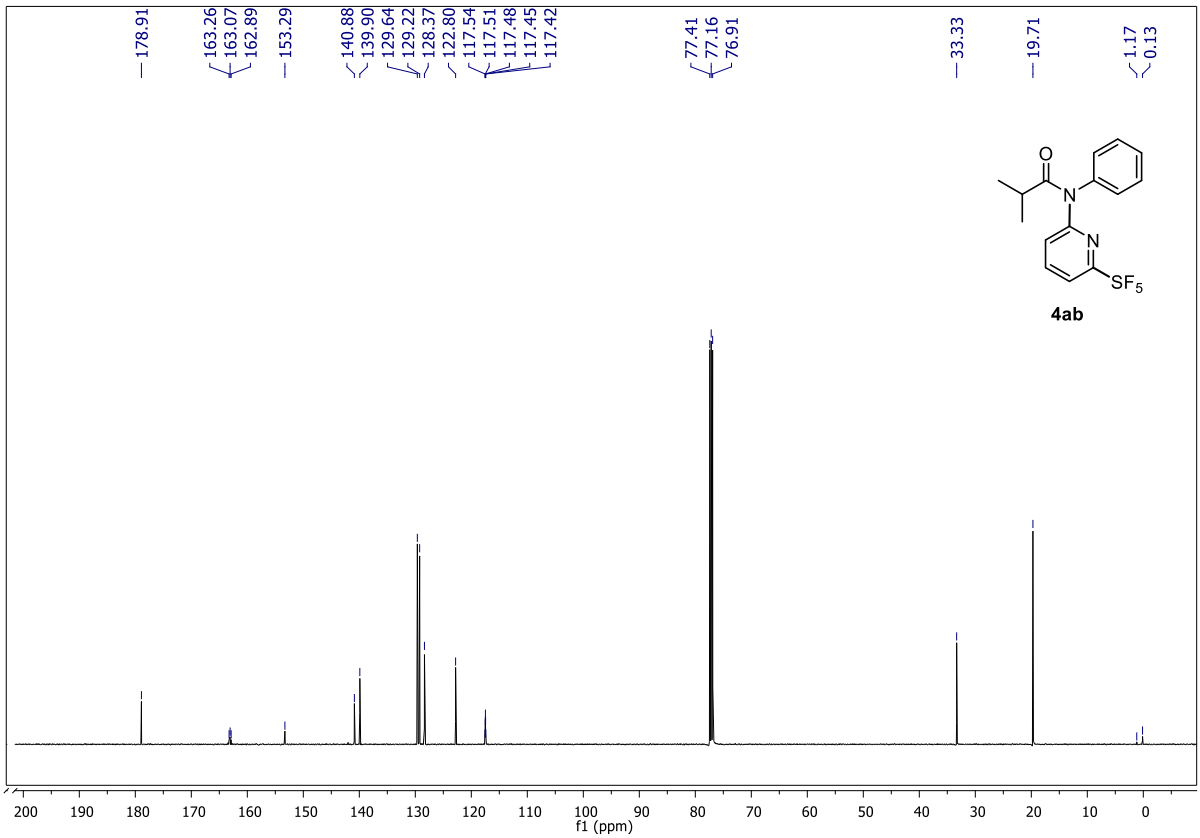
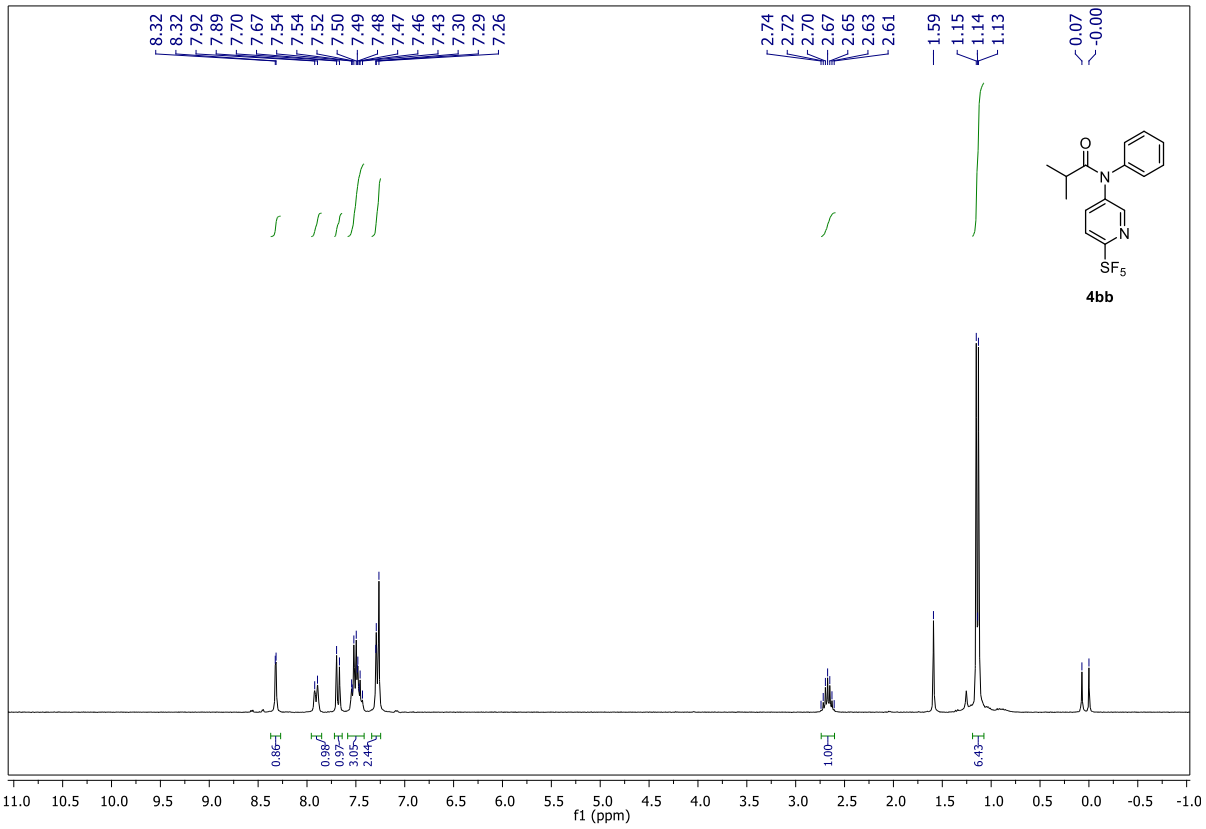
77.13
52.90
52.37
-162.20
1.00
3.84
f1 (ppm)
4ba


170.98
143.97
141.67
141.29
130.72
129.31
128.87
121.41
77.41
77.16
76.91
24.34
1.17
0.14
4ba


7.86
7.84
7.80
7.77
7.48
7.45
7.43
7.38
7.28
7.26
2.83
2.81
2.78
2.76
2.74
1.62
1.17
1.15
0.07
-0.00
4ab
1.99
3.93
2.07
1.00
5.99


78.62
78.08
77.55
77.02
76.49
51.92
51.39
-162.20
1.00
4.11
f1 (ppm)
4ab


178.91
163.26
163.07
162.89
153.29
140.88
139.90
129.64
129.22
128.37
122.80
117.54
117.51
117.48
117.45
117.42
77.41
77.16
76.91
33.33
19.71
1.17
0.13
f1 (ppm)
4ab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7.67
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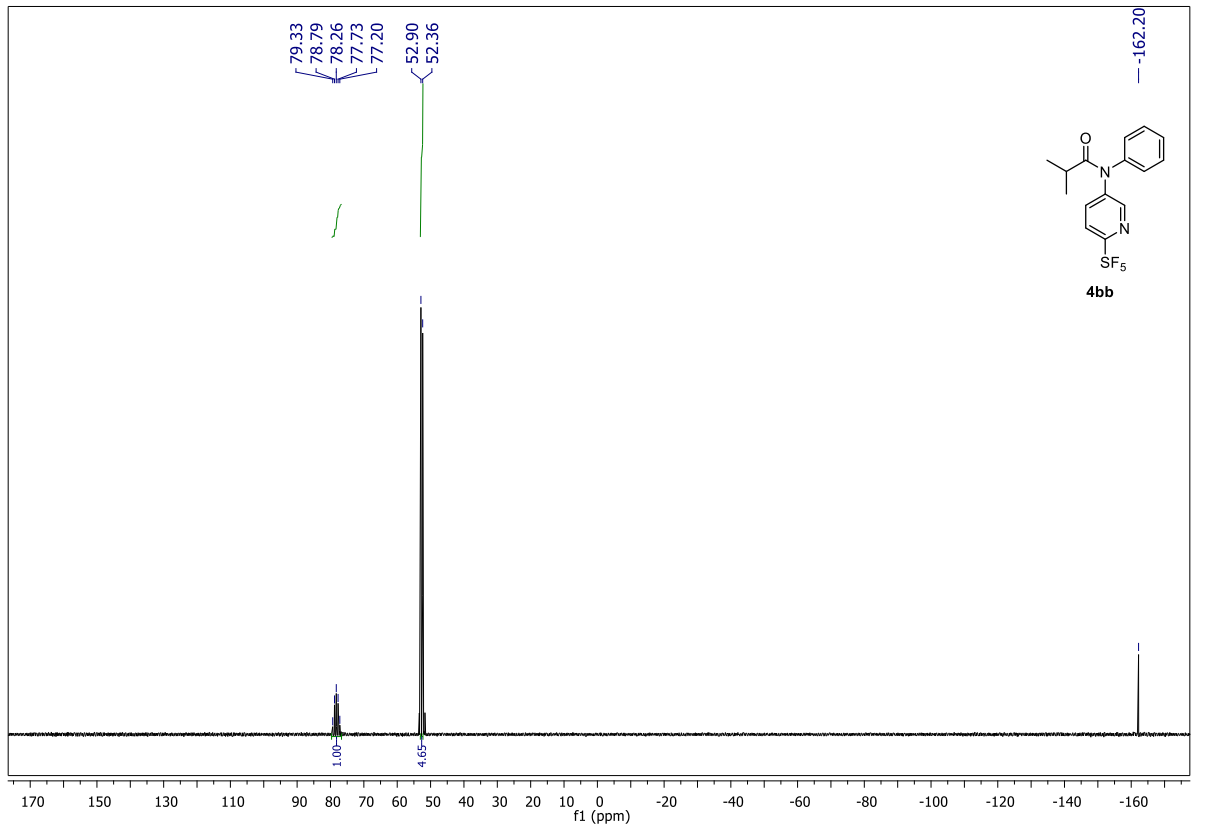
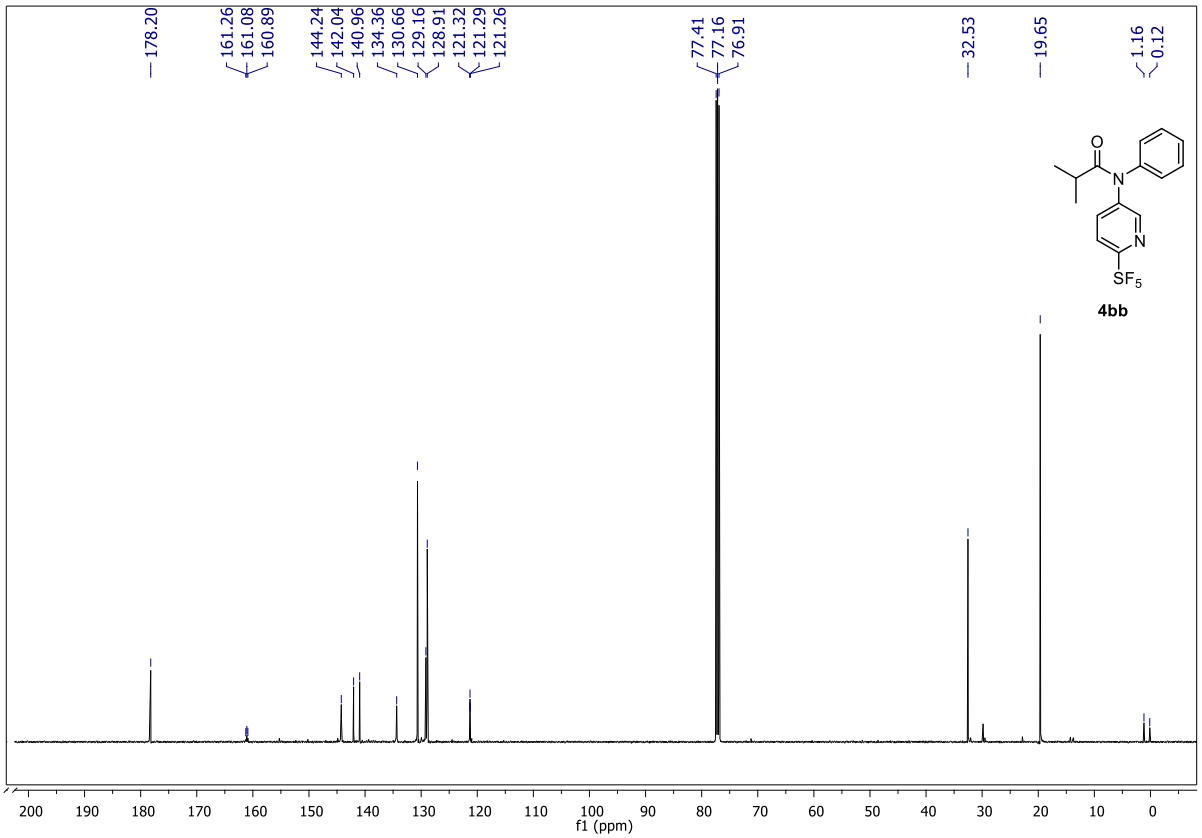
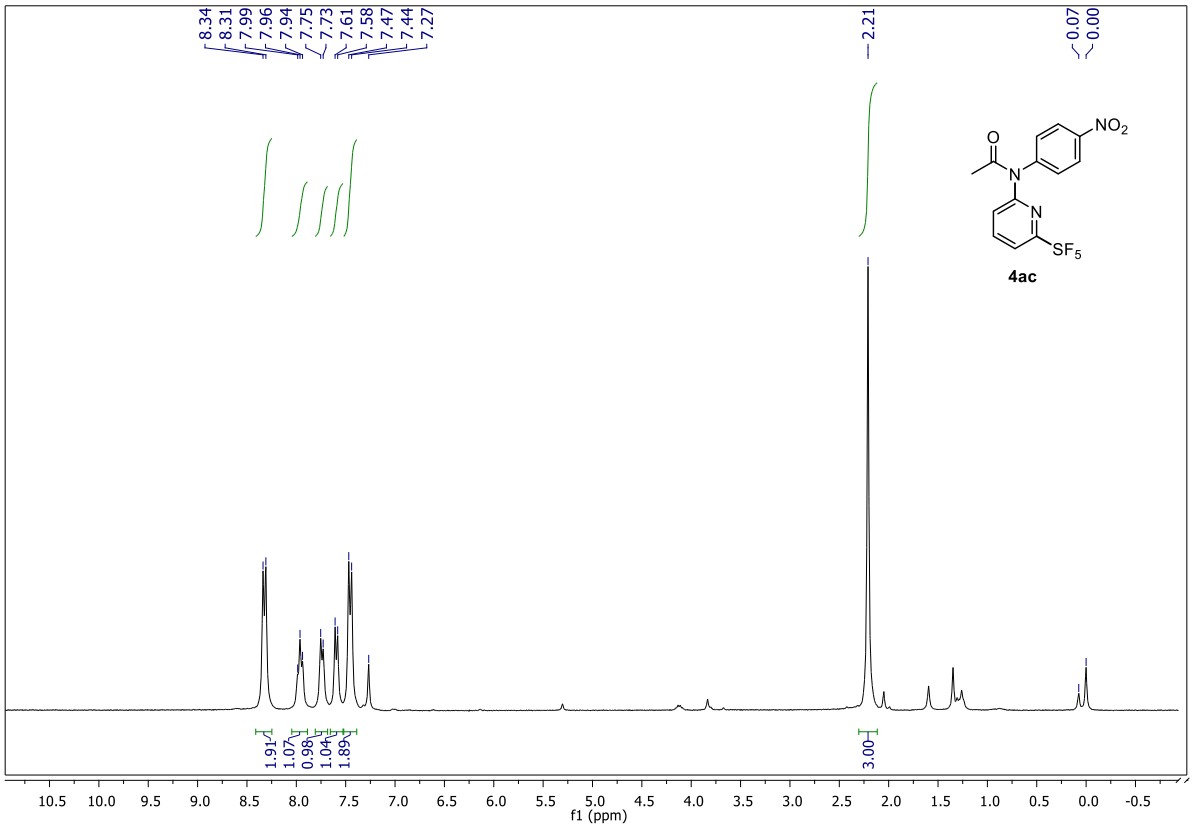
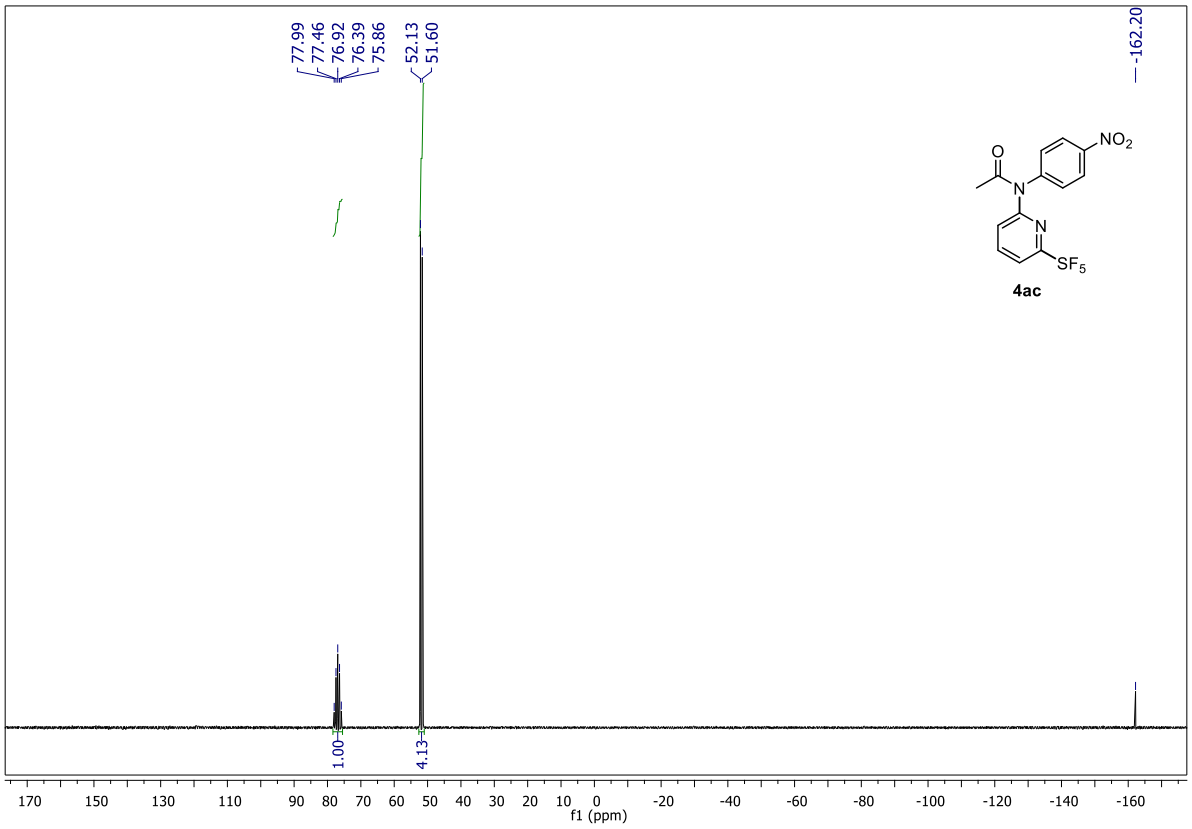
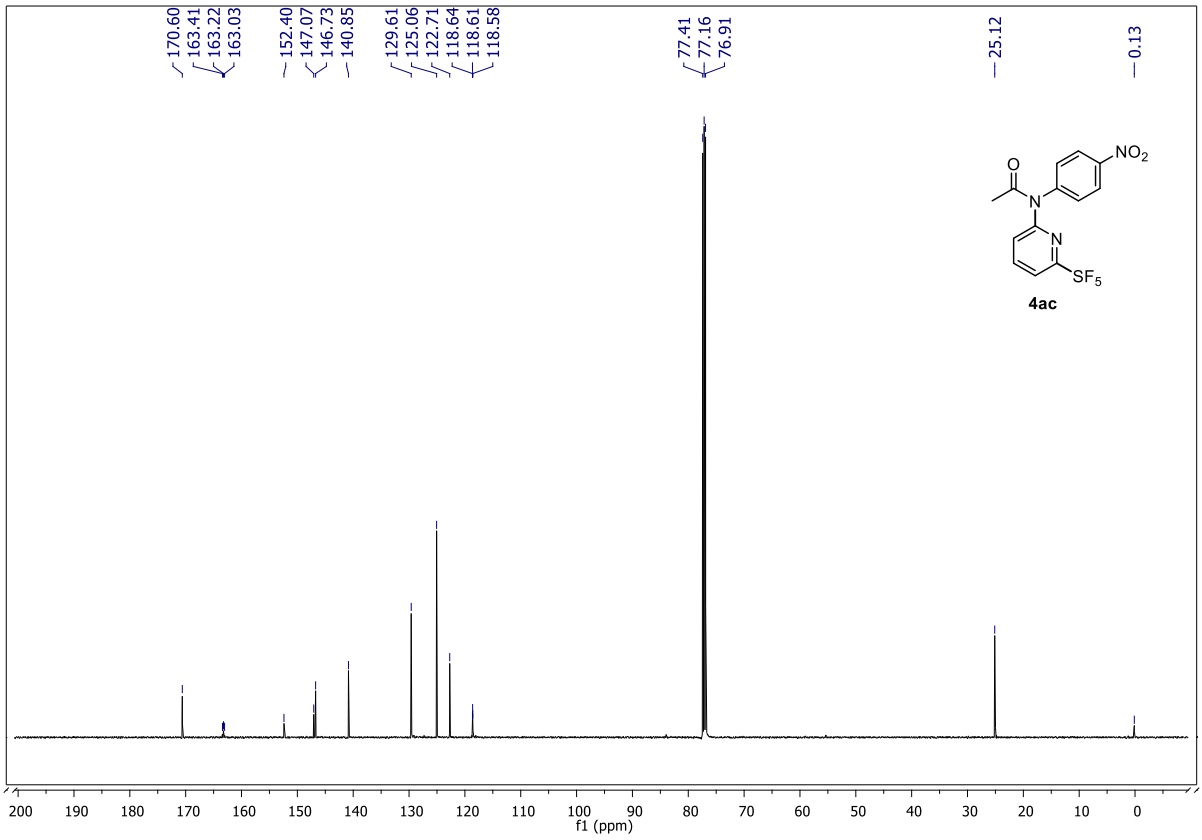
7.54
7.52
7.50
7.49
7.48
7.47
7.46
7.43
7.30
7.29
7.26
2.74
2.72
2.70
2.67
2.65
2.63
2.61
1.59
1.15
1.14
1.13
0.07
-0.00
0.86
0.98
0.97
3.05
2.44
1.00
6.43
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)
O
N
N
SF5
4bb


79.33
78.79
78.26
77.73
77.20
52.90
52.36
-162.20
1.00
4.65
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)
O
N
N
SF5
4bb


178.20
161.26
161.08
160.89
144.24
142.04
140.96
134.36
130.66
129.16
128.91
121.32
121.29
121.26
77.41
77.16
76.91
32.53
19.65
1.16
0.12
4bb
f1 (ppm)


8.34
8.31
7.99
7.96
7.94
7.75
7.73
7.61
7.58
7.47
7.44
7.27
2.21
0.07
0.00
4ac
1.91
1.07
0.98
1.04
1.89
3.00
f1 (ppm)


77.99
77.46
76.92
76.39
75.86
52.13
51.60
-162.20
1.00
4.13
f1 (ppm)
4ac


170.60
163.41
163.22
163.03
152.40
147.07
146.73
140.85
129.61
125.06
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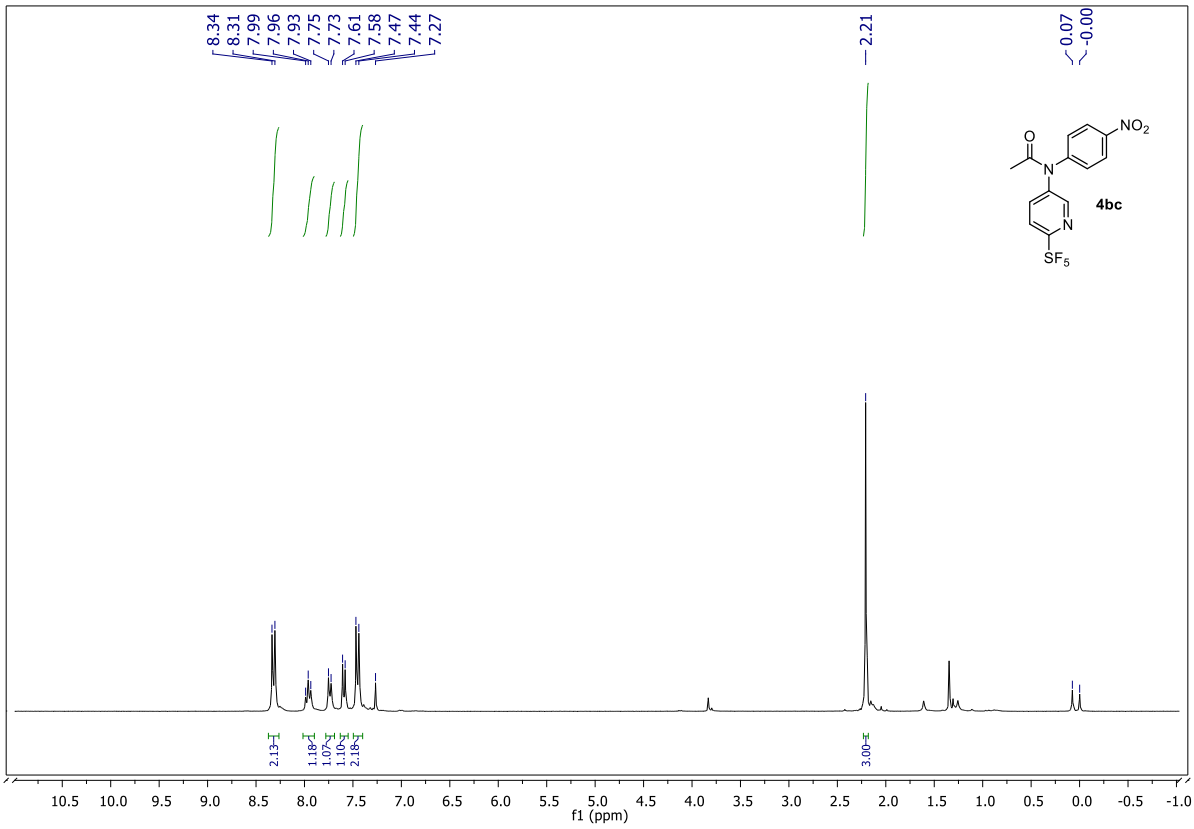
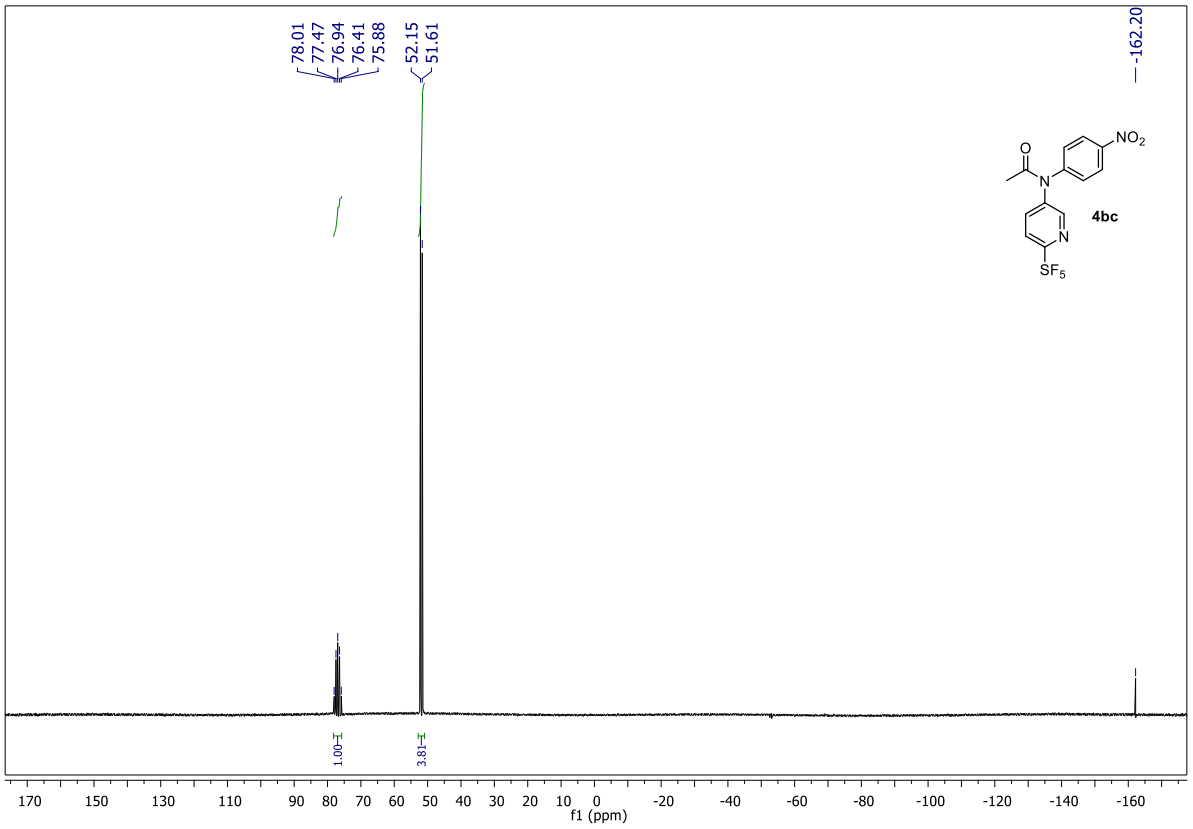
118.61
118.58
77.41
77.16
76.91
25.12
0.13
f1 (ppm)
4ac


8.34
8.31
7.99
7.96
7.93
7.75
7.73
7.61
7.58
7.47
7.44
7.27
2.21
0.07
-0.00
4bc
2.13
1.18
1.07
1.10
2.18
3.00
f1 (ppm)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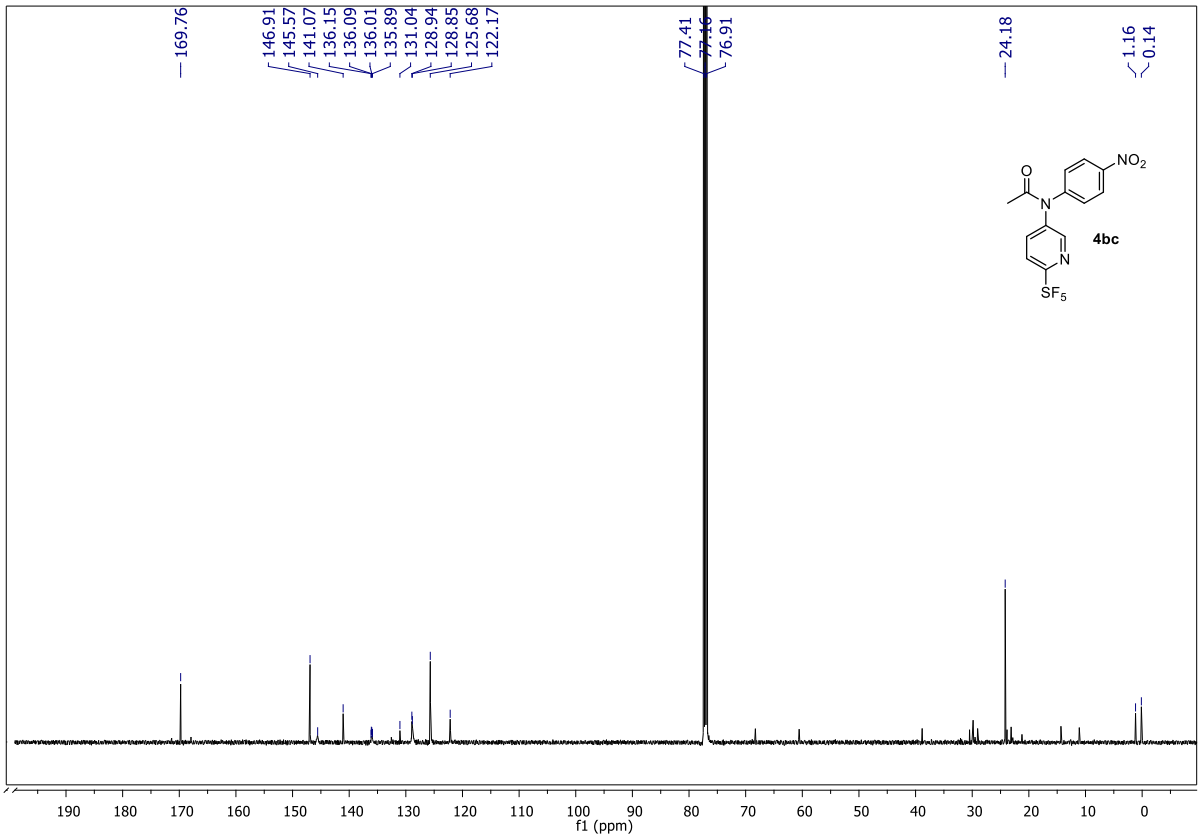
75.88
52.15
51.61
-162.20
4bc
1.00
3.81
f1 (ppm)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146.91
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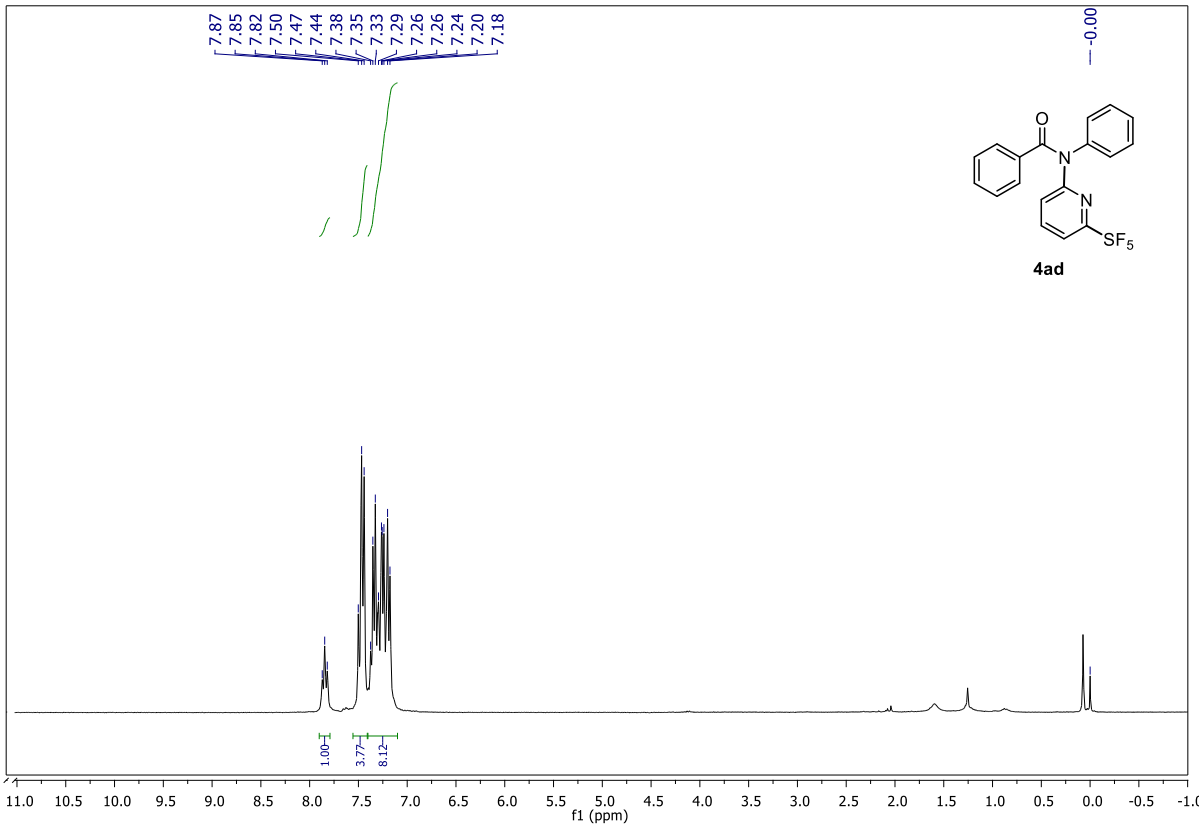
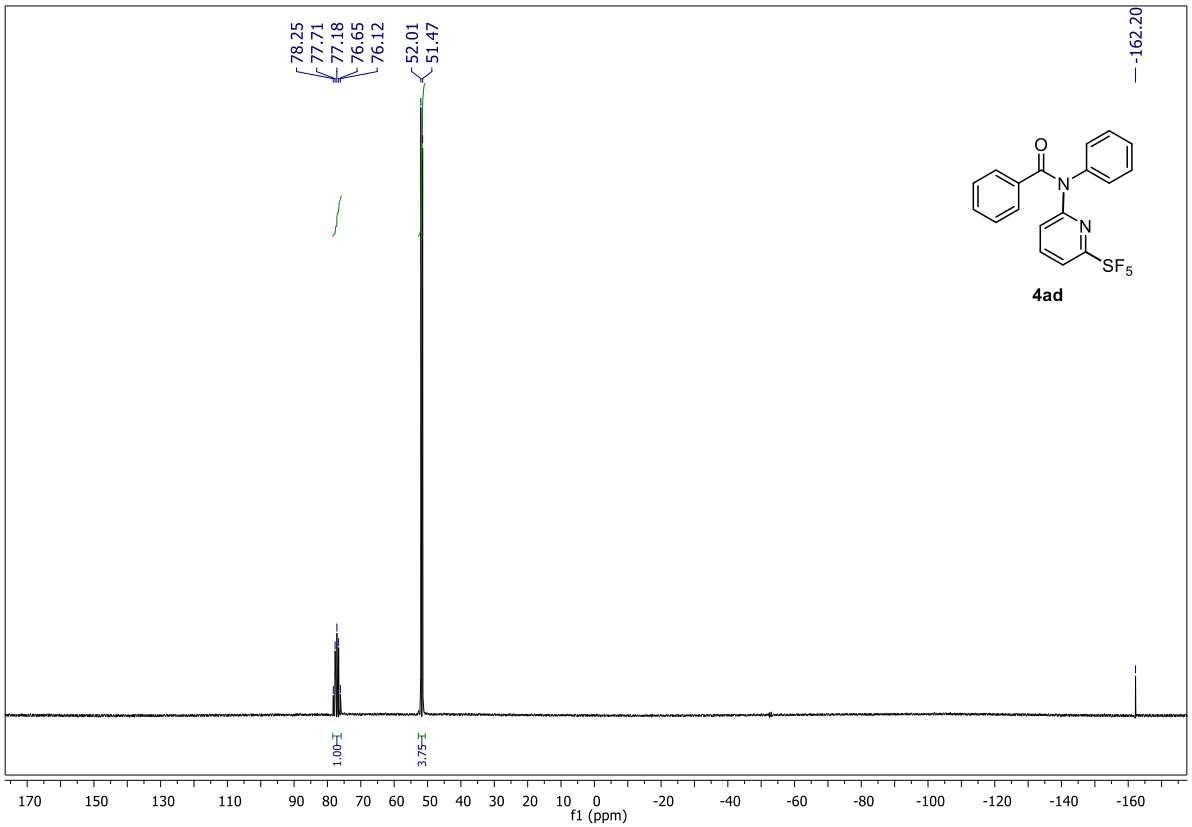
141.07
136.15
136.09
136.01
135.89
131.04
128.94
128.85
125.68
122.17
77.41
77.16
76.91
24.18
1.16
0.14
NO2
O
N
N
SF5
4bc
f1 (ppm)


7.87
7.85
7.82
7.50
7.47
7.44
7.38
7.35
7.33
7.29
7.26
7.26
7.24
7.20
7.18
0.00
O
N
N
SF5
4ad
1.00
3.77
8.12
f1 (ppm)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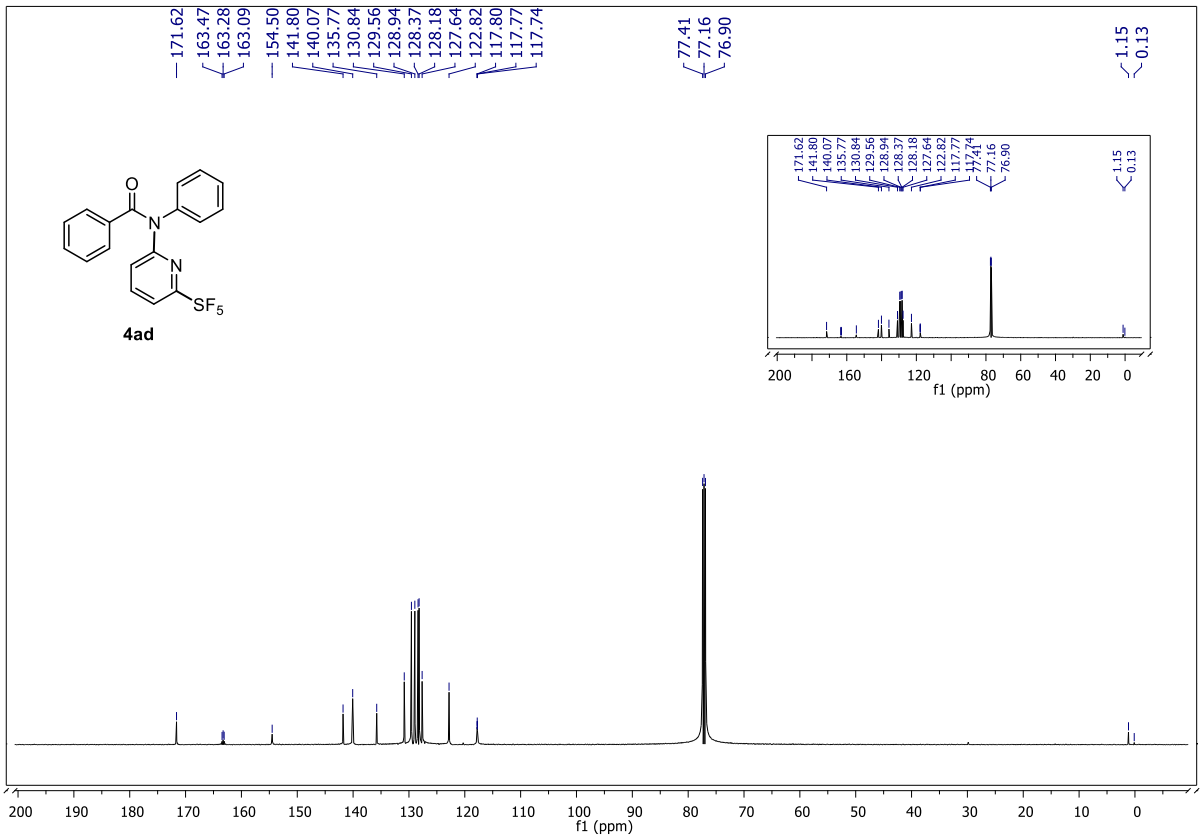
76.65
76.12
52.01
51.47
-162.20
1.00
3.75
f1 (ppm)
4ad


171.62
163.47
163.28
163.09
154.50
141.80
140.07
135.77
130.84
129.56
128.94
128.37
128.18
127.64
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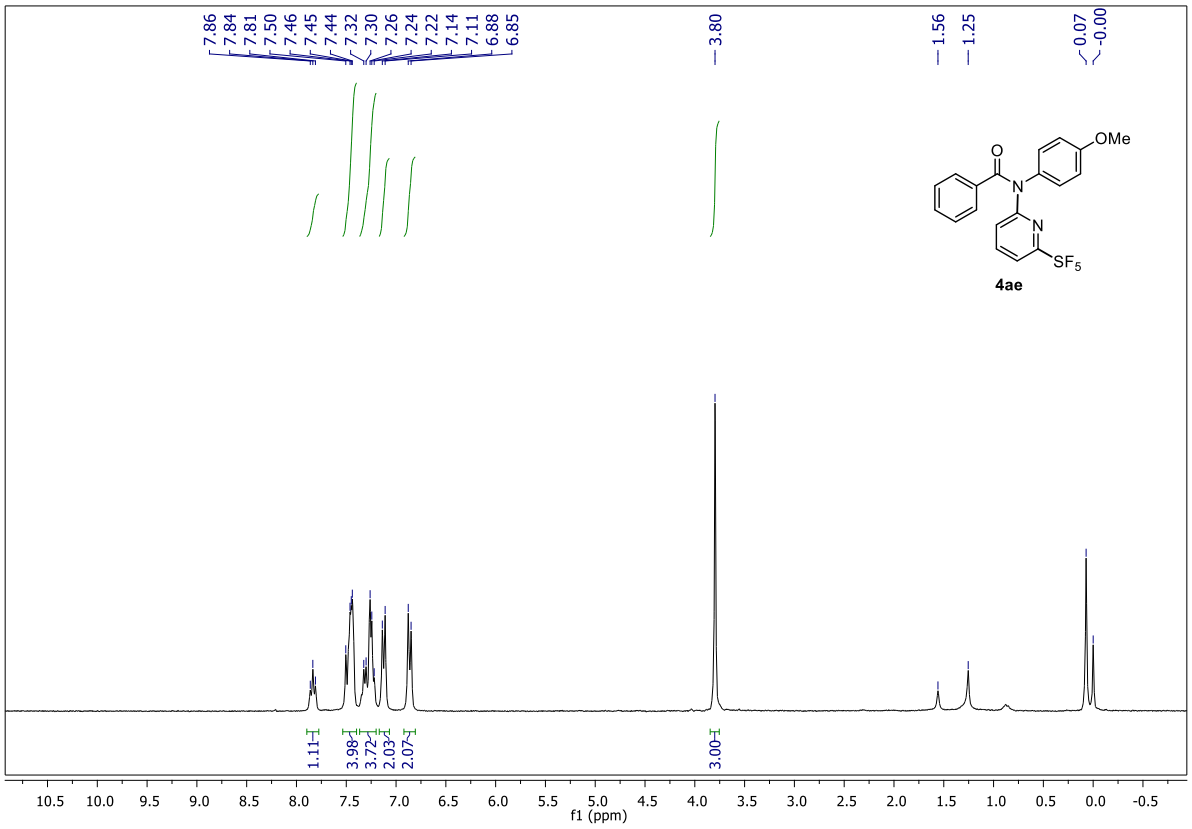
117.77
117.74
77.41
77.16
76.90
1.15
0.13
f1 (ppm)
4ad


7.86
7.84
7.81
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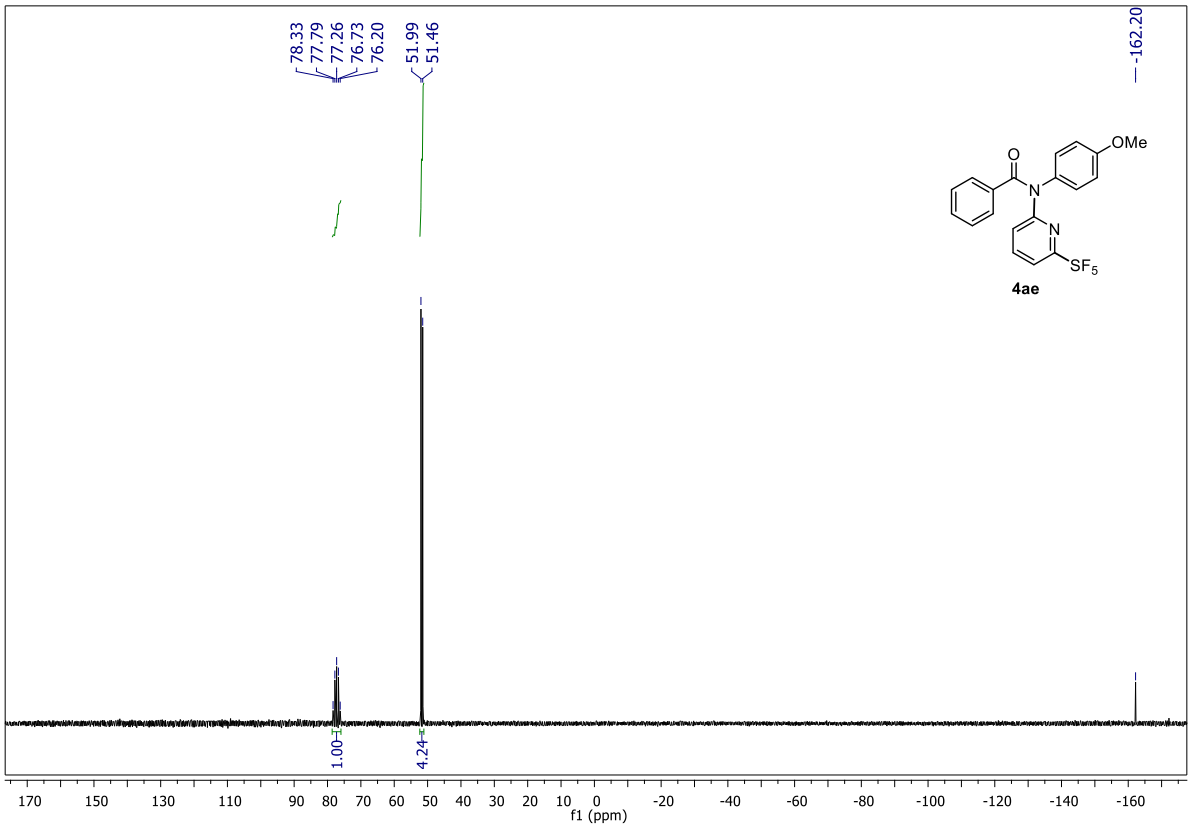
7.46
7.45
7.44
7.32
7.30
7.26
7.24
7.22
7.14
7.11
6.88
6.85
3.80
1.56
1.25
0.07
-0.00
OMe
O
N
N
SF5
4ae
1.11
3.98
3.72
2.03
2.07
3.00
f1 (ppm)


78.33
77.79
77.26
76.73
76.20
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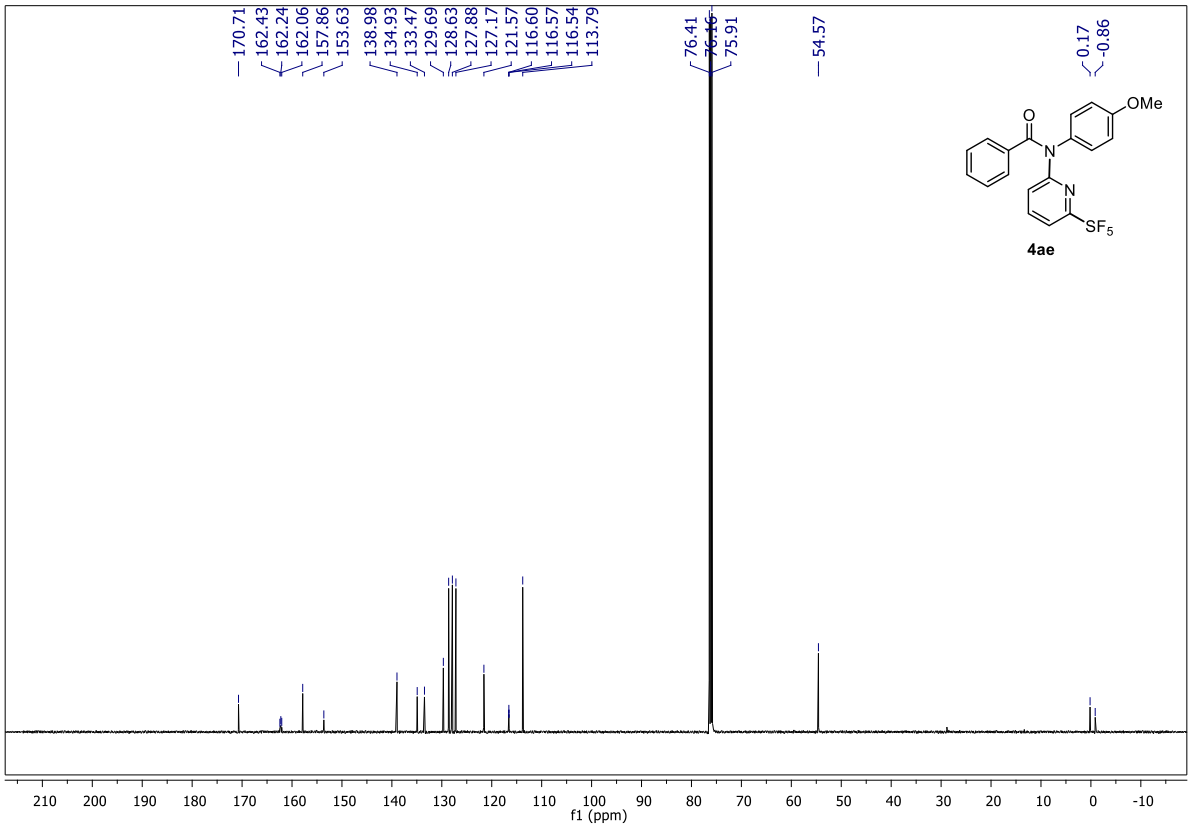
51.46
-162.20
OMe
O
N
N
SF5
4ae
1.00
4.24
f1 (ppm)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162.24
162.06
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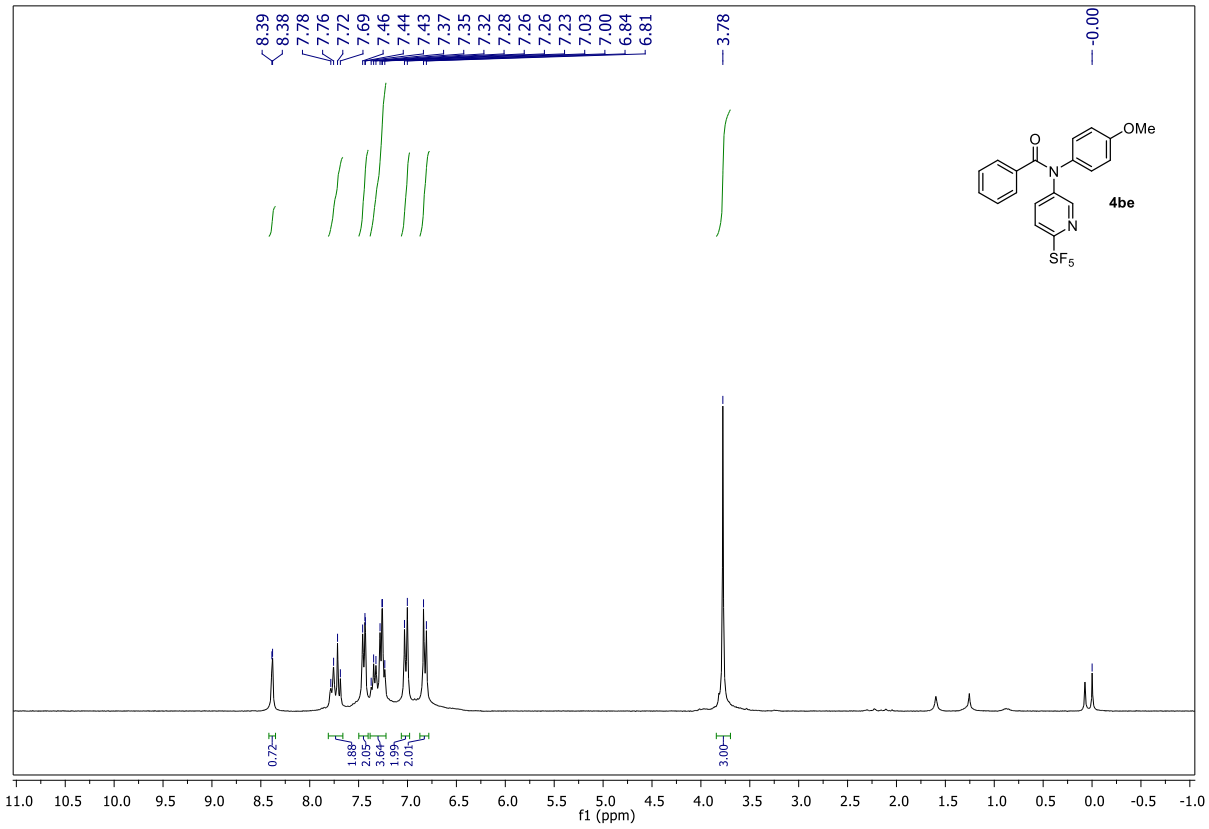
153.63
138.98
134.93
133.47
129.69
128.63
127.88
127.17
121.57
116.60
116.57
116.54
113.79
76.41
76.16
75.91
54.57
0.17
-0.86
OMe
O
N
N
SF5
4ae
f1 (ppm)


8.39
8.38
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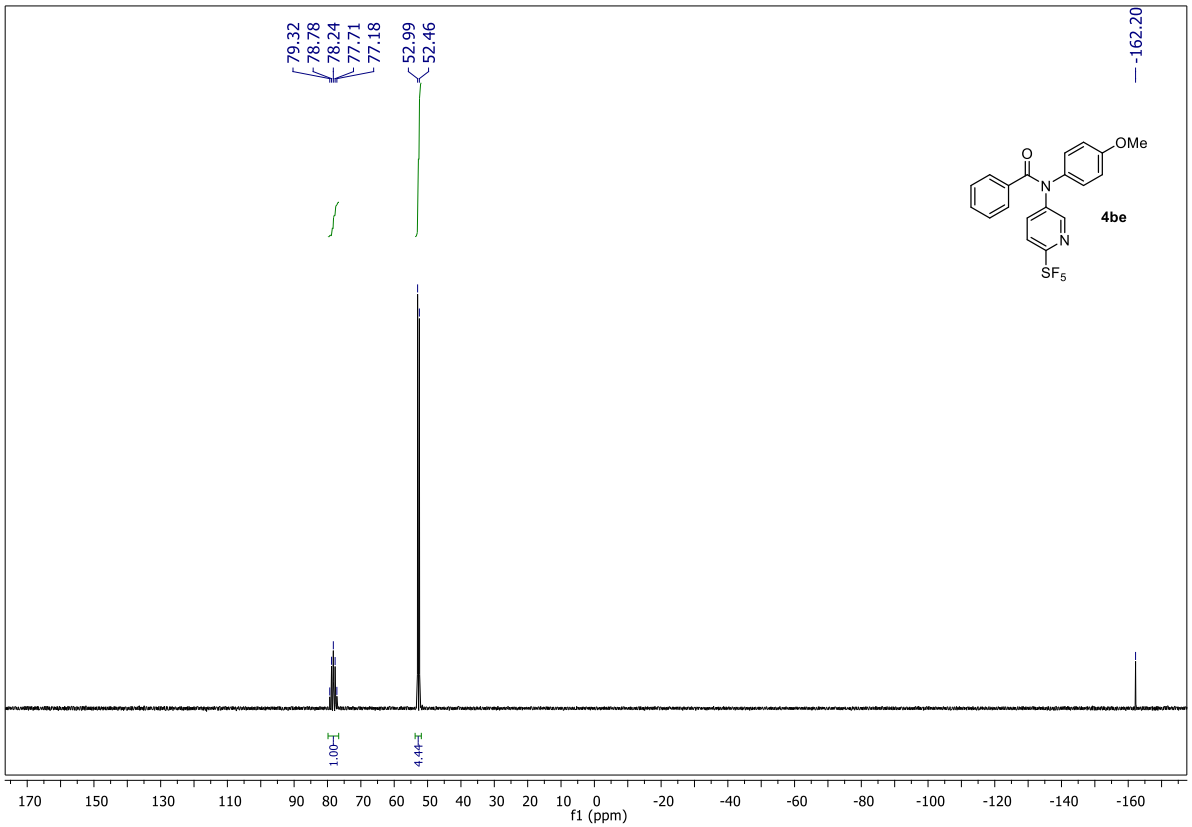
7.76
7.72
7.69
7.46
7.44
7.43
7.37
7.35
7.32
7.28
7.26
7.26
7.23
7.03
7.00
6.84
6.81
3.78
-0.00
OMe
O
N
N
SF5
4be
0.72
1.89
2.05
3.64
1.99
2.01
3.00
f1 (ppm)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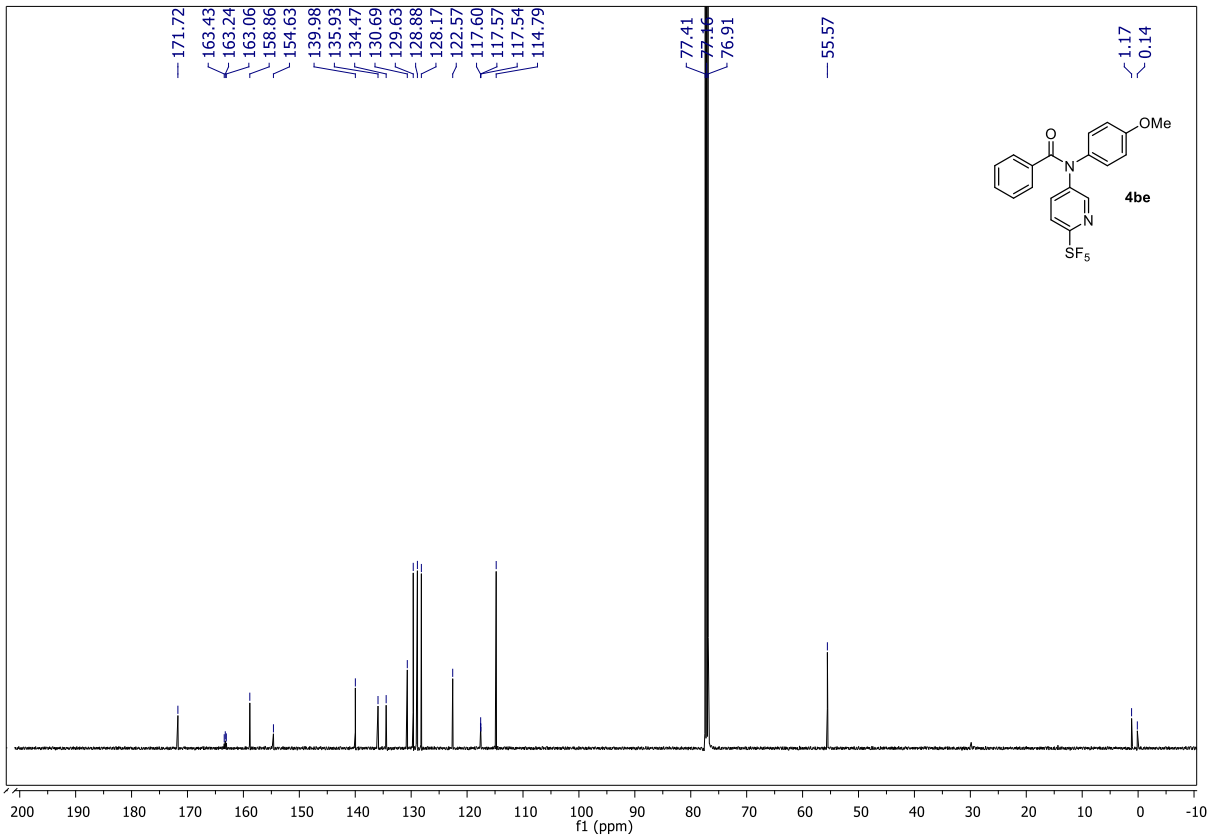
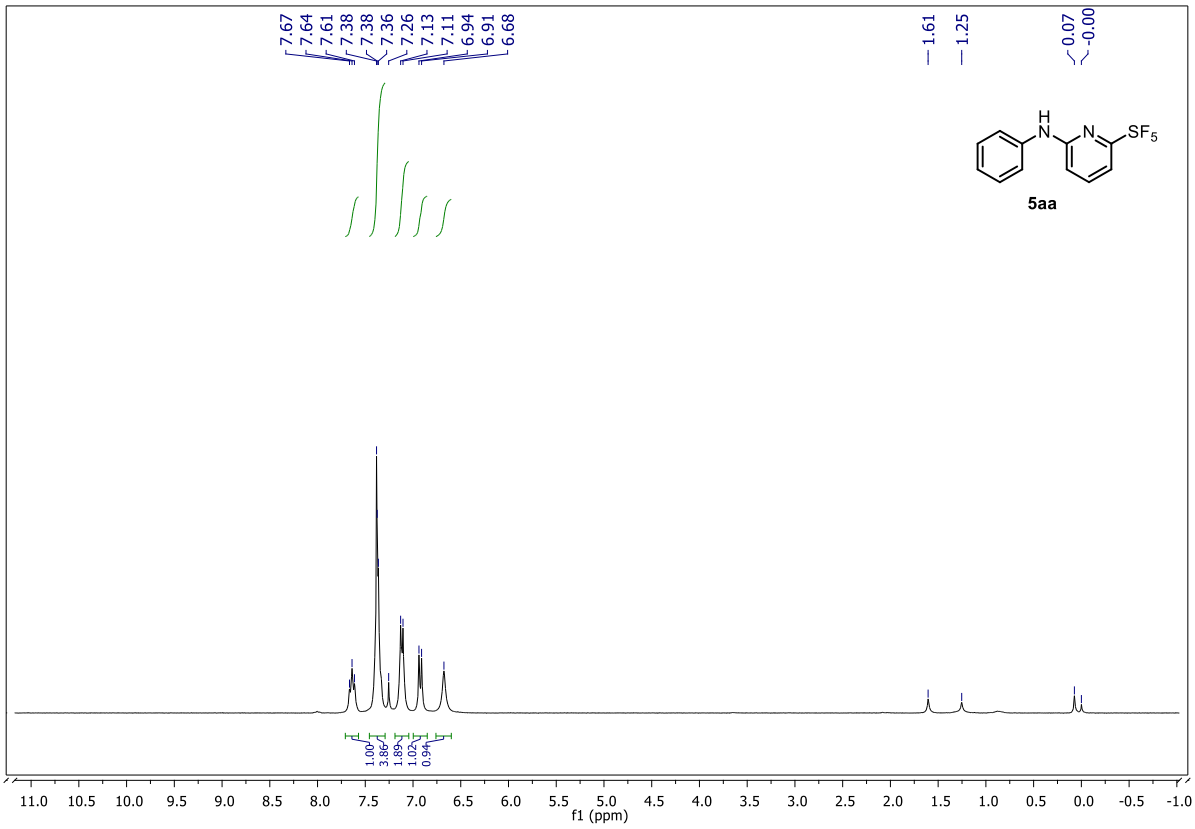
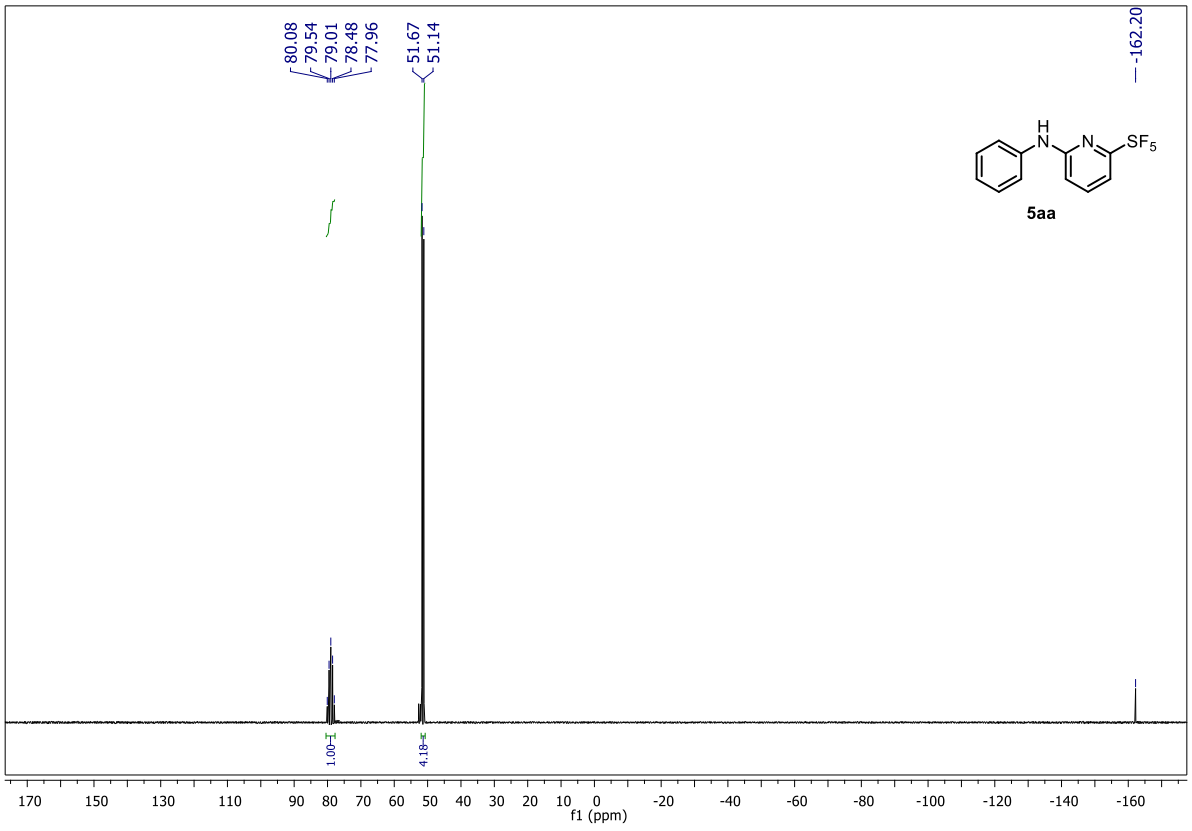
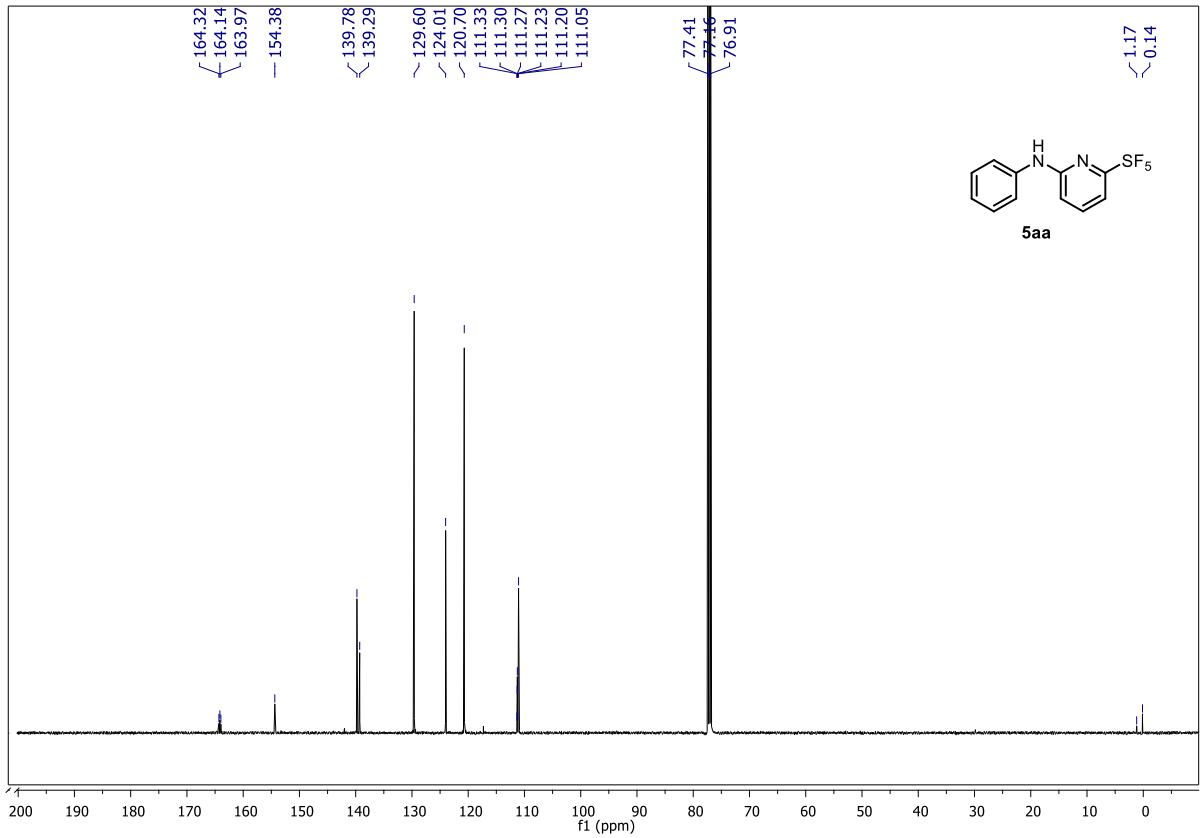
78.78
78.24
77.71
77.18
52.99
52.46
-162.20
OMe
4be
N
SF5
1.00
4.44
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)


171.72
163.43
163.24
163.06
158.86
154.63
139.98
135.93
134.47
130.69
129.63
128.88
128.17
122.57
117.60
117.57
117.54
114.79
77.41
77.16
76.91
55.57
1.17
0.14
OMe
4be
N
SF5
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.67
7.64
7.61
7.38
7.38
7.36
7.26
7.13
7.11
6.94
6.91
6.68
1.61
1.25
0.07
-0.00
1.00
3.86
1.89
1.02
0.94
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)
H
N
N
SF5
5aa


80.08
79.54
79.01
78.48
77.96
51.67
51.14
-162.20
1.00
4.18
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)
H
N
N
SF5
5aa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139.78
139.29
129.60
124.01
120.70
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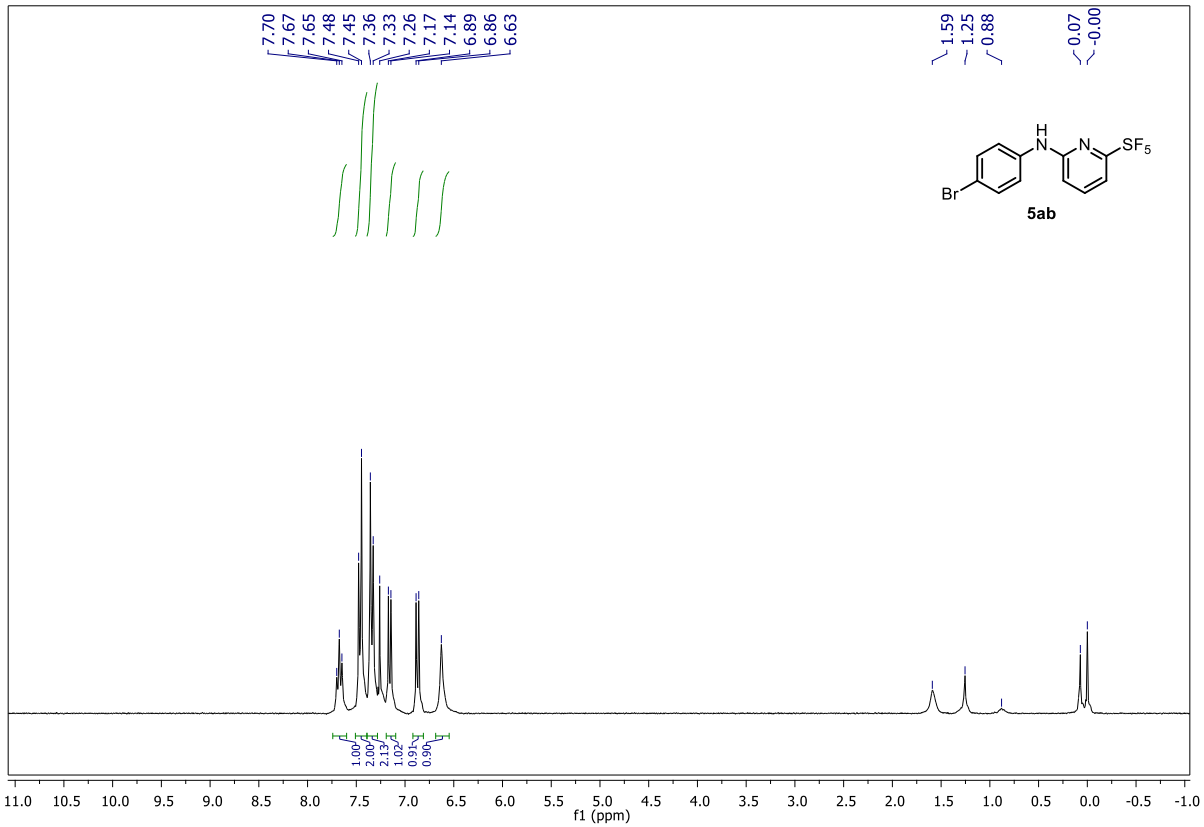
111.30
111.27
111.23
111.20
111.05
77.41
77.16
76.91
1.17
0.14
H
N
N
SF5
5aa
f1 (ppm)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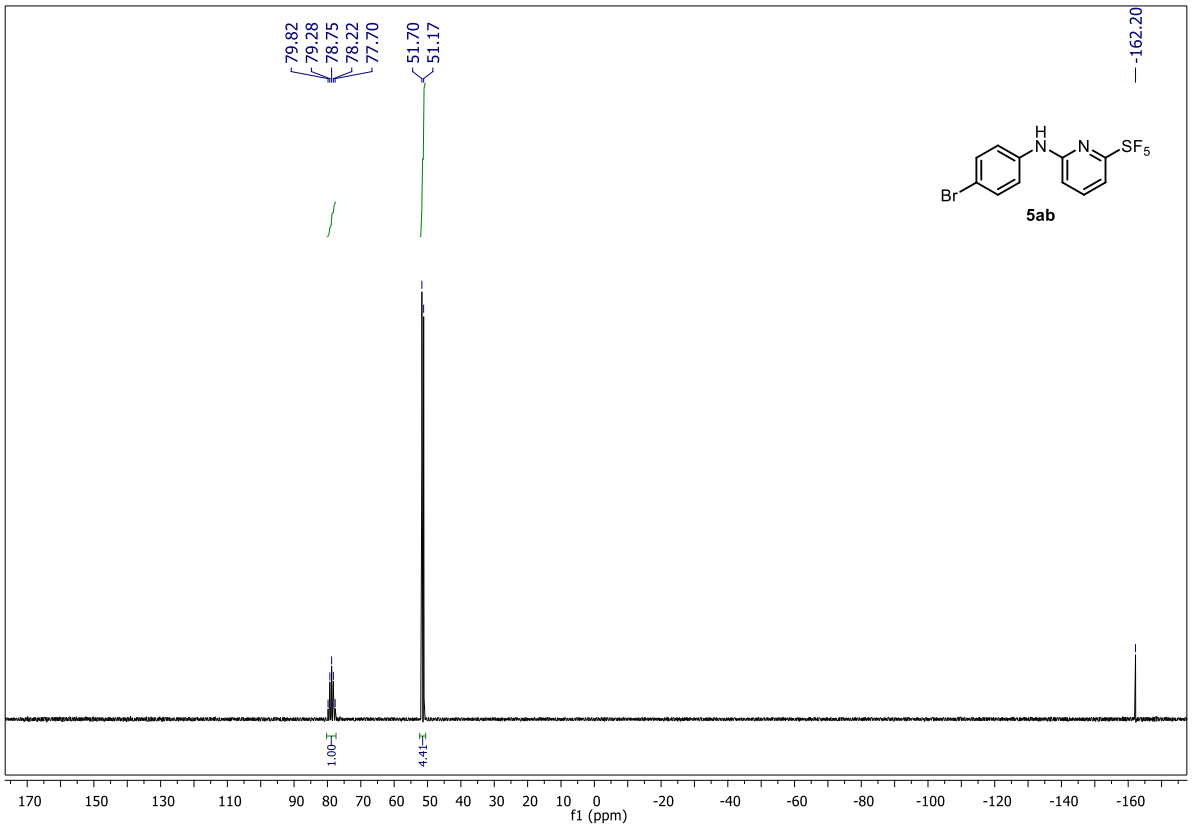
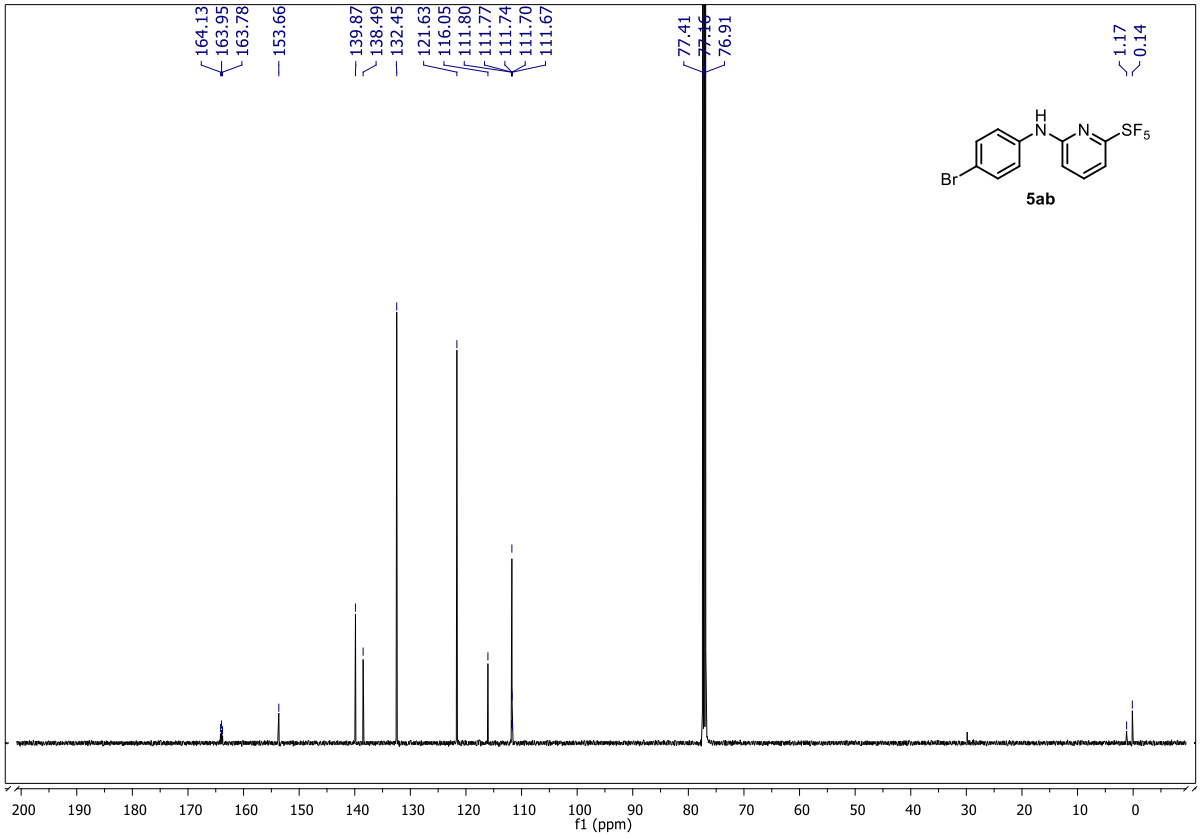
7.45
7.36
7.33
7.26
7.17
7.14
6.89
6.86
6.63
1.59
1.25
0.88
0.07
-0.00
H
N
N
SF5
Br
5ab
1.00
2.00
2.13
1.02
0.91
0.90
f1 (ppm)


79.82
79.28
78.75
78.22
77.70
51.70
51.17
-162.20
H
N
N
SF5
Br
5ab
1.00
4.41
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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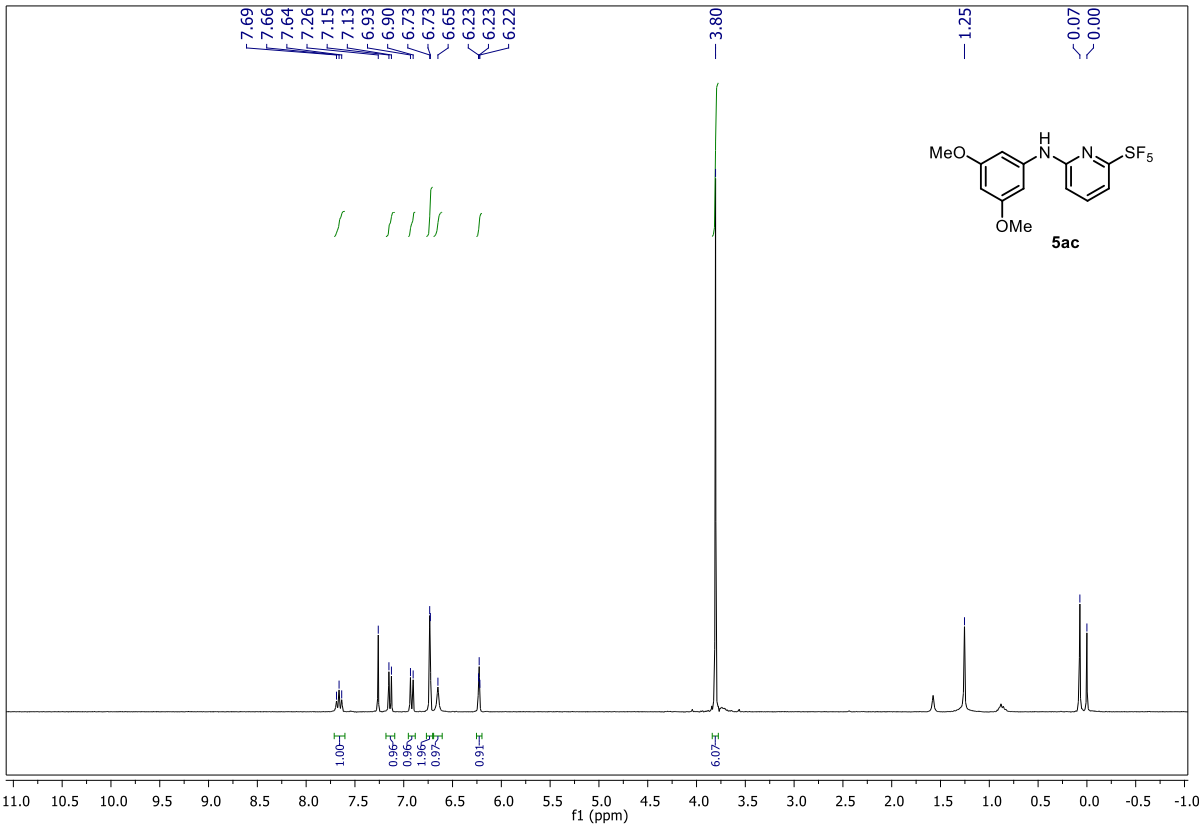
163.95
163.78
153.66
139.87
138.49
132.45
121.63
116.05
111.80
111.77
111.74
111.70
111.67
77.41
77.16
76.91
1.17
0.14
H
N
N
SF5
Br
5ab
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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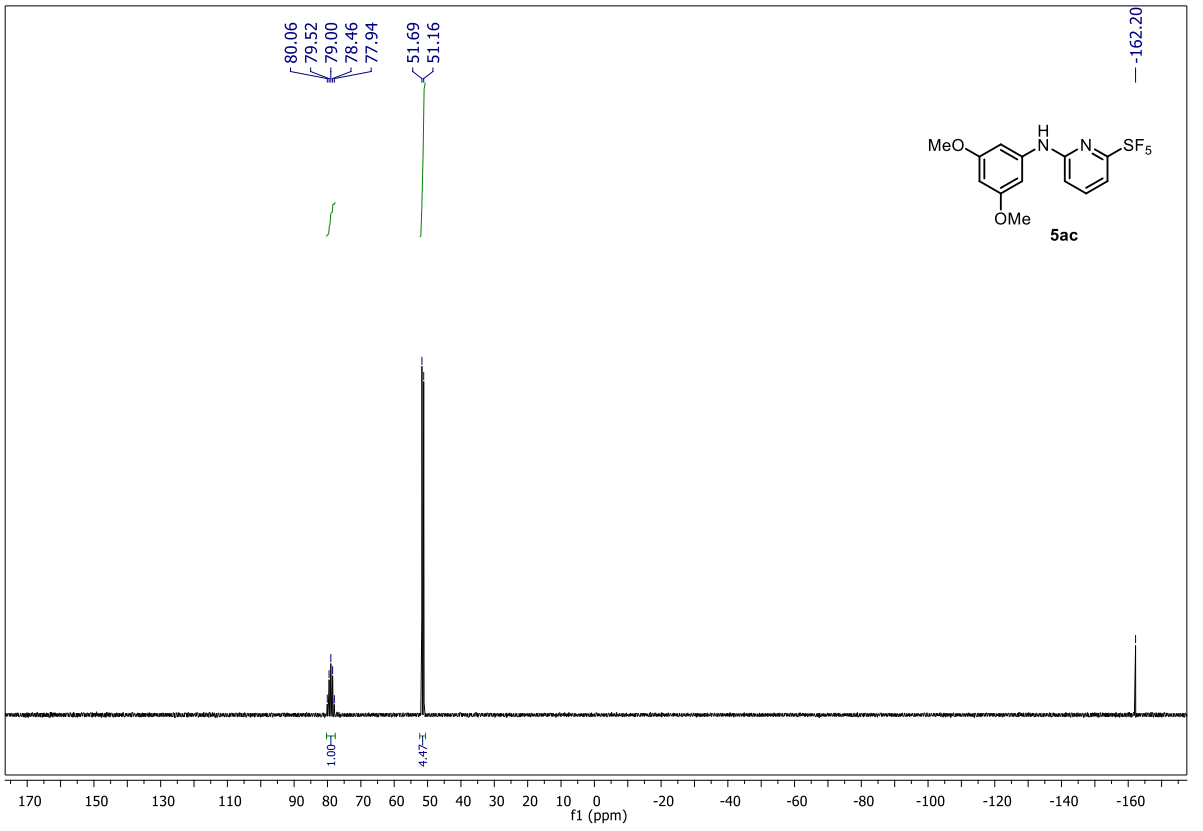
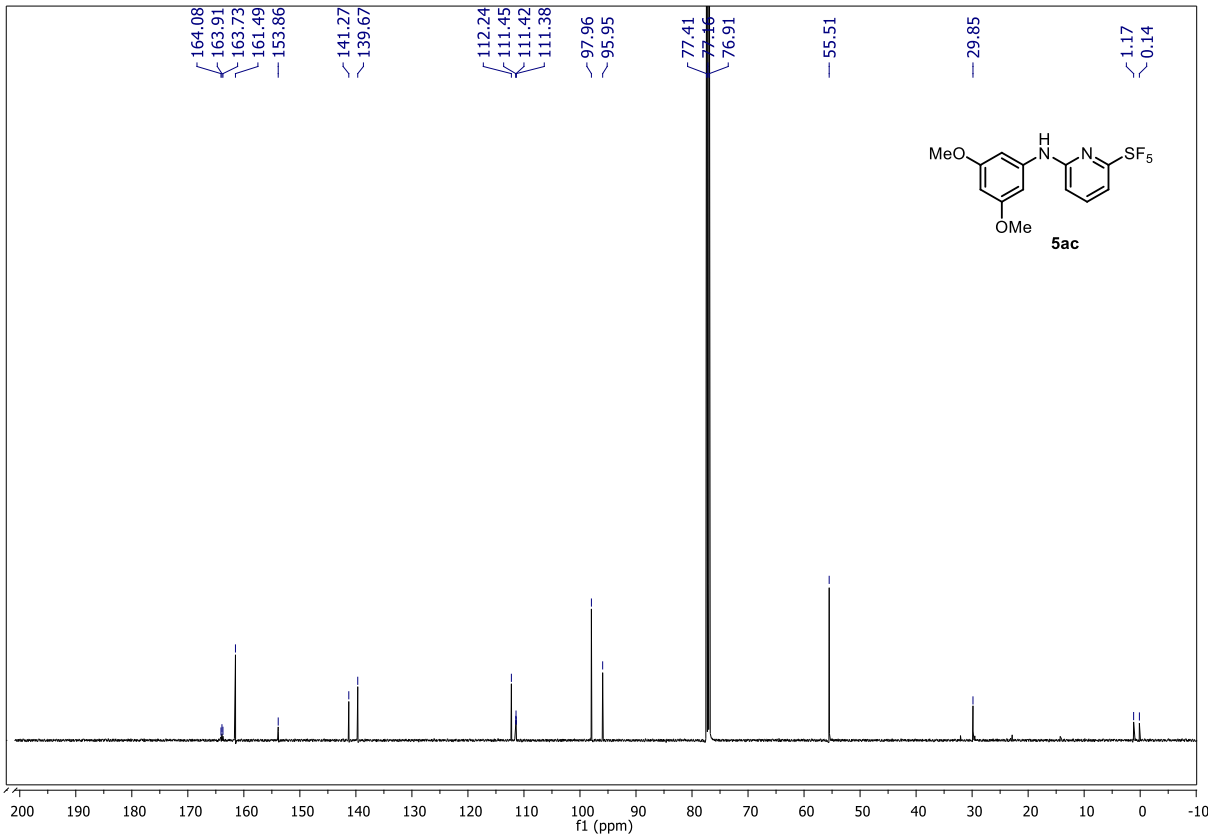
7.66
7.64
7.26
7.15
7.13
6.93
6.90
6.73
6.73
6.65
6.23
6.23
6.22
3.80
1.25
0.07
0.00
MeO
H
N
N
SF5
OMe
5ac
1.00
0.96
0.96
1.96
0.97
0.91
6.07
f1 (ppm)


80.06
79.52
79.00
78.46
77.94
51.69
51.16
-162.20
MeO
H
N
N
SF5
OMe
5ac
1.00
4.47
f1 (ppm)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163.73
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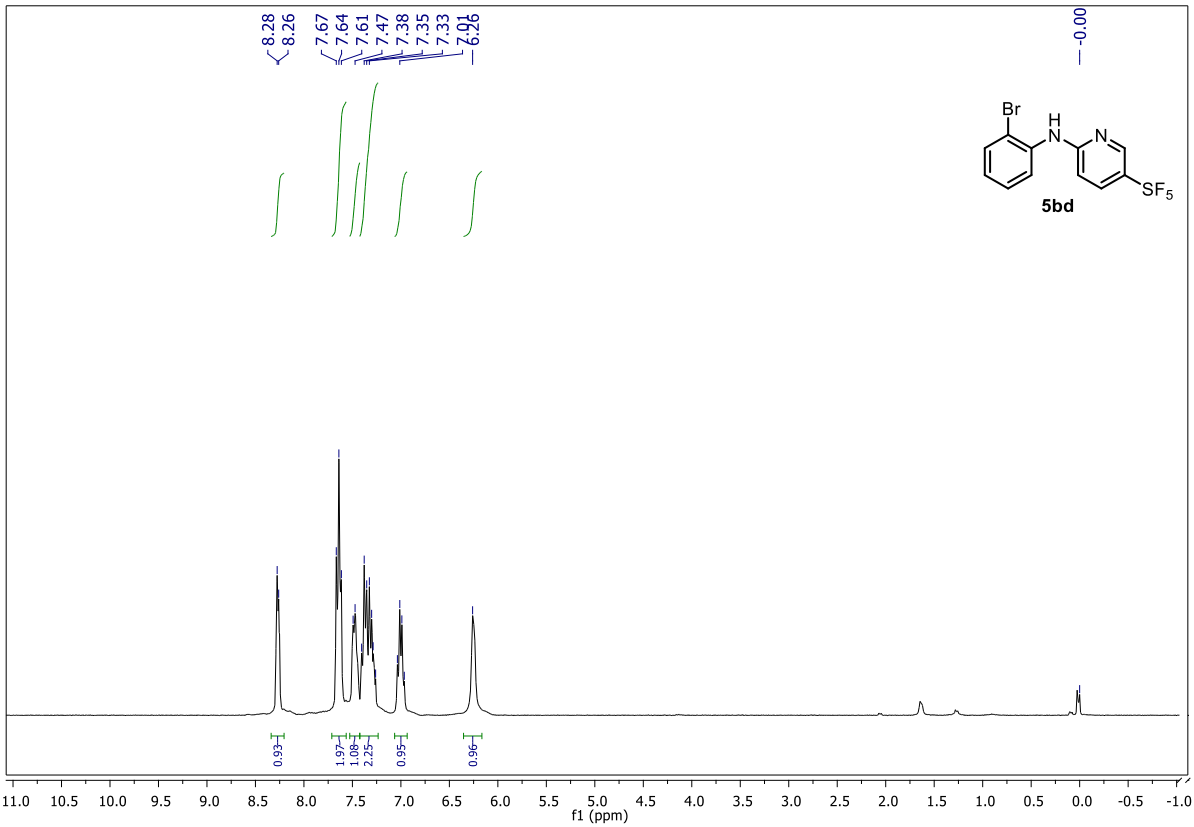
153.86
141.27
139.67
112.24
111.45
111.42
111.38
97.96
95.95
77.41
77.16
76.91
55.51
29.85
1.17
0.14
MeO
H
N
N
SF5
OMe
5ac
f1 (ppm)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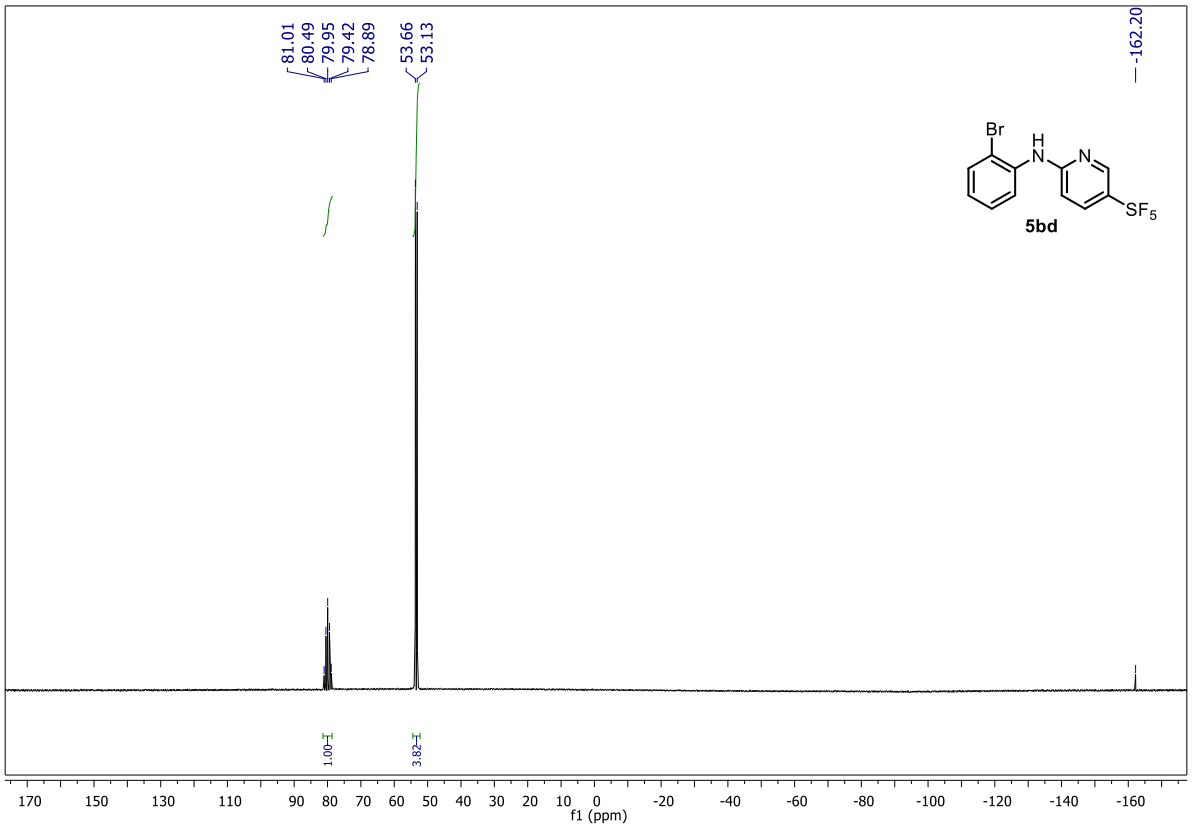
8.26
7.67
7.64
7.61
7.47
7.38
7.35
7.33
7.01
6.26
-0.00
Br
H
N
N
SF5
5bd
0.93
1.97
1.08
2.25
0.95
0.96
f1 (ppm)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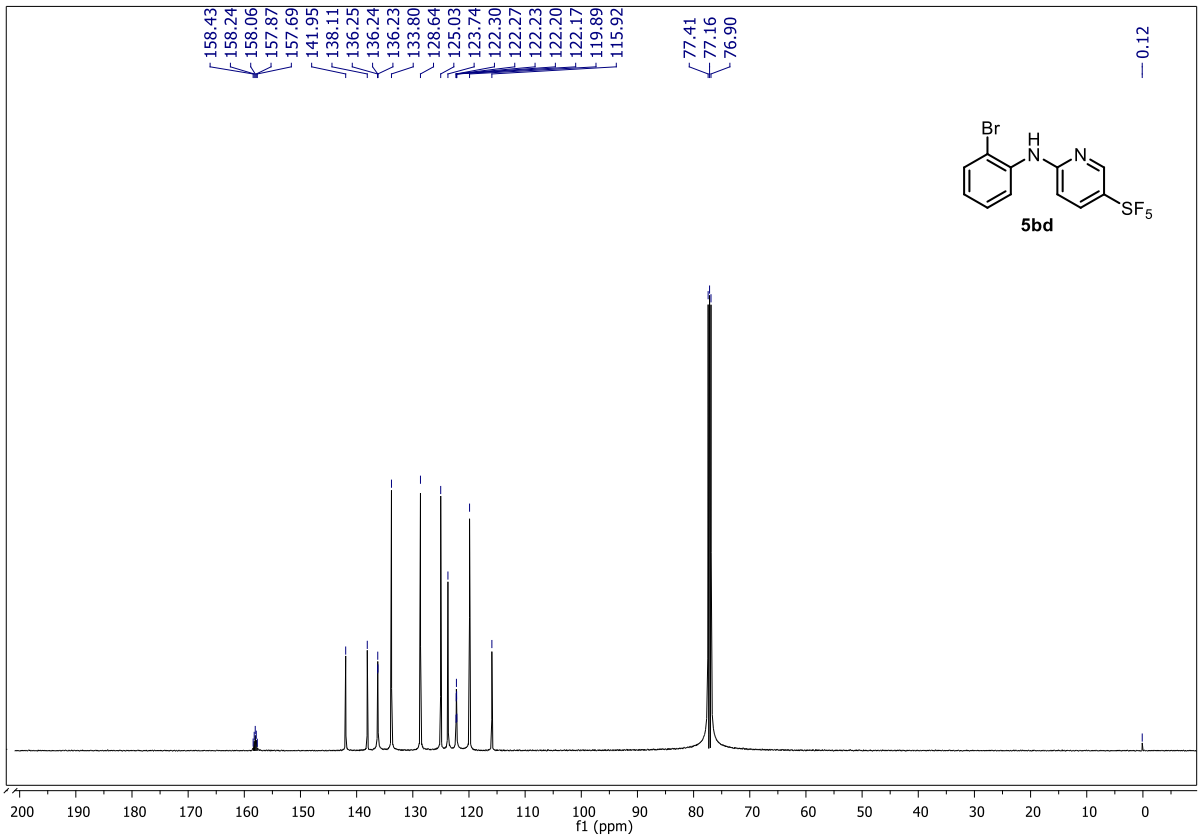
80.49
79.95
79.42
78.89
53.66
53.13
-162.20
Br
H
N
N
SF5
5bd
1.00
3.82
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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158.06
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157.69
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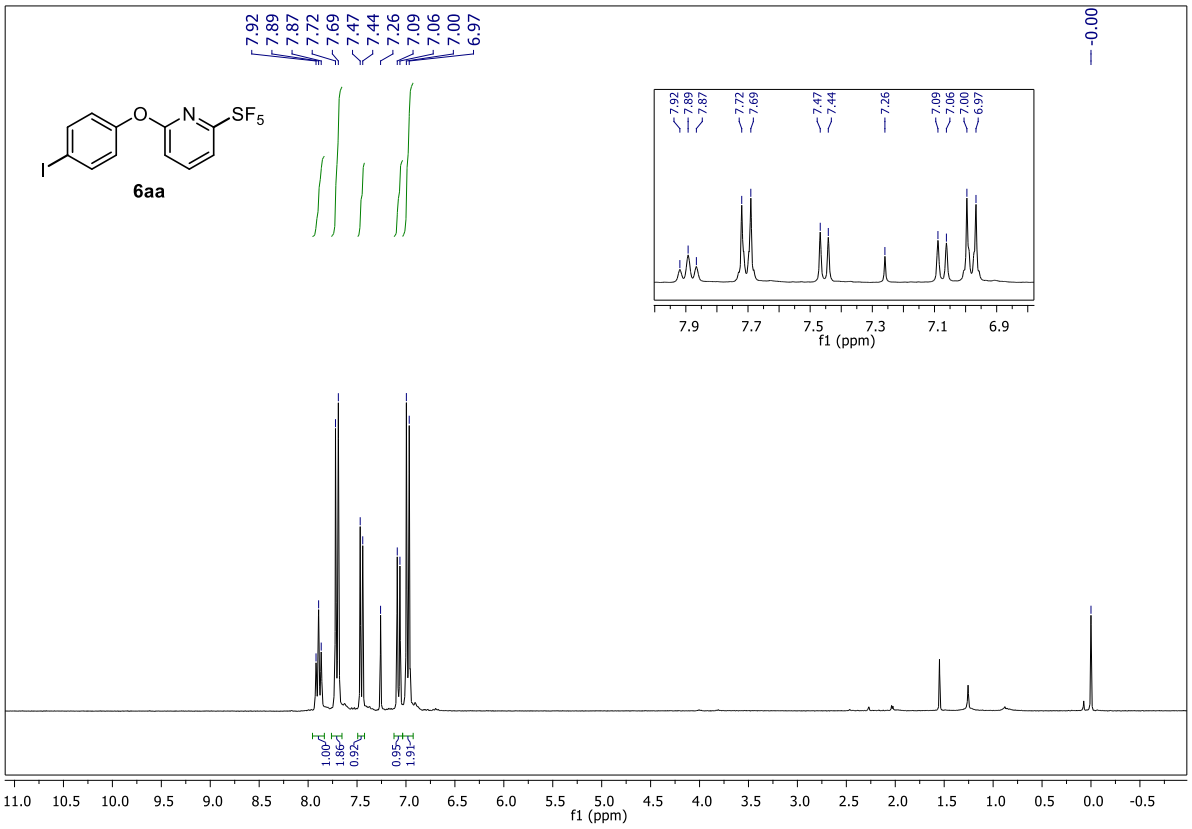
136.25
136.24
136.23
133.80
128.64
125.03
123.74
122.30
122.27
122.23
122.20
122.17
119.89
115.92
77.41
77.16
76.90
0.12
Br
H
N
N
SF5
5bd
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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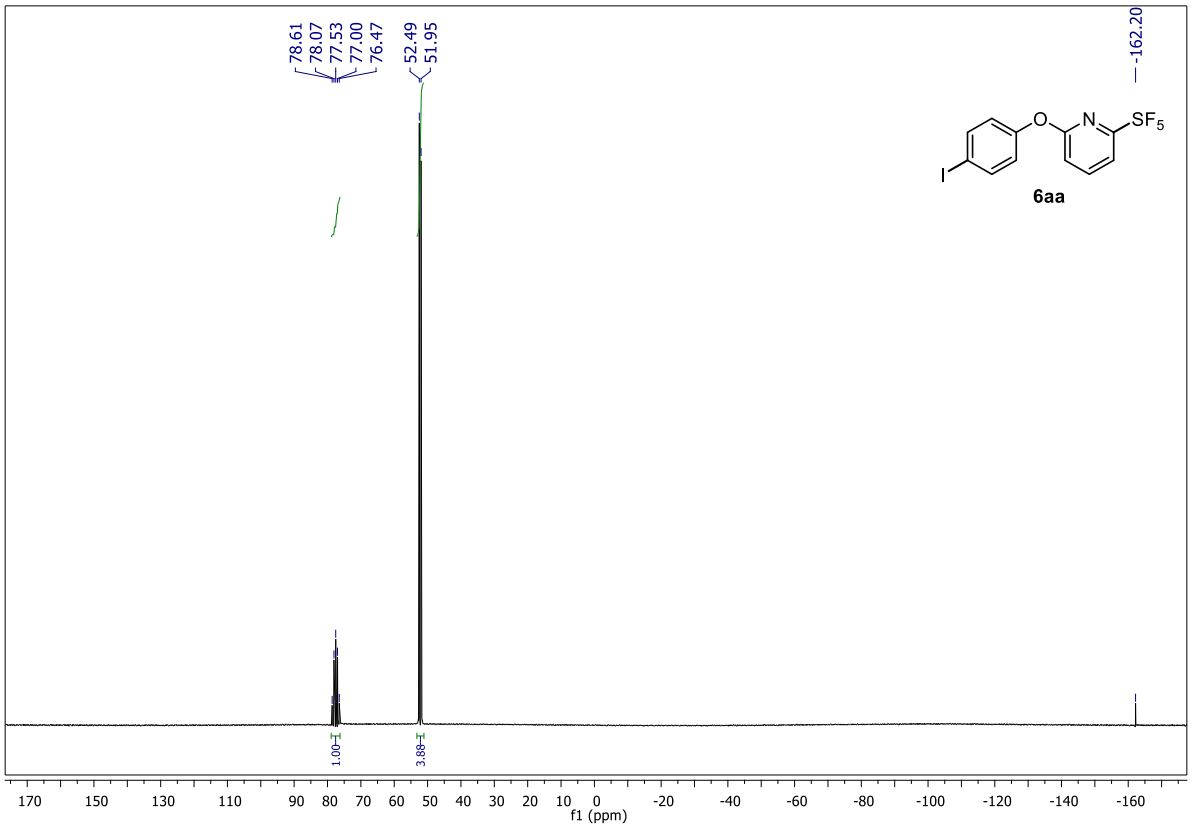
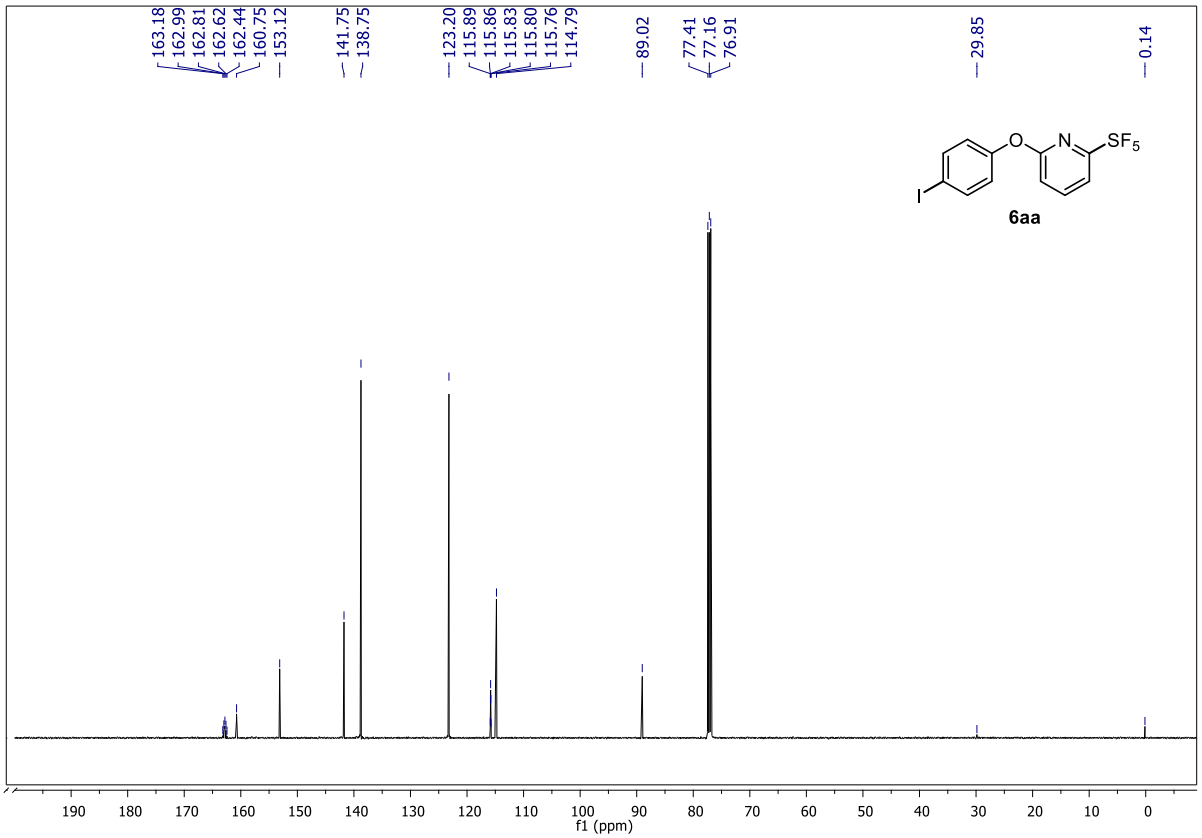
7.89
7.87
7.72
7.69
7.47
7.44
7.26
7.09
7.06
7.00
6.97
-0.00
O
N
SF5
I
6aa
f1 (ppm)
1.00
1.86
0.92
0.95
1.91


78.61
78.07
77.53
77.00
76.47
52.49
51.95
-162.20
O
N
SF5
I
6aa
f1 (ppm)
1.00
3.88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160.75
153.12
141.75
138.75
123.20
115.89
115.86
115.83
115.80
115.76
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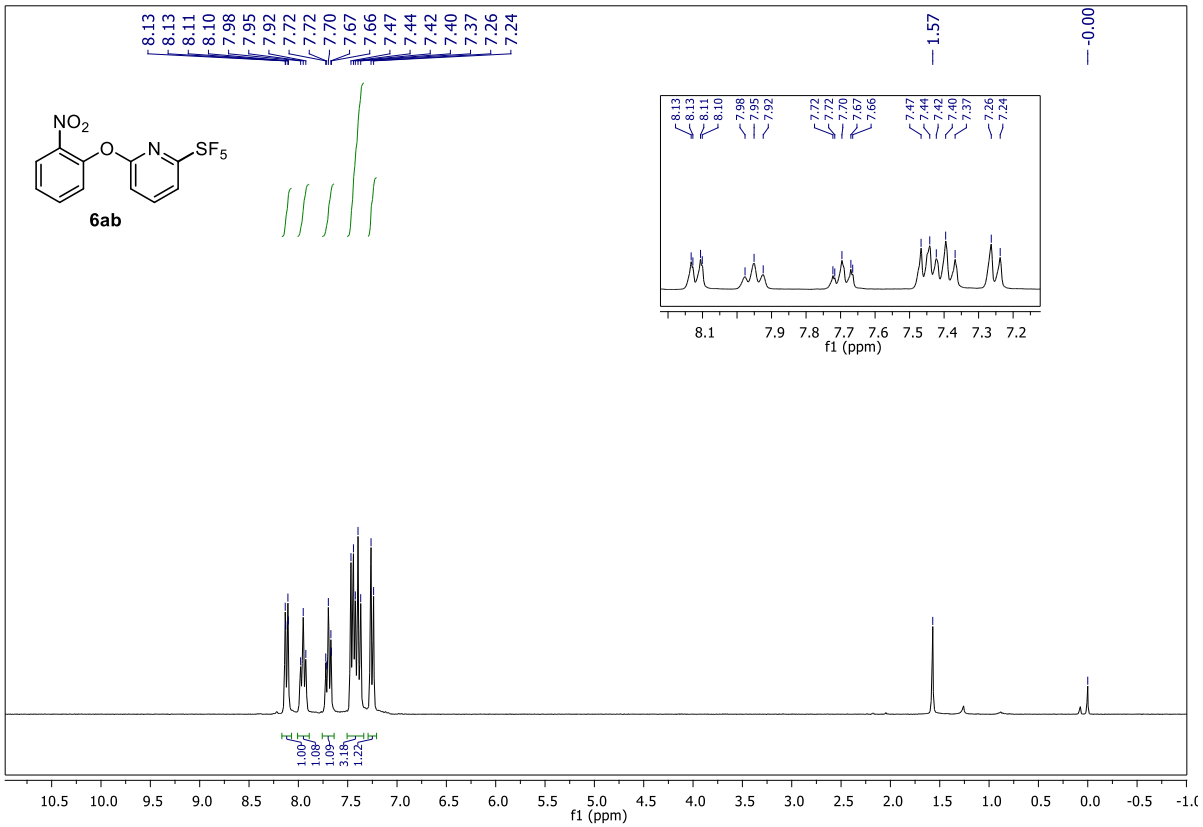
77.41
77.16
76.91
29.85
0.14
O
N
SF5
I
6aa
f1 (ppm)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8.13
8.11
8.10
7.98
7.95
7.92
7.72
7.72
7.70
7.67
7.66
7.47
7.44
7.42
7.40
7.37
7.26
7.24
1.57
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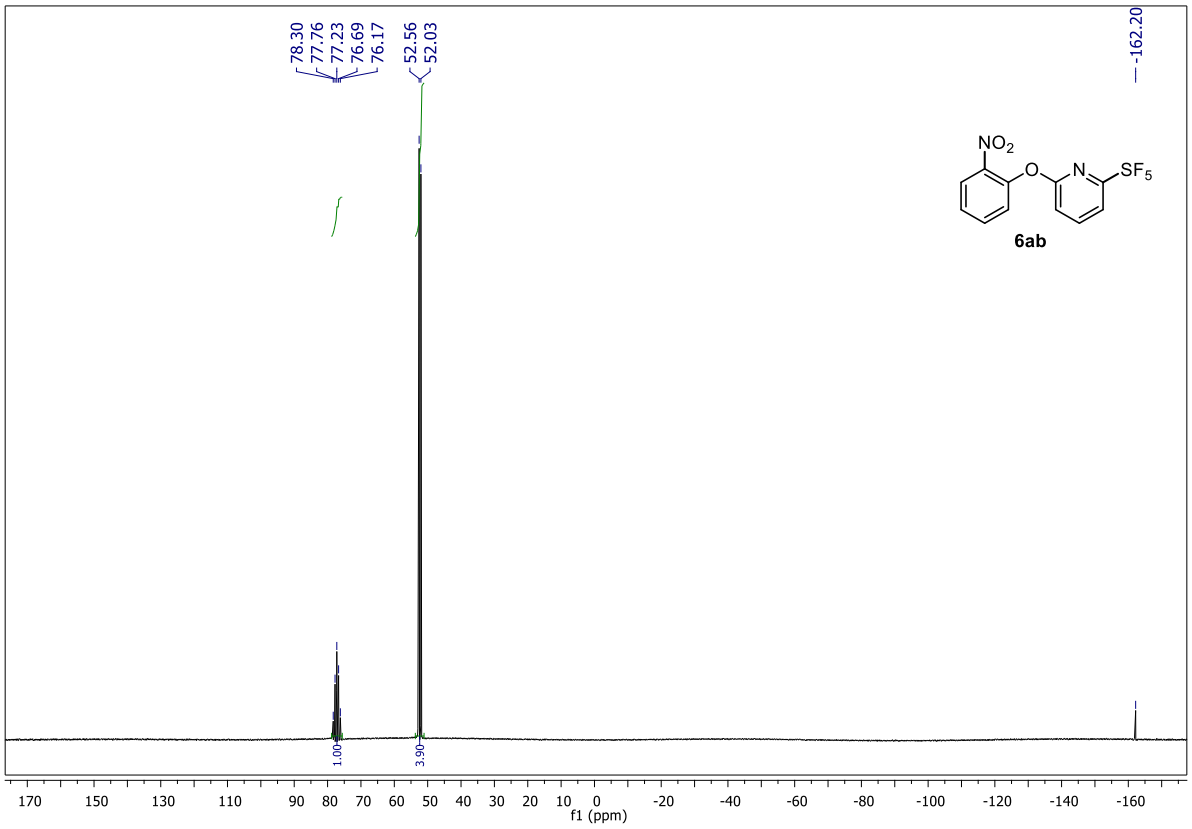
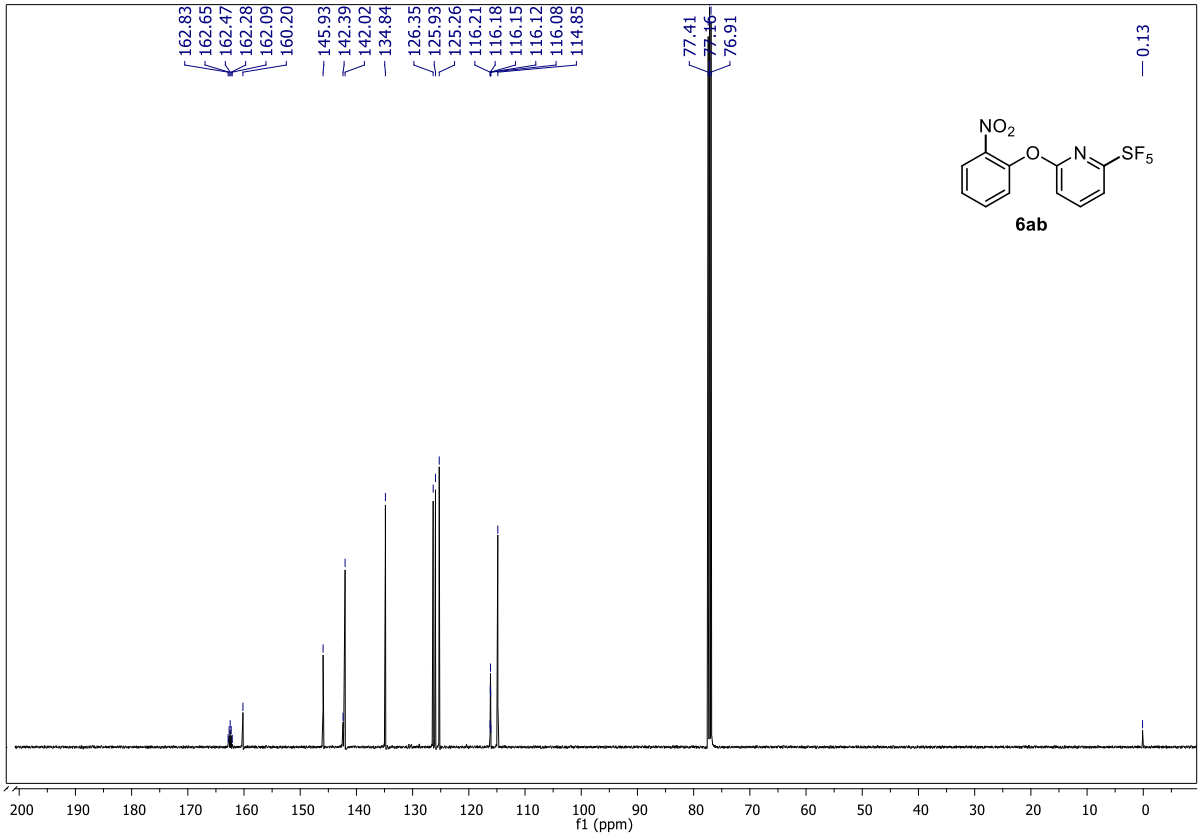
NO2
O
N
SF5
6ab
1.00
1.08
1.09
3.18
1.22
f1 (ppm)


78.30
77.76
77.23
76.69
76.17
52.56
52.03
-162.20
NO2
O
N
SF5
6ab
1.00
3.90
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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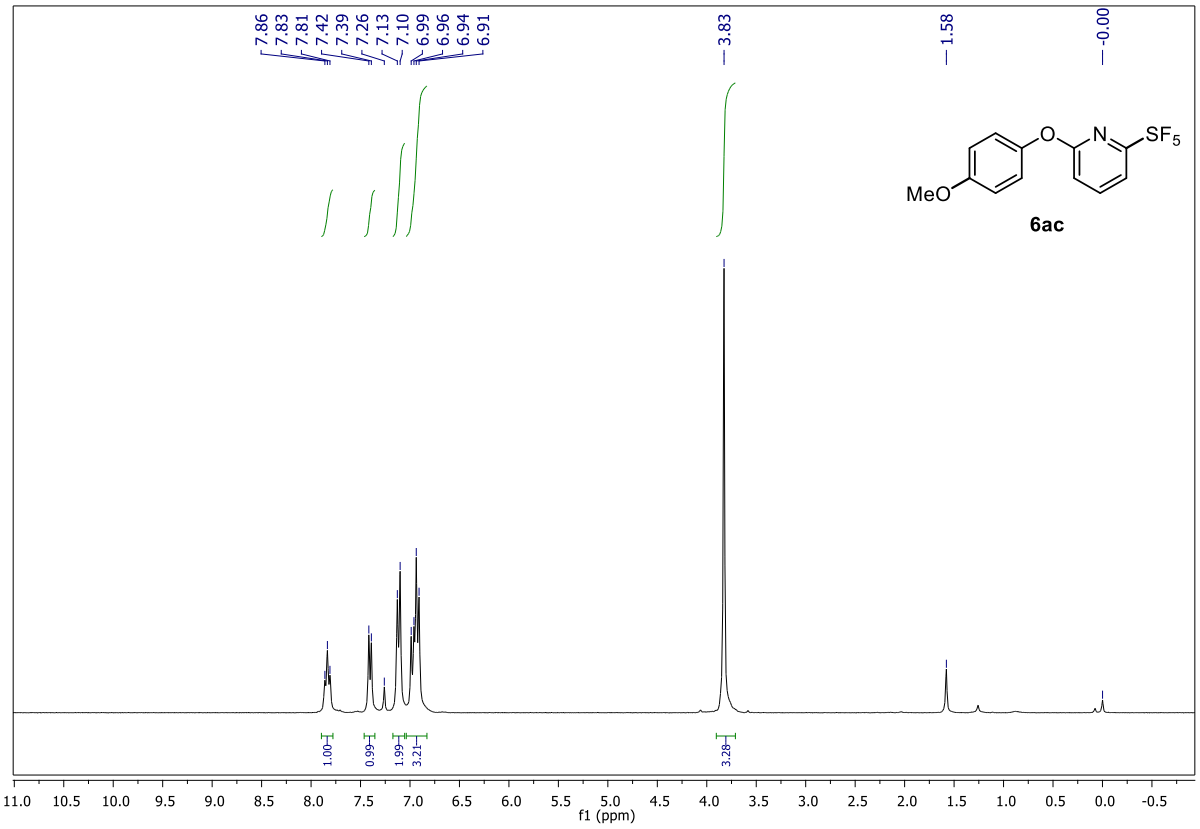
162.65
162.47
162.28
162.09
160.20
145.93
142.39
142.02
134.84
126.35
125.93
125.26
116.21
116.18
116.15
116.12
116.08
114.85
77.41
77.16
76.91
0.13
NO2
O
N
SF5
6ab
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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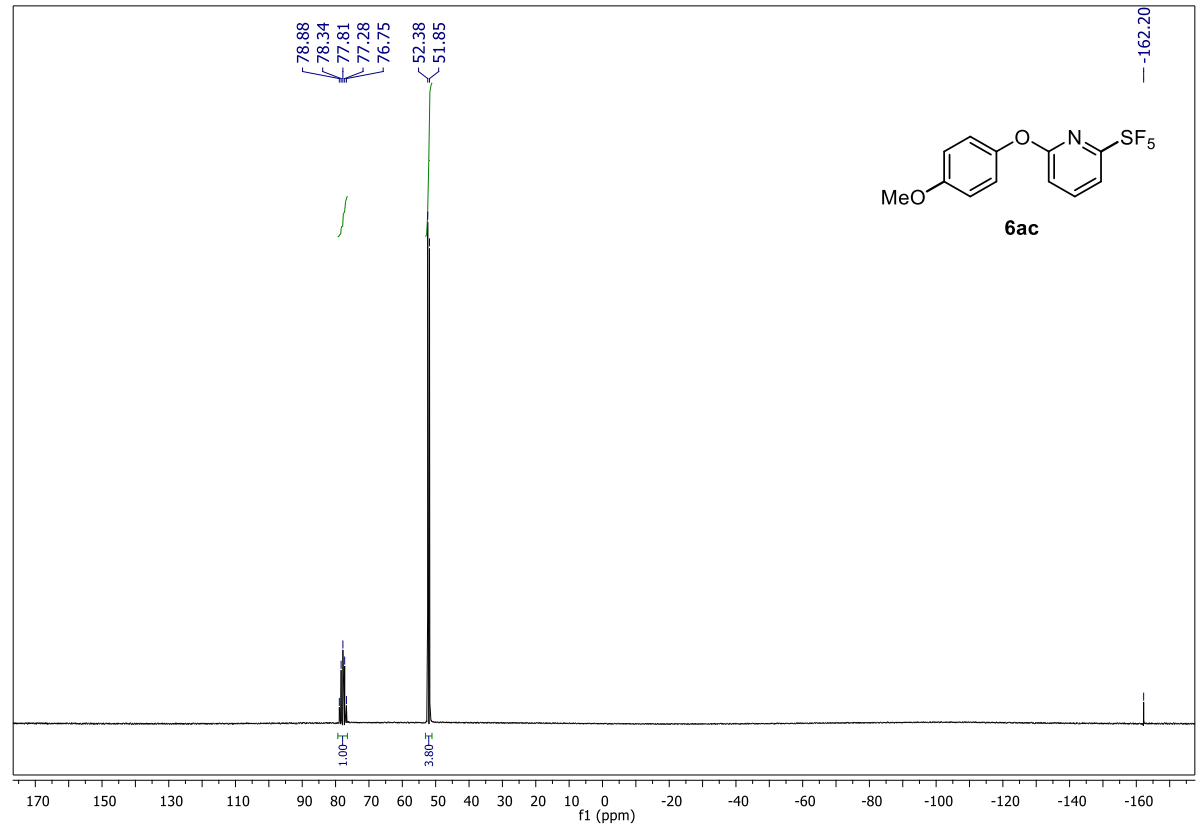
7.42
7.39
7.26
7.13
7.10
6.99
6.96
6.94
6.91
3.83
1.58
-0.00
1.00
0.99
1.99
3.21
3.28
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
O
N
SF5
MeO
6ac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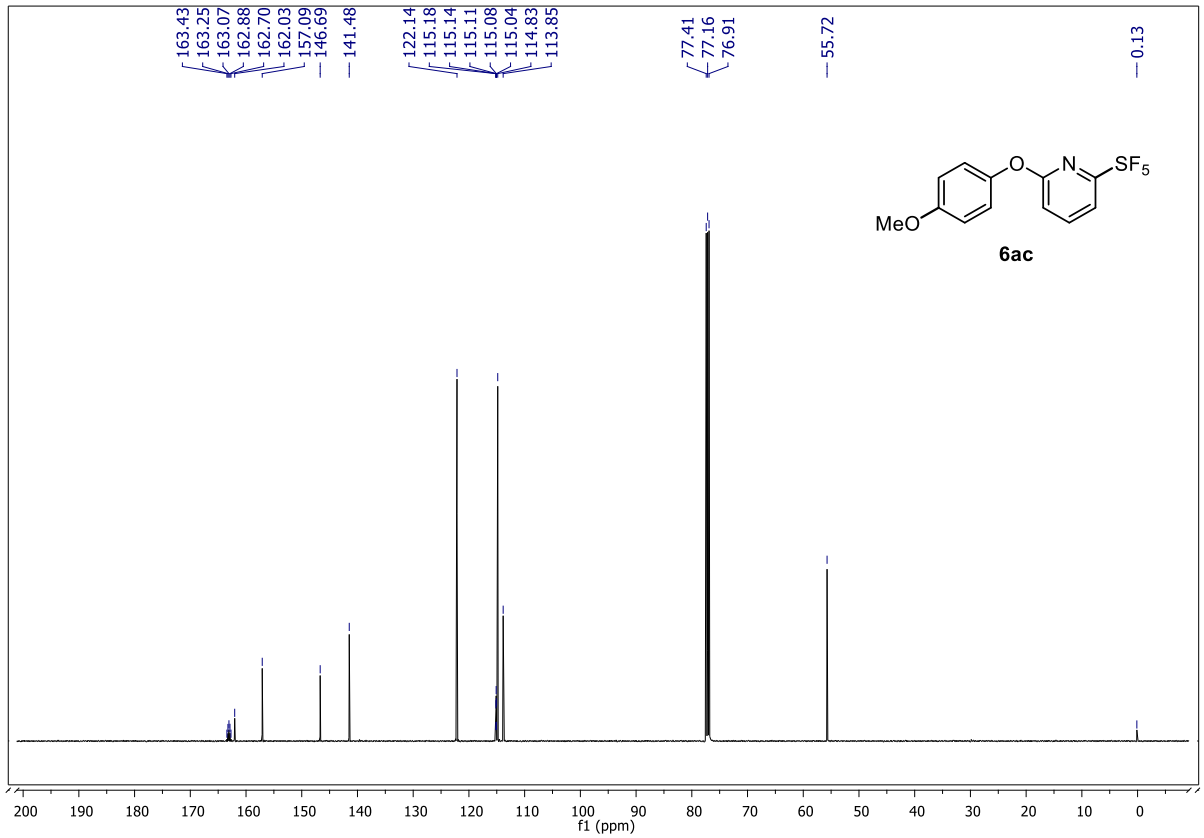
-162.20
1.00
3.80
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)
O
N
SF5
MeO
6ac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163.07
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157.09
146.69
141.48
122.14
115.18
115.14
115.11
115.08
115.04
114.83
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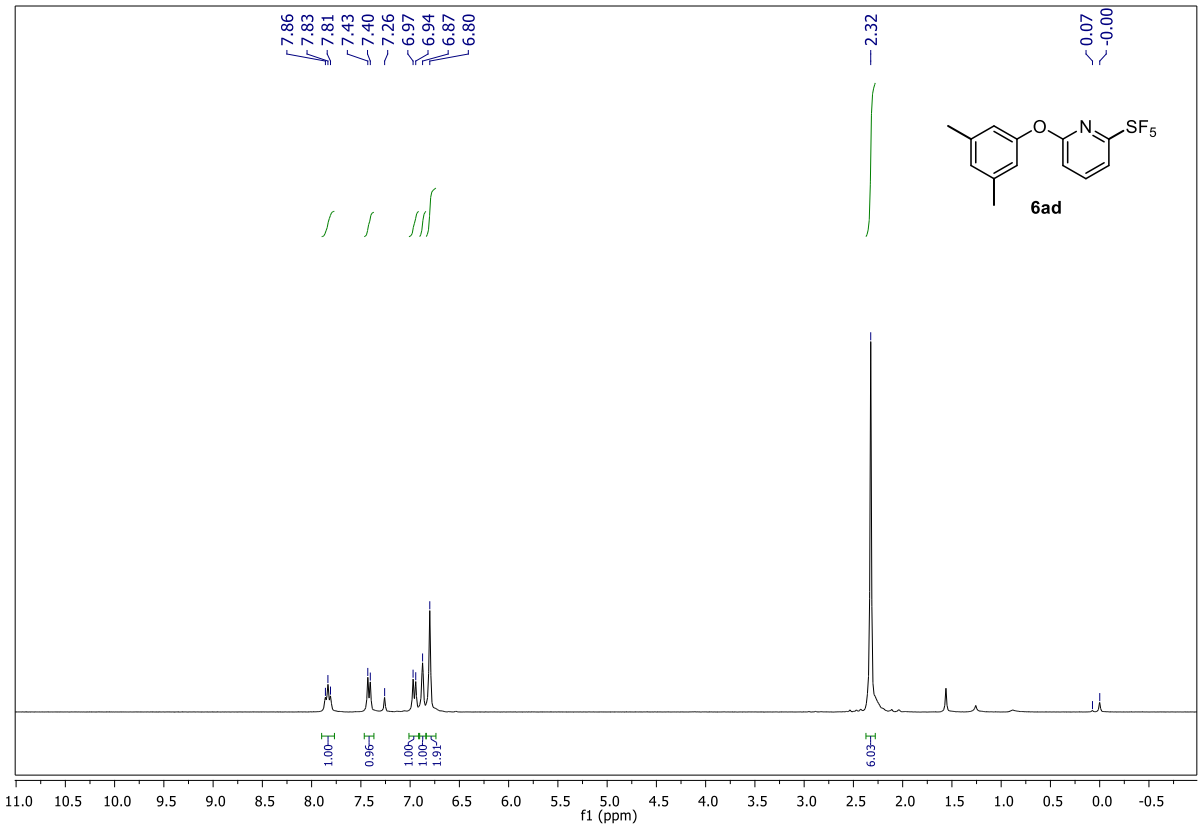
77.41
77.16
76.91
55.72
0.13
O
N
SF5
MeO
6ac
f1 (ppm)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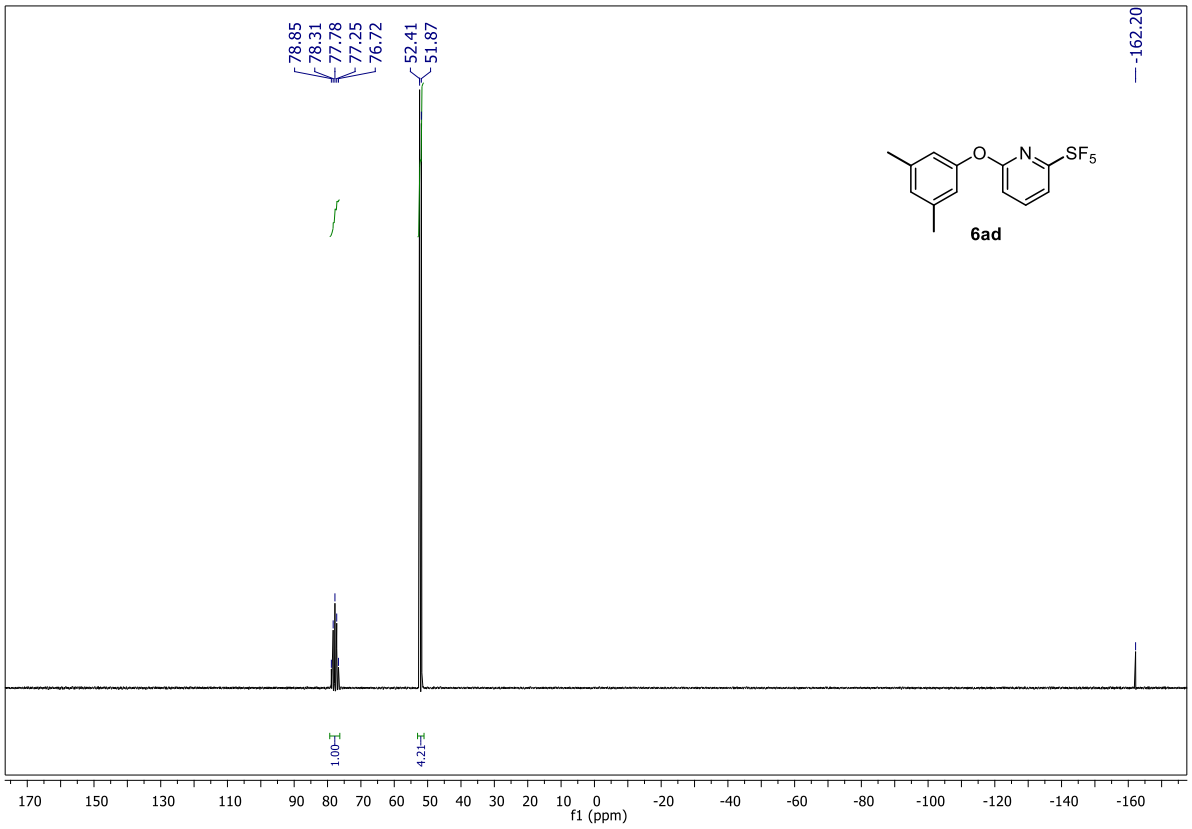
7.83
7.81
7.43
7.40
7.26
6.97
6.94
6.87
6.80
2.32
0.07
-0.00
O
N
SF5
6ad
1.00
0.96
1.00
1.00
1.91
6.03
f1 (ppm)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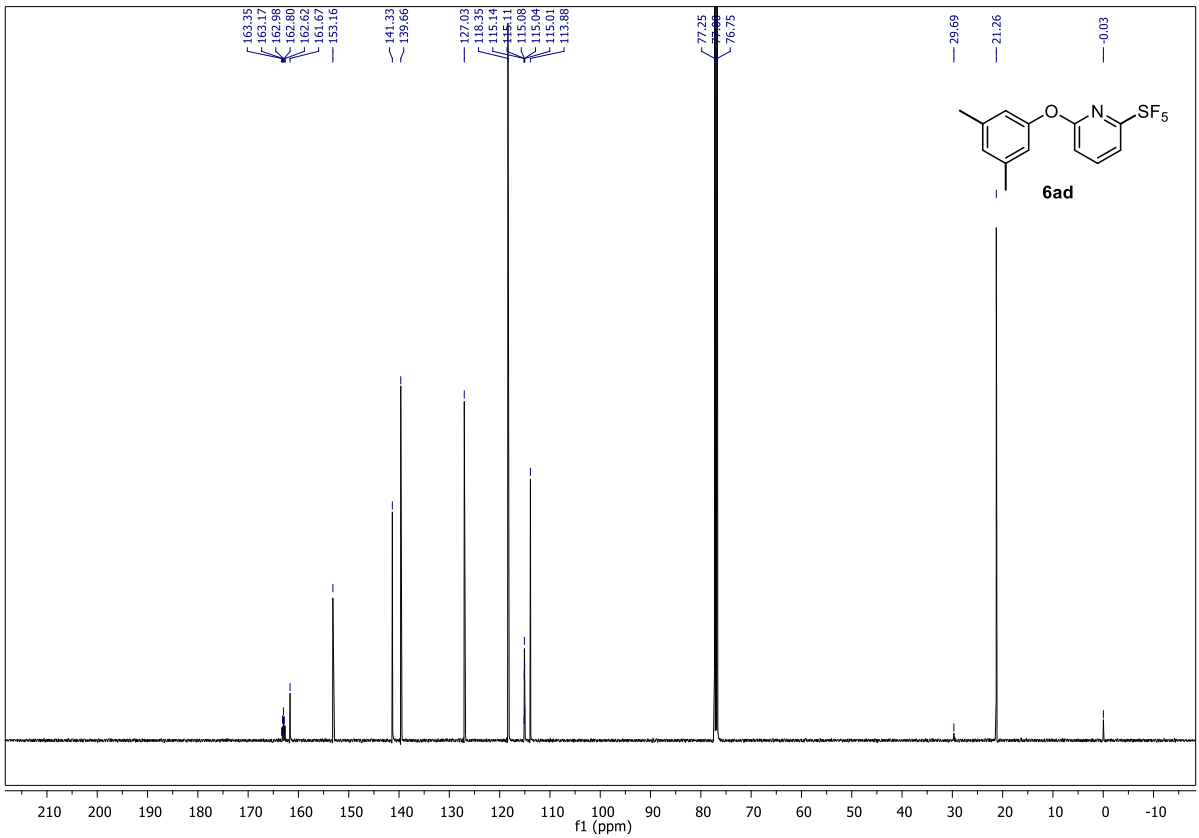
76.72
52.41
51.87
-162.20
O
N
SF5
6ad
1.00
4.21
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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163.17
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153.16
141.33
139.66
127.03
118.35
115.14
115.11
115.08
115.04
115.01
113.88
77.25
76.75
29.69
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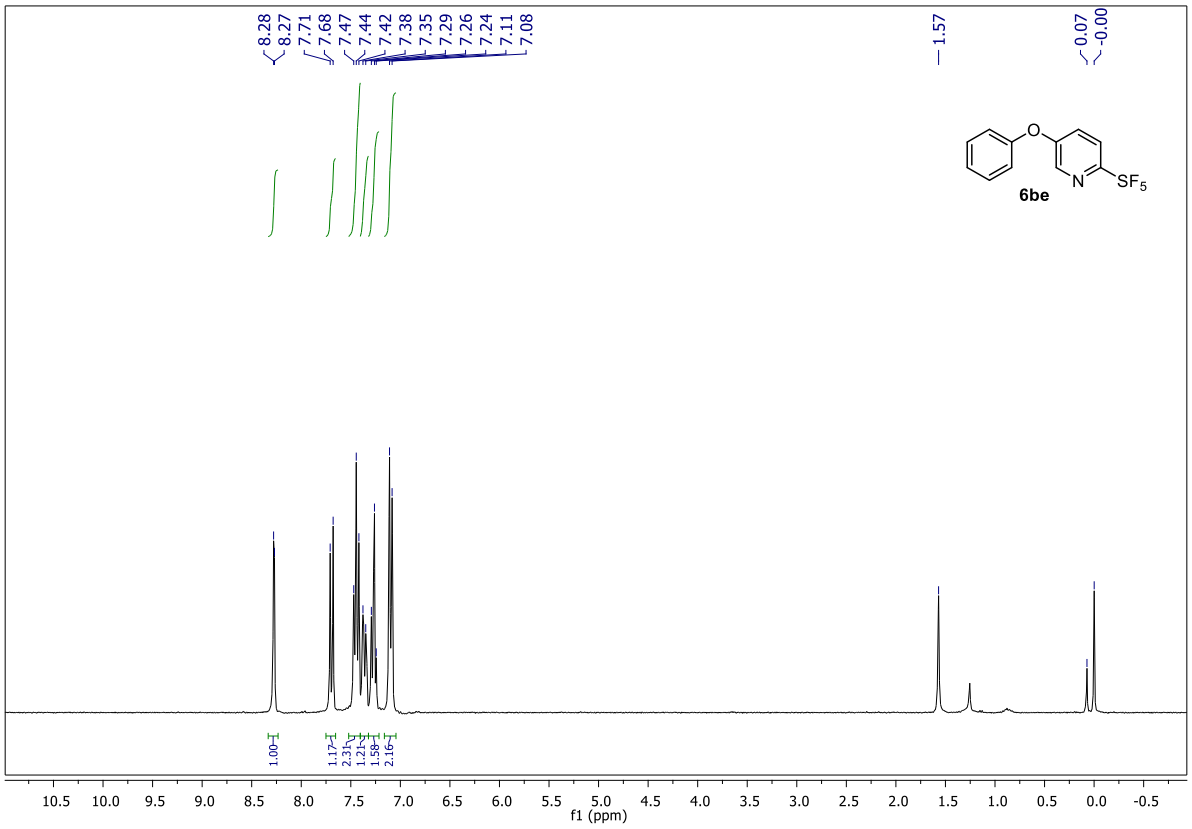
O
N
SF5
6ad
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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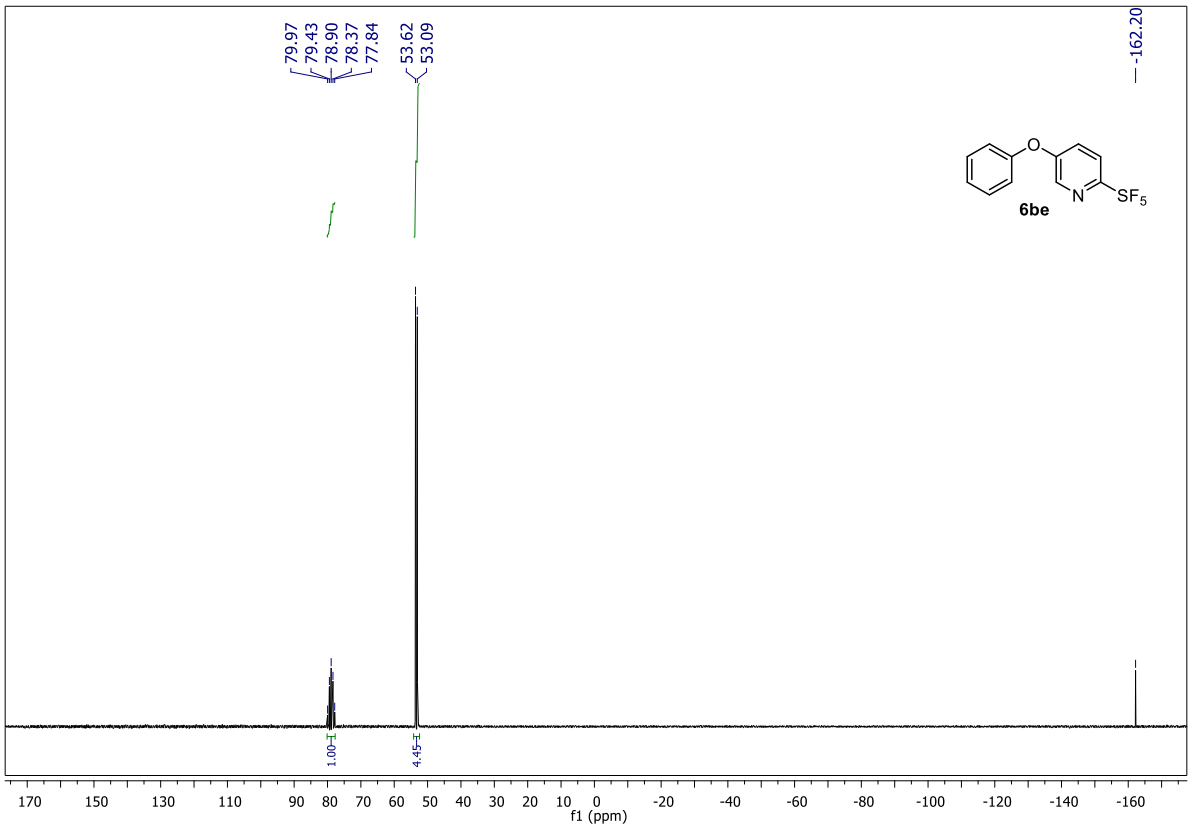
7.71
7.68
7.47
7.44
7.42
7.38
7.35
7.29
7.26
7.24
7.11
7.08
1.57
0.07
-0.00
O
N
SF5
6be
1.00
1.17
2.31
1.21
1.58
2.16
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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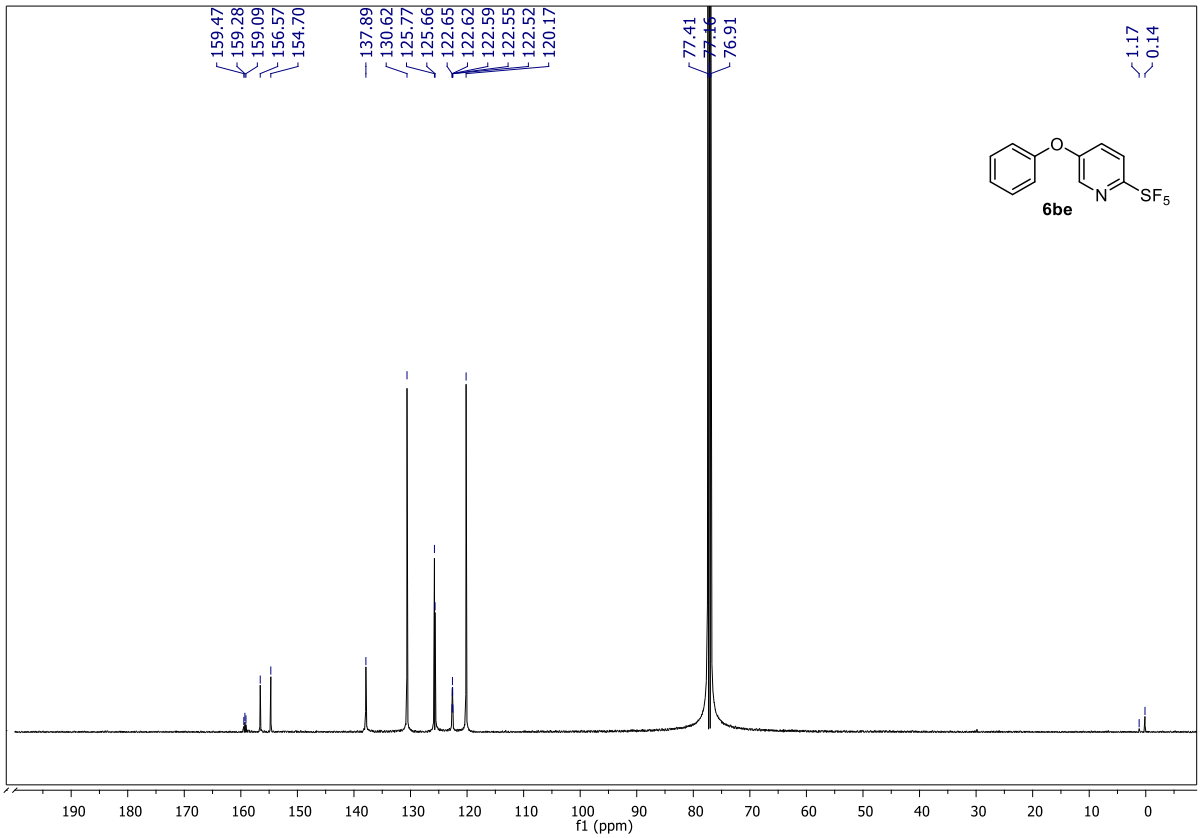
77.84
53.62
53.09
-162.20
O
N
SF5
6be
1.00
4.45
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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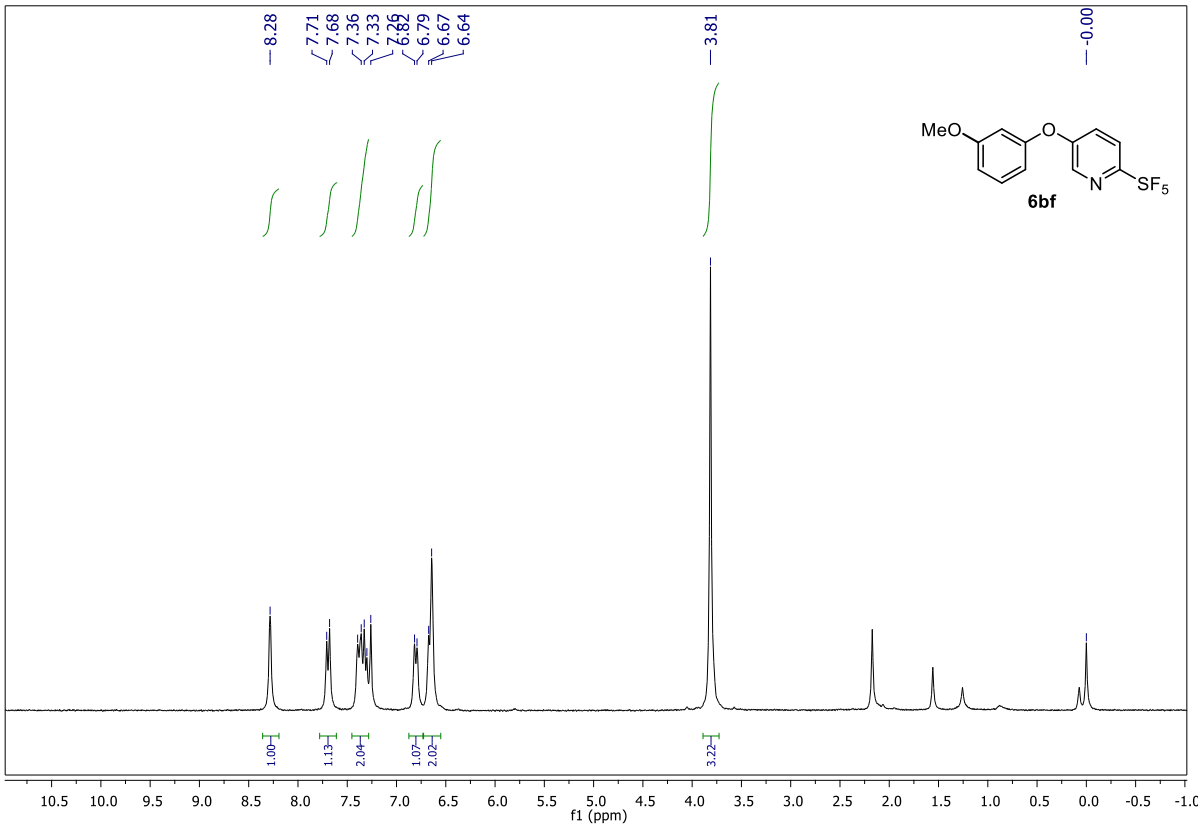
137.89
130.62
125.77
125.66
122.65
122.62
122.59
122.55
122.52
120.17
77.41
77.16
76.91
1.17
0.14
O
N
SF5
6be
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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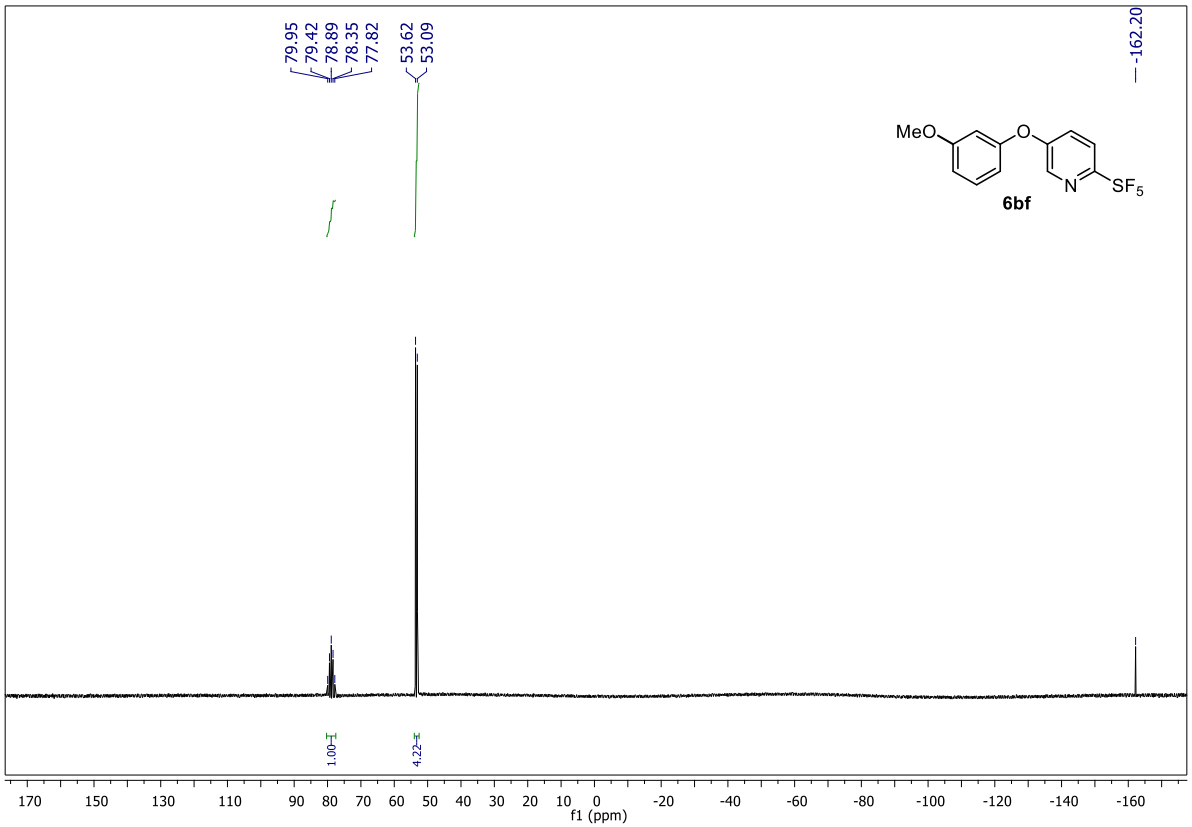
7.71
7.68
7.36
7.33
6.82
6.79
6.67
6.64
3.81
-0.00
MeO
O
N
SF5
6bf
1.00
1.13
2.04
1.07
2.02
3.22
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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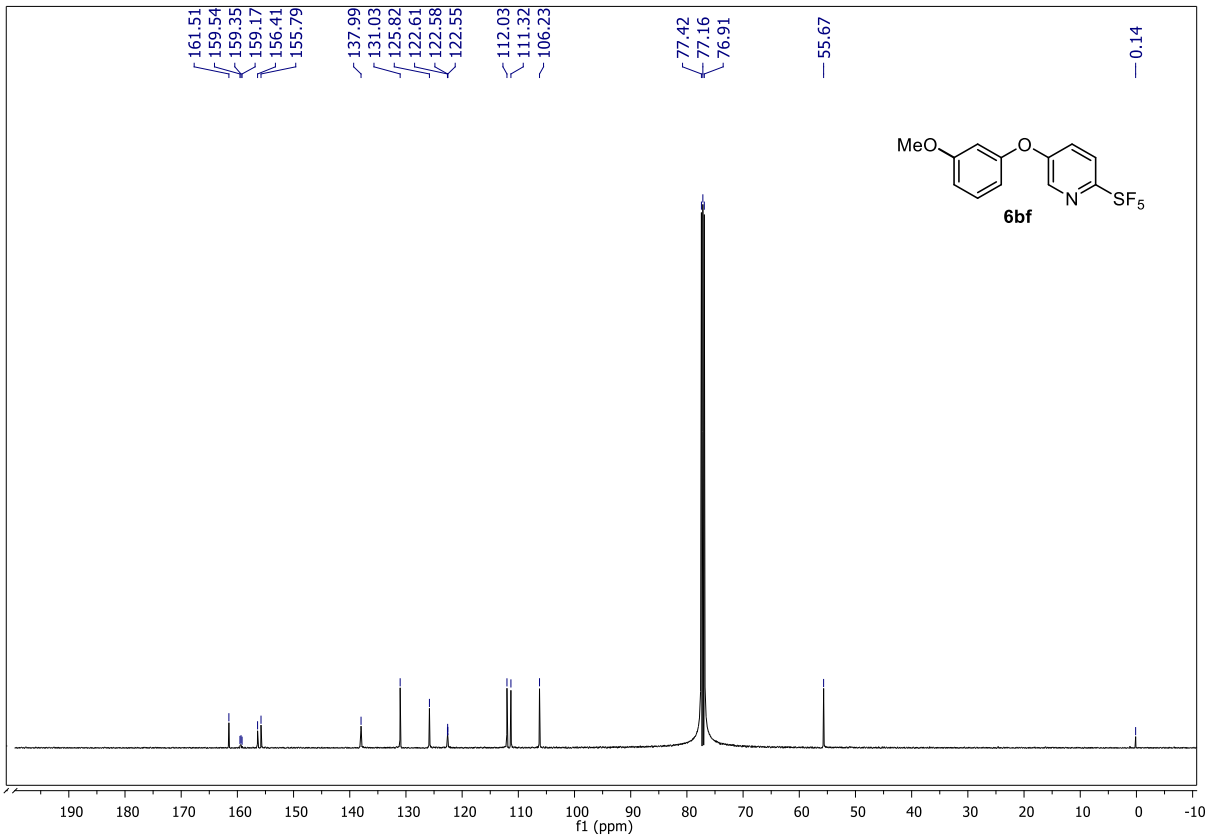
79.42
78.89
78.35
77.82
53.62
53.09
-162.20
MeO
O
N
SF5
6bf
1.00
4.22
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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159.54
159.35
159.17
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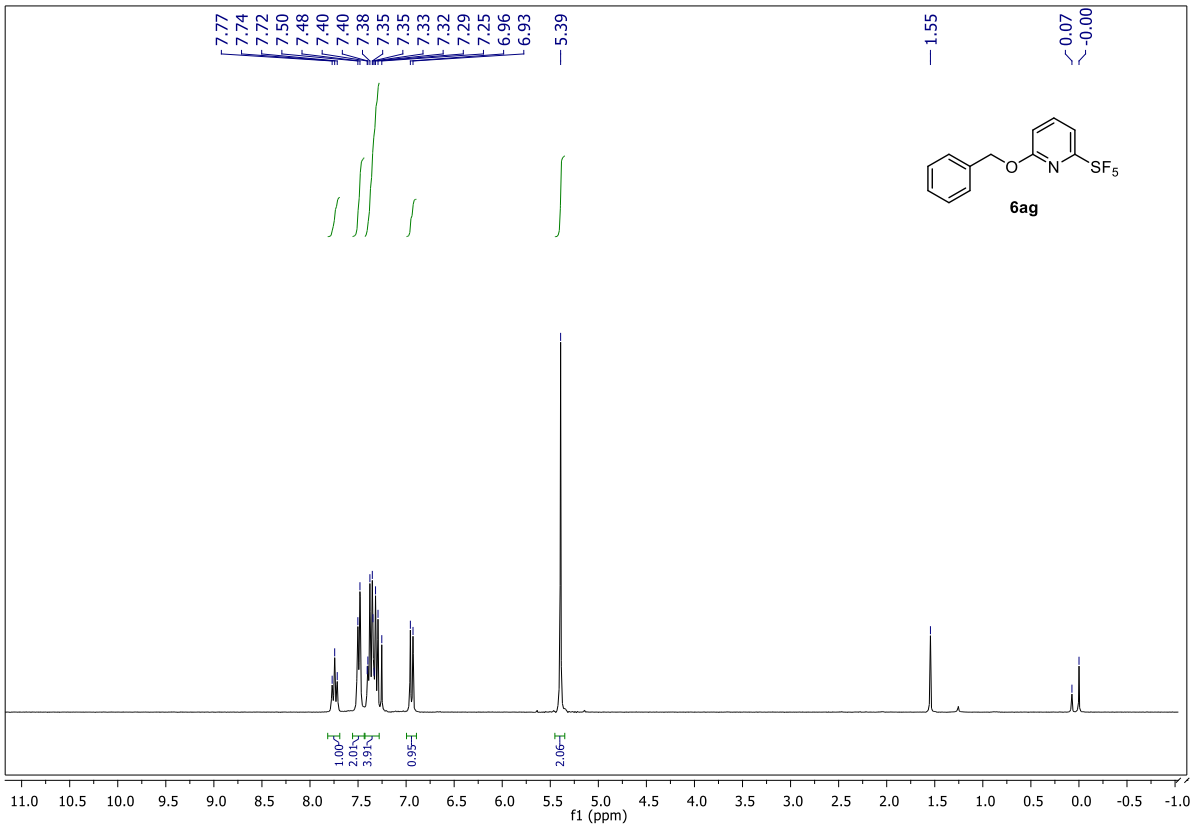
155.79
137.99
131.03
125.82
122.61
122.58
122.55
112.03
111.32
106.23
77.42
77.16
76.91
55.67
0.14
MeO
O
N
SF5
6bf
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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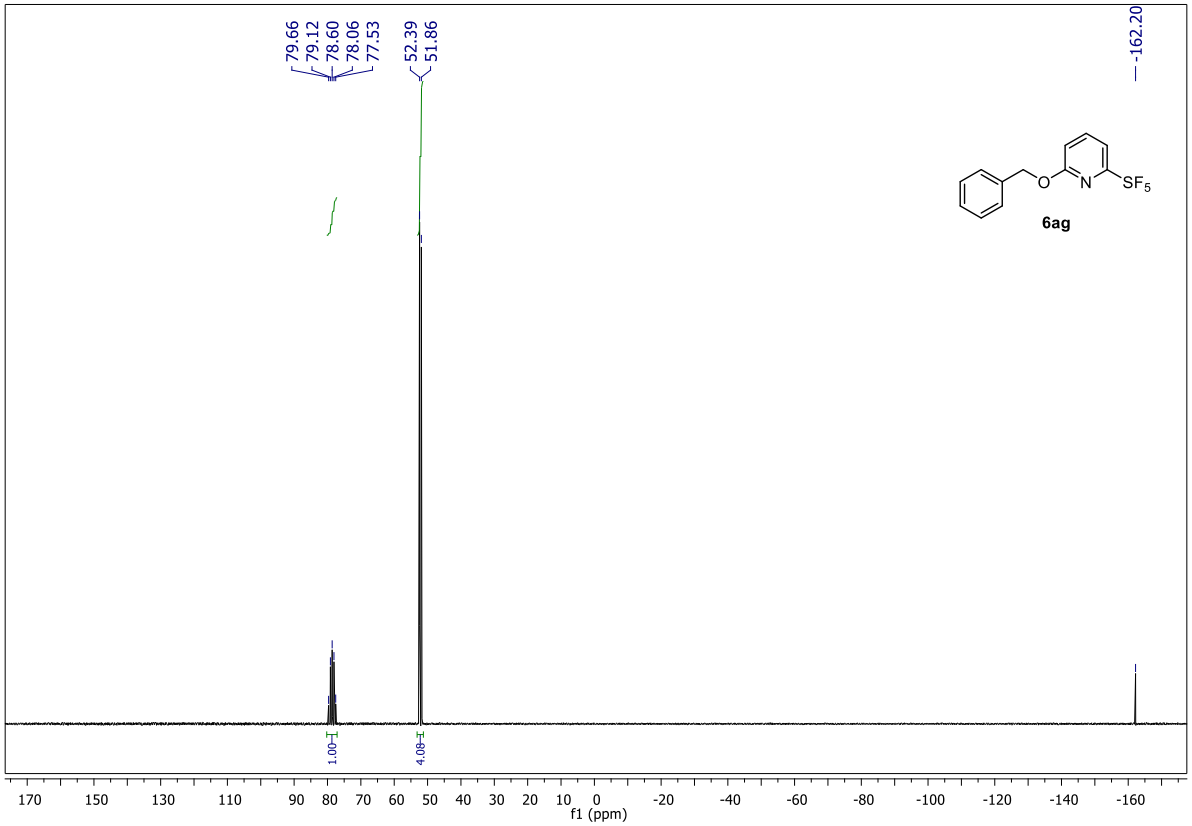
7.48
7.40
7.40
7.38
7.35
7.35
7.33
7.32
7.29
7.25
6.96
6.93
5.39
1.55
0.07
-0.00
O
N
SF5
6ag
1.00
2.01
3.91
0.95
2.06
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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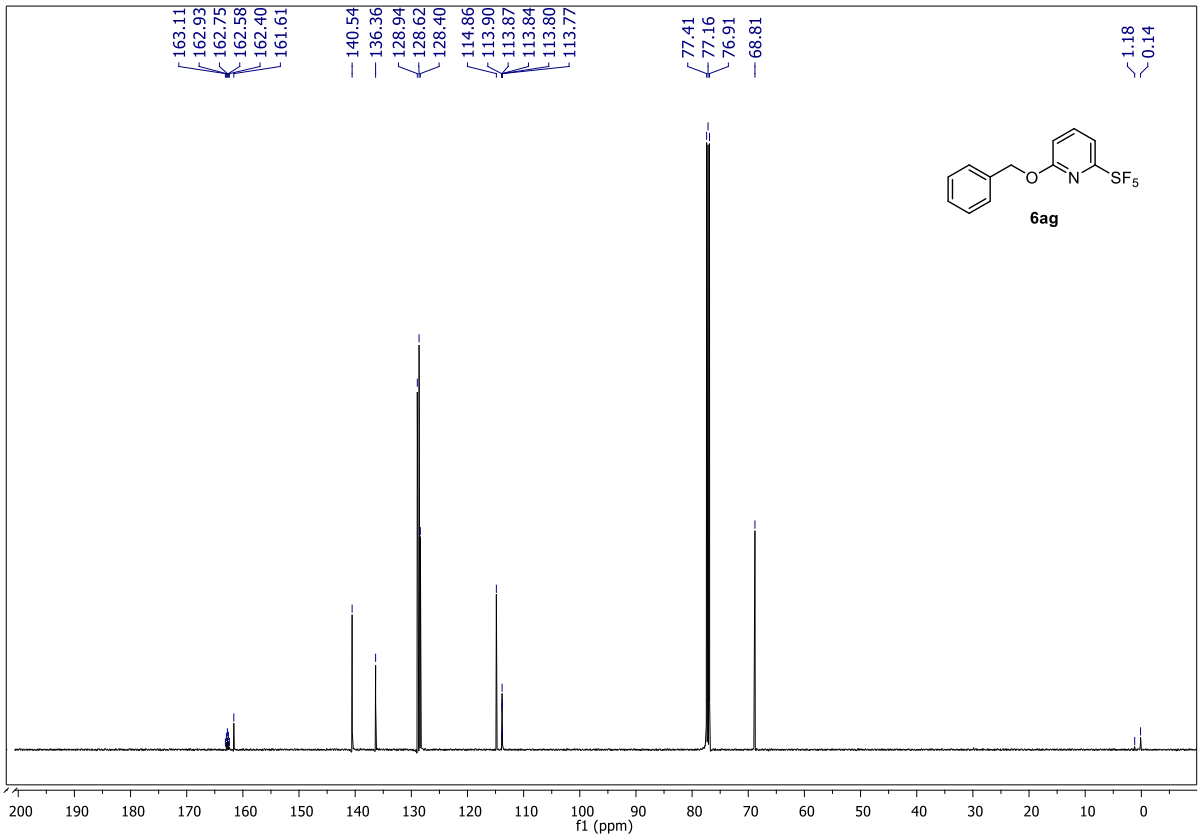
79.12
78.60
78.06
77.53
52.39
51.86
-162.20
O
N
SF5
6ag
1.00
4.08
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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162.75
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136.36
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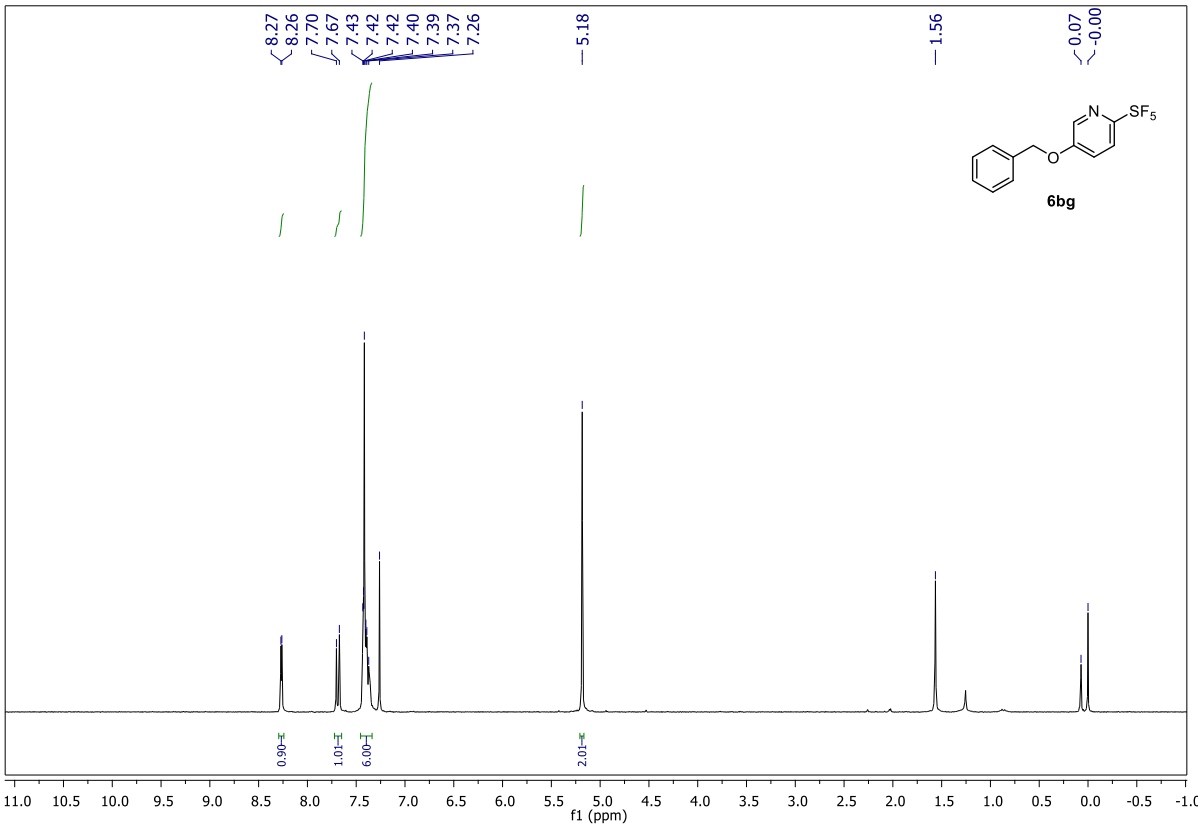
128.62
128.40
114.86
113.90
113.87
113.84
113.80
113.77
77.41
77.16
76.91
68.81
1.18
0.14
O
N
SF5
6ag
f1 (ppm)


8.27
8.26
7.70
7.67
7.43
7.42
7.42
7.40
7.39
7.37
7.26
5.18
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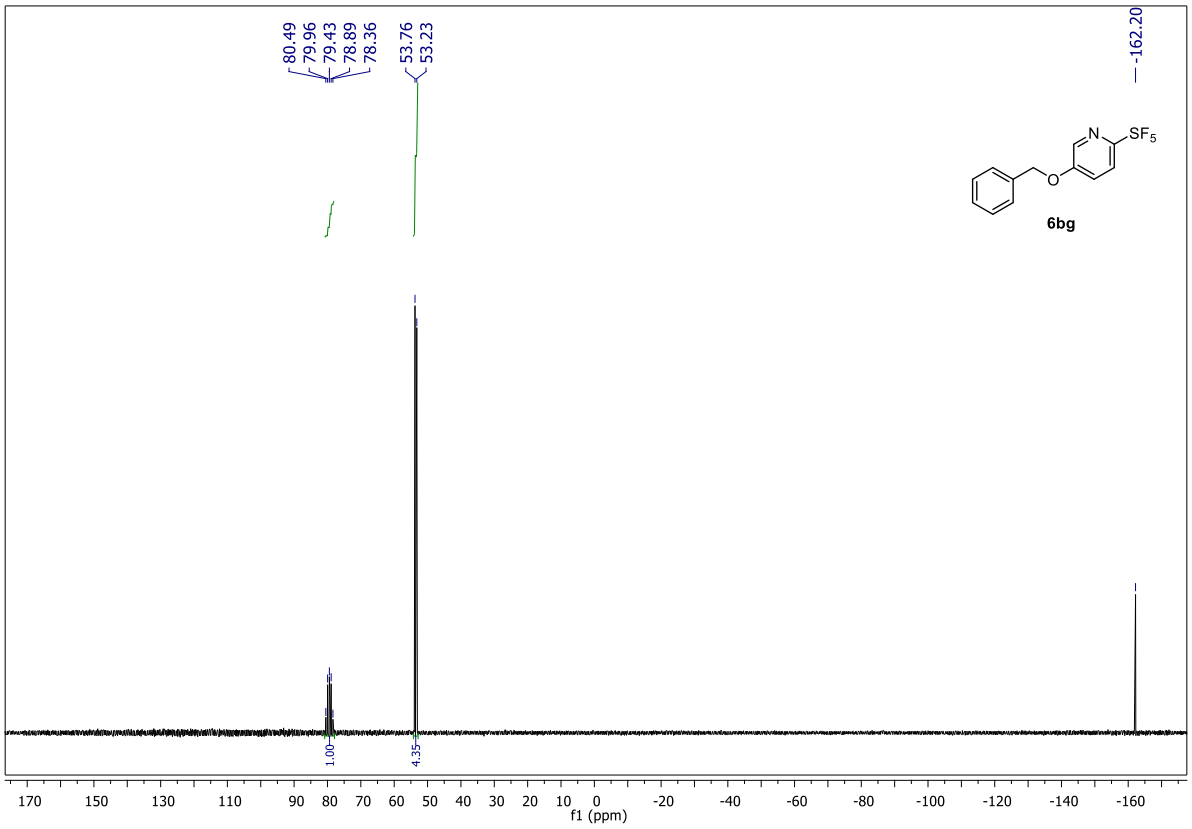
-0.00
N
SF5
O
6bg
0.90
1.01
6.00
2.01
f1 (ppm)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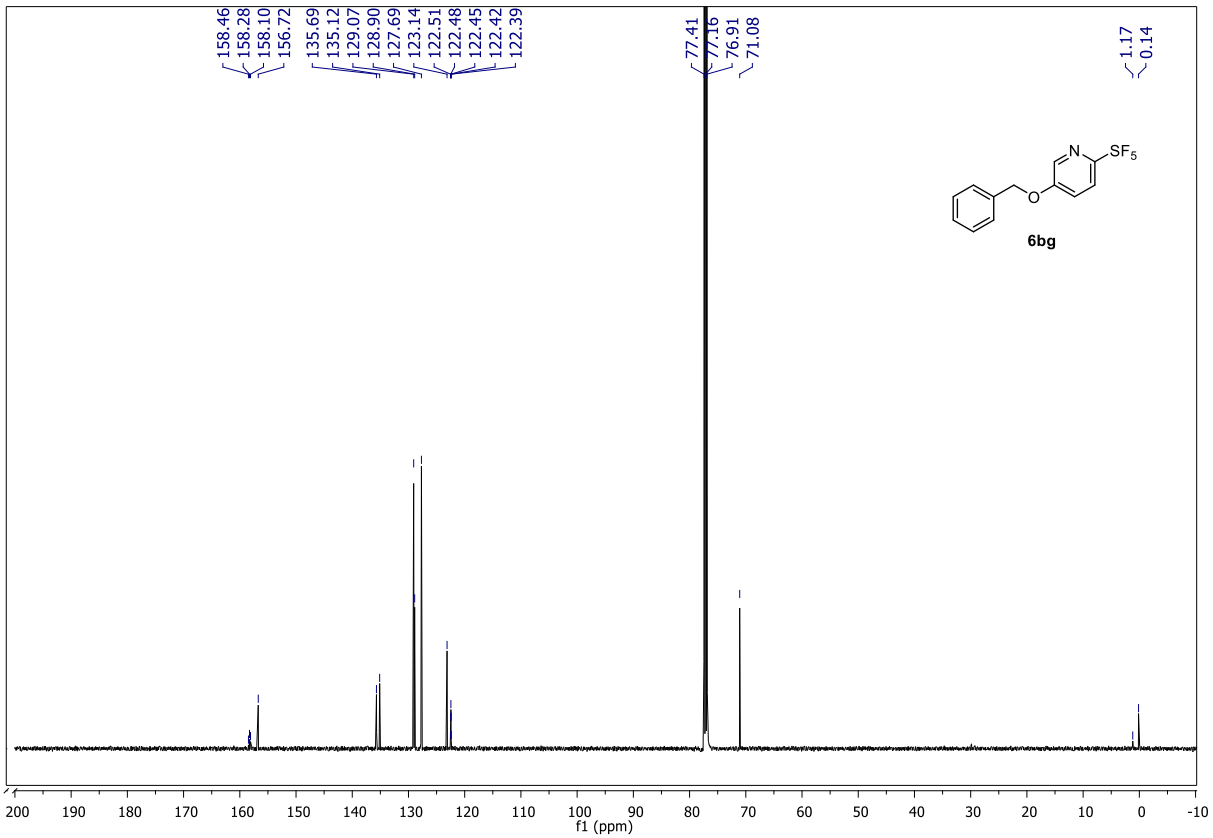
79.96
79.43
78.89
78.36
53.76
53.23
-162.20
N
SF5
O
6bg
1.00
4.35
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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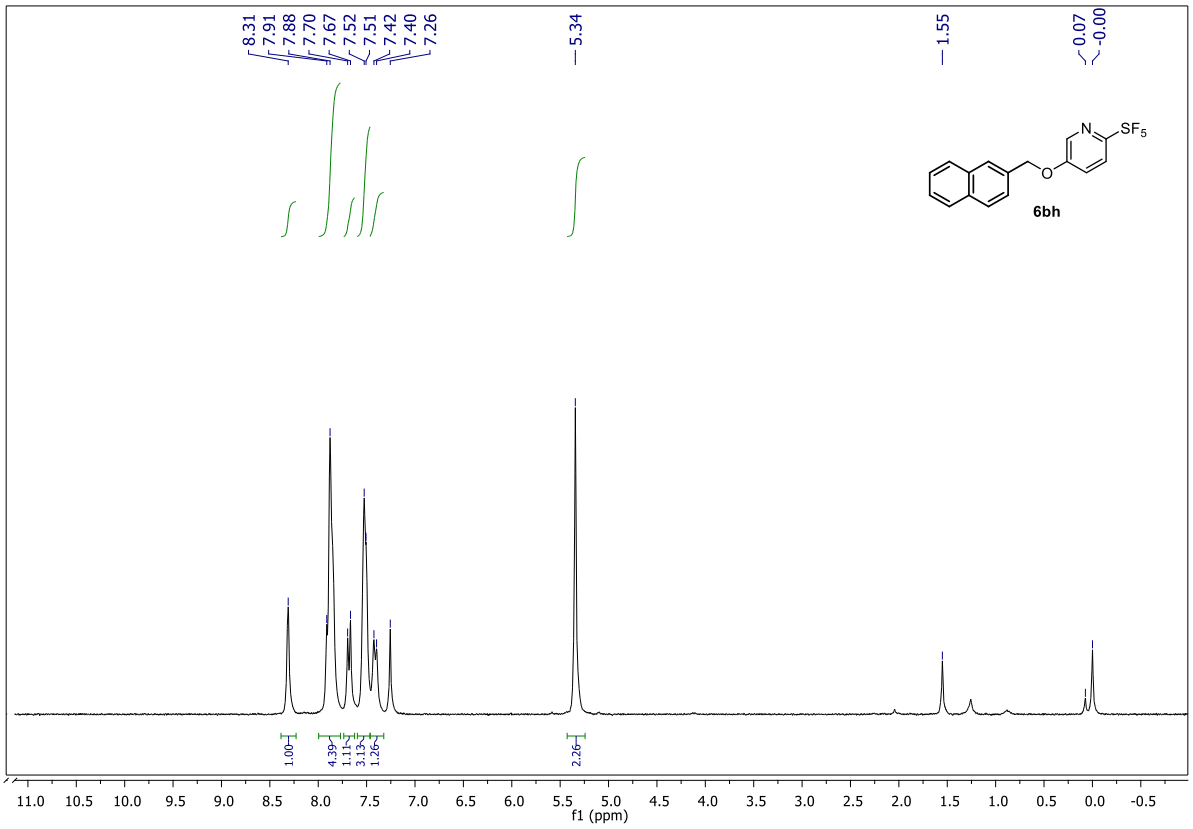
158.10
156.72
135.69
135.12
129.07
128.90
127.69
123.14
122.51
122.48
122.45
122.42
122.39
77.41
77.16
76.91
71.08
1.17
0.14
N
SF5
O
6bg
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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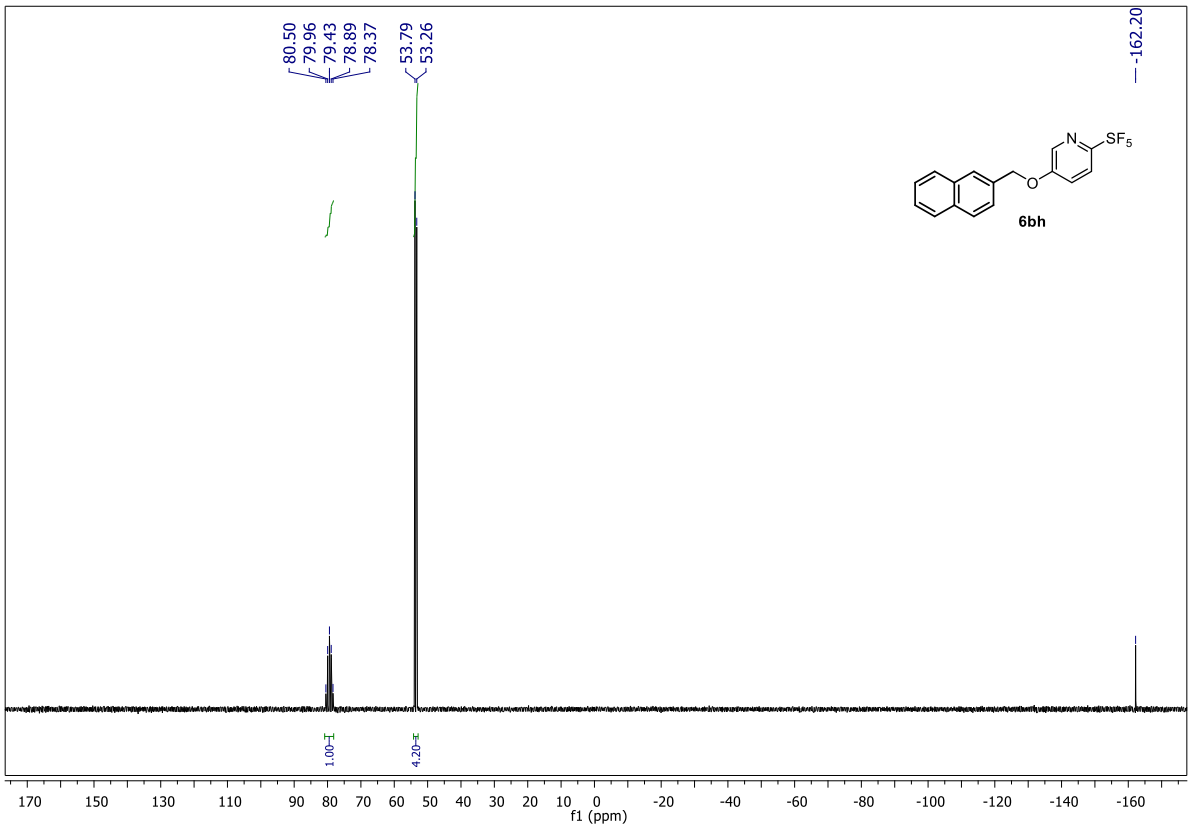
7.88
7.70
7.67
7.52
7.51
7.42
7.40
7.26
5.34
1.55
0.07
-0.00
N
SF5
O
6bh
1.00
4.39
1.11
3.13
1.26
2.26
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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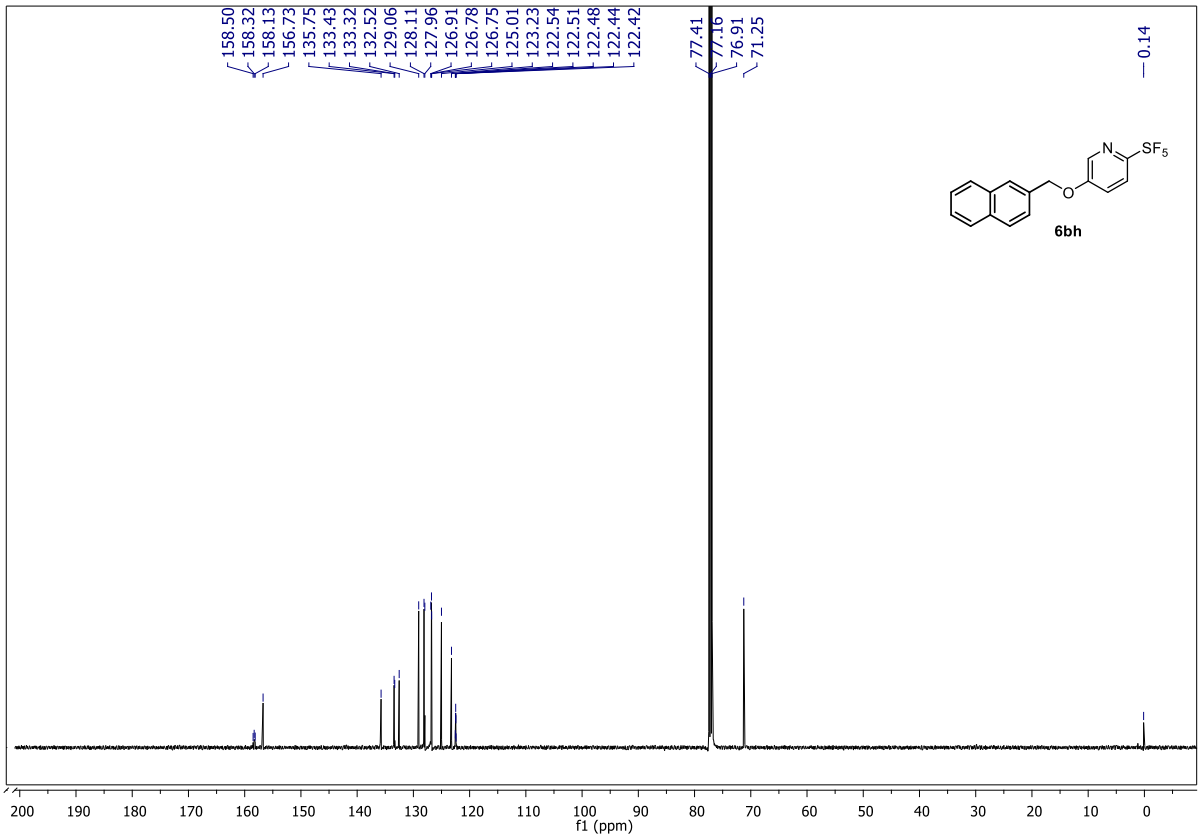
79.96
79.43
78.89
78.37
53.79
53.26
-162.20
N
SF5
O
6bh
1.00
4.20
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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129.06
128.11
127.96
126.91
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126.75
125.01
123.23
122.54
122.51
122.48
122.44
122.42
77.41
77.16
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N
SF5
O
6bh
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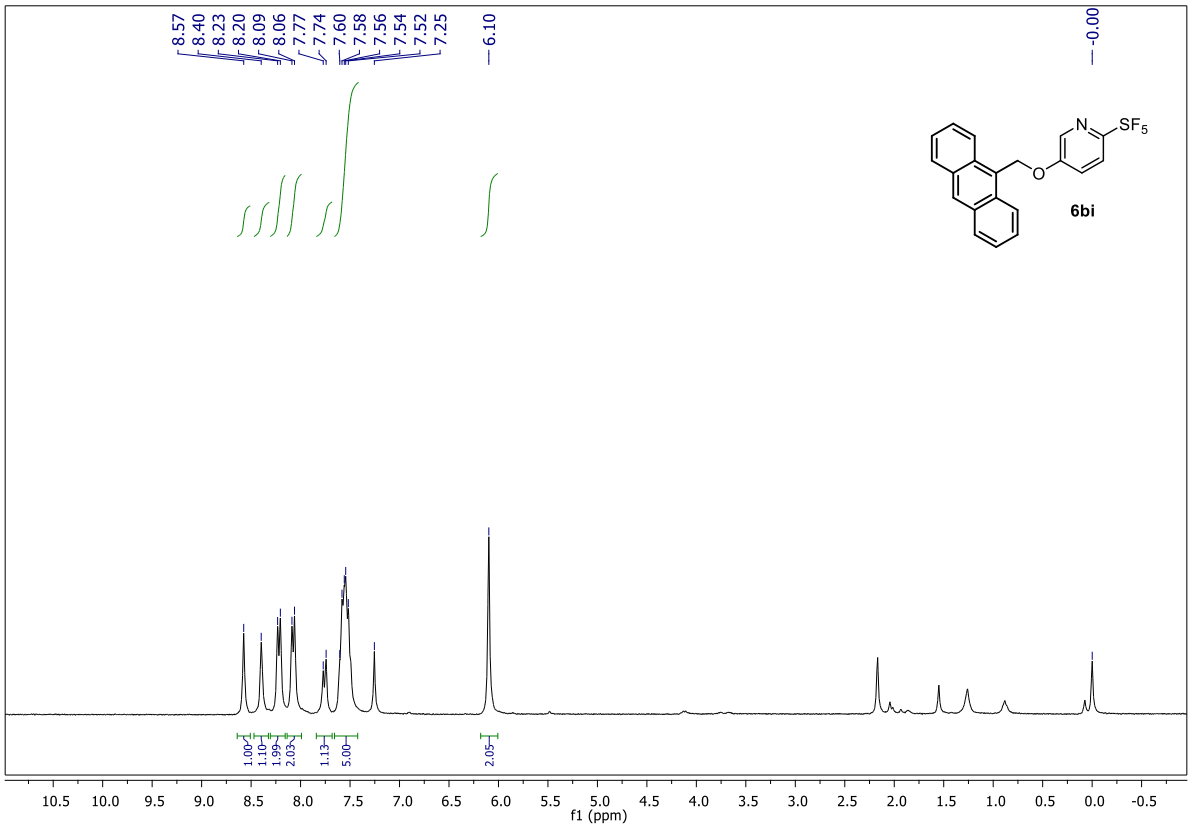
f1 (ppm)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8.06
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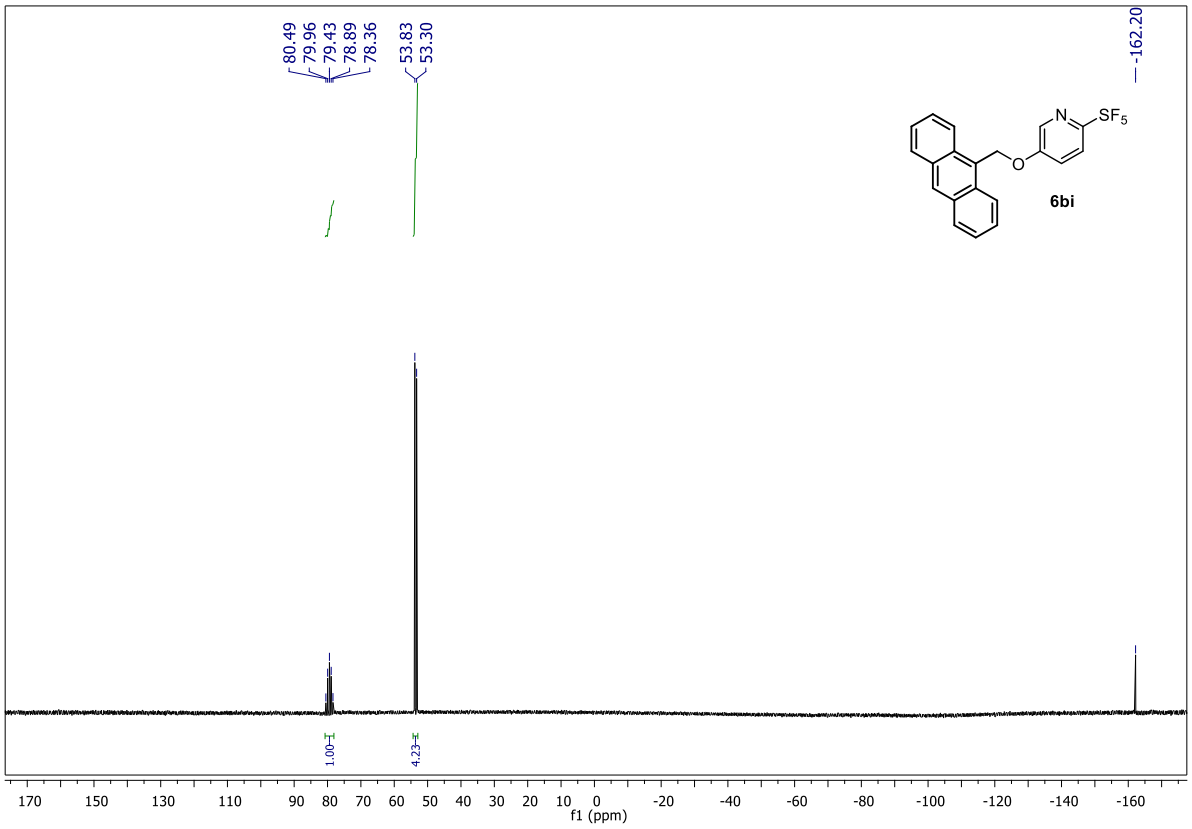
7.74
7.60
7.58
7.56
7.54
7.52
7.25
6.10
0.00
N
SF5
O
6bi
1.00
1.10
1.99
2.03
1.13
5.00
2.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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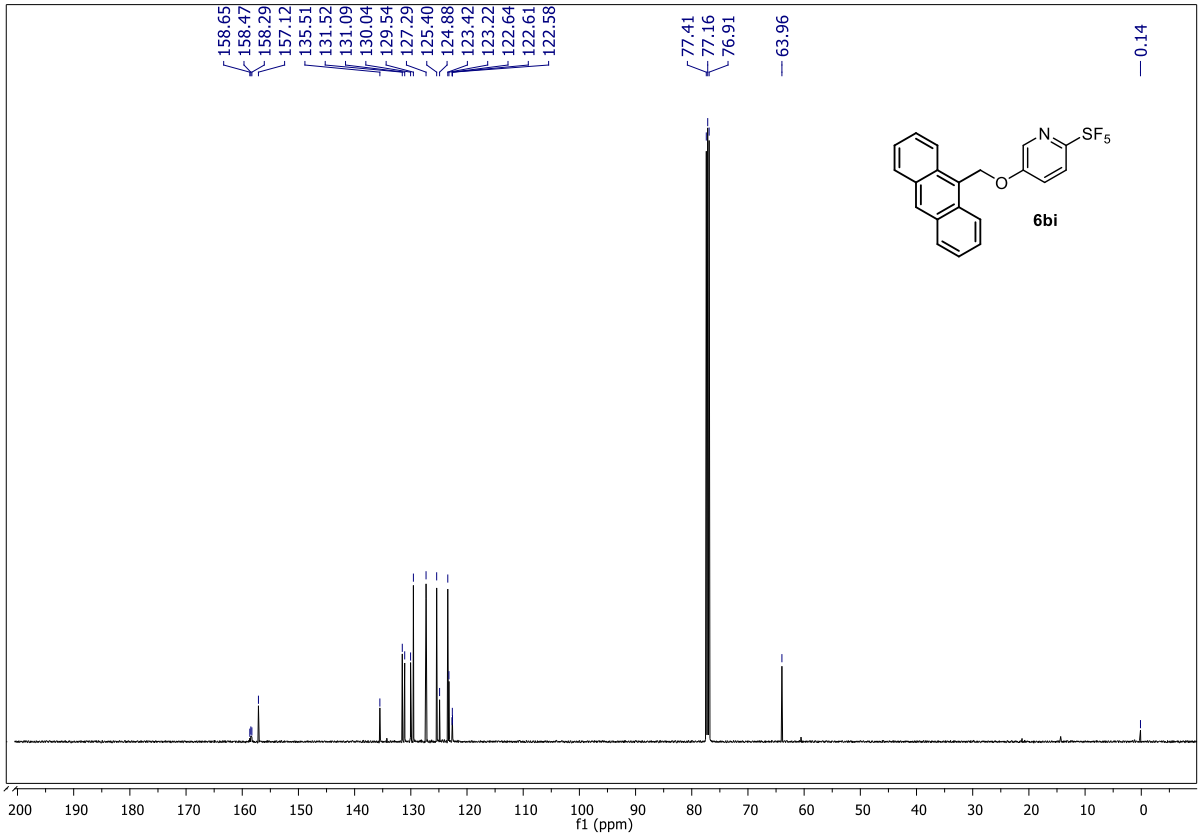
79.43
78.89
78.36
53.83
53.30
-162.20
N
SF5
O
6bi
1.00
4.23
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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127.29
125.40
124.88
123.42
123.22
122.64
122.61
122.58
77.41
77.16
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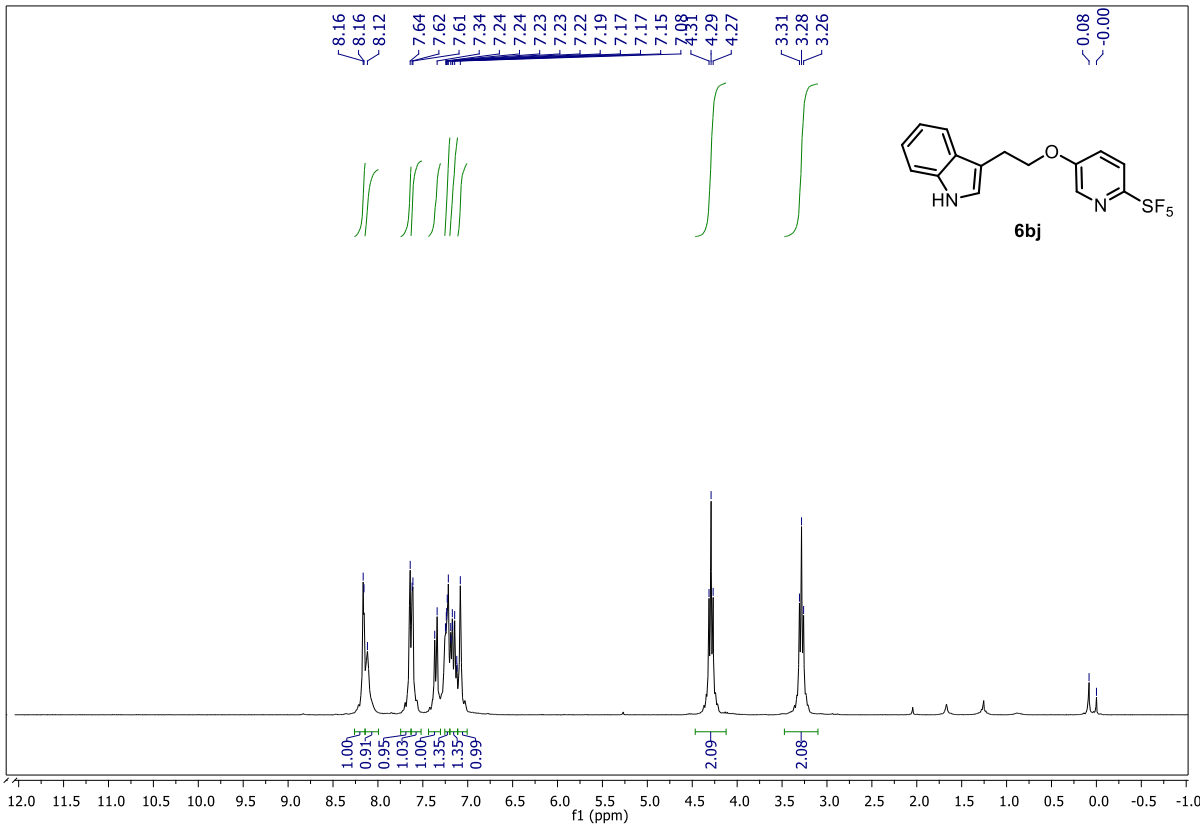
0.14
N
SF5
O
6bi
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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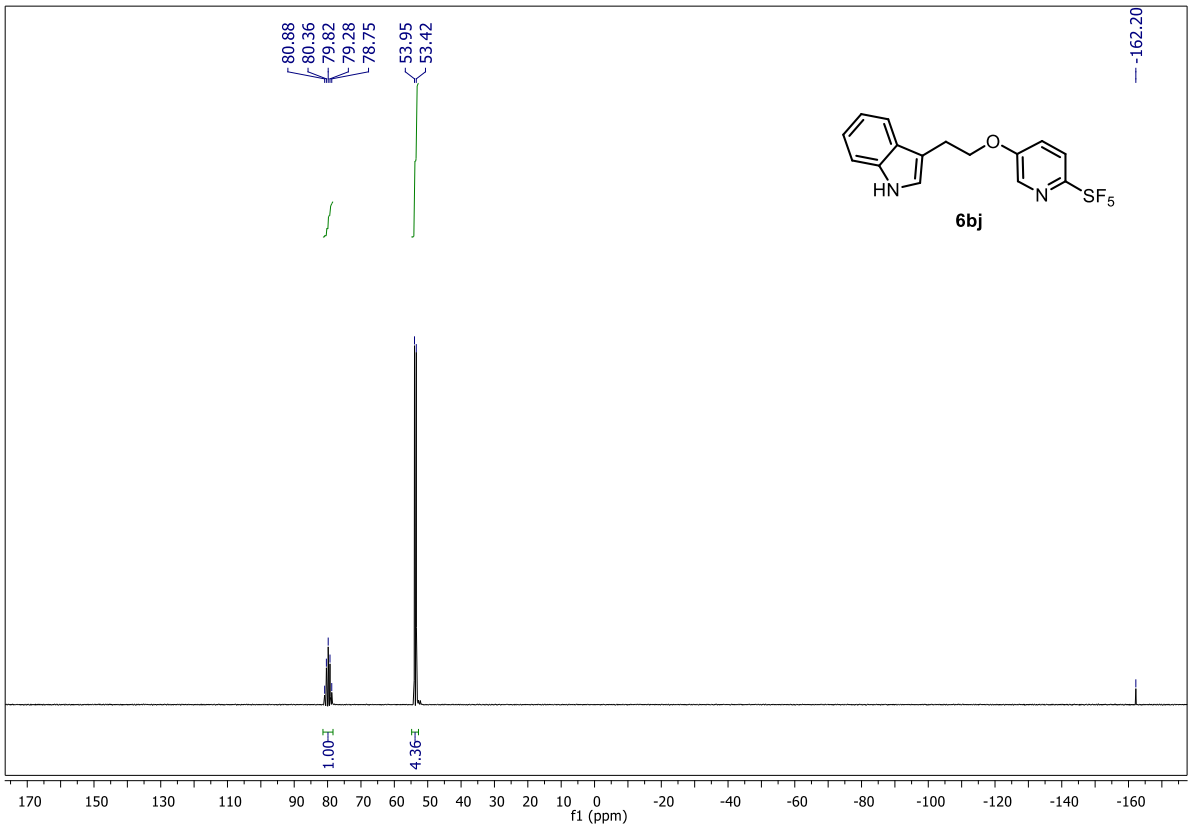
7.61
7.34
7.24
7.24
7.23
7.23
7.22
7.19
7.17
7.17
7.15
7.08
4.31
4.29
4.27
3.31
3.28
3.26
0.08
-0.00
HN
O
N
SF5
6bj
1.00
0.91
0.95
1.03
1.00
1.35
1.35
0.99
2.09
2.08
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


80.88
80.36
79.82
79.28
78.75
53.95
53.42
-162.20
HN
O
N
SF5
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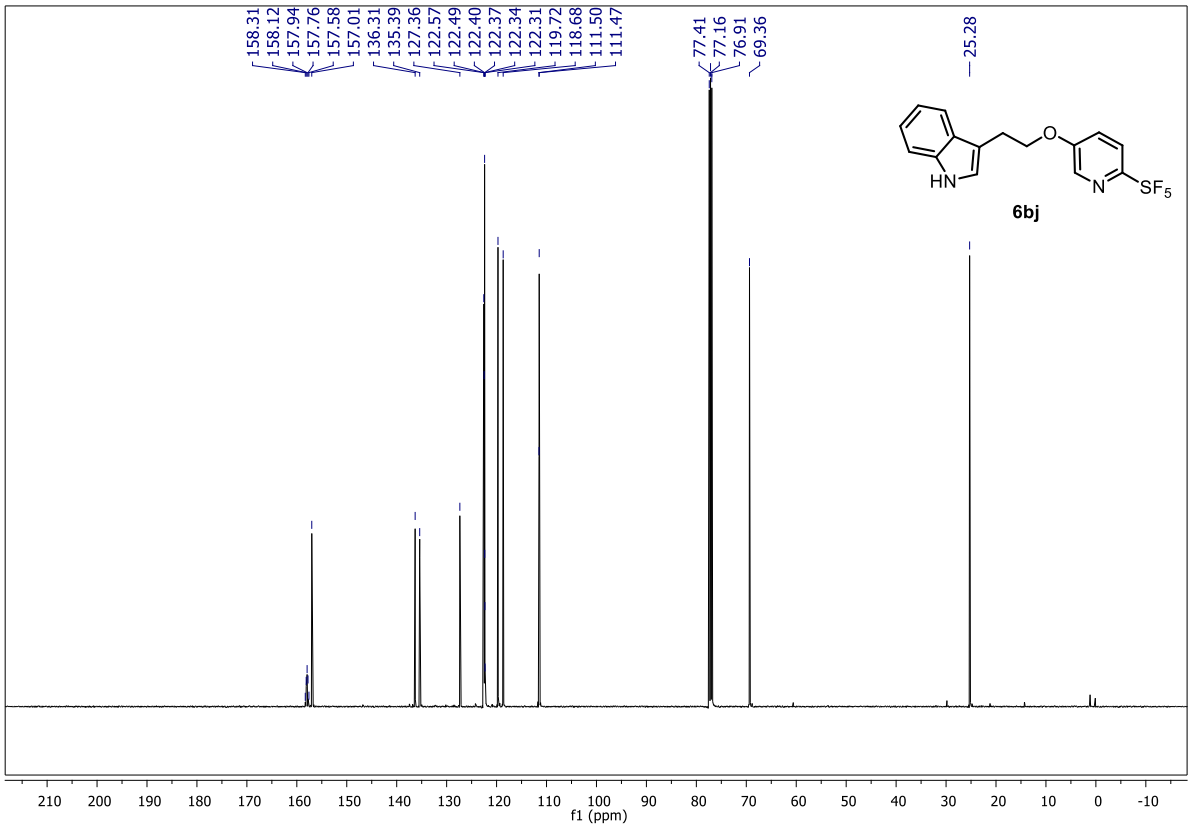
1.00
4.36
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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122.57
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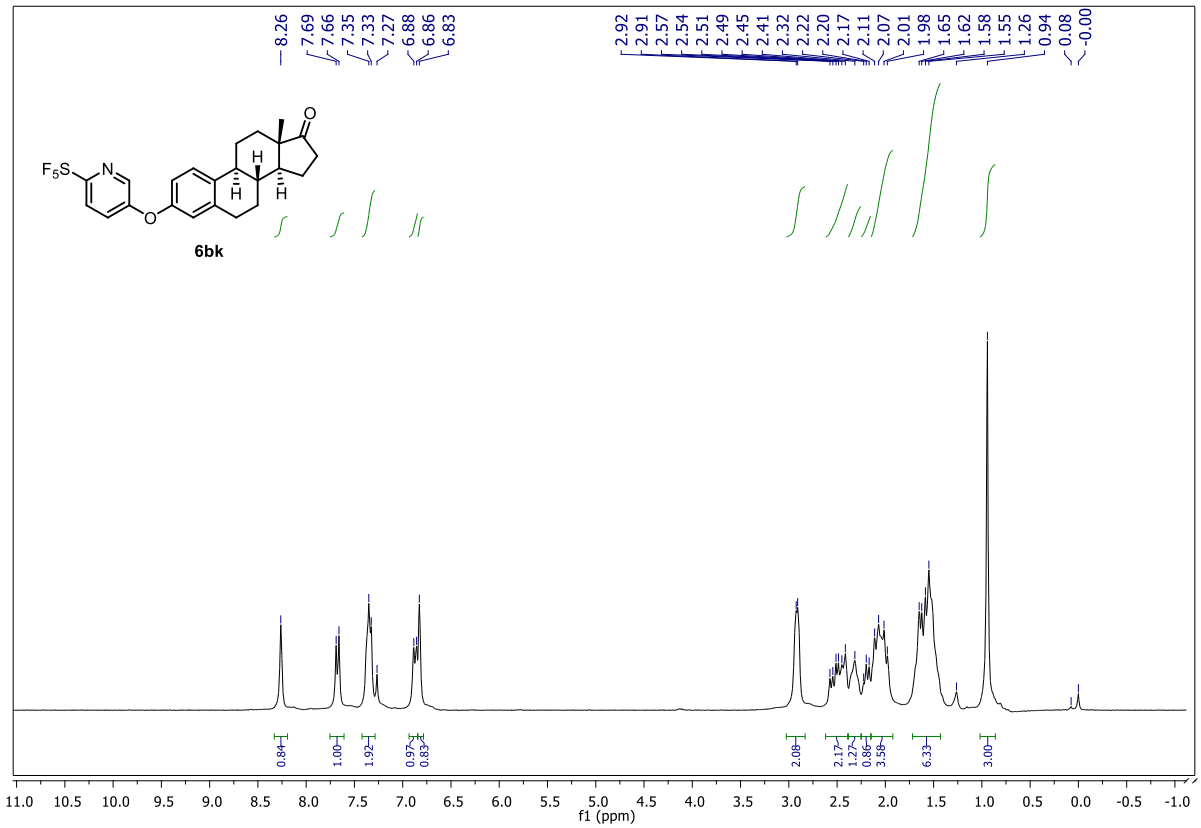
HN
O
N
SF5
6bj
f1 (ppm)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7.27
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6.86
6.83
2.92
2.91
2.57
2.54
2.51
2.49
2.45
2.41
2.32
2.22
2.20
2.17
2.11
2.07
2.01
1.98
1.65
1.62
1.58
1.55
1.26
0.94
0.08
-0.00
F5S
N
O
H
H
H
O
6bk
0.84
1.00
1.92
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0.83
2.08
2.17
1.27
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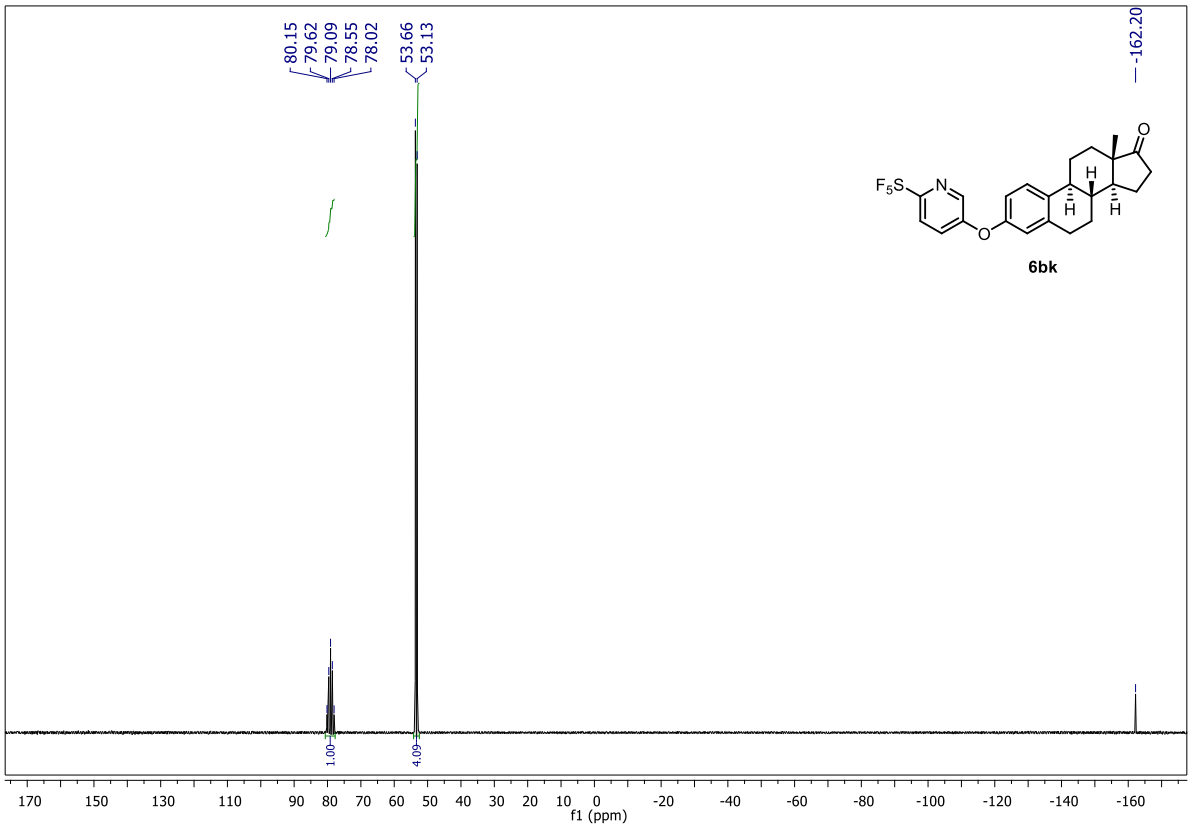
3.59
6.33
3.00
f1 (ppm)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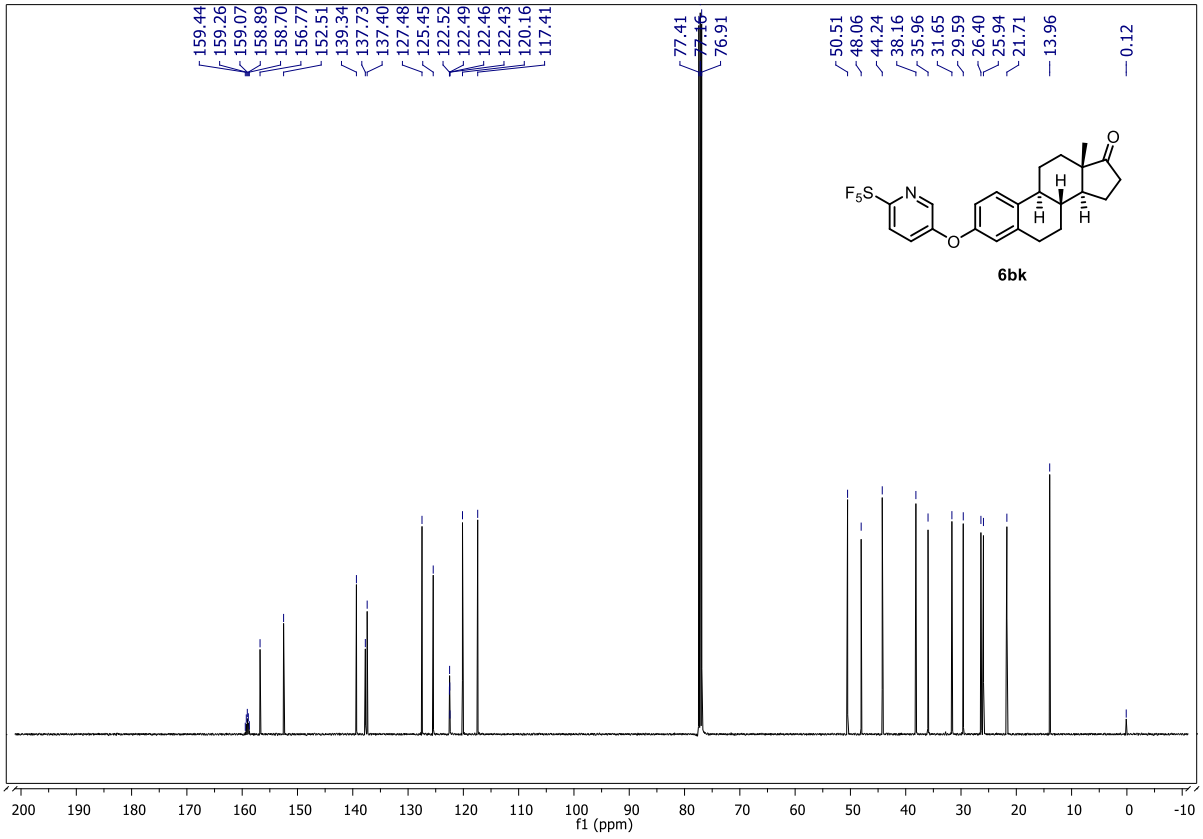
79.62
79.09
78.55
78.02
53.66
53.13
-162.20
F5S
N
O
H
H
H
O
6bk
1.00
4.09
170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)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127.48
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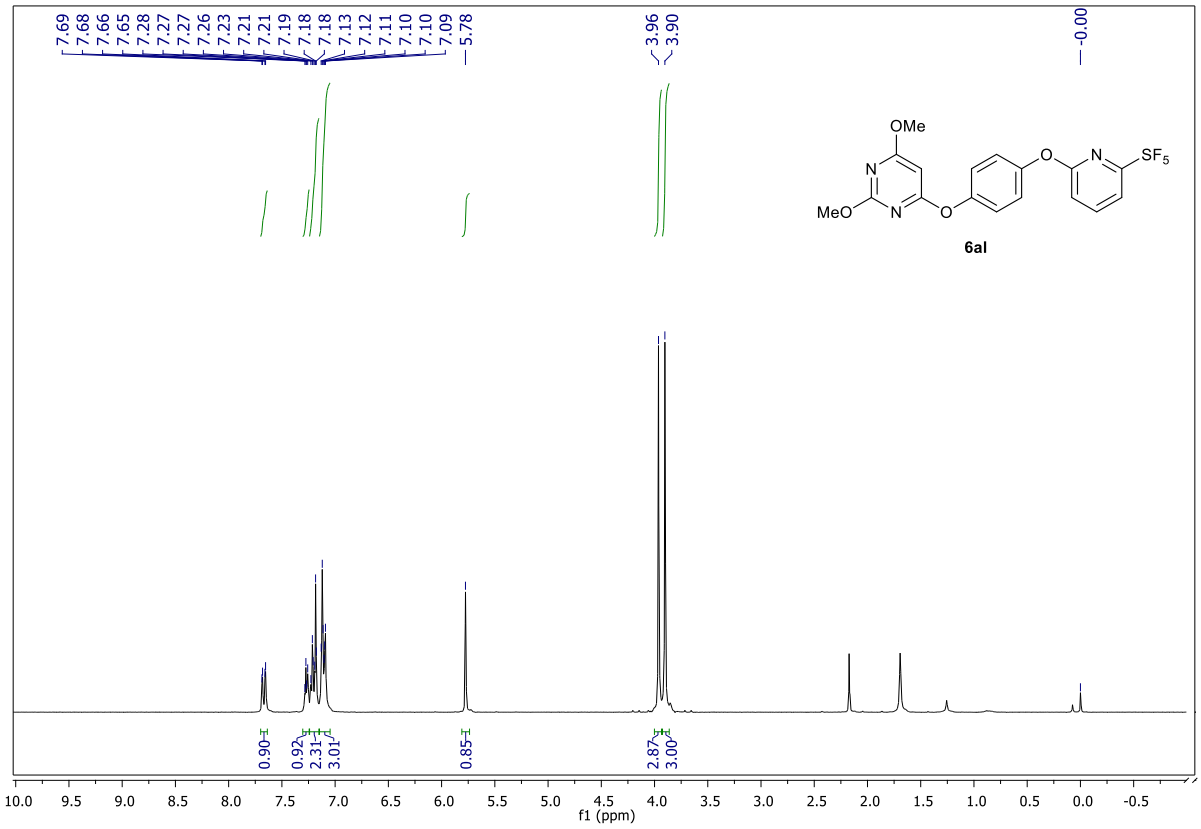
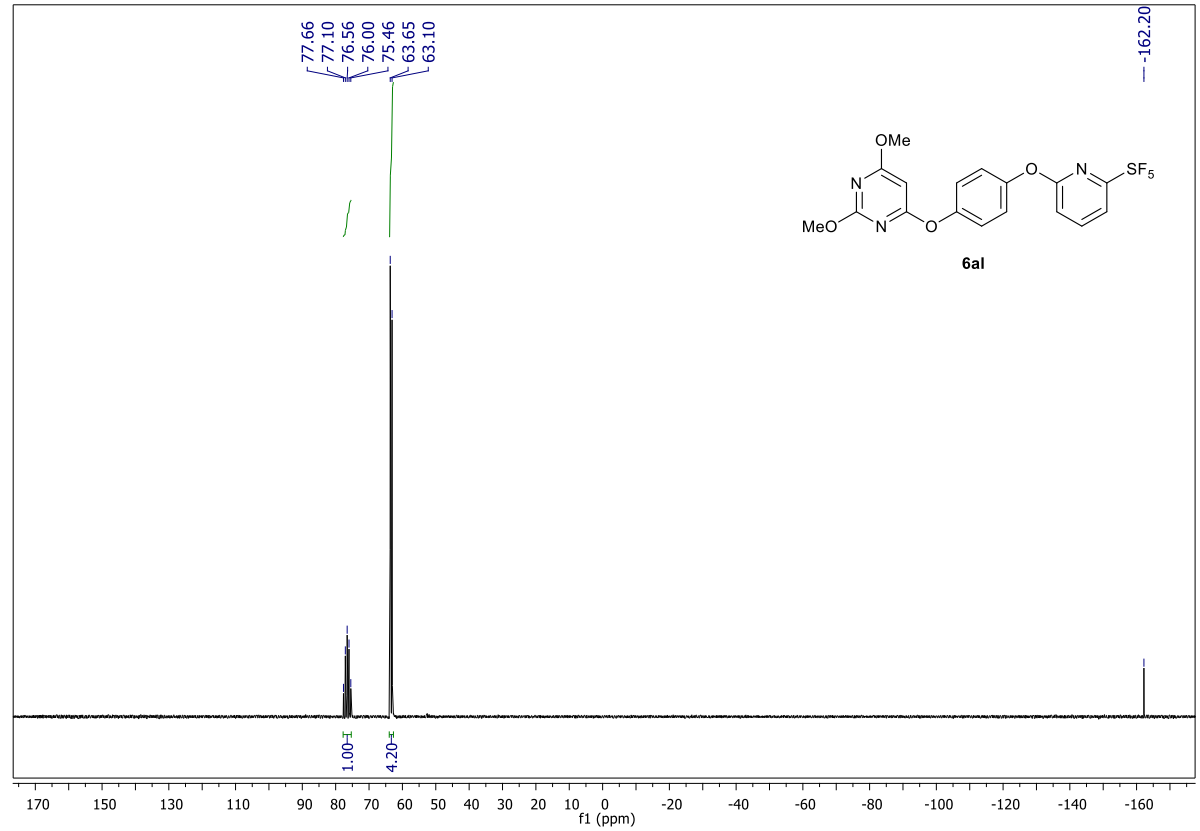
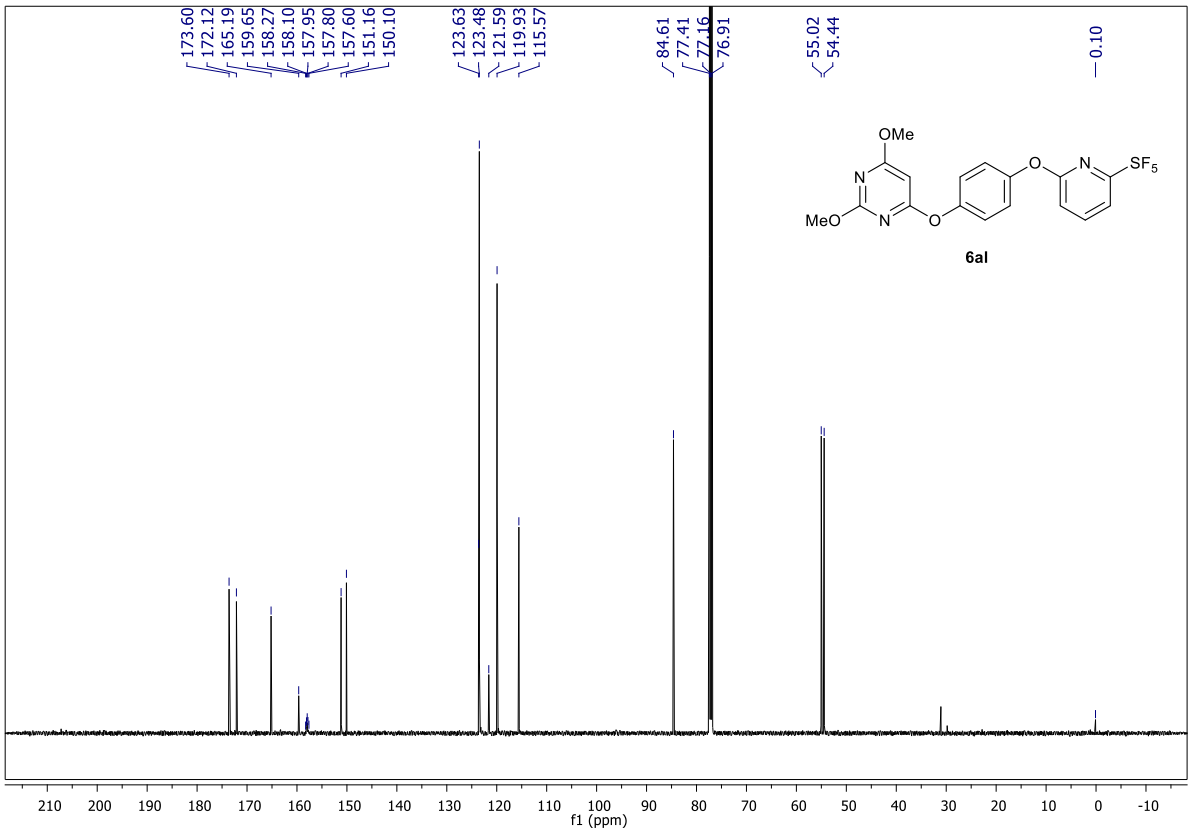
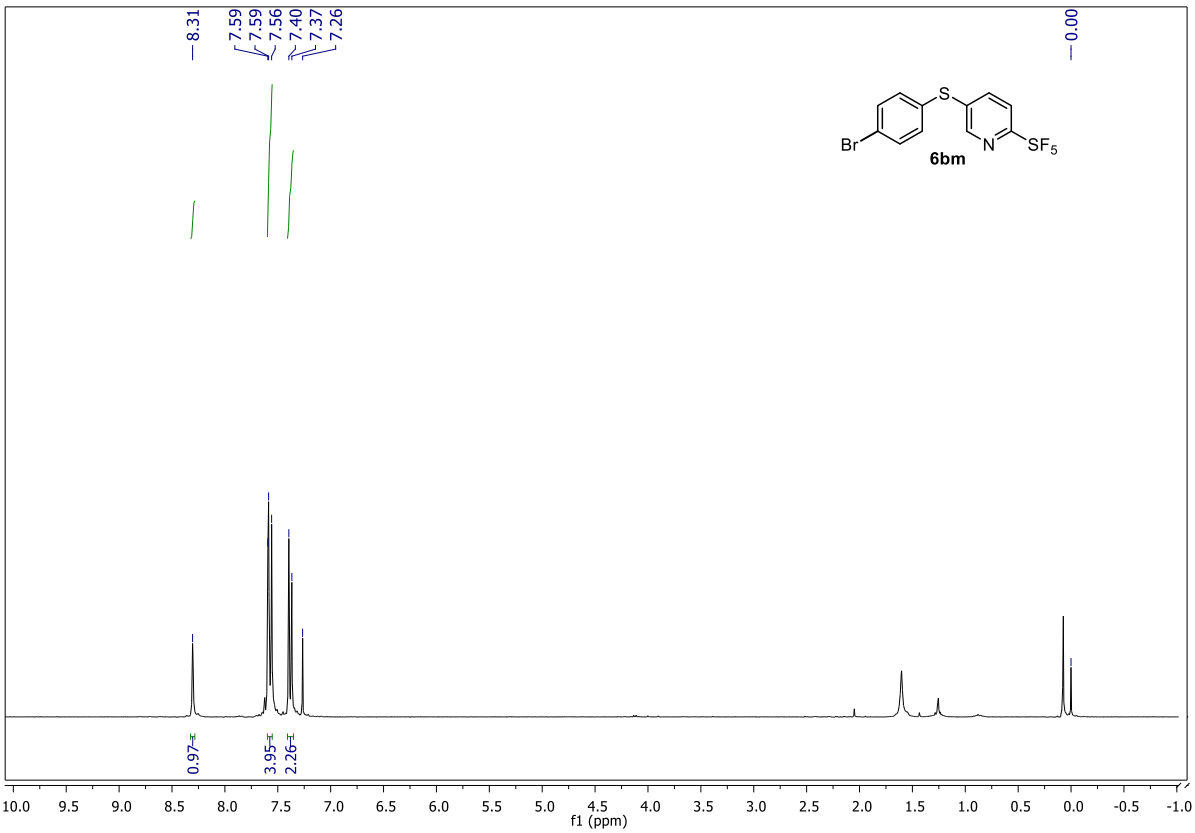
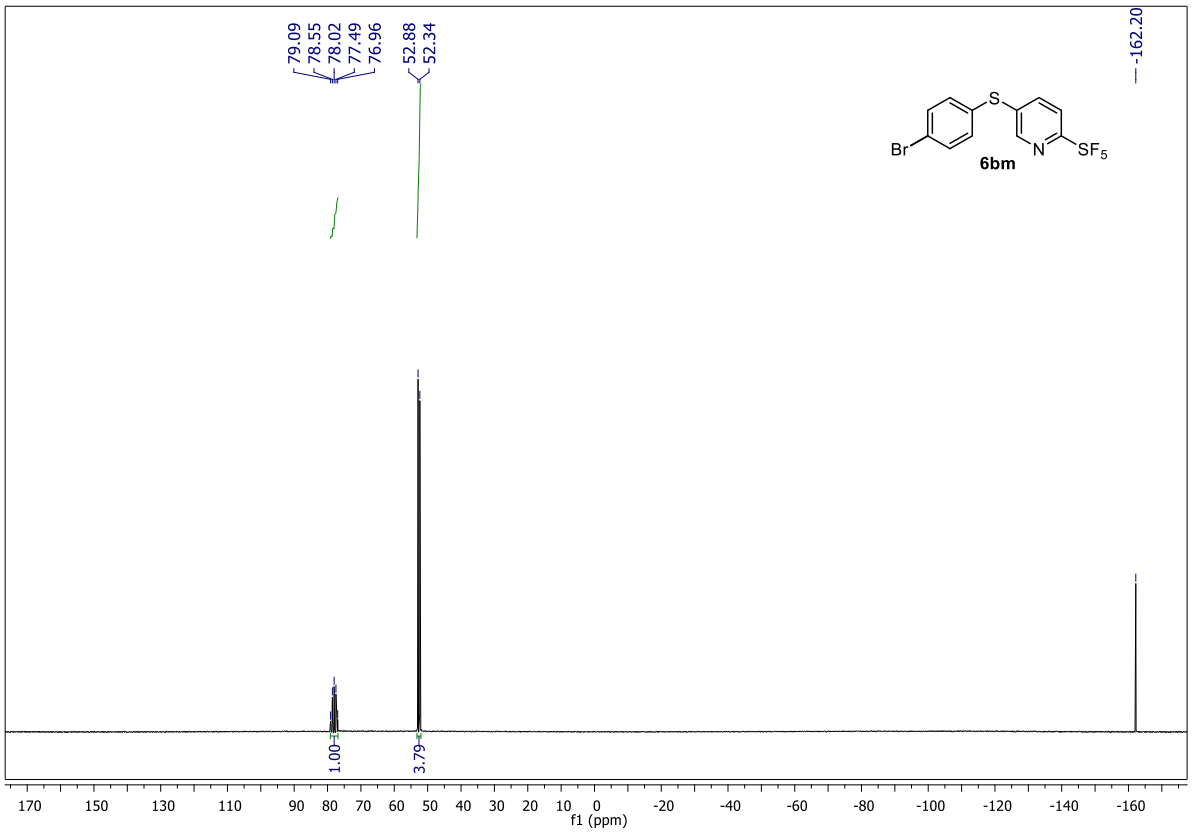
122.52
122.49
122.46
122.43
120.16
117.41
77.41
77.16
76.91
50.51
48.06
44.24
38.16
35.96
31.65
29.59
26.40
25.94
21.71
13.96
0.12
F5S
N
O
H
H
H
O
6bk
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

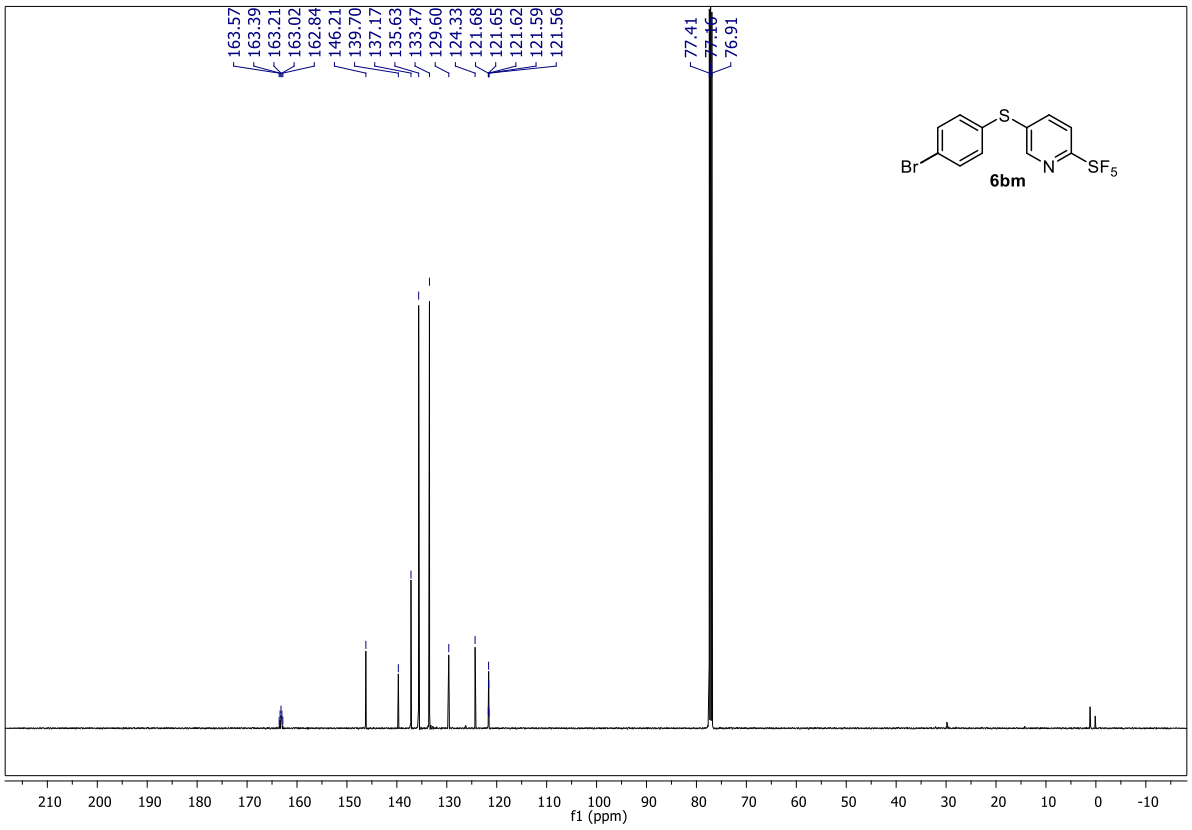

7.69
7.68
7.66
7.65
7.28
7.27
7.27
7.26
7.23
7.21
7.21
7.19
7.18
7.18
7.13
7.12
7.11
7.10
7.10
7.09
5.78
3.96
3.90
-0.00
OMe
N
MeO
N
O
O
N
SF5
6al
0.90
0.92
2.31
3.01
0.85
2.87
3.00
f1 (ppm)


77.66
77.10
76.56
76.00
75.46
63.65
63.10
-162.20
OMe
N
MeO
N
O
O
N
SF5
6al
1.00
4.20
f1 (ppm)


173.60
172.12
165.19
159.65
158.27
158.10
157.95
157.80
157.60
151.16
150.10
123.63
123.48
121.59
119.93
115.57
84.61
77.41
77.16
76.91
55.02
54.44
0.10
OMe
MeO
N
O
SF5
6al
f1 (ppm)


8.31
7.59
7.59
7.56
7.40
7.37
7.26
0.00
S
Br
N
SF5
6bm
0.97
3.95
2.26
f1 (ppm)


79.09
78.55
78.02
77.49
76.96
52.88
52.34
-162.20
S
Br
N
SF5
6bm
1.00
3.79
f1 (ppm)


163.57
163.39
163.21
163.02
162.84
146.21
139.70
137.17
135.63
133.47
129.60
124.33
121.68
121.65
121.62
121.59
121.56
77.41
77.16
76.91
S
Br
N
SF5
6bm
f1 (ppm)