Supporting Information for

Pd-Catalyzed Direct Arylation of Nitro-(pentafluorosulfanyl)benzenes with Aryl Bromides

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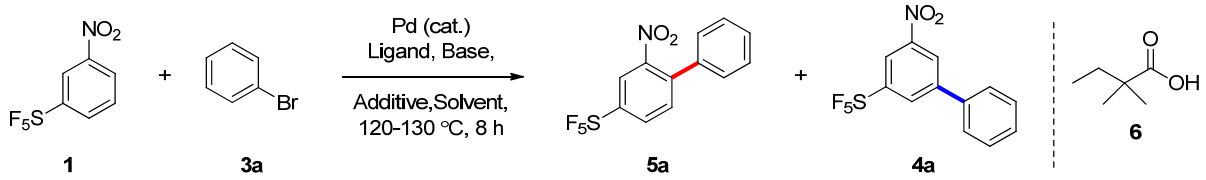
General Information: ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker AM 300 and AM 400 spectrometer. The peaks were internally referenced to TMS (0.00 ppm). ^{19}F NMR was recorded on Bruker AM 400 spectrometer ($CFCl_3$ as external reference standard and low field is positive). Chemical shifts (δ) are reported in ppm, and coupling constants (*J*) are in Hertz (Hz). NMR yield was determined by ^{19}F NMR using fluorobenzene as an internal standard before working up the reaction. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, p = pentad, m = multiplet, br = broad.

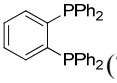
Materials: All commercial reagents were purchased from J&K, Energy Chemical, TCI, Alfa Aesar, Sigma-Aldrich of the highest purity grade. All reagents were weighed and handled in air, and refilled with an inert atmosphere of N_2 at room temperature. Toluene (from Sinopharm Chemical Reagent CO., LTD) was distilled from sodium and benzophenone before use. Phenyl Bromide **3a** (from Shanghai Lingfeng Chemical Reagent CO., LTD) was distilled before use. Other aryl bromides **3** were purchased from Energy Chemical，but 6-bromoquinoline was purchased from J&K. $(AllylPdCl)_2$ and PCy_3HBF_4 were also purchased from Energy Chemical. Compounds **1** and **2** (*m*/*p*-nitro-(pentafluorosulfanyl)benzene) were prepared according to the corresponding literatures as reported[1].

1) Optimization of Pd-Catalyzed Direct Arylation of *m/p*-Nitro-(pentafluorosulfanyl)benzene 1 with Phenyl Bromide 3a (Table S1 and S2).

A 25 mL Schlenk tube equipped with a magnetic stir bar was charged with [Pd] (10 -5 mol %), phosphane ligand (15-7.5 mol %), base (2.4-1.2 equiv.), The reaction tube was evacuated and backfilled with N_2 (4 times), then additive (0.3-1.0 equiv), **3a** (2.0-1.5 equiv), toluene (0.8-1 mL) and (**1** or **2**) (0.2-0.3 mmol, 1.0 equiv) were added subsequently. The sealed tube was screw capped and heated to 120 - 130 ℃ for 8 h (oil bath). The yield was determined by ^{19}F NMR before working up. If necessary, the reaction vessel was cooled to room temperature, and the reaction mixture was concentrated *in vacuo* directly. The resulting residue was purified with silica gel chromatography to afford the pure products (**5a** and **4a**).

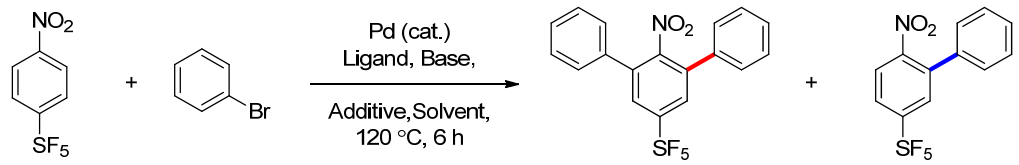
Table S1. Optimization of Pd-Catalyzed Direct Arylation of *meta*-Nitro-(pentafluorosulfanyl)benzene 1 with Phenyl Bromide 3a.[a]



entry	[Pd] (mol %)	Ligand (mol %)	Additive (equiv)	Base (equiv)	Solvent (mL)	Temp (^{o}C)	Yield (%)[b] **5a**/**4a**
1	$Pd(OAc)_2$ (10)	$P(Cy)_3.HBF_4$ (15)	PivOH (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	31/8
2	$Pd(OAc)_2$ (10)	 (7.5)	PivOH (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	22/6
3	$Pd(OAc)_2$ (10)	Dave-Phos (15)	PivOH (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	5/16
4	$Pd(OAc)_2$ (10)	Me-Phos (15)	PivOH (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	14/14
5	$Pd(OAc)_2$ (10)	$P(Cy)_3.HBF_4$ (15)	PivOH (1.0)	Cs_2CO_3 (1.2)	Tol.(1.0)	120	38/7
6	$Pd(OAc)_2$ (10)	$P(Cy)_3.HBF_4$ (15)	PivOH (1.0)	K_3PO_4 (1.2)	Tol.(1.0)	120	1/Trace
7	$Pd(OAc)_2$ (10)	$P(Cy)_3.HBF_4$ (15)	AcOH (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	2/Trace
8	$Pd(OAc)_2$ (10)	$P(Cy)_3.HBF_4$ (15)	AdCOOH (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	3/2
9	$Pd(OAc)_2$ (10)	$P(Cy)_3.HBF_4$ (15)	*o*-Me-PhCOOH (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	1/1
10	$PdCl_2$ (10)	$P(Cy)_3.HBF_4$ (15)	PivOH (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	38/3
11	$(allylPdCl)_2$ (5)	$P(Cy)_3.HBF_4$ (15)	PivOH (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	55/4
12	$Pd(dppf)Cl_2$ (10)	$P(Cy)_3.HBF_4$ (15)	PivOH (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	51/6
13	$Pd(MeCN)_2Cl_2$ (10)	$P(Cy)_3.HBF_4$ (15)	PivOH (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	38/4
14	$Pd(PPh_3)_2Cl_2$ (10)	$P(Cy)_3.HBF_4$ (15)	PivOH (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	42/4
15	$Pd(PhCN)_2Cl_2$ (10)	$P(Cy)_3.HBF_4$ (15)	PivOH (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	40/4
16	$(allylPdCl)_2$ (5)	$P(Cy)_3.HBF_4$ (15)	**6** (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	130	71/0
17	$(allylPdCl)_2$ (5)	$P(Cy)_3.HBF_4$ (15)	**6** (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	140	62/8
18	$(allylPdCl)_2$ (5)	$P(Cy)_3.HBF_4$ (15)	**6** (0.5)	K_2CO_3 (2.4)	Tol.(1.0)	130	(82)/(7)
19	$(allylPdCl)_2$ (2.5)	$P(Cy)_3.HBF_4$ (7.5)	**6** (0.3)	K_2CO_3 (1.8)	Tol.(1.0)	130	(74)/(7)
20[c]	$(allylPdCl)_2$ (2.5)	$P(Cy)_3.HBF_4$ (7.5)	**6** (0.3)	K_2CO_3 (1.8)	Tol.(0.8)	130	(79)/(7)
21[c]	$(allylPdCl)_2$ (2.5)	$P(Cy)_3.HBF_4$ (7.5)	PivOH (0.3)	K_2CO_3 (1.8)	Tol.(0.8)	130	61/8

[a]Reaction conditions: **1** (0.3 mmol) and **3a** (2.0 equiv), 8 h. [b]NMR yield determined by ^{19}F NMR using fluorobenzene as an internal standard (isolated yield in parentheses). [c]**1** (0.5 mmol), **3a** (1.5 equiv), 8 h.

Table S2. Optimization of Pd-Catalyzed Direct Arylation of *para*-Nitro-(pentafluorosulfanyl)benzene 1 with Phenyl Bromide 3a.[a]

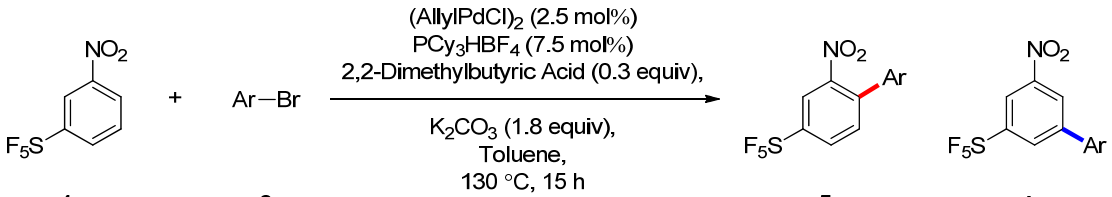


2 **3a** **6a** **7a**

entry	[Pd] (mol %)	Ligand (mol %)	Additive (equiv)	Base (equiv)	Solvent (mL)	Temp (°C)	Yield (%)[b] **6a**/**7a**
1	$Pd(OAc)_2$ (10)	$P(Cy)_3.HBF_4$ (15)	PivOH (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	3/19
2	$(allylPdCl)_2$ (5)	$P(Cy)_3.HBF_4$ (15)	*o*-Me-PhCOOH (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	3/25
3	$(allylPdCl)_2$ (5)	$P(Cy)_3.HBF_4$ (15)	**6** (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	15/30
4	$(allylPdCl)_2$ (5)	$P(Cy)_3.HBF_4$ (15)	PivOH (1.0)	Cs_2CO_3 (1.2)	Tol.(1.0)	120	21/32
5	$Pd(dppf)Cl_2$ (10)	$P(Cy)_3.HBF_4$ (15)	PivOH (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	10/27
6	$(allylPdCl)_2$ (5)	 (7.5)	PivOH (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	5/27
7	$(allylPdCl)_2$ (5)	BINAP (7.5)	PivOH (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	1/20
8	$(allylPdCl)_2$ (5)	$P(tBu)_2Me.HBF_4$ (15)	PivOH (1.0)	K_2CO_3 (1.2)	Tol.(1.0)	120	10/28
9[c]	$(allylPdCl)_2$ (5)	$P(Cy)_3.HBF_4$ (15)	**6** (1.0)	Cs_2CO_3 (1.2)	Tol.(1.0)	130	19/37
10[c,d]	$(allylPdCl)_2$ (2.5)	$P(Cy)_3.HBF_4$ (7.5)	**6** (1.0)	Cs_2CO_3 (1.2)	Tol.(1.0)	130	18/41
11[e]	$(allylPdCl)_2$ (2.5)	$P(Cy)_3.HBF_4$ (7.5)	**6** (0.3)	K_2CO_3 (1.8)	Tol.(1.0)	130	85/13
12	$(allylPdCl)_2$ (2.5)	$P(Cy)_3.HBF_4$ (7.5)	**6** (0.3)	Cs_2CO_3 (1.8)	Tol.(1.0)	130	60/28
13[f]	$(allylPdCl)_2$ (2.5)	$P(Cy)_3.HBF_4$ (7.5)	**6** (0.3)	K_2CO_3 (1.8)	Tol.(1.0)	130	(87)/(4)

[a]Reaction conditions (unless otherwise specified): **2** (0.2 mmol, 1.0 equiv), **3a** (2.0 equiv), 8 h. [b]NMR yield determined by ^{19}F NMR using fluorobenzene as an internal standard (isolated yield in parentheses). [c]**3a** (1.0 equiv). [d]Reaction conducted for 12 h. [e]**3a** (3.0 equiv). [f]**3a** (2.5 equiv) and reaction conducted for 15 h.

2) General Procedure for Pd-catalyzed Direct Arylation of *m*-Nitro-(pentafluorosulfanyl)benzene 1 with Various Aryl bromides 3.

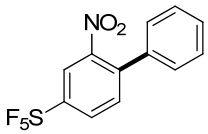


1 1.0eq. **3** 1.5 eq. **5** **4**

A 25 mL Schlenk tube equipped with a magnetic stir bar was charged with $(allylPdCl)_2$ (2.5 mol%), PCy_3HBF_4 (7.5 mol%), K_2CO_3 (1.8 equiv.), The reaction tube was evacuated and backfilled with N_2 (4 times), then 2,2-dimethylbutyric acid (0.3 equiv), **3** (1.5 equiv), toluene (0.8 mL) and **1** (0.5 mmol, 1.0 equiv) were added subsequently. The sealed tube was screw capped and heated to 130 ℃ for 15h (oil bath). The reaction vessel was then cooled to room temperature, and the reaction mixture was concentrated *in vacuo* directly. The resulting residue was purified with silica gel chromatography to afford the pure products (**5** and **4**).

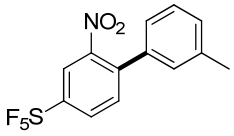
Note: The column length and diameter for the purification of compounds **5-7** are 15 cm and 2 cm respectively.

3) Data for Compounds 5 and 4.



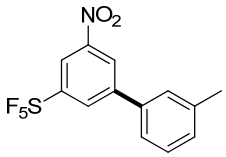
5a

2-Nitro-[1,1'-biphenyl]-4-yl sulfurpentafluoride 5a: The product (140 mg, 86％ yield as a mixture of **5a** and **4a**, **5a**/**4a** = 65:6 determined by ^{19}F NMR) as a slightly green oil was purified by silica gel column chromatography (dichloromethane/petroleum ether = 1:50). ^1H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 2.1 Hz, 1H), 7.98 (dd, *J* = 8.5, 2.1 Hz, 1H), 7.56 (d, *J* = 8.5, 1H), 7.43 (m, 3H), 7.30 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.5 (p, *J* = 19.0 Hz), 148.6, 139.7, 135.5, 132.6, 129.4 (m), 129.2, 129.0, 127.7, 122.3 (m); ^{19}F NMR (376 MHz, $CDCl_3$) δ 81.38 (p, *J* = 151 Hz, SF_{ax}, 1F), 63.15 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3107, 3032, 2925, 2879, 1612, 1538, 1478, 1448, 1351, 1120, 1099, 898 (S-F/NO_2), 830 (S-F/NO_2), 757, 728, 699, 600; MS (ESI): *m/z* 326 ($(M+H)^+$, 100), 306, 296; HRMS (ESI) *m/z* Calculated for $C_{12}H_9F_5NO_2S$ $(M+H)^+$: 326.0276, found: 326.02687.



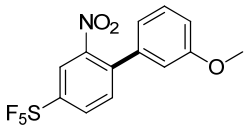
5b

3'-Methyl-2-nitro-[1,1'-biphenyl]-4-yl sulfurpentafluoride 5b: The product (142 mg, 84% yield) as a slightly green oil was purified by silica gel column chromatography (dichloromethane/petroleum ether = 3:100). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 2.0 Hz, 1H), 7.98 (dd, *J* = 8.5, 2.1 Hz, 1H), 7.56 (d, *J* = 8.5, 1H), 7.33 (t, *J* = 7.5, 1H), 7.26 (d, *J* = 7.5, 1H), 7.15-7.06 (m, 2H), 2.39 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.5 (p, *J* = 19.5 Hz), 148.7, 139.9, 138.9, 135.5, 132.5, 130.1, 129.3 (m), 128.9, 128.4, 124.8, 122.3 (m), 21.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ 81.46 (p, *J* = 151 Hz, SF_{ax}, 1F), 63.15 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3107, 2926, 1607, 1567, 1538, 1478, 1356, 1120, 1099, 904 (S-F/NO_2), 831 (S-F/NO_2), 789, 742, 671, 601; MS (EI): *m/z* 339 $(M)^+$, 311, 249 (100); HRMS (EI) *m/z* Calculated for $C_{13}H_{10}F_5NO_2S$ $(M)^+$: 339.0350, found: 339.0352.



4b

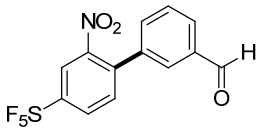
3'-Methyl-5-nitro-[1,1'-biphenyl]-3-yl sulfurpentafluoride 4b: The product (12 mg, 7% yield) as a slightly yellow oil was purified by silica gel column chromatography (dichloromethane/petroleum ether = 1:50). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (s, 2H), 8.26 (s, 1H), 7.42 (m, 3H), 7.32 (m, 1H), 2.47 (s, 3H).



5c

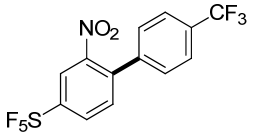
3'-Methoxy-2-nitro-[1,1'-biphenyl]-4-yl sulfurpentafluoride 5c: The product (151 mg, 90% yield) as a slightly green solid was purified by silica gel column chromatography (dichloromethane/petroleum ether = 1:20). m.p. 75.9 – 76.8 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 2.0 Hz, 1H), 7.99 (dd, *J* = 8.5, 2.1 Hz, 1H), 7.59 (d, *J* = 8.5, 1H), 7.36 (t, *J* = 8.0, 1H), 6.99 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.91 – 6.82 (m, 2H), 3.82 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.8, 152.5 (p, *J* = 20.2 Hz), 148.6, 139.4, 136.7, 132.4, 130.1, 129.3 (m), 122.2 (m), 120.0, 114.6, 113.5, 55.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ 81.37 (p, *J* = 151 Hz, SF_{ax}, 1F), 63.13 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3096, 3023, 2984, 2950, 2846, 1607, 1583, 1568, 1535, 1357, 1212, 1173, 905

(S-F/NO_2), 867 (S-F/NO_2), 827 (S-F/NO_2), 784, 739, 671; MS (EI): *m/z* 355 (M^+ ,100), 327, 139; HRMS (EI) *m/z* Calculated for $C_{13}H_{10}F_5NO_3S$ $(M)^+$: 355.0303, found: 355.0302.



5d

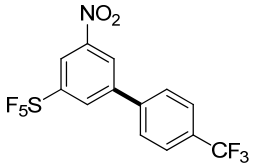
3'-Formyl-2-nitro-[1,1'-biphenyl]-4-yl sulfurpentafluoride 5d: The product (94 mg, 53％ yield) as a slightly yellow solid was purified by silica gel column chromatography (ethyl acetate/petroleum ether = 1:20). m.p. 89.8 − 93.0 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.05 (s, 1H), 8.38 (d, *J* = 2.0 Hz, 1H), 8.08 (dd, *J* = 8.5, 2.1 Hz, 1H), 7.98 (d, *J* = 7.6 Hz, 1H), 7.86 (s, 1H), 7.68 – 7.63 (m, 2H), 7.58 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.3, 153.0 (p, *J* = 20.4 Hz), 148.2, 138.5, 136.8, 136.7, 133.5, 132.6, 130.5, 129.9 (m), 129.7, 128.5, 122.7 (m); ^{19}F NMR (376 MHz, $CDCl_3$) δ 80.90 (p, *J* = 151 Hz, SF_{ax}, 1F), 63.07 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3101, 2864, 1692, 1616, 1599, 1527, 1354, 1180, 1168, 918 (S-F/NO_2), 874 (S-F/NO_2), 843 (S-F/NO_2), 827 (S-F/NO_2), 744, 683, 601; MS (EI): *m/z* 353 $(M)^+$, 325, 308, 168 (100), 151; HRMS (EI) *m/z* Calculated for $C_{13}H_8F_5NO_3S$ $(M)^+$: 353.0144, found: 353.0145.



5e

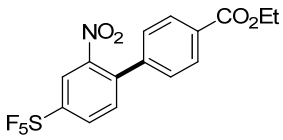
2-Nitro-4'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl sulfurpentafluoride 5e: The product (126 mg, 64 ％ yield) as a white solid was purified by silica gel column chromatography (dichloromethane/petroleum ether = 1:100). m.p. 118.3 – 119.4 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 2.0 Hz, 1H), 8.06 (dd, *J* = 8.5, 2.1 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 2H), 7.58 (d, *J* = 8.4 Hz, 1H), 7.45 (d, *J* = 8.1 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.2 (p, *J* = 20.4 Hz), 148.3, 139.3, 138.4, 132.4, 131.3 (q, *J* = 24.7 Hz), 129.8 (p, *J* = 4.5 Hz), 128.2, 125.9 (q, *J* = 3.8 Hz), 126.5 (q, *J* = 273.7 Hz), 122.7 (p, *J* = 4.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 80.85 (p, *J* = 151 Hz, SF_{ax}, 1F), 63.05 (d, *J* = 151 Hz, 4×SF_{eq}, 4F), -62.86 (s, 3F); IR (neat, cm^{-1}) 3113, 1612, 1567, 1528, 1352, 1329, 1170, 1121, 1110, 1072, 900 (S-F/NO_2), 875 (S-F/NO_2), 848 (S-F/NO_2), 825 (S-F/NO_2), 603; MS (ESI): *m/z* 416 $(M+Na)^+$, 374 (100), 331; HRMS (ESI) *m/z* Calculated for $C_{13}H_8F_8NO_2S$

$(M+H)^+$: 394.0149, found: 394.01425.



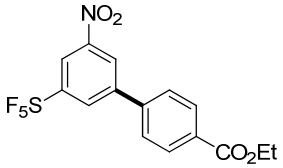
4e

5-Nitro-4'-(trifluoromethyl)-[1,1'-biphenyl]-3-yl sulfurpentafluoride 4e: The product (10 mg, 5% yield) as a white solid was purified by silica gel column chromatography (dichloromethane/petroleum ether = 1:100). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (t, *J* = 1.8 Hz, 1H), 8.62 (s, 1H), 8.28 (s, 1H), 7.82 (d, *J* = 8.0 Hz, 2H), 7.75 (d, *J* = 8.0 Hz, 2H).



5f

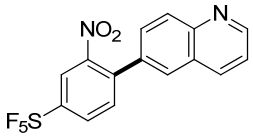
Ethyl 4'-(pentafluorothio)-2'-nitro-[1,1'-biphenyl]-4-carboxylate 5f: The product (144 mg, 72% yield) as a colorless oil was purified by silica gel column chromatography (ethyl acetate/petroleum ether = 1:20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 2.0 Hz, 1H), 8.14 (d, *J* = 8.2 Hz, 2H), 8.04 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.60 (d, *J* = 8.4 Hz, 1H), 7.39 (d, *J* = 8.2 Hz, 2H), 4.41 (q, *J* = 7.1 Hz, 2H), 1.41 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.8, 153.0 (p, *J* = 19.7 Hz), 148.3, 139.9, 138.9, 132.4, 131.1, 130.1, 129.7 (m), 127.8, 122.6 (m), 61.3, 14.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ 81.01 (p, *J* = 151 Hz, SF_{ax}, 1F), 63.05 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3109, 2985, 2934, 1717, 1608, 1541, 1479, 1355, 1278, 1182, 1110, 899 (S-F/NO_2), 834 (S-F/NO_2), 776, 761, 704, 671, 602; MS (ESI): *m/z* 398 ($(M+H)^+$,100), 269; HRMS (ESI) *m/z* Calculated for $C_{15}H_{12}F_5NO_4SNa$ $(M+Na)^+$: 420.02807, found: 420.02994.



4f

Ethyl 3'-(pentafluorothio)-5'-nitro-[1,1'-biphenyl]-4-carboxylate 4f: The product (15 mg, 8% yield) as a colorless oil was purified by silica gel column chromatography (ethyl acetate/petroleum

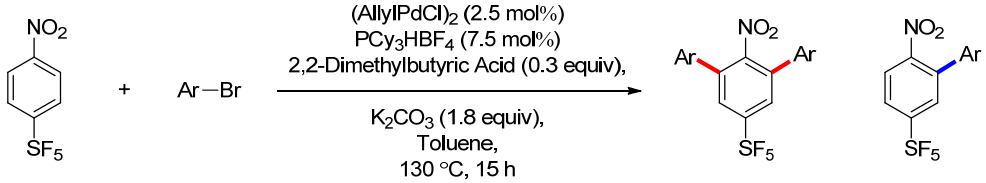
ether = 1:20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 – 8.59 (m, 2H), 8.30 (s, 1H), 8.21 (d, *J* = 8.3 Hz, 2H), 7.71 (d, *J* = 8.3 Hz, 2H), 4.44 (q, *J* = 7.2 Hz, 2H), 1.44 (t, *J* = 7.1 Hz, 3H).



5g

3-Nitro-4-(quinolin-6-yl)phenyl sulfurpentafluoride 5g: The product (70 mg, 37% yield) as a slightly yellow oil was purified by silica gel column chromatography (ethyl acetate/petroleum ether = 1:10). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.98 (d, *J* = 2.7 Hz, 1H), 8.37 (d, *J* = 2.1 Hz, 1H), 8.22 – 8.17 (m, 2H), 8.06 (dd, *J* = 8.5, 2.2 Hz, 1H), 7.79 (d, *J* = 1.8 Hz, 1H), 7.68 (d, *J* = 8.4 Hz, 1H), 7.62 (dd, *J* = 8.7, 2.0 Hz, 1H), 7.47 (dd, *J* = 8.3, 4.2 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.0 (p, *J* = 21.4 Hz), 151.7, 148.6, 148.1, 139.2, 136.5, 134.0, 133.0, 130.5, 129.8 (m), 128.9, 128.2, 127.3, 122.8 (m), 122.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ 81.13 (p, *J* = 151 Hz, SF_{ax}, 1F), 63.14 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3079, 3043, 1594, 1572, 1537, 1487, 1356, 908 (S-F/NO_2), 885 (S-F/NO_2), 847 (S-F/NO_2), 837 (S-F/NO_2), 827 (S-F/NO_2), 739, 670, 590; MS (ESI): *m/z* 377 ($(M+H)^+$, 100), 341, 251; HRMS (ESI) *m/z* Calculated for $C_{15}H_9F_5N_2O_2SNa$ $(M+Na)^+$: 399.01837, found: 399.01971.

4) General Procedure for Pd-catalyzed Direct Arylation of *p*-Nitro-(pentafluorosulfanyl)benzene 2 with Various Aryl bromides 3.



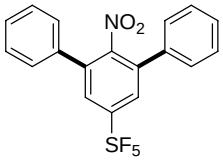
2 1.0eq. **3** 2.5 eq. **6** **7**

A 25 mL Schlenk tube equipped with a magnetic stir bar was charged with $(allylPdCl)_2$ (2.5 mol%), PCy_3HBF_4 (7.5 mol%), K_2CO_3 (1.8 equiv.). The reaction tube was evacuated and backfilled with N_2 (4 times), then 2,2-dimethylbutyric acid (0.3 equiv), **3** (2.5 equiv), toluene (1.0 mL) and **2** (0.2-0.3 mmol, 1.0 equiv) were added subsequently. The sealed tube was screw capped and heated to 130 ℃ for 15h (oil bath). The reaction vessel was then cooled to room temperature, and the reaction

mixture was concentrated *in vacuo* directly. The resulting residue was purified with silica gel chromatography to afford the pure products (**6** and **7**).

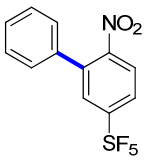
Note: For **6(a, e, f, h, j, k)** and **7(a, e, f, h, j, k)**, 0.3 mmol of **2** was used; for **6(b, c, d, g, i)** and **7(b, c, d, g, i)**, 0.2 mmol of **2** was used.

5) Data for Compounds 6 and 7.



6a

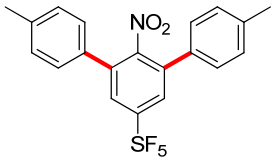
2'-Nitro-[1,1':3',1''-terphenyl]-5'-yl sulfurpentafluoride 6a: The product (105 mg, 87% yield) as a white solid was purified by silica gel column chromatography (dichloromethane/petroleum ether = 1:50). m.p. 182.1 – 182.9 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84 (s, 2H), 7.48 – 7.46 (m, 6H), 7.42 – 7.39 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.7 (p, *J* = 18.7 Hz), 150.6, 135.5, 134.7, 129.4, 129.1, 128.1, 127.8 (m); ^{19}F NMR (376 MHz, $CDCl_3$) δ 81.85 (p, *J* = 151 Hz, SF_{ax}, 1F), 63.14 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3067, 2919, 2850, 1538, 1496, 1369, 892 (S-F/NO_2), 865 (S-F/NO_2), 833 (S-F/NO_2), 755, 701, 599, 544; MS (EI): *m/z* 401 $(M)^+$, 257, 244, 226 (100), 217; HRMS (EI) *m/z* Calculated for $C_{18}H_{12}F_5NO_2S$ $(M)^+$: 401.0506, found: 401.0509.



7a

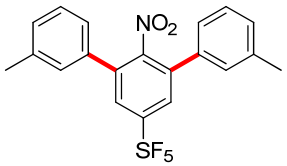
6-Nitro-[1,1'-biphenyl]-3-yl sulfurpentafluoride 7a: The product (4 mg, 4% yield) as a white solid was purified by silica gel column chromatography (dichloromethane/petroleum ether = 1:50). m.p. 107.6 – 108.4 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.87 (m, 3H), 7.48 – 7.46 (m, 3H), 7.35 – 7.33 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$)) δ 153.1 (p, *J* = 19.2 Hz), 150.40, 137.1, 135.4, 129.8 (m), 129.2, 129.0, 127.8, 126.1 (m), 124.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ 81.41 (p, *J* = 151 Hz, SF_{ax}, 1F), 62.75 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3071, 1528, 1474, 1448, 1371,

1090, 890 (S-F/NO_2), 829 (S-F/NO_2), 774, 756, 697, 601, 538; MS (EI): *m/z* 325 $(M)^+$, 297, 168, 152 (100), 139; HRMS (EI) *m/z* Calculated for $C_{12}H_8F_5NO_2S$ $(M)^+$: 325.0201, found: 325.0196.



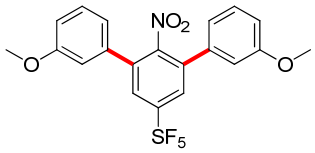
6b

4,4''-Dimethyl-2'-nitro-[1,1':3',1''-terphenyl]-5'-yl sulfurpentafluoride 6b: The product (61 mg, 71 % yield) as a white solid was purified by silica gel column chromatography (dichloromethane/petroleum ether = 1:50). m.p. 123.0 − 124.6 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (s, 2H), 7.31 – 7.26 (m, 8H), 2.41 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.7 (p, *J* = 18.2 Hz), 150.7, 139.6, 135.5, 131.9, 129.8, 127.8, 127.6 (m), 21.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ 82.05 (p, *J* = 151 Hz, SF_{ax}, 1F), 62.95 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3077, 3040, 2924, 2853, 1614, 1541, 1515, 1372, 893 (S-F/NO_2), 865 (S-F/NO_2), 840 (S-F/NO_2), 820 (S-F/NO_2), 798, 750, 666, 603, 535; MS (EI): *m/z* 429 (M^+, 100), 285; HRMS (EI) *m/z* Calculated for $C_{20}H_{16}F_5NO_2S$ $(M)^+$: 429.0819, found: 429.0822.



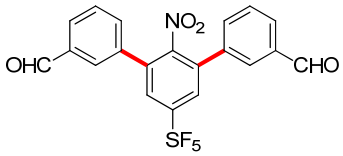
6c

3,3''-Dimethyl-2'-nitro-[1,1':3',1''-terphenyl]-5'-yl sulfurpentafluoride 6c: The product (82 mg, 95 % yield) as a white solid was purified by silica gel column chromatography (dichloromethane/petroleum ether = 1:25). m.p. 142.1 − 143.0 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.81 (s, 2H), 7.36 – 7.25 (m, 4H), 7.20 – 7.17 (m, 4H), 2.40 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.6 (p, *J* = 18.7 Hz), 150.5, 138.9, 135.6, 134.7, 130.2, 128.9, 128.8, 127.7 (m), 125.10, 21.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ 82.00 (p, *J* = 151 Hz, SF_{ax}, 1F), 63.01 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3020, 2919, 1560, 1537, 1375, 1086, 909 (S-F/NO_2), 844 (S-F/NO_2), 820 (S-F/NO_2), 820 (S-F/NO_2), 746, 701, 666, 599; MS (EI): *m/z* 429 $(M)^+$, 401, 386, 285, 239 (100); HRMS (EI) *m/z* Calculated for $C_{20}H_{16}F_5NO_2S$ $(M)^+$: 429.0818, found: 429.0822.



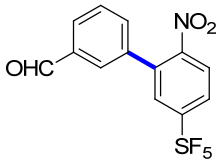
6d

3,3''-Dimethoxy-2'-nitro-[1,1':3',1''-terphenyl]-5'-yl sulfurpentafluoride 6d: The product (85 mg, 92 % yield) as a white solid was purified by silica gel column chromatography (dichloromethane/petroleum ether = 1:20). m.p. 122.7 – 124.3 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84 (s, 2H), 7.37 (t, *J* = 7.9 Hz, 2H), 7.01 – 6.93 (m, 6H), 3.83 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 153.6 (p, *J* = 18.8 Hz), 150.4, 135.8, 135.3, 130.1, 127.6 (m), 120.3, 115.0, 113.7, 55.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ 81.83 (p, *J* = 151 Hz, SF_{ax}, 1F), 63.01 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3073, 3033, 2966, 2944, 2838, 1602, 1591, 1532, 1464, 1238, 1030, 911 (S-F/NO_2), 861 (S-F/NO_2), 843 (S-F/NO_2), 822 (S-F/NO_2), 763, 698, 666, 599; MS (EI): *m/z* 461 $(M)^+$, 202 (100); HRMS (EI) *m/z* Calculated for $C_{20}H_{16}F_5NO_4S$ $(M)^+$: 461.0722, found: 461.0720.



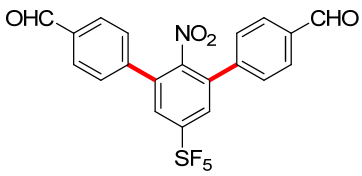
6e

3,3''-Diformyl-2'-nitro-[1,1':3',1''-terphenyl]-5'-yl sulfurpentafluoride 6e: The product (79 mg, 58 % yield) as a white solid was purified by silica gel column chromatography (ethyl acetate/petroleum ether = 1:20). m.p. 194.7 – 195.3 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.08 (s, 2H), 8.03 – 8.01 (m, 2H), 7.94 – 7.91 (m, 4H), 7.68 – 7.67 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.2, 154.0 (p, *J* = 19.2 Hz), 150.5, 136.9, 135.4, 134.4, 133.7, 130.8, 130.0, 129.2, 128.4 (m); ^{19}F NMR (376 MHz, $CDCl_3$) δ 81.06 (p, *J* = 151 Hz, SF_{ax}, 1F), 63.12 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3074, 2862, 1695, 1528, 1375, 1187, 900 (S-F/NO_2), 857 (S-F/NO_2), 828 (S-F/NO_2), 757, 696, 601; MS (EI): *m/z* 457 $(M)^+$, 244, 226 (100); HRMS (EI) *m/z* Calculated for $C_{20}H_{12}F_5NO_4S$ $(M)^+$: 457.0412, found: 457.0407.



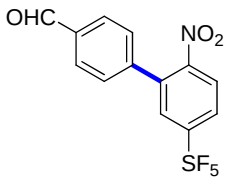
7e

3'-Formyl-6-nitro-[1,1'-biphenyl]-3-yl sulfurpentafluoride 7e: The product (20 mg, 18% yield) as a white solid was purified by silica gel column chromatography (ethyl acetate/petroleum ether = 1:20). m.p. 135.5 – 136.9 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.07 (s, 1H), 8.04 – 7.95 (m, 3H), 7.87 (s, 2H), 7.66 (t, *J* = 7.6 Hz, 1H), 7.59 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.2, 155.5 (p, *J* = 19.0 Hz), 150.1, 136.9, 136.6, 136.0, 133.6, 130.5, 129.8 (m), 129.7, 128.7, 126.9 (m), 124.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ 80.97 (p, *J* = 151 Hz, SF_{ax}, 1F), 62.81 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3110, 3059, 3037, 2857, 2753, 1698, 1537, 1367, 1182, 1166, 901 (S-F/NO_2), 851 (S-F/NO_2), 830 (S-F/NO_2), 765, 752, 694, 666, 650; MS (EI): *m/z* 353 $(M)^+$, 259, 168, 151 (100), 139; HRMS (EI) *m/z* Calculated for $C_{13}H_8F_5NO_3S$ $(M)^+$: 353.0141, found: 353.0145.



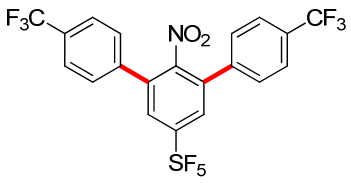
6f

4,4''-Diformyl-2'-nitro-[1,1':3',1''-terphenyl]-5'-yl sulfurpentafluoride 6f: The product (44 mg, 32 % yield) as a white solid was purified by silica gel column chromatography (ethyl acetate/petroleum ether = 1:20). m.p. 226.3 – 227.5 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.1 (s, 2H), 8.00 (d, *J* = 7.8 Hz, 4H), 7.92 (s, 2H), 7.59 (d, *J* = 7.9 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.2, 154.1 (p, *J* = 19.7 Hz), 150.2, 140.0, 136.8, 134.6, 130.3, 128.9, 128.3 (m); ^{19}F NMR (376 MHz, $CDCl_3$) δ 80.92 (p, *J* = 151 Hz, SF_{ax}, 1F), 62.79 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3080, 2823, 2732, 1702, 1600, 1608, 1532, 1372, 1209, 896 (S-F/NO_2), 870 (S-F/NO_2), 833 (S-F/NO_2), 796, 756, 603, 560; MS (EI): *m/z* 457 $(M)^+$, 428, 400, 226 (100); HRMS (EI) *m/z* Calculated for $C_{20}H_{12}F_5NO_4S$ $(M)^+$: 457.0406, found: 457.0407.



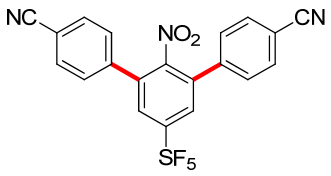
7f

4'-formyl-6-nitro-[1,1'-biphenyl]-3-yl sulfurpentafluoride 7f: The product (22 mg, 21% yield) as a white solid was purified by silica gel column chromatography (ethyl acetate/petroleum ether = 1:50). m.p. 105.6 – 106.9 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.10 (s, 1H), 8.05 – 7.96 (m, 4H), 7.87 (d, *J* = 1.9 Hz, 1H), 7.52 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.3, 155.7 (p, *J* = 19.1 Hz), 145.0, 141.4, 136.5, 136.1, 130.2, 129.5 (m), 128.7, 127.0 (m), 124.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ 80.92 (p, *J* = 151 Hz, SF_{ax}, 1F), 62.79 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3110, 3067, 2822, 2732, 1702, 1606, 1533, 1367, 1210, 888 (S-F/NO_2), 863 (S-F/NO_2), 831 (S-F/NO_2), 822 (S-F/NO_2), 760, 602; MS (ESI): *m/z* 354 $(M+H)^+$, 274; HRMS (ESI) *m/z* Calculated for $C_{13}H_9F_5NO_3S$ $(M+H)^+$: 354.0229, found: 354.02178.



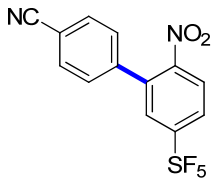
6g

2'-Nitro-4,4''-bis(trifluoromethyl)-[1,1':3',1''-terphenyl]-5'-yl sulfurpentafluoride 6g: The product (71 mg, 66% yield) as a white solid was purified by silica gel column chromatography (dichloromethane/petroleum ether = 1:50). m.p. 212.4 – 213.8 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.88 (s, 2H), 7.76 (d, *J* = 8.1 Hz, 4H), 7.54 (d, *J* = 8.1 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.0 (p, *J* = 19.5 Hz), 150.3, 137.8, 134.4, 131.8 (q, *J* = 33.2 Hz), 128.7, 128.4 (m), 126.2 (m), 123.6 (q, *J* = 273.8 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 80.99 (p, *J* = 151 Hz, SF_{ax}, 1F), 63.04 (d, *J* = 151 Hz, 4×SF_{eq}, 4F), -62.98 (s, 6F); IR (neat, cm^{-1}) 1537, 1330, 1170, 1123, 1110, 1069, 1019, 901 (S-F/NO_2), 867 (S-F/NO_2), 849 (S-F/NO_2), 822 (S-F/NO_2), 786, 755, 603; MS (EI): *m/z* 537 $(M)^+$, 393, 380, 285 (100); HRMS (EI) *m/z* Calculated for $C_{20}H_{10}F_{11}NO_2S$ $(M)^+$: 537.0255, found: 537.0257.



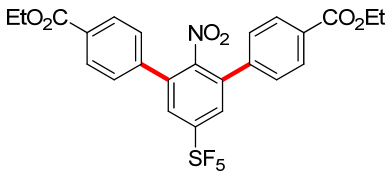
6h

4,4''-Dicyano-2'-nitro-[1,1':3',1''-terphenyl]-5'-yl sulfurpentafluoride 6h: The product (80 mg, 59 % yield) as a white solid was purified by silica gel column chromatography (ethyl acetate/petroleum ether = 1:5). m.p. 234.5 – 236.2 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (s, 2H), 7.79 (d, *J* = 7.9 Hz, 4H), 7.53 (d, *J* = 7.9 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.2 (p, *J* = 19.9 Hz), 150.0, 138.5, 134.1, 132.9, 128.9, 128.5 (m), 117.8, 113.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ 80.65 (p, *J* = 151 Hz, SF_{ax}, 1F), 63.09 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3411, 3072, 2231, 1533, 1506, 1398, 1370, 903 (S-F/NO_2), 869 (S-F/NO_2), 844 (S-F/NO_2), 828 (S-F/NO_2), 786, 603, 575; MS (ESI): *m/z* 452 $(M+H)^+$, 401, 274, 269 (100); HRMS (ESI) *m/z* Calculated for $C_{20}H_{10}F_5N_3O_2SNa$ $(M+Na)^+$: 474.02936, found: 474.03061.



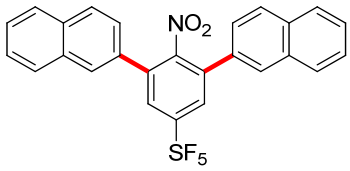
7h

4'-Cyano-6-nitro-[1,1'-biphenyl]-3-yl sulfurpentafluoride 7h: The product (25 mg, 24% yield) as a white solid was purified by silica gel column chromatography (ethyl acetate/petroleum ether = 1:5). m.p. 122.6 – 124.4 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.9 Hz, 1H), 7.99 (dd, *J* = 8.9, 2.2 Hz, 1H), 7.83 (d, *J* = 2.4 Hz, 1H), 7.78 (d, *J* = 8.4 Hz, 2H), 7.47 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.8 (p, *J* = 20.1 Hz), 149.8, 140.2, 135.5, 132.7, 129.5 (m), 128.8, 127.3 (m), 125.0, 118.0, 113.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ 80.74 (p, *J* = 151 Hz, SF_{ax}, 1F), 62.80 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3111, 3090, 3067, 2877, 2227, 1532, 1358, 884 (S-F/NO_2), 873 (S-F/NO_2), 839 (S-F/NO_2), 826 (S-F/NO_2), 791, 600; MS (EI): *m/z* 350 $(M)^+$, 322, 193 (100), 177; HRMS (ESI) *m/z* Calculated for $C_{13}H_7F_5N_2O_2S$ (M^+): 350.0149, found: 350.0148.



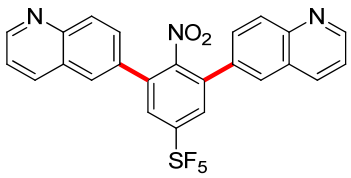
6i

Diethyl 5'-(pentafluorothio)-2'-nitro-[1,1':3',1''-terphenyl]-4,4''-dicarboxylate 6i: The product (94 mg, 86% yield) as a white solid was purified by silica gel column chromatography (ethyl acetate/petroleum ether = 1:20). m.p. 201.2 – 202.3 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.5 Hz, 4H), 7.88 (s, 2H), 7.48 (d, *J* = 8.5 Hz, 4H), 4.41 (q, *J* = 7.1 Hz, 4H), 1.41 (t, *J* = 7.1 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.7, 153.9 (p, *J* = 19.6 Hz), 150.3, 138.6, 134.82, 131.6, 130.3, 128.2, 61.4, 14.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ 81.26 (p, *J* = 151 Hz, SF_{ax}, 1F), 63.05 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3077, 3000, 2914, 2852, 1713, 1537, 1368, 1294, 1267, 1129, 1118, 893 (S-F/NO_2), 867 (S-F/NO_2), 842 (S-F/NO_2), 832 (S-F/NO_2), 759, 703, 599, 557; MS (EI): *m/z* 545 $(M)^+$, 500, 244, 226 (100); HRMS (EI) *m/z* Calculated for $C_{24}H_{20}F_5NO_6S$ $(M)^+$: 545.0993, found: 545.0932.



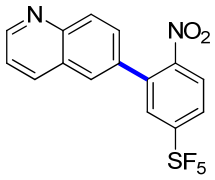
6j

3,5-Di(naphthalen-2-yl)-4-nitrophenyl sulfurpentafluoride 6j: The product (113 mg, 75% yield) as a white solid was purified by silica gel column chromatography (dichloromethane/petroleum ether = 1:100). m.p. 147.2 – 149.1 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (s, 2H), 7.97 – 7.90 (m, 8H), 7.59 – 7.57 (m, 4H), 7.54 – 7.52 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.8 (p, *J* = 19.2 Hz), 151.0, 135.7, 133.3, 133.0, 132.0, 129.1, 128.4, 128.1 (m), 128.0, 127.8, 127.3, 127.0, 125.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ 81.85 (p, *J* = 151 Hz, SF_{ax}, 1F), 63.08 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3062, 1541, 1369, 896 (S-F/NO_2), 866 (S-F/NO_2), 827 (S-F/NO_2), 755, 665, 603, 478; MS (EI): *m/z* 501 $(M)^+$, 357, 163 (100); HRMS (EI) *m/z* Calculated for $C_{26}H_{16}F_5NO_2S$ $(M)^+$: 501.0820, found: 501.0822.



6k

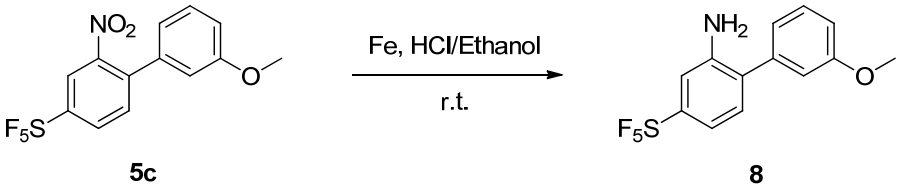
4-Nitro-3,5-di(quinolin-6-yl)phenyl sulfurpentafluoride 6k: The product (57 mg, 38% yield) as a grey white solid was purified by silica gel column chromatography (ethyl acetate/petroleum ether = 1:5). m.p. 218.7 – 219.3 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.00 (d, *J* = 2.7 Hz, 2H), 8.22 (dd, *J* = 12.0, 8.8 Hz, 4H), 8.00 (s, 2H), 7.91 (s, 2H), 7.76 (dd, *J* = 8.8, 1.6 Hz, 2H), 7.47 (dd, *J* = 8.2, 4.2 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.9 (p, *J* = 18.6 Hz), 151.8, 150.9, 148.1, 136.4, 135.1, 132.6, 130.8, 128.9, 128.4 (m), 127.9, 127.9, 122.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ 81.42 (p, *J* = 151 Hz, SF_{ax}, 1F), 63.11 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3426, 3046, 1539, 1498, 1373, 903 (S-F/NO_2), 865 (S-F/NO_2), 838 (S-F/NO_2), 602; MS (ESI): *m/z* 504 $(M+H)^+$, 253 (100); HRMS (ESI) *m/z* Calculated for $C_{24}H_{16}F_5N_3O_2S$ $(M+H)^+$: 504.07829, found: 504.07996.



7k

4-Nitro-3-(quinolin-6-yl)phenyl sulfurpentafluoride 7k: The product (32 mg, 28% yield) as a slightly green solid was purified by silica gel column chromatography (ethyl acetate/petroleum ether = 1:10). m.p. 149.8 – 151.0 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.00 (s, 1H), 8.21 (d, *J* = 8.4 Hz, 2H), 8.02 (d, *J* = 8.8 Hz, 1H), 7.97 – 7.94 (m, 2H), 7.83 (d, *J* = 1.6 Hz, 1H), 7.65 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.49 (dd, *J* = 8.3, 4.1 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.6 (p, *J* = 19.2 Hz), 151.5, 150.3, 147.9, 136.5, 136.4, 133.8, 130.4, 130.0 (m), 128.9, 128.1, 127.2, 126.6 (m), 124.7, 122.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ 81.15 (p, *J* = 151 Hz, SF_{ax}, 1F), 62.81 (d, *J* = 151 Hz, 4×SF_{eq}, 4F); IR (neat, cm^{-1}) 3064, 2869, 1523, 1496, 1482, 1353, 901 (S-F/NO_2), 887 (S-F/NO_2), 856 (S-F/NO_2), 842 (S-F/NO_2), 820 (S-F/NO_2), 771, 742, 661, 599; MS (EI): *m/z* 376 (M^+, 100), 359, 219; HRMS (EI) *m/z* Calculated for $C_{15}H_9F_5N_2O_2S$ $(M)^+$: 376.0307, found: 376.0305.

6) Preparation of Compound 8[2]

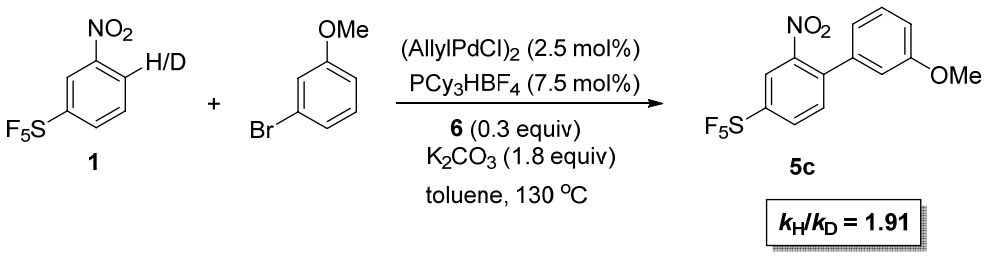


5c **8** 71%

To a stirred solution of **5c** (177 mg, 0.5 mmol, 1.0 eq.) in ethanol (5 mL) was added Fe powder (173 mg, 3 mmol, 6.0 equiv), followed by the addition of concentrated hydrochloric acid (0.25 mL) at 0 ˚C. After the reaction mixture was stirred for 1h at room temperature, the reaction was neutralized with sodium carbonate until alkaline, then extracted with EtOAc (3×20 mL). The combined extracts were dried over anhydrous Na_2SO_4, filtered and concentrated *in cacuo* to give a yellow oil. This crude product was purified by column chromatography (silica gel, 5% dichloromethane in hexane) to give the product **8** (115 mg, 71%) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (t, *J* = 7.7 Hz, 1H), 7.15-7.11 (m, 3H), 6.98 (d, *J* = 7.7 Hz, 1H), 6.94-6.92 (m, 2H), 3.97(br, 2H), 3.82 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.1, 153.8 (p, *J* = 16.6 Hz), 143.9, 140.0, 130.2, 130.19, 130.16, 121.0, 115.5 (m), 114.4, 113.6, 112.6 (m), 55.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ 85.40 (p, *J* = 150 Hz, SF_{ax}, 1F), 62.74 (d, *J* = 150 Hz, 4F); IR (neat, cm^{-1}) 3485, 3387, 2940, 2839, 1620, 1581, 1482, 1414, 1317, 1295, 1213, 1048, 1019, 928 (S-F/NO_2), 841 (S-F/NO_2), 803 (S-F/NO_2), 738, 703, 670, 641, 596; MS (EI): *m/z* 325 $(M)^+$, 85, 83 (100); HRMS (EI) *m/z* Calculated for $C_{13}H_{12}F_5NOS$ $(M)^+$: 325.0561, found: 325.0560.

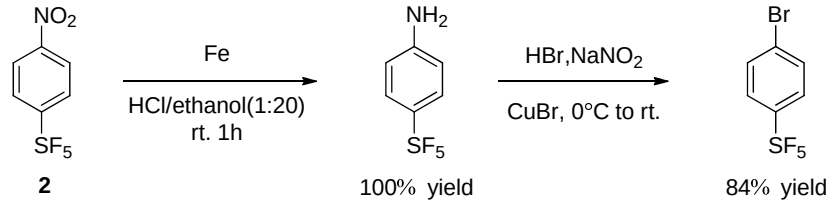
7) Kinetic Isotope Effects Study.

Two sets of reactions were carried out in a parallel manner, in each case 3-bromoanisole was allowed to react with **1** and *d*-**1** respectively.



Experimental Procedure：A 25 mL Schlenk tube equipped with a magnetic stir bar was charged with $(allylPdCl)_2$ (2.5 mol%), PCy_3HBF_4 (7.5 mol%), and K_2CO_3 (1.8 equiv.). The reaction tube was evacuated and backfilled with N_2 (4 times), then 2,2-dimethylbutyric acid (0.3 equiv), 3-bromoanisole (1.5 equiv), toluene (0.5 mL) and (**1** or *d*-**1**) (0.1 mmol, 1.0 equiv) were added subsequently. The sealed tube was screw capped and heated in oil bath of 130 ℃ for 40 min. The reaction vessel was then quenched to room temperature by ice bath, and the yield was analyzed by GC.

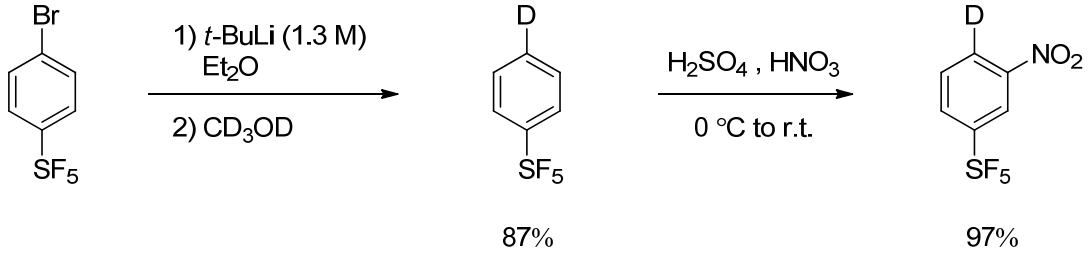
Preparation of *d*-1：



1-Amino-4-pentafluorosulfanylbenzene.[2] To a stirred solution of **2** (1.25 g, 5 mmol) in ethanol (50 mL) was added Fe powder (1.73 g), followed by the slow addition of concentrated hydrochloric acid (2.5 mL) at 0 ℃. After the reaction mixture was stirred for 1 h at room temperature, the reaction was poured into ice water and neutralized with sodium carbonate until alkaline, then extracted with dichloromethane (3×20 mL). The combined extracts were dried over anhydrous Na_2SO_4, filtered, concentrated *in vacuo* and purified by column chromatography (silica gel, 10% dichloromethane in hexane) to give the product (1.096 g, 100% yield) as a white solid.

1-Bromo-4-pentafluorosulfanylbenzene.[2] To a stirred solution of 1-amino-4-pentafluorosulfanylbenzene (1.096 g, 5 mmol) in CH_3CN (5 mL) was slowly added aqueous HBr (40%) (2.5 mL), followed by the slow addition of $NaNO_2$ (380 mg) in water (2.2 mL) between -30 ℃ – -25 ℃. The reaction mixture was continually stirred for 30 min between -30 ℃ – -25 ℃. CuBr (1.09 g) was slowly added to this reaction mixture and then stirred for overnight at room temperature. After that, the reaction was quenched by slow addition of ice water (15 mL) and neutralized with sodium carbonate until alkaline, then extracted with dichloromethane (3×20 mL).

The combined extracts were dried over anhydrous Na_2SO_4, filtered, concentrated *in vacuo* and purified by column chromatography (silica gel, hexane) to give the product (1.18 g, 83% yield) as a slightly yellow oil.



4-Deuterio-pentafluorosulfanylbenzene. In N_2 atmosphere, to a stirred solution of 1-bromo-4-pentafluorosulfanylbenzene (56 μL, 0.35 mmol, 1 equiv.) in anhydrous diethyl ether (2 mL) was slowly added *t*-BuLi (0.4 mL, 1.3 M, 1.5 equiv.) at about -70 ˚C, and was continually stirred for 1 h at the same low temperature. After that, the reaction mixture was quenched by slow addition of CH_3OD (0.5 mL) at about -40 ˚C, then extracted with EtOAc (3×5 mL). The combined extracts were dried over anhydrous Na_2SO_4, filtered, concentrated *in cacuo* and purified by column chromatography (silica gel, 5% dichloromethane in hexane) to give the product (63 mg, 87% yield) as a colorless oil.

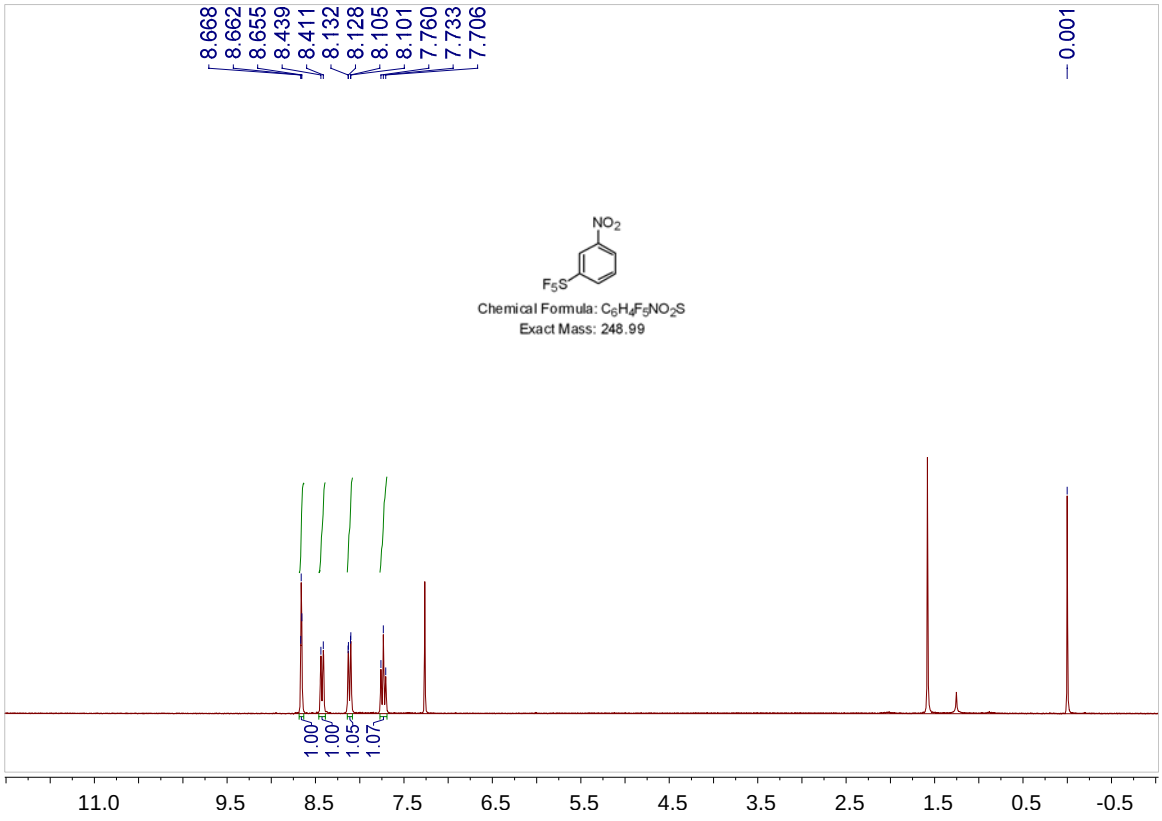
4-Deuterio-3-nitro-pentafluorosulfanylbenzene (*d*-1). To a stirred solution of 4-Deuterio-pentafluorosulfanylbenzene (62 mg, 0.3 mmol), concentrated H_2SO_4 (1.0 mL), and ten drops of trifluoroacetic acid, was added the mixture of concentrated H_2SO_4 (0.5 mL) and 60% of HNO_3 (1.0 mL) at 0 ˚C, after stirred for 2 h at the same temperature, the same mixture of concentrated H_2SO_4 (0.5 mL) and 60% of HNO_3 (1.0 mL) were refilled. After that, the reaction mixture was quenched by poured into ice water, then extracted with dichloromethane (3×5 mL). The combined extracts were dried over anhydrous Na_2SO_4, filtered, concentrated *in cacuo* and purified by column chromatography (silica gel, 3% of dichloromethane in hexane) to give the product (73 mg, 97% yield, the purity of *d*-**1** is 96% by ^{1}H NMR) as a slightly yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, J = 1.8 Hz, 1H), 8.11 (dd, J = 8.2, 1.9 Hz, 1H), 7.73 (d, J = 8.2 Hz, 1H); ^{19}F NMR (376 MHz, $CDCl_3$) δ 81.09 (p, J = 151 Hz, SF_{ax}, 1F), 62.82 (d, J = 151 Hz, 4F);

8) References

(1) Roy D. Bowden, Paul J. Comina, Martin P. Greenhall, Benson M. Kariuki, Amanda Loveday, Douglas Philp. *Tetrahedron*, **2000**, *56*, 3399-3408

(2) John T. Welch and Dong Sung Lim, *Bioorganic & Medicinal Chemistry*, **2007**, *15*, 6659-6666.

Compound 1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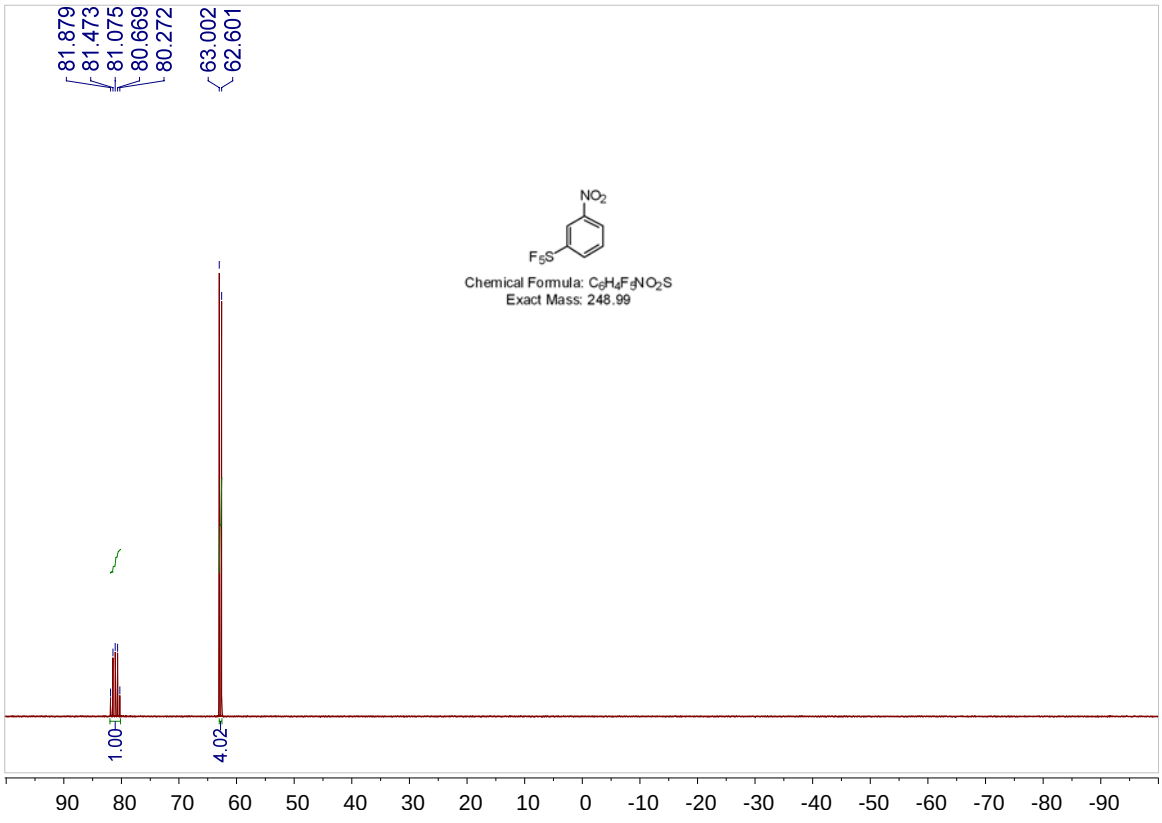
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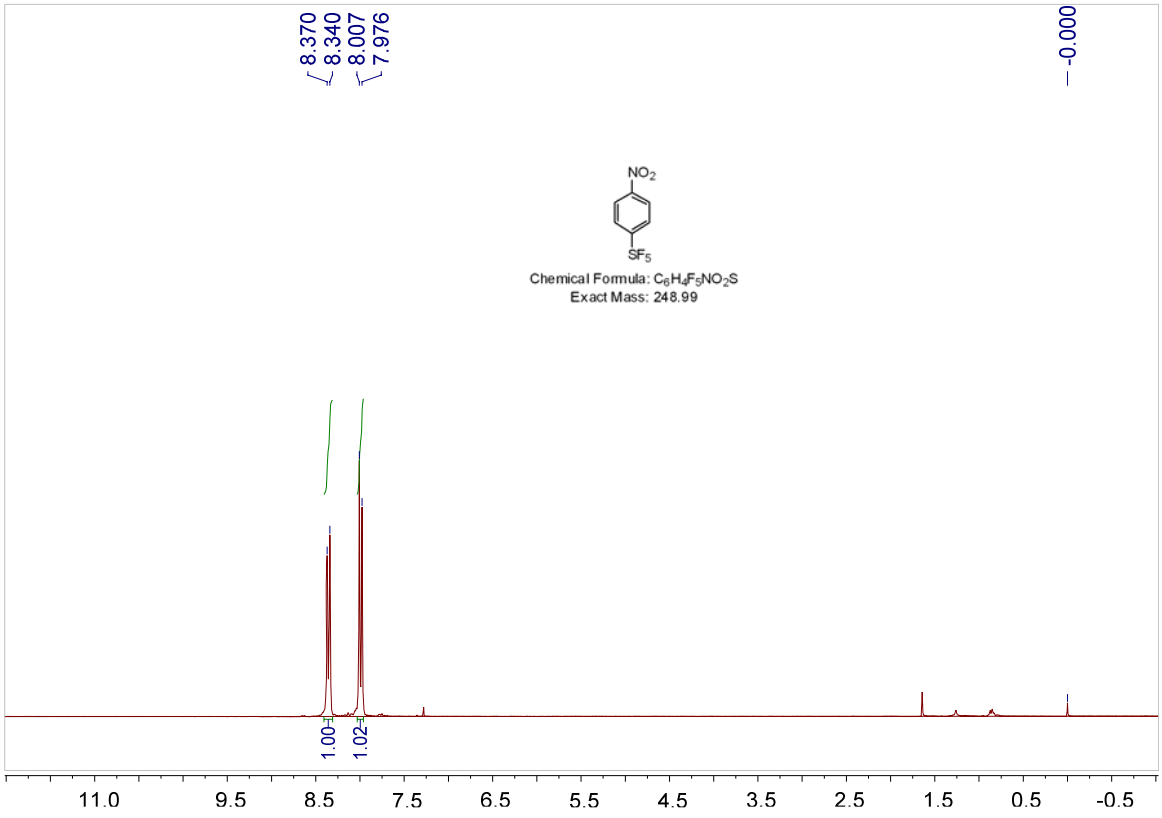
Compound 2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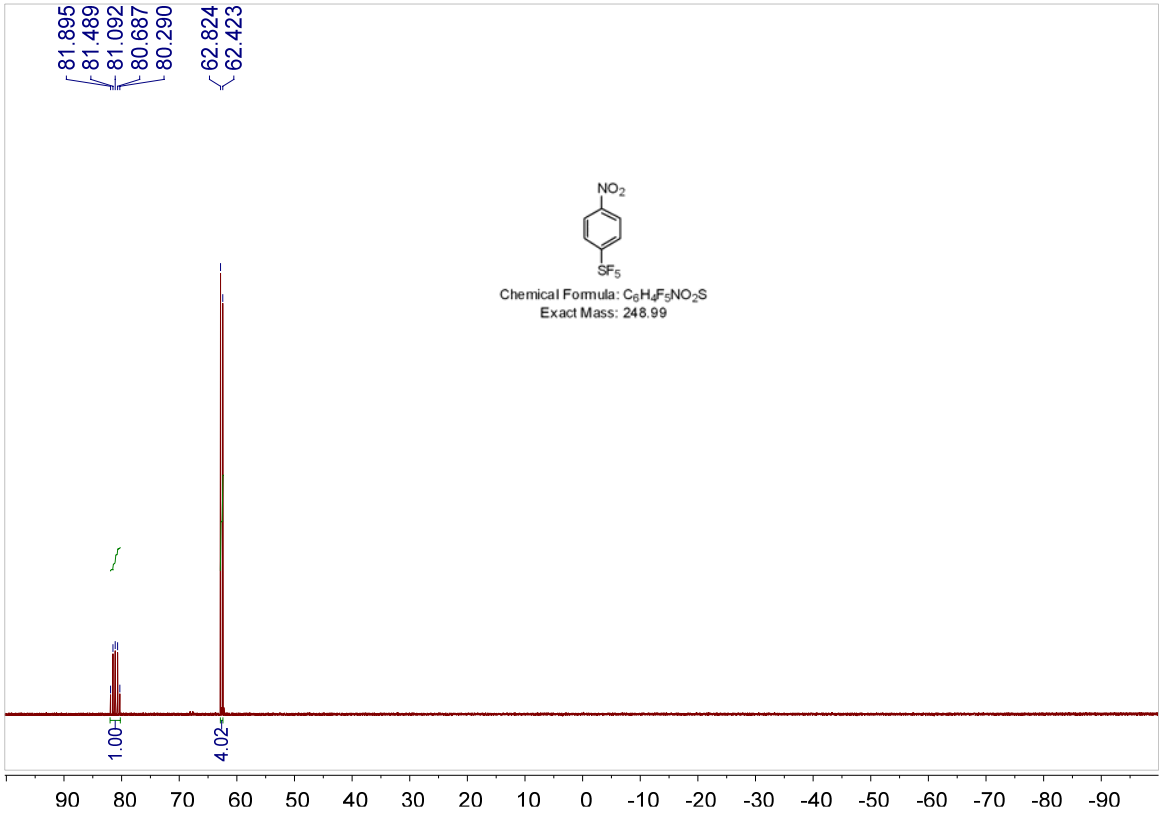
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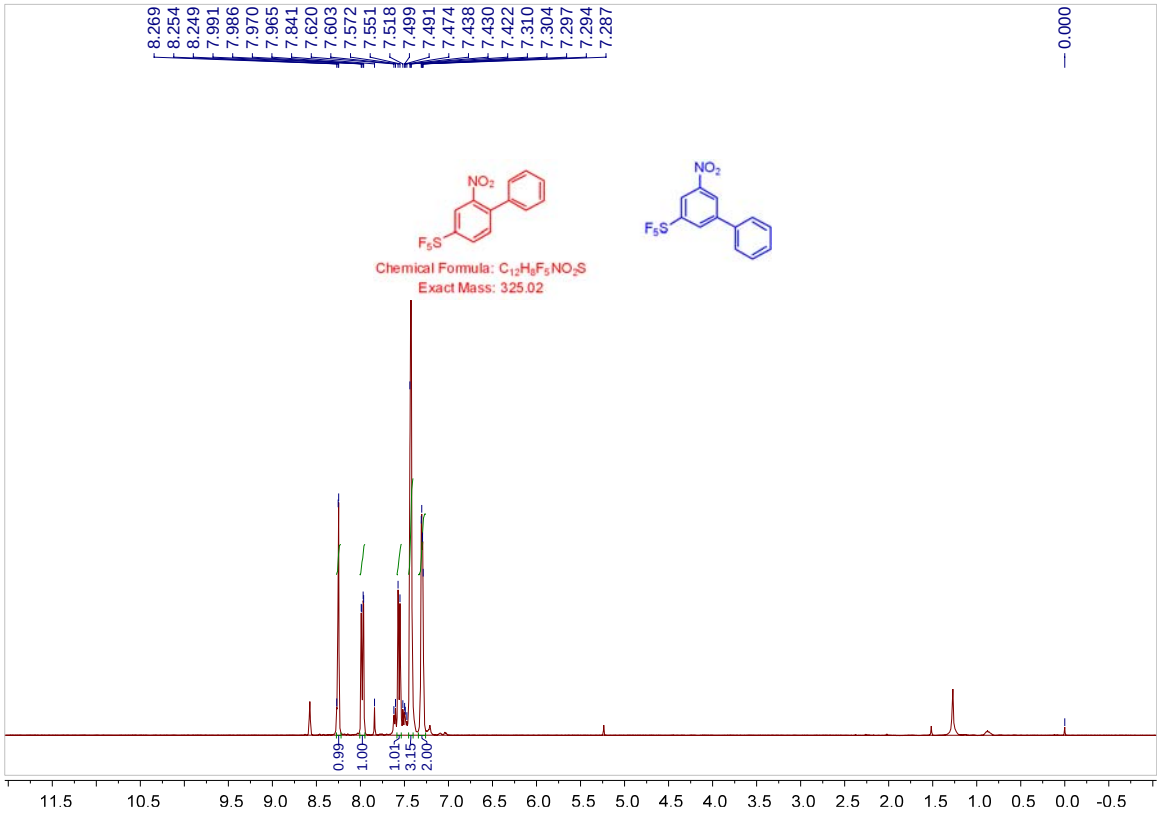
Compound 5a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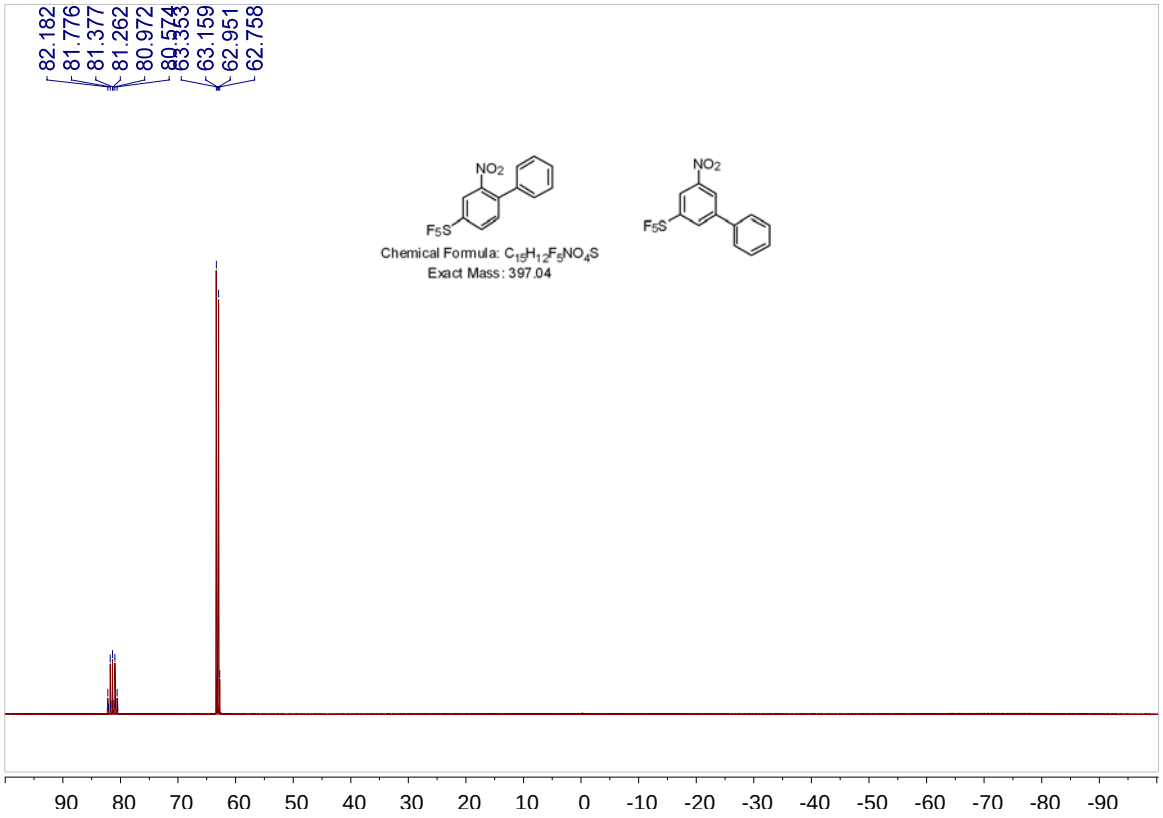
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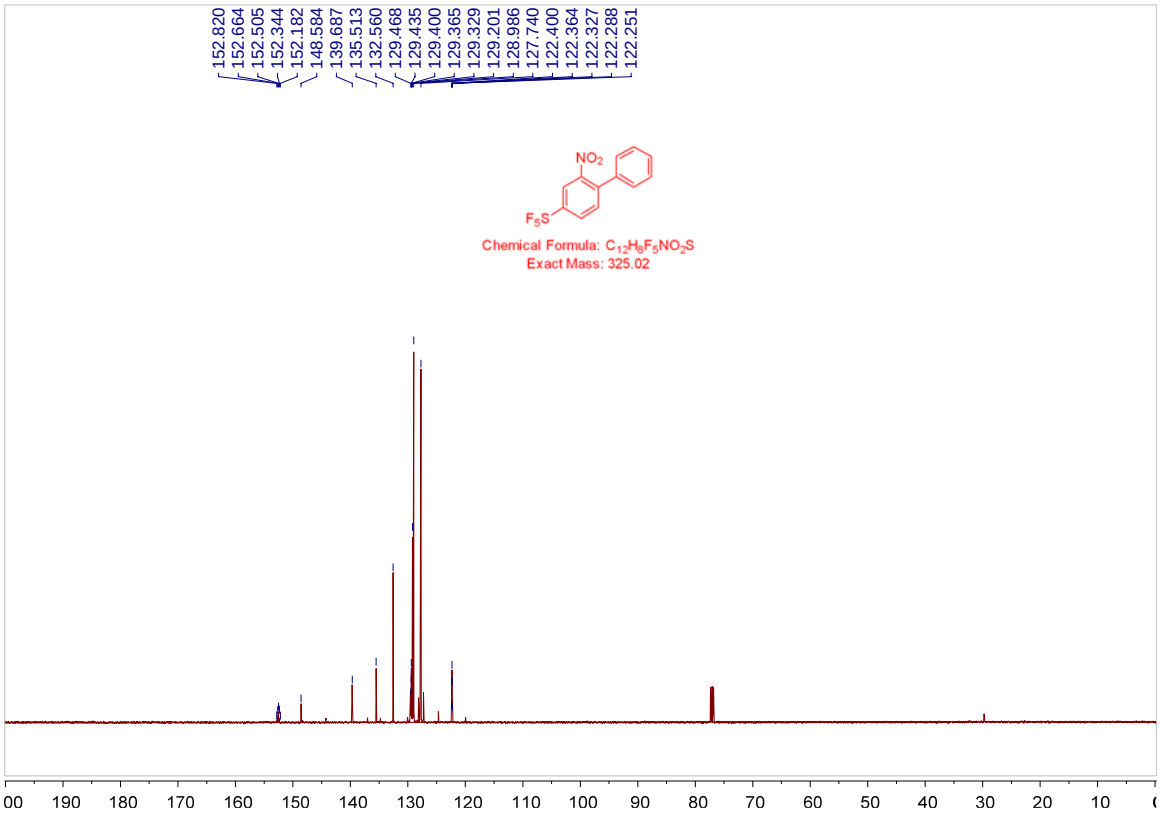
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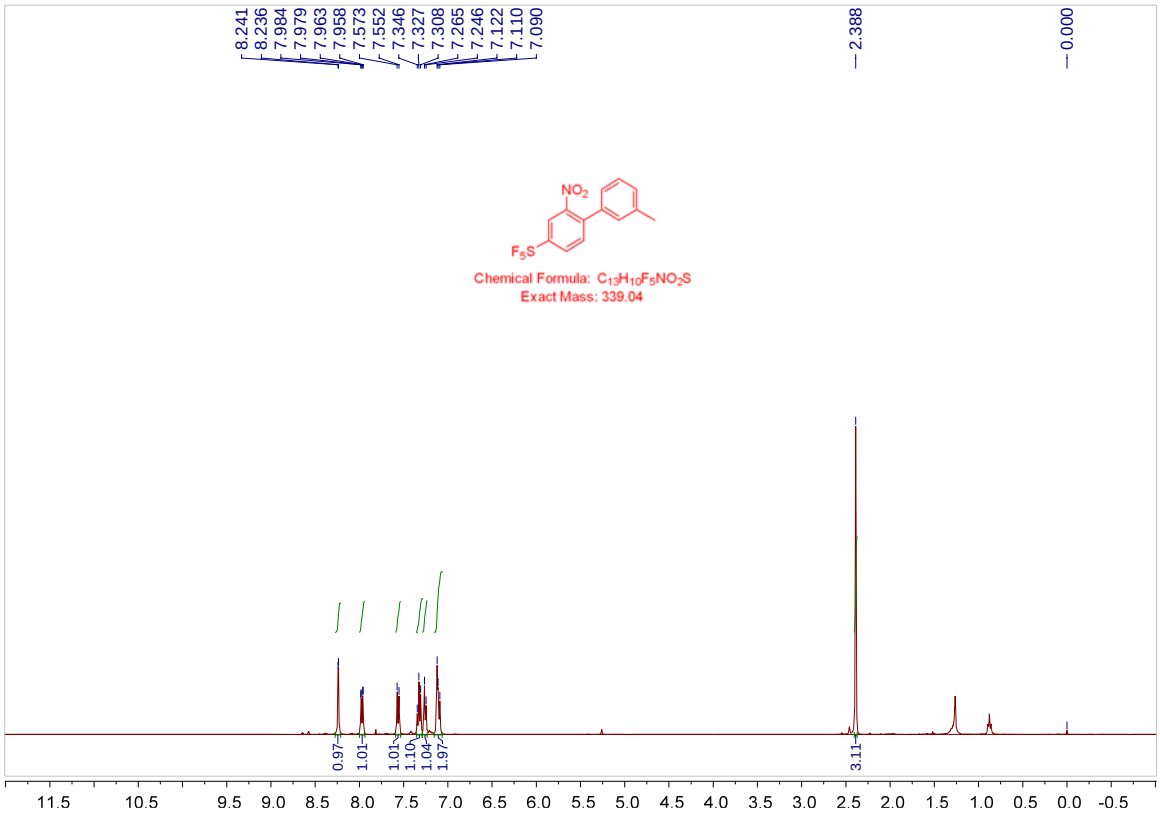
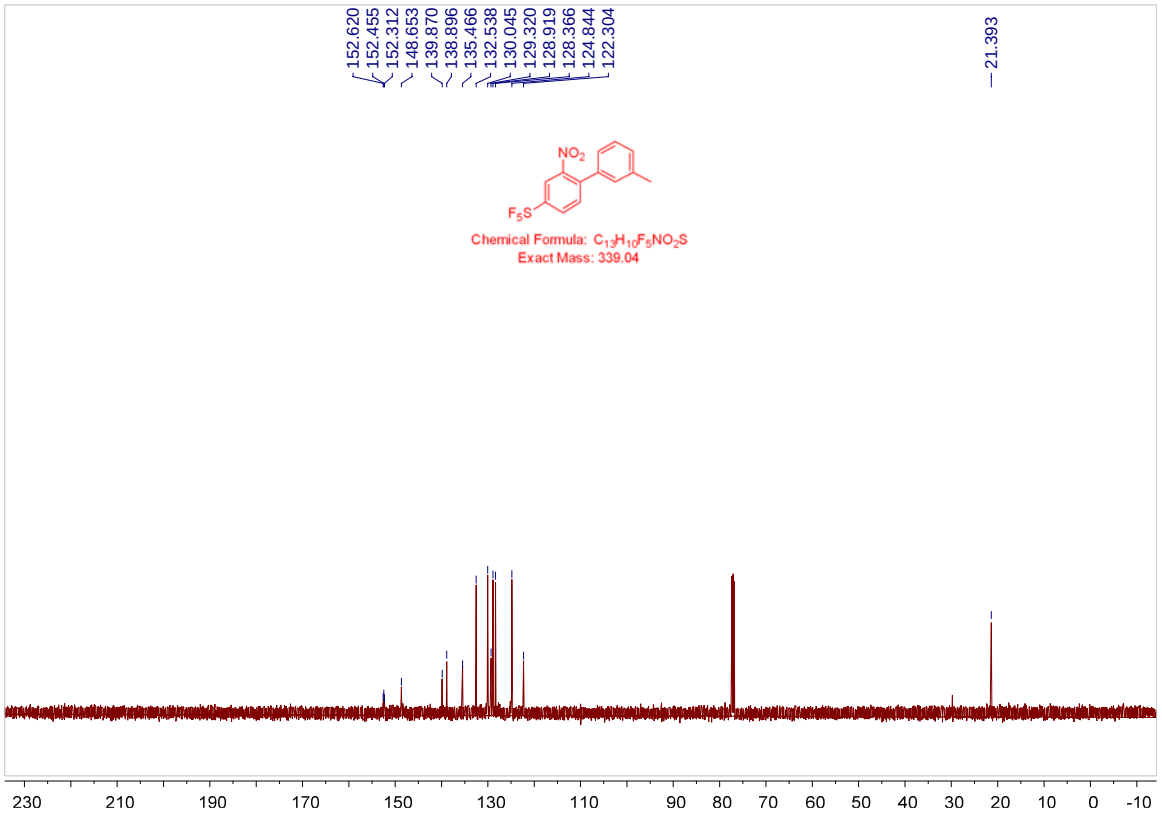
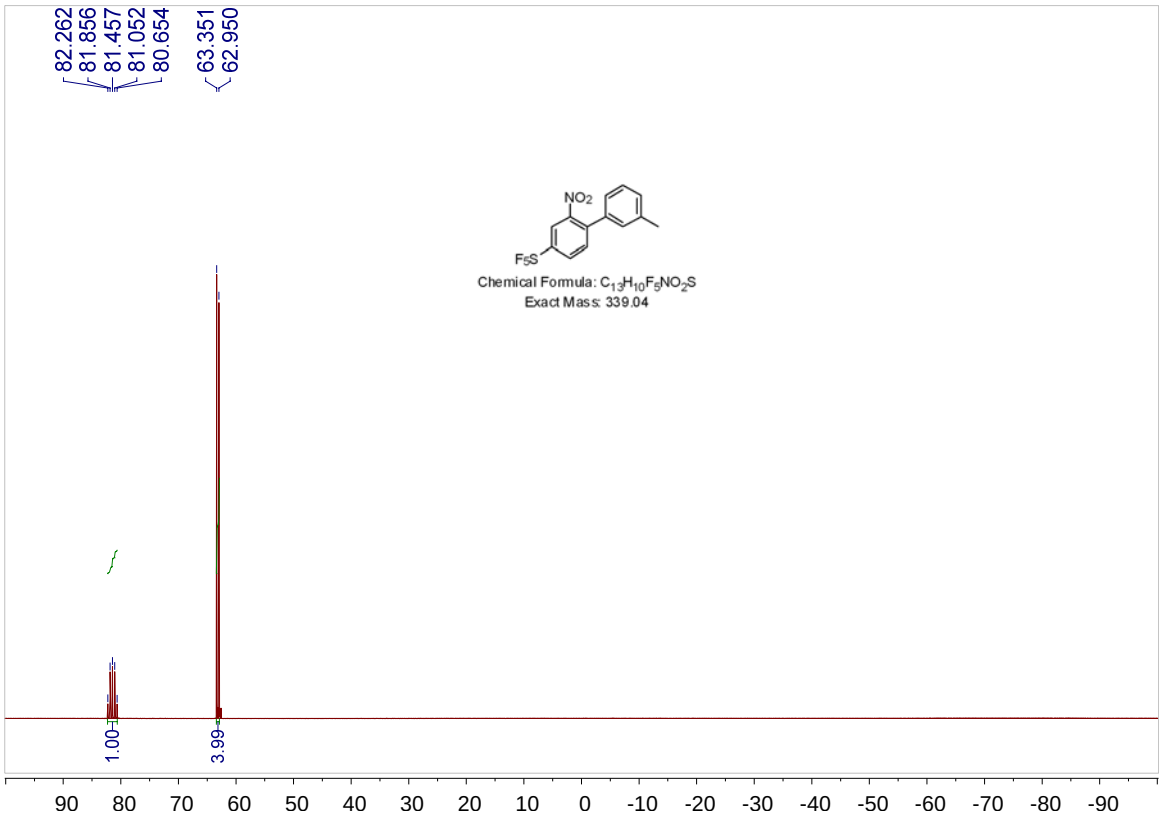
129.329
129.201
128.986
127.740
122.400
122.364
122.327
122.288
122.251
NO2
F5S
Chemical Formula: C12H6F5NO2S
Exact Mass: 325.02

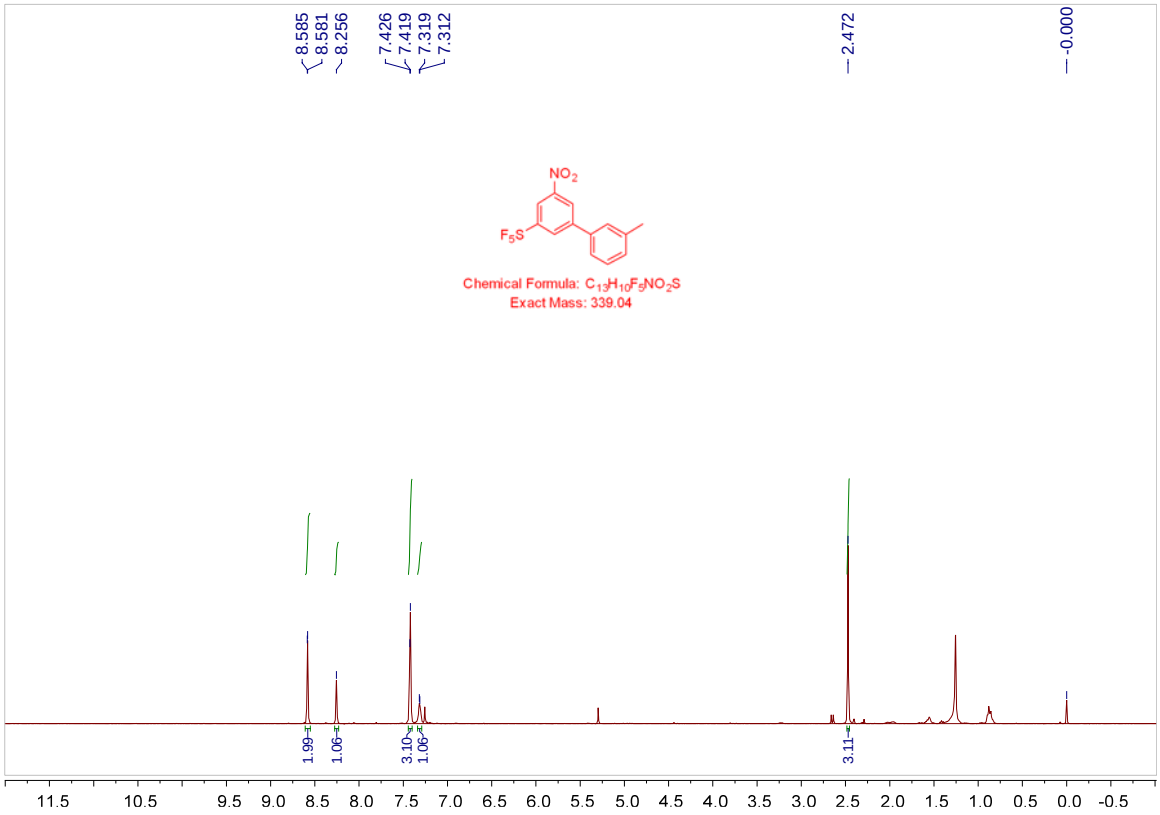
Compound 5b


8.241
8.236
7.984
7.979
7.963
7.958
7.573
7.552
7.346
7.327
7.308
7.265
7.246
7.122
7.110
7.090
2.388
0.000
NO2
F5S
Chemical Formula: C13H10F5NO2S
Exact Mass: 339.04
0.97
1.01
1.01
1.10
1.04
1.97
3.11

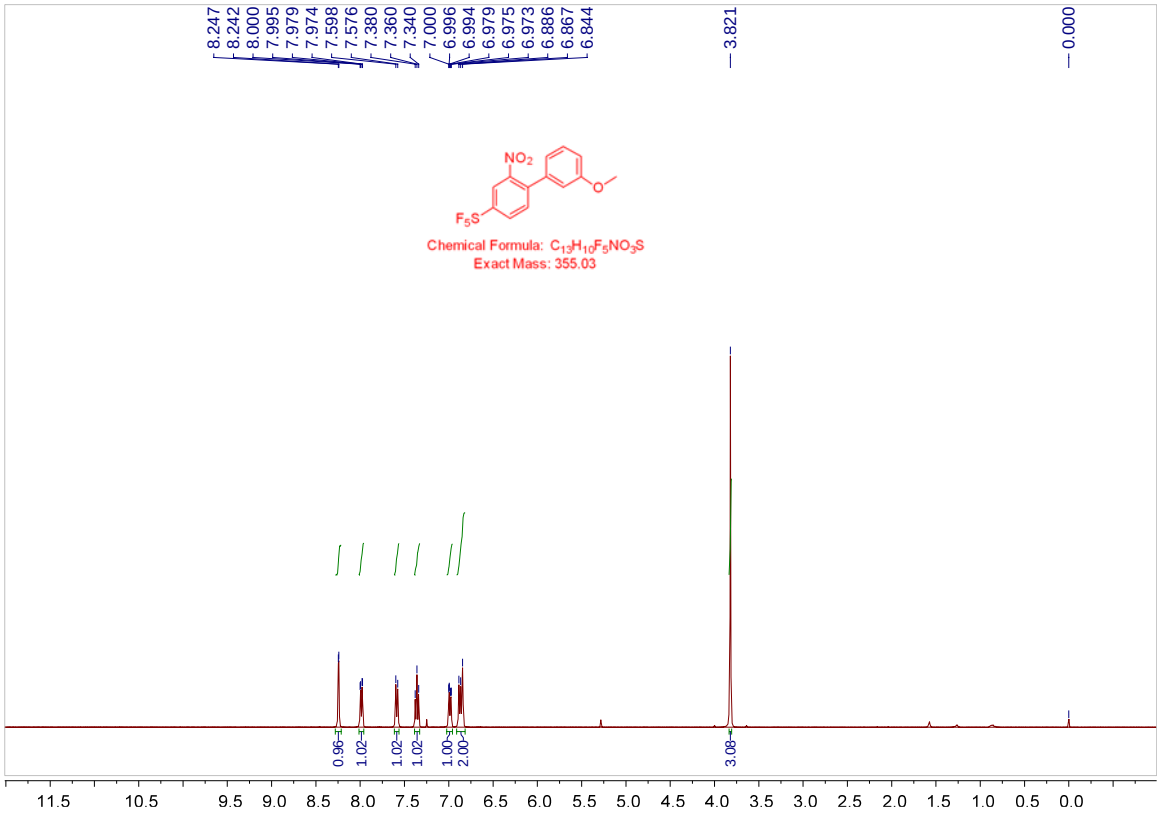

152.620
152.455
152.312
148.653
139.870
138.896
135.466
132.538
130.045
129.320
128.919
128.366
124.844
122.304
21.393
NO2
F5S
Chemical Formula: C13H10F5NO2S
Exact Mass: 339.04
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10

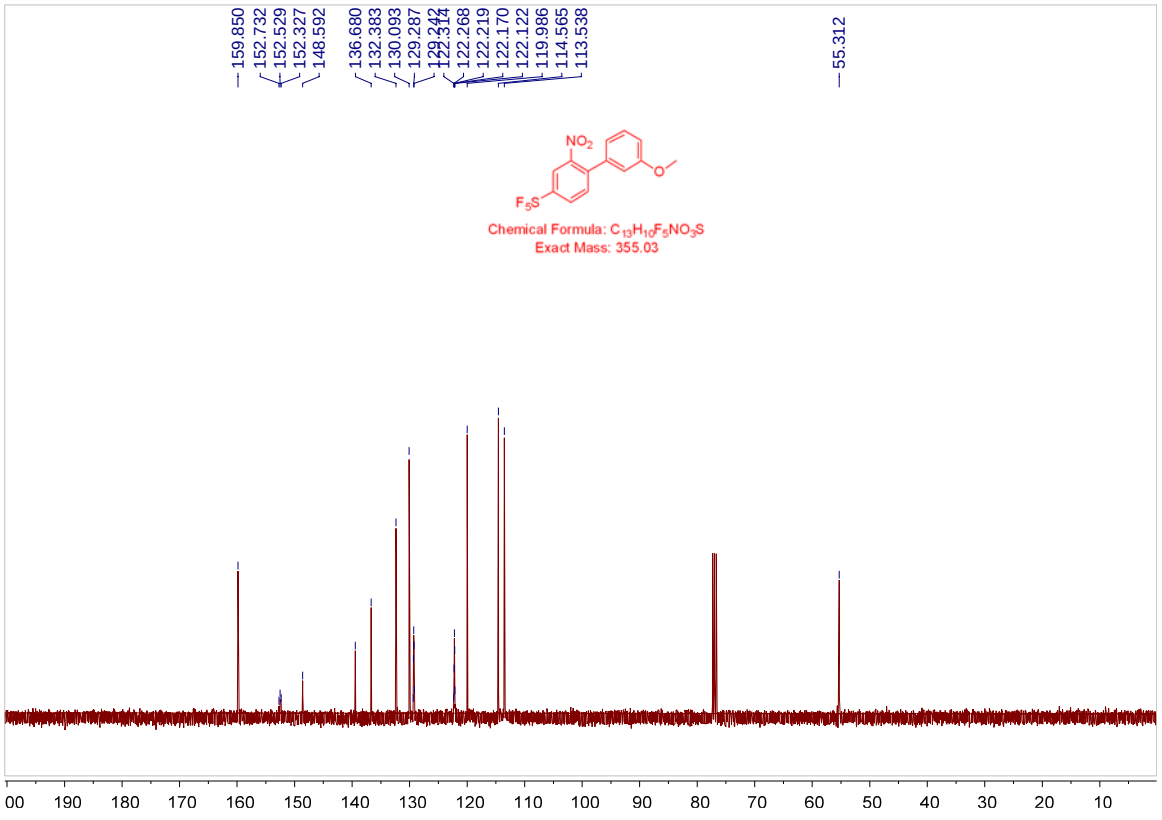

82.262
81.856
81.457
81.052
80.654
63.351
62.950
NO2
F5S
Chemical Formula: C13H10F5NO2S
Exact Mass: 339.04
1.00
3.99
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90

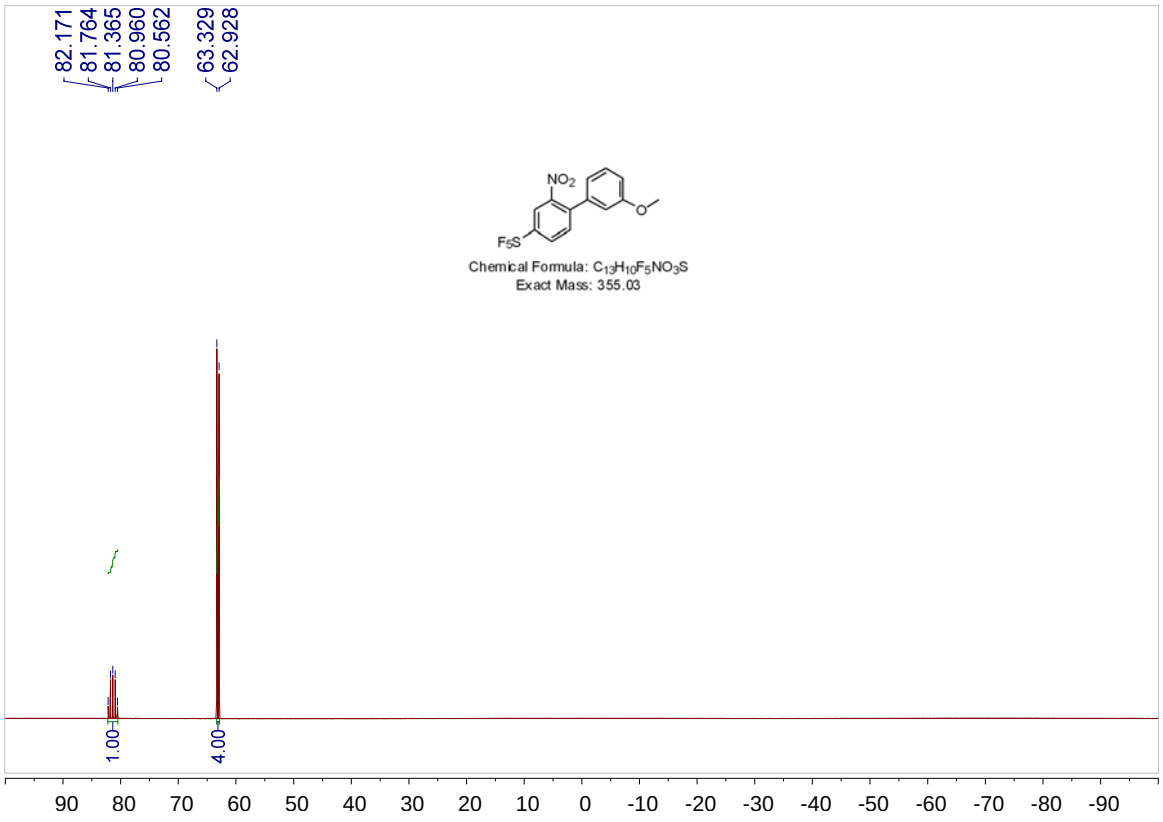
Compound 4b



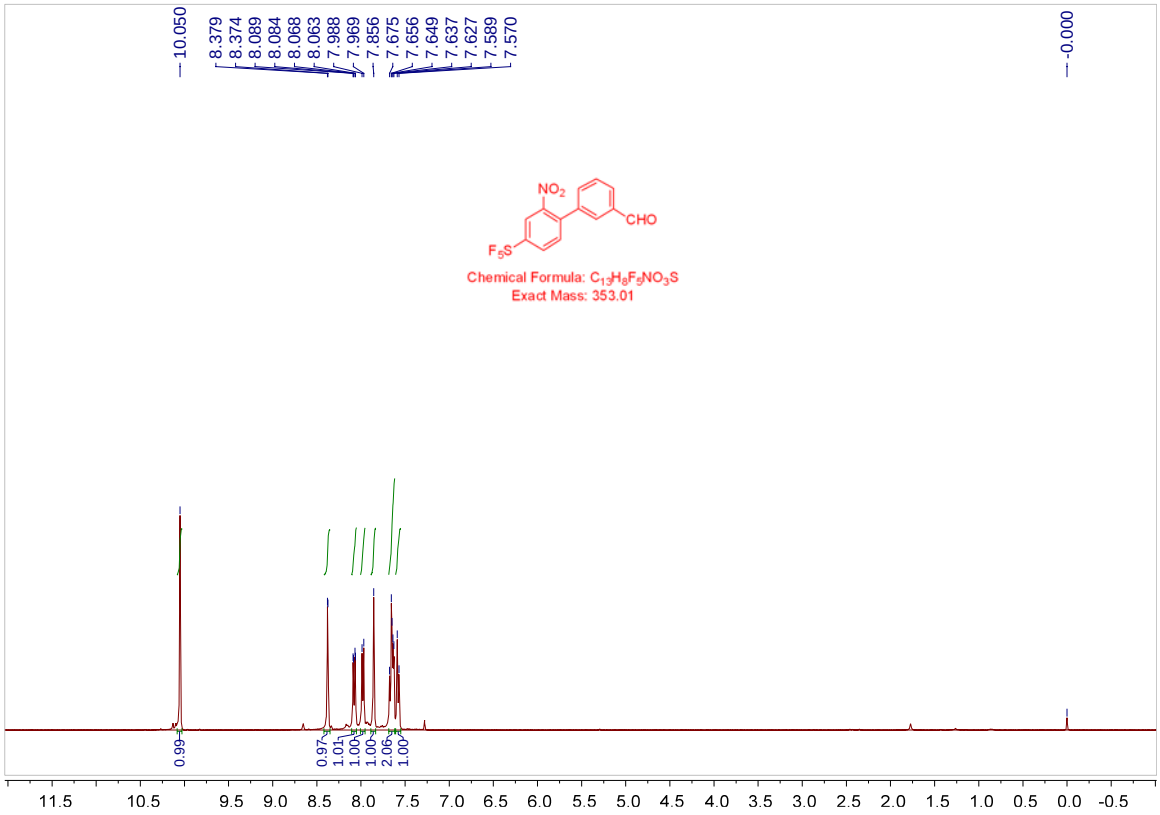
Compound 5c

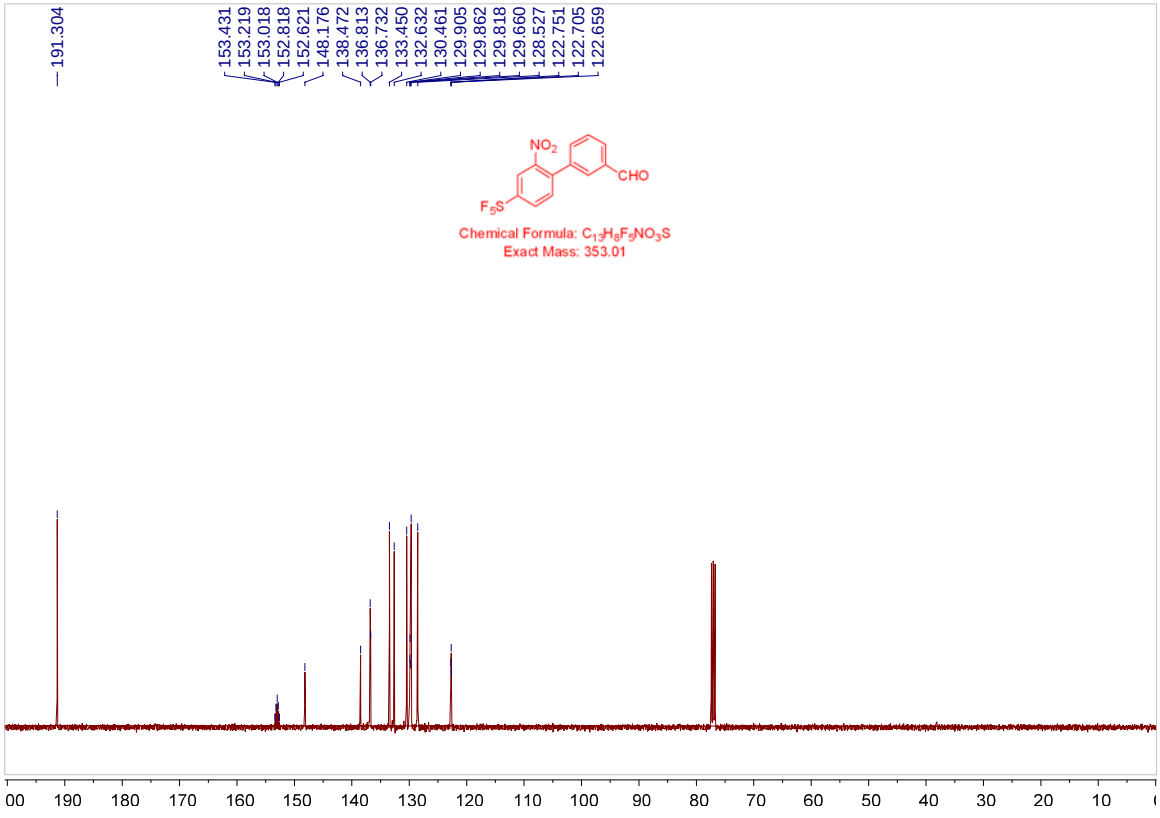


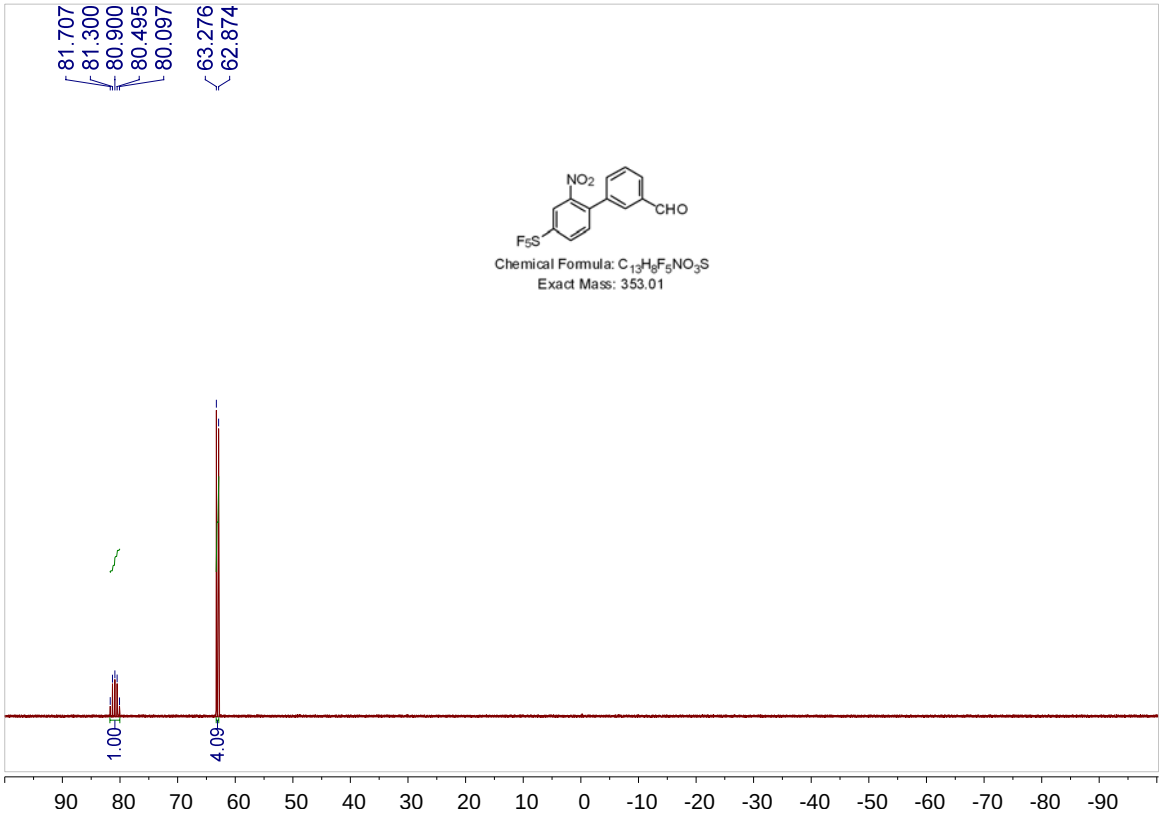

159.850
152.732
152.529
152.327
148.592
136.680
132.383
130.093
129.287
122.268
122.219
122.170
122.122
119.986
114.565
113.538
55.312
NO2
F5S
Chemical Formula: C13H10F5NO3S
Exact Mass: 355.03
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10


82.171
81.764
81.365
80.960
80.562
63.329
62.928
NO2
F5S
Chemical Formula: C13H10F5NO3S
Exact Mass: 355.03
1.00
4.00
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90

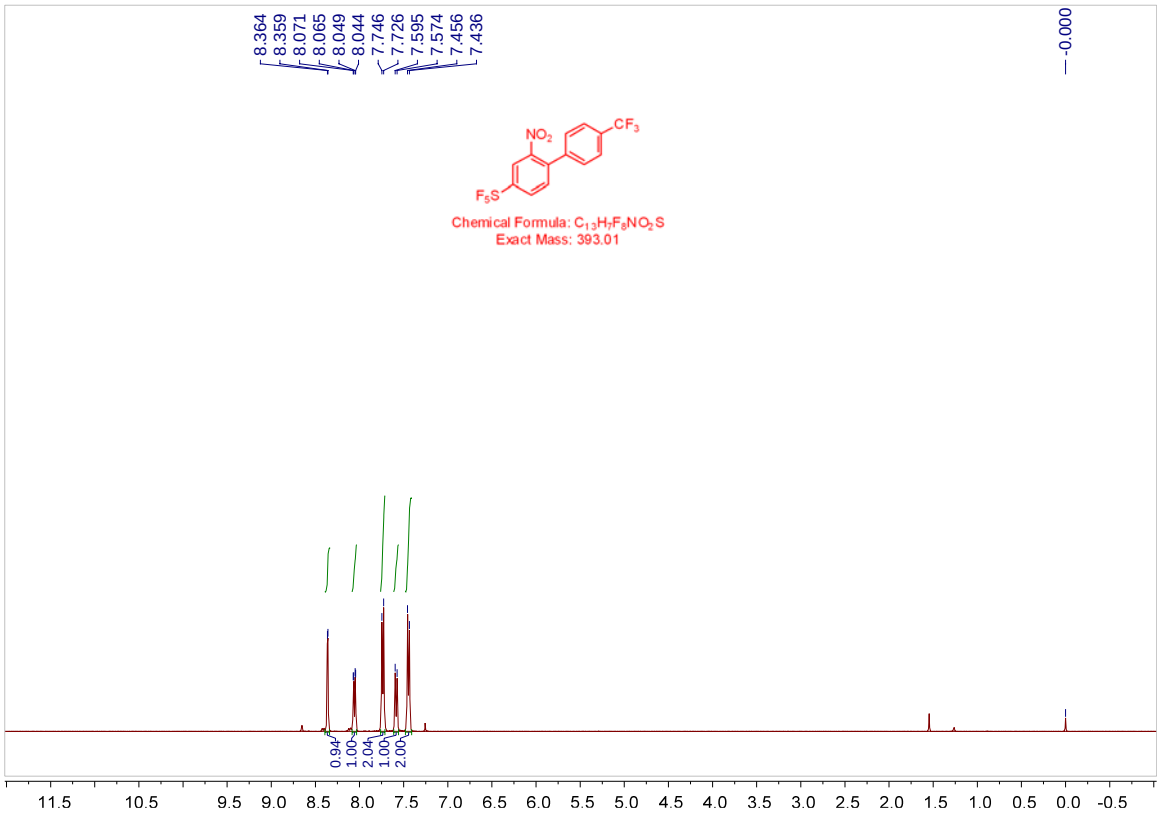
Compound 5d

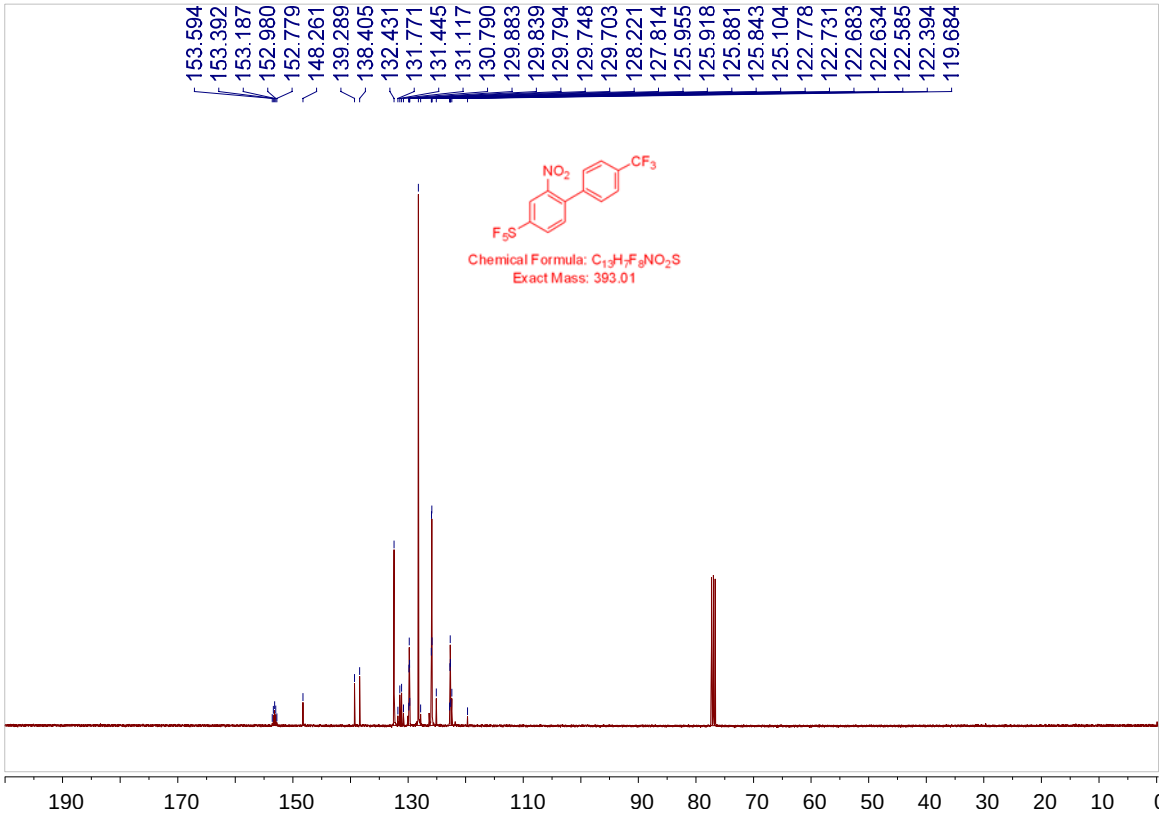

10.050
8.379
8.374
8.089
8.084
8.068
8.063
7.988
7.969
7.856
7.675
7.656
7.649
7.637
7.627
7.589
7.570
-0.000
NO2
CHO
F5S
Chemical Formula: C13H8F5NO3S
Exact Mass: 353.01
0.99
0.97
1.01
1.00
1.00
2.06
1.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

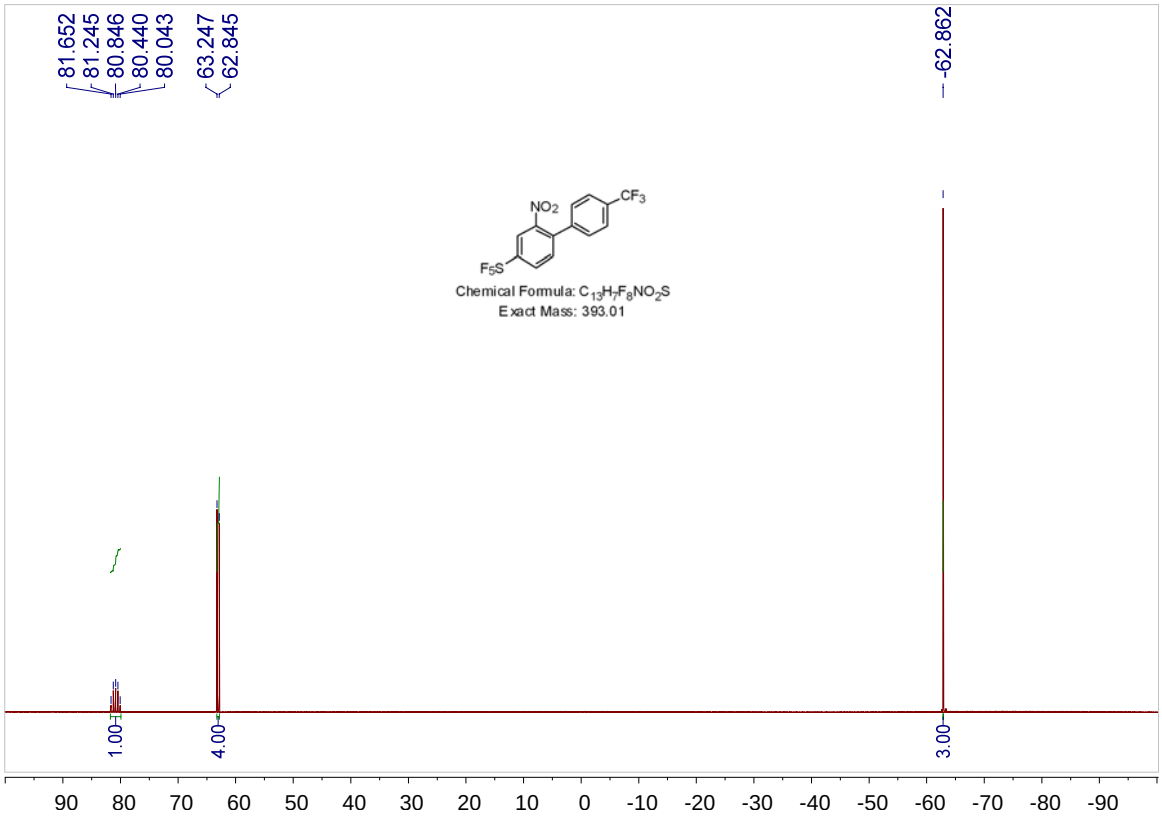

191.304
153.431
153.219
153.018
152.818
152.621
148.176
138.472
136.813
136.732
133.450
132.632
130.461
129.905
129.862
129.818
129.660
128.527
122.751
122.705
122.659
NO2
CHO
F5S
Chemical Formula: C13H8F5NO3S
Exact Mass: 353.01
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


81.707
81.300
80.900
80.495
80.097
63.276
62.874
NO2
CHO
F5S
Chemical Formula: C13H8F5NO3S
Exact Mass: 353.01
1.00
4.09
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90

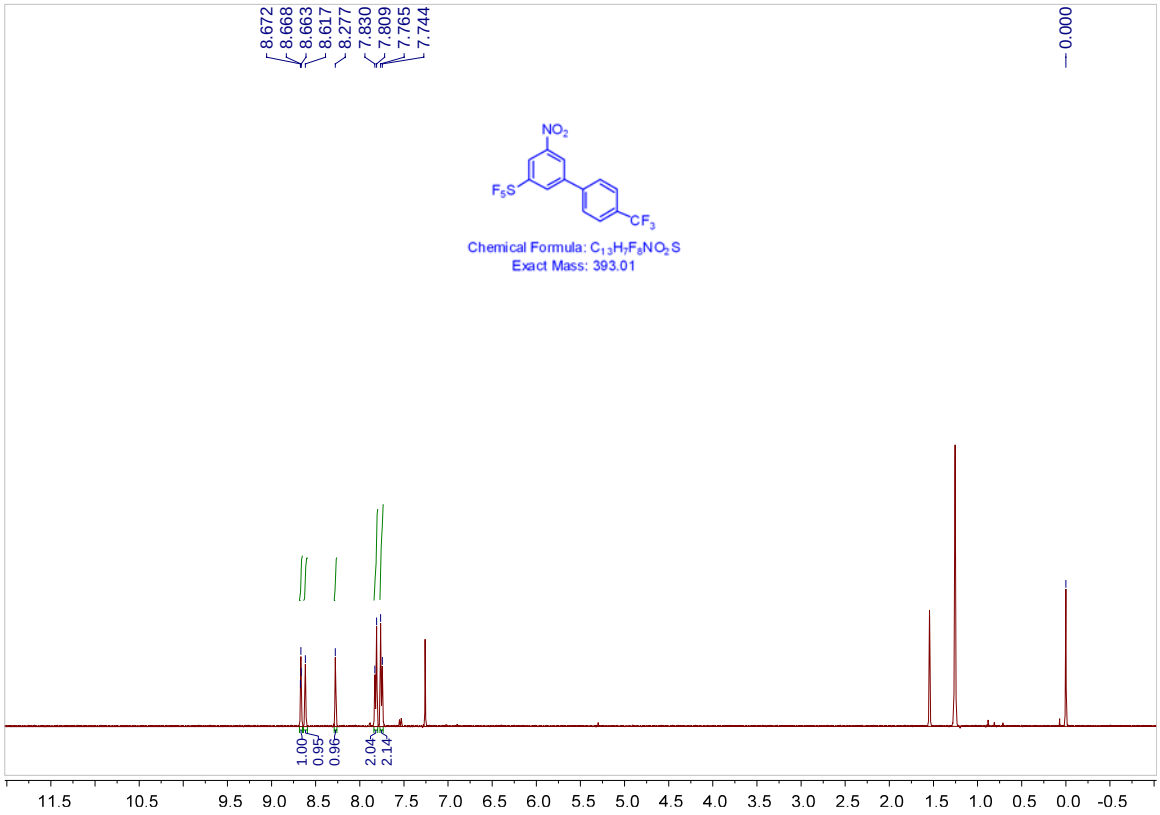
Compound 5e


8.364
8.359
8.071
8.065
8.049
8.044
7.746
7.726
7.595
7.574
7.456
7.436
-0.000
NO2
CF3
F5S
Chemical Formula: C13H7F8NO2S
Exact Mass: 393.01
0.94
1.00
2.04
1.00
2.00
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

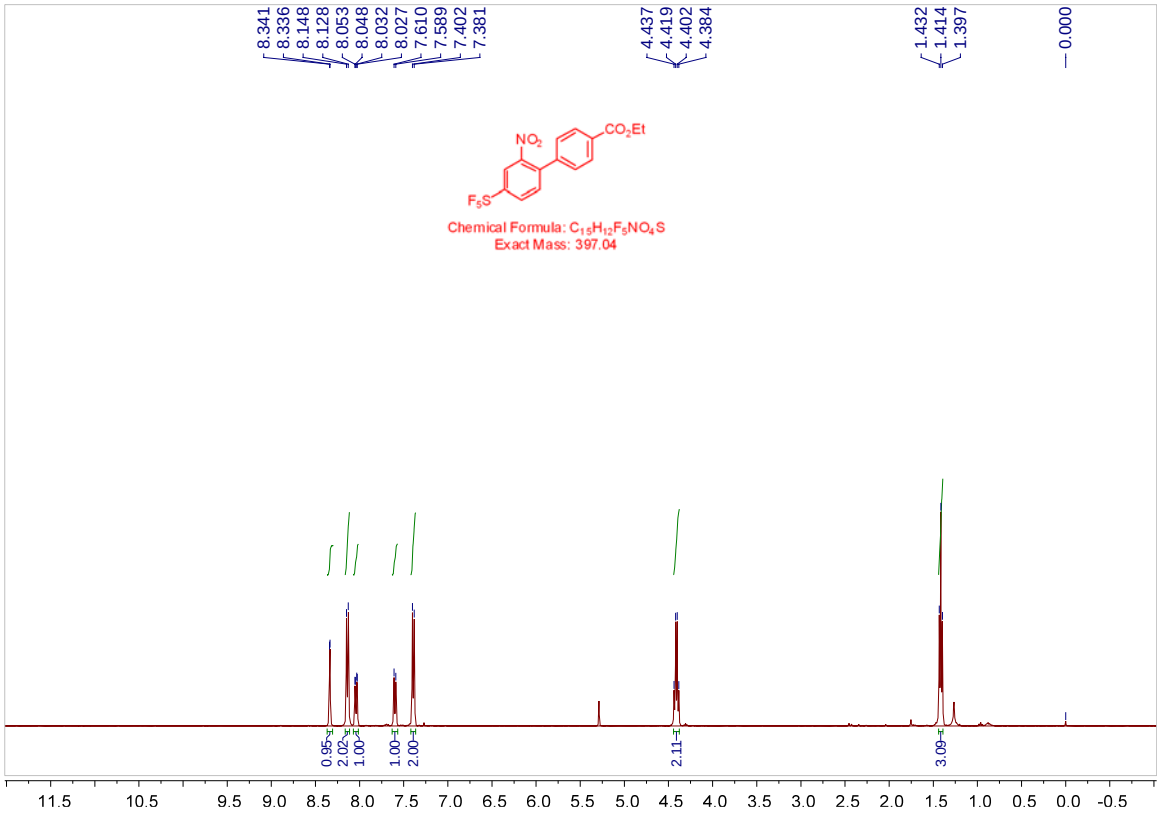

153.594
153.392
153.187
152.980
152.779
148.261
139.289
138.405
132.431
131.771
131.445
131.117
130.790
129.883
129.839
129.794
129.748
129.703
128.221
127.814
125.955
125.918
125.881
125.843
125.104
122.778
122.731
122.683
122.634
122.585
122.394
119.684
NO2
CF3
F5S
Chemical Formula: C13H7F8NO2S
Exact Mass: 393.01
190
170
150
130
110
90
80
70
60
50
40
30
20
10

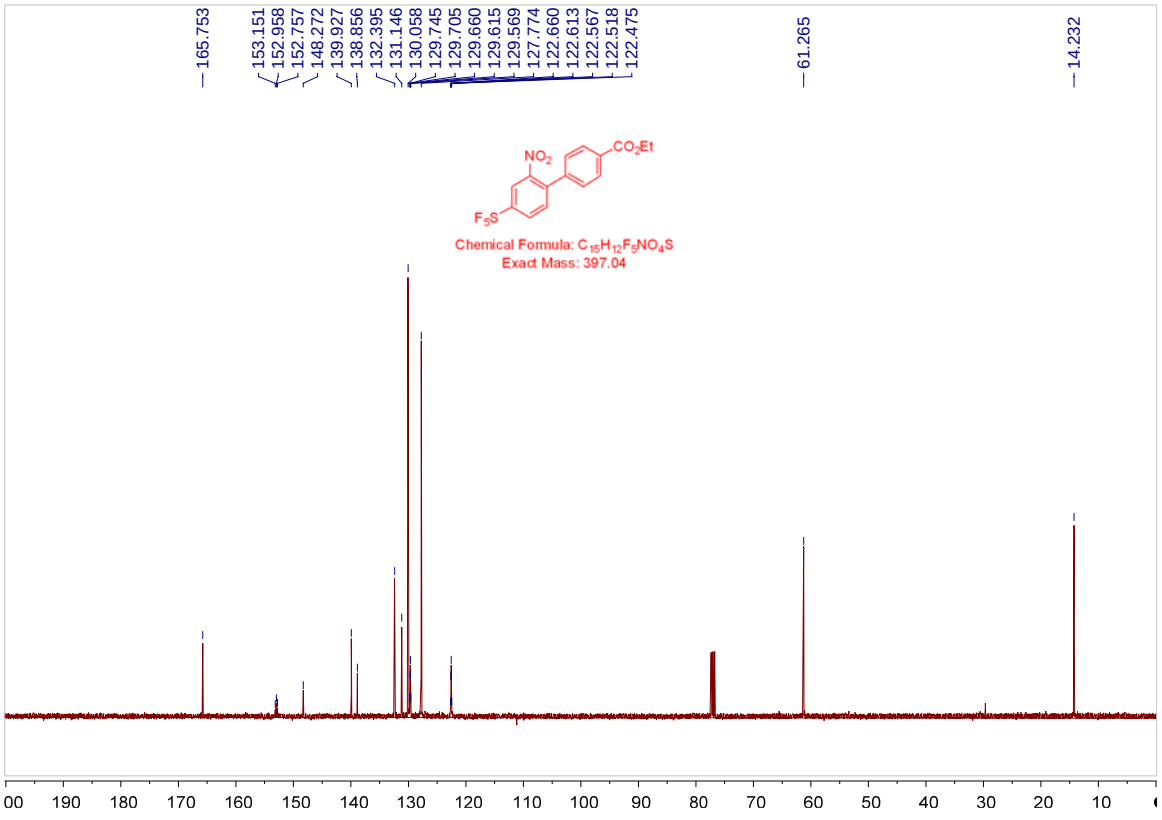

81.652
81.245
80.846
80.440
80.043
63.247
62.845
-62.862
NO2
CF3
F5S
Chemical Formula: C13H7F8NO2S
Exact Mass: 393.01
1.00
4.00
3.00
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90

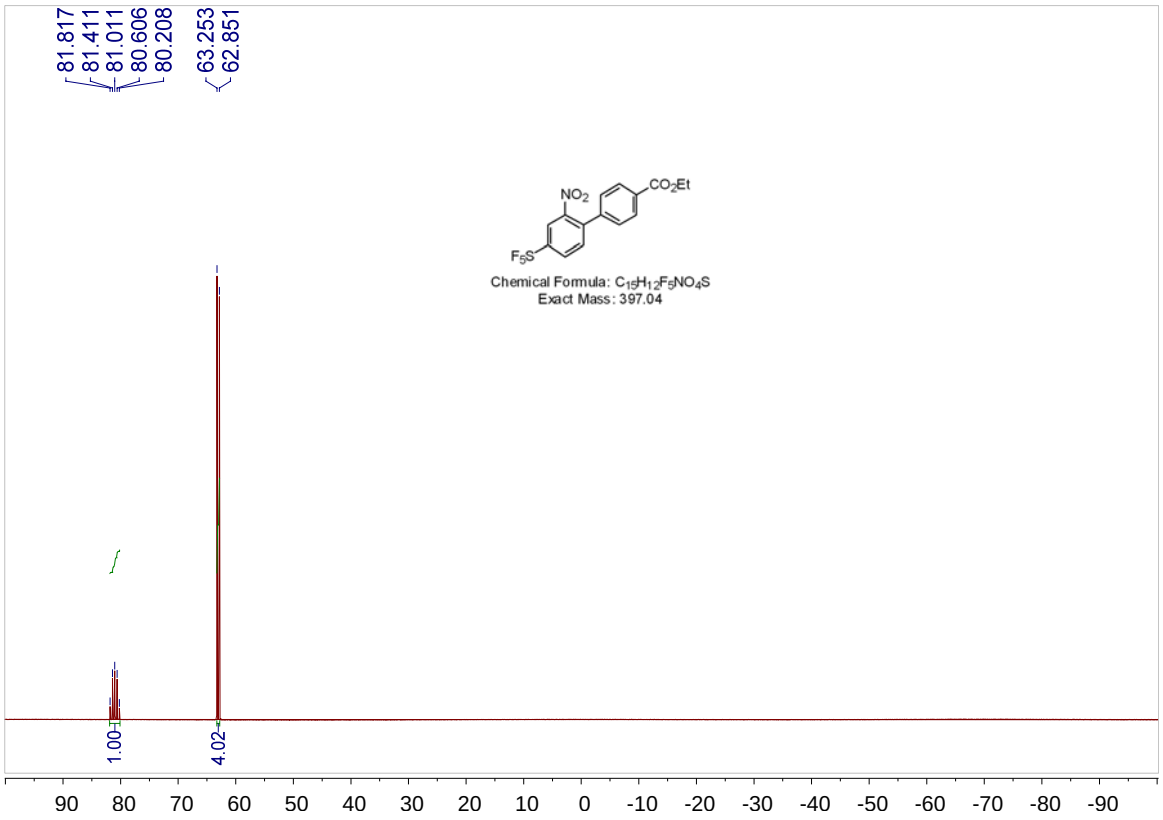
Compound 4e



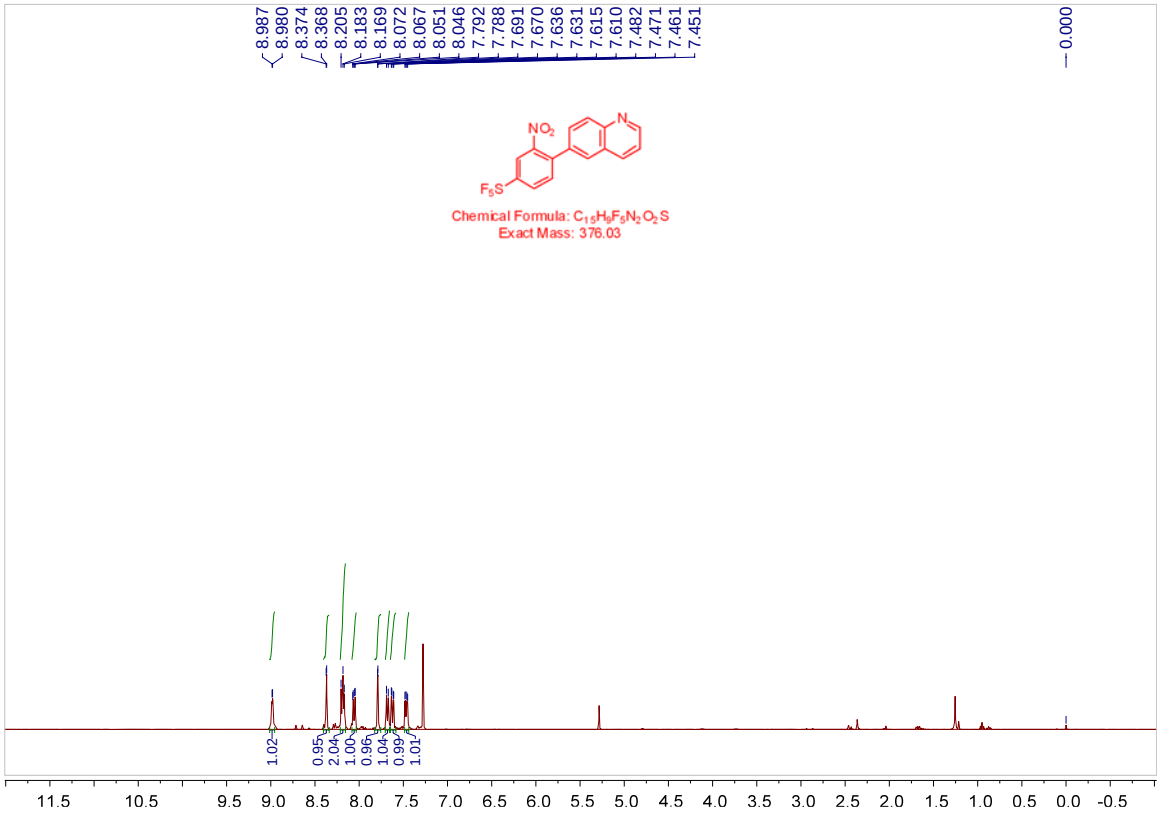
Compound 5f

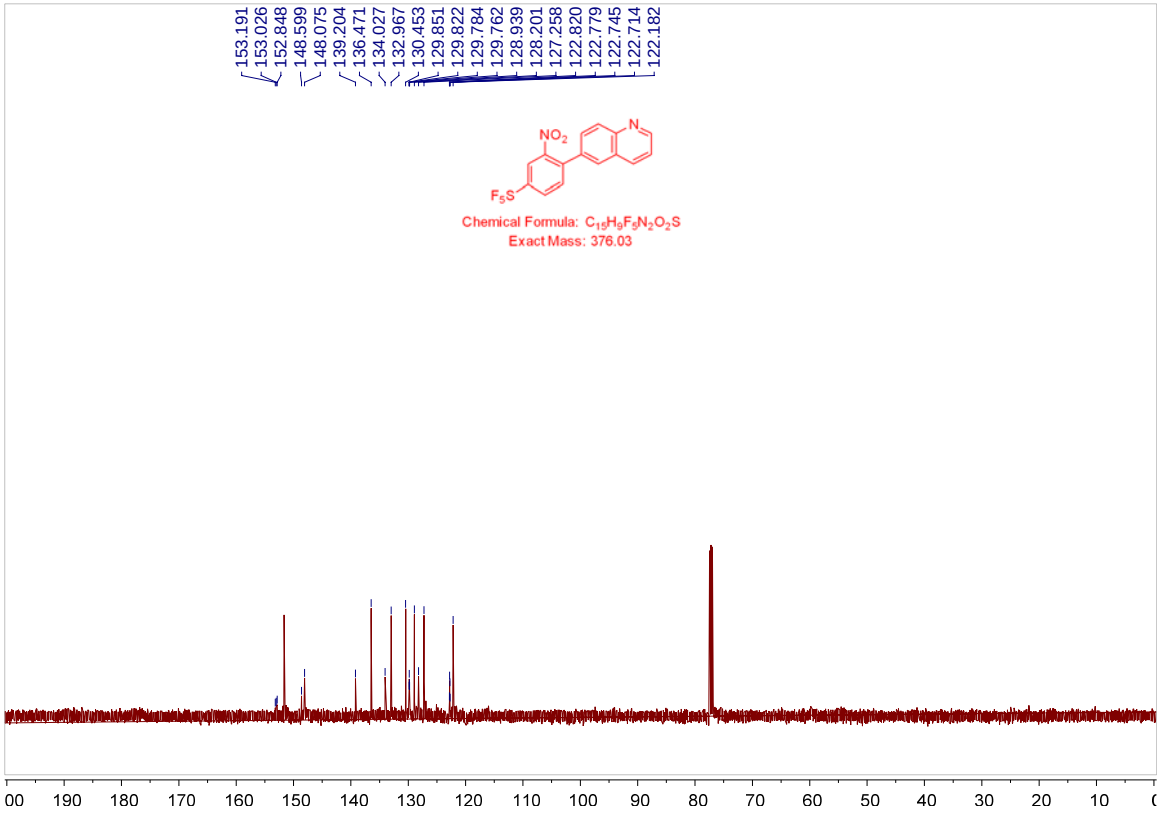


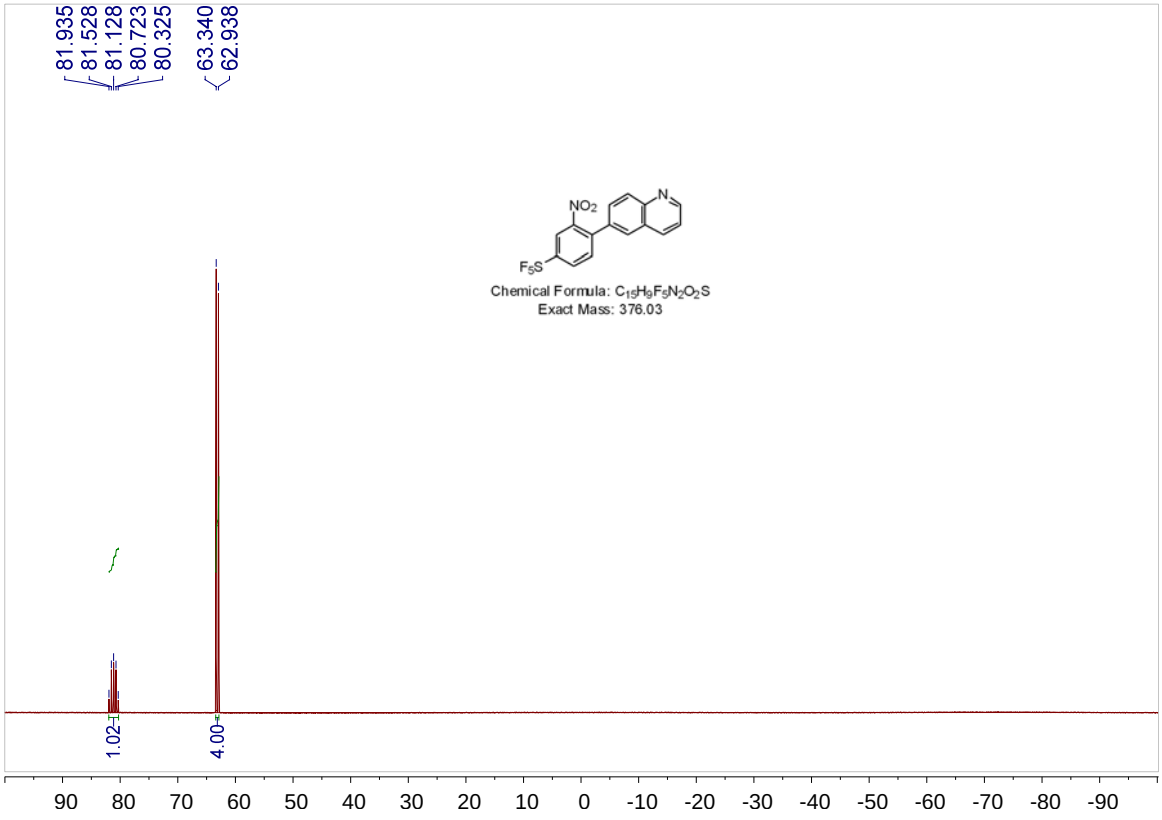

165.753
153.151
152.958
152.757
148.272
139.927
138.856
132.395
131.146
130.058
129.745
129.705
129.660
129.615
129.569
127.774
122.660
122.613
122.567
122.518
122.475
61.265
14.232
NO2
CO2Et
F5S
Chemical Formula: C15H12F5NO4S
Exact Mass: 397.04


81.817
81.411
81.011
80.606
80.208
63.253
62.851
NO2
CO2Et
F5S
Chemical Formula: C15H12F5NO4S
Exact Mass: 397.04
1.00
4.02

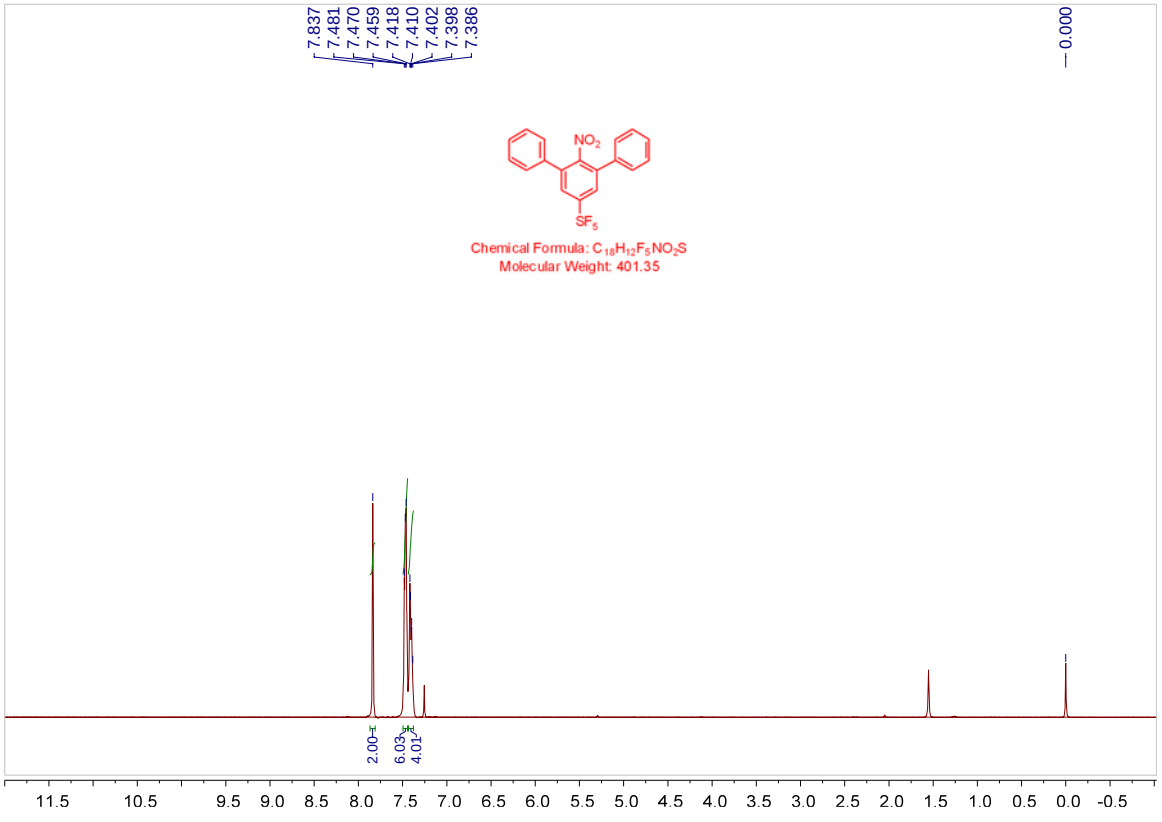
Compound 5g

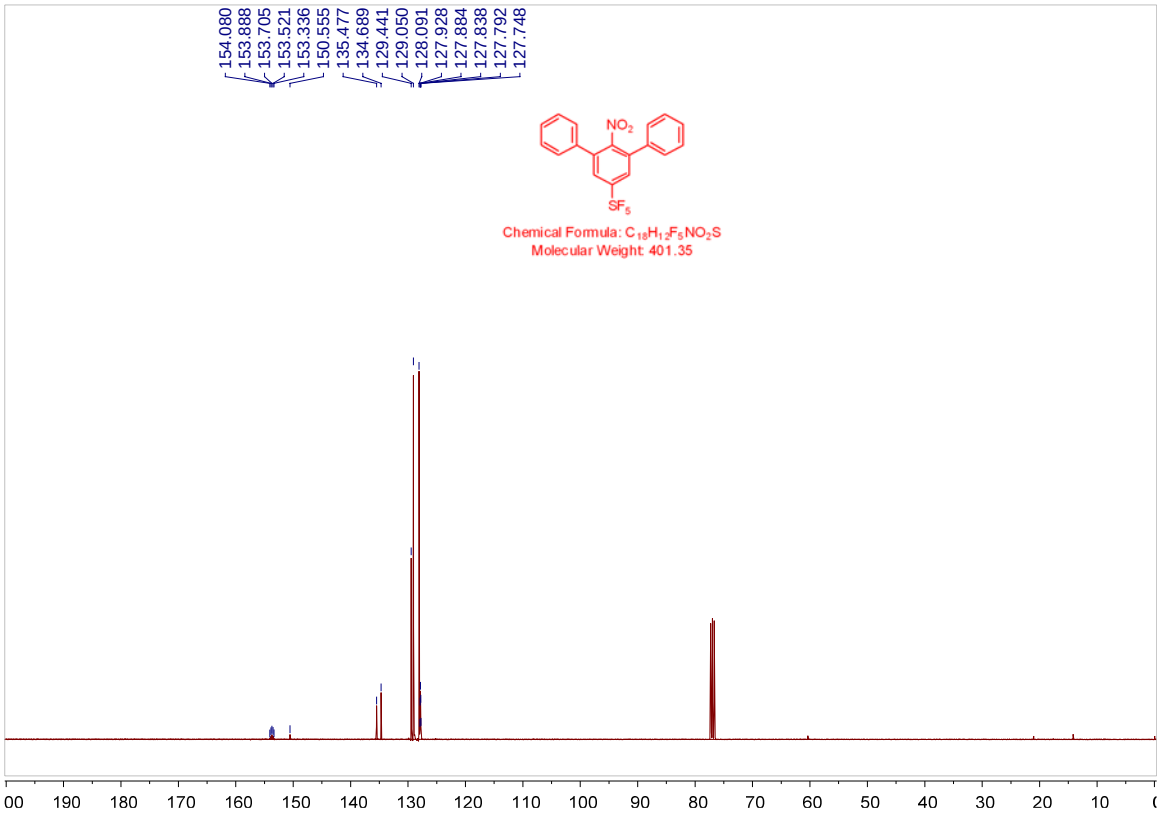

8.987
8.980
8.374
8.368
8.205
8.183
8.169
8.072
8.067
8.051
8.046
7.792
7.788
7.691
7.670
7.636
7.631
7.615
7.610
7.482
7.471
7.461
7.451
0.000
NO2
N
F5S
Chemical Formula: C15H9F5N2O2S
Exact Mass: 376.03
1.02
0.95
2.04
1.00
0.96
1.04
0.99
1.01
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

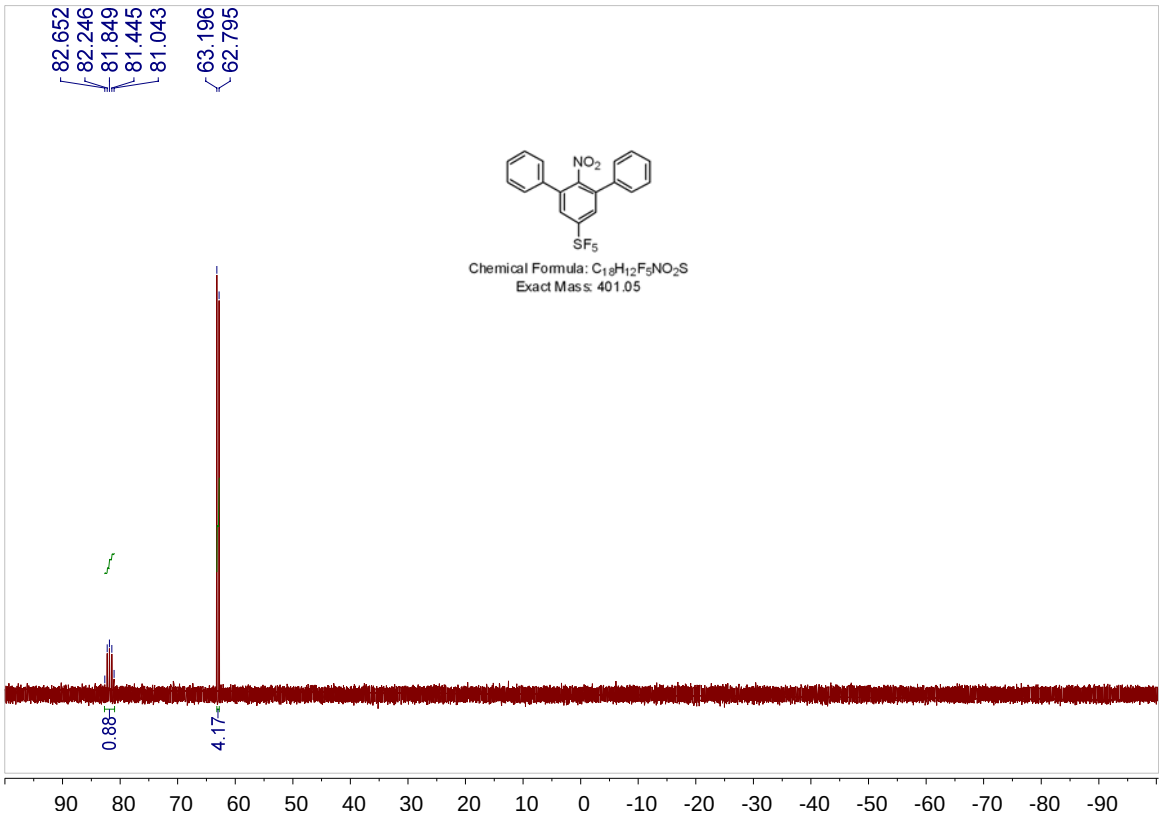

153.191
153.026
152.848
148.599
148.075
139.204
136.471
134.027
132.967
130.453
129.851
129.822
129.784
129.762
128.939
128.201
127.258
122.820
122.779
122.745
122.714
122.182
NO2
N
F5S
Chemical Formula: C15H9F5N2O2S
Exact Mass: 376.03
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


81.935
81.528
81.128
80.723
80.325
63.340
62.938
NO2
N
F5S
Chemical Formula: C15H9F5N2O2S
Exact Mass: 376.03
1.02
4.00
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90

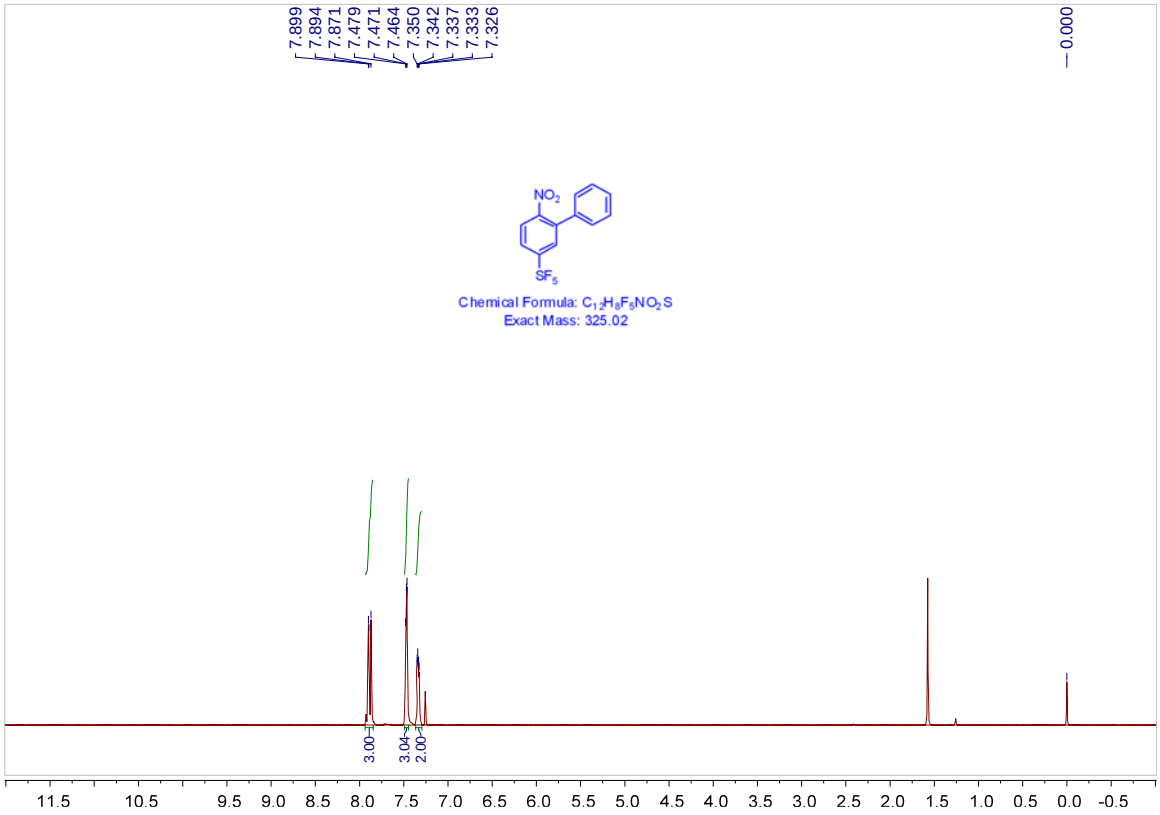
Compound 6a

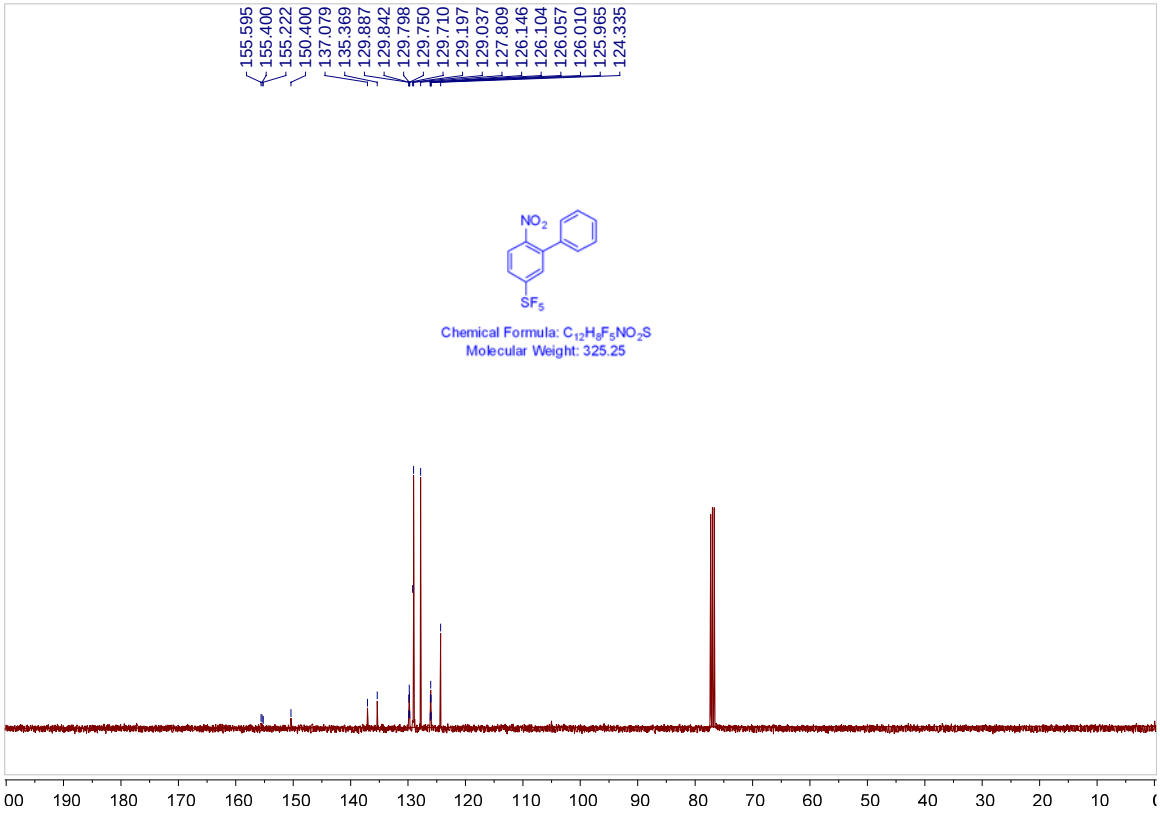

7.837
7.481
7.470
7.459
7.418
7.410
7.402
7.398
7.386
0.000
NO2
SF5
Chemical Formula: C18H12F5NO2S
Molecular Weight: 401.35
2.00
6.03
4.01
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

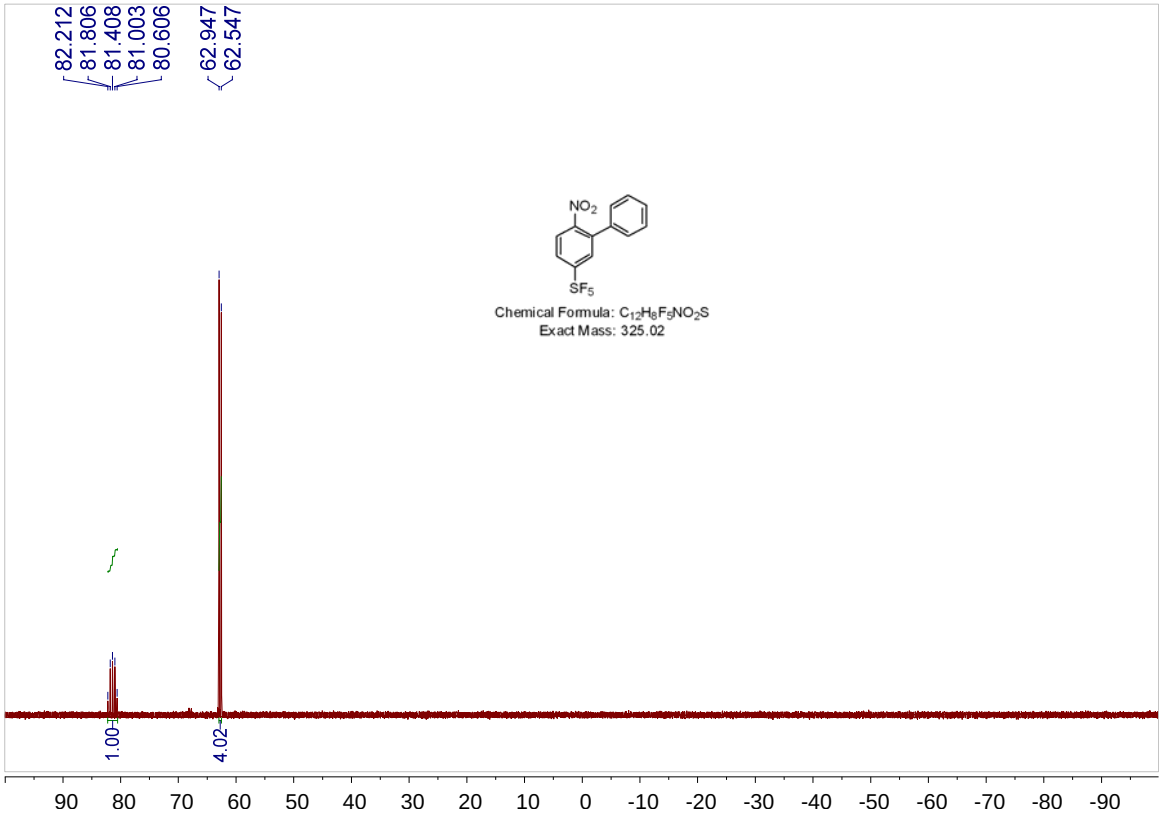

154.080
153.888
153.705
153.521
153.336
150.555
135.477
134.689
129.441
129.050
128.091
127.928
127.884
127.838
127.792
127.748
NO2
SF5
Chemical Formula: C18H12F5NO2S
Molecular Weight: 401.35
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10


82.652
82.246
81.849
81.445
81.043
63.196
62.795
NO2
SF5
Chemical Formula: C18H12F5NO2S
Exact Mass: 401.05
0.88
4.17
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90

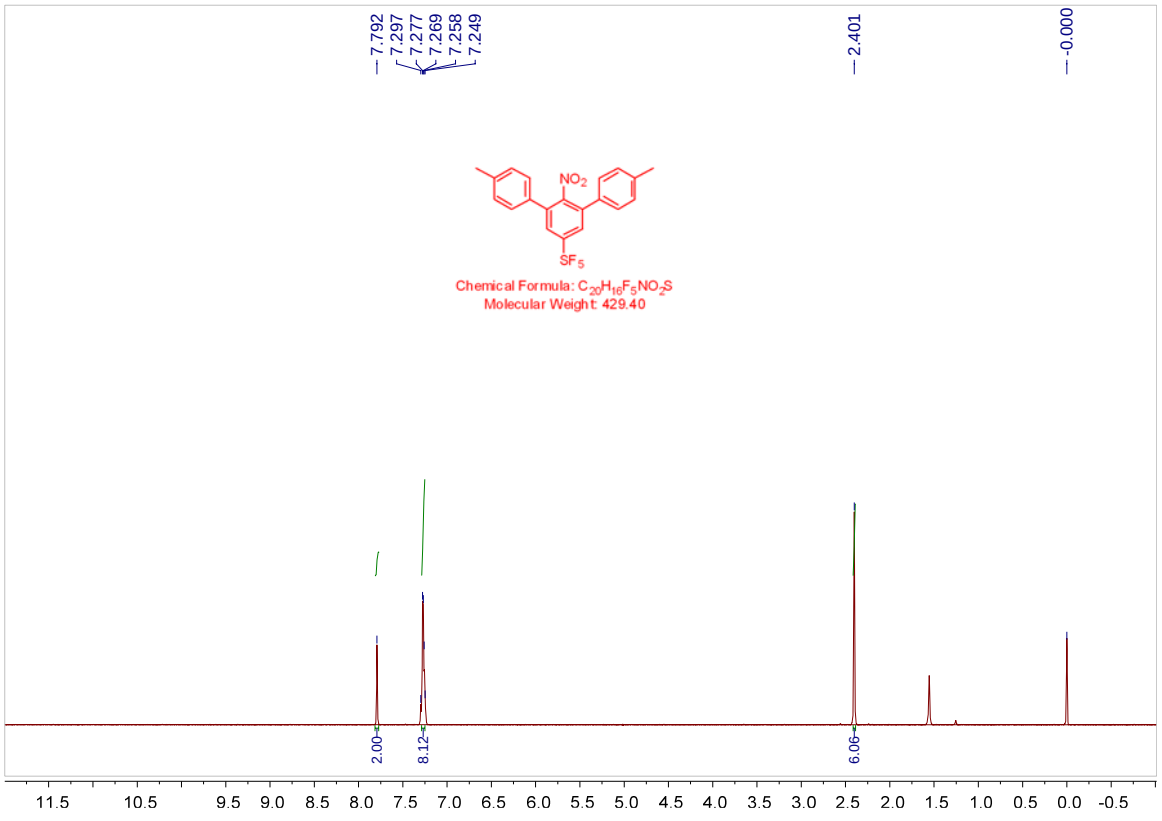
Compound 7a

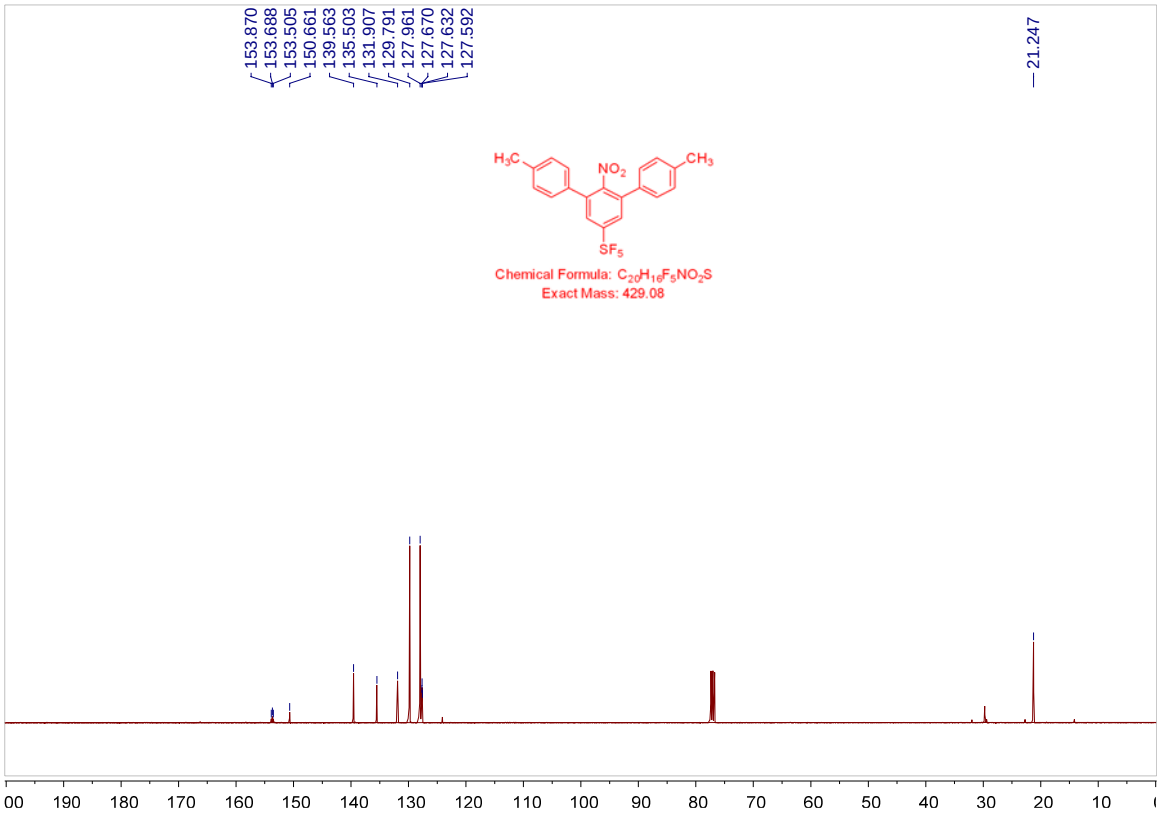

7.899
7.894
7.871
7.479
7.471
7.464
7.350
7.342
7.337
7.333
7.326
0.000
NO2
SF5
Chemical Formula: C12H8F5NO2S
Exact Mass: 325.02
3.00
3.04
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

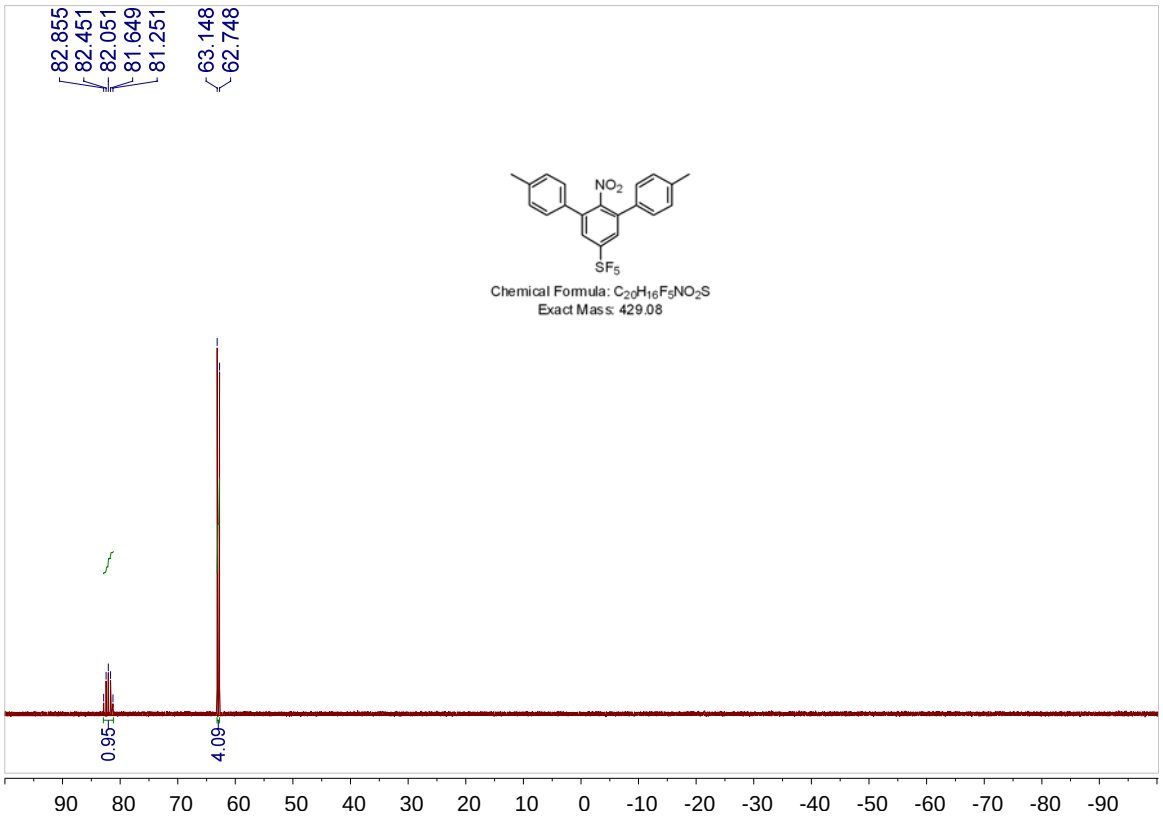

155.595
155.400
155.222
150.400
137.079
135.369
129.887
129.842
129.798
129.750
129.710
129.197
129.037
127.809
126.146
126.104
126.057
126.010
125.965
124.335
NO2
SF5
Chemical Formula: C12H8F5NO2S
Molecular Weight: 325.25
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


82.212
81.806
81.408
81.003
80.606
62.947
62.547
NO2
SF5
Chemical Formula: C12H8F5NO2S
Exact Mass: 325.02
1.00
4.02
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90

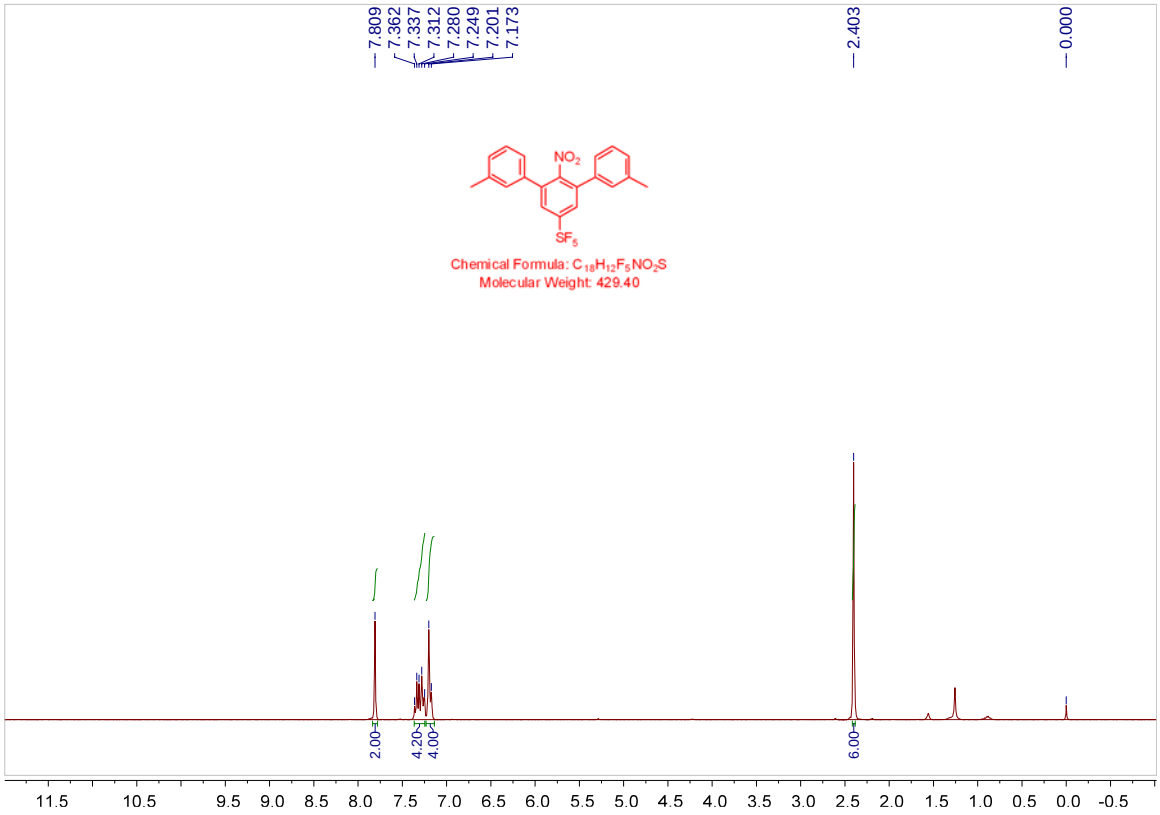
Compound 6b

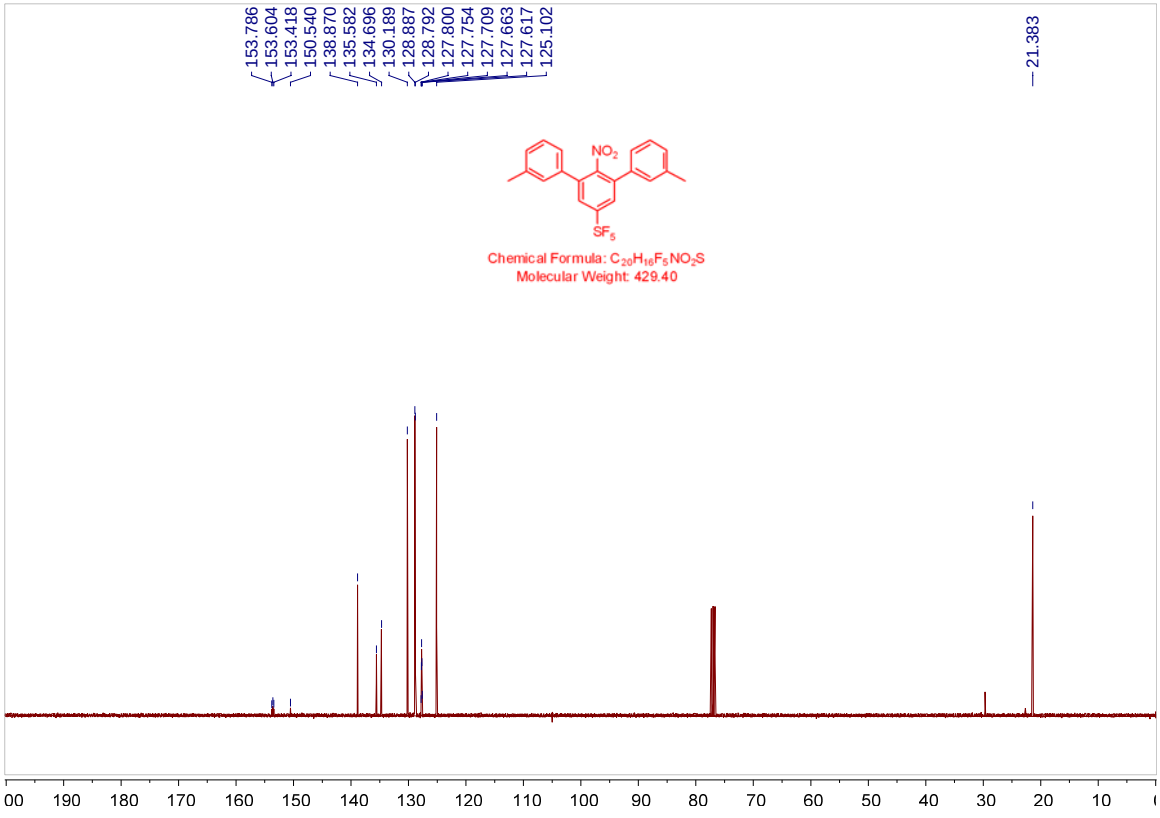

7.792
7.297
7.277
7.269
7.258
7.249
2.401
-0.000
NO2
SF5
Chemical Formula: C20H16F5NO2S
Molecular Weight: 429.40
2.00
8.12
6.06
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

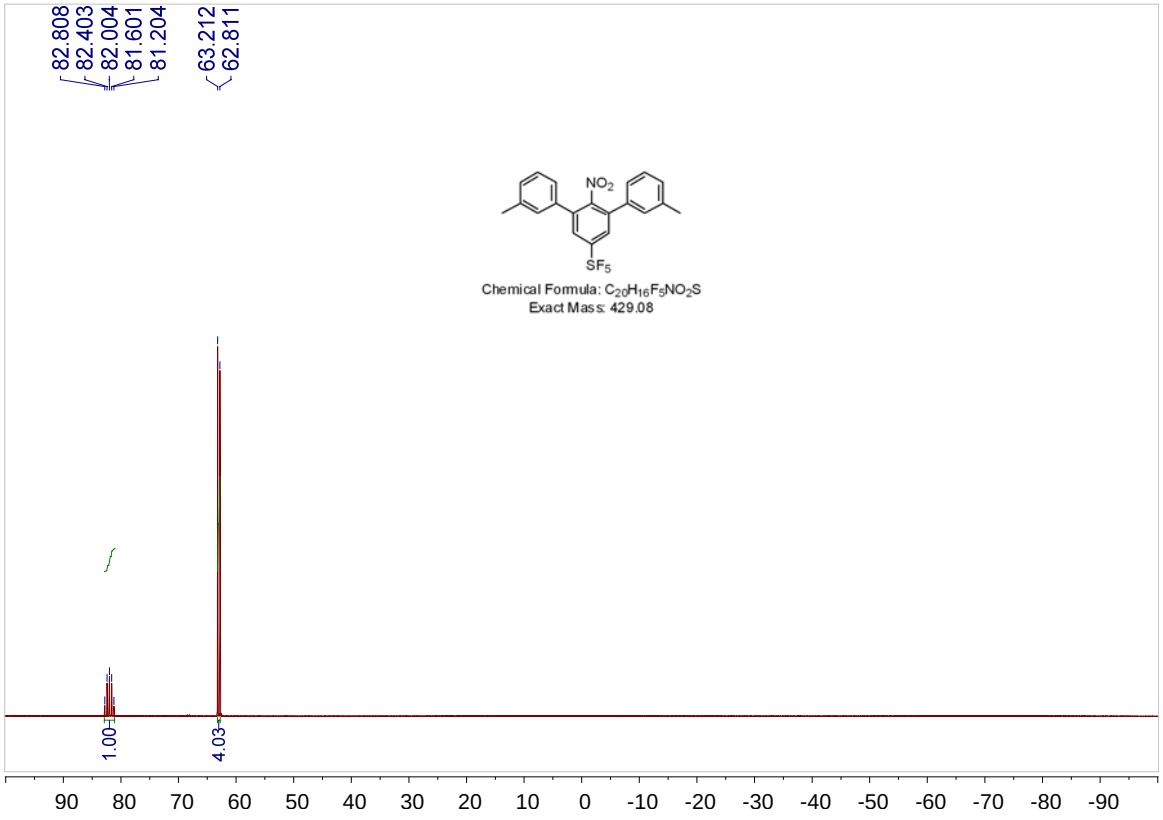

153.870
153.688
153.505
150.661
139.563
135.503
131.907
129.791
127.961
127.670
127.632
127.592
21.247
H3C
NO2
CH3
SF5
Chemical Formula: C20H16F5NO2S
Exact Mass: 429.08
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10


82.855
82.451
82.051
81.649
81.251
63.148
62.748
NO2
SF5
Chemical Formula: C20H16F5NO2S
Exact Mass: 429.08
0.95
4.09
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90

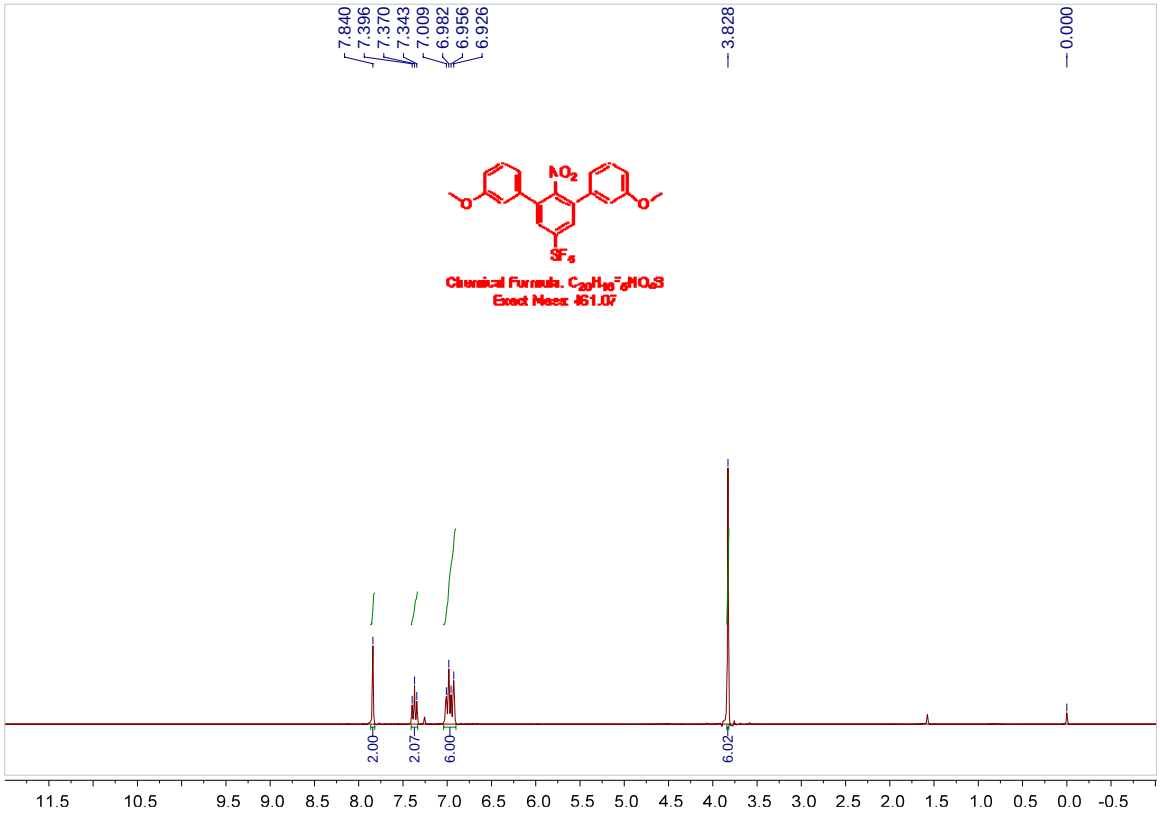
Compound 6c

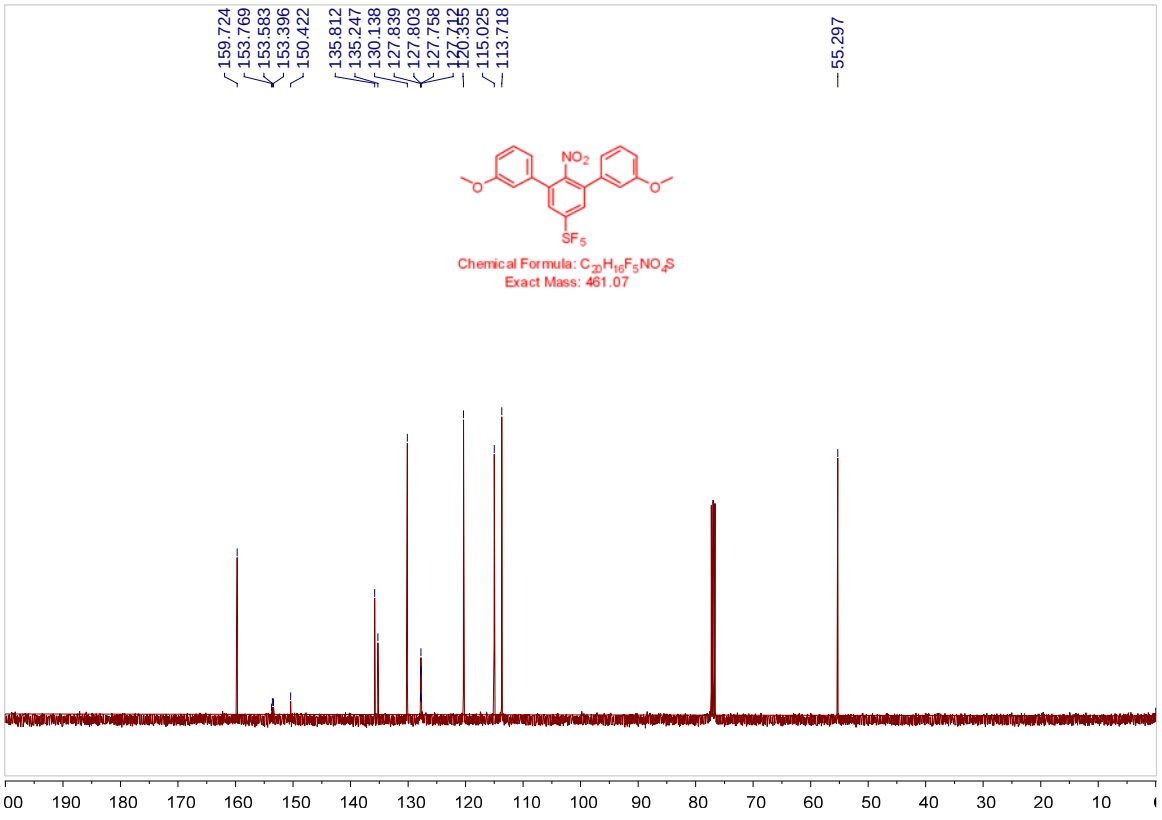

7.809
7.362
7.337
7.312
7.280
7.249
7.201
7.173
2.403
0.000
NO2
SF5
Chemical Formula: C18H12F5NO2S
Molecular Weight: 429.40
2.00
4.20
4.00
6.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

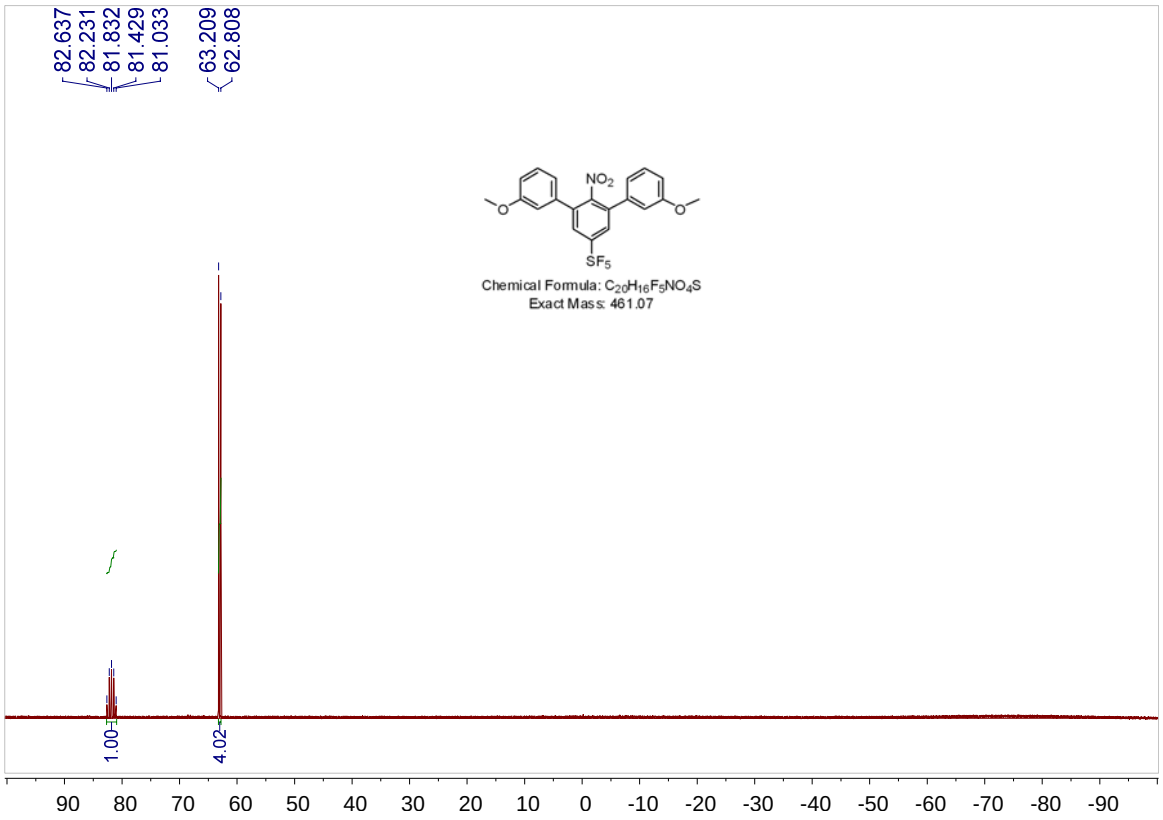

153.786
153.604
153.418
150.540
138.870
135.582
134.696
130.189
128.887
128.792
127.800
127.754
127.709
127.663
127.617
125.102
21.383
NO2
SF5
Chemical Formula: C20H16F5NO2S
Molecular Weight: 429.40
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


82.808
82.403
82.004
81.601
81.204
63.212
62.811
NO2
SF5
Chemical Formula: C20H16F5NO2S
Exact Mass: 429.08
1.00
4.03
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90

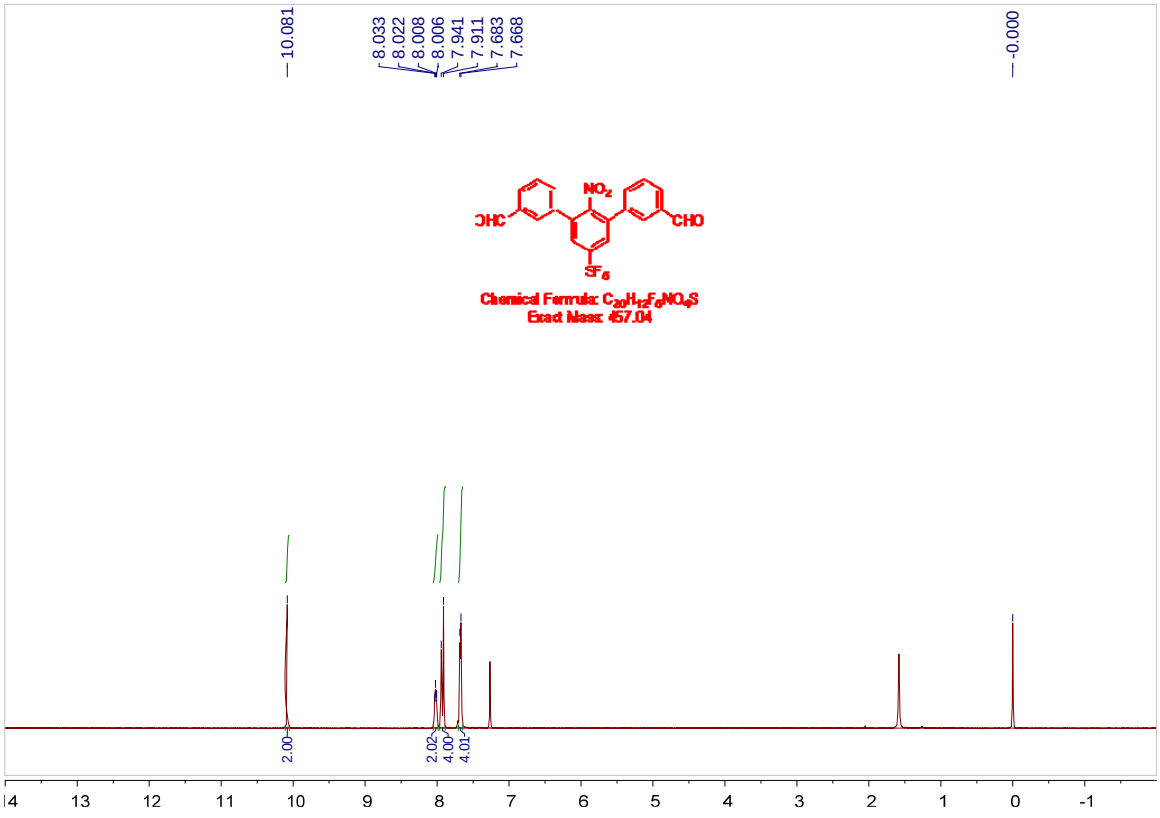
Compound 6d

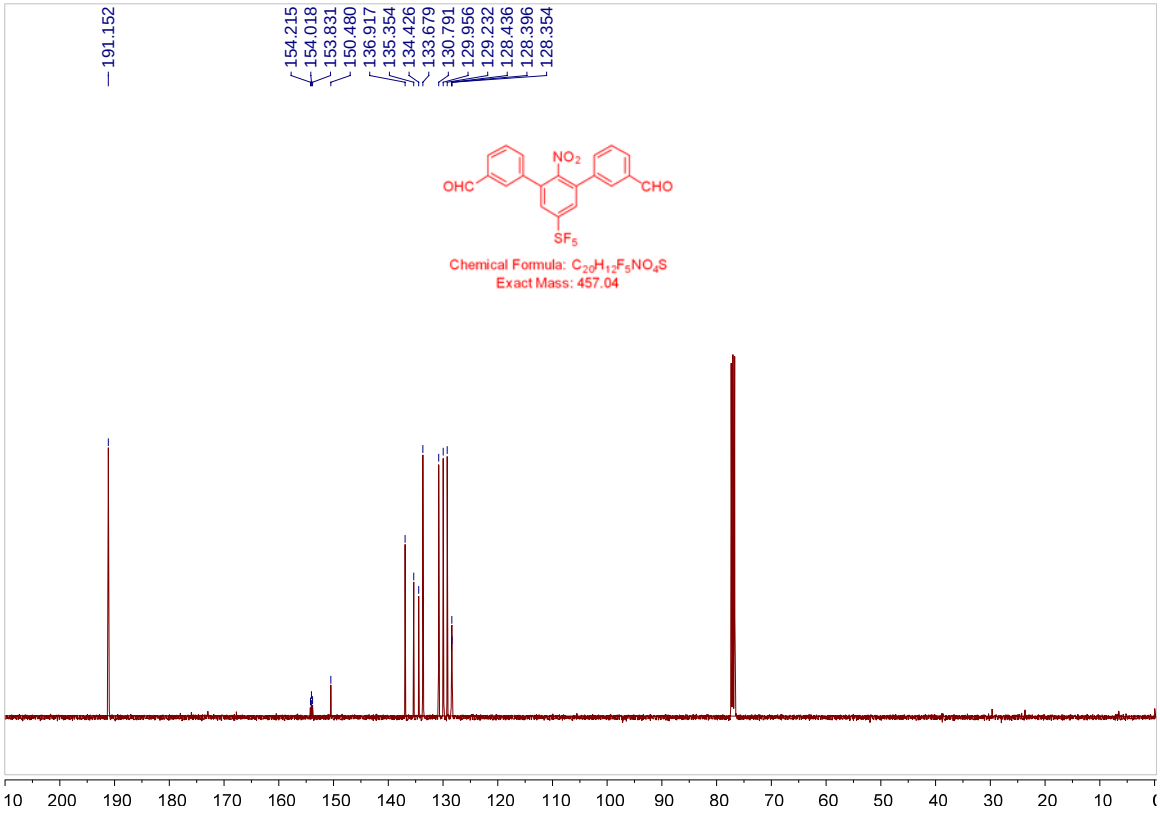

7.840
7.396
7.370
7.343
7.009
6.982
6.956
6.926
3.828
0.000
NO2
SF5
2.00
2.07
6.00
6.02
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

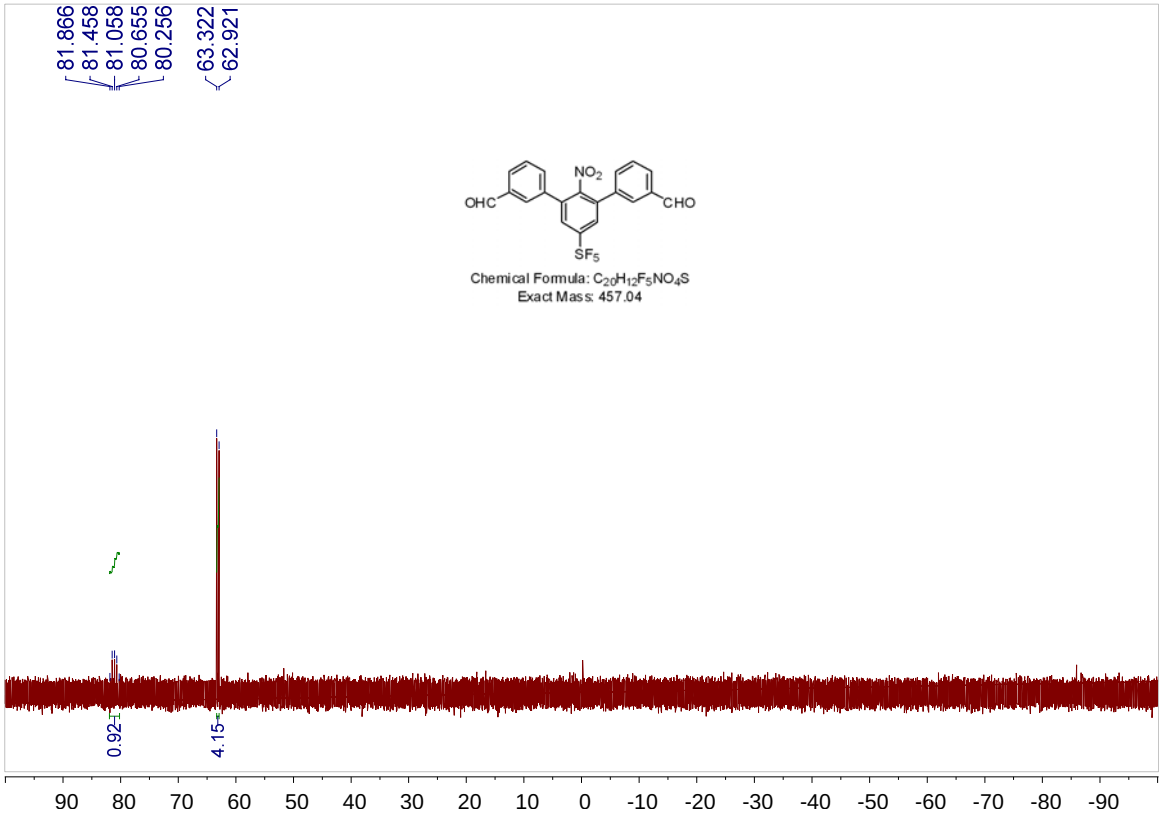

159.724
153.769
153.583
153.396
150.422
135.812
135.247
130.138
127.839
127.803
127.758
120.355
115.025
113.718
55.297
NO2
SF5
Chemical Formula: C20H16F5NO4S
Exact Mass: 461.07


82.637
82.231
81.832
81.429
81.033
63.209
62.808
NO2
SF5
Chemical Formula: C20H16F5NO4S
Exact Mass: 461.07
1.00
4.02

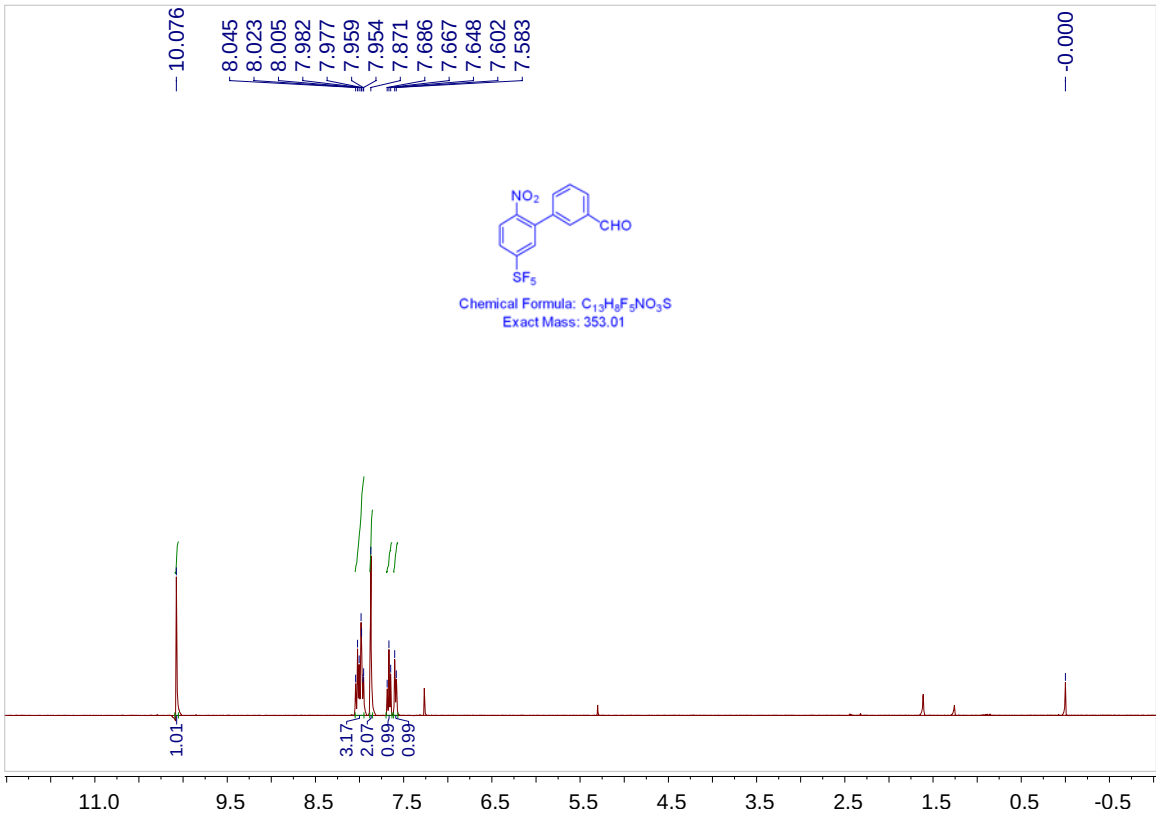
Compound 6e

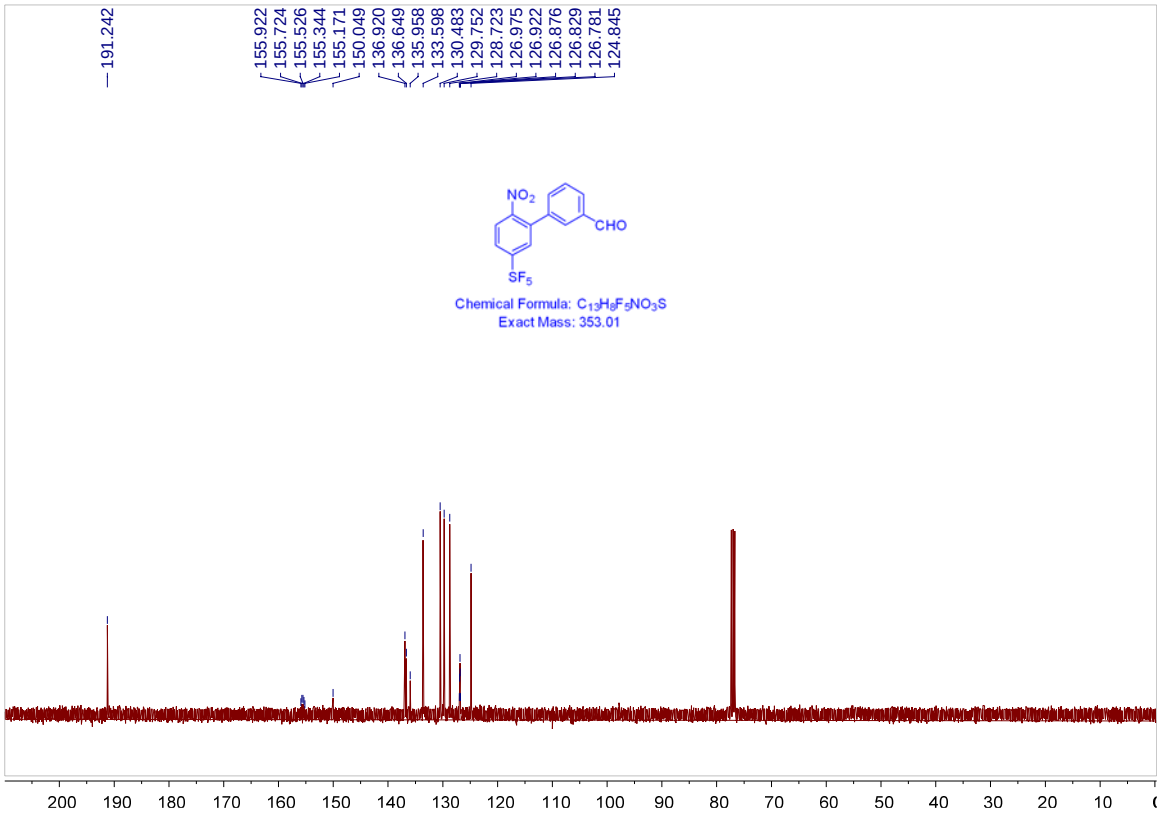

10.081
8.033
8.022
8.008
8.006
7.941
7.911
7.683
7.668
-0.000
NO2
OHC
CHO
SF5
Chemical Formula: C20H12F5NO4S
Exact Mass: 457.04
2.00
2.02
4.00
4.01

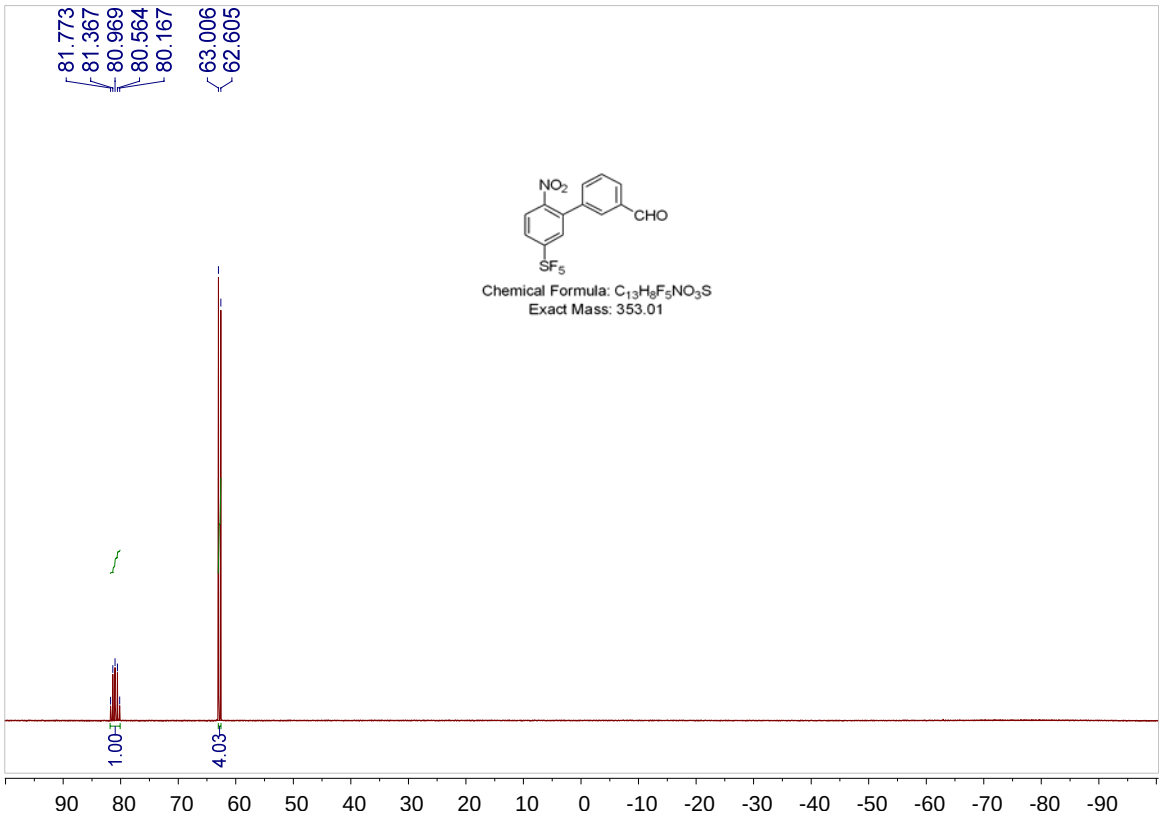

191.152
154.215
154.018
153.831
150.480
136.917
135.354
134.426
133.679
130.791
129.956
129.232
128.436
128.396
128.354
NO2
OHC
CHO
SF5
Chemical Formula: C20H12F5NO4S
Exact Mass: 457.04


81.866
81.458
81.058
80.655
80.256
63.322
62.921
NO2
OHC
CHO
SF5
Chemical Formula: C20H12F5NO4S
Exact Mass: 457.04
0.92
4.15
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90

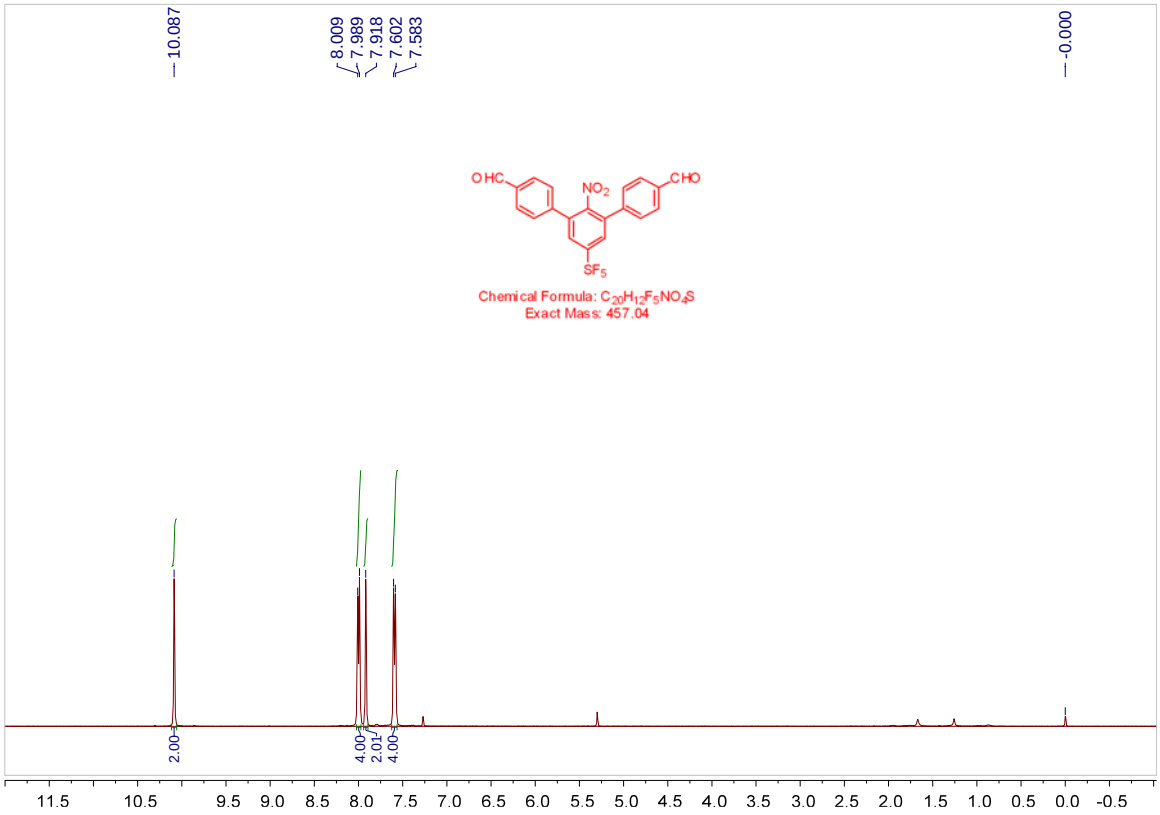
Compound 7e

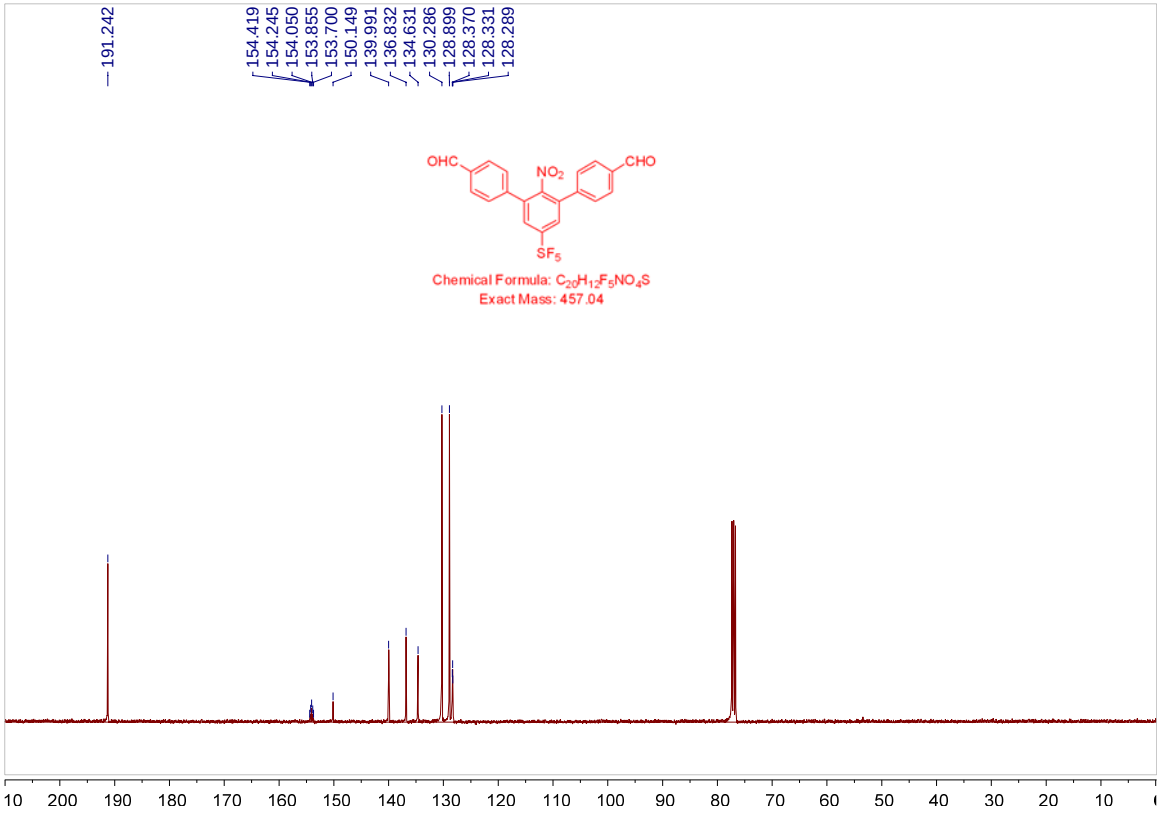

10.076
8.045
8.023
8.005
7.982
7.977
7.959
7.954
7.871
7.686
7.667
7.648
7.602
7.583
-0.000
NO2
CHO
SF5
Chemical Formula: C13H8F5NO3S
Exact Mass: 353.01
1.01
3.17
2.07
0.99
0.99
11.0 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5

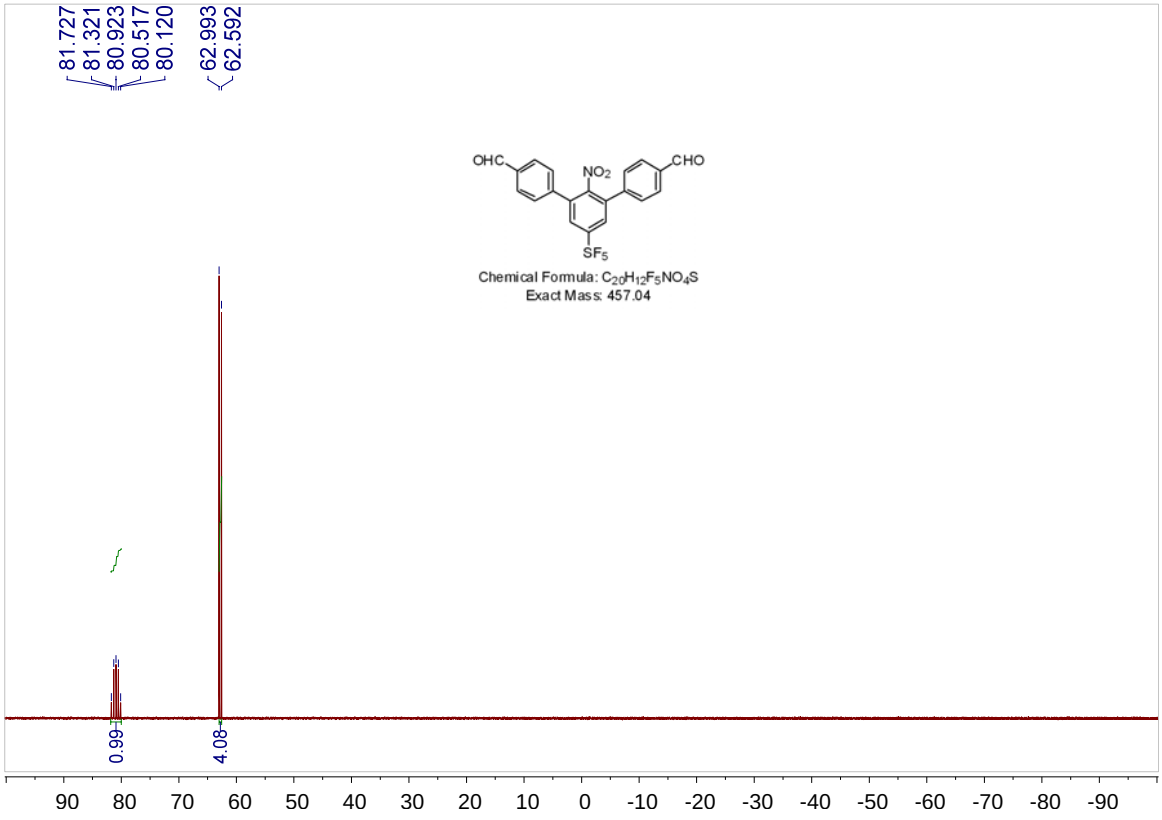

191.242
155.922
155.724
155.526
155.344
155.171
150.049
136.920
136.649
135.958
133.598
130.483
129.752
128.723
126.975
126.922
126.876
126.829
126.781
124.845
NO2
CHO
SF5
Chemical Formula: C13H8F5NO3S
Exact Mass: 353.01
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10


81.773
81.367
80.969
80.564
80.167
63.006
62.605
NO2
CHO
SF5
Chemical Formula: C13H8F5NO3S
Exact Mass: 353.01
1.00
4.03
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90

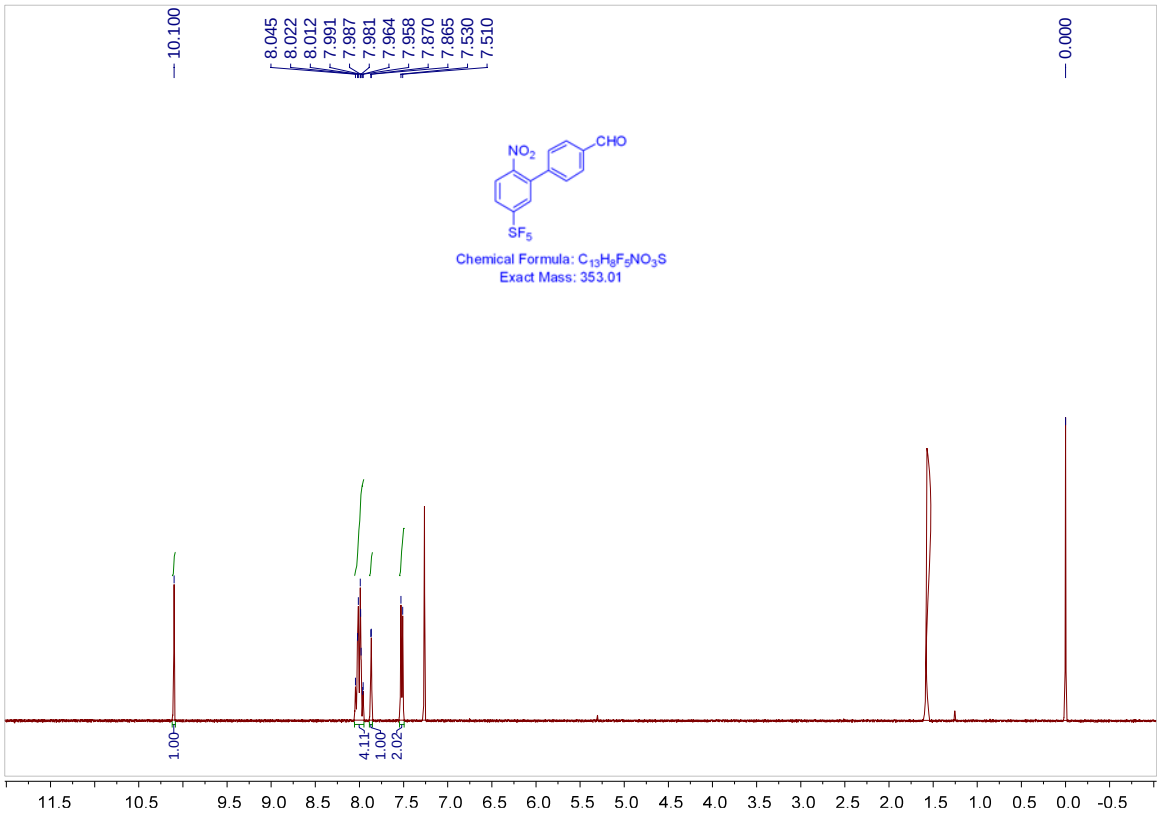
Compound 6f

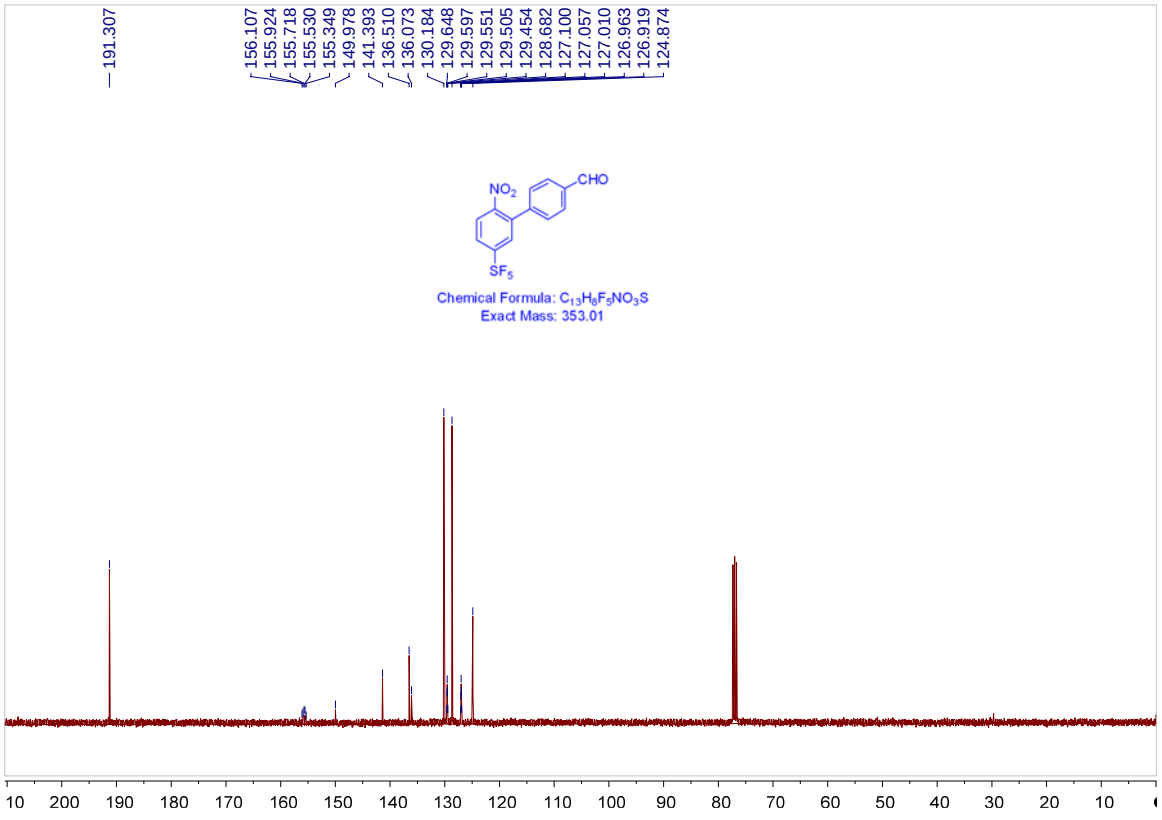

10.087
8.009
7.989
7.918
7.602
7.583
-0.000
OHC
NO2
CHO
SF5
Chemical Formula: C20H12F5NO4S
Exact Mass: 457.04
2.00
4.00
2.01
4.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

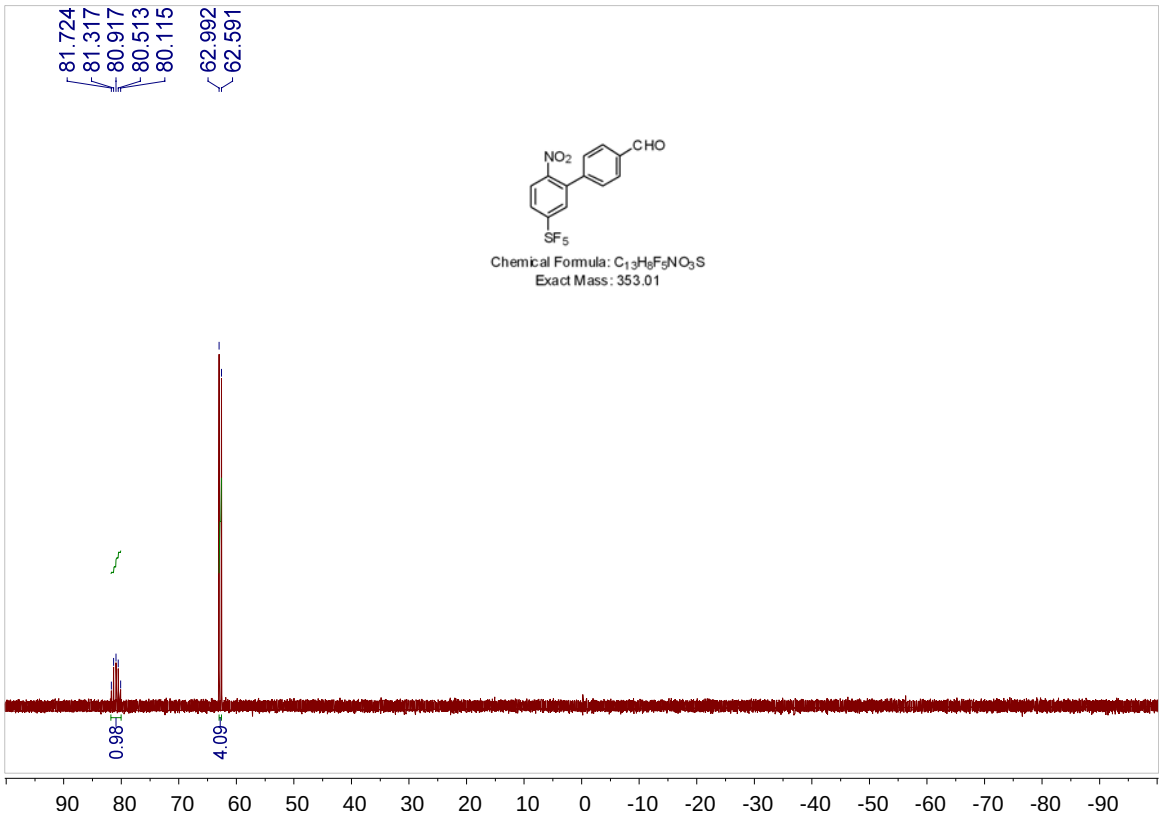

191.242
154.419
154.245
154.050
153.855
153.700
150.149
139.991
136.832
134.631
130.286
128.899
128.370
128.331
128.289
OHC
NO2
CHO
SF5
Chemical Formula: C20H12F5NO4S
Exact Mass: 457.04
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


81.727
81.321
80.923
80.517
80.120
62.993
62.592
OHC
NO2
CHO
SF5
Chemical Formula: C20H12F5NO4S
Exact Mass: 457.04
0.99
4.08
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90

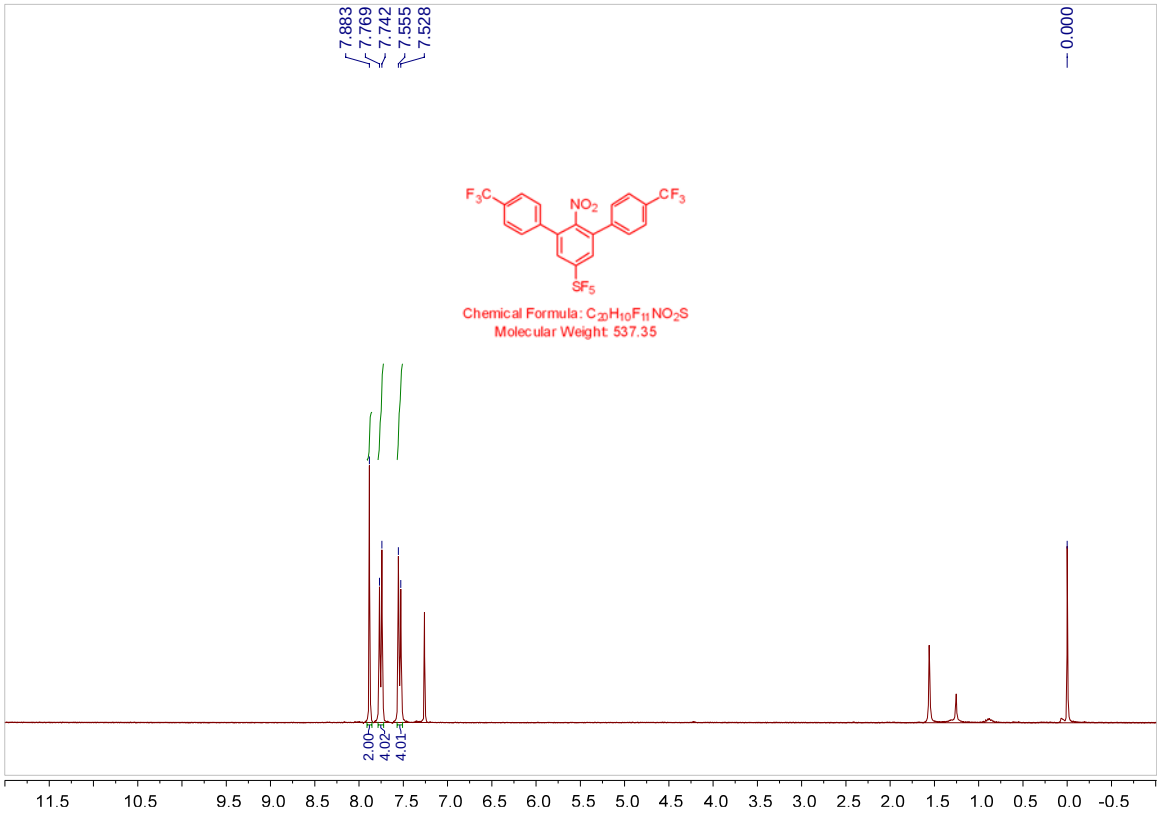
Compound 7f

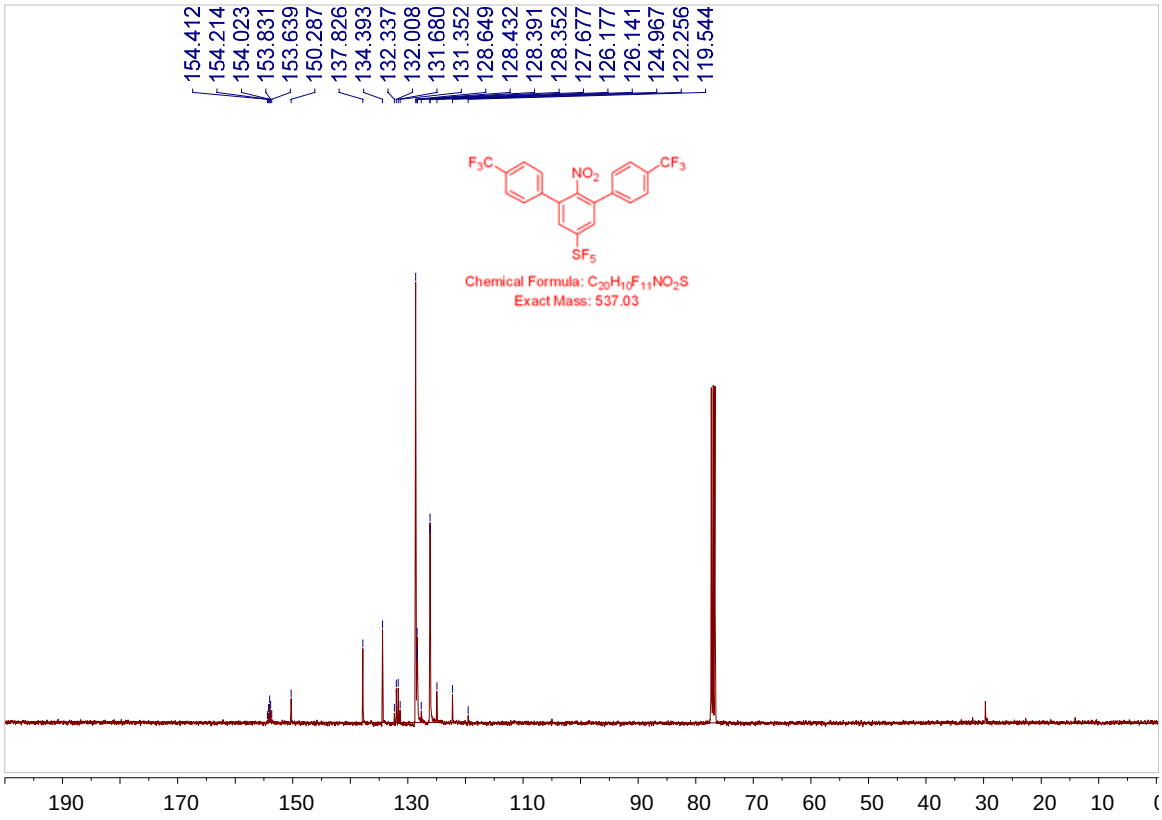

10.100
8.045
8.022
8.012
7.991
7.987
7.981
7.964
7.958
7.870
7.865
7.530
7.510
0.000
NO2
CHO
SF5
Chemical Formula: C13H8F5NO3S
Exact Mass: 353.01
1.00
4.11
1.00
2.02
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

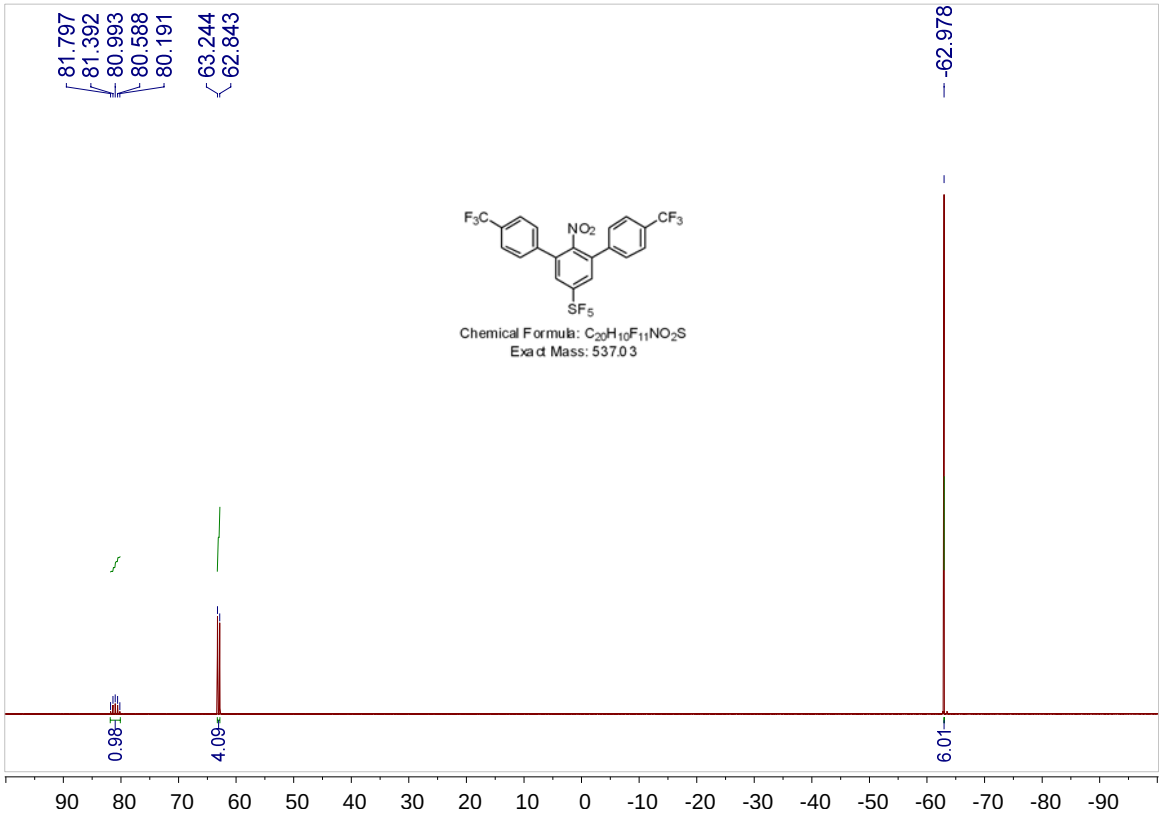

191.307
156.107
155.924
155.718
155.530
155.349
149.978
141.393
136.510
136.073
130.184
129.648
129.597
129.551
129.505
129.454
128.682
127.100
127.057
127.010
126.963
126.919
124.874
NO2
CHO
SF5
Chemical Formula: C13H8F5NO3S
Exact Mass: 353.01
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10


81.724
81.317
80.917
80.513
80.115
62.992
62.591
NO2
CHO
SF5
Chemical Formula: C13H8F5NO3S
Exact Mass: 353.01
0.98
4.09
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90

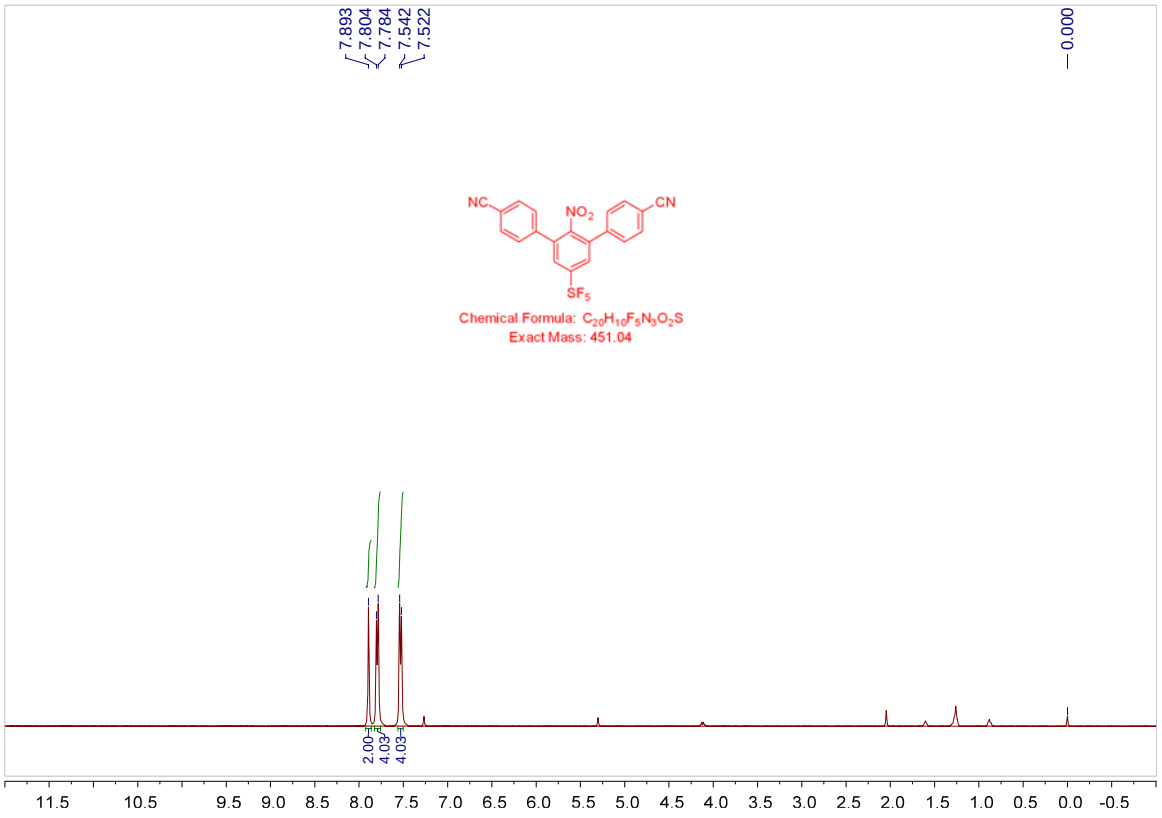
Compound 6g

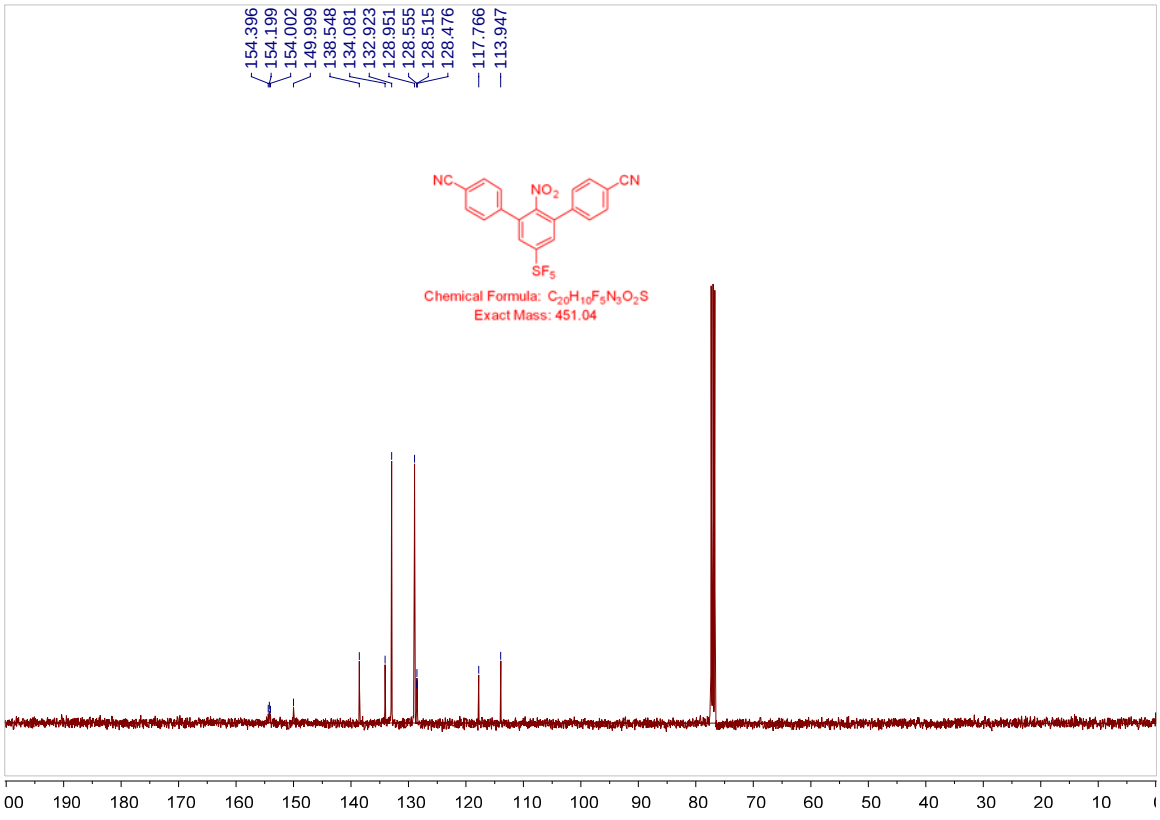

7.883
7.769
7.742
7.555
7.528
0.000
Chemical Formula: C20H10F11NO2S
Molecular Weight: 537.35
2.00
4.02
4.01

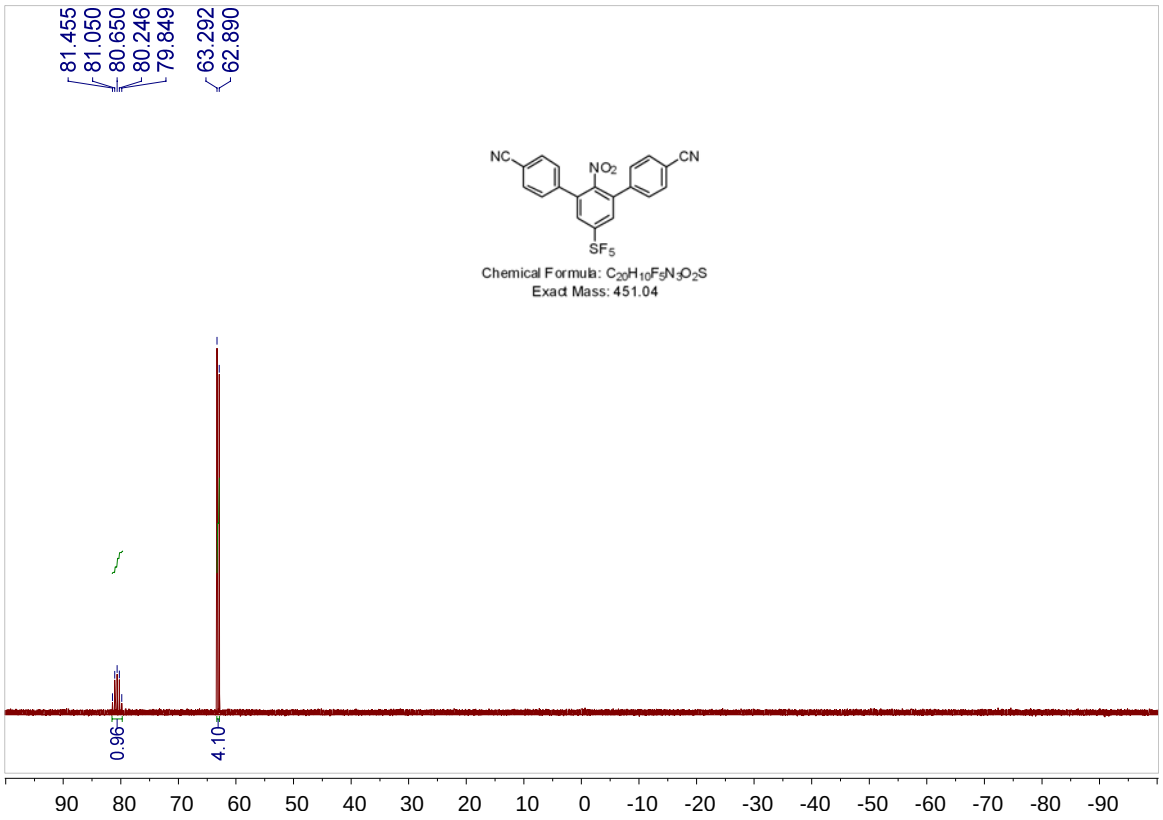

154.412
154.214
154.023
153.831
153.639
150.287
137.826
134.393
132.337
132.008
131.680
131.352
128.649
128.432
128.391
128.352
127.677
126.177
126.141
124.967
122.256
119.544
Chemical Formula: C20H10F11NO2S
Exact Mass: 537.03


81.797
81.392
80.993
80.588
80.191
63.244
62.843
-62.978
F3C
NO2
CF3
SF5
Chemical Formula: C20H10F11NO2S
Exact Mass: 537.03
0.98
4.09
6.01
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90

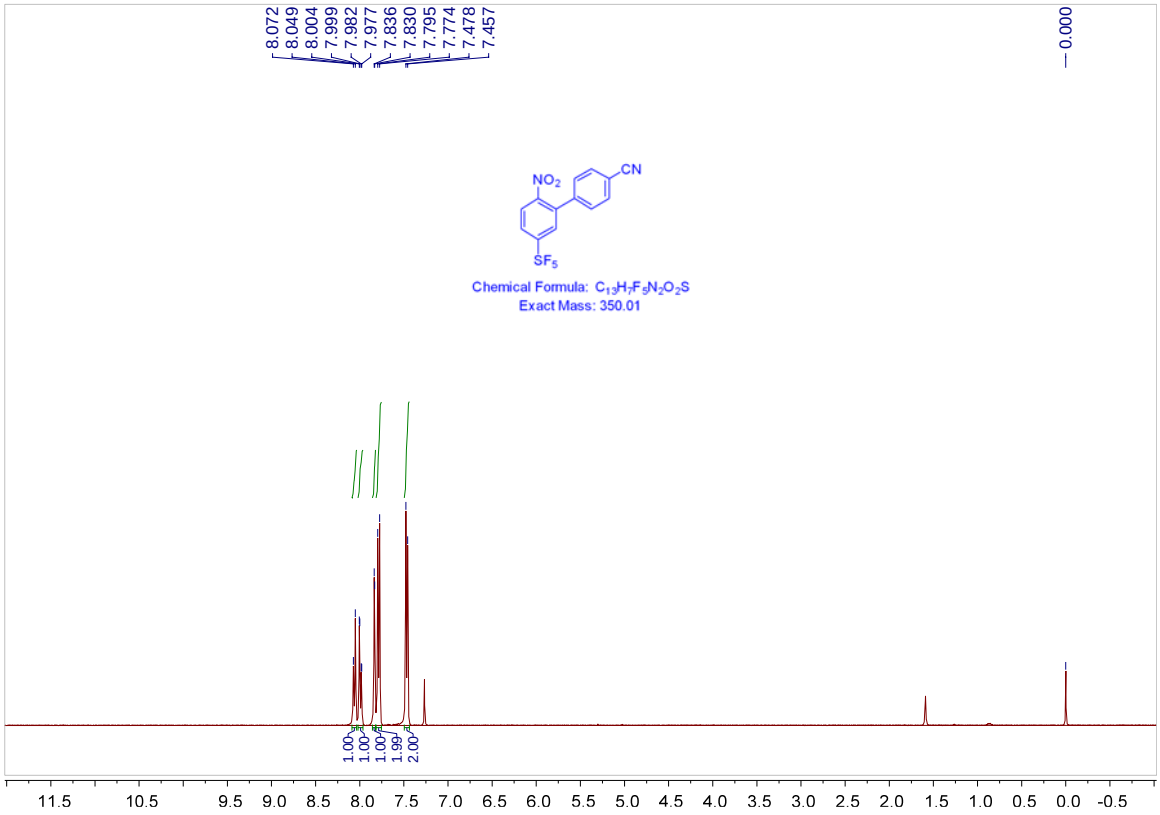
Compound 6h

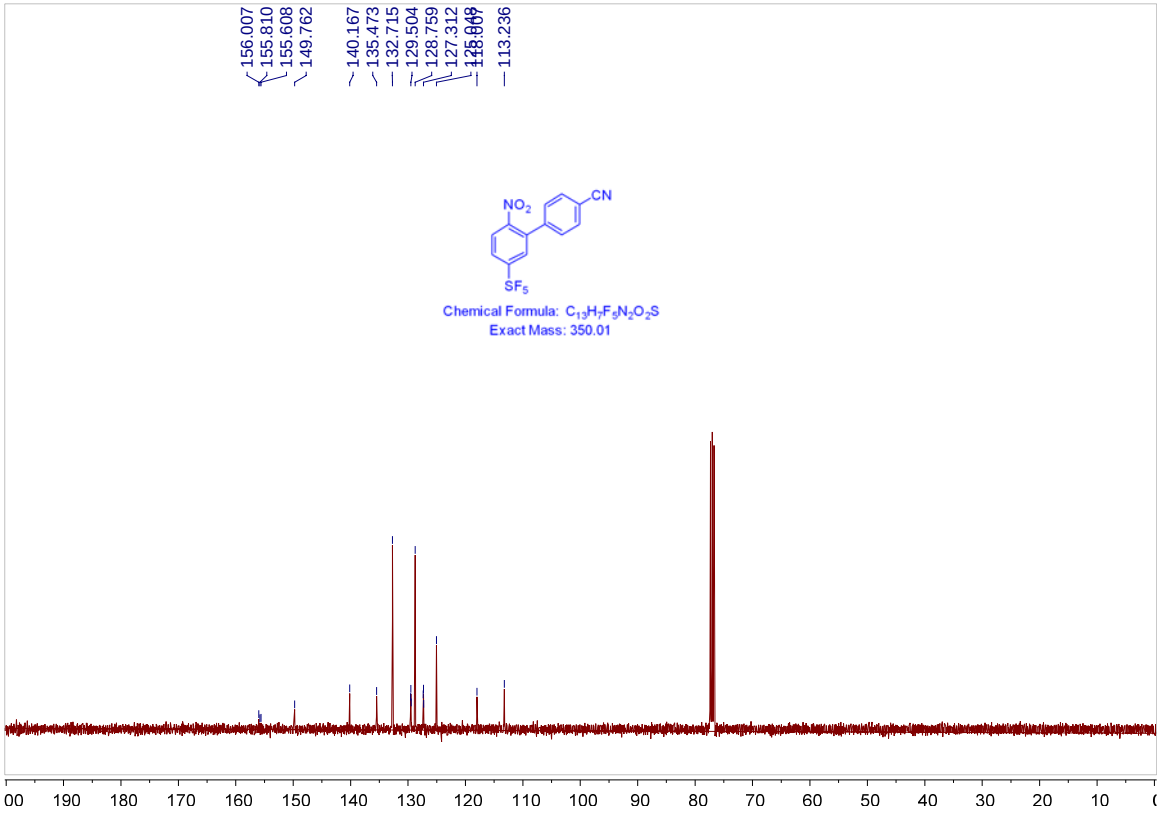

7.893
7.804
7.784
7.542
7.522
0.000
NC
NO2
CN
SF5
Chemical Formula: C20H10F5N3O2S
Exact Mass: 451.04
2.00
4.03
4.03
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

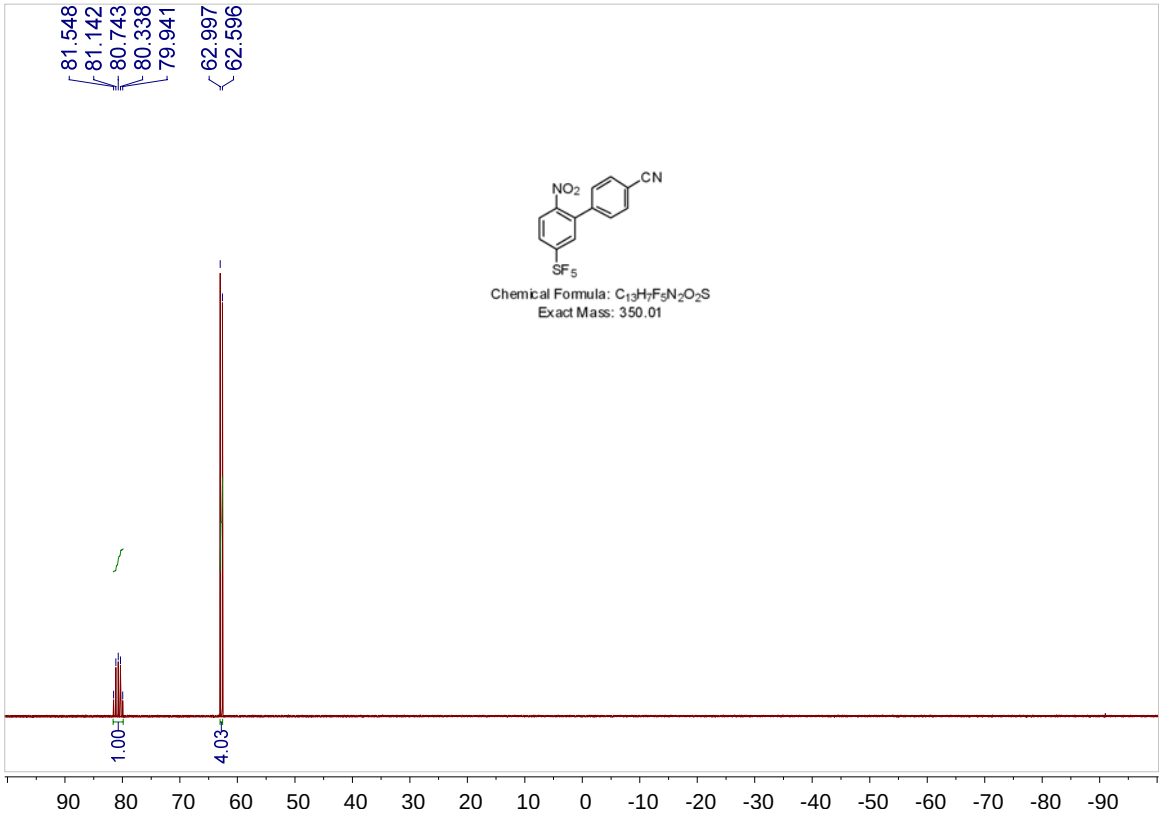

154.396
154.199
154.002
149.999
138.548
134.081
132.923
128.951
128.555
128.515
128.476
117.766
113.947
NC
NO2
CN
SF5
Chemical Formula: C20H10F5N3O2S
Exact Mass: 451.04
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10


81.455
81.050
80.650
80.246
79.849
63.292
62.890
NC
NO2
CN
SF5
Chemical Formula: C20H10F5N3O2S
Exact Mass: 451.04
0.96
4.10
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90

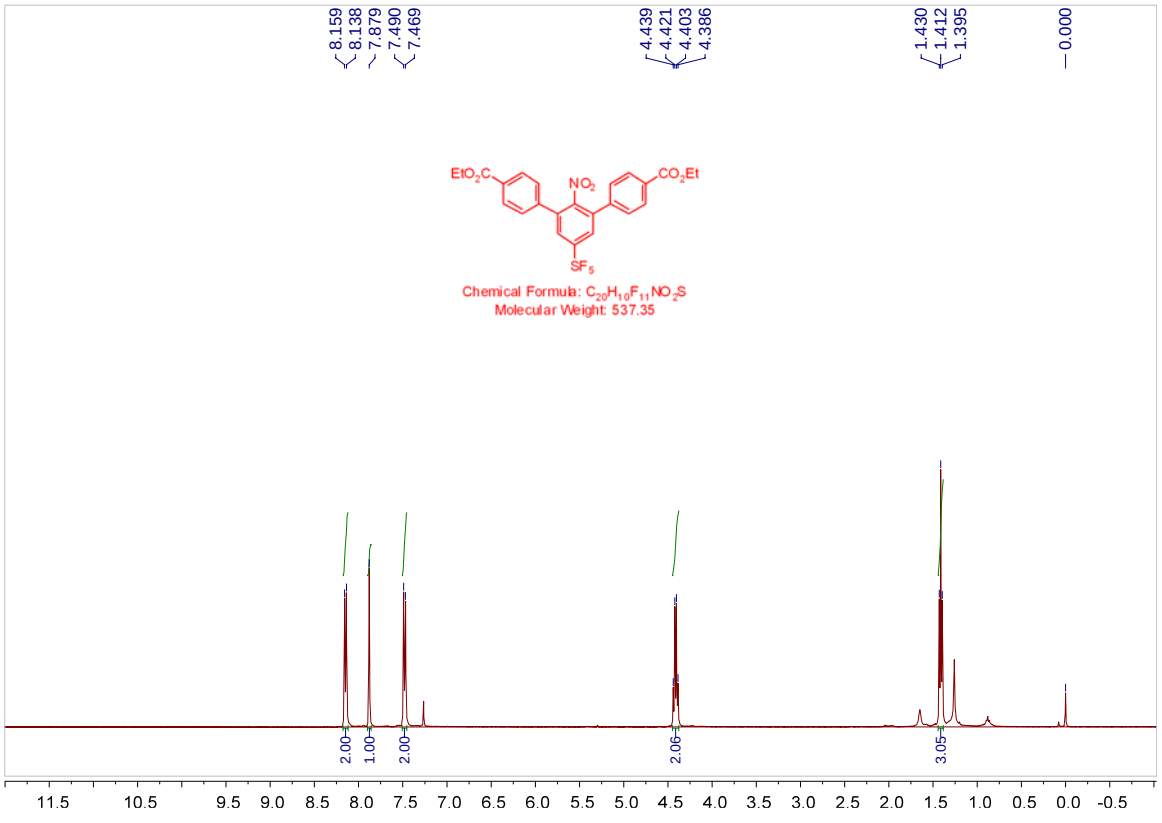
Compound 7h

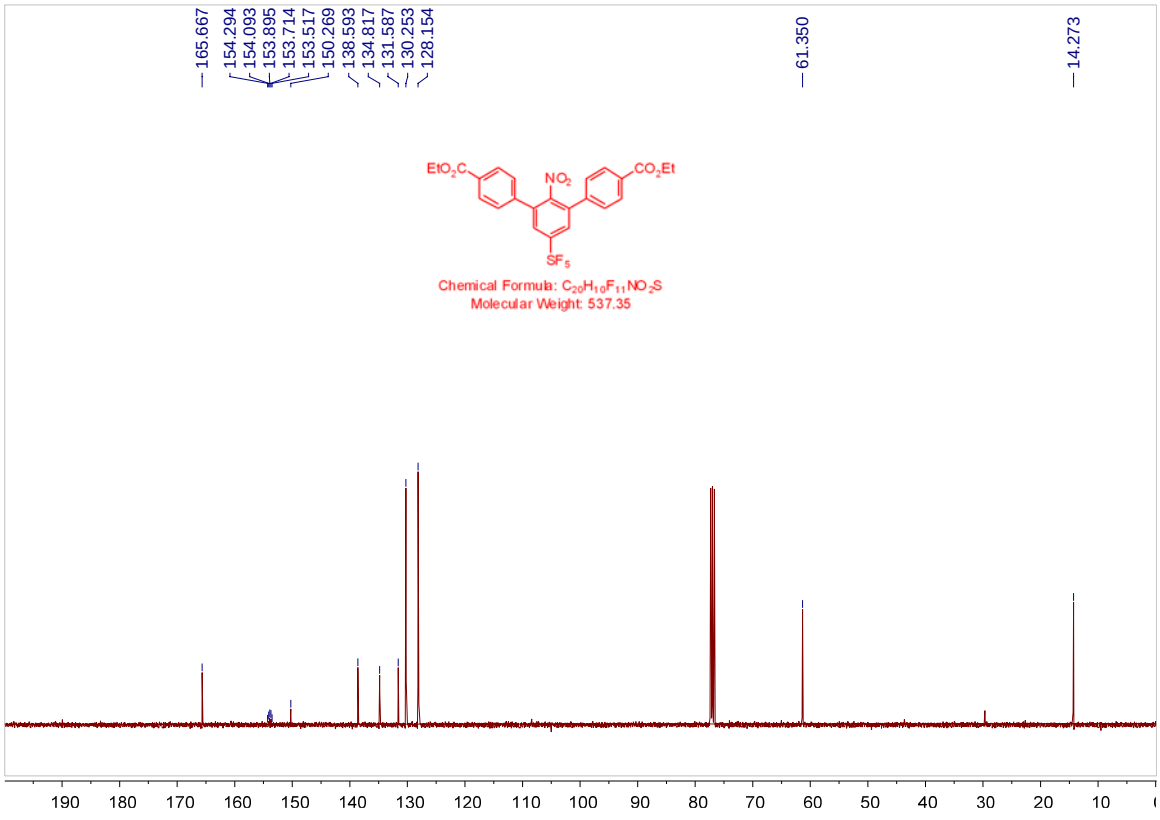

8.072
8.049
8.004
7.999
7.982
7.977
7.836
7.830
7.795
7.774
7.478
7.457
0.000
NO2
CN
SF5
Chemical Formula: C13H7F5N2O2S
Exact Mass: 350.01
1.00
1.00
1.00
1.99
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

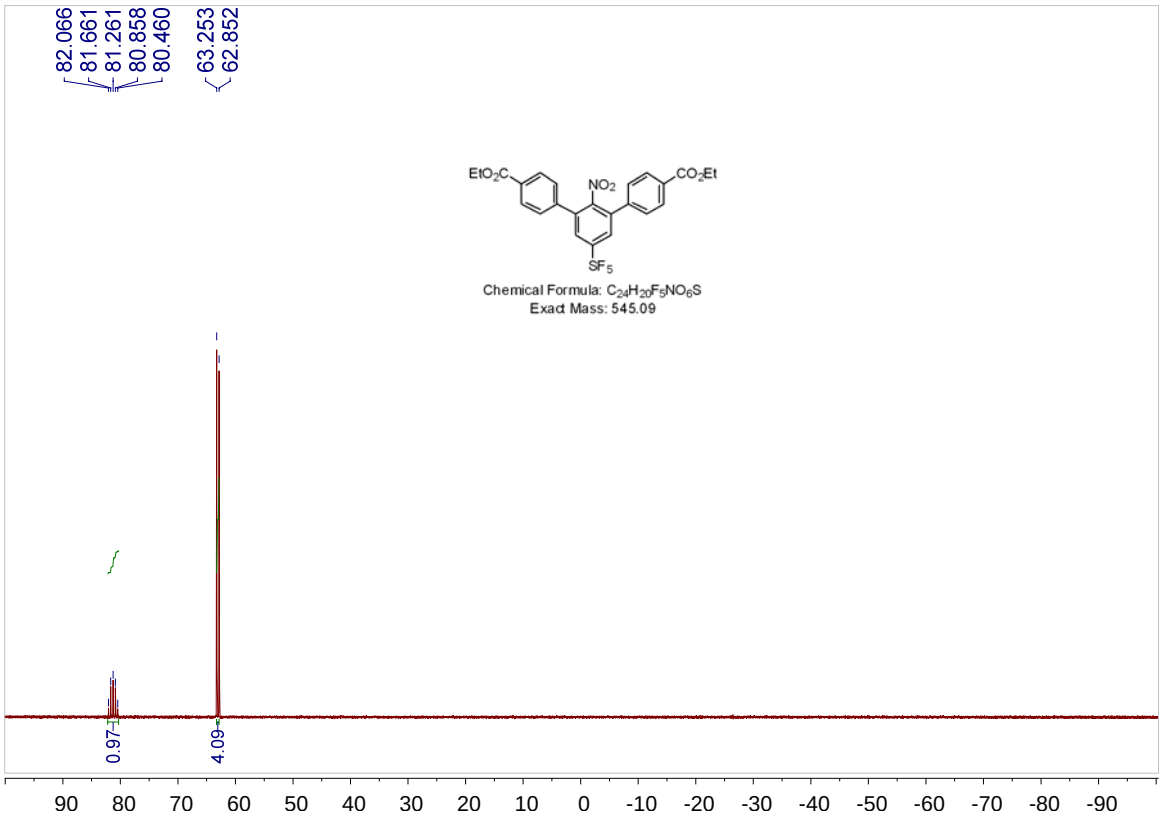

156.007
155.810
155.608
149.762
140.167
135.473
132.715
129.504
128.759
127.312
113.236
NO2
CN
SF5
Chemical Formula: C13H7F5N2O2S
Exact Mass: 350.01
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


81.548
81.142
80.743
80.338
79.941
62.997
62.596
NO2
CN
SF5
Chemical Formula: C13H7F5N2O2S
Exact Mass: 350.01
1.00
4.03
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90

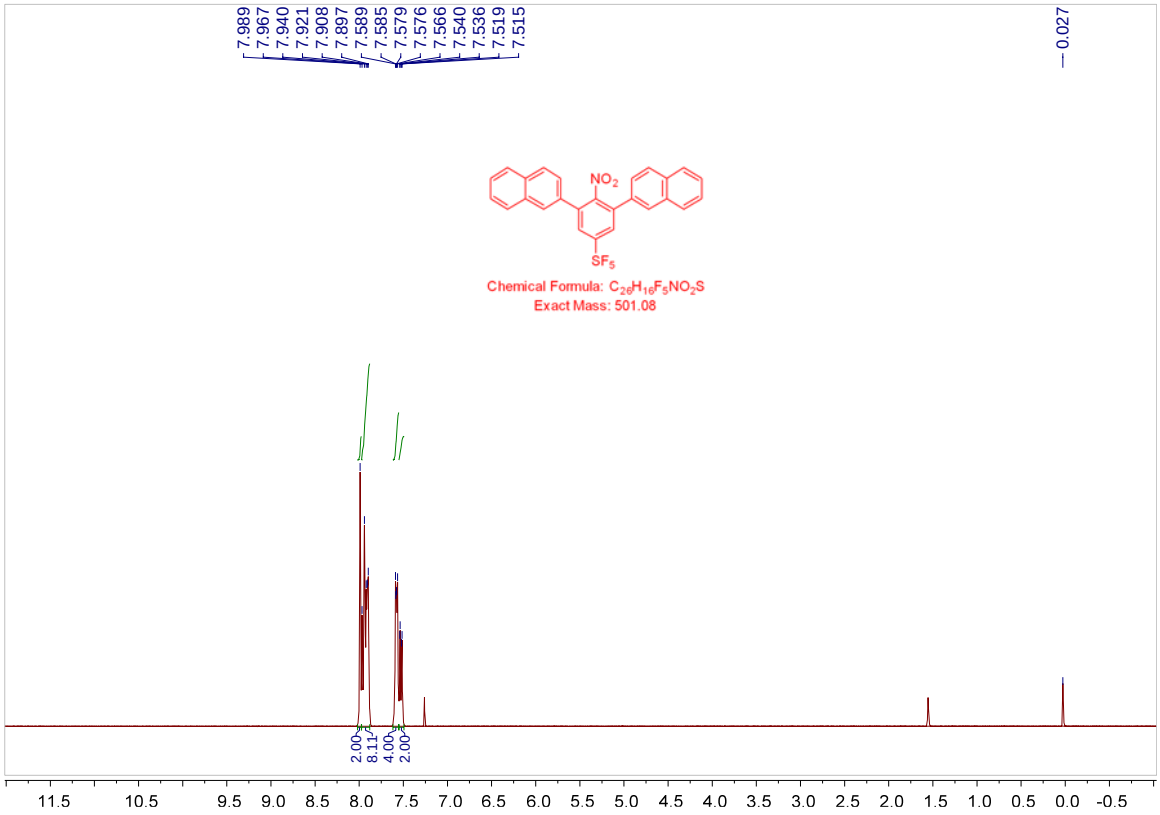
Compound 6i

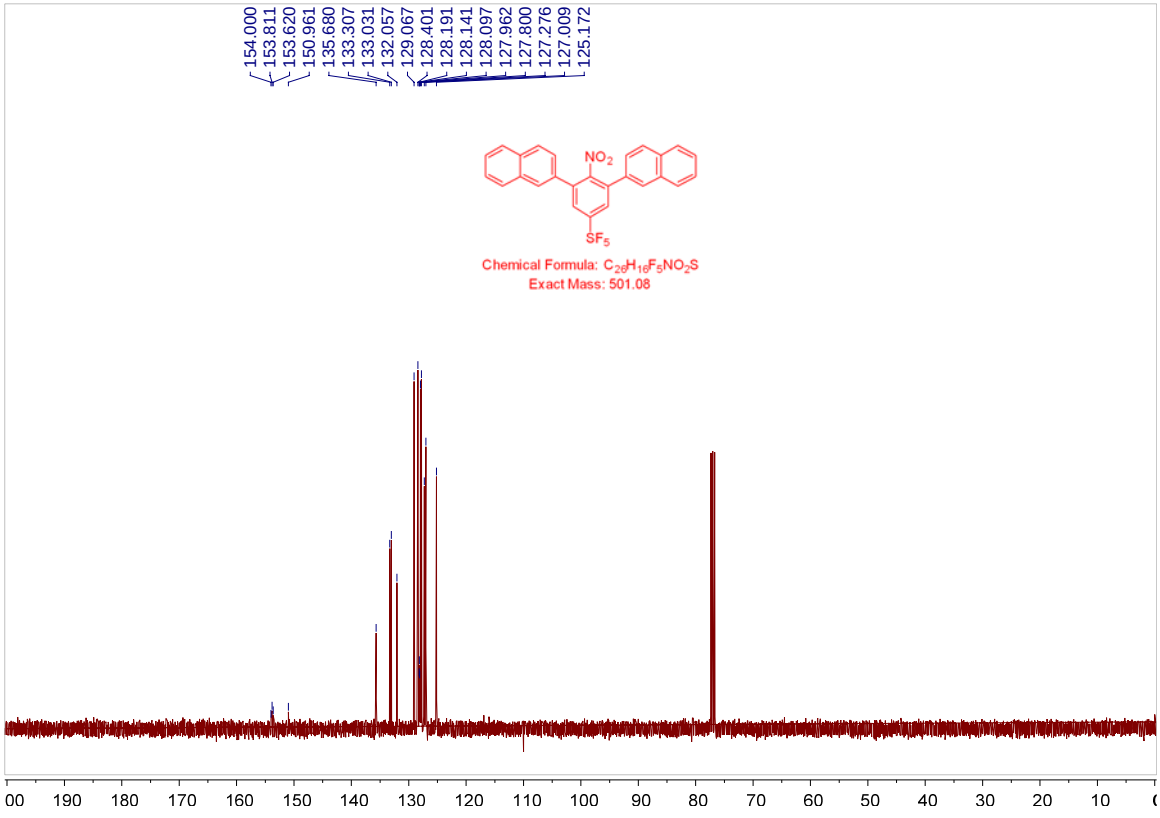

8.159
8.138
7.879
7.490
7.469
4.439
4.421
4.403
4.386
1.430
1.412
1.395
0.000
EtO2C
NO2
CO2Et
SF5
Chemical Formula: C20H10F11NO2S
Molecular Weight: 537.35
2.00
1.00
2.00
2.06
3.05
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

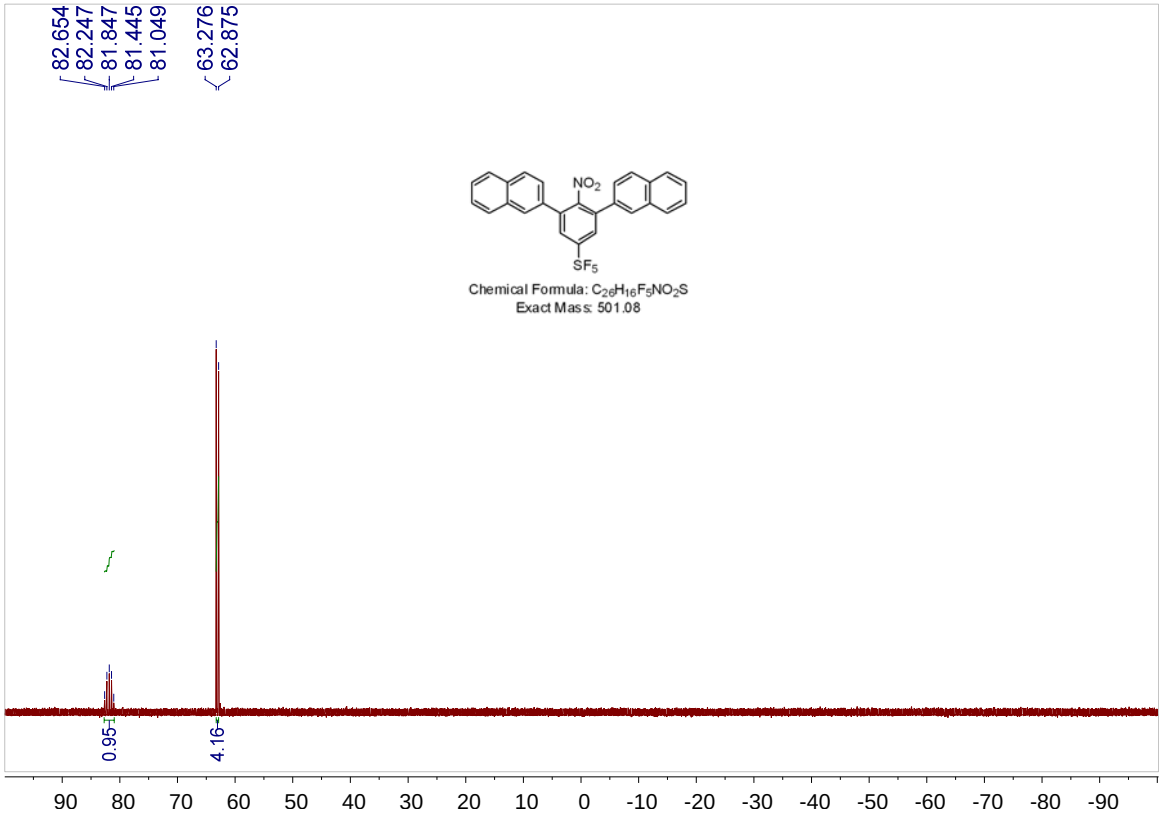

165.667
154.294
154.093
153.895
153.714
153.517
150.269
138.593
134.817
131.587
130.253
128.154
61.350
14.273
EtO2C
NO2
CO2Et
SF5
Chemical Formula: C20H10F11NO2S
Molecular Weight: 537.35
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10


82.066
81.661
81.261
80.858
80.460
63.253
62.852
EtO2C
NO2
CO2Et
SF5
Chemical Formula: C24H20F5NO6S
Exact Mass: 545.09
0.97
4.09
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90

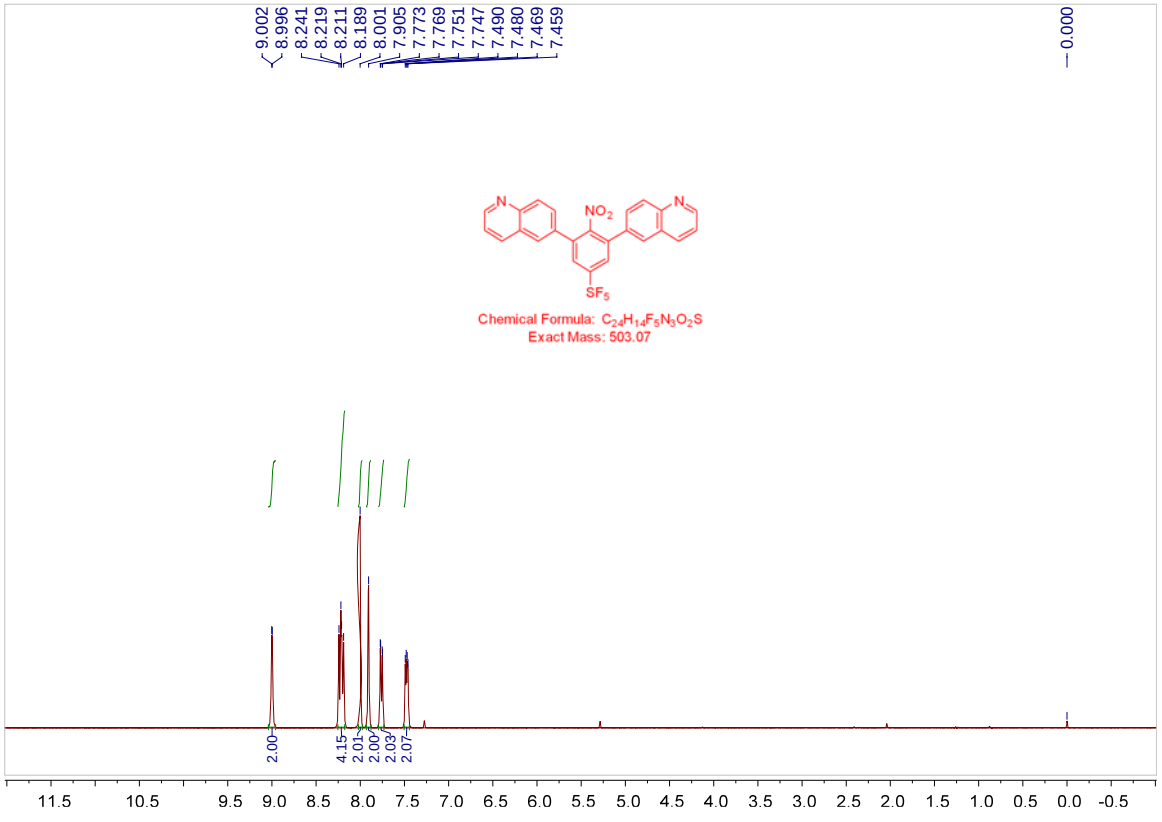
Compound 6j

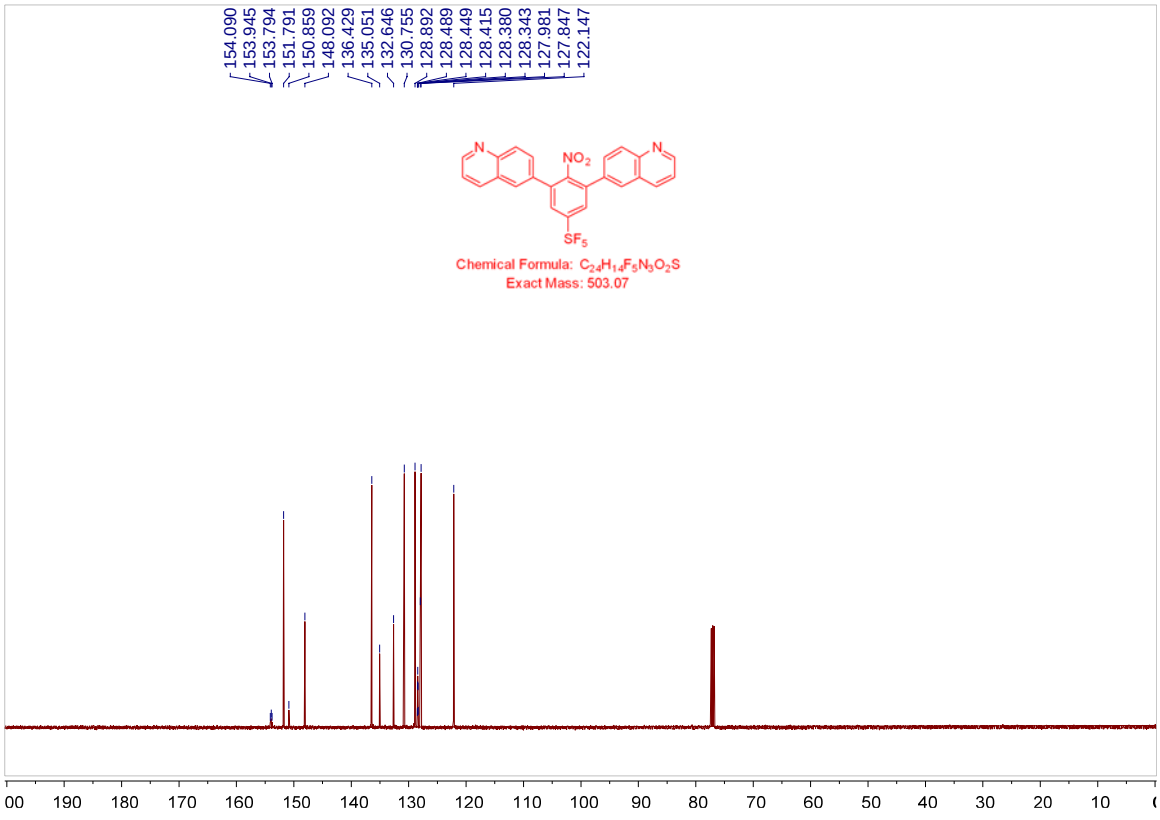

7.989
7.967
7.940
7.921
7.908
7.897
7.589
7.585
7.579
7.576
7.566
7.540
7.536
7.519
7.515
0.027
NO2
SF5
Chemical Formula: C26H16F5NO2S
Exact Mass: 501.08
2.00
8.11
4.00
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

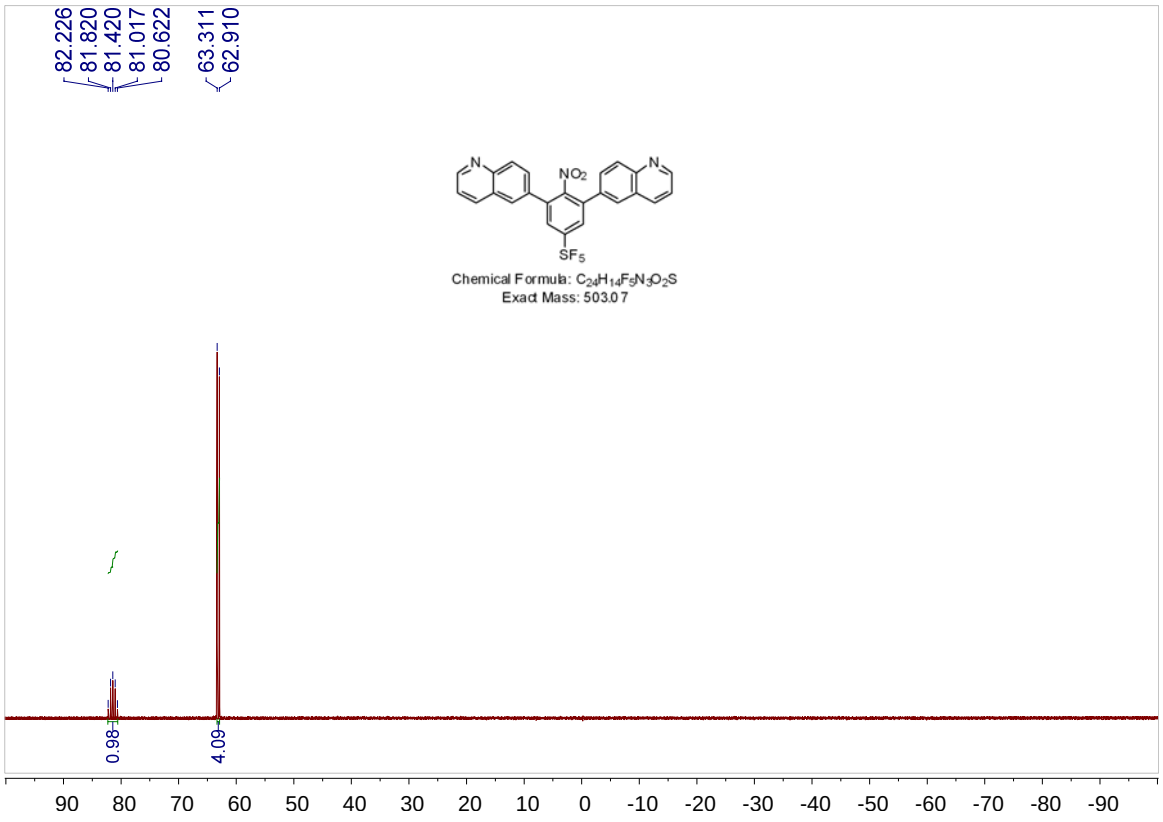

154.000
153.811
153.620
150.961
135.680
133.307
133.031
132.057
129.067
128.401
128.191
128.141
128.097
127.962
127.800
127.276
127.009
125.172
NO2
SF5
Chemical Formula: C26H16F5NO2S
Exact Mass: 501.08
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


82.654
82.247
81.847
81.445
81.049
63.276
62.875
NO2
SF5
Chemical Formula: C26H16F5NO2S
Exact Mass: 501.08
0.95
4.16
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90

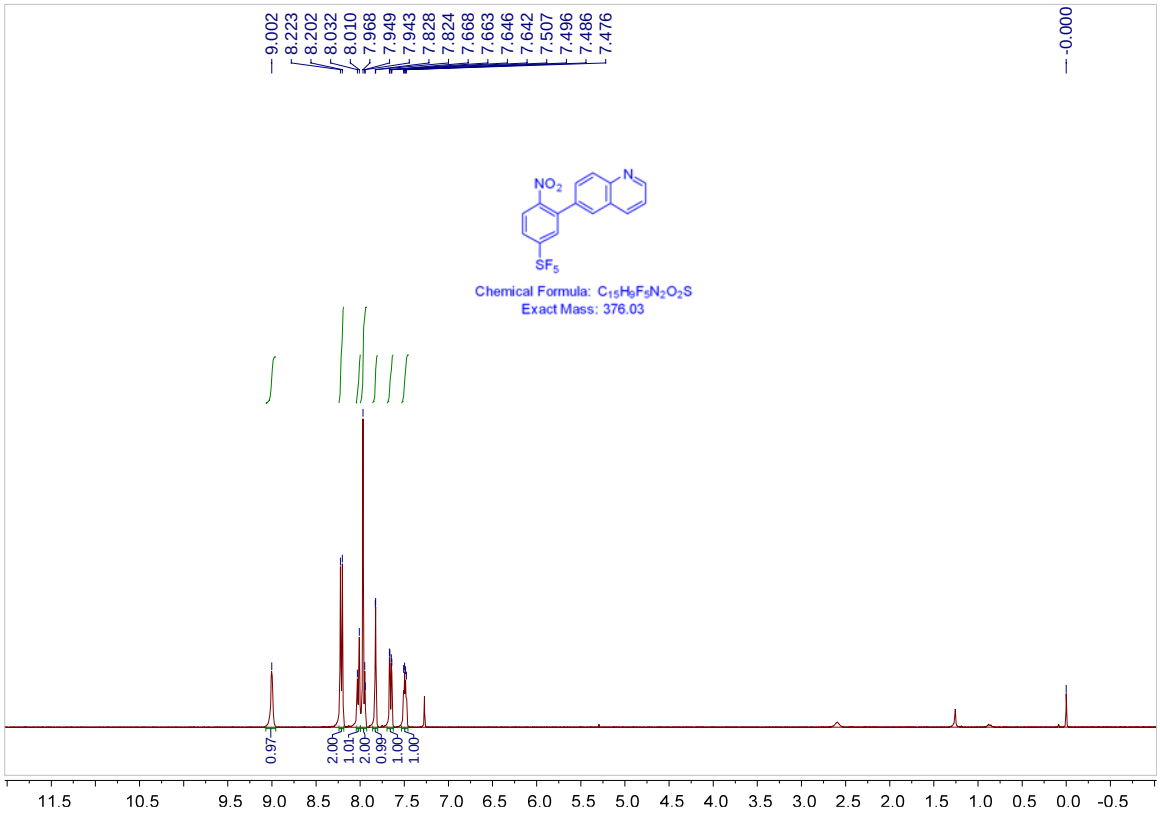
Compound 6k

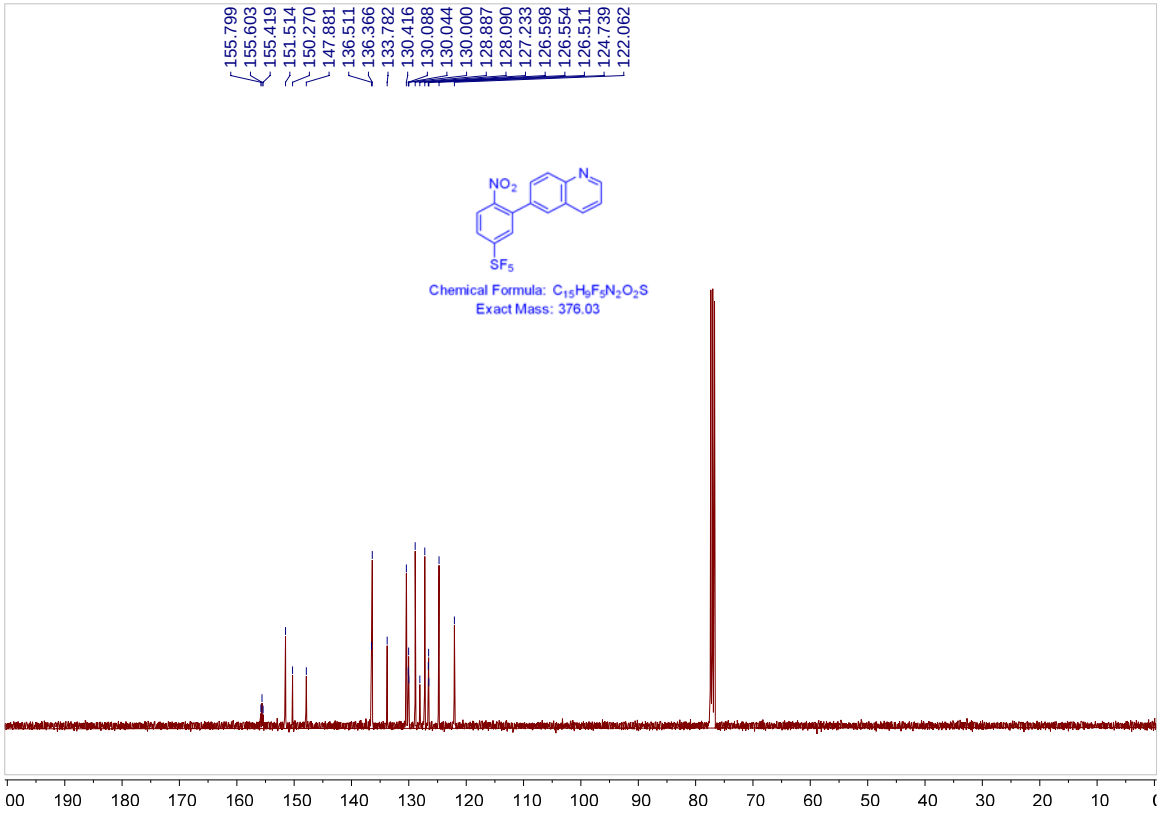

9.002
8.996
8.241
8.219
8.211
8.189
8.001
7.905
7.773
7.769
7.751
7.747
7.490
7.480
7.469
7.459
0.000
N
NO2
N
SF5
Chemical Formula: C24H14F5N3O2S
Exact Mass: 503.07
2.00
4.15
2.01
2.00
2.03
2.07
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

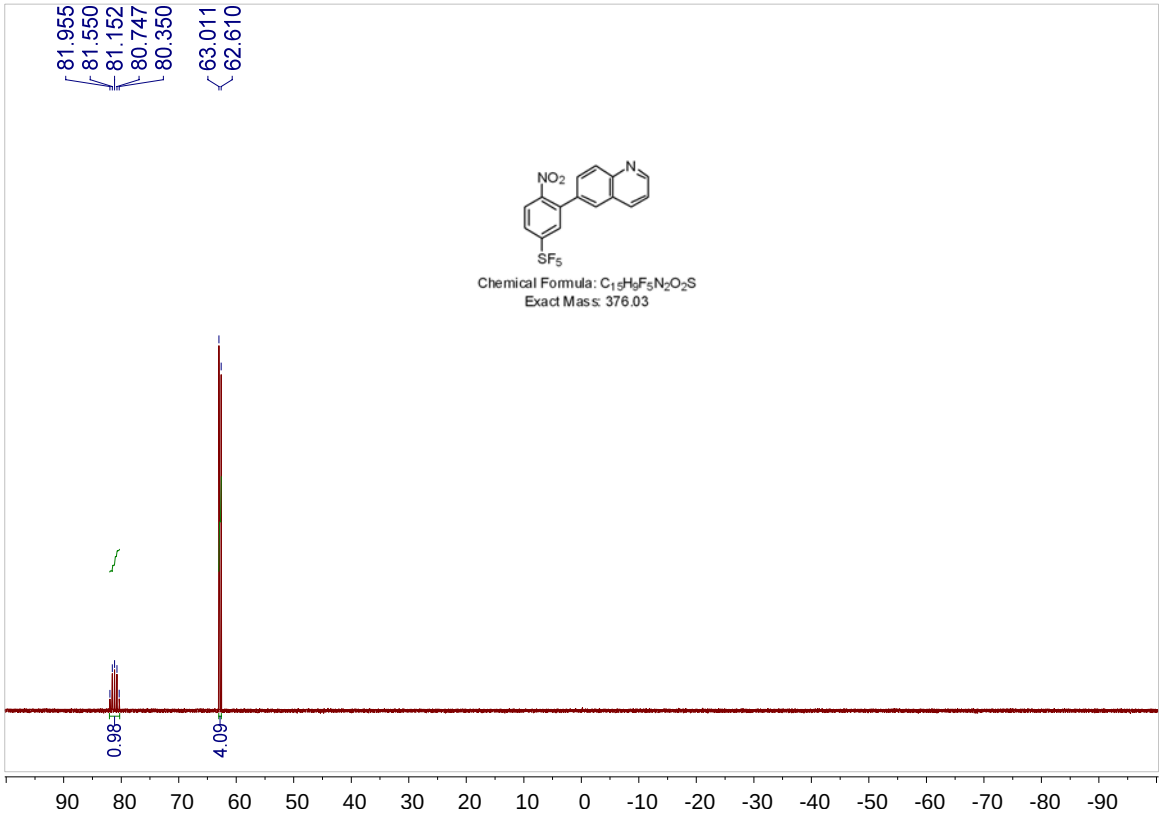

154.090
153.945
153.794
151.791
150.859
148.092
136.429
135.051
132.646
130.755
128.892
128.489
128.449
128.415
128.380
128.343
127.981
127.847
122.147
NO2
SF5
Chemical Formula: C24H14F5N3O2S
Exact Mass: 503.07


82.226
81.820
81.420
81.017
80.622
63.311
62.910
NO2
SF5
Chemical Formula: C24H14F5N3O2S
Exact Mass: 503.07
0.98
4.09

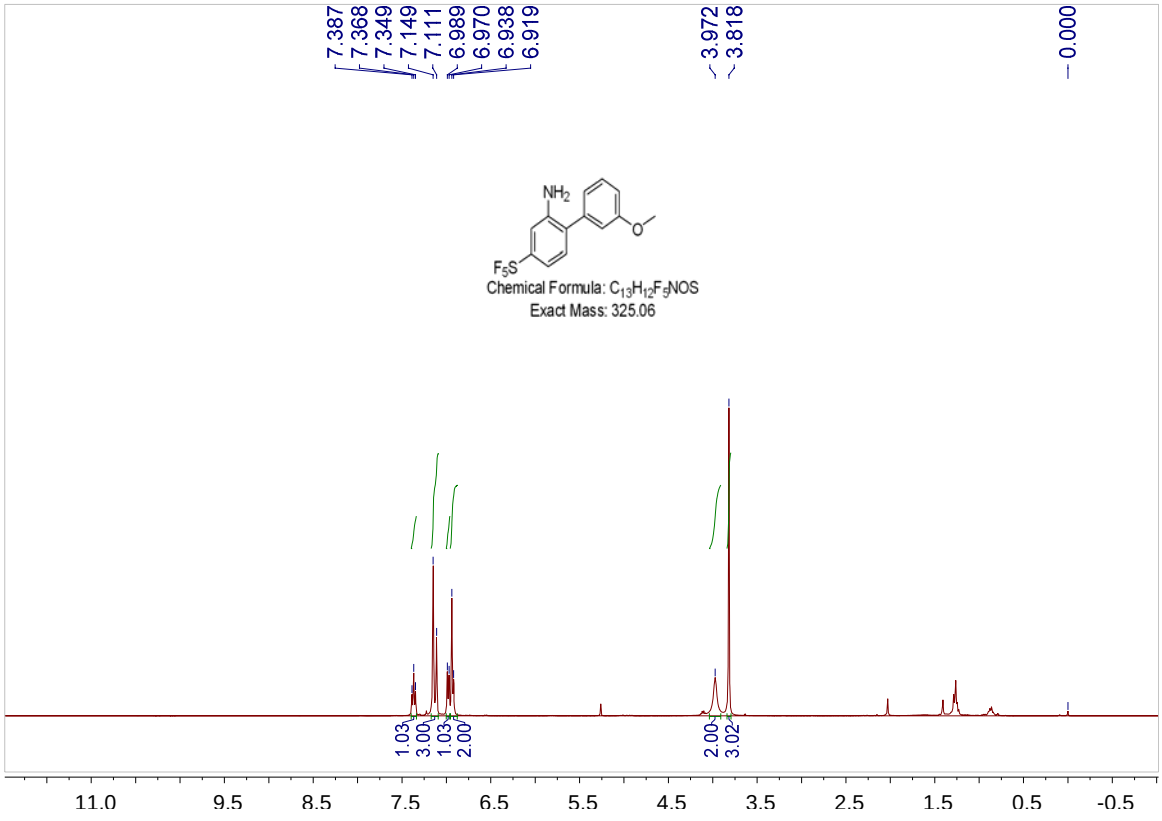
Compound 7k

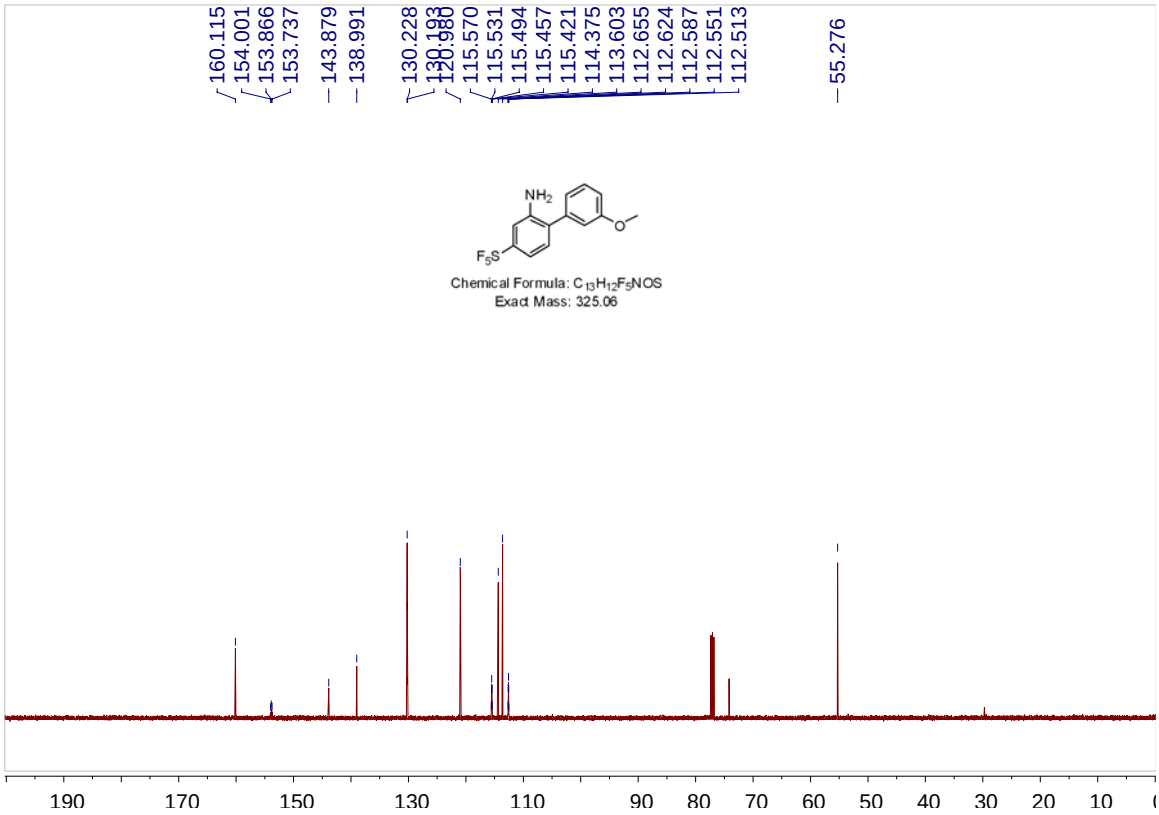

9.002
8.223
8.202
8.032
8.010
7.968
7.949
7.943
7.828
7.824
7.668
7.663
7.646
7.642
7.507
7.496
7.486
7.476
-0.000
NO2
N
SF5
Chemical Formula: C15H9F5N2O2S
Exact Mass: 376.03
0.97
2.00
1.01
2.00
0.99
1.00
1.00
1.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

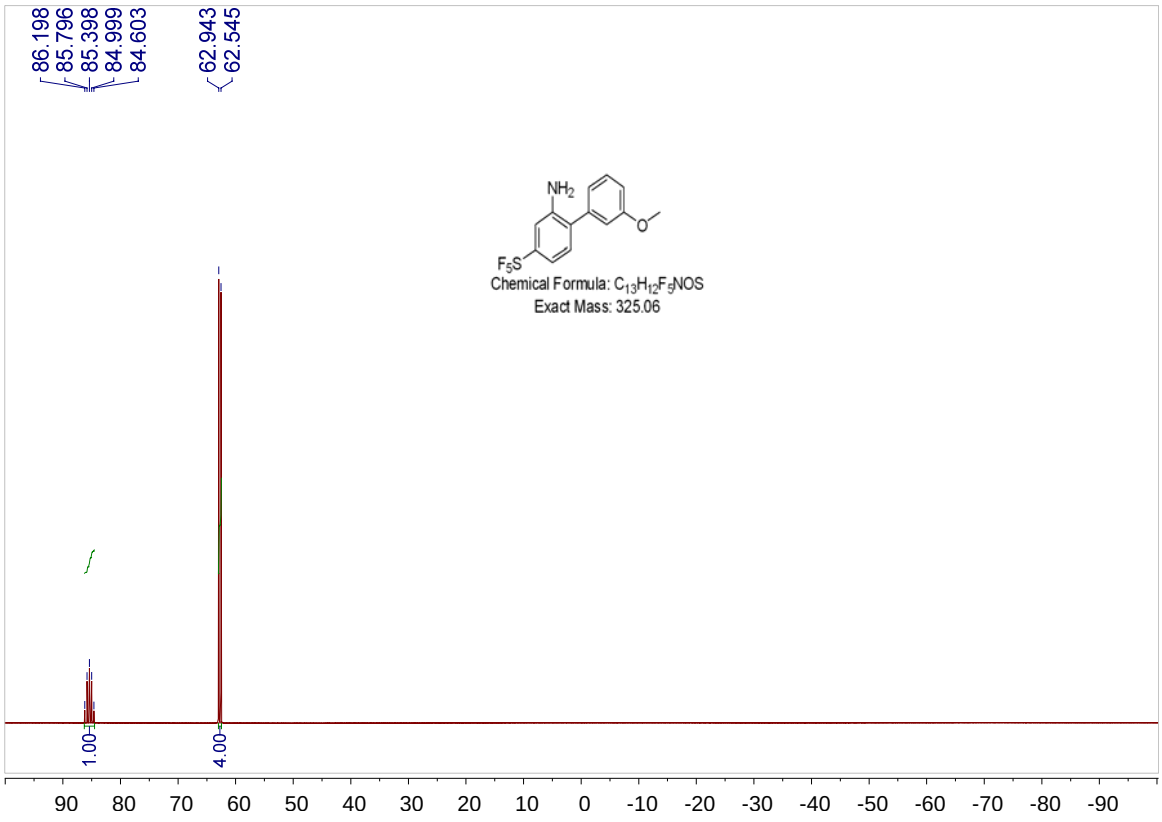

155.799
155.603
155.419
151.514
150.270
147.881
136.511
136.366
133.782
130.416
130.088
130.044
130.000
128.887
128.090
127.233
126.598
126.554
126.511
124.739
122.062
NO2
N
SF5
Chemical Formula: C15H9F5N2O2S
Exact Mass: 376.03
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


81.955
81.550
81.152
80.747
80.350
63.011
62.610
NO2
N
SF5
Chemical Formula: C15H9F5N2O2S
Exact Mass: 376.03
0.98
4.09
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90

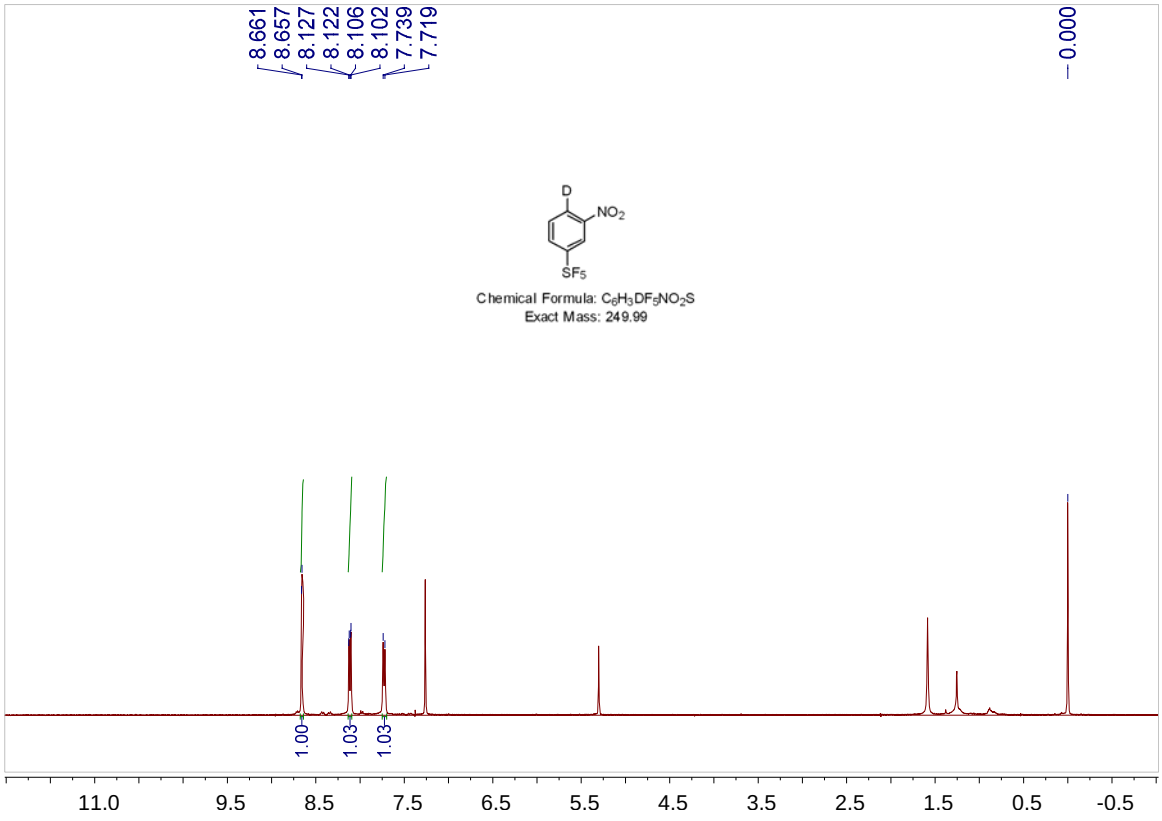
Compound 8

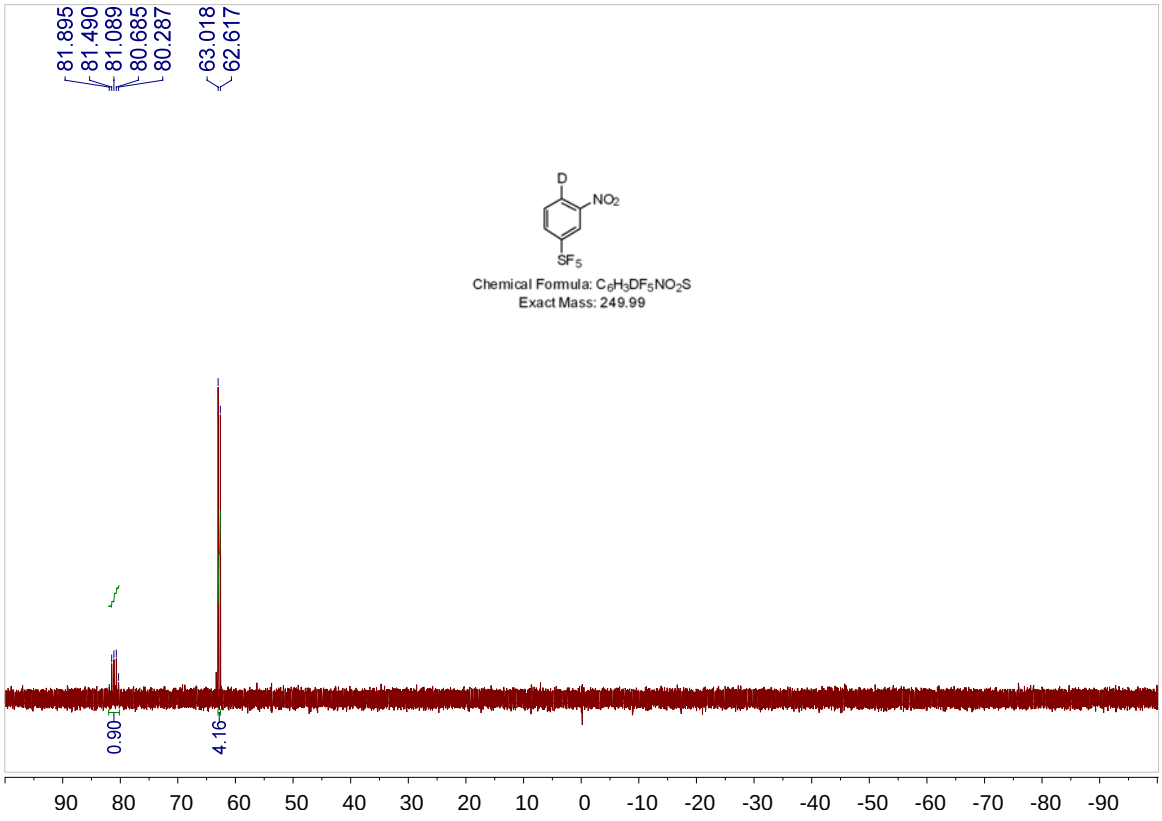

7.387
7.368
7.349
7.149
7.111
6.989
6.970
6.938
6.919
3.972
3.818
0.000
NH2
O
F5S
Chemical Formula: C13H12F5NOS
Exact Mass: 325.06
1.03
3.00
1.03
2.00
2.00
3.02
11.0 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5


160.115
154.001
153.866
153.737
143.879
138.991
130.228
130.193
120.980
115.570
115.531
115.494
115.457
115.421
114.375
113.603
112.655
112.624
112.587
112.551
112.513
55.276
NH2
O
F5S
Chemical Formula: C13H12F5NOS
Exact Mass: 325.06
190
170
150
130
110
90
80
70
60
50
40
30
20
10


86.198
85.796
85.398
84.999
84.603
62.943
62.545
NH2
O
F5S
Chemical Formula: C13H12F5NOS
Exact Mass: 325.06
1.00
4.00
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90

***d*-1**


8.661
8.657
8.127
8.122
8.106
8.102
7.739
7.719
0.000
D
NO2
SF5
Chemical Formula: C6H3DF5NO2S
Exact Mass: 249.99
1.00
1.03
1.03
11.0
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5


81.895
81.490
81.089
80.685
80.287
63.018
62.617
D
NO2
SF5
Chemical Formula: C6H3DF5NO2S
Exact Mass: 249.99
0.90
4.16
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90