Supporting Information

For

Identification of Monodentate Oxazoline as a Ligand for Copper-Promoted *ortho*-C–H Hydroxylation and Amination

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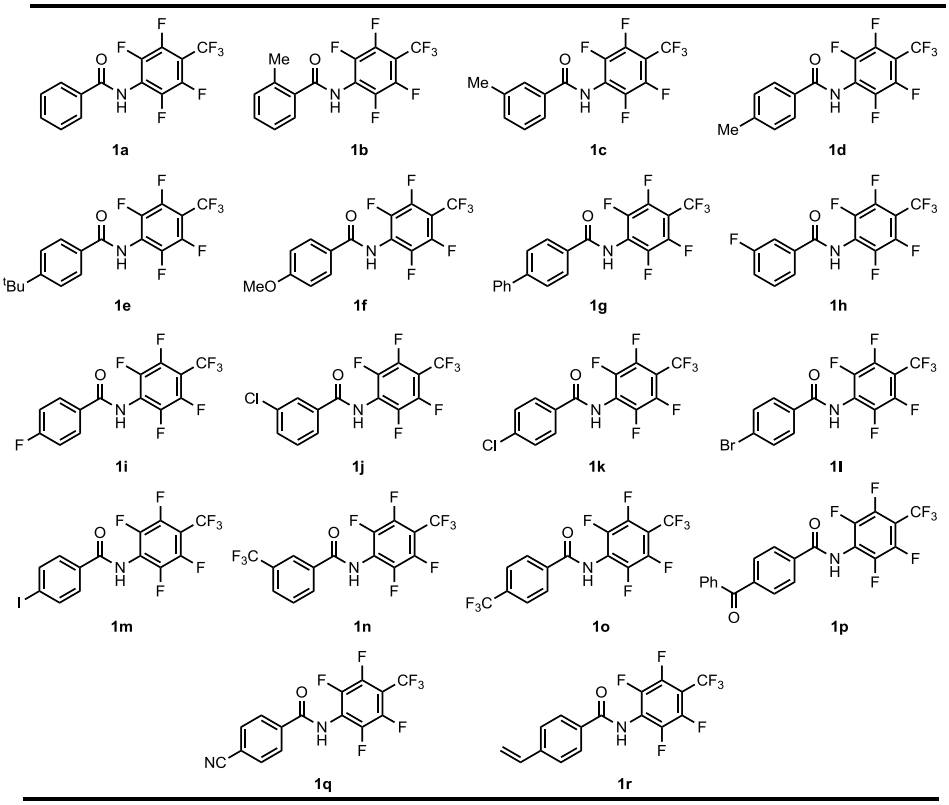
1. General Information

All commercial reagents were purchased from TCI, Sigma-Aldrich, Adamas-beta and Energy Chemical of the highest purity grade. They were used without further purification unless specified. ^{1}H and ^{13}C NMR spectra were recorded on Agilent AV 400, Varian Inova 400 (400 MHz and 100 MHz, respectively), and Agilent AV 600 (600 MHz and 150 MHz, respectively) instruments. ^{19}F NMR spectra were recorded on Agilent AV 400, Varian Inova 400 (375 MHz) instrument and are reported relative to the $CFCl_3$ as the internal standard. The peaks were internally referenced to TMS (0.00 ppm) or residual undeuterated solvent signal. The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, and br = broad. High resolution mass spectra were recorded at the Center for Mass Spectrometry, Shanghai Institute of Organic Chemistry.

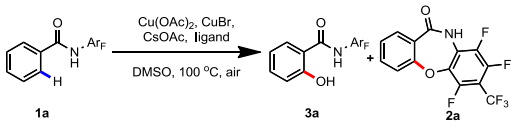
2. Experimental Section

2.1 Preparation of Substrates 1a-1r. [1]



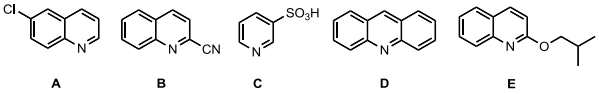
2.2 Optimization Studies.

Table 1. Screening of Pyridine and Quinoline Ligand.[a,b]



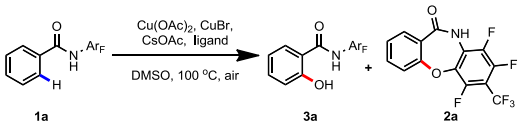
Entry	ligand	yield **3a**(%)	yield **2a**(%)	SM(%)
1	Pyridine	22	12	6
2	**A**	23	11	5
3	**B**	26	10	6
4	**C**	19	8	8
5	**D**	23	11	10
6	**E**	27	10	8

[a] **1a** (0.1 mmol), $Cu(OAc)_2$ (0.2 mmol), CuBr (0.08 mmol), CsOAc (0.2 mmol), ligand (0.1 mmol), DMSO(1 mL), 100°C, air, 6h. [b] the yield was determined by ^1H NMR analysis of crude product using CH_2Br_2 as an internal standard.



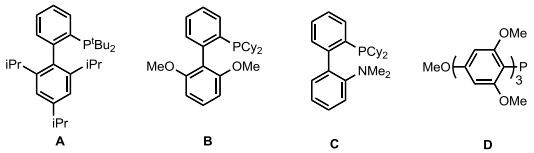
A **B** **C** **D** **E**

Table 2. Screening of Phosphine Ligand.[a,b]



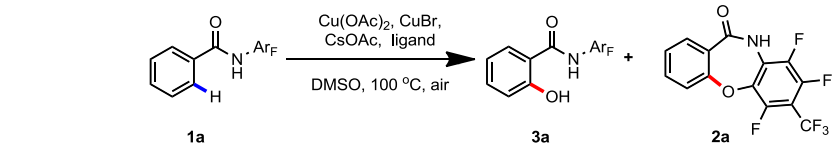
Entry	ligand	yield **3a**(%)
1	**PPh_3**	25
2	**A**	30
3	**B**	40
4	**C**	39
5	**D**	32
6	**PCy_3**	34

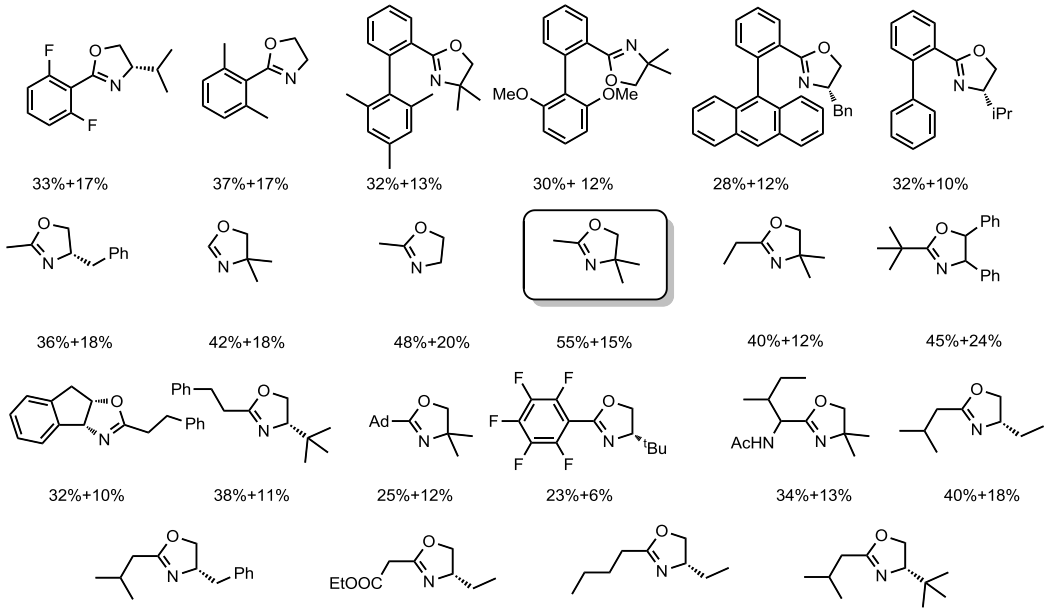
[a] **1a** (0.1 mmol), $Cu(OAc)_2$ (0.2 mmol), CuBr (0.08 mmol), CsOAc (0.2 mmol), ligand (0.1 mmol), DMSO(1 mL), 100°C, air, 6h. [b] the yield was determined by ^1H NMR analysis of crude product using CH_2Br_2 as an internal standard.



A **B** **C** **D**

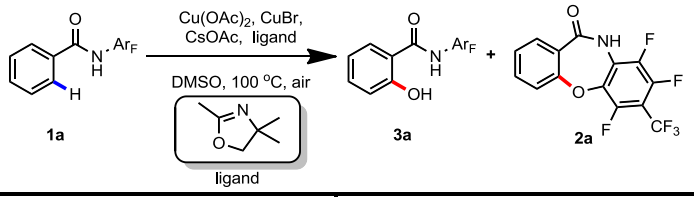
Table 3. Screening of Oxazoline Ligand.[a,b]





[a] Reaction conditions: **1a** (0.1 mmol), $Cu(OAc)_2$ (0.2 mmol), CuBr (0.08 mmol), CsOAc (0.2 mmol), ligand (0.1 mmol), DMSO (1.0 mL), 100 °C, air, 6 h. [b] Yield determined by ^1H NMR analysis of crudereaction mixture using CH_2Br_2 as an internal standard.

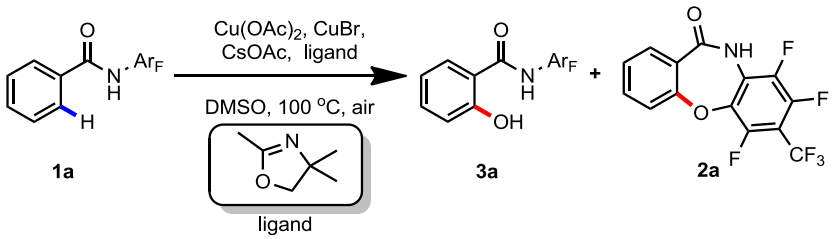
Table 4. Screening the Loading of CuBr.[a,b]



Entry	CuBr (eq)	yield(%, **3a**+**2a**, SM)	Entry	CuBr (eq)	yield(%, **3a**+**2a**, SM)
1	0	35+12 ,12	5	1.0	50+17, 12
2	0.2	41+14, 12	6	1.5	52+19, 10
3	0.5	43+16, 10	7	2.0	51+18, 12
4	0.8	55+15, 15			

[a] **1a** (0.1 mmol), $Cu(OAc)_2$ (0.2 mmol), CuBr (x eq), CsOAc (0.2 mmol), ligand (0.1 mmol), DMSO (1 mL), 100°C, air, 6h. [b] the yield was determined by ^1H NMR analysis of crude product using CH_2Br_2 as an internal standard.

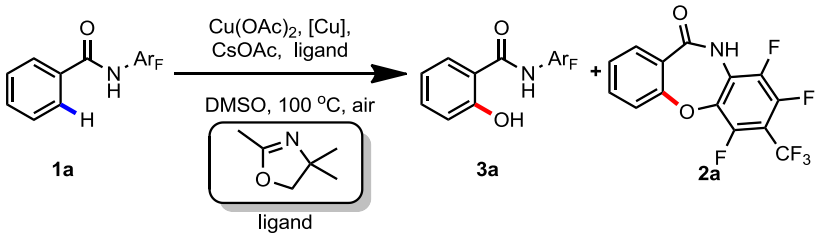
Table 5. Screening the Loading of $Cu(OAc)_2$.[a,b]



Entry	$Cu(OAc)_2$ (eq)	yield(%, **3a**+**2a**, SM)	Entry	$Cu(OAc)_2$ (eq)	yield(%, **3a**+**2a**, SM)
1	0	26+11 ,32	4	1.5	49+18, 20
2	0.5	41+15, 18	5	2.0	55+15, 15
3	1	44+16, 12			

[a] **1a** (0.1 mmol), $Cu(OAc)_2$ (x eq), CuBr (0.08 mmol), CsOAc (0.2 mmol), ligand (0.1 mmol), DMSO (1 mL), 100°C, air, 6h. [b] the yield was determined by ^{1}H NMR analysis of crude product using CH_2Br_2 as an internal standard.

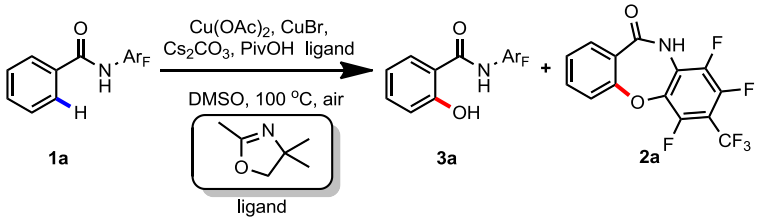
Table 6. The Effect of Combination Other Copper(I) Salts with $Cu(OAc)_2$.[a,b]



Entry	[Cu]	yield(%, **3a**+**2a**, SM)
1	CuOAc	32+14, 9
2	CuI	43+14, 14
3	CuTc	26+10, 20
4	$Cu(MeCN)_4PF_6$	34+12, 12
5	$Cu(OH)_2CO_3$	39+13, 18

[a] **1a** (0.1 mmol), $Cu(OAc)_2$ (0.2 mmol), [Cu] (0.08 mmol), CsOAc (0.2 mmol), ligand (0.1 mmol), DMSO (1 mL), 100°C, air, 6h. [b] the yield was determined by ^{1}H NMR analysis of crude product using CH_2Br_2 as an internal standard.

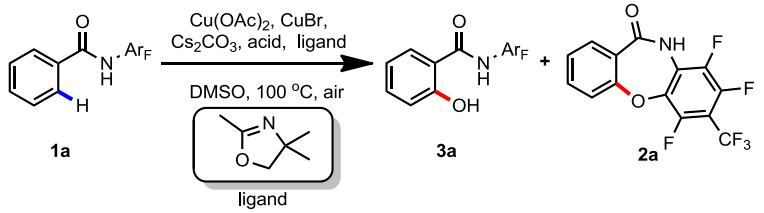
Table 7. Screening the Effect of Base and Acid.[a,b]



Entry	Cs_2CO_3+PivOH	yield(%, **3a**+**2a**, SM)
1	0.5 eq + 0.5 eq	44+10, 26
2	0.5 eq + 1.0 eq	42+9, 30
3	1.0 eq + 1.0 eq	57+14, 7
4	0.8 eq + 0.8 eq	47+12, 8
5	1.2 eq + 1.2 eq	57+16, 5
6	1.5 eq + 1.5 eq	59+12, 6
7	1.0 eq + 0.5 eq	54+17, 4
8	1.5 eq + 0.5 eq	52+19, 7
9	1.0 eq + 1.5 eq	55+12, 10

[a] **1a** (0.1 mmol), $Cu(OAc)_2$ (0.2 mmol), CuBr (0.08 mmol), Cs_2CO_3 (x eq), PivOH (x eq), ligand (0.1 mmol), DMSO (1 mL), 100°C, air, 6h. [b] the yield was determined by ^1H NMR analysis of crude product using CH_2Br_2 as an internal standard.

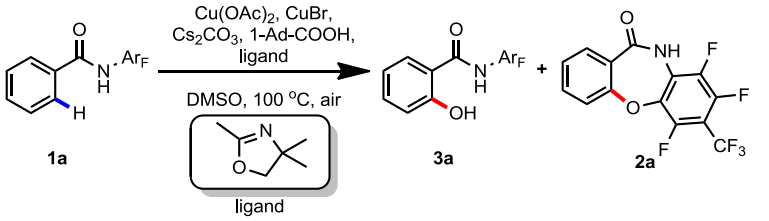
Table 8. Screening the Effect of Different Acids.[a,b]



Entry	acid	yield(%, **3a**+**2a**, SM)
1	-	37+17, 14
2	HOAc	49+17, 10
3	2,3,4,5,6-pentafluorobenzoic acid	41+21, 7
4	$TsOH{\cdot}H_2O$	48+12, 18
5	1-Ad-COOH	61+13, 6
6	1-Ad-COOH (1.8 eq)	63+12, 6

[a] **1a** (0.1 mmol), $Cu(OAc)_2$ (0.2 mmol), CuBr (0.08 mmol), Cs_2CO_3 (0.15 mmol), Acid (0.15 mmol), ligand (0.1 mmol), DMSO (1 mL), 100°C, air, 6h. [b] the yield was determined by ^1H NMR analysis of crude product using CH_2Br_2 as an internal standard.

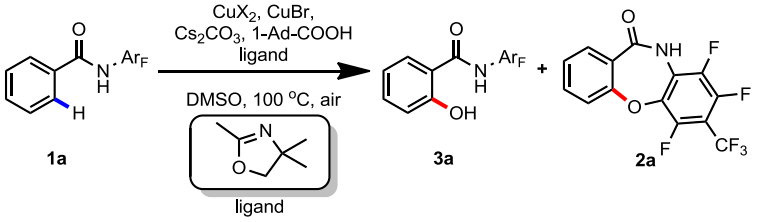
Table 9. Further Optimization of Reaction Parameter. [a,b]



Entry	DMSO	loading of $Cu(OAc)_2$	yield(%, **3a**+**2a**, SM)
1	1 mL	2 eq	63+12, 14
2	1 mL	1.5 eq	63+11, 12
3	0.5 mL	1.5 eq	66+8, trace
4[c]	0.5 mL	1.5 eq	67+8, trace

[a] **1a** (0.1 mmol), $Cu(OAc)_2$ (x eq), CuBr (0.08 mmol), Cs_2CO_3 (0.15 mmol), 1-Ad-COOH (0.18 mmol), ligand (0.1 mmol), DMSO (y mL), 100°C, air, 6h. [b] the yield was determined by ^1H NMR analysis of crude product using CH_2Br_2 as an internal standard. [c] 0.4 eq ligand

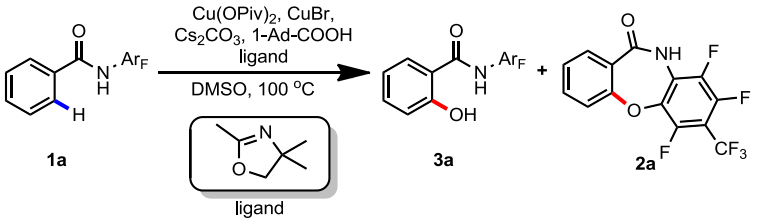
Table 10. Screening the Effect of CuX_2 salt. [a,b]



Entry	CuX_2	yield(%, **3a**+**2a**, SM)
1	$Cu(OPiv)_2$	75+0, 8
2	$Cu(^iPrCOO)_2$	68+0, trace
3	$Cu(1\text{-}AdCOO)_2$	45+trace, 15
4[c]	$Cu(OPiv)_2$	80+0, trace

[a] **1a** (0.1 mmol), CuX_2 (0.15 mmol), CuBr (0.08mmol), Cs_2CO_3 (0.15 mmol), 1-Ad-COOH (0.18 mmol), ligand (0.04 mmol), DMSO (0.5 mL), 100°C, air, 6h. [b] the yield was determined by ^1H NMR analysis of crude product using CH_2Br_2 as an internal standard [c] 105°C

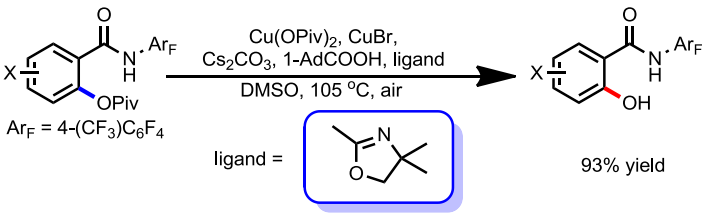
Table 11. Screening the Effect of Atmosphere. [a,b]



Entry	atmosphere	yield(%, **3a**+**2a**, SM)
1	Ar	56+0, 30
2	O_2	42+0, 30
3	air	80+0, trace

[a] **1a** (0.1 mmol), $Cu(OPiv)_2$ (0.15 mmol), CuBr (0.08 mmol), Cs_2CO_3 (0.15 mmol), 1-Ad-COOH (0.18 mmol), ligand (0.04 mmol), DMSO (0.5 mL), 105°C, atmosphere, 6h. [b] the yield was determined by ^1H NMR analysis of crude product using CH_2Br_2 as an internal standard.

2.3 Control Experiment.



2.4 Typical Procedure for Copper Promoted *ortho*- C–H Hydroxylation.

To a 15 mL sealed tube was added substrates **1** (0.1 mmol, 1 equiv), $Cu(OPiv)_2$ (0.15 mmol), CuBr (0.08 mmol), Cs_2CO_3 (0.15 mmol), 1-Ad-COOH (0.18 mmol), ligand **L15** (0.04 mmol) and DMSO (0.5 mL). The reaction tube was then placed into a pre-heated oil bath and stirred at 105°C for 6h under air. Upon completion, EtOAc was added to dilute the mixture and then washed with $NH_3 \cdot H_2O$ and saturated NaCl(aq). The organic fraction was dried over Na_2SO_4, evaporated and purified by preparative TLC (EtOAc/hexane) to provide the corresponding products as white solids.

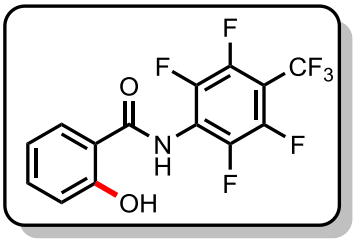
2.5 Typical Procedure for Copper Promoted *ortho*-C–H Amination.

To a 15 mL sealed tube was added substrates **1** (0.1 mmol, 1 equiv), alkyl amine **4** (0.3 mmol), $Cu(OAc)_2$ (0.2 mmol), CuBr (0.1 mmol), CsOAc (0.2 mmol), LiOAc (0.1 mmol), ligand **L15** (0.05 mmol) and DMSO (1 mL). The reaction tube was then

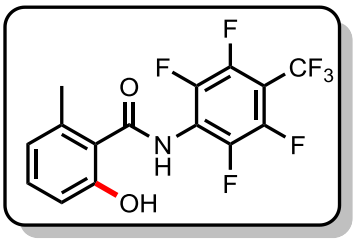
placed into a pre-heated oil bath and stirred at 100°C for 6h under air. Upon completion, EtOAc was added to dilute the mixture and then washed with NH_3 H_2O and saturated NaCl(aq). The organic fraction was dried over Na_2SO_4, evaporated and purified by preparative TLC (EtOAc/hexane) to provide the corresponding products as white solids.

3. Analytical Data.

3.1 Characterization of Products 3a-3r, 5a-5k.

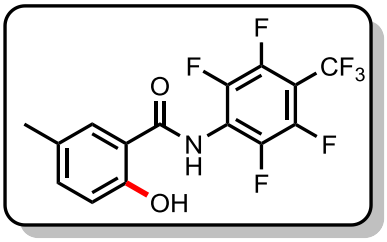


2-hydroxy-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (3a): white solid. Mp = 165 – 167 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 11.04 (s, 1H), 7.81 (s, 1H), 7.63 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.57 – 7.51 (m, 1H), 7.08 (d, *J* = 7.8 Hz, 1H), 6.99 (t, *J* = 7.6 Hz, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 167.75, 161.72, 136.05, 126.61, 119.59, 119.06, 113.00. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -56.08 (t, *J* = 21.7 Hz), -139.95 – -140.25 (m), -142.35 – -142.56 (m). **IR** (film): 3265, 1645, 1612, 1476, 1336, 1221, 994, 755. **HRMS** (DART) m/z Calcd for $C_{14}H_7F_7NO_2$ $[M]^+$ 354.0365, found 354.0359.

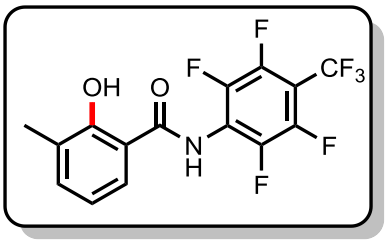


2-hydroxy-6-methyl-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (3b): white solid. Mp = 167 – 168 °C. **^{1}H NMR** (400 MHz, acetone-d_6) δ 9.43 (s, 1H),

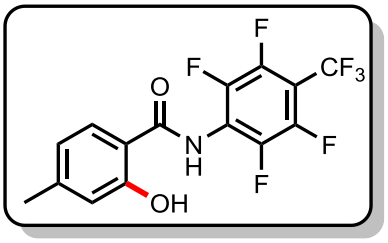
7.19 (t, *J* = 7.9 Hz, 1H), 6.82 (dd, *J* = 13.0, 7.9 Hz, 2H), 2.41 (s, 3H). **^{13}C NMR** (150 MHz, acetone-d_6) δ 166.09, 155.20, 138.35, 131.37, 123.38, 122.33, 113.91, 19.58. **^{19}F NMR** (376 MHz, acetone-d_6) δ -56.69 – -56.80 (m), -143.63, -144.12 – -144.44 (m). **IR** (film): 3348, 2857, 1738, 1514, 1335, 1030, 792, 708. **HRMS** (DART) m/z Calcd for $C_{15}H_9F_7NO_2$ $[M]^+$ 368.0522, found 368.0515.



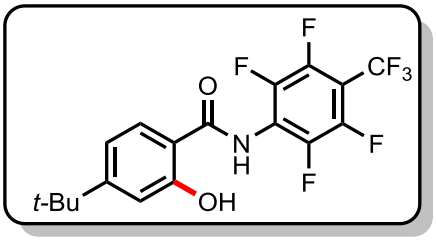
2-hydroxy-5-methyl-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (3c): white solid. Mp = 174 – 175 °C. **^{1}H NMR** (400 MHz, acetone-d_6) δ 7.85 (s, 1H), 7.37 (dd, *J* = 8.4, 1.8 Hz, 1H), 6.95 (d, *J* = 8.4 Hz, 1H), 2.30 (s, 3H). **^{13}C NMR** (150 MHz, acetone-d_6) δ 167.30, 158.13, 136.03, 128.75, 128.69, 117.61, 114.10, 19.46. **^{19}F NMR** (376 MHz, acetone-d_6) δ -56.78 – -56.90 (m), -143.90 – -143.93 (m). **IR** (film): 3286, 2924, 2855, 1663, 1479, 1142, 993, 751. **HRMS** (DART) m/z Calcd for $C_{15}H_9F_7NO_2$ $[M]^+$ 368.0522, found 368.0509.



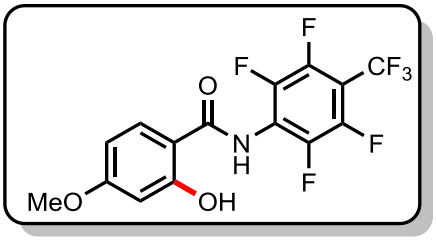
2-hydroxy-3-methyl-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (3c'): white solid. **^{1}H NMR** (400 MHz, acetone-d_6) δ 11.89 (s, 1H), 10.21 (s, 1H), 7.87 (d, *J* = 8.2 Hz, 1H), 7.45 (d, *J* = 7.3 Hz, 1H), 6.90 (t, *J* = 7.7 Hz, 1H), 2.25 (s, 3H). **^{13}C NMR** (150 MHz, acetone-d_6) δ 169.49, 160.25, 136.27, 127.19, 125.25, 118.59, 112.43, 14.79. **^{19}F NMR** (376 MHz, acetone-d_6) δ -56.83 – -56.94 (m), -143.89 – -143.94 (m). **IR** (film): 2922, 1682, 1473, 1335, 1130, 798, 714. **HRMS** (DART) m/z Calcd for $C_{15}H_9F_7NO_2$ $[M]^+$ 368.0522, found 368.0511.



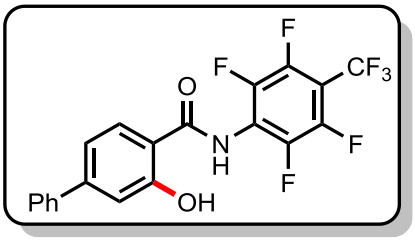
2-hydroxy-4-methyl-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (3d): white solid. Mp = 178 – 180 °C. **^{1}H NMR** (400 MHz, acetone-d_6) δ 7.93 (d, *J* = 8.1 Hz, 1H), 6.87 (s, 1H), 6.81 (d, *J* = 8.1 Hz, 1H), 2.34 (s, 3H). **^{13}C NMR** (100 MHz, acetone-d_6) δ 167.49, 160.80, 146.43, 128.63, 120.39, 117.98, 111.89, 20.68. **^{19}F NMR** (376 MHz, acetone-d_6) δ -56.79 (t, J = 21.7 Hz), -143.86 – -144.14 (m). **IR** (film): 2922, 1630, 1472, 1336, 1177, 1058, 711. **HRMS** (DART) m/z Calcd for $C_{15}H_9F_7NO_2$ $[M]^+$ 368.0522, found 368.0513.



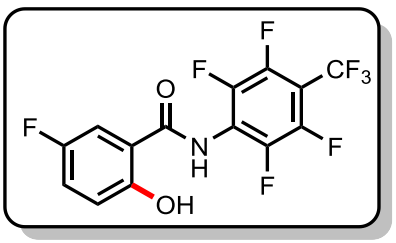
4-(tert-butyl)-2-hydroxy-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (3e): white solid. Mp = 152 – 154 °C. **^{1}H NMR** (400 MHz, acetone-d_6) δ 10.71 (s, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.10 (dd, *J* = 8.5, 1.4 Hz, 1H), 7.06 (d, *J* = 1.7 Hz, 1H), 1.33 (s, 9H). **^{13}C NMR** (100 MHz, acetone-d_6) δ 168.58, 161.68, 160.57, 129.34, 118.10, 115.57, 112.55, 35.82, 31.20. **^{19}F NMR** (376 MHz, acetone-d_6) δ -56.82 (m), -143.88 (m). **IR** (film): 2968, 1627, 1471, 1338, 1143, 998, 709. **HRMS** (DART) m/z Calcd for $C_{18}H_{15}F_7NO_2$ $[M]^+$ 410.0991, found 410.0983.



2-hydroxy-4-methoxy-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (3f): white solid. Mp = 166 – 167 °C. **^{1}H NMR** (400 MHz, acetone-d_6) δ 7.97 (d, *J* = 8.9 Hz, 1H), 6.58 (dd, J = 8.9, 2.5 Hz, 1H), 6.54 (d, *J* = 2.5 Hz, 1H), 3.88 (s, 3H). **^{13}C NMR** (100 MHz, acetone-d_6) δ 167.88, 165.50, 163.48, 129.80, 107.27, 106.74, 101.26, 55.13. **^{19}F NMR** (376 MHz, acetone-d_6) δ -56.67 – -56.85 (m), -144.14 (d, *J* = 11.2 Hz). **IR** (film): 3145, 1625, 1475, 1335, 1214, 1144, 993, 861, 706. **HRMS** (DART) m/z Calcd for $C_{15}H_9F_7NO_3$ $[M]^+$ 384.0471, found 384.0462.

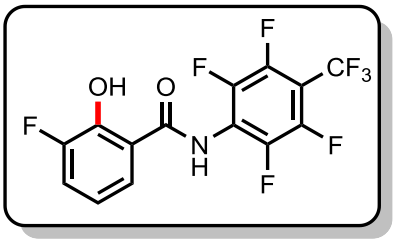


3-hydroxy-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)-[1,1'-biphenyl]-4-carboxamide (3g): white solid. Mp =242 – 244 °C. **^{1}H NMR** (400 MHz, acetone-d_6) δ 8.14 (d, *J* = 8.2 Hz, 1H), 7.74 (d, *J* = 7.5 Hz, 2H), 7.51 (t, *J* = 7.5 Hz, 2H), 7.45 (d, *J* = 7.0 Hz, 1H), 7.34 (d, *J* = 7.8 Hz, 2H). **^{13}C NMR** (150 MHz, acetone-d_6) δ 167.34, 160.87, 147.83, 139.17, 129.39, 128.97, 128.55, 127.02, 118.19, 115.69, 113.24. **^{19}F NMR** (376 MHz, acetone-d_6) δ -56.71 – -56.97 (m), -143.65 – -144.00 (m). **IR** (film): 2975, 1638, 1470, 1338, 1140, 996, 713. **HRMS** (DART) m/z Calcd for $C_{20}H_{11}F_7NO_2$ $[M]^+$ 430.0678, found 430.0662.

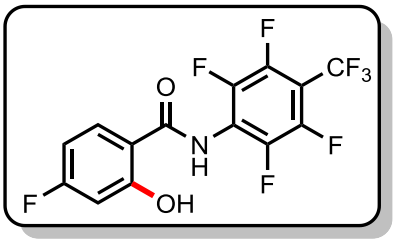


5-fluoro-2-hydroxy-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (3h): white solid. Mp = 188 – 189 °C. **^{1}H NMR** (400 MHz, acetone-d_6) δ 7.86 (dt, *J* = 8.1, 1.3 Hz, 1H), 7.44 (m, 1H), 7.00 (td, *J* = 8.1, 4.8 Hz, 1H). **^{13}C NMR** (100 MHz, acetone-d_6) δ 166.70 (d, *J* = 3.3 Hz), 151.80 (d, *J* = 243.5 Hz), 148.87, 124.05 (d, *J* =

3.6 Hz), 120.78 (d, *J* = 17.9 Hz), 118.94 (d, *J* = 7.0 Hz), 116.89 (d, *J* = 2.8 Hz). **^{19}F NMR** (376 MHz, acetone-d_6) δ -56.65 – -57.08 (m), -137.29 (dd, *J* = 10.7, 4.0 Hz), -143.74 (d, *J* = 11.0 Hz). **IR** (film): 2918, 1663, 1472, 1334, 1145, 996, 748. **HRMS** (DART) m/z Calcd for $C_{14}H_6F_8NO_2$ $[M]^+$ 372.0271, found 372.0264.

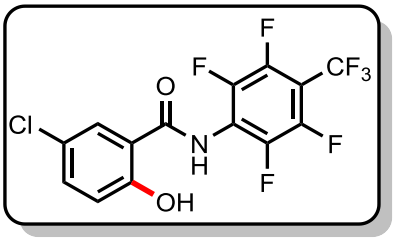


3-fluoro-2-hydroxy-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (3h'): white solid. **^{1}H NMR** (400 MHz, acetone-d_6) δ 7.82 (dd, *J* = 9.4, 3.2 Hz, 1H), 7.37 (ddd, *J* = 9.0, 7.9, 3.1 Hz, 1H), 7.11 (dd, *J* = 9.1, 4.6 Hz, 1H). **^{13}C NMR** (100 MHz, acetone-d_6) δ 166.07, 156.37 (d, *J* = 1.7 Hz), 156.16 (d, *J* = 236.8 Hz), 122.76 (d, *J* = 23.7 Hz), 119.75 (d, *J* = 7.6 Hz), 116.07 (d, *J* = 6.9 Hz), 115.29 (d, *J* = 24.9 Hz). **^{19}F NMR** (376 MHz, acetone-d_6) δ -56.93 (t, *J* = 22.0 Hz), -125.34 (ddd, *J* = 9.3, 8.1, 4.6 Hz), -143.65 – -144.01 (m). **IR** (film): 3273, 2974, 1640, 1478, 1335, 1146, 1001, 773. **HRMS** (DART) m/z Calcd for $C_{14}H_6F_8NO_2$ $[M]^+$ 372.0271, found 372.0267.

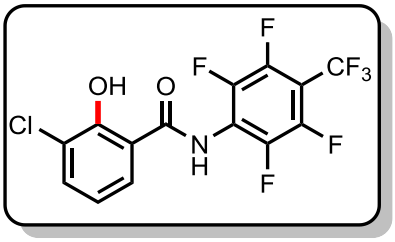


4-fluoro-2-hydroxy-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (3i): white solid. Mp = 205 – 206 ^{o}C. **^{1}H NMR** (400 MHz, acetone-d_6) δ 8.17 – 8.12 (m, 1H), 6.88 – 6.78 (m, 2H). **^{13}C NMR** (150 MHz, acetone-d_6) δ 167.64 (d, *J* = 252.7 Hz), 167.76, 163.57 (d, *J* = 13.5 Hz), 132.41 (d, *J* = 11.6 Hz), 112.42 (d, *J* = 2.5 Hz), 108.26 (d, *J* = 22.8 Hz), 105.32 (d, *J* = 24.3 Hz). **^{19}F NMR** (376 MHz, acetone-d_6) δ -56.76 – -56.95 (m), -104.08 – -104.26 (m), -143.71 – -143.90 (m). **IR**

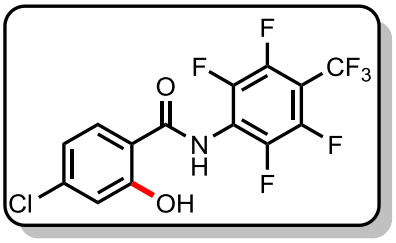
(film): 3223, 2971, 1640, 1476, 1336, 1229, 1150, 991, 714. **HRMS** (DART) m/z Calcd for $C_{14}H_6F_8NO_2$ $[M]^+$ 372.0271, found 372.0263.



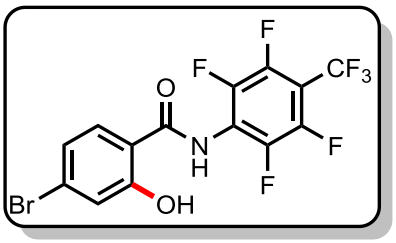
5-chloro-2-hydroxy-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (3j): white solid. Mp = 163 – 164 ^oC. **^{1}H NMR** (400 MHz, acetone-d_6) δ 8.07 (d, *J* = 2.6 Hz, 1H), 7.55 (dd, *J* = 8.9, 2.6 Hz, 1H), 7.11 (d, *J* = 8.9 Hz, 1H). **^{13}C NMR** (100 MHz, acetone-d_6) δ 165.77, 158.75, 134.80, 128.57, 123.81, 119.68, 116.21. **^{19}F NMR** (376 MHz, acetone-d_6) δ -56.83 (t, *J* = 21.6 Hz), -143.57 – -143.91 (m). **IR** (film): 3054, 1625, 1470, 1329, 1144, 995, 709. **HRMS** (DART) m/z Calcd for $C_{14}H_6ClF_7NO_2$ $[M]^+$ 387.9975, found 387.9968.



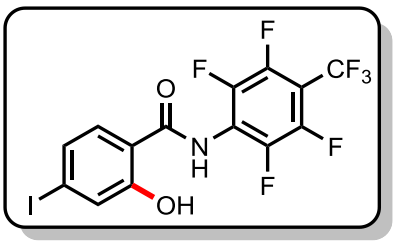
3-chloro-2-hydroxy-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (3j'): white solid. **^{1}H NMR** (400 MHz, acetone-d_6) δ 7.91 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.33 (dd, *J* = 7.6, 1.4 Hz, 1H), 6.48 (t, *J* = 7.7 Hz, 1H). **^{13}C NMR** (100 MHz, acetone-d_6) δ 168.16, 157.86, 135.07, 127.13, 122.54, 118.79, 115.64. **^{19}F NMR** (376 MHz, acetone-d^6) δ -56.16 (t, *J* = 21.5 Hz), -145.18 (d, *J* = 13.2 Hz), -145.91 – -146.17 (m). **IR** (film): 2904, 1671, 1648, 1545, 1508, 1338, 1248, 1149, 998, 878, 738, 632. **HRMS** (DART) m/z Calcd for $C_{14}H_6ClF_7NO_2$ $[M]^+$ 387.9975, found 387.9968.



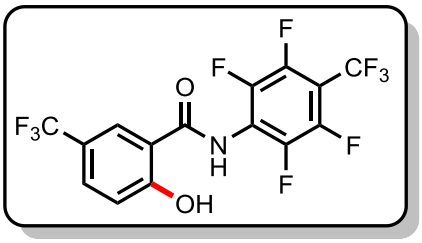
4-chloro-2-hydroxy-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (3k): white solid. Mp = 200 – 201 ^{o}C. **^{1}H NMR** (400 MHz, acetone-d^{6}) δ 8.07 (d, *J* = 8.6 Hz, 1H), 7.12 (d, *J* = 2.0 Hz, 1H), 7.10 – 7.05 (m, 1H). **^{13}C NMR** (100 MHz, acetone-d_6) δ 166.51, 160.92, 140.07, 130.46, 119.83, 117.55, 113.58. **^{19}F NMR** (376 MHz, acetone-d_6) δ -56.76 – -56.92 (m), -143.66 – -143.82 (m). **IR** (film): 3114, 1633, 1474, 1336, 1152, 997, 718. **HRMS** (DART) m/z Calcd for $C_{14}H_6ClF_7NO_2$ $[M]^+$ 387.9975, found 387.9967.



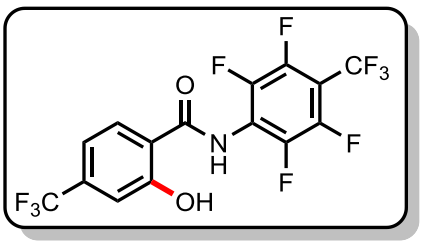
4-bromo-2-hydroxy-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (3l): white solid. Mp = 210 – 211 ^{o}C. **^{1}H NMR** (400 MHz, acetone-d^{6}) δ 7.99 (d, *J* = 8.5 Hz, 1H), 7.28 (d, *J* = 1.9 Hz, 1H), 7.21 (dd, *J* = 8.5, 1.9 Hz, 1H). **^{13}C NMR** (100 MHz, acetone-d_6) δ 166.54, 160.90, 130.57, 128.50, 122.70, 120.69, 114.12. **^{19}F NMR** (376 MHz, acetone-d_6) δ -56.75 – -56.90 (m), -143.59 – -143.84 (m). **IR** (film): 3104, 1631, 1578, 1478, 1331, 1216, 1147, 992, 908, 865, 736. **HRMS** (DART) m/z Calcd for $C_{14}H_6BrF_7NO_2$ $[M]^+$ 431.9470, found 431.9462.



2-hydroxy-4-iodo-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (3m): white solid. Mp = 212 – 213 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 11.12 (s, 1H), 7.70 (s, 1H), 7.51 (d, *J* = 1.5 Hz, 1H), 7.33 (dt, *J* = 18.3, 5.0 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 167.47, 161.68, 128.82, 128.41, 127.20, 112.44, 102.92. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -56.09 (t, *J* = 21.7 Hz), -139.90 (dd, *J* = 21.7, 11.3 Hz), -141.91 – -142.72 (m). **IR** (film): 3283, 2923, 1662, 1479, 1371, 1143, 993, 750. **HRMS** (DART) m/z Calcd for $C_{14}H_6F_7INO_2$ $[M]^+$ 479.9331, found 479.9320.

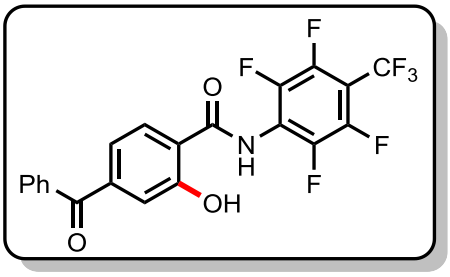


2-hydroxy-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)-5-(trifluoromethyl)benzamide (3n): white solid. Mp = 161 – 162 °C. **^{1}H NMR** (400 MHz, acetone-d^6) δ 8.41 (d, *J* = 1.3 Hz, 1H), 7.87 (dd, *J* = 8.7, 1.9 Hz, 1H), 7.27 (d, *J* = 8.8 Hz, 1H). **^{13}C NMR** (100 MHz, acetone-d^6) δ 165.97, 162.78, 131.61 (d, *J* = 3.5 Hz), 126.92 (d, *J* = 4.1 Hz), 124.23 (q, *J* = 270.7 Hz), 121.08 (q, *J* = 32.9 Hz), 118.83, 115.05. **^{19}F NMR** (376 MHz, acetone-d^6) δ -56.88 – -56.93 (m), -62.28 (s), -143.66 – -143.69 (m). **IR** (film): 3234, 2920, 1642, 1479, 1170, 1001, 771, 717. **HRMS** (DART) m/z Calcd for $C_{15}H_6F_{10}NO_2$ $[M]^+$ 422.0239, found 422.0231.

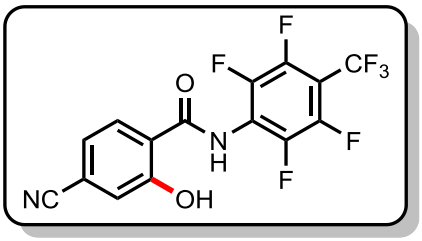


2-hydroxy-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)-4-(trifluoromethyl)benzamide (3o): white solid. Mp = 166 – 167 °C. **^{1}H NMR** (400 MHz, acetone-d^6) δ 8.27 (d, *J* = 8.1 Hz, 1H), 7.39 – 7.33 (m, 2H). **^{13}C NMR** (150 MHz, acetone-d^6) δ 167.31, 161.31, 136.95 (q, *J* = 32.6 Hz), 132.09, 124.92 (q, *J* = 272.1 Hz), 119.83,

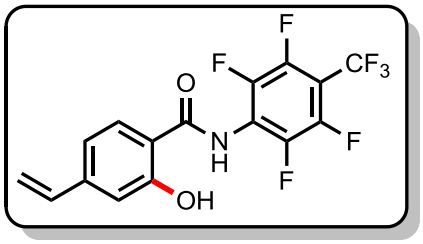
117.30 (q, *J* = 3.7 Hz), 116.11 (q, *J* = 3.9 Hz). **^{19}F NMR** (376 MHz, acetone-d^6) δ -56.87, -64.18, -143.62. **IR** (film): 3253, 1669, 1476, 1328, 1141, 925, 703. **HRMS** (DART) m/z Calcd for $C_{15}H_6F_{10}NO_2$ $[M]^+$ 422.0239, found 422.0233.



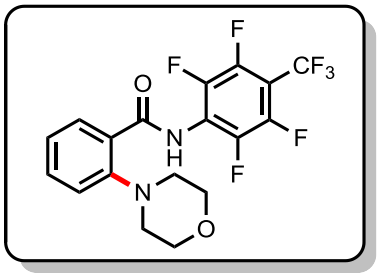
4-benzoyl-2-hydroxy-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (3p): white solid. **^{1}H NMR** (400 MHz, acetone-d^6) δ 8.16 (d, *J* = 8.1 Hz, 1H), 7.79 (d, *J* = 7.2 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.39 (s, 1H), 7.14 (d, *J* = 8.0 Hz, 1H). **^{13}C NMR** (100 MHz, acetone-d^6) δ 195.26, 165.25, 161.50, 142.41, 137.13, 132.54, 130.21, 129.70, 128.27, 119.79, 119.39, 117.97. **^{19}F NMR** (376 MHz, acetone-d^6) δ -51.31 – -51.42 (m), -139.14 – -139.76 (m). **IR** (film): 2930, 1649, 1433, 1135, 991, 718. **HRMS** (DART) m/z Calcd for $C_{21}H_{11}F_7NO_3$ $[M]^+$ 458.0627, found 458.0614.



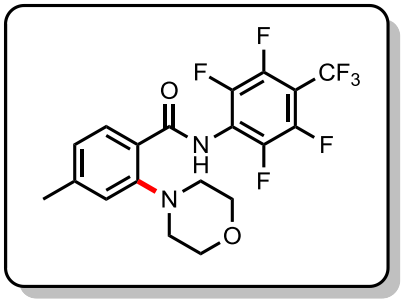
4-cyano-2-hydroxy-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (3q): white solid. **^{1}H NMR** (400 MHz, acetone-d^6) δ 8.11 (d, *J* = 8.0 Hz, 1H), 7.28 (s, 1H), 6.97 (d, *J* = 7.8 Hz, 1H). **^{13}C NMR** (150 MHz, acetone-d^6) δ 165.54, 164.71, 132.26, 123.49, 121.54, 119.34, 119.01, 116.59. **^{19}F NMR** (376 MHz, acetone-d^6) δ -56.36 (t, *J* = 21.6 Hz), -144.58 (s), -145.28 (s). **IR** (film): 2917, 1647, 1474, 1329, 1150, 995, 777, 703. **HRMS** (DART) m/z Calcd for $C_{15}H_6F_7N_2O_2$ $[M]^+$ 379.0317, found 379.0312.



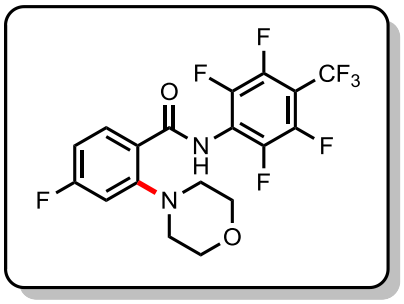
2-hydroxy-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)-4-vinylbenzamide (3r): white solid. Mp = 179 – 180 ^{o}C. **^{1}H NMR** (400 MHz, acetone-d_6) δ 8.02 (d, *J* = 8.3 Hz, 1H), 7.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.11 (d, *J* = 1.7 Hz, 1H), 6.78 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.98 (dd, *J* = 17.6, 0.7 Hz, 1H), 5.44 (d, *J* = 0.6 Hz, 1H). **^{13}C NMR** (150 MHz, acetone-d_6) δ 166.88, 161.22, 143.94, 136.00, 129.40, 116.59, 116.40, 115.34, 114.48. **^{19}F NMR** (376 MHz, acetone-d_6) δ -54.44 – -58.77 (m), -142.42 – -144.93 (m). **IR** (film): 3138, 1680, 1638, 1572, 1473, 1313, 1291, 1246, 1028, 873, 736, 676. **HRMS** (DART) m/z Calcd for $C_{16}H_9F_7NO_2$ $[M]^+$ 380.0522, found 380.0513.



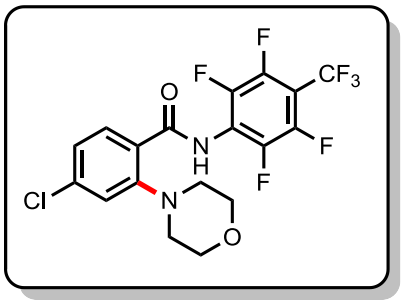
2-morpholino-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (5a): (Known compound)[2] white solid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.11 (brs, 1H), 8.36 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.65-7.61 (m, 1H), 7.45-7.41 (m, 2H), 3.92-3.90 (m, 4H), 3.12-3.10 (m, 4H).



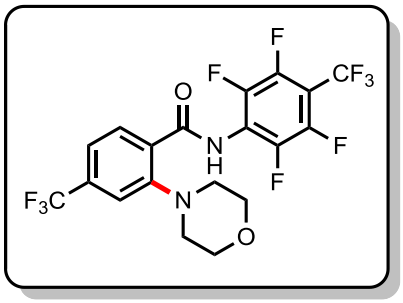
4-methyl-2-morpholino-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (5b): (Known compound)[2] white solid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.09 (brs, 1H), 8.24 (d, *J* = 8.0 Hz, 1H), 7.26-7.20 (m, 2H), 4.05-3.69 (m, 4H), 3.28-2.92 (m, 4H), 2.45 (s, 3H).



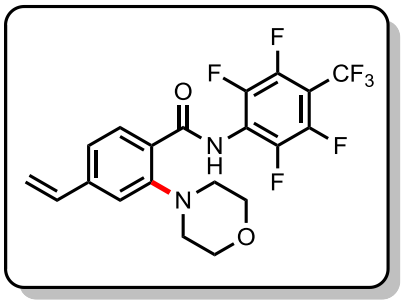
4-fluoro-2-morpholino-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (5c): (Known compound)[2] white solid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.56 (brs, 1H), 8.37 (dd, *J* = 8.8, 6.7 Hz, 1H), 7.11 (m, 2H), 3.91-3.90 (m, 4H), 3.10-3.08 (m, 4H).



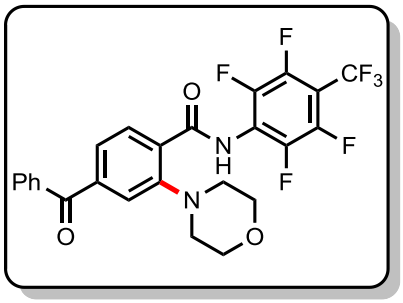
4-chloro-2-morpholino-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (5d): (Known compound)[2] white solid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.60 (brs, 1H), 8.28 (d, *J* = 8.5 Hz, 1H), 7.42-736 (m, 2H), 3.92-3.89 (m, 4H), 3.11-3.09 (m, 4H).



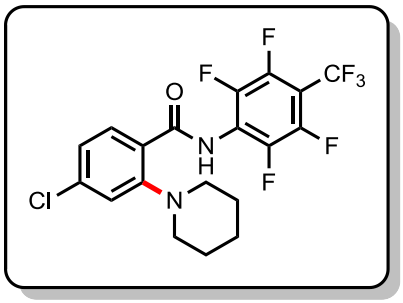
2-morpholino-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)-4-(trifluoromethyl)benzamide (5e): (Known compound)[3] white solid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.60 (brs, 1H), 8.47 (d, *J* = 8.2 Hz, 1H), 7.67 (s, 1H), 7.65 (d, *J* = 8.6 Hz, 1H), 3.95 – 3.90 (m, 4H), 3.18 – 3.12 (m, 4H).



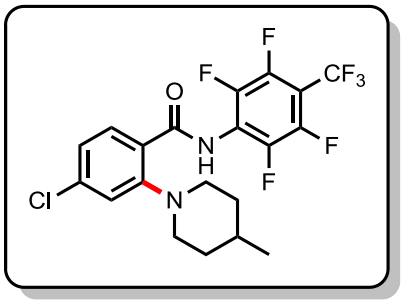
2-morpholino-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)-4-(trifluoromethyl)benzamide (5f): white solid. Mp = 100 – 102 ^{o}C. **^{1}H NMR** (400 MHz, acetone-d_6) δ 12.83 (brs, 1H), 8.16 (d, *J* = 8.2 Hz, 1H), 7.73 (s, 1H), 7.53 (d, *J* = 8.5 Hz, 1H), 6.88 (dd, *J* = 17.7, 11.1 Hz, 1H), 6.08 (d, *J* = 17.7 Hz, 1H), 5.46 (d, *J* = 11.0 Hz, 1H), 3.93 – 3.88 (m, 4H), 3.19 – 3.13 (m, 4H). **^{13}C NMR** (150 MHz, acetone-d_6) δ 163.54, 152.43, 143.33, 136.12, 132.10, 131.88, 123.71, 121.00, 117.10, 67.00, 53.94 . **^{19}F NMR** (376 MHz, acetone-d_6) δ -56.61 – -56.73 (m), -143.55 – -143.65 (m), -144.24 – -144.38 (m). **IR** (film): 2921, 2853, 1691, 1651, 1501, 1336, 1141, 991, 716. **HRMS** (ESI-TOF) m/z Calcd for $C_{20}H_{16}F_7N_2O_2$ $[M]^+$ 449.1095, found 449.1097.



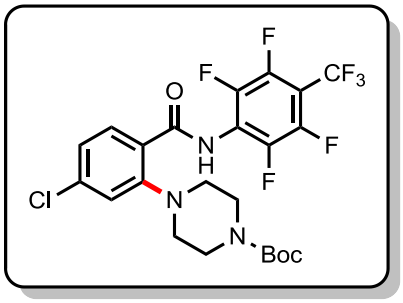
4-benzoyl-2-morpholino-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benza mide (5g): white solid. Mp = 189 – 191 ^{o}C. **^{1}H NMR** (400 MHz, acetone-d_6) δ 12.30 (brs, 1H), 8.23 (d, *J* = 8.0 Hz, 1H), 7.88 – 7.85 (m, 3H), 7.74 – 7.67 (m, 2H), 7.63 – 7.58 (m, 2H), 3.92 – 3.89 (m, 4H), 3.20 – 3.17 (m, 4H). **^{13}C NMR** (150 MHz, acetone-d_6) δ 195.26, 152.03, 142.42, 137.41, 133.51, 131.84, 130.53, 130.36, 129.09, 126.50, 123.20, 66.93, 53.90. **^{19}F NMR** (376 MHz, acetone-d_6) δ -56.66 – -56.78 (m), -143.42 – -143.52 (m), -143.97 – -144.16 (m). **IR** (film): 2920, 2853, 1650, 1490, 1332, 1142, 989, 715. **HRMS** (DART) m/z Calcd for $C_{25}H_{18}F_7N_2O_3$ $[M]^+$ 527.1187, found 527.1199.



4-chloro-2-(piperidin-1-yl)-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benz amide (5h): white solid. Mp = 132 – 134 ^{o}C. **^{1}H NMR** (400 MHz, acetone-d_6) δ 12.95 (brs, 1H), 8.19 – 8.16 (m, 1H), 7.62 (d, *J* = 1.9 Hz, 1H), 7.42 (dd, *J* = 8.5, 2.0 Hz, 1H), 3.12 – 3.07 (m, 4H), 1.84 – 1.79 (m, 4H), 1.67 – 1.60 (m, 2H). **^{13}C NMR** (150 MHz, acetone-d_6) δ 163.11, 154.80, 139.22, 133.27, 126.24, 125.83, 123.74, 55.14, 26.51, 23.67. **^{19}F NMR** (376 MHz, acetone-d_6) δ -56.73 – -56.85 (m), -143.69 – -143.81 (m), -144.16 – -144.44 (m). **IR** (film): 2942, 1651, 1484, 1336, 1143, 992, 714. **HRMS** (DART) m/z Calcd for $C_{19}H_{15}ClF_7N_2O$ $[M]^+$ 455.0756, found 455.0757.

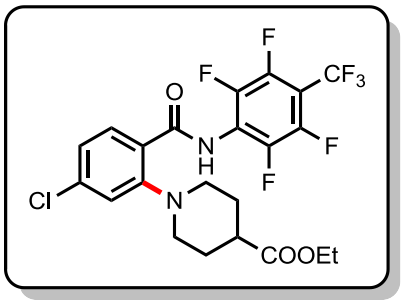


4-chloro-2-(4-methylpiperidin-1-yl)-N-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)benzamide (5i): white solid. Mp = 194 – 198 °C. **^{1}H NMR** (400 MHz, acetone-d_6) δ 12.86 (brs, 1H), 8.16 (d, *J* = 8.5 Hz, 1H), 7.62 (d, *J* = 1.9 Hz, 1H), 7.41 (dd, *J* = 8.5, 2.0 Hz, 1H), 3.23 (d, *J* = 11.6 Hz, 2H), 3.01 (t, *J* = 11.7 Hz, 2H), 1.86 (d, *J* = 13.0 Hz, 2H), 1.72 – 1.59 (m, 1H), 1.47 (td, *J* = 15.4, 3.7 Hz, 2H), 0.98 (d, *J* = 6.5 Hz, 3H). **^{13}C NMR** (150 MHz, acetone-d_6) δ 163.18, 154.59, 139.20, 133.30, 126.21, 125.93, 123.69, 54.60, 34.81, 30.29, 21.58. **^{19}F NMR** (376 MHz, acetone-d_6) δ -51.45 – -51.57 (m), -138.42. – -138.52 (m), -138.89 – -139.15 (m). **IR** (film): 2961, 1673, 1451, 1332, 1052, 989, 709. **HRMS** (DART) m/z Calcd for $C_{20}H_{17}ClF_7N_2O$ $[M]^+$ 468.0912, found 468.0915.

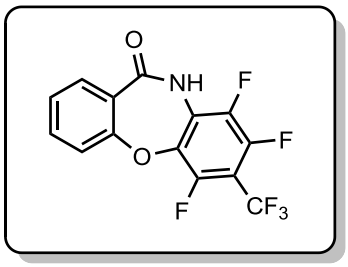


tert-butyl4-(5-chloro-2-((2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)carbamoyl)phenyl)piperazine-1-carboxylate (5j): white solid. Mp = 132 – 134 °C. **^{1}H NMR** (400 MHz, acetone-d_6) δ 12.08 (brs, 1H), 8.10 (d, *J* = 8.5 Hz, 1H), 7.58 (d, *J* = 2.0 Hz, 1H), 7.42 (dd, *J* = 8.4, 2.0 Hz, 1H), 3.67 – 3.65 (m, 4H), 3.16 – 3.11 (m, 4H), 1.46 (s, 9H). **^{13}C NMR** (150 MHz, acetone-d_6) δ 163.54, 154.54, 153.47, 139.15, 133.36, 126.32, 126.06, 123.13, 79.71, 53.57, 28.15. **^{19}F NMR** (376 MHz, acetone-d_6) δ -51.45 – -51.57 (m), -138.42. – -138.52 (m), -138.89 – -139.15 (m). **IR** (film): 2969,

1695, 1424, 1127, 998, 704. **HRMS** (DART) m/z Calcd for $C_{23}H_{22}ClF_7N_3O_3$ $[M]^+$ 556.1232, found 556.1235.

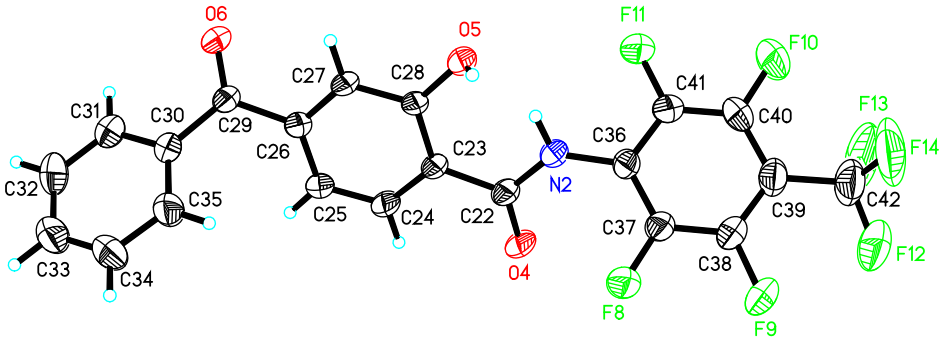


ethyl1-(5-chloro-2-((2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)carbamoyl)phenyl)piperidine-4-carboxylate (5k): white solid. Mp = 102 – 104 ^oC. **^{1}H NMR** (400 MHz, acetone-d_6) δ 12.48 (brs, 1H), 8.14 (d, *J* = 8.5 Hz, 1H), 7.59 (d, *J* = 1.9 Hz, 1H), 7.41 (dd, *J* = 8.5, 2.0 Hz, 1H), 4.12 (q, *J* = 7.1 Hz, 2H), 3.32 – 3.29 (m, 2H), 3.08 (td, *J* = 11.7, 2.5 Hz, 2H), 2.62 – 2.54 (m, 1H), 2.17 – 2.08 (m, 2H), 2.02 – 1.89 (m, 2H), 1.23 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (150 MHz, acetone-d_6) δ 174.19, 163.34, 154.21, 139.17, 133.35, 126.15, 126.08, 123.41, 60.52, 53.59, 40.22, 28.87, 14.13. **^{19}F NMR** (376 MHz, acetone-d_6) δ -51.47 – -51.59 (m), -138.34 – -138.44 (m), -138.89 – -139.13 (m). **IR** (film): 2976, 1665, 1459, 1333, 1138, 1051, 937, 710. **HRMS** (DART) m/z Calcd for $C_{22}H_{19}ClF_7N_2O_3$ $[M]^+$ 527.0967, found 527.0970.



6,8,9-trifluoro-7-(trifluoromethyl)dibenzo[b,f][1,4]oxazepin-11(10H)-one (2a): white solid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.98 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.66 – 7.60 (m, 1H), 7.39 – 7.33 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 164.81, 157.98, 135.67, 132.61, 126.51, 123.92, 121.17. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -55.76 – -55.88 (t), -134.22 – -134.53 (m), -139.35 (pd, *J* = 21.7 Hz, 4.7Hz), -153.50 (dd, *J* = 21.7, 10.9 Hz). **HRMS** (DART) m/z Calcd for $C_{14}H_5F_6NO_2$ $[M]^+$ 333.0224, found 333.0220.

3.2 X-ray Crystallographic Data of 3p and 2a.



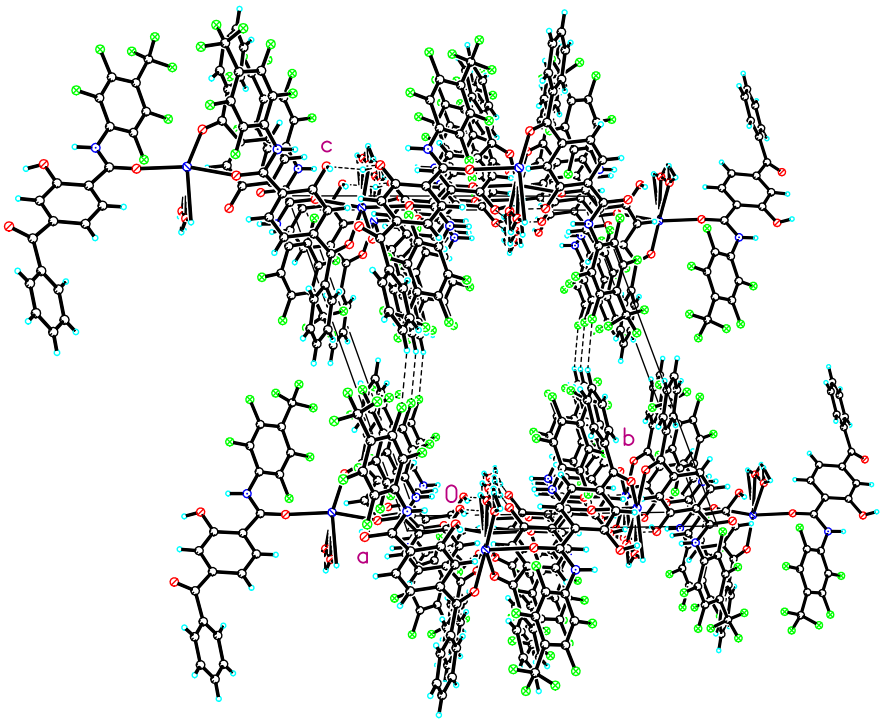


Table 12. Crystal data and structure refinement for cd15058.

Identification code	cd15058
Empirical formula	C42 H22 F14 N2 Na O7
Formula weight	955.60
Temperature	293(2) K

Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.857(2) Å	α= 108.566(4) °.
	b = 15.141(3) Å	β= 96.630(4) °.
	c = 17.359(3) Å	γ = 96.910(4) °.
Volume	2649.3(9) $Å^3$	
Z	2	
Density (calculated)	1.198 Mg/m^3	
Absorption coefficient	0.121 mm^{-1}	
F(000)	962	
Crystal size	0.220 x 0.170 x 0.120 mm^3	
Theta range for data collection	1.254 to 25.500 °.	
Index ranges	-12<=h<=13, -18<=k<=18, -21<=l<=20	
Reflections collected	15334	
Independent reflections	9835 [R(int) = 0.0480]	
Completeness to theta = 25.242 °	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.5874	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9835 / 11 / 614	
Goodness-of-fit on F^2	0.872	
Final R indices [I>2sigma(I)]	R1 = 0.0695, wR2 = 0.1813	
R indices (all data)	R1 = 0.1361, wR2 = 0.2064	

Extinction coefficient	n/a
Largest diff. peak and hole	0.323 and -0.272 e.Å^{-3}

Table 13. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for cd15058. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Na(1)	7495(2)	7672(1)	465(1)	83(1)
O(1)	7334(2)	6143(2)	415(2)	84(1)
O(2)	7438(3)	3474(2)	533(2)	83(1)
O(3)	10591(3)	2256(2)	-1331(2)	92(1)
O(4)	2336(2)	10949(2)	-210(1)	72(1)
O(5)	2655(2)	8164(2)	-495(1)	72(1)
O(6)	6505(2)	8456(2)	1587(1)	74(1)
O(7)	5659(8)	6917(5)	-711(5)	177(3)
O(7')	6873(14)	7049(8)	-966(7)	184(4)
N(1)	6779(3)	5098(2)	1034(2)	75(1)
N(2)	1606(3)	9406(2)	-915(2)	66(1)
C(1)	7317(3)	5348(2)	455(2)	66(1)
C(2)	7932(3)	4629(2)	-92(2)	58(1)
C(3)	8540(3)	4885(2)	-678(2)	74(1)
C(4)	9165(3)	4278(2)	-1205(2)	71(1)
C(5)	9236(3)	3390(2)	-1132(2)	63(1)

C(6)	8679(3)	3136(2)	-548(2)	65(1)
C(7)	7991(3)	3732(2)	-32(2)	62(1)
C(8)	9996(3)	2732(2)	-1632(2)	69(1)
C(9)	10034(3)	2659(2)	-2512(3)	75(1)
C(10)	9048(4)	2843(3)	-2991(3)	96(1)
C(11)	9096(5)	2722(4)	-3815(3)	119(2)
C(12)	10122(6)	2419(4)	-4151(3)	119(2)
C(13)	11090(5)	2244(4)	-3659(4)	120(2)
C(14)	11037(4)	2354(3)	-2867(3)	93(1)
C(15)	6274(4)	5692(2)	1671(2)	71(1)
C(16)	6602(5)	5711(3)	2468(3)	94(1)
C(17)	6132(5)	6253(3)	3104(3)	100(1)
C(18)	5299(4)	6858(3)	3009(3)	86(1)
C(19)	4946(4)	6832(3)	2203(3)	80(1)
C(20)	5408(3)	6258(2)	1558(2)	69(1)
C(21)	4823(6)	7454(5)	3743(4)	117(2)
C(22)	2372(3)	10110(2)	-300(2)	56(1)
C(23)	3256(3)	9809(2)	244(2)	52(1)
C(24)	4058(3)	10510(2)	889(2)	65(1)
C(25)	4908(3)	10321(2)	1433(2)	64(1)
C(26)	5013(3)	9378(2)	1329(2)	56(1)
C(27)	4253(3)	8667(2)	684(2)	58(1)
C(28)	3365(3)	8860(2)	129(2)	55(1)
C(29)	5969(3)	9109(2)	1875(2)	59(1)

C(30)	6241(3)	9645(2)	2775(2)	67(1)
C(31)	7402(4)	9662(3)	3214(3)	83(1)
C(32)	7657(5)	10122(4)	4056(3)	110(2)
C(33)	6785(5)	10579(4)	4473(3)	112(2)
C(34)	5640(5)	10552(4)	4043(3)	116(2)
C(35)	5357(4)	10105(3)	3200(2)	90(1)
C(36)	768(3)	9505(2)	-1551(2)	59(1)
C(37)	-116(3)	10096(2)	-1431(2)	61(1)
C(38)	-918(3)	10151(3)	-2083(2)	69(1)
C(39)	-887(3)	9614(3)	-2893(2)	80(1)
C(40)	-18(4)	8988(3)	-3003(2)	87(1)
C(41)	782(4)	8950(3)	-2359(2)	77(1)
C(42)	-1712(6)	9673(5)	-3618(3)	117(2)
F(1)	7489(3)	5189(2)	2615(2)	141(1)
F(2)	6519(3)	6231(2)	3871(2)	154(1)
F(3)	4106(2)	7359(2)	2045(2)	109(1)
F(4)	4976(2)	6254(2)	804(1)	93(1)
F(5)	5721(4)	7954(3)	4316(2)	209(2)
F(6)	4074(4)	6971(3)	4037(2)	188(2)
F(7)	4107(4)	8047(3)	3569(2)	159(1)
F(8)	-262(2)	10596(2)	-668(1)	81(1)
F(9)	-1764(2)	10734(2)	-1910(1)	100(1)
F(10)	52(3)	8429(2)	-3756(1)	132(1)
F(11)	1623(2)	8356(2)	-2498(1)	111(1)

F(12)	-2333(3)	10373(3)	-3452(2)	153(1)
F(13)	-1076(4)	9771(4)	-4175(2)	218(2)
F(14)	-2544(5)	8964(3)	-3950(3)	236(3)

Table 14. Bond lengths [Å] and angles [°] for cd15058.

Na(1)-O(4)#1	2.258(2)
Na(1)-O(1)	2.273(3)
Na(1)-O(7')	2.342(12)
Na(1)-O(6)	2.383(3)
Na(1)-O(3)#2	2.389(3)
Na(1)-O(7)	2.544(8)
Na(1)-H(7C)	2.6139
O(1)-C(1)	1.226(4)
O(2)-C(7)	1.342(4)
O(2)-H(2)	0.8200
O(3)-C(8)	1.218(4)
O(3)-Na(1)#2	2.389(3)
O(4)-C(22)	1.237(4)
O(4)-Na(1)#1	2.258(2)
O(5)-C(28)	1.328(4)
O(5)-H(5)	0.8200
O(6)-C(29)	1.207(3)
O(7)-H(7A)	0.8854

O(7)-H(7B)	1.0979
O(7')-H(7C)	0.9268
O(7')-H(7D)	0.8725
N(1)-C(1)	1.349(5)
N(1)-C(15)	1.399(4)
N(1)-H(1)	0.91(5)
N(2)-C(22)	1.350(4)
N(2)-C(36)	1.405(4)
N(2)-H(2A)	0.84(5)
C(1)-C(2)	1.480(5)
C(2)-C(3)	1.403(5)
C(2)-C(7)	1.403(4)
C(3)-C(4)	1.378(5)
C(3)-H(3)	0.9300
C(4)-C(5)	1.401(5)
C(4)-H(4)	0.9300
C(5)-C(6)	1.368(5)
C(5)-C(8)	1.498(5)
C(6)-C(7)	1.406(5)
C(6)-H(6)	0.9300
C(8)-C(9)	1.501(5)
C(9)-C(14)	1.370(5)
C(9)-C(10)	1.388(5)
C(10)-C(11)	1.391(6)

C(10)-H(10)	0.9300
C(11)-C(12)	1.377(6)
C(11)-H(11)	0.9300
C(12)-C(13)	1.381(7)
C(12)-H(12)	0.9300
C(13)-C(14)	1.340(6)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(15)-C(16)	1.379(5)
C(15)-C(20)	1.383(5)
C(16)-C(17)	1.344(6)
C(16)-F(1)	1.369(5)
C(17)-F(2)	1.362(5)
C(17)-C(18)	1.394(6)
C(18)-C(19)	1.395(6)
C(18)-C(21)	1.496(6)
C(19)-F(3)	1.341(4)
C(19)-C(20)	1.369(5)
C(20)-F(4)	1.337(4)
C(21)-F(5)	1.277(6)
C(21)-F(6)	1.283(6)
C(21)-F(7)	1.337(6)
C(22)-C(23)	1.481(4)
C(23)-C(24)	1.390(4)

C(23)-C(28)	1.409(4)
C(24)-C(25)	1.362(4)
C(24)-H(24)	0.9300
C(25)-C(26)	1.402(4)
C(25)-H(25)	0.9300
C(26)-C(27)	1.378(4)
C(26)-C(29)	1.504(4)
C(27)-C(28)	1.404(4)
C(27)-H(27)	0.9300
C(29)-C(30)	1.489(5)
C(30)-C(31)	1.388(5)
C(30)-C(35)	1.395(5)
C(31)-C(32)	1.382(6)
C(31)-H(31)	0.9300
C(32)-C(33)	1.378(6)
C(32)-H(32)	0.9300
C(33)-C(34)	1.363(6)
C(33)-H(33)	0.9300
C(34)-C(35)	1.382(5)
C(34)-H(34)	0.9300
C(35)-H(35)	0.9300
C(36)-C(37)	1.378(4)
C(36)-C(41)	1.389(5)
C(37)-F(8)	1.339(4)

C(37)-C(38)	1.377(5)
C(38)-F(9)	1.343(4)
C(38)-C(39)	1.389(5)
C(39)-C(40)	1.402(5)
C(39)-C(42)	1.492(6)
C(40)-F(10)	1.330(4)
C(40)-C(41)	1.355(5)
C(41)-F(11)	1.346(4)
C(42)-F(14)	1.247(7)
C(42)-F(13)	1.287(6)
C(42)-F(12)	1.297(6)

O(4)#1-Na(1)-O(1)	167.14(11)
O(4)#1-Na(1)-O(7')	82.0(3)
O(1)-Na(1)-O(7')	85.7(3)
O(4)#1-Na(1)-O(6)	85.34(9)
O(1)-Na(1)-O(6)	106.17(10)
O(7')-Na(1)-O(6)	134.2(4)
O(4)#1-Na(1)-O(3)#2	106.03(11)
O(1)-Na(1)-O(3)#2	79.40(10)
O(7')-Na(1)-O(3)#2	132.0(4)
O(6)-Na(1)-O(3)#2	93.79(10)
O(4)#1-Na(1)-O(7)	91.88(19)
O(1)-Na(1)-O(7)	80.07(19)

O(6)-Na(1)-O(7)	103.1(2)
O(3)#2-Na(1)-O(7)	156.3(2)
O(4)#1-Na(1)-H(7C)	74.8
O(1)-Na(1)-H(7C)	92.4
O(7')-Na(1)-H(7C)	20.6
O(6)-Na(1)-H(7C)	148.7
O(3)#2-Na(1)-H(7C)	114.6
C(1)-O(1)-Na(1)	174.3(3)
C(7)-O(2)-H(2)	109.5
C(8)-O(3)-Na(1)#2	142.6(2)
C(22)-O(4)-Na(1)#1	160.3(2)
C(28)-O(5)-H(5)	109.5
C(29)-O(6)-Na(1)	145.7(2)
Na(1)-O(7)-H(7A)	149.4
Na(1)-O(7)-H(7B)	141.3
H(7A)-O(7)-H(7B)	68.7
Na(1)-O(7')-H(7C)	96.4
Na(1)-O(7')-H(7D)	139.6
H(7C)-O(7')-H(7D)	123.7
C(1)-N(1)-C(15)	126.2(3)
C(1)-N(1)-H(1)	114(3)
C(15)-N(1)-H(1)	118(3)
C(22)-N(2)-C(36)	126.7(3)
C(22)-N(2)-H(2A)	108(3)

C(36)-N(2)-H(2A)	124(3)
O(1)-C(1)-N(1)	121.0(3)
O(1)-C(1)-C(2)	122.7(4)
N(1)-C(1)-C(2)	116.3(3)
C(3)-C(2)-C(7)	118.4(3)
C(3)-C(2)-C(1)	117.4(3)
C(7)-C(2)-C(1)	124.1(3)
C(4)-C(3)-C(2)	122.2(3)
C(4)-C(3)-H(3)	118.9
C(2)-C(3)-H(3)	118.9
C(3)-C(4)-C(5)	118.9(4)
C(3)-C(4)-H(4)	120.6
C(5)-C(4)-H(4)	120.6
C(6)-C(5)-C(4)	119.8(3)
C(6)-C(5)-C(8)	118.4(3)
C(4)-C(5)-C(8)	121.6(4)
C(5)-C(6)-C(7)	121.8(3)
C(5)-C(6)-H(6)	119.1
C(7)-C(6)-H(6)	119.1
O(2)-C(7)-C(2)	119.8(3)
O(2)-C(7)-C(6)	121.4(3)
C(2)-C(7)-C(6)	118.8(3)
O(3)-C(8)-C(5)	120.5(4)
O(3)-C(8)-C(9)	119.6(3)

C(5)-C(8)-C(9)	119.9(3)
C(14)-C(9)-C(10)	118.9(4)
C(14)-C(9)-C(8)	119.1(4)
C(10)-C(9)-C(8)	121.9(3)
C(9)-C(10)-C(11)	119.9(4)
C(9)-C(10)-H(10)	120.0
C(11)-C(10)-H(10)	120.0
C(12)-C(11)-C(10)	119.7(5)
C(12)-C(11)-H(11)	120.2
C(10)-C(11)-H(11)	120.2
C(11)-C(12)-C(13)	119.1(5)
C(11)-C(12)-H(12)	120.5
C(13)-C(12)-H(12)	120.5
C(14)-C(13)-C(12)	121.2(5)
C(14)-C(13)-H(13)	119.4
C(12)-C(13)-H(13)	119.4
C(13)-C(14)-C(9)	121.3(5)
C(13)-C(14)-H(14)	119.4
C(9)-C(14)-H(14)	119.4
C(16)-C(15)-C(20)	115.8(3)
C(16)-C(15)-N(1)	119.9(3)
C(20)-C(15)-N(1)	124.3(3)
C(17)-C(16)-F(1)	119.3(4)
C(17)-C(16)-C(15)	122.7(4)

F(1)-C(16)-C(15)	117.9(4)
C(16)-C(17)-F(2)	118.5(4)
C(16)-C(17)-C(18)	122.4(4)
F(2)-C(17)-C(18)	119.1(4)
C(17)-C(18)-C(19)	115.3(4)
C(17)-C(18)-C(21)	119.9(5)
C(19)-C(18)-C(21)	124.8(4)
F(3)-C(19)-C(20)	118.7(4)
F(3)-C(19)-C(18)	119.7(4)
C(20)-C(19)-C(18)	121.6(4)
F(4)-C(20)-C(19)	117.2(3)
F(4)-C(20)-C(15)	120.7(3)
C(19)-C(20)-C(15)	122.2(4)
F(5)-C(21)-F(6)	109.0(6)
F(5)-C(21)-F(7)	107.1(6)
F(6)-C(21)-F(7)	102.1(5)
F(5)-C(21)-C(18)	111.9(5)
F(6)-C(21)-C(18)	113.0(5)
F(7)-C(21)-C(18)	113.2(5)
O(4)-C(22)-N(2)	121.4(3)
O(4)-C(22)-C(23)	122.7(3)
N(2)-C(22)-C(23)	115.8(3)
C(24)-C(23)-C(28)	118.2(3)
C(24)-C(23)-C(22)	117.8(3)

C(28)-C(23)-C(22)	123.9(3)
C(25)-C(24)-C(23)	123.2(3)
C(25)-C(24)-H(24)	118.4
C(23)-C(24)-H(24)	118.4
C(24)-C(25)-C(26)	119.0(3)
C(24)-C(25)-H(25)	120.5
C(26)-C(25)-H(25)	120.5
C(27)-C(26)-C(25)	119.2(3)
C(27)-C(26)-C(29)	118.3(3)
C(25)-C(26)-C(29)	122.4(3)
C(26)-C(27)-C(28)	121.9(3)
C(26)-C(27)-H(27)	119.0
C(28)-C(27)-H(27)	119.0
O(5)-C(28)-C(27)	120.8(3)
O(5)-C(28)-C(23)	120.7(3)
C(27)-C(28)-C(23)	118.4(3)
O(6)-C(29)-C(30)	120.1(3)
O(6)-C(29)-C(26)	120.2(3)
C(30)-C(29)-C(26)	119.7(3)
C(31)-C(30)-C(35)	118.8(3)
C(31)-C(30)-C(29)	118.8(3)
C(35)-C(30)-C(29)	122.4(3)
C(32)-C(31)-C(30)	119.8(4)
C(32)-C(31)-H(31)	120.1

C(30)-C(31)-H(31)	120.1
C(33)-C(32)-C(31)	121.3(4)
C(33)-C(32)-H(32)	119.3
C(31)-C(32)-H(32)	119.3
C(34)-C(33)-C(32)	118.8(4)
C(34)-C(33)-H(33)	120.6
C(32)-C(33)-H(33)	120.6
C(33)-C(34)-C(35)	121.4(4)
C(33)-C(34)-H(34)	119.3
C(35)-C(34)-H(34)	119.3
C(34)-C(35)-C(30)	119.9(4)
C(34)-C(35)-H(35)	120.1
C(30)-C(35)-H(35)	120.1
C(37)-C(36)-C(41)	116.6(3)
C(37)-C(36)-N(2)	124.5(3)
C(41)-C(36)-N(2)	118.8(3)
F(8)-C(37)-C(38)	118.1(3)
F(8)-C(37)-C(36)	120.4(3)
C(38)-C(37)-C(36)	121.5(3)
F(9)-C(38)-C(37)	117.6(3)
F(9)-C(38)-C(39)	120.3(3)
C(37)-C(38)-C(39)	122.1(3)
C(38)-C(39)-C(40)	115.8(3)
C(38)-C(39)-C(42)	123.8(4)

C(40)-C(39)-C(42)	120.4(4)
F(10)-C(40)-C(41)	118.5(4)
F(10)-C(40)-C(39)	119.8(4)
C(41)-C(40)-C(39)	121.7(4)
F(11)-C(41)-C(40)	119.5(3)
F(11)-C(41)-C(36)	118.2(3)
C(40)-C(41)-C(36)	122.3(3)
F(14)-C(42)-F(13)	107.4(6)
F(14)-C(42)-F(12)	103.9(5)
F(13)-C(42)-F(12)	105.6(6)
F(14)-C(42)-C(39)	113.1(6)
F(13)-C(42)-C(39)	111.6(5)
F(12)-C(42)-C(39)	114.6(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z #2 -x+2,-y+1,-z

Table 15. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for cd15058. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Na(1)	141(1)	44(1)	72(1)	24(1)	16(1)	38(1)
O(1)	115(2)	41(1)	103(2)	24(1)	21(2)	35(1)

O(2)	148(2)	37(1)	74(2)	21(1)	27(2)	38(1)
O(3)	99(2)	69(2)	117(2)	35(2)	15(2)	45(2)
O(4)	95(2)	43(1)	82(2)	28(1)	0(1)	28(1)
O(5)	110(2)	39(1)	65(2)	19(1)	-11(1)	21(1)
O(6)	93(2)	69(2)	67(2)	23(1)	12(1)	46(1)
O(7)	184(7)	156(5)	185(6)	54(5)	45(5)	9(5)
O(7')	219(9)	162(7)	177(8)	61(7)	52(7)	23(8)
N(1)	126(3)	37(2)	66(2)	14(2)	18(2)	32(2)
N(2)	96(2)	46(2)	58(2)	21(2)	-3(2)	25(2)
C(1)	82(2)	40(2)	76(3)	19(2)	2(2)	22(2)
C(2)	81(2)	32(2)	60(2)	12(2)	2(2)	19(2)
C(3)	92(3)	42(2)	93(3)	25(2)	9(2)	26(2)
C(4)	88(3)	60(2)	72(2)	26(2)	11(2)	27(2)
C(5)	74(2)	44(2)	66(2)	13(2)	-3(2)	21(2)
C(6)	92(3)	41(2)	61(2)	14(2)	0(2)	25(2)
C(7)	90(2)	36(2)	56(2)	11(2)	1(2)	20(2)
C(8)	68(2)	49(2)	85(3)	15(2)	2(2)	15(2)
C(9)	71(2)	60(2)	85(3)	11(2)	11(2)	21(2)
C(10)	84(3)	108(3)	91(3)	21(3)	10(2)	36(2)
C(11)	127(4)	150(5)	75(3)	28(3)	9(3)	39(3)
C(12)	140(5)	136(5)	73(3)	13(3)	34(3)	32(4)
C(13)	116(4)	132(5)	116(5)	33(4)	38(4)	46(3)
C(14)	97(3)	88(3)	93(3)	17(3)	26(3)	36(2)
C(15)	103(3)	46(2)	65(2)	17(2)	15(2)	24(2)

C(16)	139(4)	73(3)	86(3)	34(2)	23(3)	52(3)
C(17)	148(4)	101(3)	61(3)	27(3)	24(3)	46(3)
C(18)	102(3)	76(3)	79(3)	19(2)	27(2)	22(2)
C(19)	90(3)	65(2)	89(3)	23(2)	21(2)	27(2)
C(20)	84(3)	59(2)	55(2)	7(2)	3(2)	19(2)
C(21)	127(5)	134(5)	96(4)	25(4)	47(4)	52(4)
C(22)	72(2)	47(2)	58(2)	24(2)	10(2)	20(2)
C(23)	69(2)	40(2)	52(2)	21(2)	8(2)	19(2)
C(24)	86(2)	37(2)	69(2)	17(2)	-2(2)	19(2)
C(25)	84(2)	46(2)	57(2)	10(2)	1(2)	23(2)
C(26)	72(2)	52(2)	48(2)	16(2)	11(2)	24(2)
C(27)	82(2)	40(2)	55(2)	19(2)	8(2)	26(2)
C(28)	83(2)	36(2)	47(2)	12(2)	2(2)	21(2)
C(29)	72(2)	56(2)	56(2)	24(2)	12(2)	27(2)
C(30)	76(2)	68(2)	59(2)	20(2)	0(2)	26(2)
C(31)	83(3)	93(3)	78(3)	29(2)	1(2)	37(2)
C(32)	108(3)	136(4)	77(3)	32(3)	-27(3)	33(3)
C(33)	121(4)	133(4)	64(3)	7(3)	-7(3)	49(3)
C(34)	137(4)	142(4)	59(3)	6(3)	12(3)	65(3)
C(35)	87(3)	119(4)	60(3)	16(2)	5(2)	49(2)
C(36)	79(2)	51(2)	51(2)	23(2)	0(2)	15(2)
C(37)	70(2)	64(2)	56(2)	23(2)	12(2)	24(2)
C(38)	63(2)	74(2)	77(3)	32(2)	6(2)	23(2)
C(39)	74(3)	97(3)	69(3)	33(2)	-5(2)	18(2)

C(40)	103(3)	97(3)	47(2)	6(2)	0(2)	27(3)
C(41)	98(3)	69(2)	62(3)	14(2)	7(2)	38(2)
C(42)	105(4)	179(6)	75(3)	48(4)	-3(3)	50(4)
F(1)	222(3)	136(2)	104(2)	60(2)	36(2)	110(2)
F(2)	232(3)	181(3)	76(2)	57(2)	38(2)	89(3)
F(3)	106(2)	112(2)	118(2)	34(2)	27(1)	60(2)
F(4)	102(2)	105(2)	71(2)	24(1)	0(1)	40(1)
F(5)	144(3)	286(5)	104(2)	-70(3)	15(2)	64(3)
F(6)	243(4)	188(4)	180(4)	74(3)	139(3)	78(3)
F(7)	190(3)	151(3)	139(3)	21(2)	61(2)	86(3)
F(8)	95(1)	89(2)	64(1)	22(1)	18(1)	40(1)
F(9)	83(1)	118(2)	106(2)	40(2)	1(1)	53(1)
F(10)	151(2)	165(3)	56(2)	1(2)	-7(1)	61(2)
F(11)	143(2)	109(2)	72(2)	5(1)	3(1)	74(2)
F(12)	152(3)	197(3)	124(2)	72(2)	-23(2)	73(3)
F(13)	162(3)	446(8)	117(3)	163(4)	27(2)	131(4)
F(14)	231(4)	183(4)	215(4)	49(3)	-164(4)	-21(3)

Table 16. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for cd15058.

	x	y	z	U(eq)

H(2)	7037	2937	319	124
H(5)	1955	8054	-378	109
H(7A)	5357	6733	-1243	212
H(7B)	4633	6706	-828	212
H(7C)	7646	7219	-1101	221
H(7D)	6221	6713	-1329	221
H(3)	8522	5484	-712	89
H(4)	9533	4456	-1603	85
H(6)	8757	2554	-492	78
H(10)	8357	3047	-2760	115
H(11)	8437	2846	-4137	143
H(12)	10163	2333	-4702	143
H(13)	11791	2048	-3881	144
H(14)	11695	2219	-2552	112
H(24)	4013	11138	952	78
H(25)	5410	10811	1866	77
H(27)	4331	8043	613	69
H(31)	8007	9364	2941	100
H(32)	8432	10122	4346	132
H(33)	6974	10901	5037	134
H(34)	5036	10841	4324	139
H(35)	4579	10110	2916	108
H(1)	6910(40)	4520(30)	1060(30)	123(16)

H(2A)	1830(40)	8890(30)	-920(30)	118(17)

Table 17. Torsion angles [°] for cd15058.

C(15)-N(1)-C(1)-O(1)	-4.6(6)
C(15)-N(1)-C(1)-C(2)	172.3(3)
O(1)-C(1)-C(2)-C(3)	-0.7(5)
N(1)-C(1)-C(2)-C(3)	-177.6(3)
O(1)-C(1)-C(2)-C(7)	176.2(3)
N(1)-C(1)-C(2)-C(7)	-0.7(5)
C(7)-C(2)-C(3)-C(4)	1.5(5)
C(1)-C(2)-C(3)-C(4)	178.6(3)
C(2)-C(3)-C(4)-C(5)	-2.5(5)
C(3)-C(4)-C(5)-C(6)	0.6(5)
C(3)-C(4)-C(5)-C(8)	-174.4(3)
C(4)-C(5)-C(6)-C(7)	2.3(5)
C(8)-C(5)-C(6)-C(7)	177.5(3)
C(3)-C(2)-C(7)-O(2)	178.8(3)
C(1)-C(2)-C(7)-O(2)	2.0(5)
C(3)-C(2)-C(7)-C(6)	1.3(5)
C(1)-C(2)-C(7)-C(6)	-175.5(3)
C(5)-C(6)-C(7)-O(2)	179.3(3)
C(5)-C(6)-C(7)-C(2)	-3.2(5)
Na(1)#2-O(3)-C(8)-C(5)	-79.8(5)

Na(1)#2-O(3)-C(8)-C(9)	99.9(4)
C(6)-C(5)-C(8)-O(3)	-33.5(5)
C(4)-C(5)-C(8)-O(3)	141.6(4)
C(6)-C(5)-C(8)-C(9)	146.8(3)
C(4)-C(5)-C(8)-C(9)	-38.1(5)
O(3)-C(8)-C(9)-C(14)	-23.6(5)
C(5)-C(8)-C(9)-C(14)	156.1(3)
O(3)-C(8)-C(9)-C(10)	152.8(4)
C(5)-C(8)-C(9)-C(10)	-27.5(5)
C(14)-C(9)-C(10)-C(11)	-0.4(6)
C(8)-C(9)-C(10)-C(11)	-176.8(4)
C(9)-C(10)-C(11)-C(12)	0.1(8)
C(10)-C(11)-C(12)-C(13)	-0.3(8)
C(11)-C(12)-C(13)-C(14)	0.9(9)
C(12)-C(13)-C(14)-C(9)	-1.3(8)
C(10)-C(9)-C(14)-C(13)	1.0(7)
C(8)-C(9)-C(14)-C(13)	177.5(4)
C(1)-N(1)-C(15)-C(16)	-131.0(4)
C(1)-N(1)-C(15)-C(20)	51.4(6)
C(20)-C(15)-C(16)-C(17)	-1.0(7)
N(1)-C(15)-C(16)-C(17)	-178.8(4)
C(20)-C(15)-C(16)-F(1)	-177.7(4)
N(1)-C(15)-C(16)-F(1)	4.5(6)
F(1)-C(16)-C(17)-F(2)	-2.8(7)

C(15)-C(16)-C(17)-F(2)	-179.5(4)
F(1)-C(16)-C(17)-C(18)	175.0(4)
C(15)-C(16)-C(17)-C(18)	-1.7(8)
C(16)-C(17)-C(18)-C(19)	2.6(7)
F(2)-C(17)-C(18)-C(19)	-179.6(4)
C(16)-C(17)-C(18)-C(21)	-179.1(5)
F(2)-C(17)-C(18)-C(21)	-1.3(7)
C(17)-C(18)-C(19)-F(3)	177.2(4)
C(21)-C(18)-C(19)-F(3)	-1.1(7)
C(17)-C(18)-C(19)-C(20)	-0.8(6)
C(21)-C(18)-C(19)-C(20)	-179.1(5)
F(3)-C(19)-C(20)-F(4)	-0.6(5)
C(18)-C(19)-C(20)-F(4)	177.4(4)
F(3)-C(19)-C(20)-C(15)	-179.9(3)
C(18)-C(19)-C(20)-C(15)	-1.8(6)
C(16)-C(15)-C(20)-F(4)	-176.5(3)
N(1)-C(15)-C(20)-F(4)	1.2(6)
C(16)-C(15)-C(20)-C(19)	2.7(6)
N(1)-C(15)-C(20)-C(19)	-179.6(4)
C(17)-C(18)-C(21)-F(5)	54.3(8)
C(19)-C(18)-C(21)-F(5)	-127.5(6)
C(17)-C(18)-C(21)-F(6)	-69.3(7)
C(19)-C(18)-C(21)-F(6)	109.0(6)
C(17)-C(18)-C(21)-F(7)	175.4(5)

C(19)-C(18)-C(21)-F(7)	-6.4(8)
Na(1)#1-O(4)-C(22)-N(2)	-65.4(8)
Na(1)#1-O(4)-C(22)-C(23)	113.8(6)
C(36)-N(2)-C(22)-O(4)	5.1(6)
C(36)-N(2)-C(22)-C(23)	-174.1(3)
O(4)-C(22)-C(23)-C(24)	1.1(5)
N(2)-C(22)-C(23)-C(24)	-179.7(3)
O(4)-C(22)-C(23)-C(28)	-176.4(3)
N(2)-C(22)-C(23)-C(28)	2.8(5)
C(28)-C(23)-C(24)-C(25)	-2.7(5)
C(22)-C(23)-C(24)-C(25)	179.7(3)
C(23)-C(24)-C(25)-C(26)	2.0(5)
C(24)-C(25)-C(26)-C(27)	-0.3(5)
C(24)-C(25)-C(26)-C(29)	176.9(3)
C(25)-C(26)-C(27)-C(28)	-0.7(5)
C(29)-C(26)-C(27)-C(28)	-178.0(3)
C(26)-C(27)-C(28)-O(5)	179.1(3)
C(26)-C(27)-C(28)-C(23)	-0.1(5)
C(24)-C(23)-C(28)-O(5)	-177.5(3)
C(22)-C(23)-C(28)-O(5)	0.0(5)
C(24)-C(23)-C(28)-C(27)	1.7(5)
C(22)-C(23)-C(28)-C(27)	179.1(3)
Na(1)-O(6)-C(29)-C(30)	-139.6(3)
Na(1)-O(6)-C(29)-C(26)	41.1(6)

C(27)-C(26)-C(29)-O(6)	36.1(5)
C(25)-C(26)-C(29)-O(6)	-141.1(3)
C(27)-C(26)-C(29)-C(30)	-143.2(3)
C(25)-C(26)-C(29)-C(30)	39.6(5)
O(6)-C(29)-C(30)-C(31)	25.6(5)
C(26)-C(29)-C(30)-C(31)	-155.1(3)
O(6)-C(29)-C(30)-C(35)	-152.1(4)
C(26)-C(29)-C(30)-C(35)	27.2(5)
C(35)-C(30)-C(31)-C(32)	0.5(6)
C(29)-C(30)-C(31)-C(32)	-177.3(4)
C(30)-C(31)-C(32)-C(33)	-0.9(7)
C(31)-C(32)-C(33)-C(34)	1.7(8)
C(32)-C(33)-C(34)-C(35)	-2.2(9)
C(33)-C(34)-C(35)-C(30)	1.9(8)
C(31)-C(30)-C(35)-C(34)	-1.0(6)
C(29)-C(30)-C(35)-C(34)	176.7(4)
C(22)-N(2)-C(36)-C(37)	-51.7(5)
C(22)-N(2)-C(36)-C(41)	130.9(4)
C(41)-C(36)-C(37)-F(8)	174.5(3)
N(2)-C(36)-C(37)-F(8)	-3.0(5)
C(41)-C(36)-C(37)-C(38)	-1.9(5)
N(2)-C(36)-C(37)-C(38)	-179.3(3)
F(8)-C(37)-C(38)-F(9)	2.6(5)
C(36)-C(37)-C(38)-F(9)	179.0(3)

F(8)-C(37)-C(38)-C(39)	-176.0(3)
C(36)-C(37)-C(38)-C(39)	0.4(6)
F(9)-C(38)-C(39)-C(40)	-176.4(3)
C(37)-C(38)-C(39)-C(40)	2.2(6)
F(9)-C(38)-C(39)-C(42)	3.3(6)
C(37)-C(38)-C(39)-C(42)	-178.2(5)
C(38)-C(39)-C(40)-F(10)	178.3(4)
C(42)-C(39)-C(40)-F(10)	-1.4(7)
C(38)-C(39)-C(40)-C(41)	-3.3(6)
C(42)-C(39)-C(40)-C(41)	177.0(5)
F(10)-C(40)-C(41)-F(11)	0.2(6)
C(39)-C(40)-C(41)-F(11)	-178.2(4)
F(10)-C(40)-C(41)-C(36)	-179.6(4)
C(39)-C(40)-C(41)-C(36)	2.0(7)
C(37)-C(36)-C(41)-F(11)	-179.1(3)
N(2)-C(36)-C(41)-F(11)	-1.5(5)
C(37)-C(36)-C(41)-C(40)	0.7(6)
N(2)-C(36)-C(41)-C(40)	178.3(4)
C(38)-C(39)-C(42)-F(14)	-108.4(6)
C(40)-C(39)-C(42)-F(14)	71.3(7)
C(38)-C(39)-C(42)-F(13)	130.4(6)
C(40)-C(39)-C(42)-F(13)	-49.9(8)
C(38)-C(39)-C(42)-F(12)	10.5(8)
C(40)-C(39)-C(42)-F(12)	-169.9(5)

Symmetry transformations used to generate equivalent atoms:

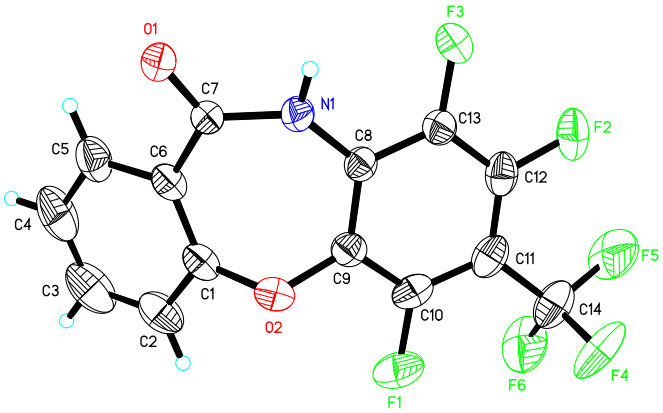
#1 -x+1,-y+2,-z #2 -x+2,-y+1,-z

Table 18. Hydrogen bonds for cd15058 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2A)...O(5)	0.84(5)	1.78(5)	2.563(4)	154(4)
N(1)-H(1)...O(2)	0.91(5)	1.76(5)	2.554(3)	144(4)
O(2)-H(2)...O(5)#3	0.82	1.85	2.448(3)	128.9
N(2)-H(2A)...O(5)	0.84(5)	1.78(5)	2.563(4)	154(4)
N(1)-H(1)...O(2)	0.91(5)	1.76(5)	2.554(3)	144(4)
O(2)-H(2)...O(5)#3	0.82	1.85	2.448(3)	128.9
O(2)-H(2)...O(5)#3	0.82	1.85	2.448(3)	128.9
N(1)-H(1)...O(2)	0.91(5)	1.76(5)	2.554(3)	144(4)
N(2)-H(2A)...O(5)	0.84(5)	1.78(5)	2.563(4)	154(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z #2 -x+2,-y+1,-z #3 -x+1,-y+1,-z



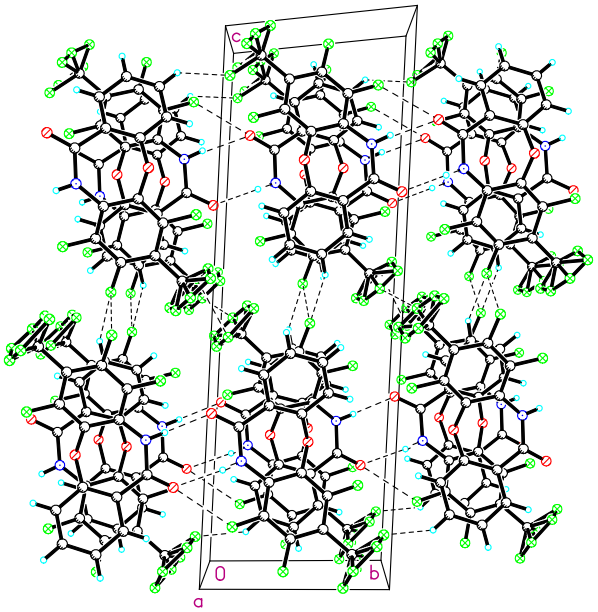


Table 19. Crystal data and structure refinement for cd16124.

Identification code	cd16124
Empirical formula	C14 H5 F6 N O2
Formula weight	333.19
Temperature	293(2) K
Wavelength	0.71073 Å

Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.5465(13) Å	α= 84.375(4) °.
	b = 7.9565(14) Å	β= 89.317(4) °.
	c = 22.733(4) Å	γ = 72.275(4) °.
Volume	1293.7(4) $Å^3$	
Z	4	
Density (calculated)	1.711 Mg/m^3	
Absorption coefficient	0.172 mm^{-1}	
F(000)	664	
Crystal size	0.200 x 0.140 x 0.080 mm^3	
Theta range for data collection	1.801 to 24.999 °.	
Index ranges	-8<=h<=8, -8<=k<=9, -20<=l<=27	
Reflections collected	7165	
Independent reflections	4540 [R(int) = 0.0274]	
Completeness to theta = 25.242 °	97.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6423	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4540 / 92 / 477	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0673, wR2 = 0.1822	
R indices (all data)	R1 = 0.0942, wR2 = 0.2054	
Extinction coefficient	n/a	

Largest diff. peak and hole	0.457 and -0.262 e.Å^{-3}

Table 20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)

for cd16124. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	3442(4)	6990(4)	2774(1)	51(1)
N(2)	699(4)	1971(3)	2289(1)	52(1)
O(1)	2361(4)	8488(3)	1907(1)	79(1)
O(2)	4381(3)	3321(3)	2573(1)	61(1)
O(3)	1120(4)	278(3)	3149(1)	74(1)
O(4)	-1542(3)	5444(3)	2534(1)	66(1)
C(1)	4996(5)	3897(5)	2033(2)	58(1)
C(2)	5967(6)	2638(6)	1681(2)	80(1)
C(3)	6455(7)	3140(9)	1127(3)	107(2)
C(4)	6003(7)	4886(9)	919(2)	102(2)
C(5)	5018(6)	6174(6)	1270(2)	76(1)
C(6)	4507(5)	5686(5)	1837(1)	55(1)
C(7)	3364(5)	7134(4)	2171(1)	54(1)
C(8)	4530(4)	5625(4)	3166(1)	47(1)
C(9)	4999(4)	3847(4)	3070(1)	51(1)
C(10)	5958(5)	2570(4)	3496(2)	63(1)
C(11)	6463(5)	2958(5)	4042(2)	66(1)
C(12)	6009(5)	4731(5)	4126(2)	62(1)

C(13)	5060(5)	6037(4)	3700(1)	54(1)
C(14)	7381(7)	1527(7)	4504(2)	86(1)
C(15)	-484(5)	5041(5)	3059(2)	58(1)
C(16)	-637(6)	6394(6)	3405(2)	82(1)
C(17)	239(8)	6009(8)	3957(3)	100(2)
C(18)	1262(7)	4302(8)	4146(2)	90(2)
C(19)	1412(5)	2963(6)	3795(2)	69(1)
C(20)	549(4)	3314(4)	3240(1)	54(1)
C(21)	790(5)	1761(4)	2894(1)	53(1)
C(22)	501(4)	3489(4)	1900(1)	48(1)
C(23)	-540(5)	5169(4)	2019(2)	56(1)
C(24)	-731(5)	6598(4)	1602(2)	69(1)
C(25)	56(6)	6439(5)	1050(2)	69(1)
C(26)	1085(5)	4747(5)	935(2)	63(1)
C(27)	1299(5)	3315(4)	1346(1)	53(1)
C(28)	-237(8)	8000(6)	597(3)	93(1)
F(1)	6328(3)	874(3)	3386(1)	92(1)
F(2)	6470(3)	5249(3)	4630(1)	85(1)
F(3)	4651(3)	7729(3)	3807(1)	74(1)
F(4)	6163(8)	963(9)	4803(3)	121(2)
F(5)	8182(11)	2177(8)	4955(3)	125(2)
F(6)	8704(13)	258(8)	4305(3)	125(3)
F(4')	7160(19)	1777(16)	5011(6)	135(3)
F(5')	9060(20)	886(18)	4463(6)	129(3)

F(6')	6856(16)	0(13)	4489(5)	132(2)
F(7)	-1795(4)	8193(3)	1738(1)	99(1)
F(8)	1898(4)	4456(3)	411(1)	87(1)
F(9)	2305(3)	1713(2)	1206(1)	72(1)
F(10)	-2162(12)	8714(12)	466(4)	116(2)
F(11)	498(9)	7601(6)	52(2)	110(2)
F(12)	262(11)	9243(11)	754(4)	107(2)
F(10')	-1520(20)	8303(19)	276(5)	113(3)
F(11')	1422(16)	8048(12)	391(4)	128(2)
F(12')	-559(18)	9605(18)	914(6)	111(3)

Table 21. Bond lengths [Å] and angles [°] for cd16124.

N(1)-C(7)	1.364(4)
N(1)-C(8)	1.391(4)
N(1)-H(1)	0.814(18)
N(2)-C(21)	1.370(4)
N(2)-C(22)	1.395(4)
N(2)-H(2A)	0.820(18)
O(1)-C(7)	1.217(4)
O(2)-C(9)	1.377(4)
O(2)-C(1)	1.391(4)
O(3)-C(21)	1.217(4)
O(4)-C(23)	1.385(4)
O(4)-C(15)	1.398(4)
C(1)-C(2)	1.369(5)
C(1)-C(6)	1.386(5)
C(2)-C(3)	1.366(7)
C(2)-H(2)	0.9300
C(3)-C(4)	1.363(8)
C(3)-H(3)	0.9300
C(4)-C(5)	1.386(6)
C(4)-H(4)	0.9300
C(5)-C(6)	1.394(5)
C(5)-H(5)	0.9300

C(6)-C(7)	1.483(5)
C(8)-C(13)	1.381(4)
C(8)-C(9)	1.389(4)
C(9)-C(10)	1.367(5)
C(10)-F(1)	1.340(4)
C(10)-C(11)	1.394(5)
C(11)-C(12)	1.379(5)
C(11)-C(14)	1.477(5)
C(12)-F(2)	1.339(4)
C(12)-C(13)	1.378(5)
C(13)-F(3)	1.333(4)
C(14)-F(4')	1.189(13)
C(14)-F(5')	1.216(15)
C(14)-F(4)	1.298(7)
C(14)-F(6)	1.299(9)
C(14)-F(6')	1.392(11)
C(14)-F(5)	1.411(8)
C(15)-C(16)	1.372(5)
C(15)-C(20)	1.382(5)
C(16)-C(17)	1.387(7)
C(16)-H(16)	0.9300
C(17)-C(18)	1.372(7)
C(17)-H(17)	0.9300
C(18)-C(19)	1.370(6)

C(18)-H(18)	0.9300
C(19)-C(20)	1.390(5)
C(19)-H(19)	0.9300
C(20)-C(21)	1.494(5)
C(22)-C(23)	1.380(4)
C(22)-C(27)	1.389(4)
C(23)-C(24)	1.380(5)
C(24)-F(7)	1.342(4)
C(24)-C(25)	1.382(6)
C(25)-C(26)	1.383(5)
C(25)-C(28)	1.497(6)
C(26)-F(8)	1.341(4)
C(26)-C(27)	1.372(5)
C(27)-F(9)	1.337(4)
C(28)-F(10')	1.166(16)
C(28)-F(12)	1.244(10)
C(28)-F(11')	1.341(11)
C(28)-F(11)	1.377(7)
C(28)-F(10)	1.413(11)
C(28)-F(12')	1.483(16)

C(7)-N(1)-C(8)	129.4(3)
C(7)-N(1)-H(1)	108(2)
C(8)-N(1)-H(1)	123(2)

C(21)-N(2)-C(22)	129.8(3)
C(21)-N(2)-H(2A)	111(2)
C(22)-N(2)-H(2A)	117(2)
C(9)-O(2)-C(1)	116.5(2)
C(23)-O(4)-C(15)	115.7(2)
C(2)-C(1)-C(6)	121.0(4)
C(2)-C(1)-O(2)	117.9(3)
C(6)-C(1)-O(2)	120.9(3)
C(3)-C(2)-C(1)	119.9(4)
C(3)-C(2)-H(2)	120.0
C(1)-C(2)-H(2)	120.0
C(4)-C(3)-C(2)	120.7(4)
C(4)-C(3)-H(3)	119.6
C(2)-C(3)-H(3)	119.6
C(3)-C(4)-C(5)	120.0(5)
C(3)-C(4)-H(4)	120.0
C(5)-C(4)-H(4)	120.0
C(4)-C(5)-C(6)	120.1(5)
C(4)-C(5)-H(5)	120.0
C(6)-C(5)-H(5)	120.0
C(1)-C(6)-C(5)	118.3(3)
C(1)-C(6)-C(7)	124.8(3)
C(5)-C(6)-C(7)	116.8(3)
O(1)-C(7)-N(1)	119.0(3)

O(1)-C(7)-C(6)	120.0(3)
N(1)-C(7)-C(6)	121.0(3)
C(13)-C(8)-C(9)	117.8(3)
C(13)-C(8)-N(1)	118.6(3)
C(9)-C(8)-N(1)	123.4(3)
C(10)-C(9)-O(2)	118.4(3)
C(10)-C(9)-C(8)	120.1(3)
O(2)-C(9)-C(8)	121.3(3)
F(1)-C(10)-C(9)	117.6(3)
F(1)-C(10)-C(11)	119.4(3)
C(9)-C(10)-C(11)	122.9(3)
C(12)-C(11)-C(10)	116.2(3)
C(12)-C(11)-C(14)	122.9(4)
C(10)-C(11)-C(14)	121.0(4)
F(2)-C(12)-C(13)	117.4(3)
F(2)-C(12)-C(11)	121.0(3)
C(13)-C(12)-C(11)	121.6(3)
F(3)-C(13)-C(12)	119.0(3)
F(3)-C(13)-C(8)	119.6(3)
C(12)-C(13)-C(8)	121.4(3)
F(4')-C(14)-F(5')	104.4(10)
F(4)-C(14)-F(6)	113.0(6)
F(4')-C(14)-F(6')	101.2(9)
F(5')-C(14)-F(6')	99.2(9)

F(4)-C(14)-F(5)	100.6(6)
F(6)-C(14)-F(5)	106.7(6)
F(4')-C(14)-C(11)	119.6(7)
F(5')-C(14)-C(11)	116.0(7)
F(4)-C(14)-C(11)	110.9(4)
F(6)-C(14)-C(11)	113.4(5)
F(6')-C(14)-C(11)	113.7(5)
F(5)-C(14)-C(11)	111.4(4)
C(16)-C(15)-C(20)	121.7(4)
C(16)-C(15)-O(4)	117.4(4)
C(20)-C(15)-O(4)	120.7(3)
C(15)-C(16)-C(17)	119.0(4)
C(15)-C(16)-H(16)	120.5
C(17)-C(16)-H(16)	120.5
C(18)-C(17)-C(16)	120.1(4)
C(18)-C(17)-H(17)	119.9
C(16)-C(17)-H(17)	119.9
C(19)-C(18)-C(17)	120.3(5)
C(19)-C(18)-H(18)	119.8
C(17)-C(18)-H(18)	119.8
C(18)-C(19)-C(20)	120.6(4)
C(18)-C(19)-H(19)	119.7
C(20)-C(19)-H(19)	119.7
C(15)-C(20)-C(19)	118.2(3)

C(15)-C(20)-C(21)	125.4(3)
C(19)-C(20)-C(21)	116.4(3)
O(3)-C(21)-N(2)	119.1(3)
O(3)-C(21)-C(20)	119.9(3)
N(2)-C(21)-C(20)	120.9(3)
C(23)-C(22)-C(27)	117.2(3)
C(23)-C(22)-N(2)	123.6(3)
C(27)-C(22)-N(2)	119.1(3)
C(22)-C(23)-C(24)	120.2(3)
C(22)-C(23)-O(4)	121.2(3)
C(24)-C(23)-O(4)	118.4(3)
F(7)-C(24)-C(23)	117.5(4)
F(7)-C(24)-C(25)	119.4(3)
C(23)-C(24)-C(25)	123.0(3)
C(24)-C(25)-C(26)	116.1(3)
C(24)-C(25)-C(28)	121.9(4)
C(26)-C(25)-C(28)	121.9(4)
F(8)-C(26)-C(27)	117.9(3)
F(8)-C(26)-C(25)	120.6(3)
C(27)-C(26)-C(25)	121.5(3)
F(9)-C(27)-C(26)	118.6(3)
F(9)-C(27)-C(22)	119.6(3)
C(26)-C(27)-C(22)	121.9(3)
F(10')-C(28)-F(11')	120.6(9)

F(12)-C(28)-F(11)	108.8(6)
F(12)-C(28)-F(10)	105.9(7)
F(11)-C(28)-F(10)	102.5(6)
F(10')-C(28)-F(12')	105.3(10)
F(11')-C(28)-F(12')	94.5(8)
F(10')-C(28)-C(25)	116.6(8)
F(12)-C(28)-C(25)	115.2(6)
F(11')-C(28)-C(25)	108.9(5)
F(11)-C(28)-C(25)	114.9(4)
F(10)-C(28)-C(25)	108.5(5)
F(12')-C(28)-C(25)	107.8(7)

Symmetry transformations used to generate equivalent atoms:

Table 22. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for cd16124. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	62(2)	47(2)	42(1)	-5(1)	5(1)	-11(1)
N(2)	69(2)	40(1)	47(2)	-8(1)	4(1)	-18(1)
O(1)	129(2)	52(1)	49(1)	-2(1)	-15(1)	-16(2)
O(2)	67(2)	53(1)	68(2)	-12(1)	1(1)	-25(1)
O(3)	108(2)	52(1)	52(1)	3(1)	15(1)	-15(1)
O(4)	54(1)	58(1)	81(2)	-9(1)	15(1)	-9(1)
C(1)	53(2)	67(2)	60(2)	-23(2)	3(2)	-23(2)
C(2)	67(2)	83(3)	93(3)	-45(2)	9(2)	-14(2)
C(3)	82(3)	131(5)	112(4)	-75(4)	27(3)	-23(3)
C(4)	96(4)	164(5)	66(3)	-51(3)	31(2)	-57(4)
C(5)	85(3)	107(3)	52(2)	-17(2)	11(2)	-51(2)
C(6)	56(2)	65(2)	52(2)	-19(2)	6(2)	-27(2)
C(7)	73(2)	48(2)	44(2)	-3(1)	-5(2)	-26(2)
C(8)	47(2)	51(2)	44(2)	-4(1)	7(1)	-18(1)
C(9)	49(2)	55(2)	54(2)	-7(2)	7(1)	-22(2)
C(10)	58(2)	48(2)	76(2)	7(2)	5(2)	-12(2)
C(11)	51(2)	78(3)	64(2)	13(2)	5(2)	-18(2)
C(12)	54(2)	89(3)	47(2)	-2(2)	5(2)	-28(2)
C(13)	60(2)	56(2)	49(2)	-5(2)	5(2)	-22(2)

C(14)	72(3)	91(3)	79(3)	25(3)	-2(2)	-12(3)
C(15)	51(2)	63(2)	67(2)	-23(2)	23(2)	-26(2)
C(16)	84(3)	75(3)	99(3)	-38(2)	37(3)	-33(2)
C(17)	102(4)	117(4)	111(4)	-73(3)	45(3)	-61(3)
C(18)	81(3)	141(5)	70(3)	-51(3)	25(2)	-55(3)
C(19)	60(2)	99(3)	54(2)	-21(2)	14(2)	-29(2)
C(20)	48(2)	64(2)	55(2)	-17(2)	14(2)	-23(2)
C(21)	55(2)	52(2)	51(2)	-7(2)	6(2)	-15(2)
C(22)	50(2)	47(2)	53(2)	-2(1)	-5(1)	-23(1)
C(23)	50(2)	53(2)	64(2)	-4(2)	5(2)	-17(2)
C(24)	63(2)	44(2)	93(3)	5(2)	-4(2)	-12(2)
C(25)	78(3)	59(2)	73(3)	14(2)	-5(2)	-29(2)
C(26)	72(2)	72(2)	52(2)	2(2)	-3(2)	-33(2)
C(27)	64(2)	48(2)	50(2)	-7(1)	2(2)	-21(2)
C(28)	104(4)	70(3)	102(4)	23(3)	-11(3)	-33(3)
F(1)	94(2)	51(1)	121(2)	11(1)	-7(1)	-15(1)
F(2)	89(2)	125(2)	45(1)	-3(1)	-6(1)	-38(1)
F(3)	101(2)	70(1)	55(1)	-18(1)	0(1)	-26(1)
F(4)	103(4)	126(4)	120(4)	67(3)	17(3)	-40(3)
F(5)	137(4)	119(4)	111(3)	42(3)	-68(4)	-42(3)
F(6)	125(5)	96(4)	102(4)	15(3)	-10(3)	37(4)
F(4')	137(5)	132(5)	109(4)	45(4)	-8(4)	-17(4)
F(5')	115(5)	126(5)	116(5)	54(4)	-12(4)	-13(4)
F(6')	139(5)	117(5)	124(4)	48(4)	-16(4)	-33(4)

F(7)	100(2)	46(1)	133(2)	6(1)	14(2)	-1(1)
F(8)	118(2)	99(2)	52(1)	2(1)	9(1)	-49(2)
F(9)	105(2)	58(1)	56(1)	-16(1)	15(1)	-25(1)
F(10)	124(5)	97(4)	106(5)	31(4)	-20(3)	-15(3)
F(11)	167(5)	92(3)	63(3)	26(2)	8(3)	-38(3)
F(12)	157(6)	79(4)	98(5)	25(3)	-26(4)	-63(4)
F(10')	153(7)	100(5)	83(6)	26(4)	-34(5)	-41(5)
F(11')	168(6)	99(4)	106(5)	45(4)	15(4)	-41(4)
F(12')	143(7)	70(4)	110(6)	29(4)	0(5)	-30(5)

Table 23. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for cd16124.

	x	y	z	U(eq)
H(2)	6292	1443	1820	97
H(3)	7104	2279	888	128
H(4)	6356	5213	543	123
H(5)	4697	7366	1126	91
H(16)	-1318	7552	3273	99
H(17)	132	6911	4199	119
H(18)	1858	4052	4515	108
H(19)	2097	1807	3929	83
H(2A)	1080(40)	1010(30)	2151(12)	43(9)
H(1)	2810(40)	7930(30)	2880(14)	55(10)

Table 24. Torsion angles [°] for cd16124.

C(9)-O(2)-C(1)-C(2)	121.4(3)
C(9)-O(2)-C(1)-C(6)	-63.9(4)
C(6)-C(1)-C(2)-C(3)	-0.4(6)
O(2)-C(1)-C(2)-C(3)	174.3(4)
C(1)-C(2)-C(3)-C(4)	0.6(7)
C(2)-C(3)-C(4)-C(5)	-0.8(8)
C(3)-C(4)-C(5)-C(6)	0.8(7)
C(2)-C(1)-C(6)-C(5)	0.4(5)
O(2)-C(1)-C(6)-C(5)	-174.1(3)
C(2)-C(1)-C(6)-C(7)	176.1(3)
O(2)-C(1)-C(6)-C(7)	1.6(5)
C(4)-C(5)-C(6)-C(1)	-0.6(5)
C(4)-C(5)-C(6)-C(7)	-176.6(4)
C(8)-N(1)-C(7)-O(1)	-176.9(3)
C(8)-N(1)-C(7)-C(6)	1.8(5)
C(1)-C(6)-C(7)-O(1)	-148.8(4)
C(5)-C(6)-C(7)-O(1)	27.0(5)
C(1)-C(6)-C(7)-N(1)	32.5(5)
C(5)-C(6)-C(7)-N(1)	-151.7(3)
C(7)-N(1)-C(8)-C(13)	149.8(3)
C(7)-N(1)-C(8)-C(9)	-35.2(5)
C(1)-O(2)-C(9)-C(10)	-122.1(3)

C(1)-O(2)-C(9)-C(8)	63.4(4)
C(13)-C(8)-C(9)-C(10)	-0.2(5)
N(1)-C(8)-C(9)-C(10)	-175.1(3)
C(13)-C(8)-C(9)-O(2)	174.2(3)
N(1)-C(8)-C(9)-O(2)	-0.7(5)
O(2)-C(9)-C(10)-F(1)	3.6(5)
C(8)-C(9)-C(10)-F(1)	178.2(3)
O(2)-C(9)-C(10)-C(11)	-172.7(3)
C(8)-C(9)-C(10)-C(11)	1.8(5)
F(1)-C(10)-C(11)-C(12)	-179.0(3)
C(9)-C(10)-C(11)-C(12)	-2.7(5)
F(1)-C(10)-C(11)-C(14)	-0.7(5)
C(9)-C(10)-C(11)-C(14)	175.7(4)
C(10)-C(11)-C(12)-F(2)	-178.4(3)
C(14)-C(11)-C(12)-F(2)	3.3(5)
C(10)-C(11)-C(12)-C(13)	1.9(5)
C(14)-C(11)-C(12)-C(13)	-176.3(4)
F(2)-C(12)-C(13)-F(3)	0.0(5)
C(11)-C(12)-C(13)-F(3)	179.7(3)
F(2)-C(12)-C(13)-C(8)	179.9(3)
C(11)-C(12)-C(13)-C(8)	-0.4(5)
C(9)-C(8)-C(13)-F(3)	179.4(3)
N(1)-C(8)-C(13)-F(3)	-5.4(5)
C(9)-C(8)-C(13)-C(12)	-0.5(5)

N(1)-C(8)-C(13)-C(12)	174.7(3)
C(12)-C(11)-C(14)-F(4')	27.6(12)
C(10)-C(11)-C(14)-F(4')	-150.6(10)
C(12)-C(11)-C(14)-F(5')	-98.8(10)
C(10)-C(11)-C(14)-F(5')	83.0(10)
C(12)-C(11)-C(14)-F(4)	94.5(7)
C(10)-C(11)-C(14)-F(4)	-83.7(7)
C(12)-C(11)-C(14)-F(6)	-137.0(6)
C(10)-C(11)-C(14)-F(6)	44.8(8)
C(12)-C(11)-C(14)-F(6')	147.1(7)
C(10)-C(11)-C(14)-F(6')	-31.1(8)
C(12)-C(11)-C(14)-F(5)	-16.6(7)
C(10)-C(11)-C(14)-F(5)	165.2(5)
C(23)-O(4)-C(15)-C(16)	119.2(3)
C(23)-O(4)-C(15)-C(20)	-66.0(4)
C(20)-C(15)-C(16)-C(17)	-1.3(5)
O(4)-C(15)-C(16)-C(17)	173.4(3)
C(15)-C(16)-C(17)-C(18)	0.9(6)
C(16)-C(17)-C(18)-C(19)	-0.7(7)
C(17)-C(18)-C(19)-C(20)	0.7(6)
C(16)-C(15)-C(20)-C(19)	1.4(5)
O(4)-C(15)-C(20)-C(19)	-173.2(3)
C(16)-C(15)-C(20)-C(21)	179.9(3)
O(4)-C(15)-C(20)-C(21)	5.3(5)

C(18)-C(19)-C(20)-C(15)	-1.0(5)
C(18)-C(19)-C(20)-C(21)	-179.7(3)
C(22)-N(2)-C(21)-O(3)	-174.0(3)
C(22)-N(2)-C(21)-C(20)	4.1(5)
C(15)-C(20)-C(21)-O(3)	-153.7(3)
C(19)-C(20)-C(21)-O(3)	24.9(5)
C(15)-C(20)-C(21)-N(2)	28.2(5)
C(19)-C(20)-C(21)-N(2)	-153.2(3)
C(21)-N(2)-C(22)-C(23)	-34.6(5)
C(21)-N(2)-C(22)-C(27)	149.2(3)
C(27)-C(22)-C(23)-C(24)	-1.1(5)
N(2)-C(22)-C(23)-C(24)	-177.3(3)
C(27)-C(22)-C(23)-O(4)	173.3(3)
N(2)-C(22)-C(23)-O(4)	-3.0(5)
C(15)-O(4)-C(23)-C(22)	65.2(4)
C(15)-O(4)-C(23)-C(24)	-120.3(3)
C(22)-C(23)-C(24)-F(7)	178.5(3)
O(4)-C(23)-C(24)-F(7)	3.9(5)
C(22)-C(23)-C(24)-C(25)	1.2(6)
O(4)-C(23)-C(24)-C(25)	-173.4(3)
F(7)-C(24)-C(25)-C(26)	-178.0(3)
C(23)-C(24)-C(25)-C(26)	-0.8(6)
F(7)-C(24)-C(25)-C(28)	0.3(6)
C(23)-C(24)-C(25)-C(28)	177.5(4)

C(24)-C(25)-C(26)-F(8)	179.8(3)
C(28)-C(25)-C(26)-F(8)	1.5(6)
C(24)-C(25)-C(26)-C(27)	0.3(6)
C(28)-C(25)-C(26)-C(27)	-178.0(4)
F(8)-C(26)-C(27)-F(9)	0.2(5)
C(25)-C(26)-C(27)-F(9)	179.7(3)
F(8)-C(26)-C(27)-C(22)	-179.8(3)
C(25)-C(26)-C(27)-C(22)	-0.2(6)
C(23)-C(22)-C(27)-F(9)	-179.3(3)
N(2)-C(22)-C(27)-F(9)	-2.9(5)
C(23)-C(22)-C(27)-C(26)	0.6(5)
N(2)-C(22)-C(27)-C(26)	177.1(3)
C(24)-C(25)-C(28)-F(10')	-89.9(10)
C(26)-C(25)-C(28)-F(10')	88.2(9)
C(24)-C(25)-C(28)-F(12)	57.9(8)
C(26)-C(25)-C(28)-F(12)	-123.9(6)
C(24)-C(25)-C(28)-F(11')	129.5(7)
C(26)-C(25)-C(28)-F(11')	-52.3(8)
C(24)-C(25)-C(28)-F(11)	-174.5(5)
C(26)-C(25)-C(28)-F(11)	3.7(8)
C(24)-C(25)-C(28)-F(10)	-60.5(7)
C(26)-C(25)-C(28)-F(10)	117.7(6)
C(24)-C(25)-C(28)-F(12')	28.2(9)
C(26)-C(25)-C(28)-F(12')	-153.6(7)

Symmetry transformations used to generate equivalent atoms:

Table 25. Hydrogen bonds for cd16124 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(3)#1	0.814(18)	2.060(19)	2.873(4)	178(3)
N(2)-H(2A)...O(1)#2	0.820(18)	2.074(19)	2.887(4)	171(3)
C(2)-H(2)...F(7)#3	0.93	2.57	3.414(5)	150.6
N(1)-H(1)...O(3)#1	0.814(18)	2.060(19)	2.873(4)	178(3)
N(2)-H(2A)...O(1)#2	0.820(18)	2.074(19)	2.887(4)	171(3)
C(2)-H(2)...F(7)#3	0.93	2.57	3.414(5)	150.6
N(1)-H(1)...O(3)#1	0.814(18)	2.060(19)	2.873(4)	178(3)
N(2)-H(2A)...O(1)#2	0.820(18)	2.074(19)	2.887(4)	171(3)
C(2)-H(2)...F(7)#3	0.93	2.57	3.414(5)	150.6
N(1)-H(1)...O(3)#1	0.814(18)	2.060(19)	2.873(4)	178(3)
N(2)-H(2A)...O(1)#2	0.820(18)	2.074(19)	2.887(4)	171(3)
C(2)-H(2)...F(7)#3	0.93	2.57	3.414(5)	150.6
C(2)-H(2)...F(7)#3	0.93	2.57	3.414(5)	150.6
N(2)-H(2A)...O(1)#2	0.820(18)	2.074(19)	2.887(4)	171(3)
N(1)-H(1)...O(3)#1	0.814(18)	2.060(19)	2.873(4)	178(3)
C(2)-H(2)...F(7)#3	0.93	2.57	3.414(5)	150.6
N(2)-H(2A)...O(1)#2	0.820(18)	2.074(19)	2.887(4)	171(3)
N(1)-H(1)...O(3)#1	0.814(18)	2.060(19)	2.873(4)	178(3)
C(2)-H(2)...F(7)#3	0.93	2.57	3.414(5)	150.6
N(2)-H(2A)...O(1)#2	0.820(18)	2.074(19)	2.887(4)	171(3)

N(1)-H(1)...O(3)#1	0.814(18)	2.060(19)	2.873(4)	178(3)

Symmetry transformations used to generate equivalent atoms:

#1 x,y+1,z #2 x,y-1,z #3 x+1,y-1,z

4. References.

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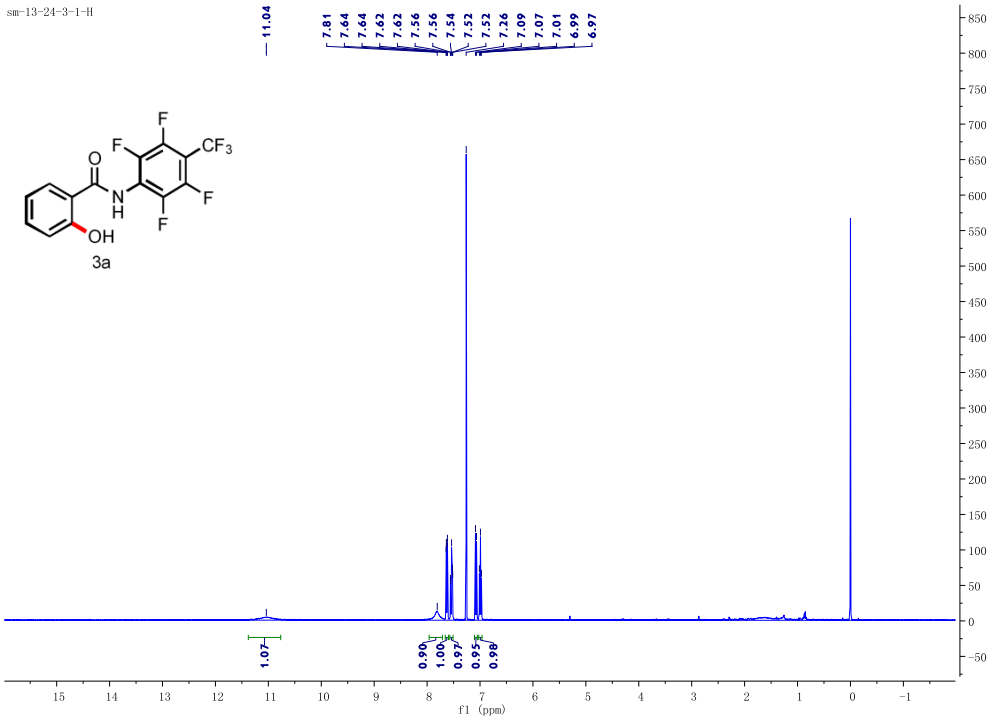
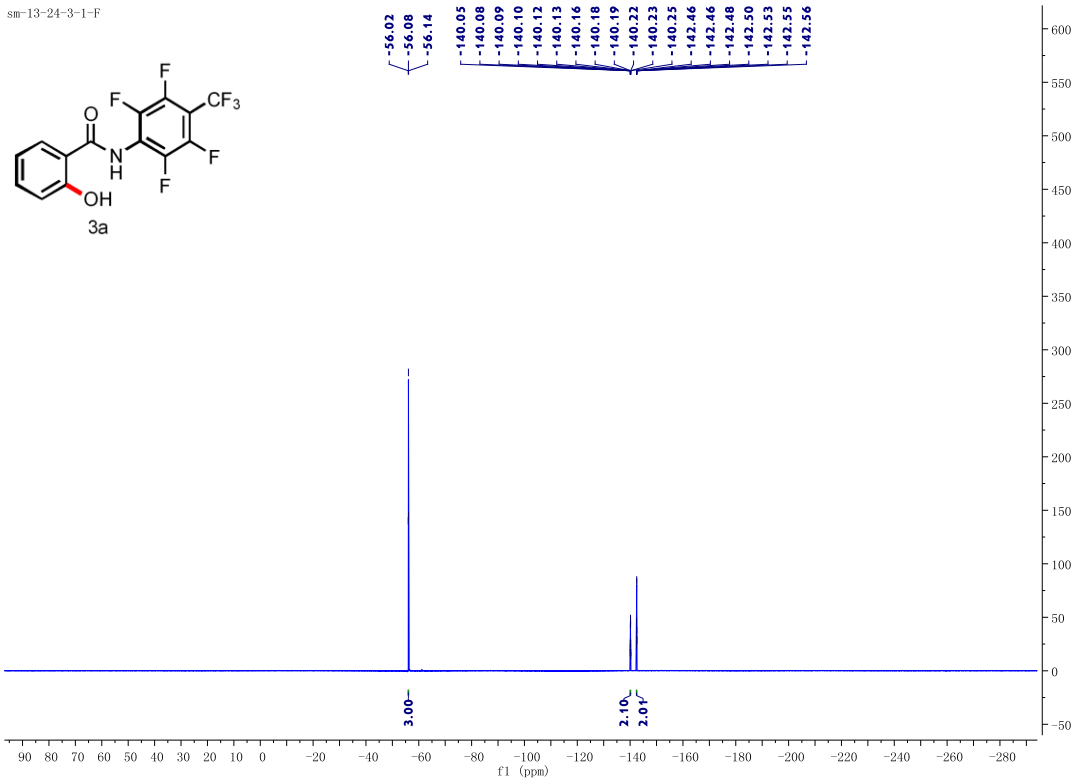
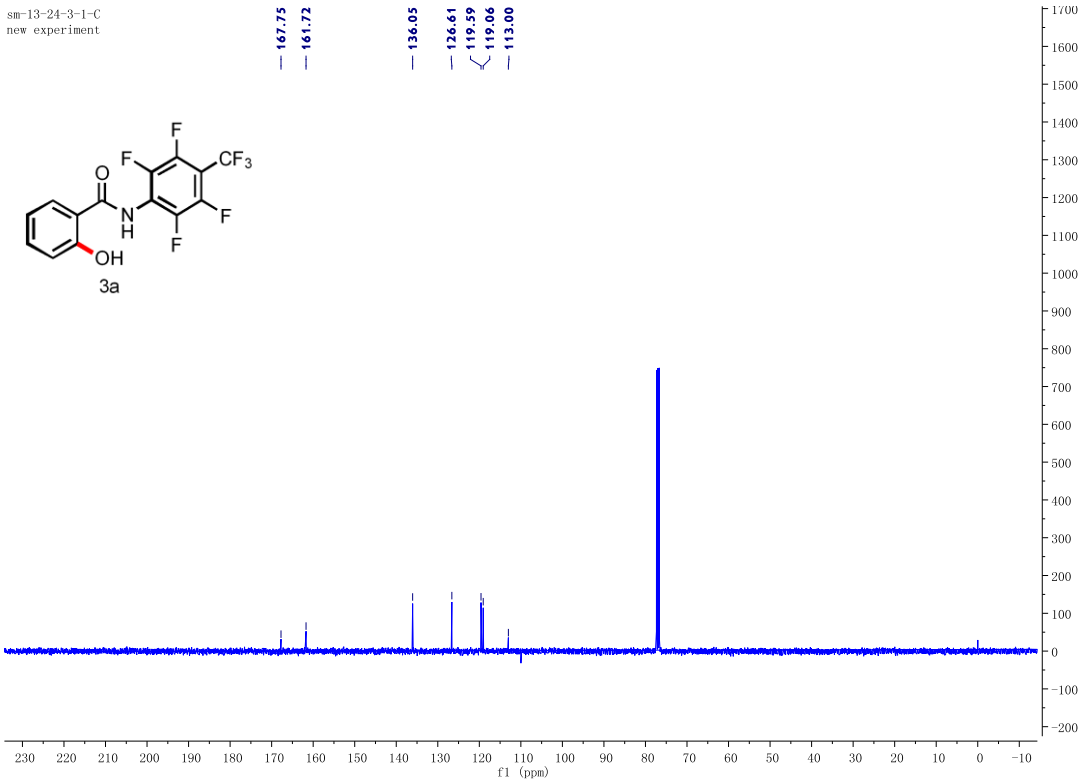
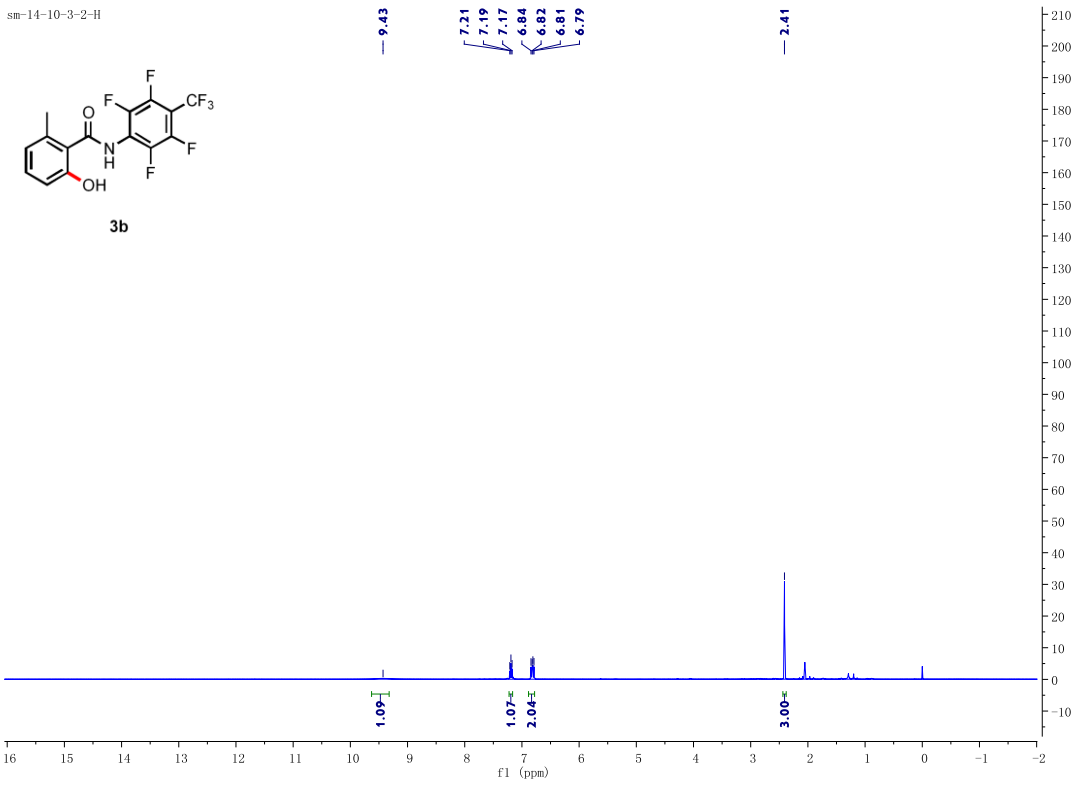
(3) Zhu, D.; Yang, G.; He, J.; Chu, L.; Chen, G.; Gong, W.; Chen, K.; Eastgate, M. D.; Yu, J.-Q. *Angew. Chem. Int. Ed.* **2015**, *54*, 2497.

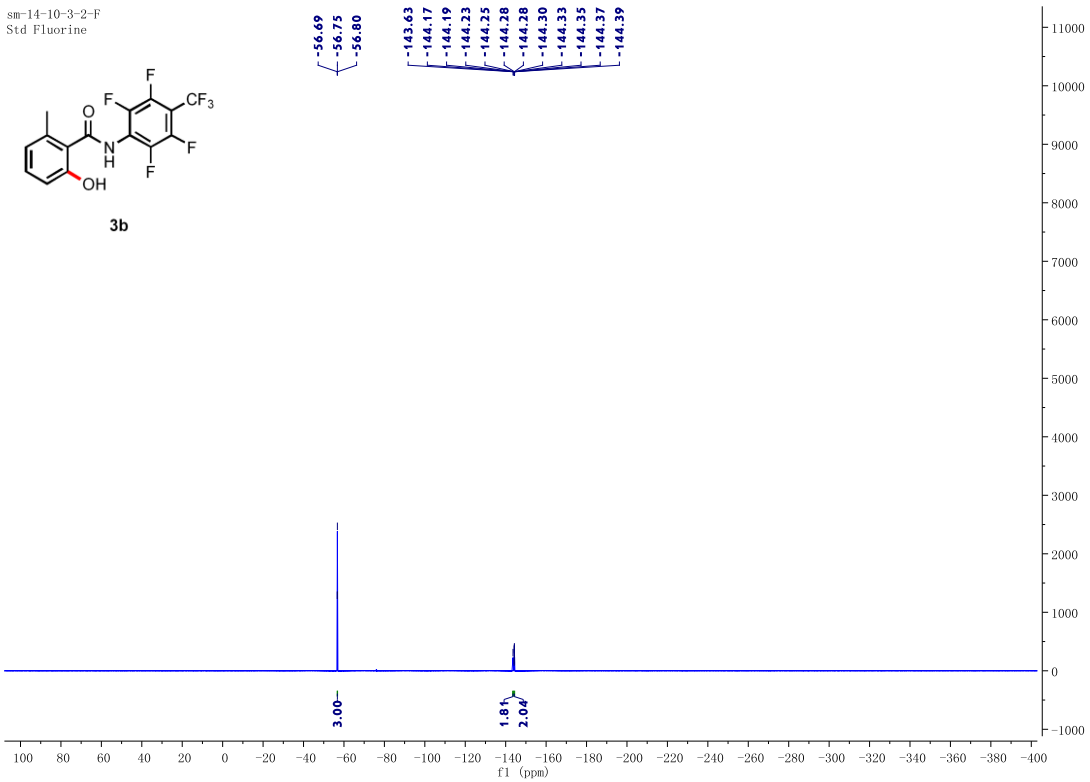
5. NMR Spectra for New Compounds. .



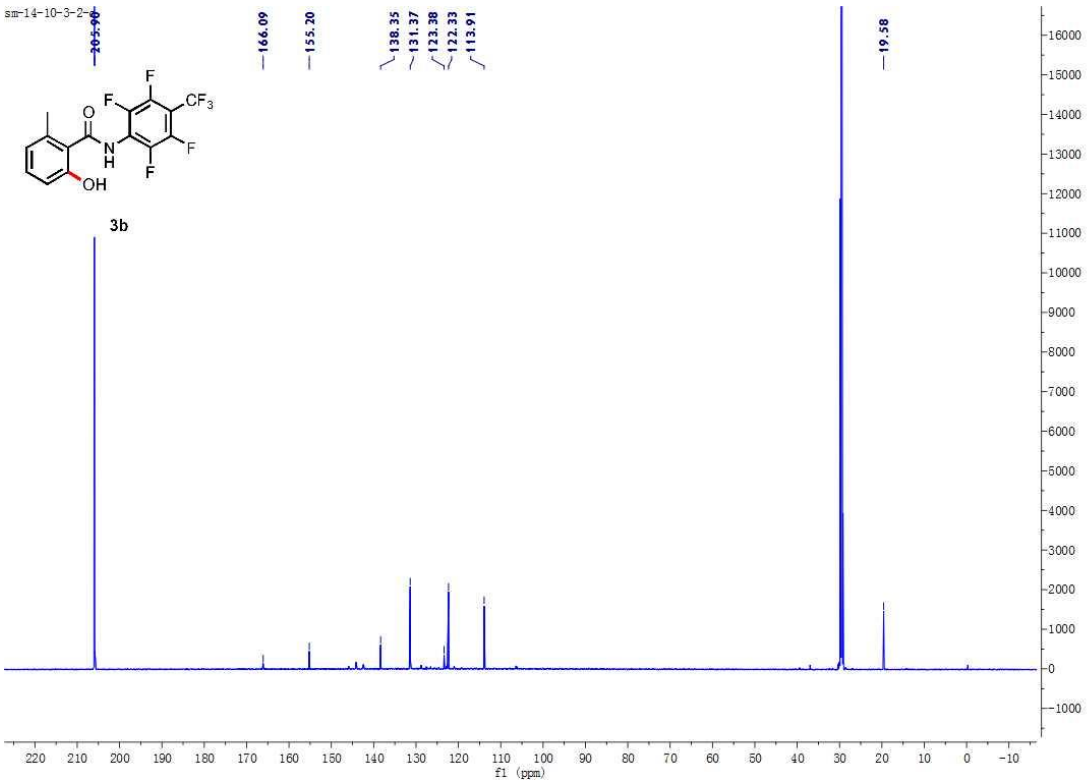



sm-13-24-3-1-C
new experiment
167.75
161.72
136.05
126.61
119.59
119.06
113.00
F
F
CF3
O
N
H
F
F
OH
3a
f1 (ppm)

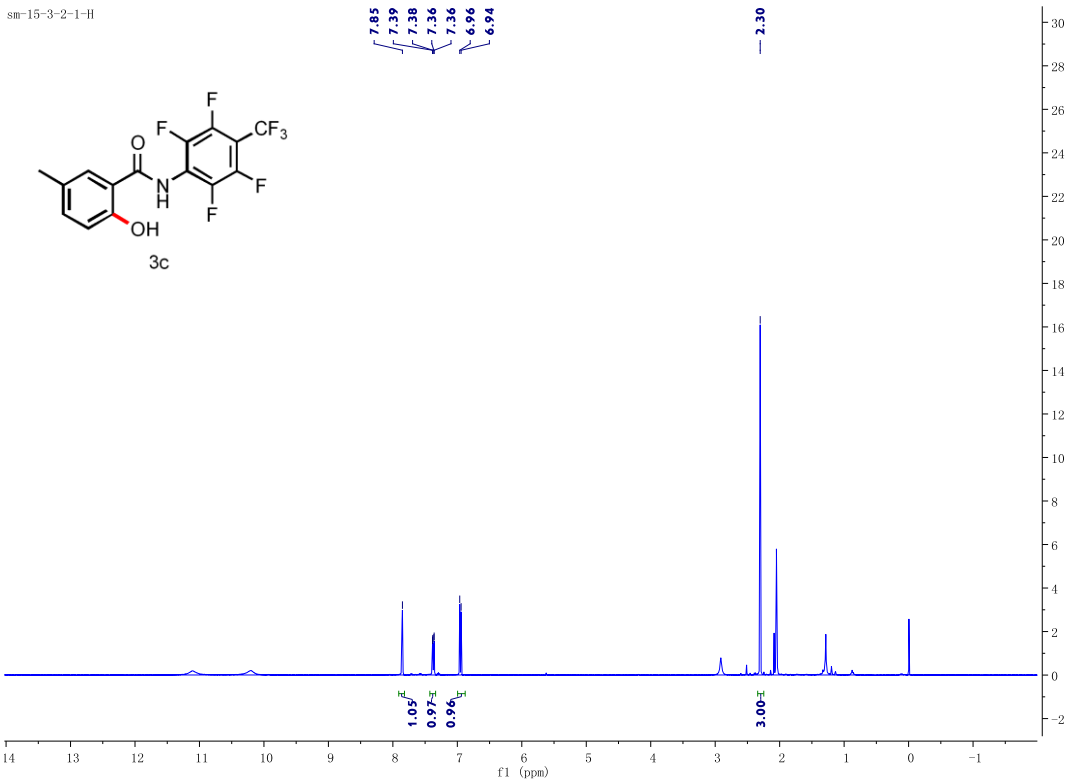

sm-14-10-3-2-H
9.43
7.21
7.19
7.17
6.84
6.82
6.81
6.79
2.41
F
F
CF3
O
N
H
F
F
OH
3b
1.09
1.07
2.04
3.00
f1 (ppm)

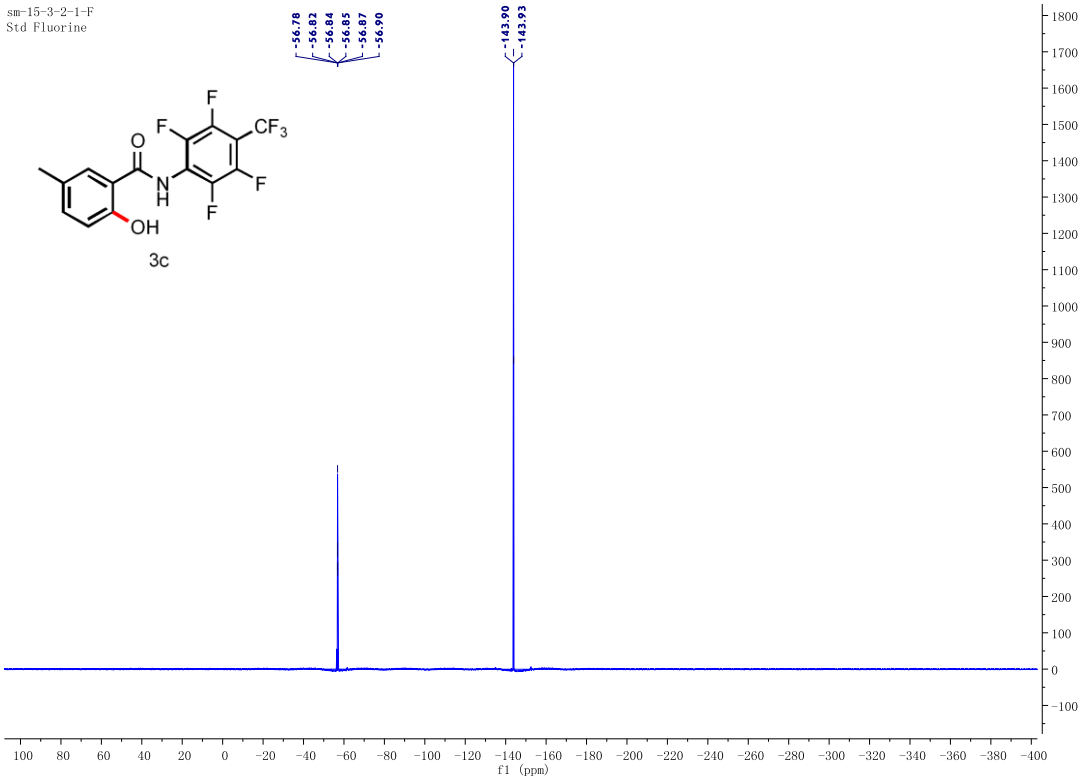

sm-14-10-3-2-F
Std Fluorine
-56.69
-56.75
-56.80
-143.63
-144.17
-144.19
-144.23
-144.25
-144.28
-144.28
-144.30
-144.33
-144.35
-144.37
-144.39
3.00
1.81
2.04
f1 (ppm)

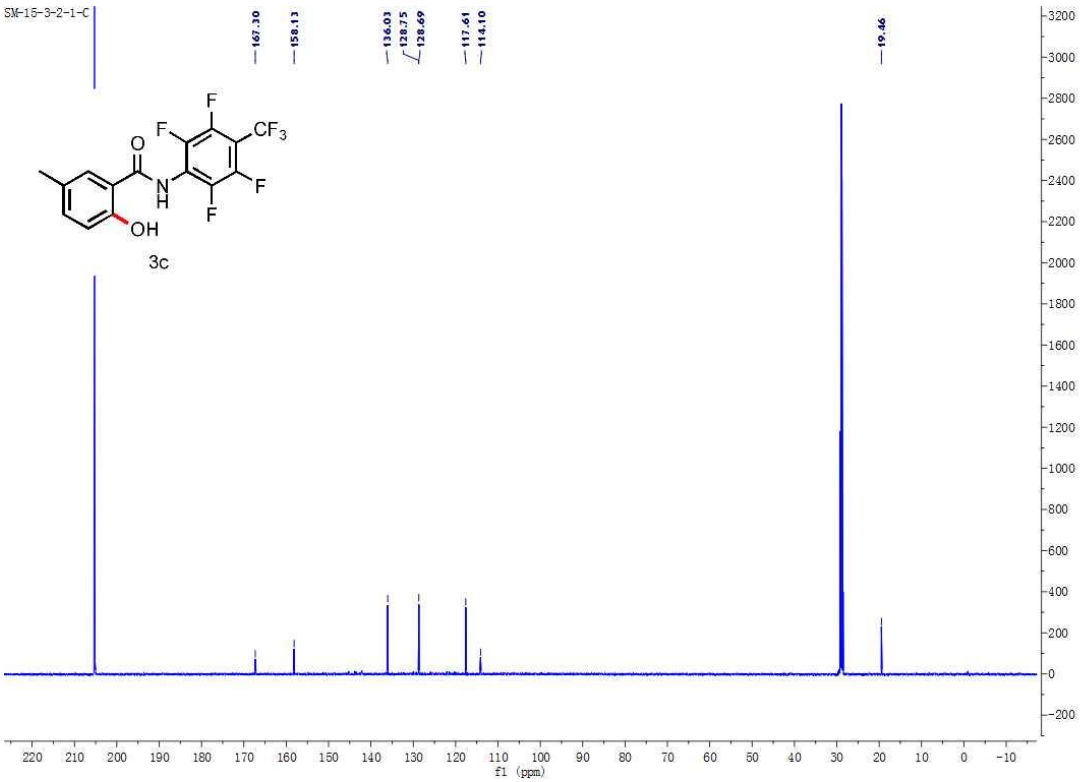
3b

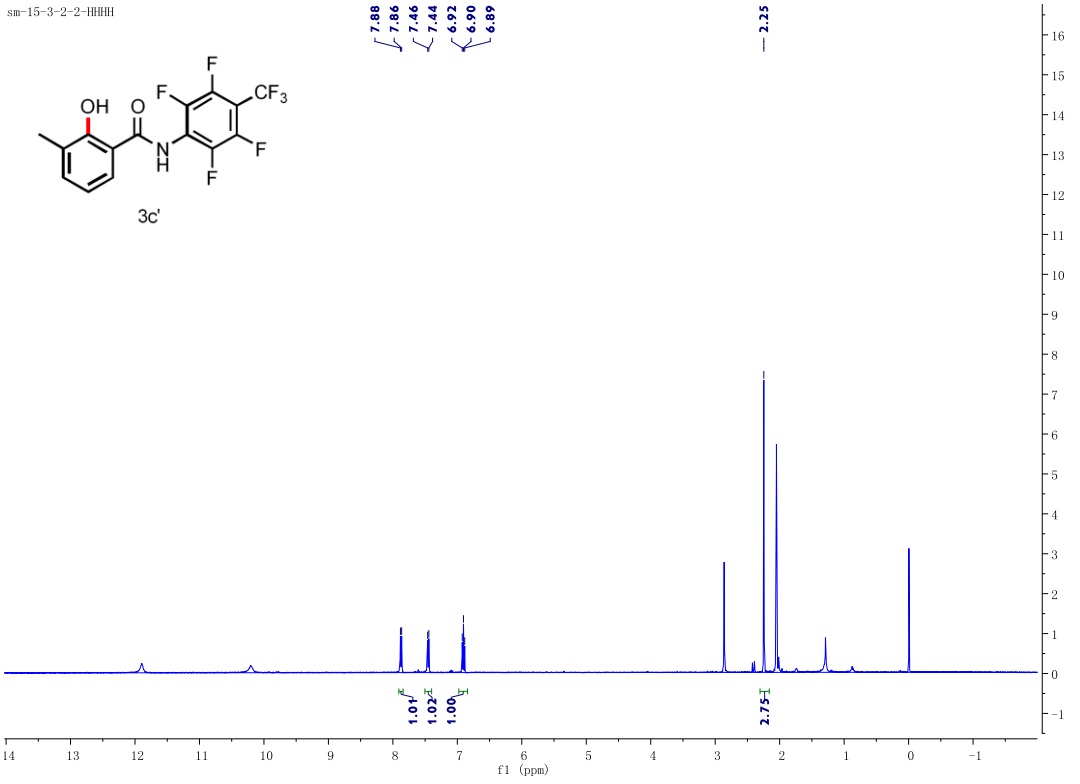

sm-14-10-3-2-
166.09
155.20
138.35
131.37
123.38
122.33
113.91
19.58
f1 (ppm)

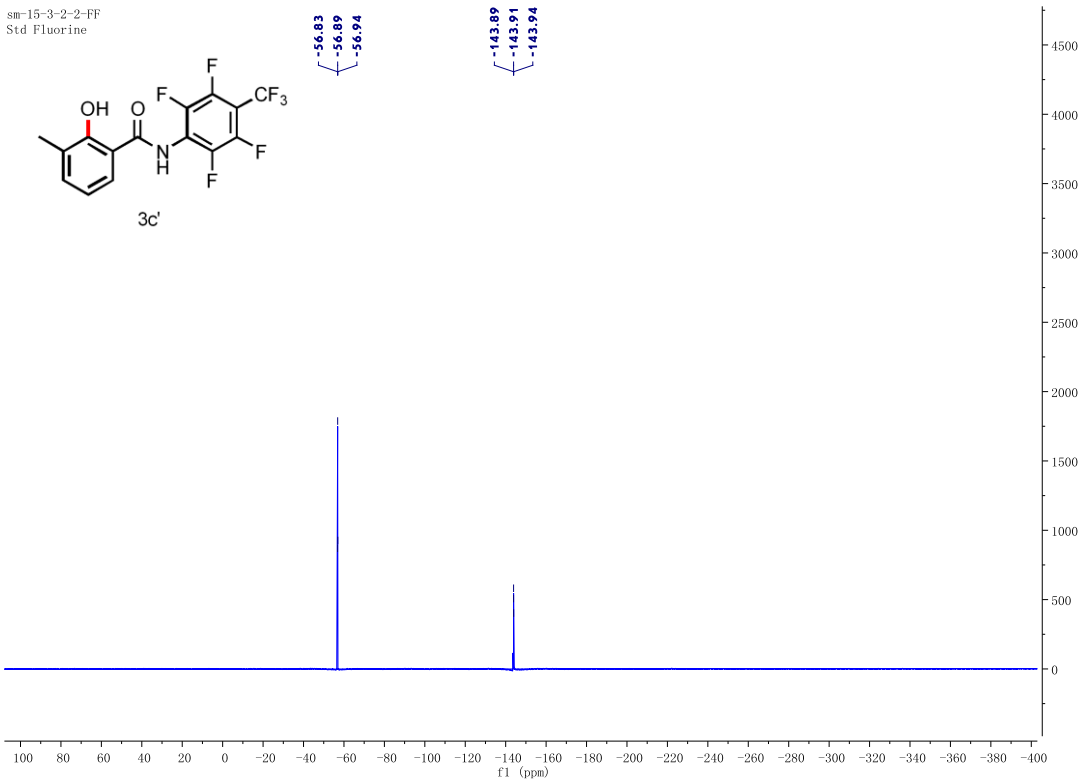
3b

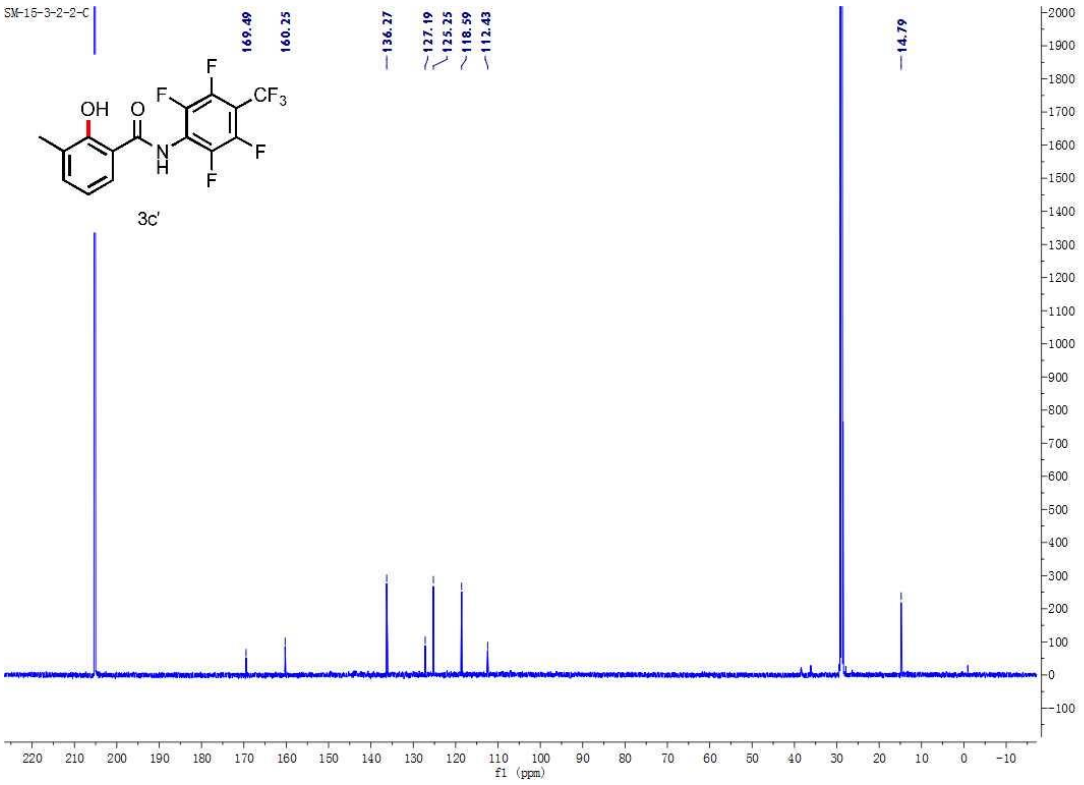

sm-15-3-2-1-H
7.85
7.39
7.38
7.36
7.36
6.96
6.94
2.30
F
F
CF3
O
N
H
F
F
OH
3c
1.05
0.97
0.96
3.00
f1 (ppm)

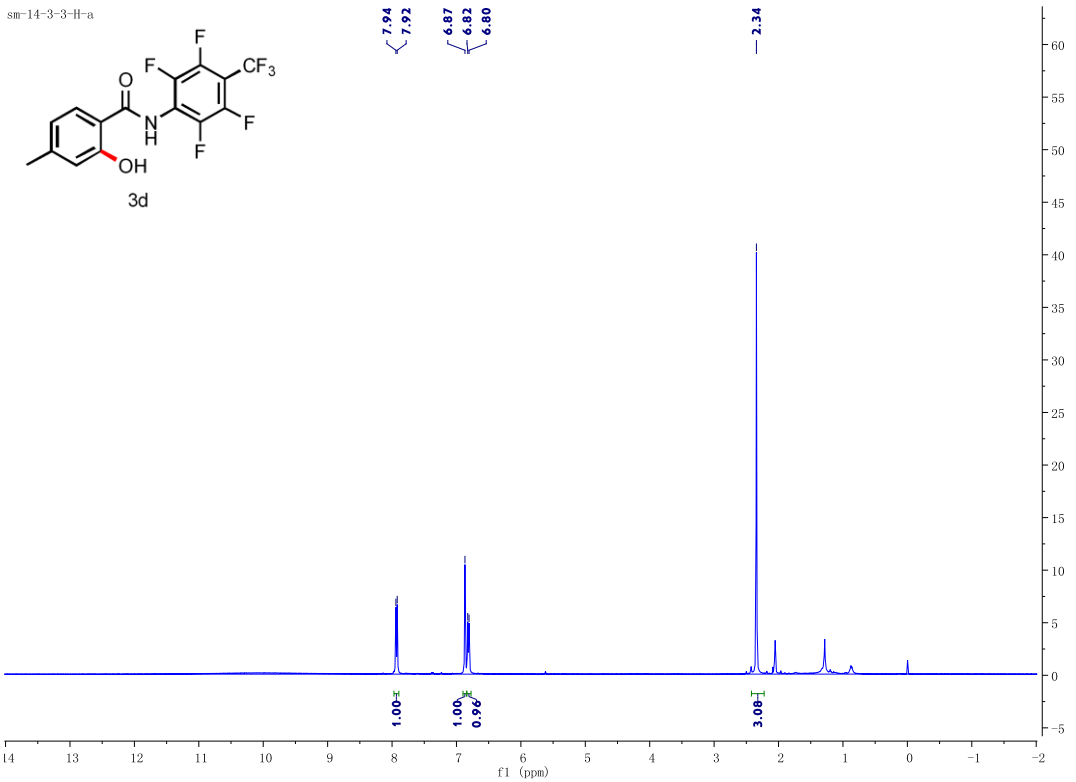

sm-15-3-2-1-F
Std Fluorine
-56.78
-56.82
-56.84
-56.85
-56.87
-56.90
-143.90
-143.93
F
F
CF3
O
N
H
F
F
OH
3c
f1 (ppm)

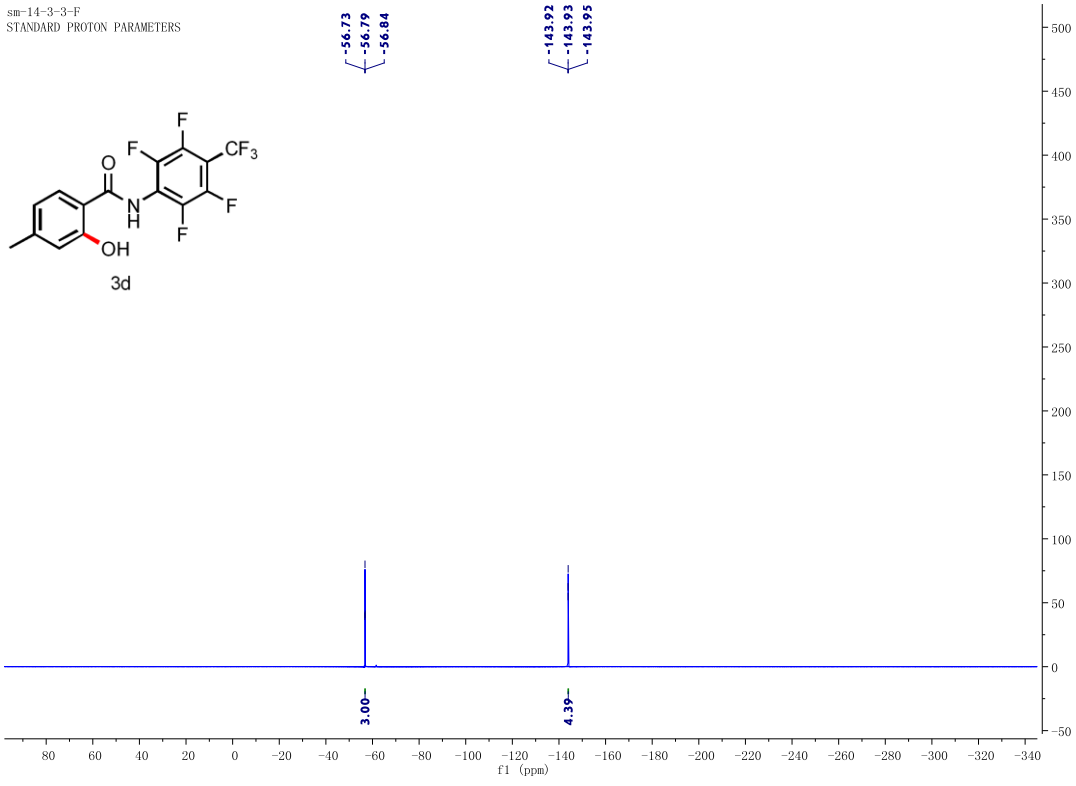

SM-15-3-2-1-C
167.30
158.13
136.03
128.75
128.69
117.61
114.10
19.46
3c
f1 (ppm)

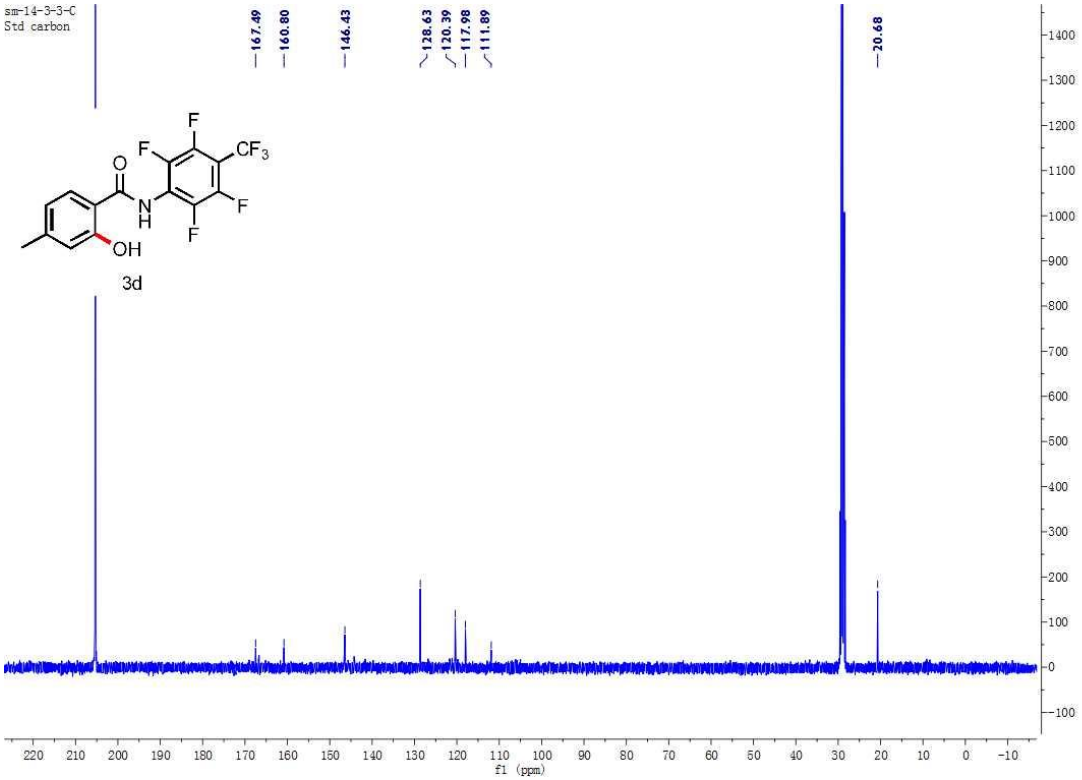

sm-15-3-2-2-HHHH
7.88
7.86
7.46
7.44
6.92
6.90
6.89
2.25
1.01
1.02
1.00
2.75
3c'
f1 (ppm)

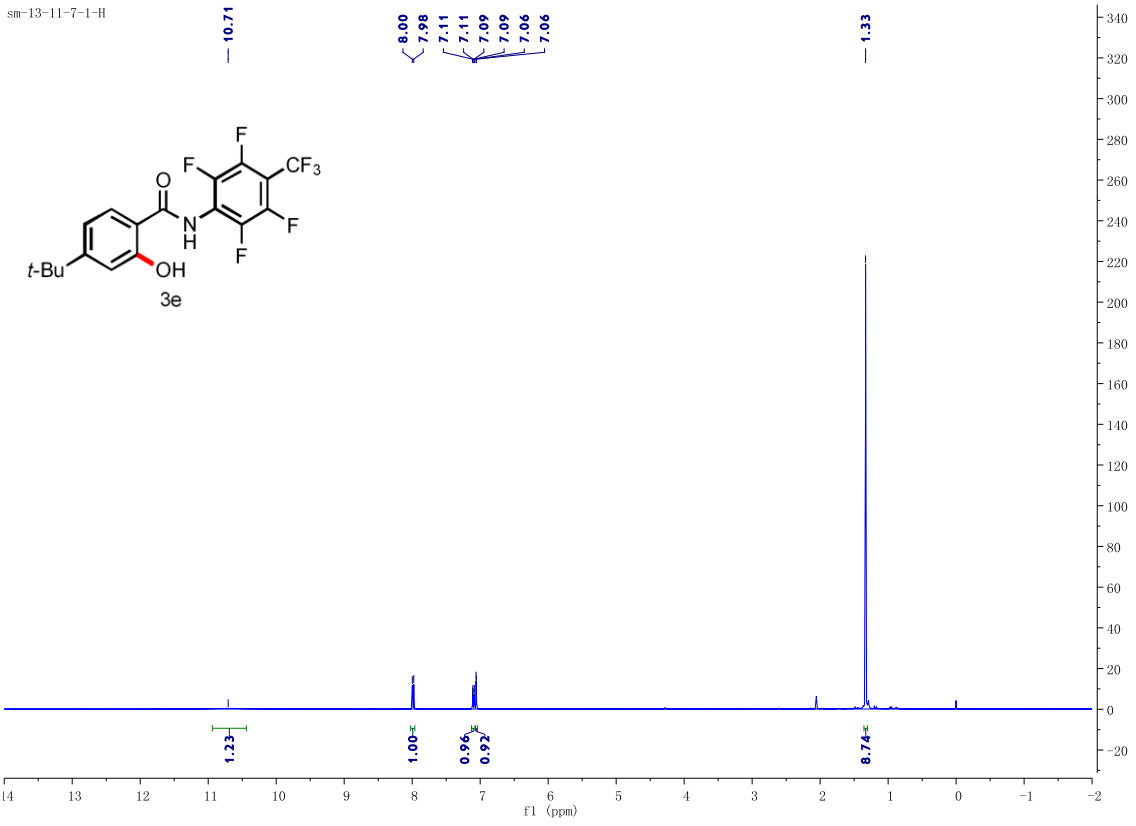

sm-15-3-2-2-FF
Std Fluorine
-56.83
-56.89
-56.94
-143.89
-143.91
-143.94
OH
O
N
H
F
CF3
3c'
f1 (ppm)

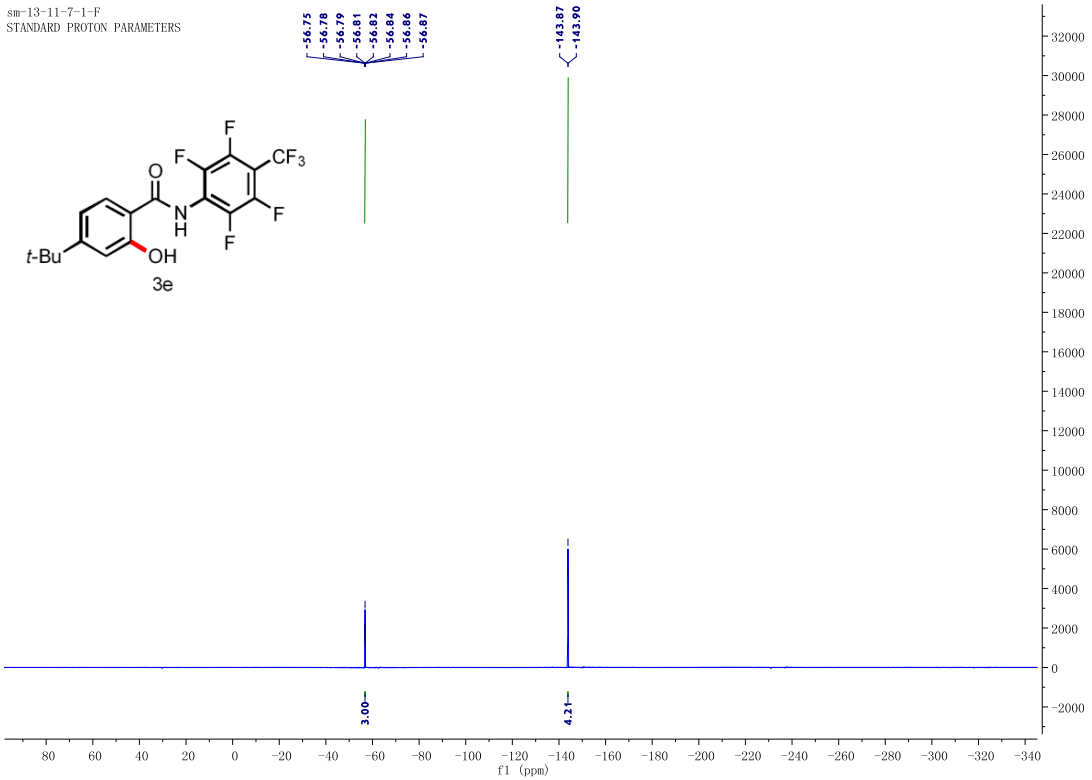

SM-15-3-2-2-C
169.49
160.25
136.27
127.19
125.25
118.59
112.43
14.79
OH
O
N
H
F
CF3
3c'
f1 (ppm)

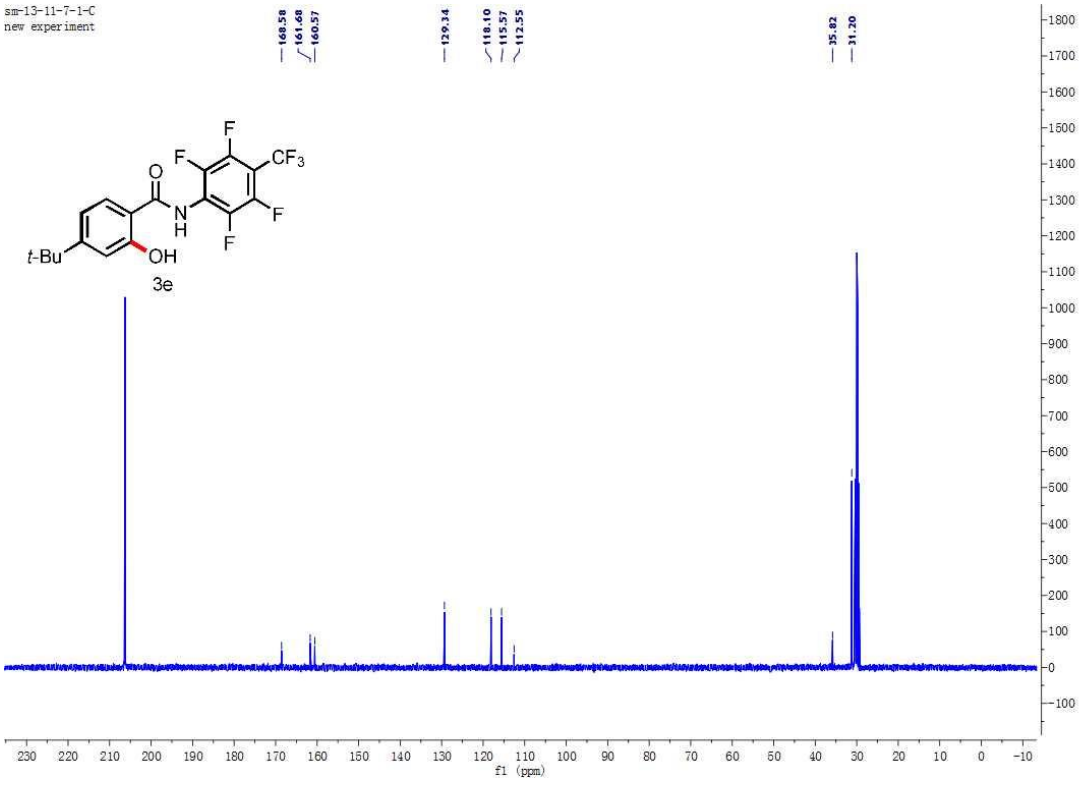

sm-14-3-3-H-a
7.94
7.92
6.87
6.82
6.80
2.34
1.00
1.00
0.96
3.08
f1 (ppm)
3d

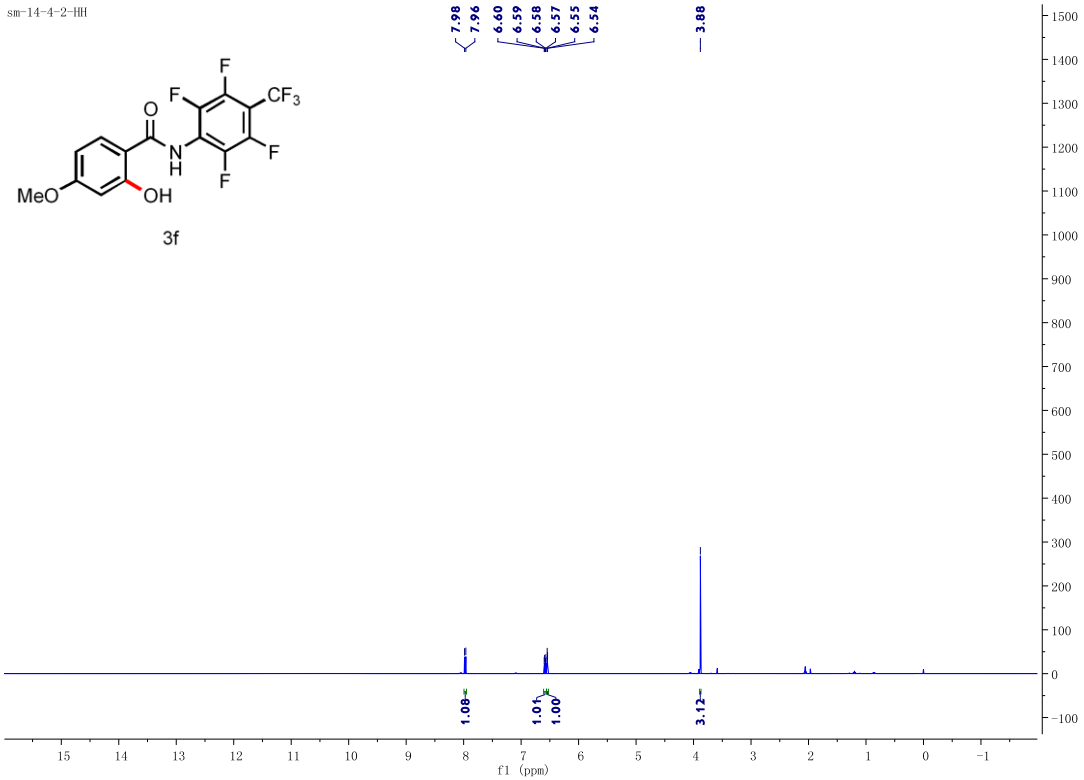

sm-14-3-3-F
STANDARD PROTON PARAMETERS
-56.73
-56.79
-56.84
-143.92
-143.93
-143.95
3.00
4.39
f1 (ppm)
3d

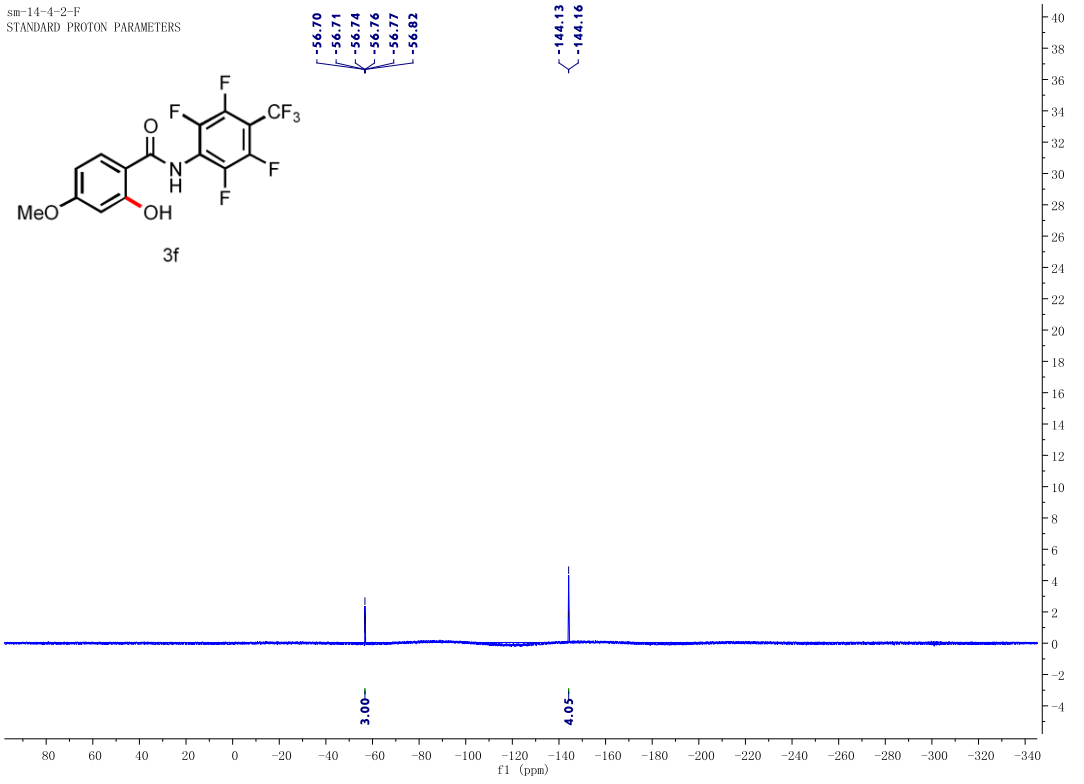

sm-14-3-3-C
Std carbon
167.49
160.80
146.43
128.63
120.39
117.98
111.89
20.68
3d
f1 (ppm)

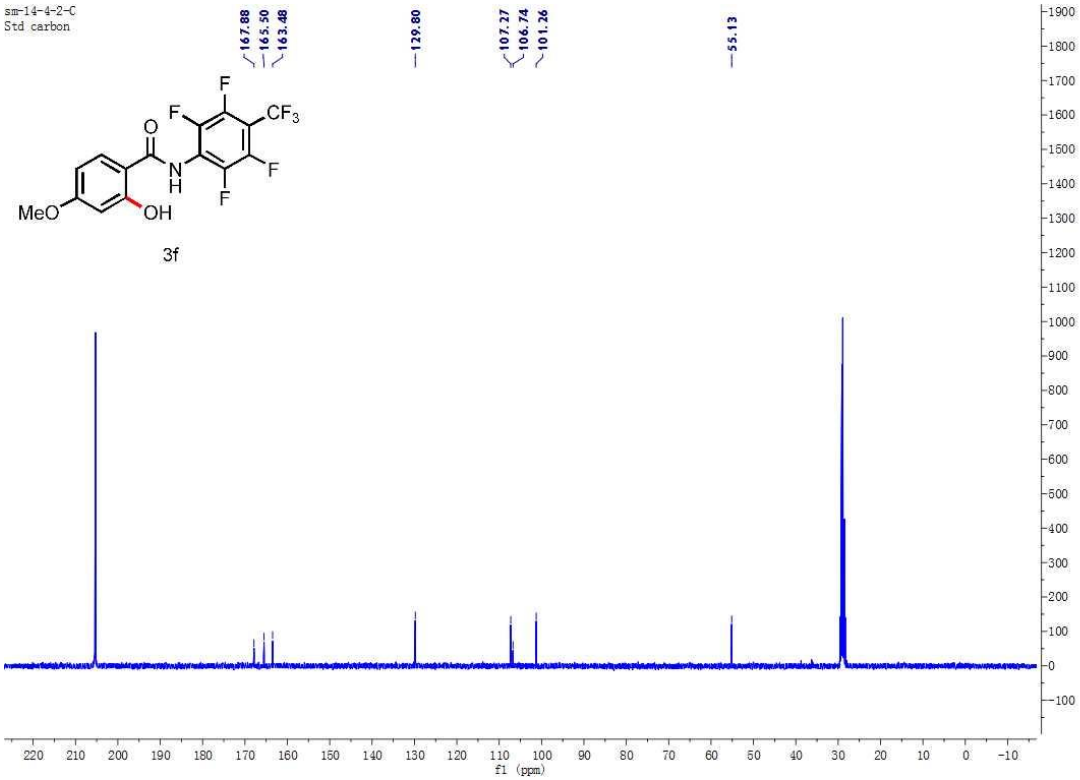

sm-13-11-7-1-H
10.71
8.00
7.98
7.11
7.11
7.09
7.09
7.06
7.06
1.33
t-Bu
3e
1.23
1.00
0.96
0.92
8.74
f1 (ppm)

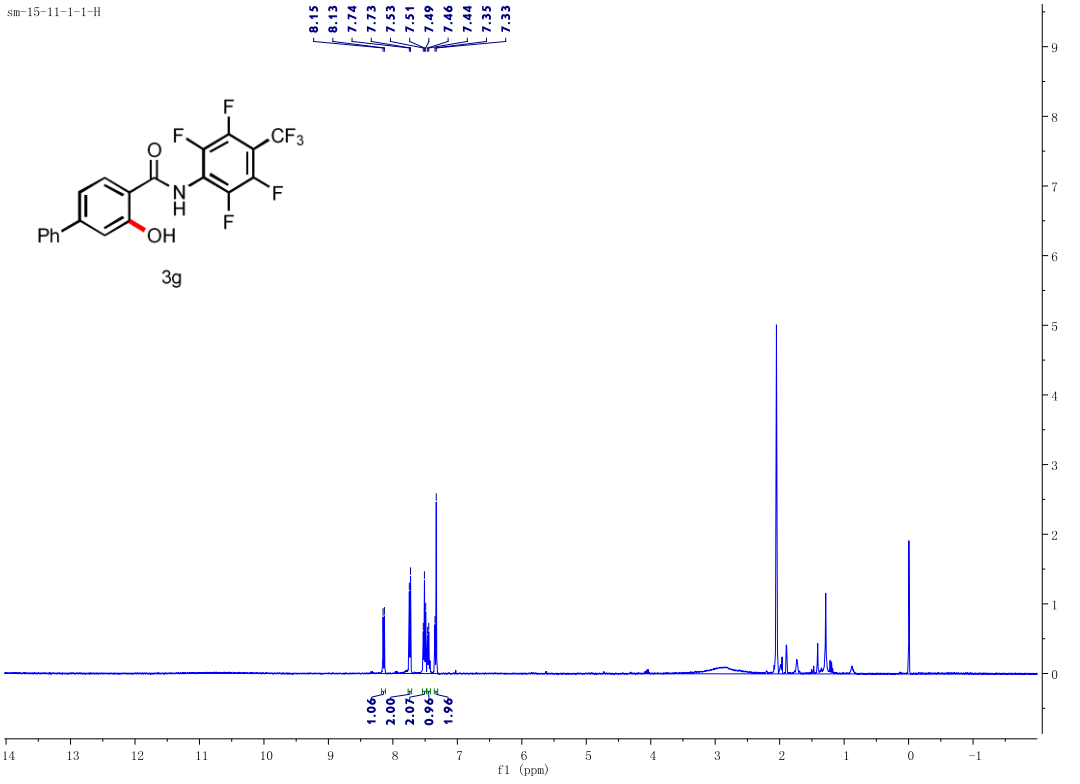

sm-13-11-7-1-F
STANDARD PROTON PARAMETERS
-56.75
-56.78
-56.79
-56.81
-56.82
-56.84
-56.86
-56.87
-143.87
-143.90
3.00
4.21
f1 (ppm)
3e

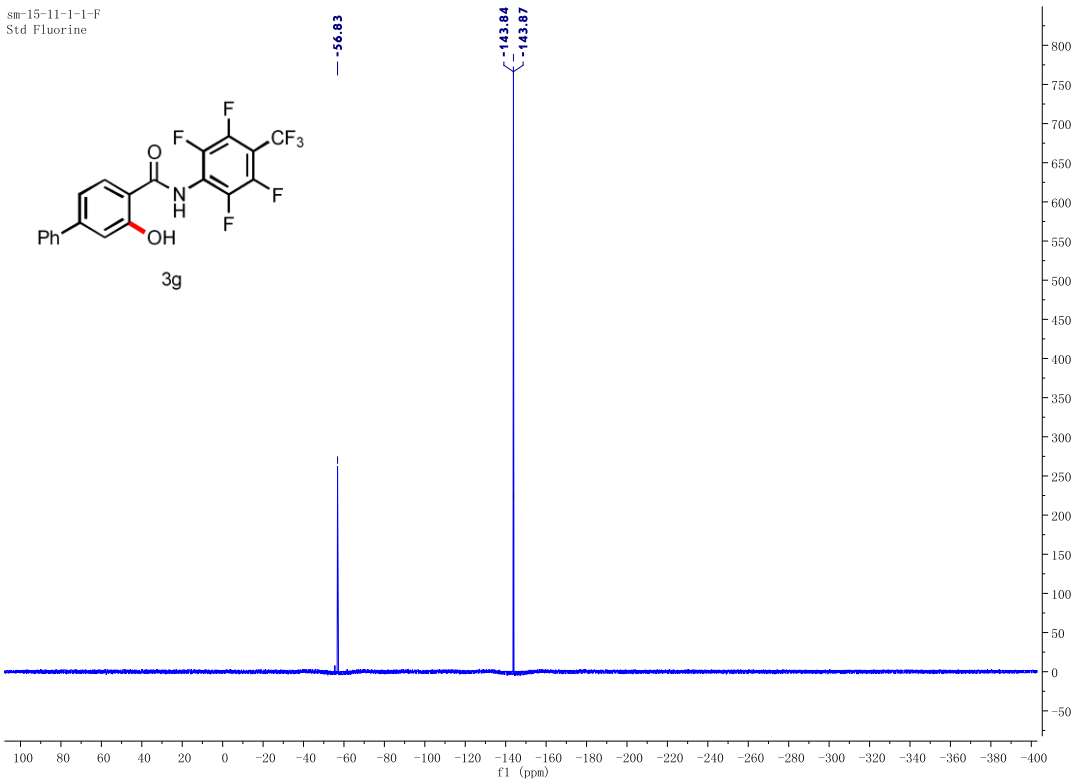

sm-13-11-7-1-C
new experiment
168.58
161.68
160.57
129.34
118.10
115.57
112.55
35.82
31.20
f1 (ppm)
3e

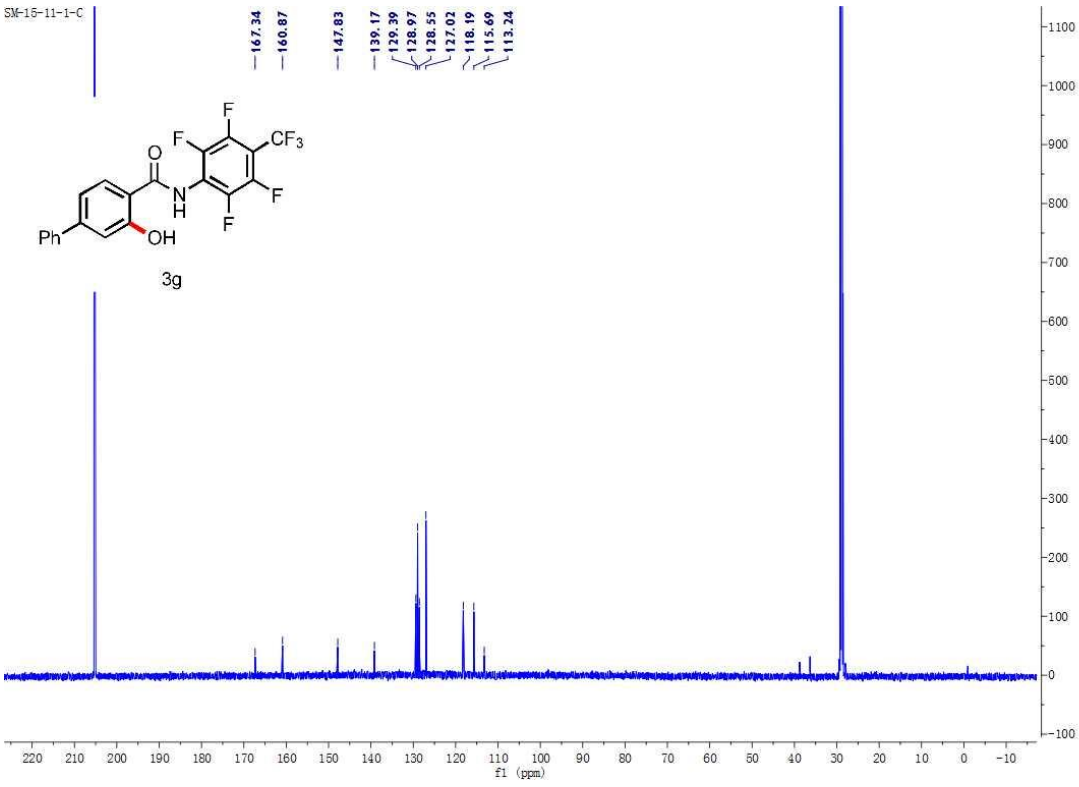

sm-14-4-2-HH
7.98
7.96
6.60
6.59
6.58
6.57
6.55
6.54
3.88
F
F
CF3
O
N
H
F
F
MeO
OH
3f
1.08
1.01
1.00
3.12
f1 (ppm)

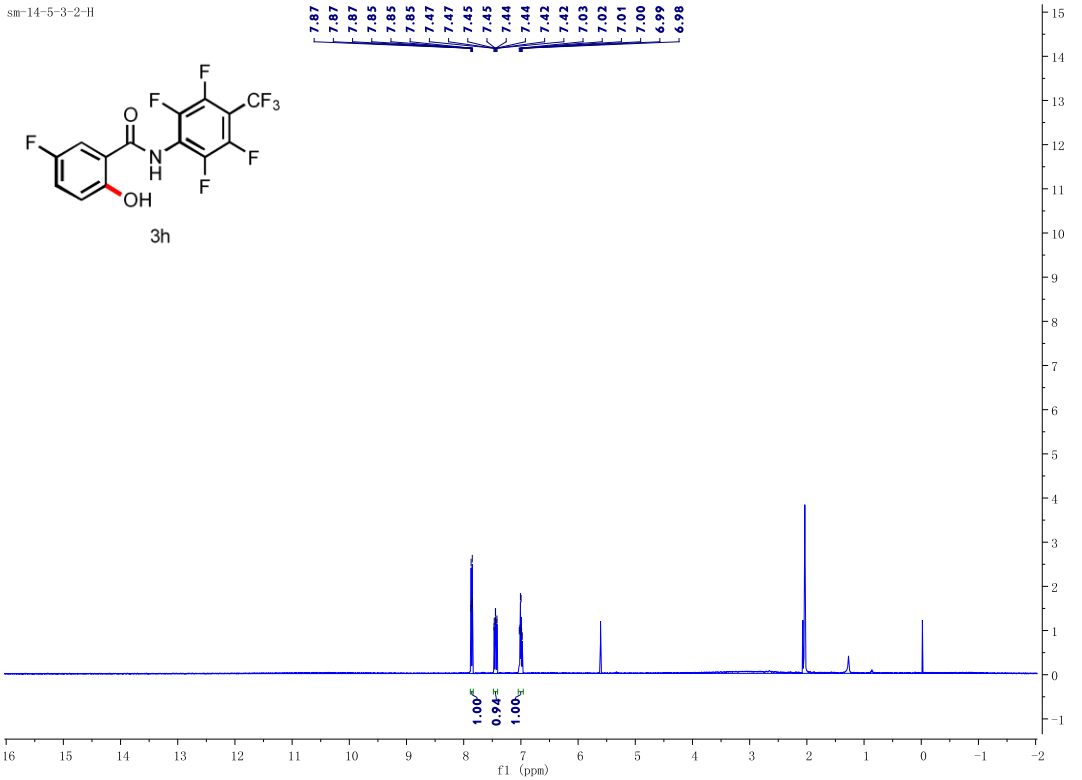

sm-14-4-2-F
STANDARD PROTON PARAMETERS
-56.70
-56.71
-56.74
-56.76
-56.77
-56.82
-144.13
-144.16
F
F
CF3
O
N
H
F
F
MeO
OH
3f
3.00
4.05
f1 (ppm)

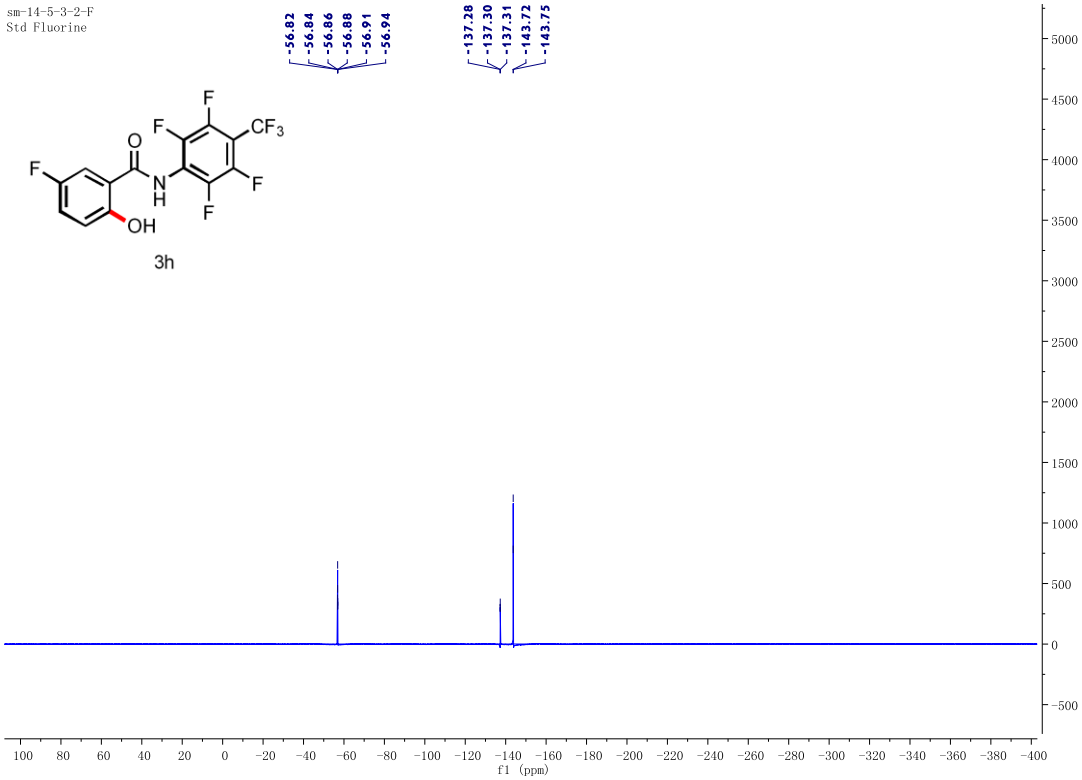

sm-14-4-2-C
Std carbon
167.88
165.50
163.48
129.80
107.27
106.74
101.26
55.13
MeO
OH
3f
f1 (ppm)

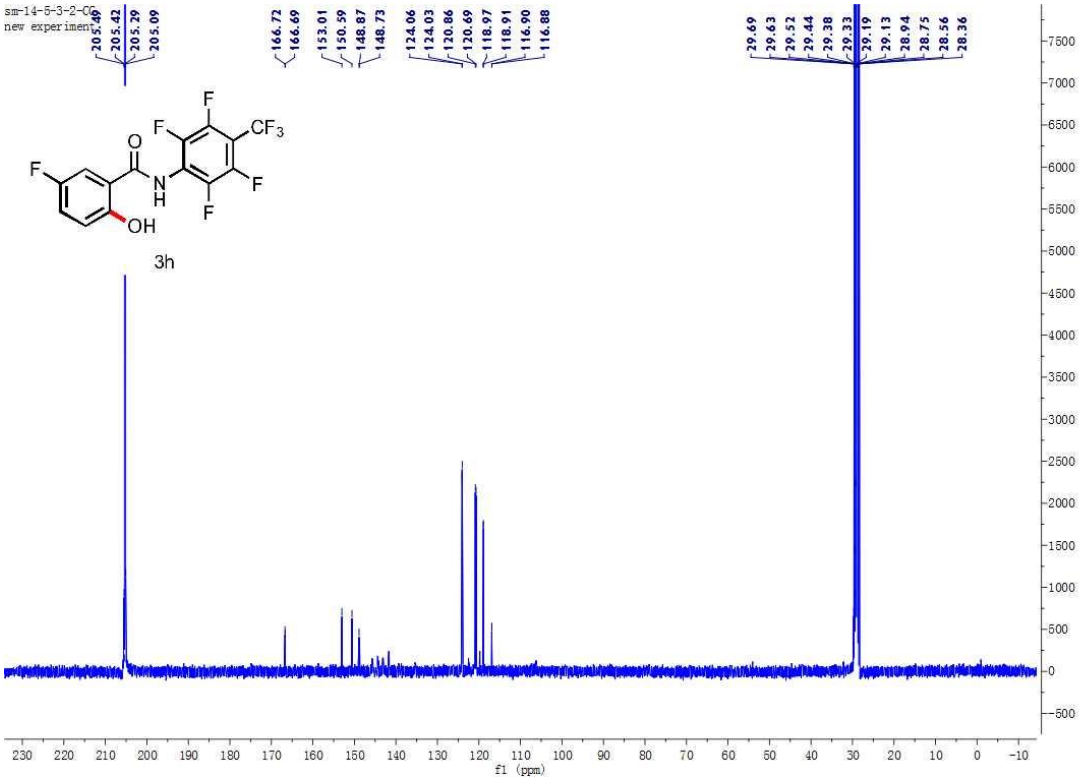

sm-15-11-1-1-H
8.15
8.13
7.74
7.73
7.53
7.51
7.49
7.46
7.44
7.35
7.33
Ph
OH
3g
1.06
2.00
2.07
0.96
1.96
f1 (ppm)

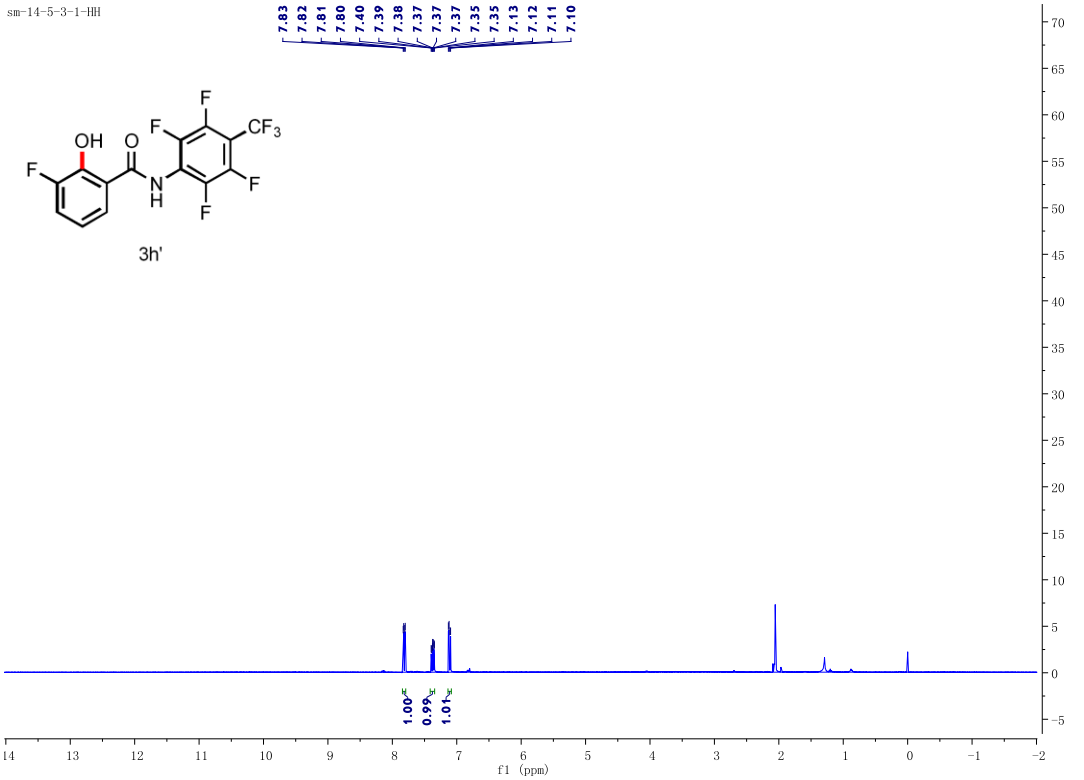

sm-15-11-1-F
Std Fluorine
-56.83
-143.84
-143.87
3g
f1 (ppm)

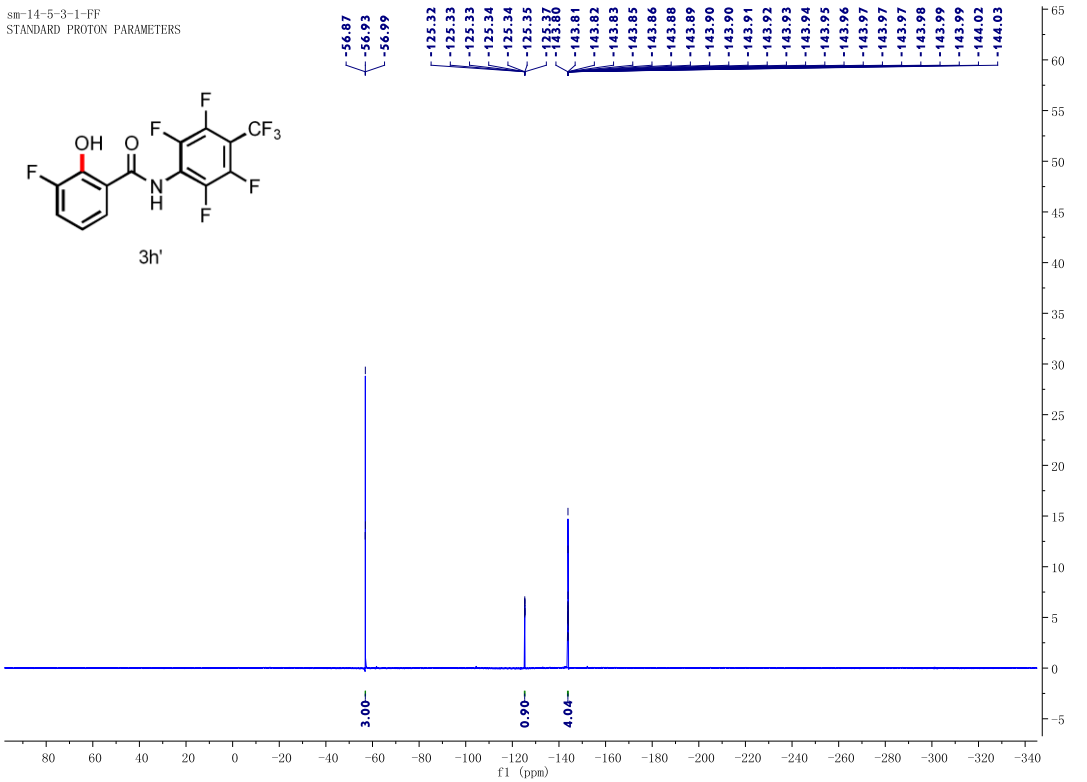

SM-15-11-1-C
167.34
160.87
147.83
139.17
129.39
128.97
128.55
127.02
118.19
115.69
113.24
3g
f1 (ppm)

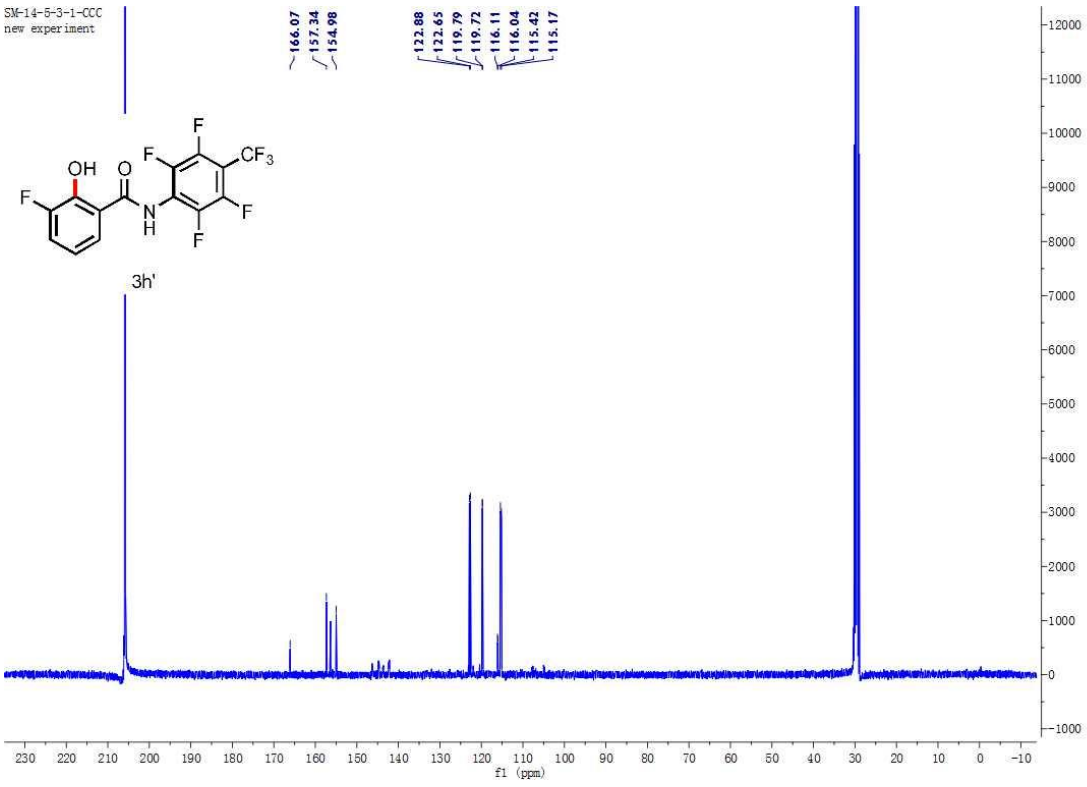

sm-14-5-3-2-H
7.87
7.87
7.87
7.85
7.85
7.85
7.47
7.47
7.45
7.45
7.44
7.44
7.42
7.42
7.03
7.02
7.01
7.00
6.99
6.98
F
F
CF3
O
N
H
F
F
F
OH
3h
1.00
0.94
1.00
f1 (ppm)

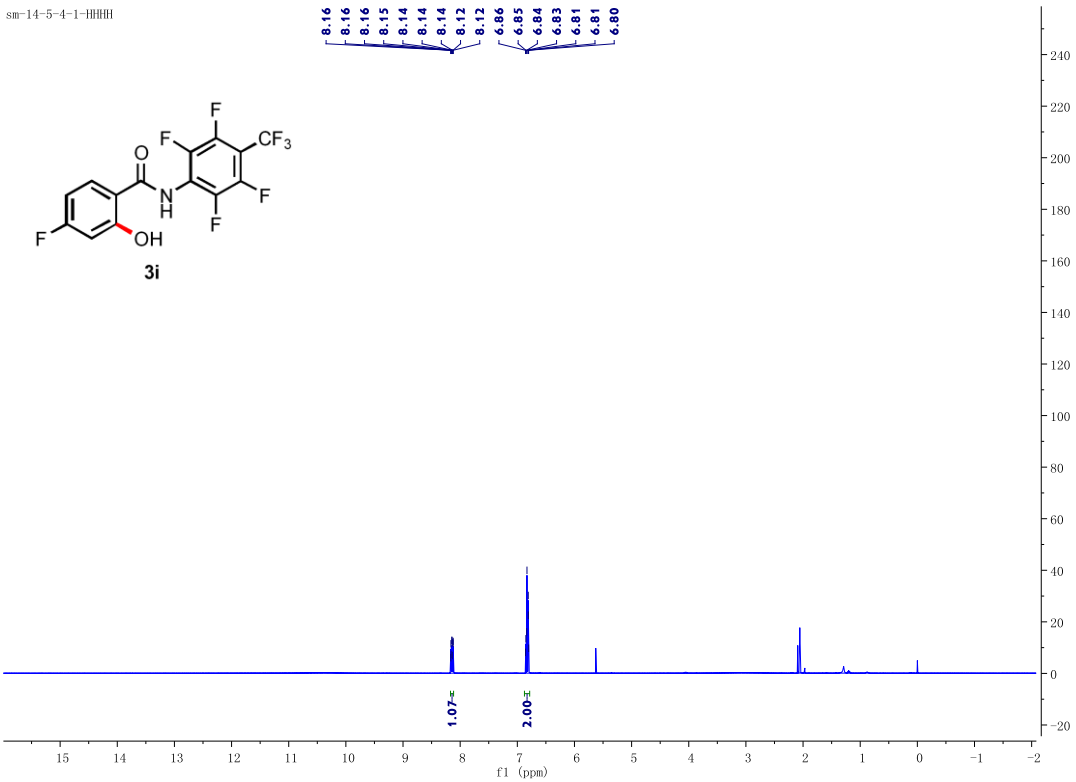

sm-14-5-3-2-F
Std Fluorine
-56.82
-56.84
-56.86
-56.88
-56.91
-56.94
-137.28
-137.30
-137.31
-143.72
-143.75
F
F
CF3
O
N
H
F
F
F
OH
3h
f1 (ppm)

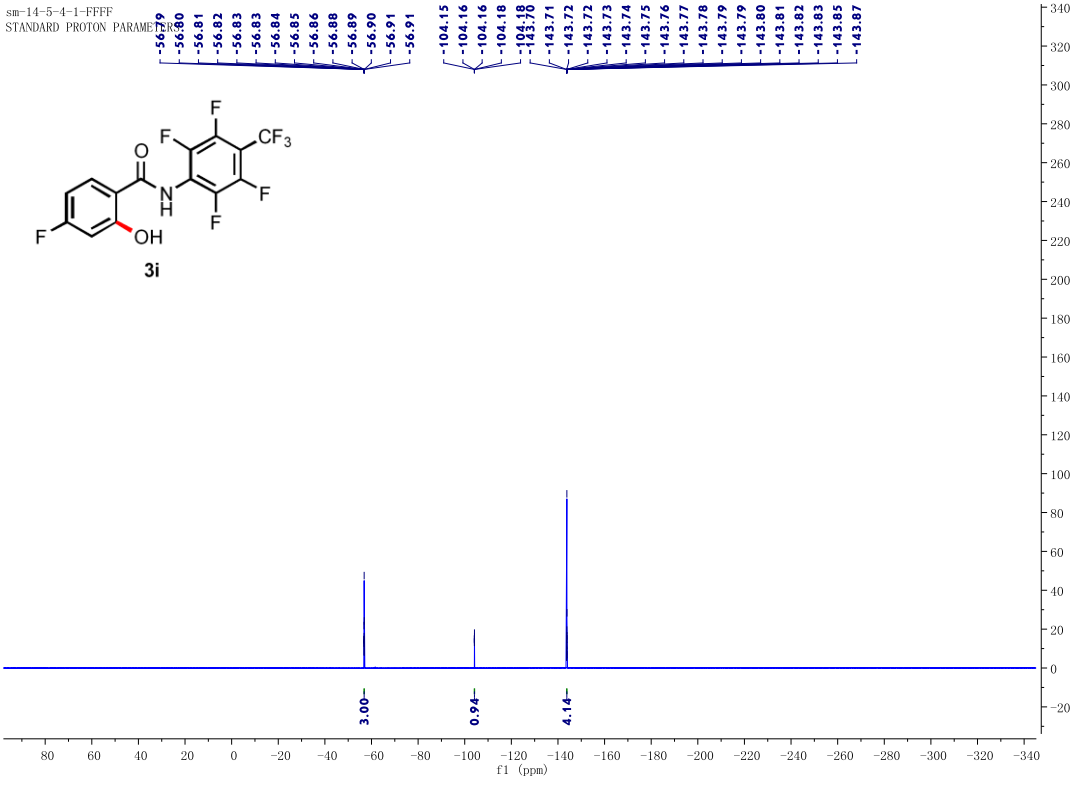

sm-14-5-3-2-CC
new experiment
205.49
205.42
205.29
205.09
166.72
166.69
153.01
150.59
148.87
148.73
124.06
124.03
120.86
120.69
118.97
118.91
116.90
116.88
29.69
29.63
29.52
29.44
29.38
29.33
29.19
29.13
28.94
28.75
28.56
28.36
F
F
CF3
O
N
H
F
F
OH
3h
f1 (ppm)

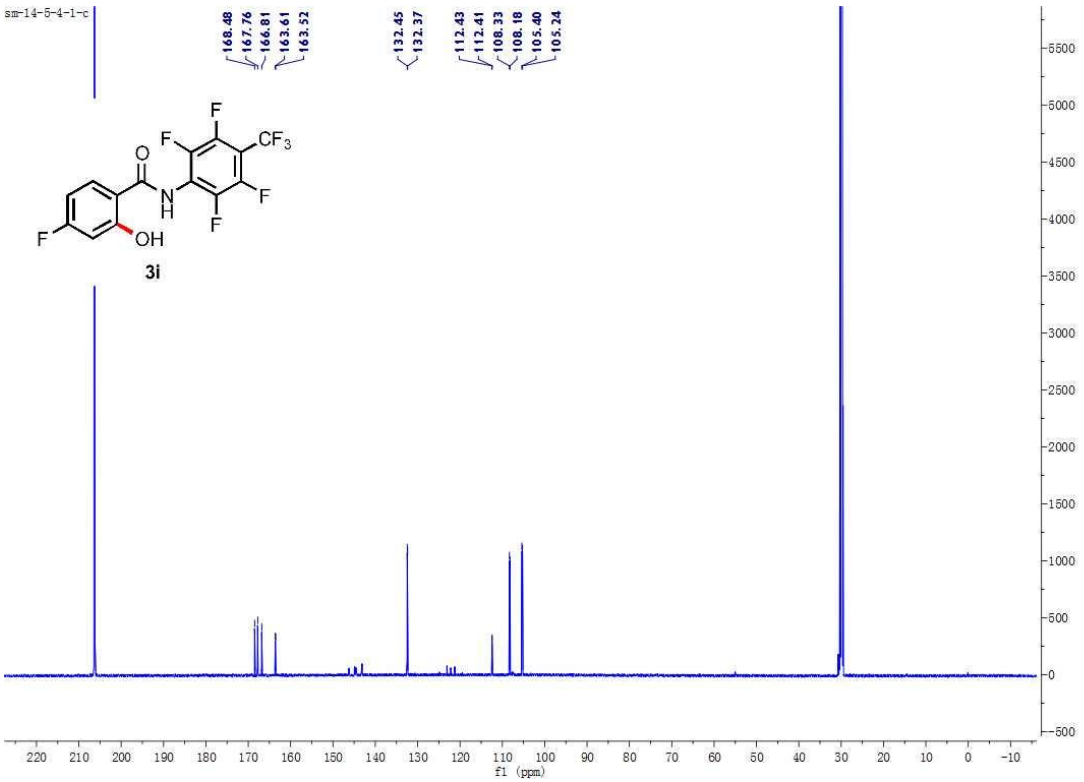

sm-14-5-3-1-HH
7.83
7.82
7.81
7.80
7.40
7.39
7.38
7.37
7.37
7.37
7.35
7.35
7.13
7.12
7.11
7.10
F
F
CF3
OH
O
N
H
F
F
F
3h'
1.00
0.99
1.01
f1 (ppm)

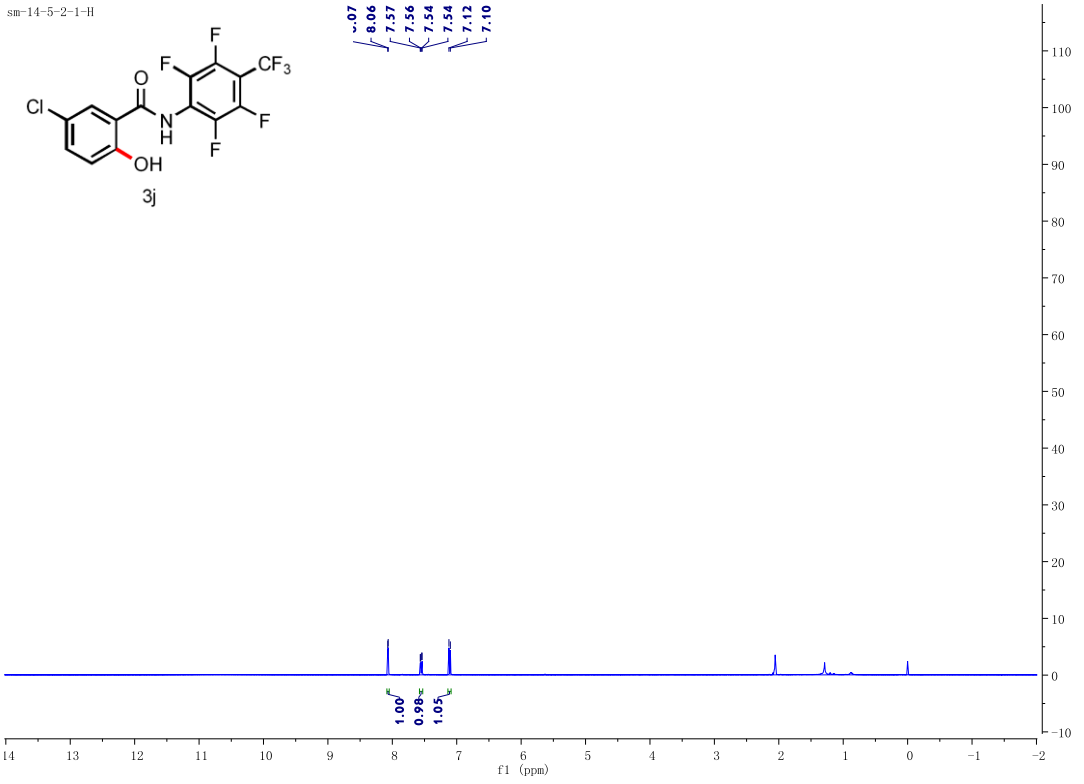

sm-14-5-3-1-FF
STANDARD PROTON PARAMETERS
-56.87
-56.93
-56.99
-125.32
-125.33
-125.33
-125.34
-125.34
-125.35
-125.37
-143.80
-143.81
-143.82
-143.83
-143.85
-143.86
-143.88
-143.89
-143.90
-143.90
-143.91
-143.92
-143.93
-143.94
-143.95
-143.96
-143.97
-143.97
-143.97
-143.98
-143.99
-143.99
-144.02
-144.03
OH
O
F
F
CF3
F
N
H
F
F
3h'
3.00
0.90
4.04
f1 (ppm)

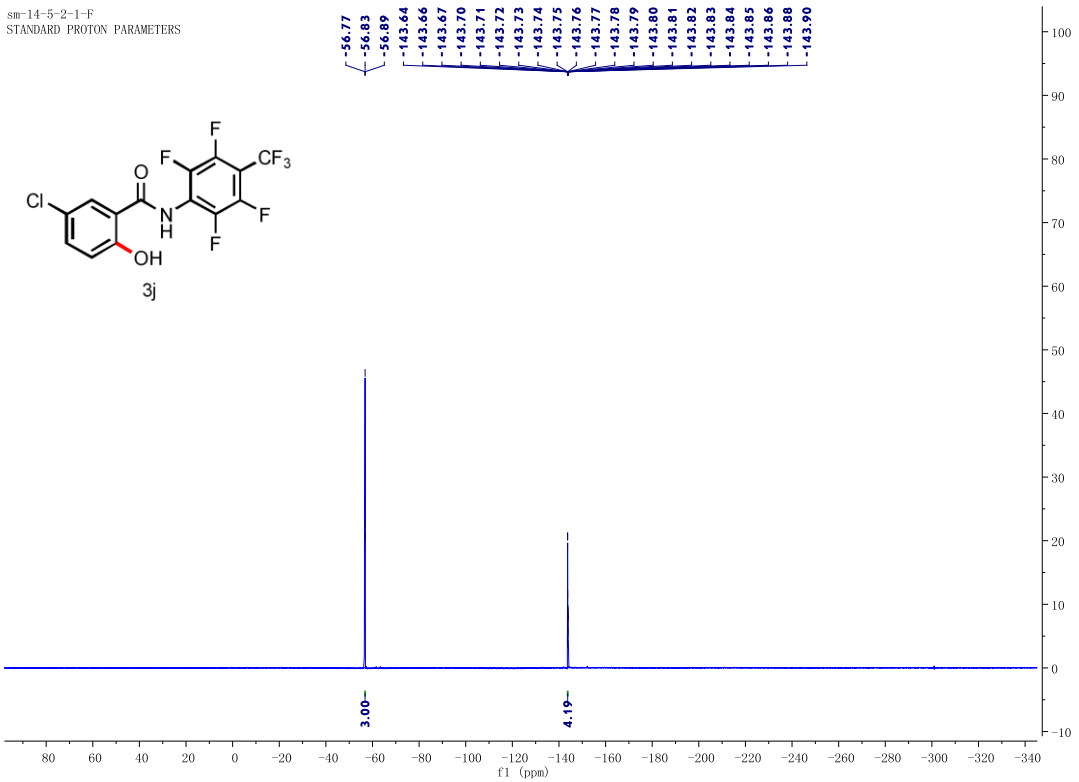

SM-14-5-3-1-CCC
new experiment
166.07
157.34
154.98
122.88
122.65
119.79
119.72
116.11
116.04
115.42
115.17
OH
O
F
F
CF3
F
N
H
F
F
3h'
f1 (ppm)

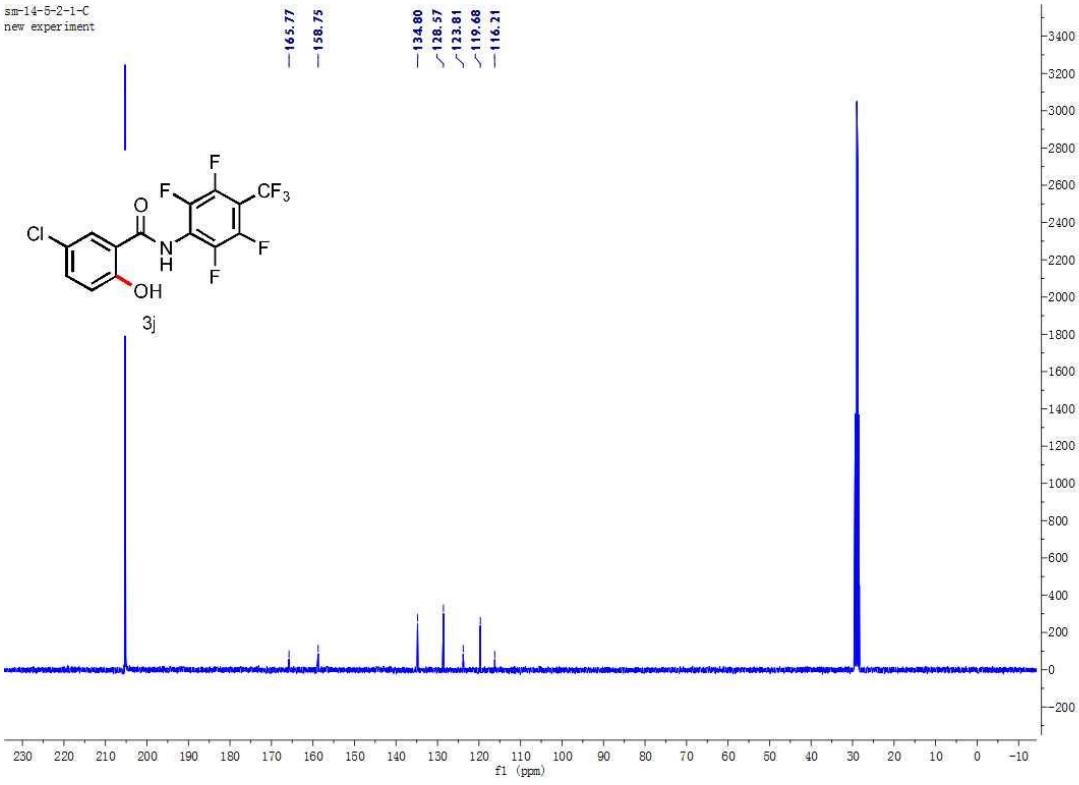

sm-14-5-4-1-HHHH
8.16
8.16
8.16
8.15
8.14
8.14
8.14
8.12
8.12
6.86
6.85
6.84
6.83
6.81
6.81
6.80
F
F
CF3
O
N
H
F
F
OH
3i
1.07
2.00
f1 (ppm)

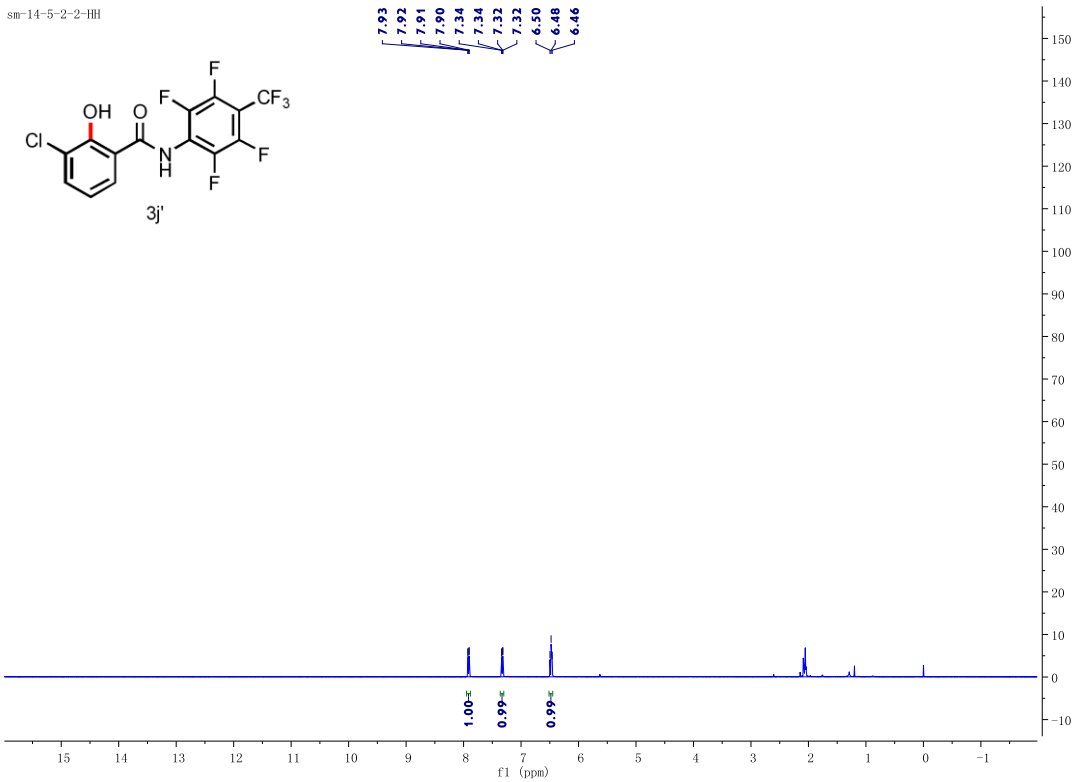

sm-14-5-4-1-FFFF
STANDARD PROTON PARAMETER
-56.79
-56.80
-56.81
-56.82
-56.83
-56.83
-56.84
-56.85
-56.86
-56.88
-56.89
-56.90
-56.91
-104.15
-104.16
-104.16
-104.18
-104.18
-143.71
-143.72
-143.72
-143.73
-143.74
-143.75
-143.76
-143.77
-143.78
-143.79
-143.79
-143.80
-143.81
-143.82
-143.83
-143.85
-143.87
F
F
CF3
O
N
H
F
F
OH
3i
3.00
0.94
4.14
f1 (ppm)

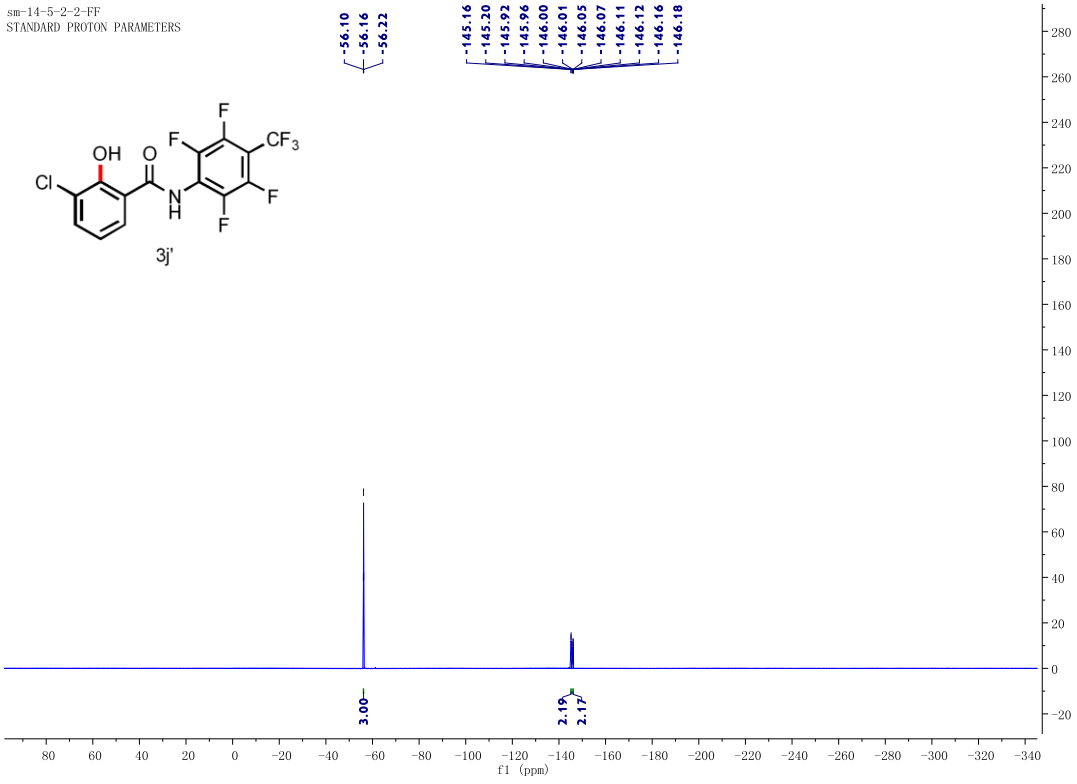

sm-14-5-4-1-c
168.48
167.76
166.81
163.61
163.52
132.45
132.37
112.43
112.41
108.33
108.18
105.40
105.24
F
F
CF3
O
N
H
F
F
OH
3i
f1 (ppm)

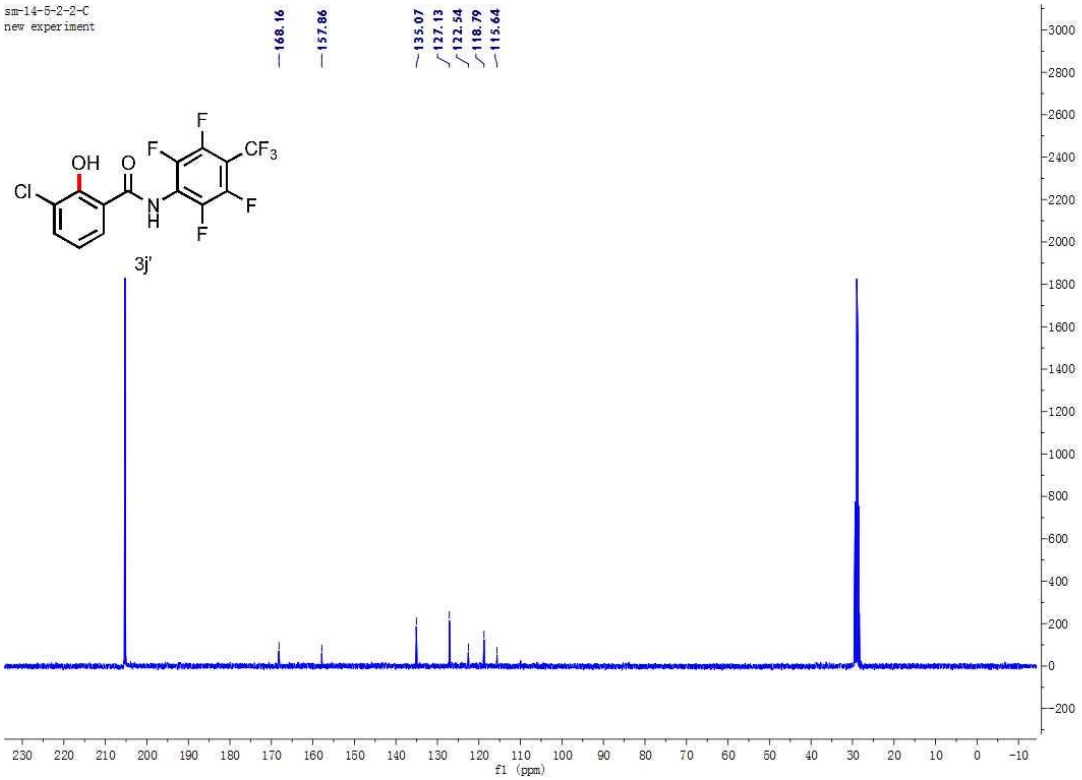

sm-14-5-2-1-H
8.07
8.06
7.57
7.56
7.54
7.54
7.12
7.10
F
F
CF3
O
N
H
Cl
F
F
OH
3j
1.00
0.98
1.05
f1 (ppm)

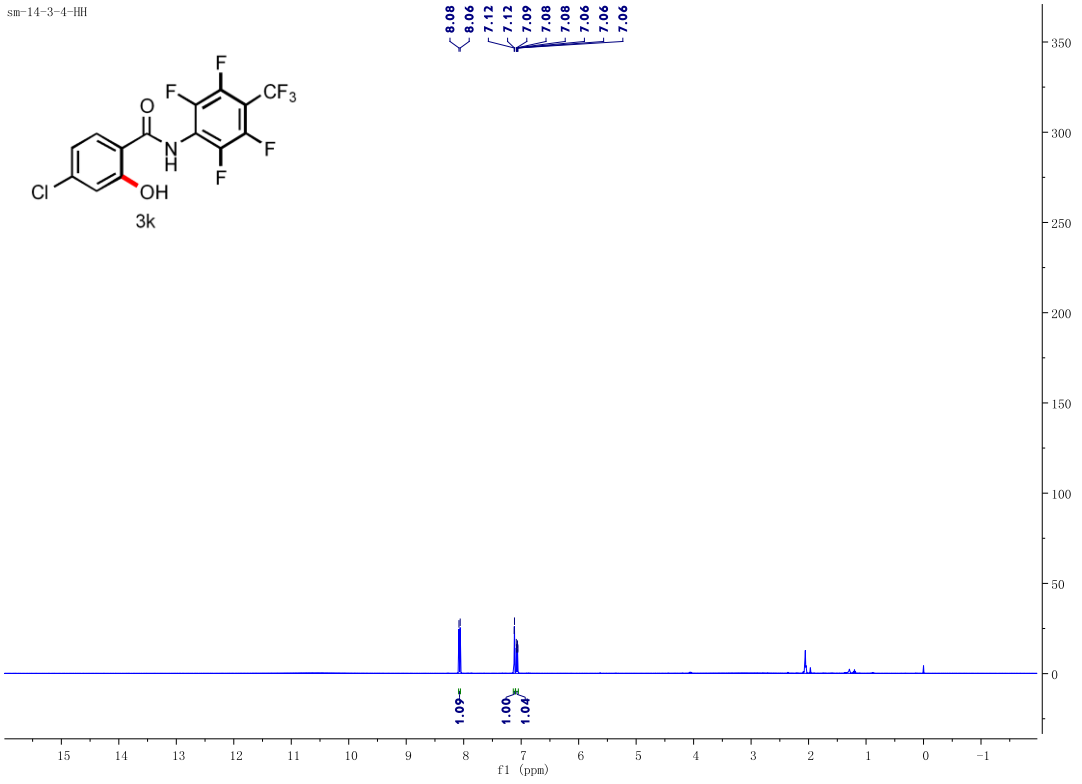

sm-14-5-2-1-F
STANDARD PROTON PARAMETERS
-56.77
-56.83
-56.89
-143.64
-143.66
-143.67
-143.70
-143.71
-143.72
-143.73
-143.74
-143.75
-143.76
-143.77
-143.78
-143.79
-143.80
-143.81
-143.82
-143.83
-143.84
-143.85
-143.86
-143.88
-143.90
F
F
CF3
O
N
H
Cl
F
OH
3j
3.00
4.19
f1 (ppm)

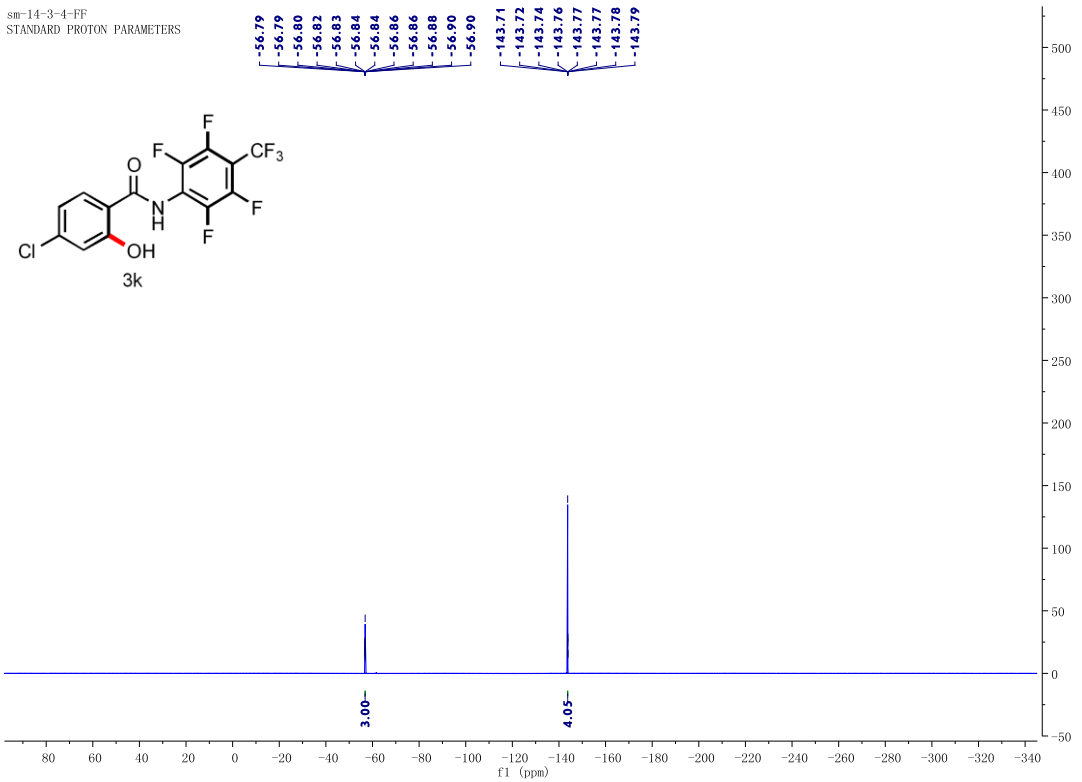

sm-14-5-2-1-C
new experiment
165.77
158.75
134.80
128.57
123.81
119.68
116.21
F
F
CF3
O
N
H
Cl
F
OH
3j
f1 (ppm)

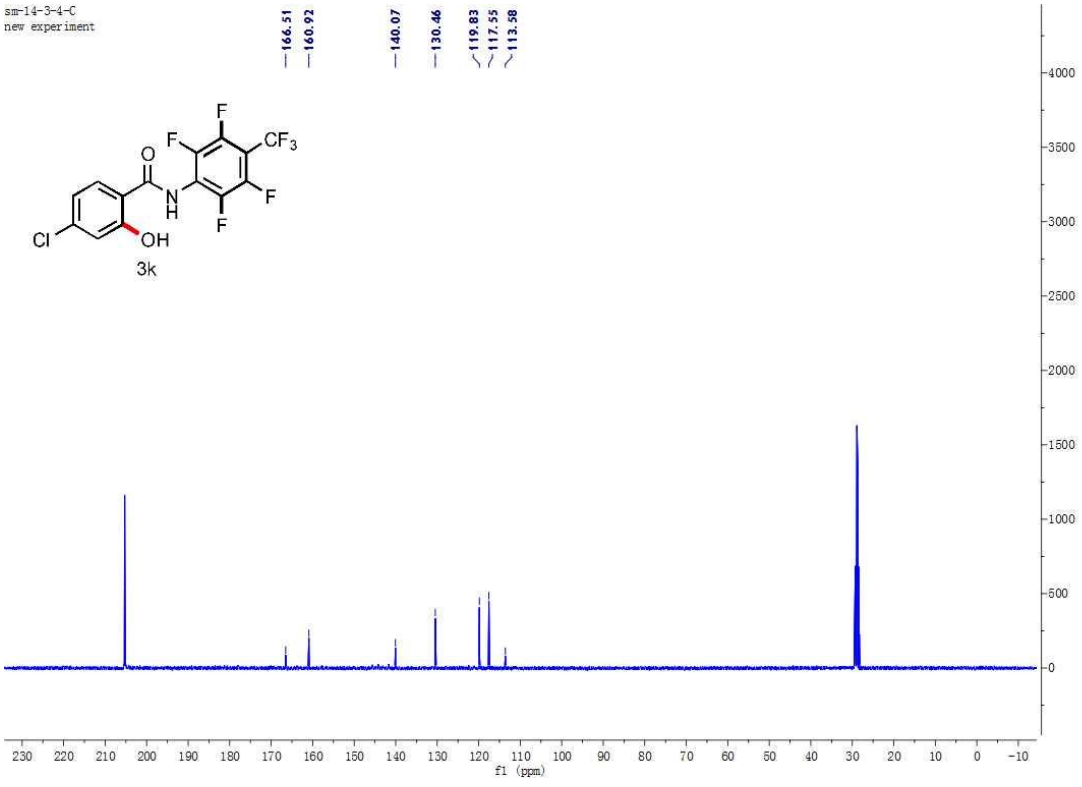

sm-14-5-2-2-HH
7.93
7.92
7.91
7.90
7.34
7.34
7.32
7.32
6.50
6.48
6.46
OH
O
Cl
N
H
F
F
F
F
CF3
3j'
1.00
0.99
0.99
f1 (ppm)

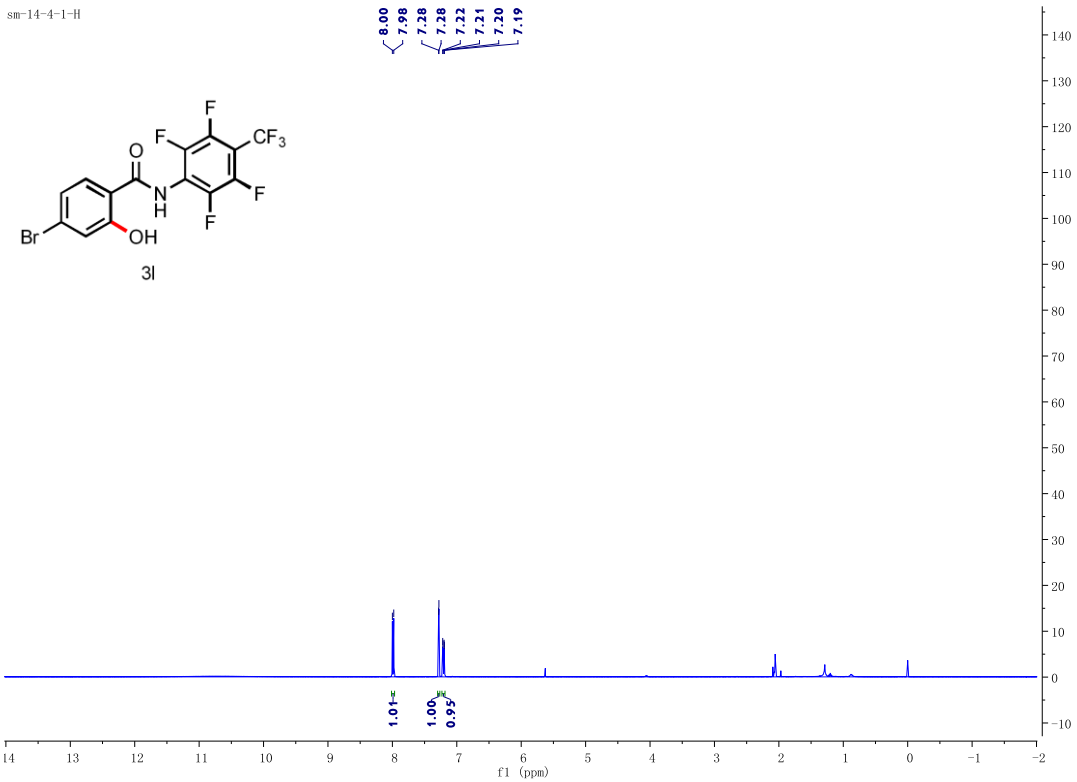

sm-14-5-2-2-FF
STANDARD PROTON PARAMETERS
-56.10
-56.16
-56.22
-145.16
-145.20
-145.92
-145.96
-146.00
-146.01
-146.05
-146.07
-146.11
-146.12
-146.16
-146.18
OH
O
Cl
N
H
F
F
F
F
CF3
3j'
3.00
2.19
2.17
f1 (ppm)

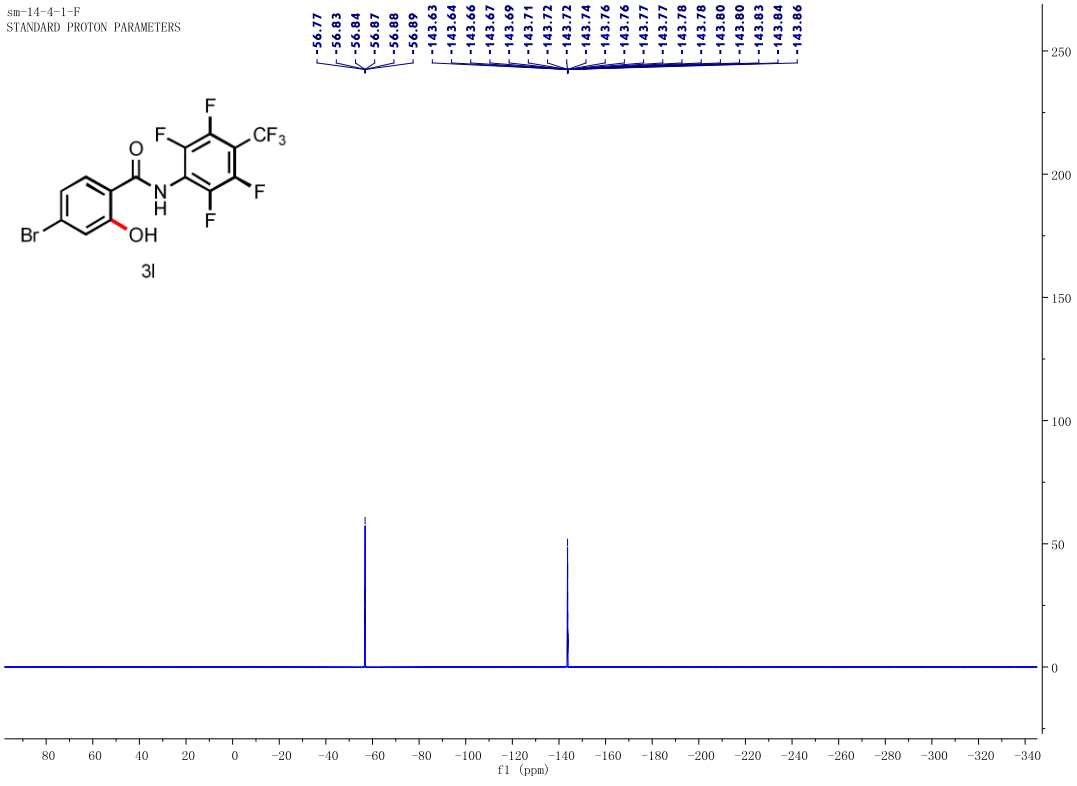

sm-14-5-2-2-C
new experiment
168.16
157.86
135.07
127.13
122.54
118.79
115.64
OH
O
Cl
N
H
F
F
CF3
F
F
3j'
f1 (ppm)

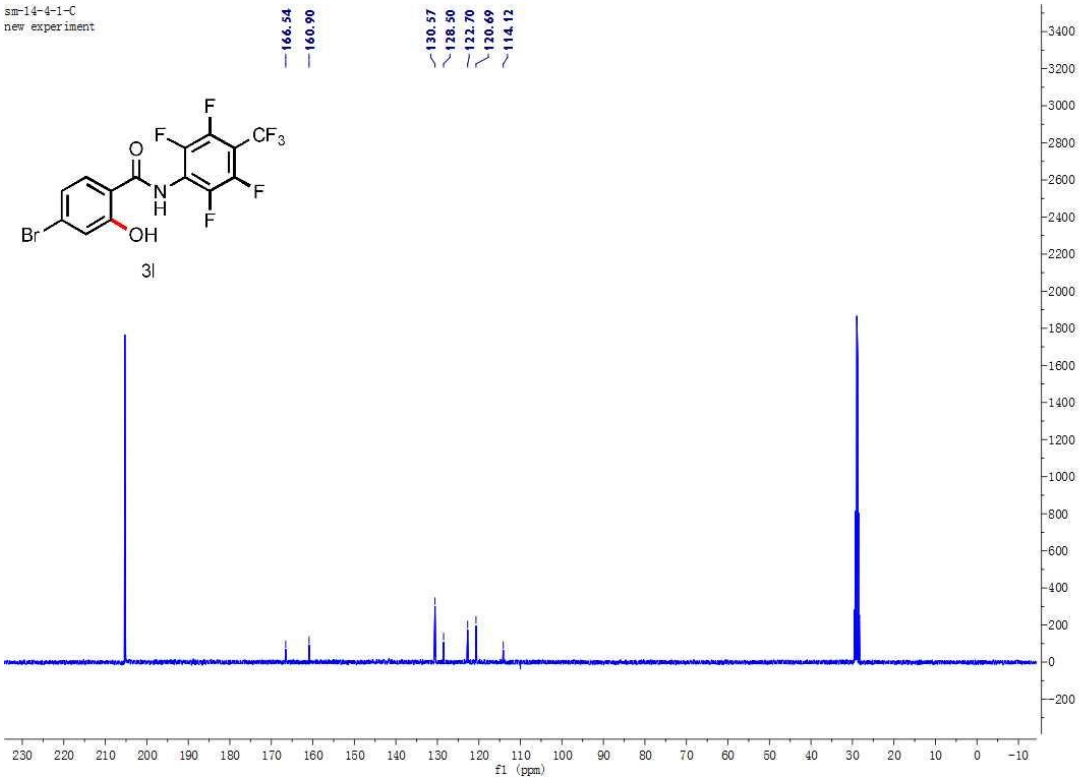

sm-14-3-4-HH
8.08
8.06
7.12
7.12
7.09
7.08
7.08
7.06
7.06
7.06
O
N
H
F
F
CF3
F
F
Cl
OH
3k
1.09
1.00
1.04
f1 (ppm)

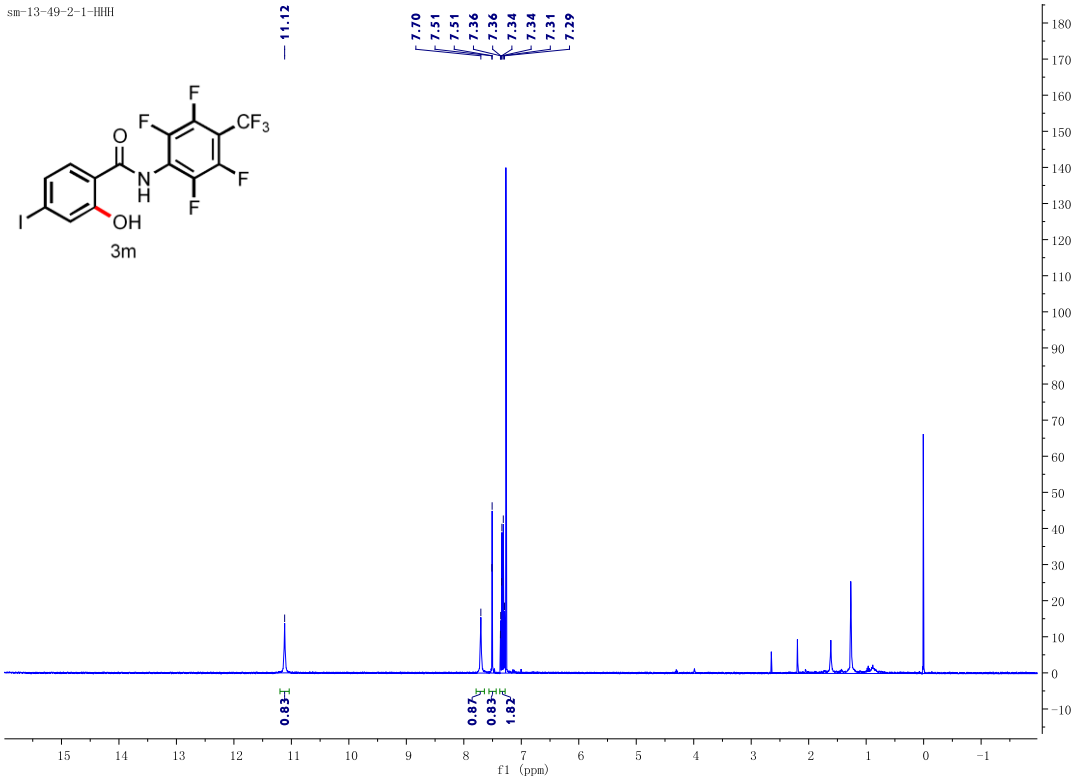

sm-14-3-4-FF
STANDARD PROTON PARAMETERS
-56.79
-56.79
-56.80
-56.82
-56.83
-56.84
-56.84
-56.86
-56.86
-56.88
-56.90
-56.90
-143.71
-143.72
-143.74
-143.76
-143.77
-143.77
-143.78
-143.79
F
F
CF3
O
N
H
F
F
Cl
OH
3k
3.00
4.05
f1 (ppm)

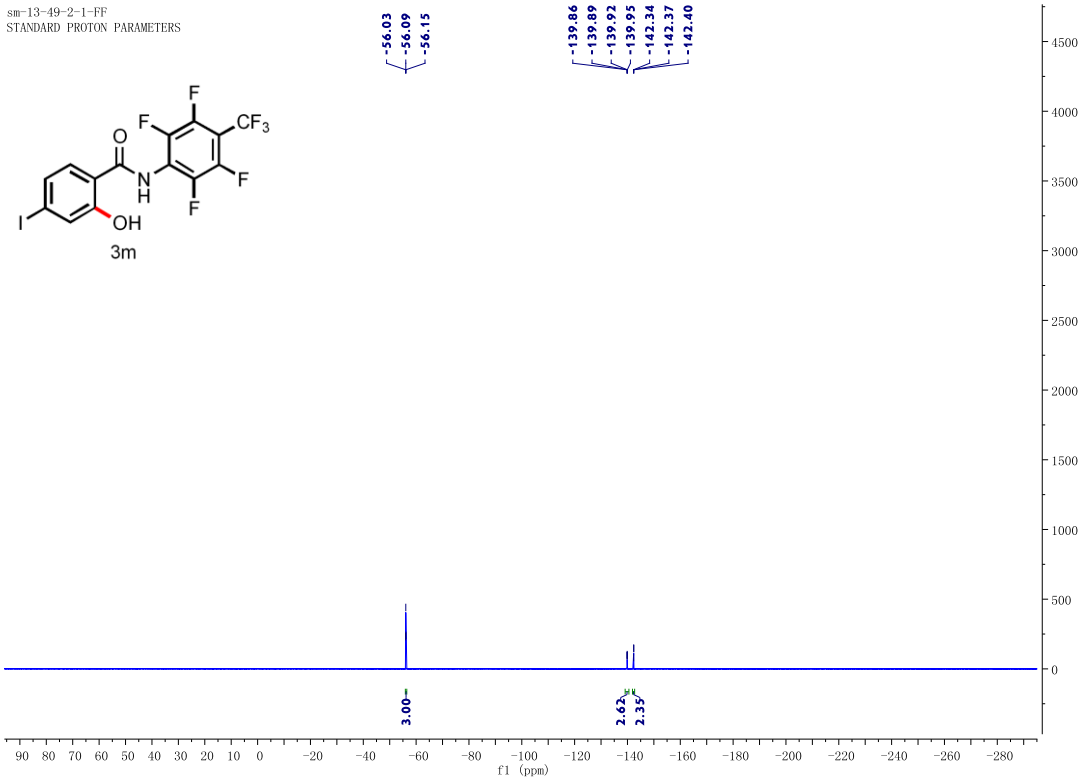

sm-14-3-4-C
new experiment
166.51
160.92
140.07
130.46
119.83
117.55
113.58
F
F
CF3
O
N
H
F
F
Cl
OH
3k
f1 (ppm)

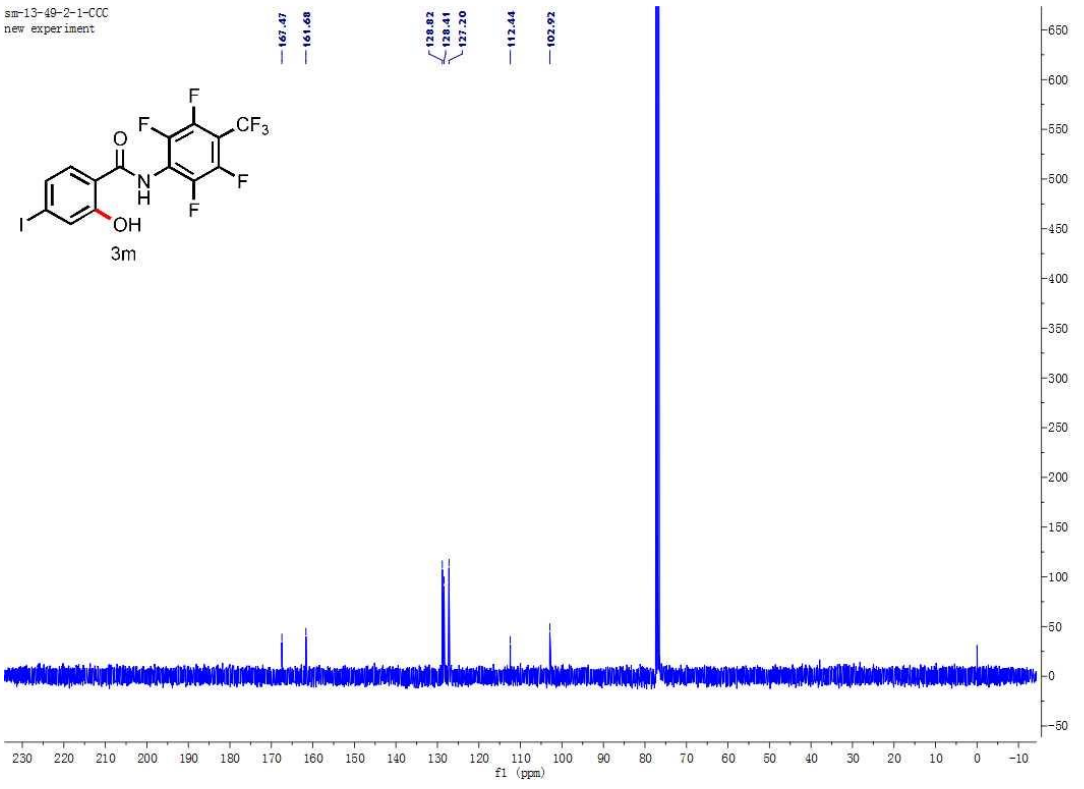

sm-14-4-1-H
8.00
7.98
7.28
7.28
7.22
7.21
7.20
7.19
F
F
CF3
O
N
H
F
F
Br
OH
3l
1.01
1.00
0.95
f1 (ppm)

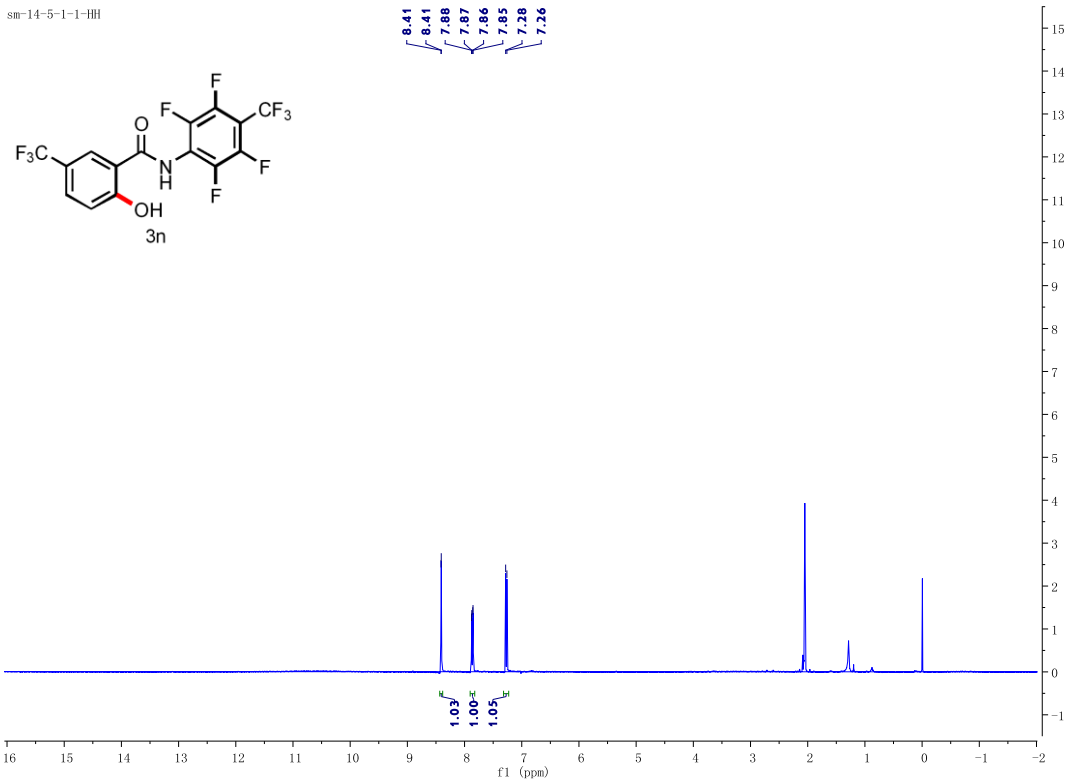

sm-14-4-1-F
STANDARD PROTON PARAMETERS
-56.77
-56.83
-56.84
-56.87
-56.88
-56.89
-143.63
-143.64
-143.66
-143.67
-143.69
-143.71
-143.72
-143.72
-143.74
-143.76
-143.76
-143.77
-143.77
-143.78
-143.78
-143.80
-143.80
-143.83
-143.84
-143.86
F
F
CF3
O
N
H
F
F
Br
OH
3l
f1 (ppm)

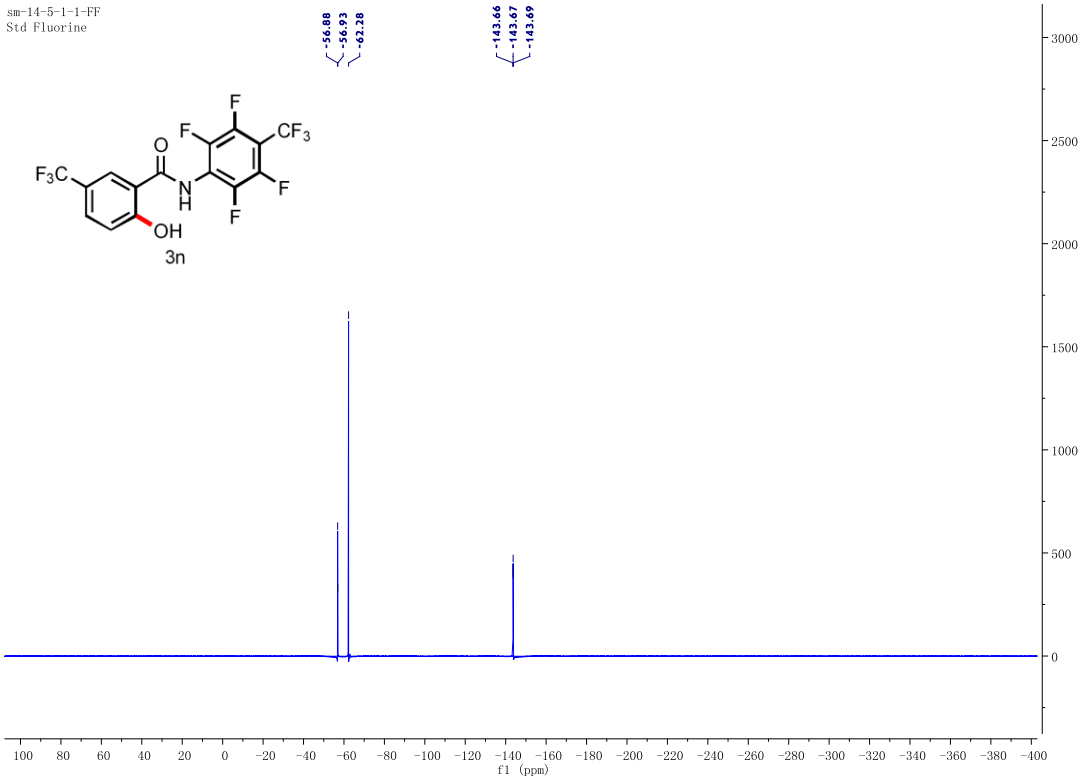

sm-14-4-1-C
new experiment
166.54
160.90
130.57
128.50
122.70
120.69
114.12
F
F
CF3
O
N
H
F
F
Br
OH
3l
f1 (ppm)

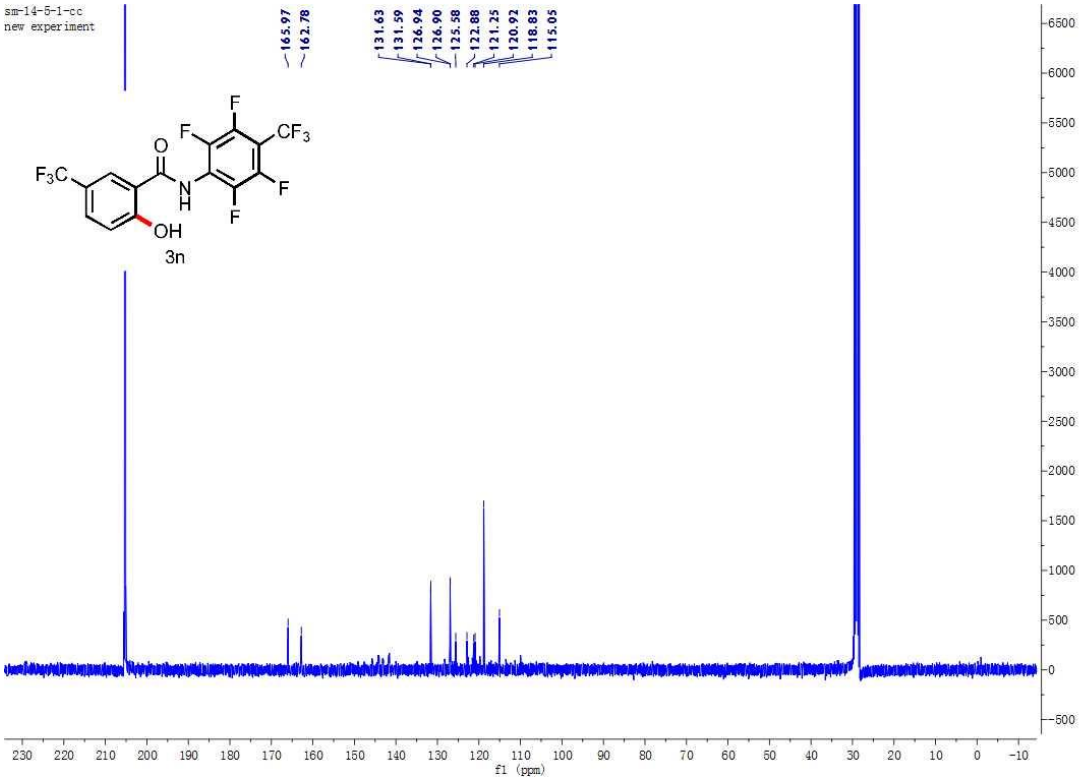

sm-13-49-2-1-HHH
11.12
7.70
7.51
7.51
7.36
7.36
7.34
7.34
7.31
7.29
F
F
CF3
O
N
H
F
F
I
OH
3m
0.83
0.87
0.83
1.82
f1 (ppm)

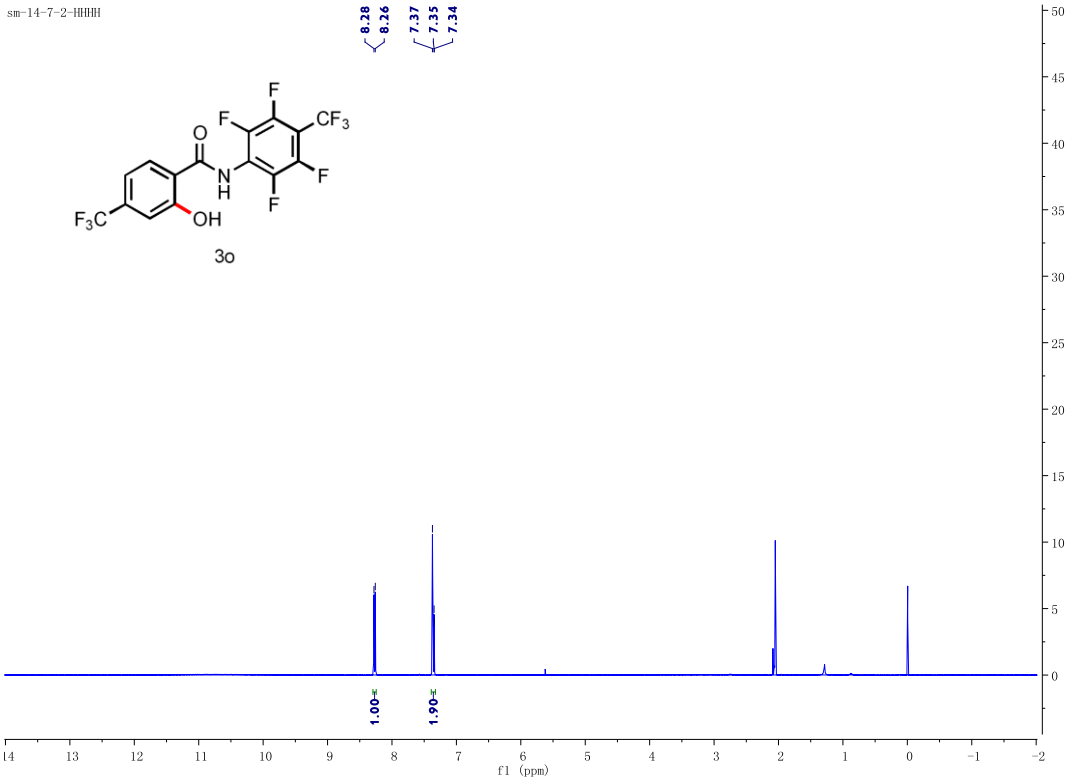

sm-13-49-2-1-FF
STANDARD PROTON PARAMETERS
-56.03
-56.09
-56.15
-139.86
-139.89
-139.92
-139.95
-142.34
-142.37
-142.40
3m
3.00
2.62
2.35
f1 (ppm)

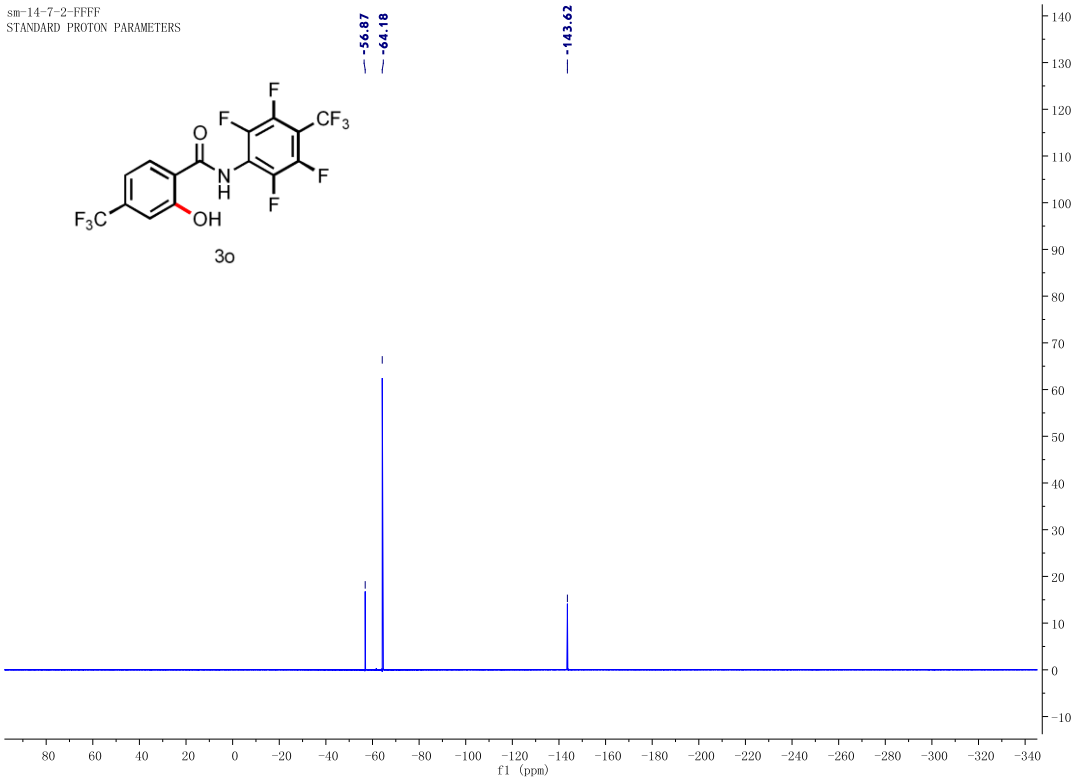

sm-13-49-2-1-CCC
new experiment
167.47
161.68
128.82
128.41
127.20
112.44
102.92
3m
f1 (ppm)

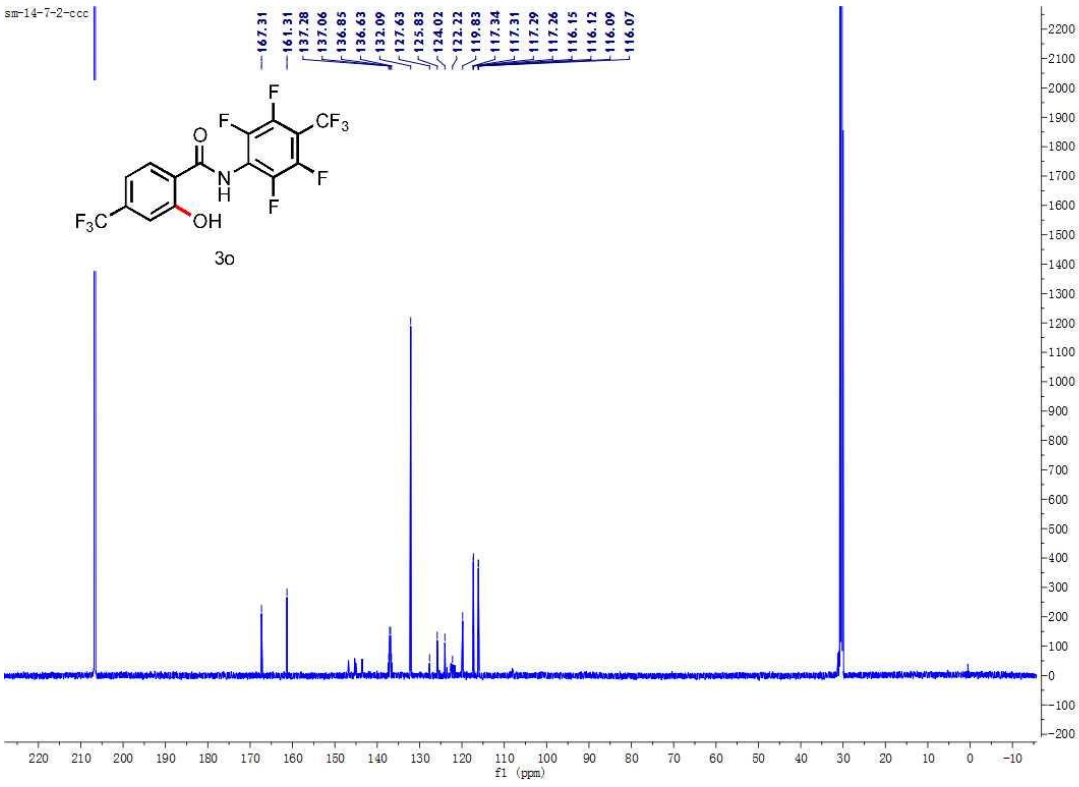

sm-14-5-1-1-HH
8.41
8.41
7.88
7.87
7.86
7.85
7.28
7.26
F
F
CF3
O
F3C
N
H
F
OH
3n
1.03
1.00
1.05
f1 (ppm)

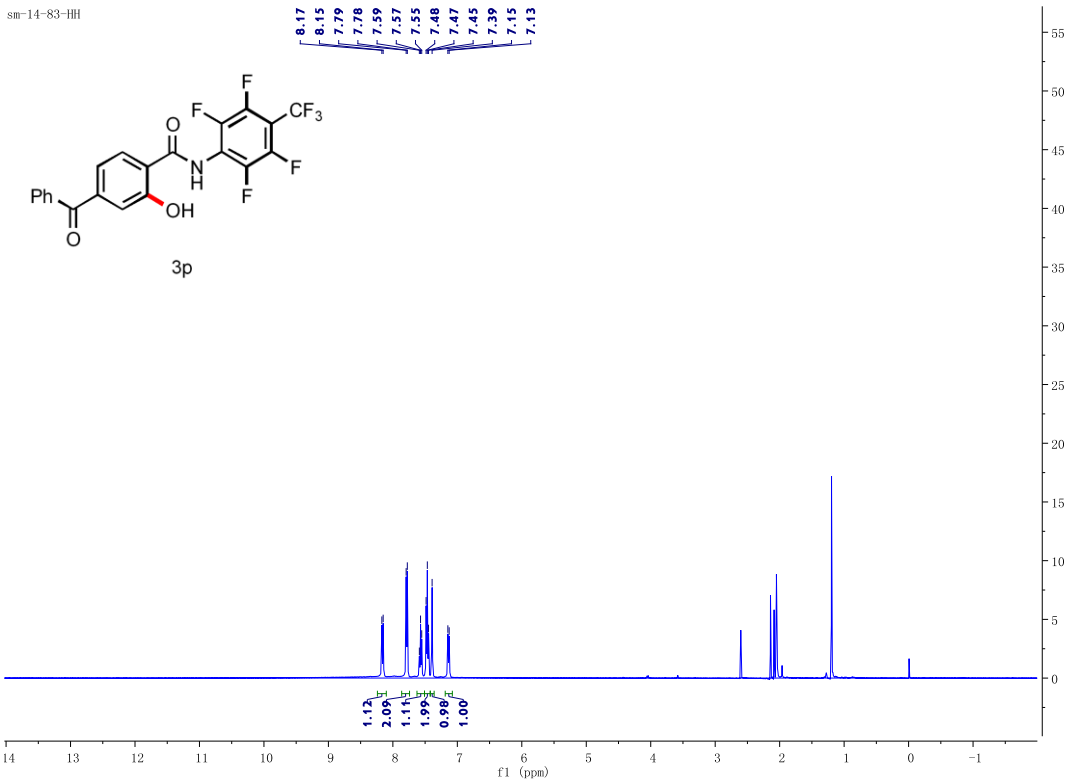

sm-14-5-1-1-FF
Std Fluorine
-56.88
-56.93
-62.28
-143.66
-143.67
-143.69
F
F
CF3
O
F3C
N
H
F
OH
3n
f1 (ppm)

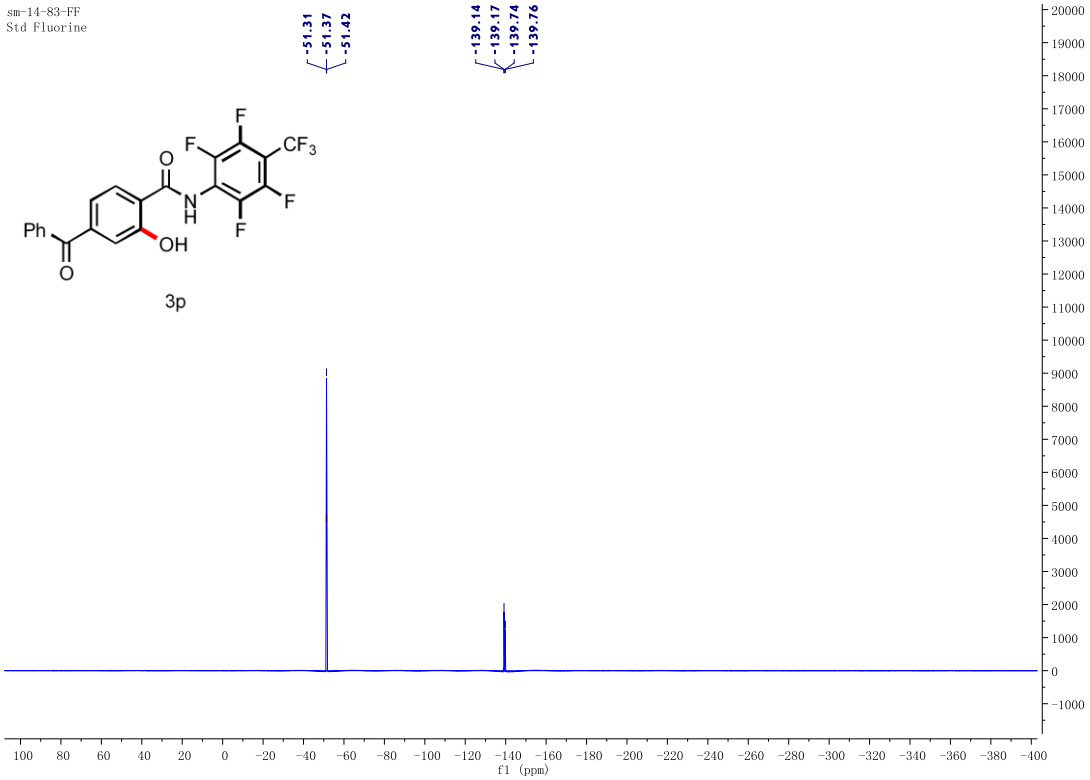

sm-14-5-1-cc
new experiment
165.97
162.78
131.63
131.59
126.94
126.90
125.58
122.88
121.25
120.92
118.83
115.05
F
F
CF3
O
F3C
N
H
F
F
OH
3n
f1 (ppm)

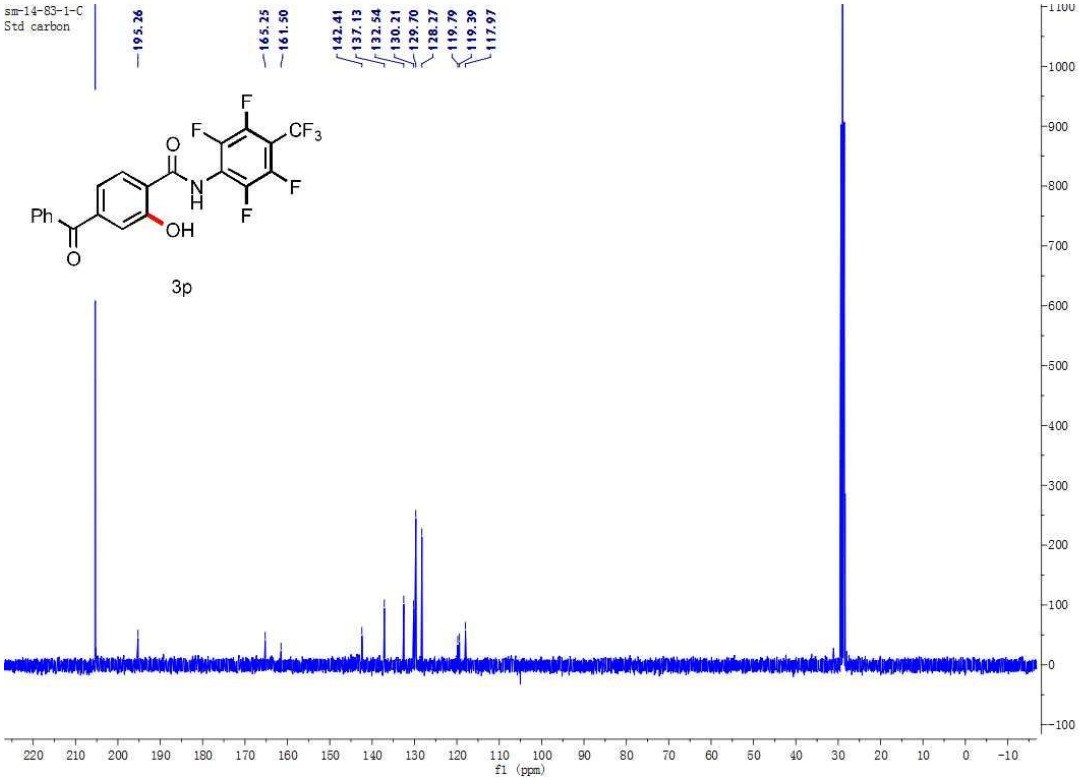

sm-14-7-2-HHHH
8.28
8.26
7.37
7.35
7.34
F
F
CF3
O
N
H
F
F3C
OH
3o
1.00
1.90
f1 (ppm)

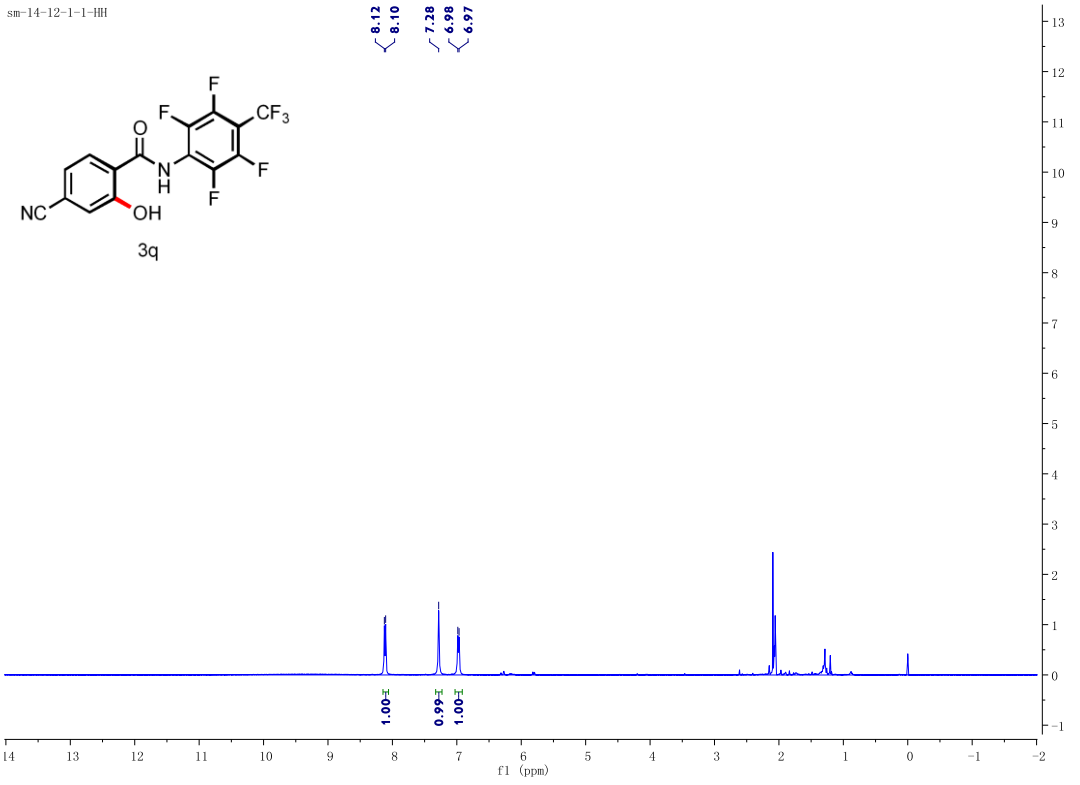

sm-14-7-2-FFFF
STANDARD PROTON PARAMETERS
-56.87
-64.18
-143.62
3o
f1 (ppm)

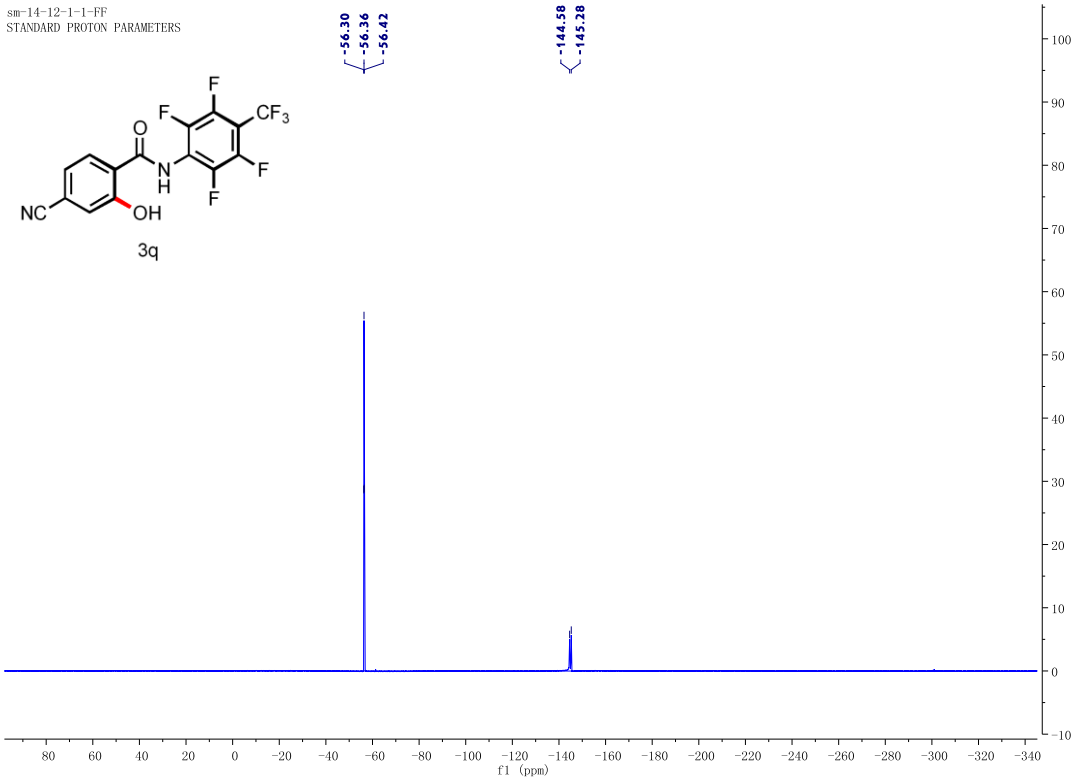

sm-14-7-2-ccc
167.31
161.31
137.28
137.06
136.85
136.63
132.09
127.63
125.83
124.02
122.22
119.83
117.34
117.31
117.29
117.26
116.15
116.12
116.09
116.07
3o
f1 (ppm)

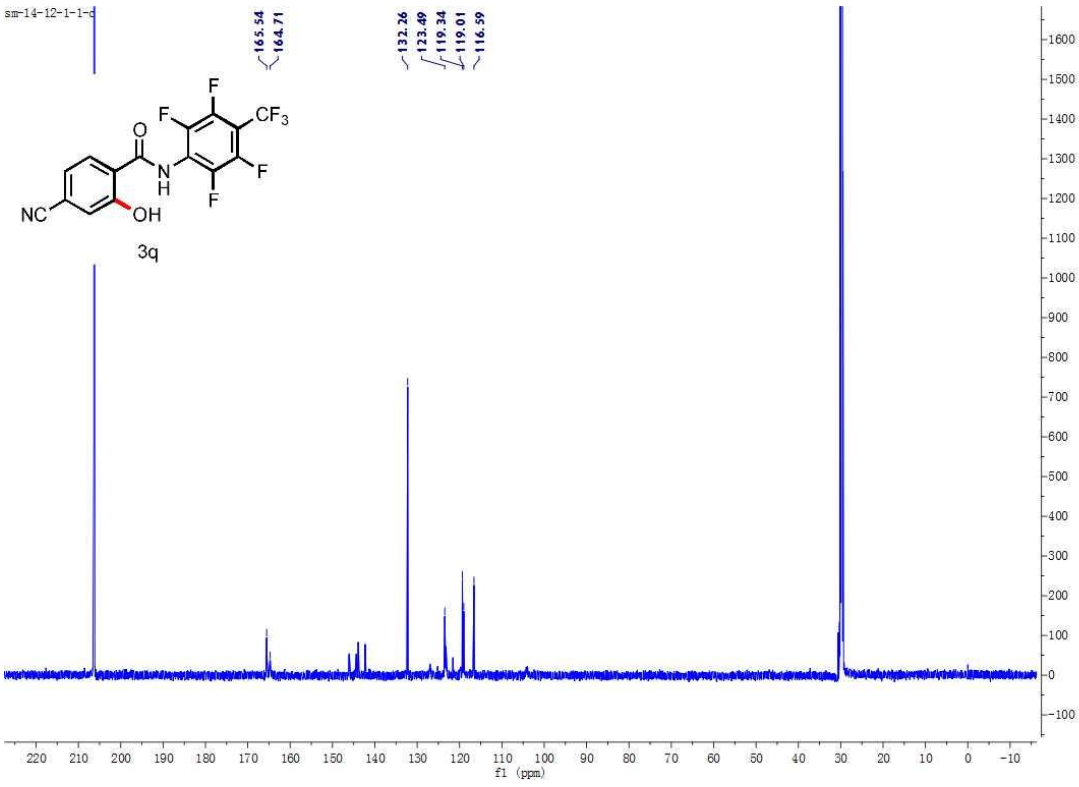

sm-14-83-HH
8.17
8.15
7.79
7.78
7.59
7.57
7.55
7.48
7.47
7.45
7.39
7.15
7.13
F
F
CF3
O
N
H
F
F
Ph
OH
O
3p
1.12
2.09
1.11
1.99
0.98
1.00
f1 (ppm)

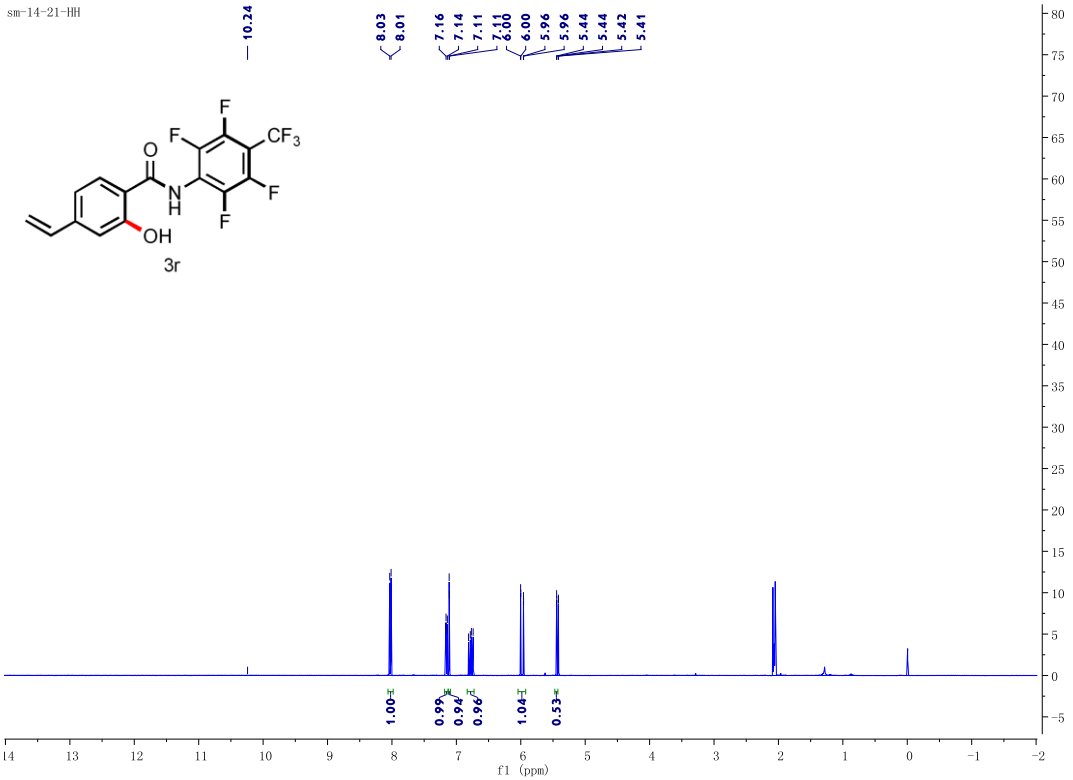

sm-14-83-FF
Std Fluorine
-51.31
-51.37
-51.42
-139.14
-139.17
-139.74
-139.76
F
F
CF3
O
N
H
F
F
Ph
OH
O
3p
f1 (ppm)

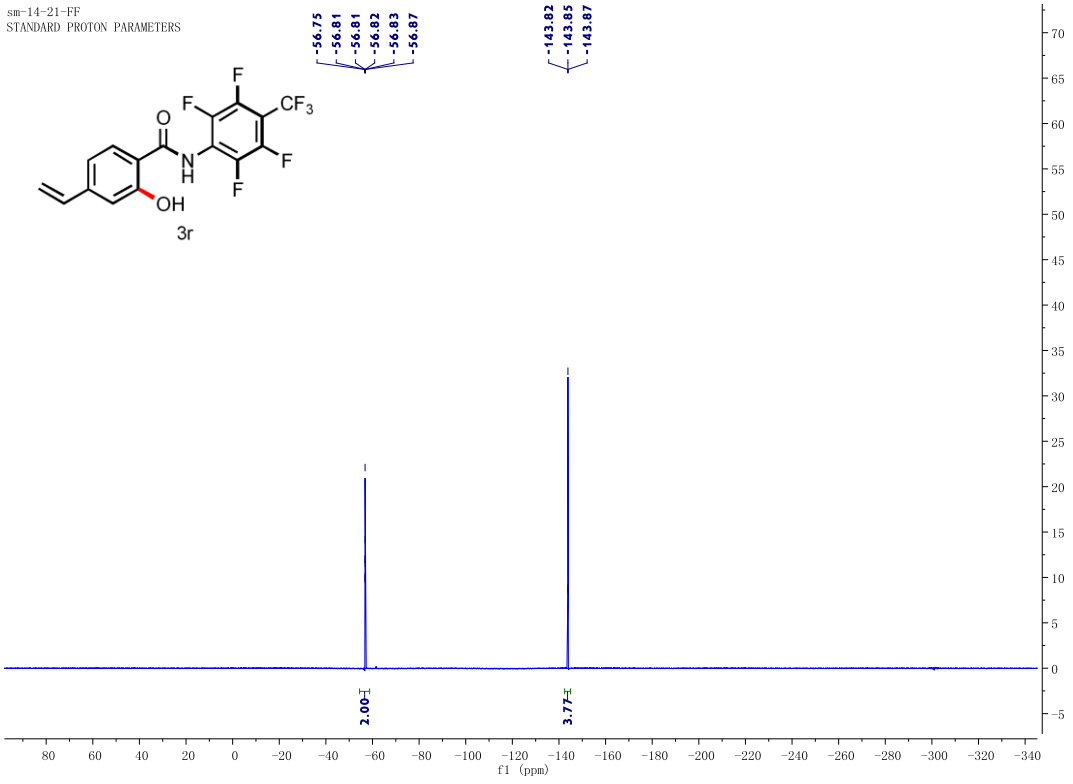

sm-14-83-1-C
Std carbon
195.26
165.25
161.50
142.41
137.13
132.54
130.21
129.70
128.27
119.79
119.39
117.97
F
F
CF3
O
N
H
F
F
Ph
O
OH
3p
f1 (ppm)

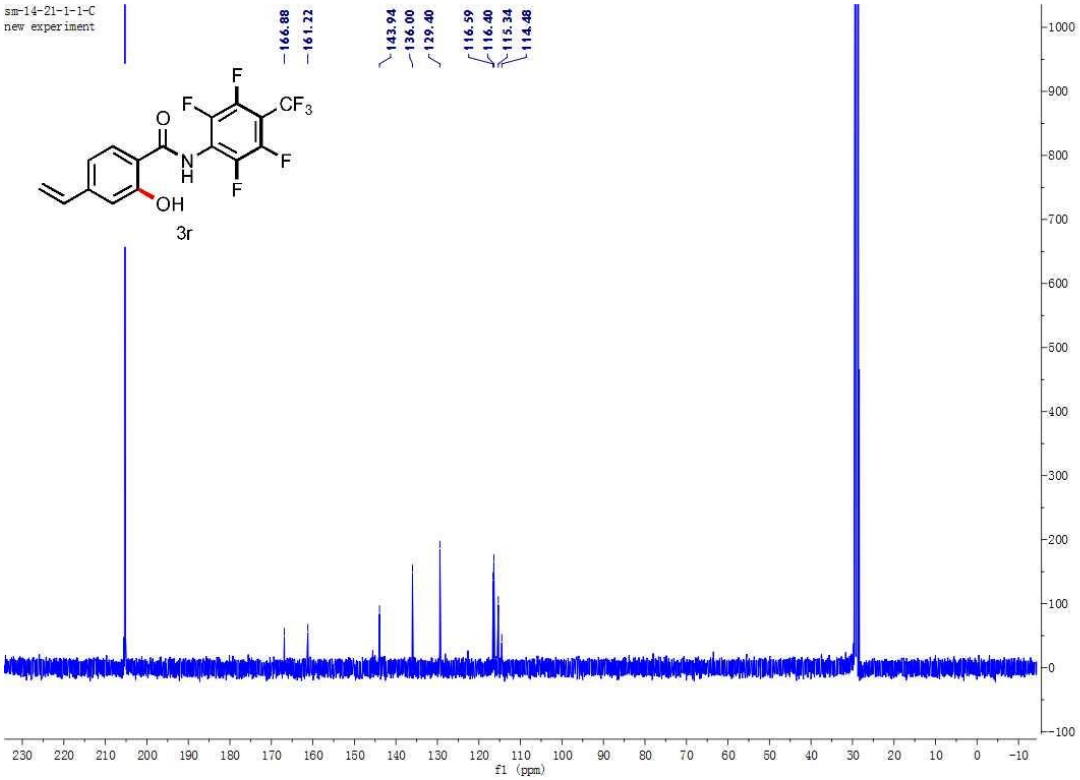

sm-14-12-1-1-HH
8.12
8.10
7.28
6.98
6.97
F
F
CF3
O
N
H
F
F
NC
OH
3q
1.00
0.99
1.00
f1 (ppm)

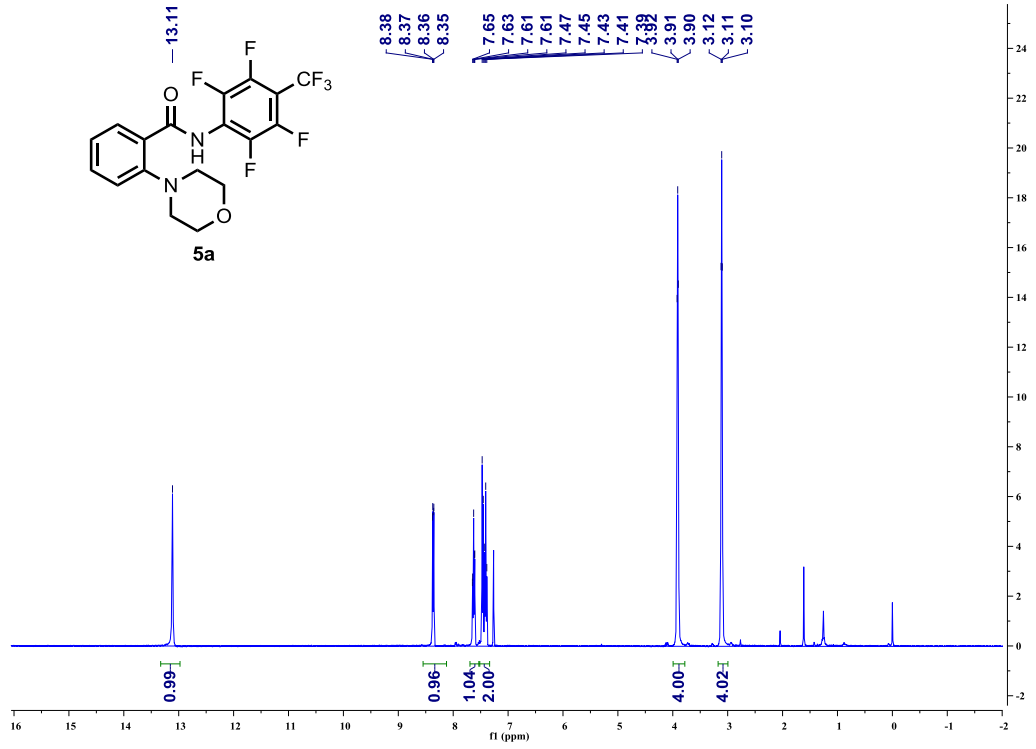

sm-14-12-1-1-FF
STANDARD PROTON PARAMETERS
-56.30
-56.36
-56.42
-144.58
-145.28
F
F
CF3
O
N
H
F
F
NC
OH
3q
f1 (ppm)

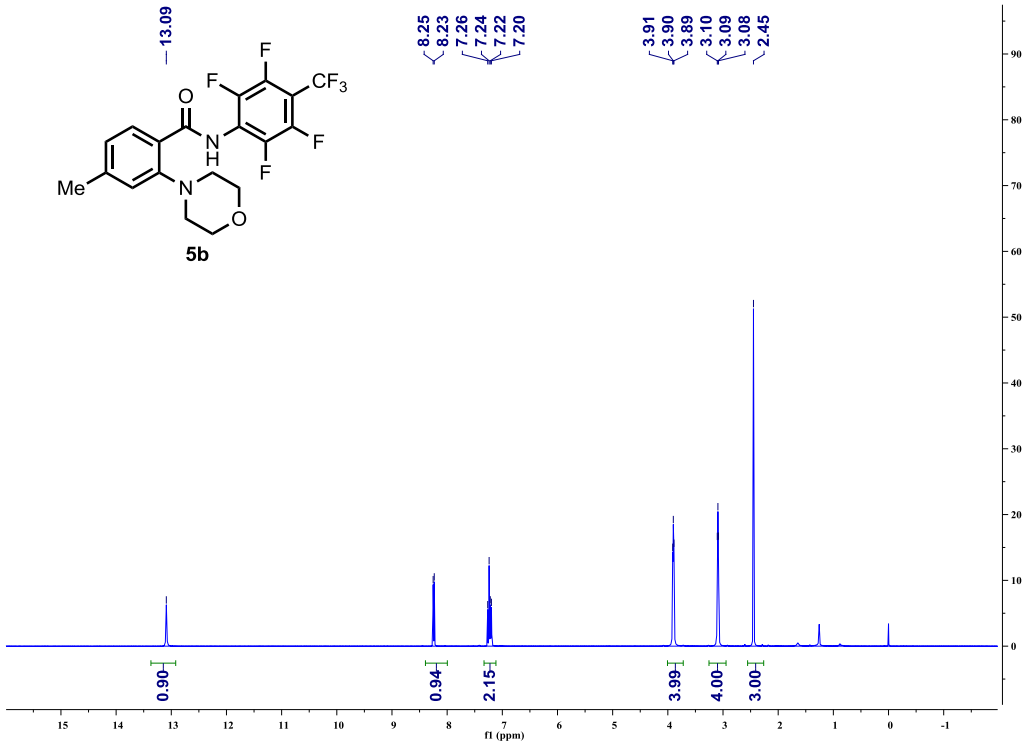

sm-14-12-1-1-d
165.54
164.71
132.26
123.49
119.34
119.01
116.59
F
F
CF3
O
N
H
F
F
NC
OH
3q
f1 (ppm)


sm-14-21-HH
10.24
8.03
8.01
7.16
7.14
7.11
7.11
6.00
6.00
5.96
5.96
5.44
5.44
5.42
5.41
F
F
CF3
O
N
H
F
F
OH
3r
1.00
0.99
0.94
0.96
1.04
0.53
f1 (ppm)

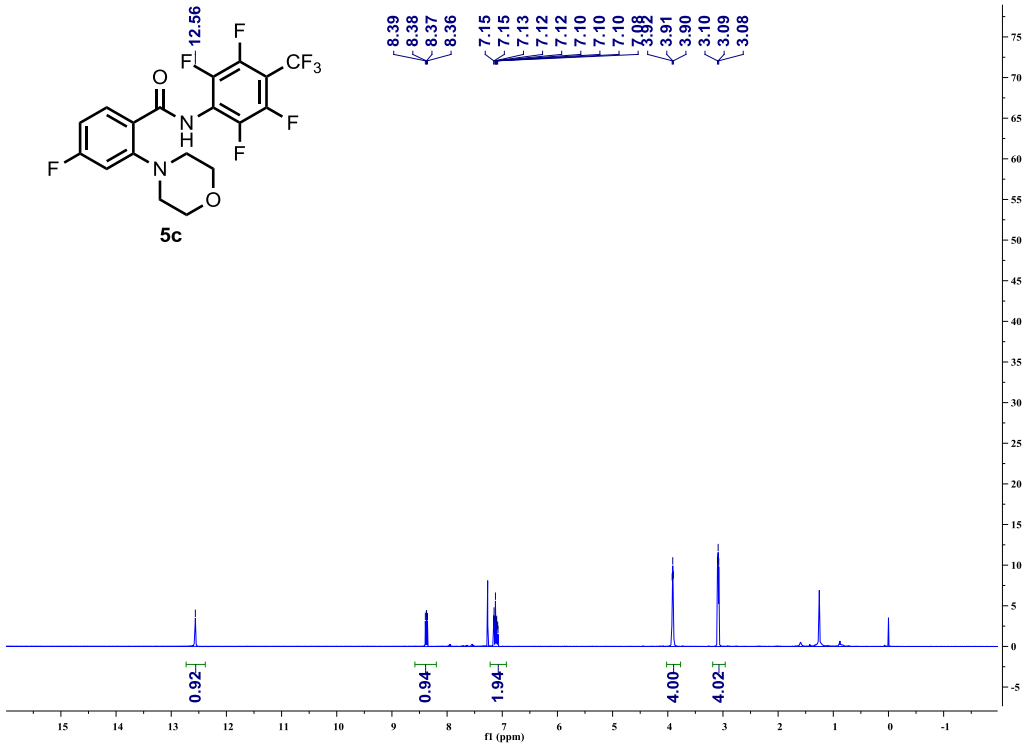

sm-14-21-FF
STANDARD PROTON PARAMETERS
-56.75
-56.81
-56.81
-56.82
-56.83
-56.87
-143.82
-143.85
-143.87
F
F
CF3
O
N
H
F
F
OH
3r
2.00
3.77
f1 (ppm)


sm-14-21-1-1-C
new experiment
166.88
161.22
143.94
136.00
129.40
116.59
116.40
115.34
114.48
3r
f1 (ppm)

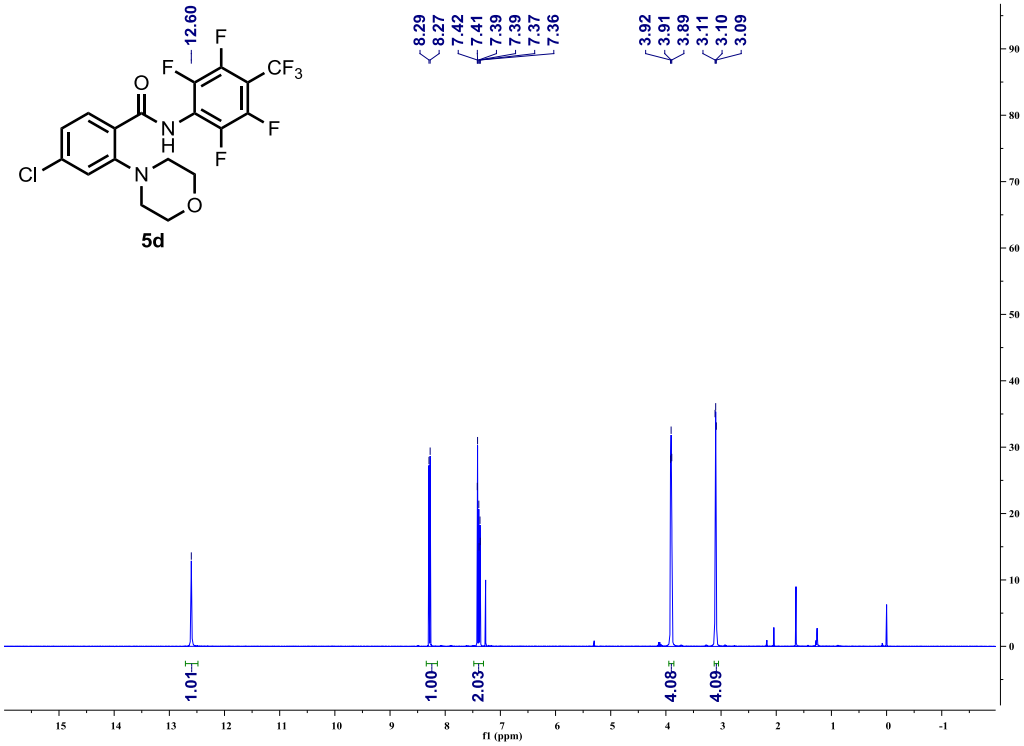

13.11
8.38
8.37
8.36
8.35
7.65
7.63
7.61
7.61
7.47
7.45
7.43
7.41
3.91
3.90
3.12
3.11
3.10
5a
0.99
0.96
1.04
2.00
4.00
4.02
f1 (ppm)

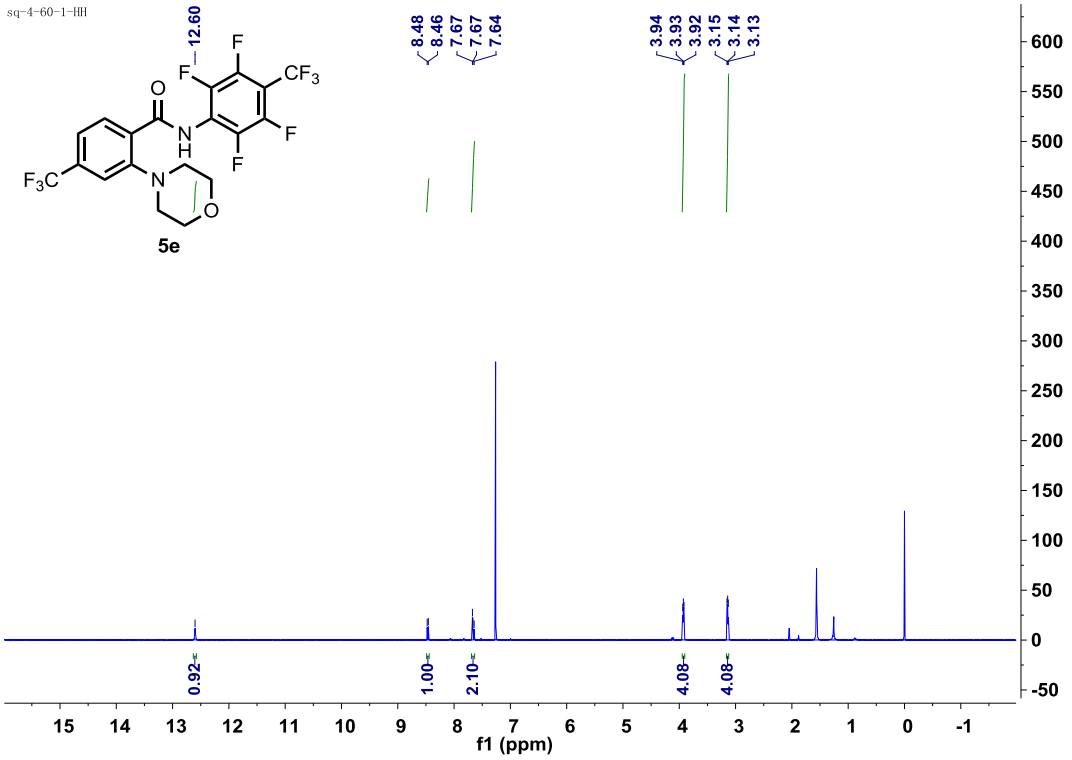

13.09
8.25
8.23
7.26
7.24
7.22
7.20
3.91
3.90
3.89
3.10
3.09
3.08
2.45
F
F
CF3
O
N
H
F
F
Me
N
O
0.90
0.94
2.15
3.99
4.00
3.00
f1 (ppm)

5b


12.56
8.39
8.38
8.37
8.36
7.15
7.15
7.13
7.12
7.12
7.10
7.10
7.10
7.08
3.91
3.90
3.10
3.09
3.08
F
F
CF3
O
N
H
F
F
F
N
O
0.92
0.94
1.94
4.00
4.02
f1 (ppm)

5c


12.60
8.29
8.27
7.42
7.41
7.39
7.39
7.37
7.36
3.92
3.91
3.89
3.11
3.10
3.09
1.01
1.00
2.03
4.08
4.09
f1 (ppm)
5d


sq-4-60-1-HH
12.60
8.48
8.46
7.67
7.67
7.64
3.94
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3.14
3.13
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2.10
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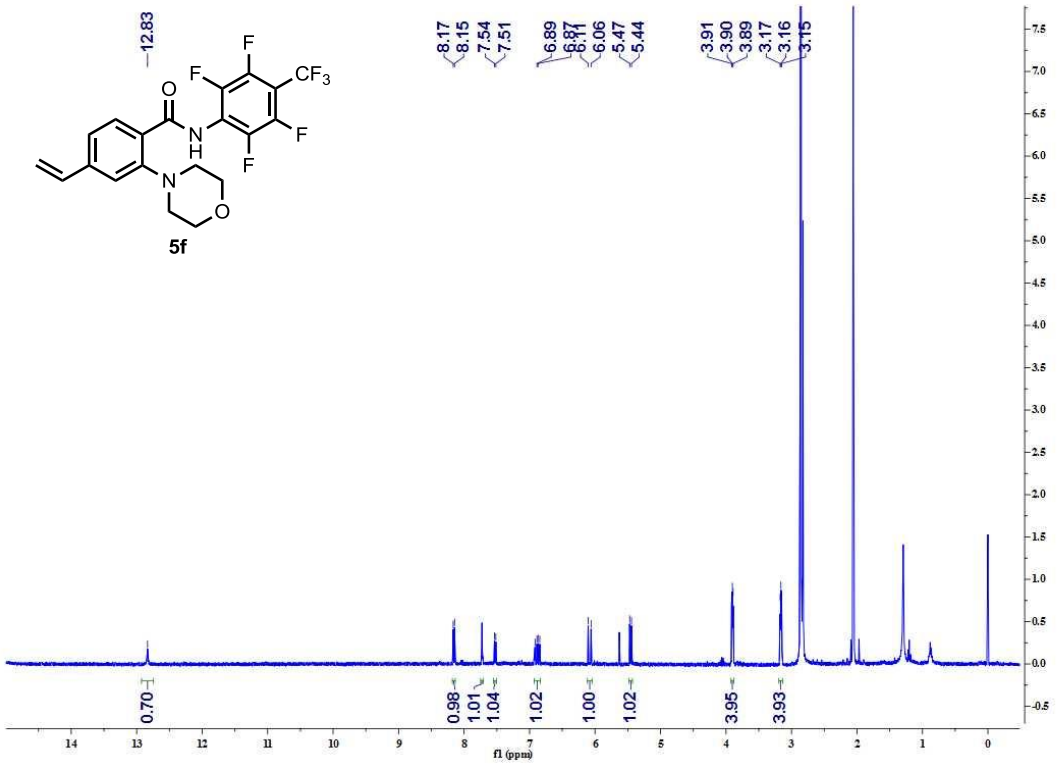
4.08
f1 (ppm)
5e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6.87
6.11
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5.44
3.91
3.90
3.89
3.17
3.16
3.15
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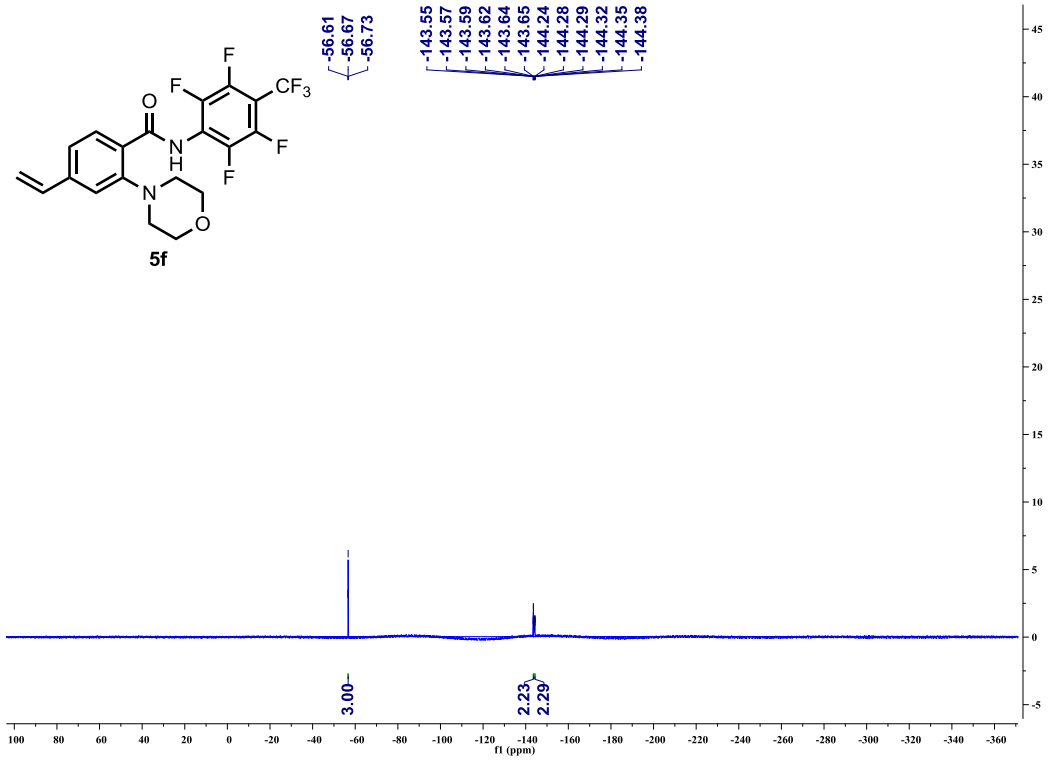
1.04
1.02
1.00
1.02
3.95
3.93
f1 (ppm)
5f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-143.65
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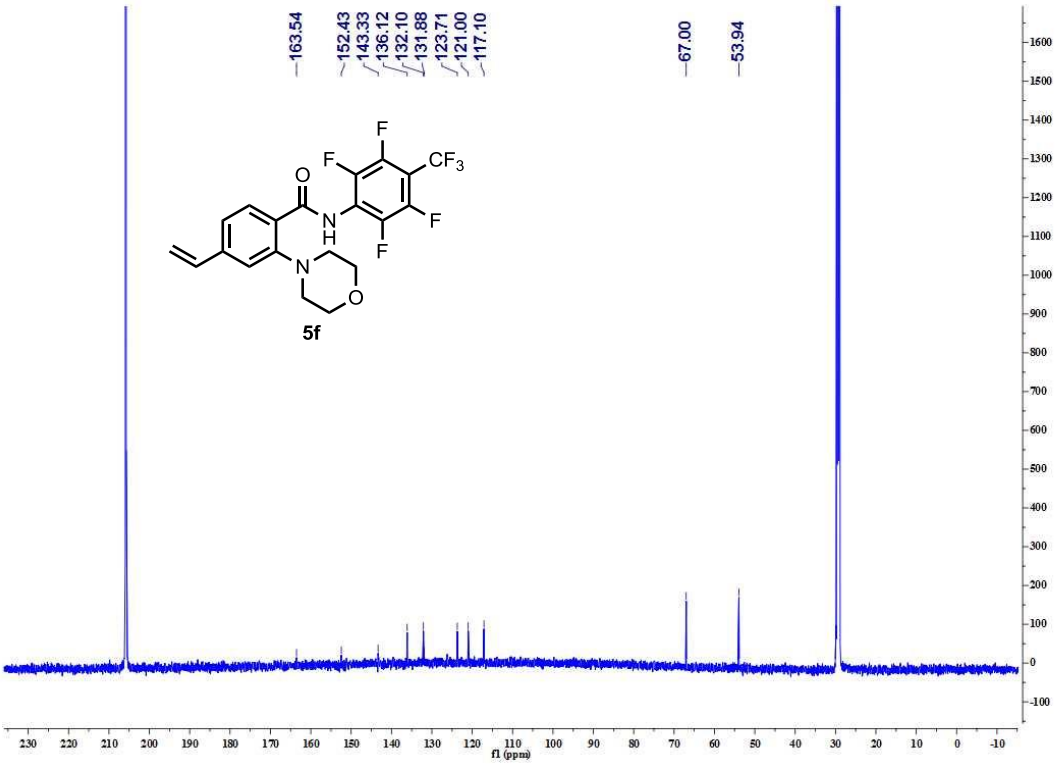
2.23
2.29
f1 (ppm)
5f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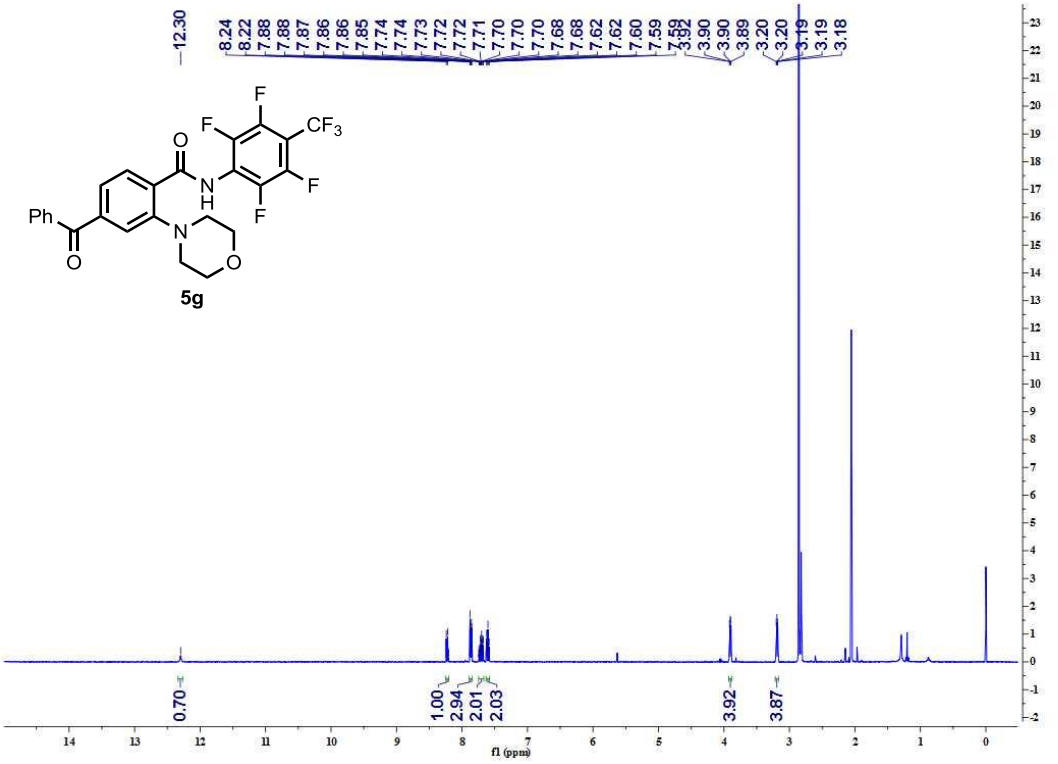
143.33
136.12
132.10
131.88
123.71
121.00
117.10
67.00
53.94
F
F
CF3
O
N
H
F
F
N
O
5f
f1 (ppm)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8.22
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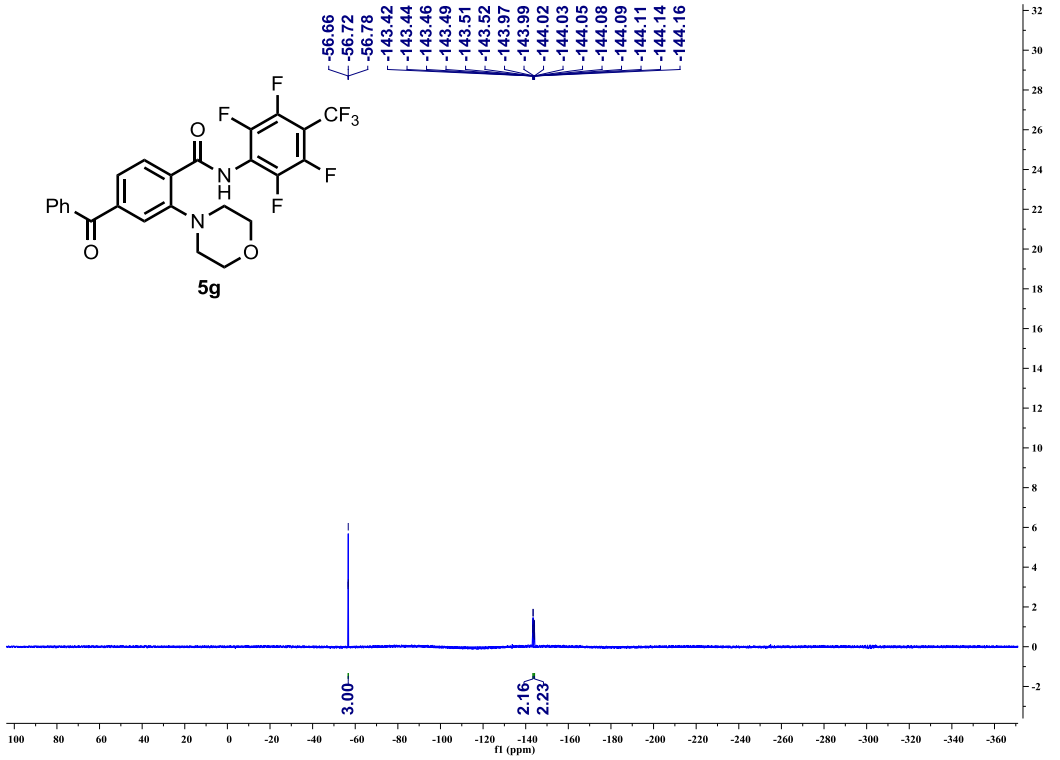
7.88
7.87
7.86
7.86
7.85
7.74
7.74
7.73
7.72
7.72
7.71
7.70
7.70
7.70
7.68
7.68
7.62
7.62
7.60
7.59
7.59
3.92
3.90
3.90
3.89
3.20
3.20
3.19
3.19
3.18
F
F
CF3
O
N
H
F
F
Ph
O
N
O
5g
0.70
1.00
2.94
2.01
2.03
3.92
3.87
f1 (ppm)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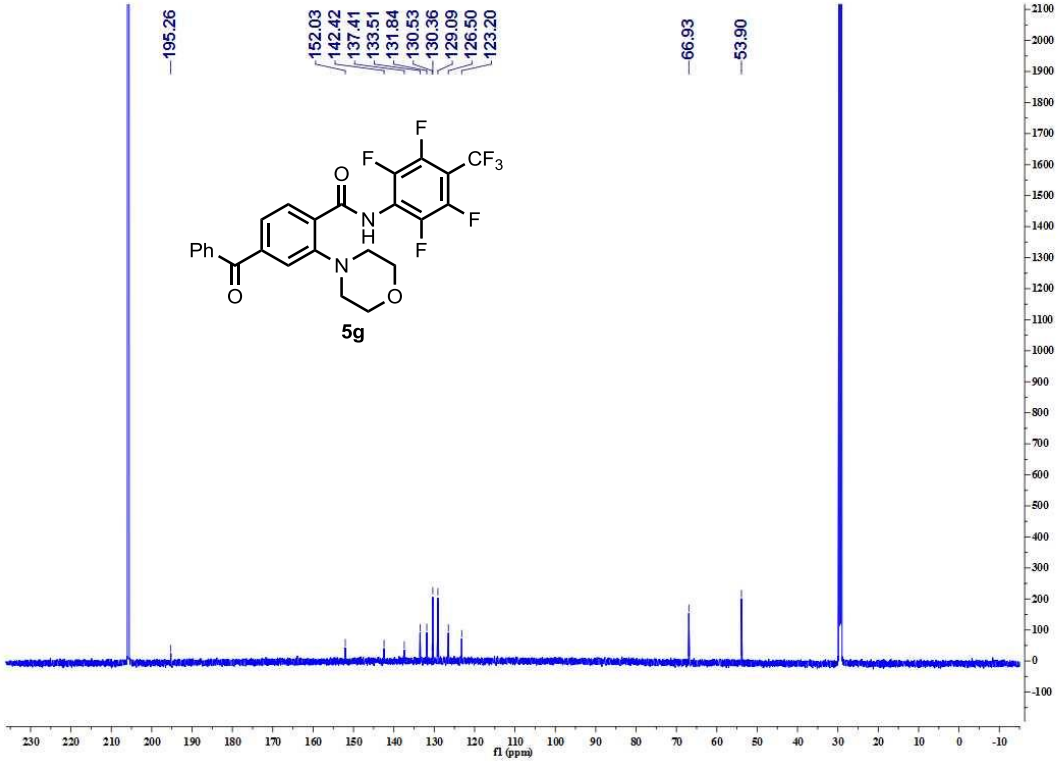
-143.52
-143.97
-143.99
-144.02
-144.03
-144.05
-144.08
-144.09
-144.11
-144.14
-144.16
F
F
CF3
O
N
H
F
F
Ph
O
N
O
5g
3.00
2.16
2.23
fl (ppm)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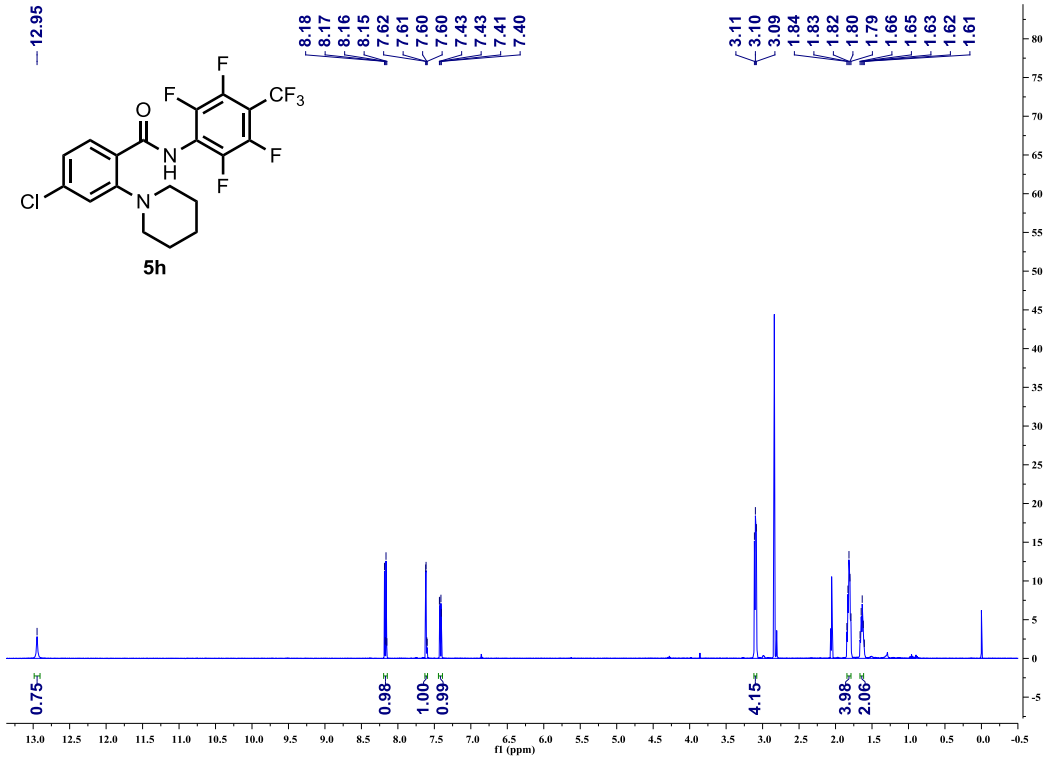
152.03
142.42
137.41
133.51
131.84
130.53
130.36
129.09
126.50
123.20
66.93
53.90
F
F
CF3
O
N
H
F
F
Ph
O
N
O
5g
fl (ppm)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8.18
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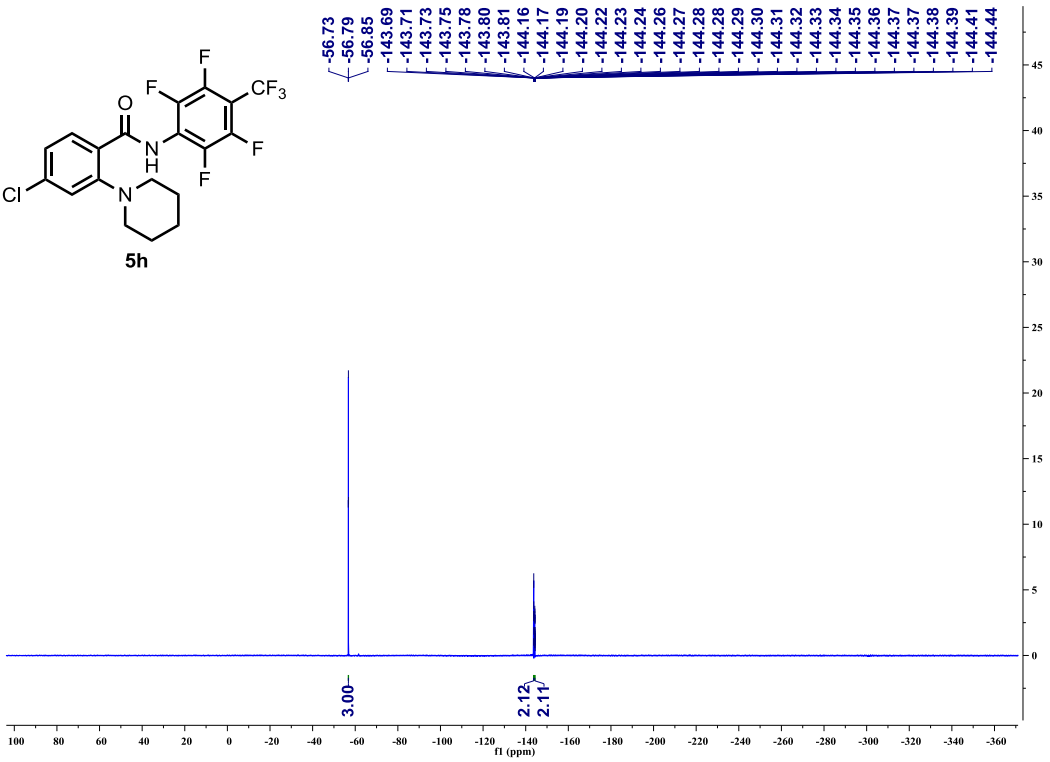
8.16
8.15
7.62
7.61
7.60
7.60
7.43
7.43
7.41
7.40
3.11
3.10
3.09
1.84
1.83
1.82
1.80
1.79
1.66
1.65
1.63
1.62
1.61
F
F
CF3
O
N
H
F
Cl
N
5h
0.75
0.98
1.00
0.99
4.15
3.98
2.06
f1 (ppm)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-144.17
-144.19
-144.20
-144.22
-144.23
-144.24
-144.26
-144.27
-144.28
-144.28
-144.29
-144.30
-144.31
-144.32
-144.33
-144.34
-144.35
-144.36
-144.37
-144.37
-144.38
-144.39
-144.41
-144.44
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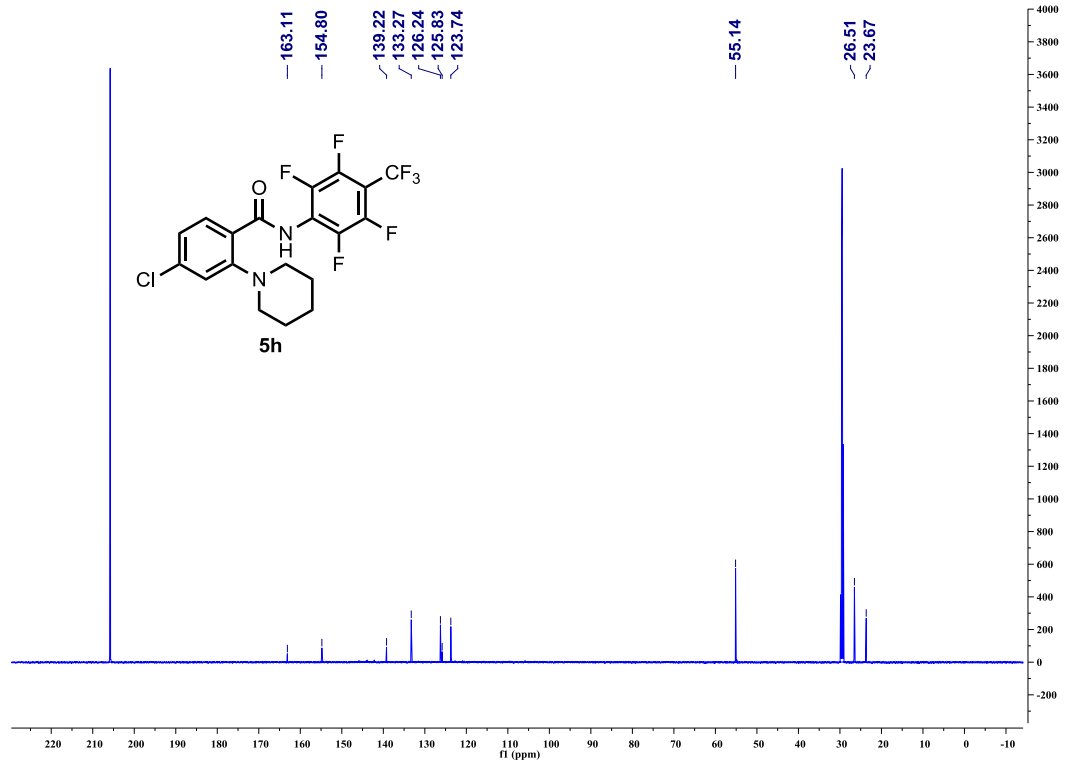
F
CF3
O
N
H
F
Cl
N
5h
3.00
2.12
2.11
f1 (ppm)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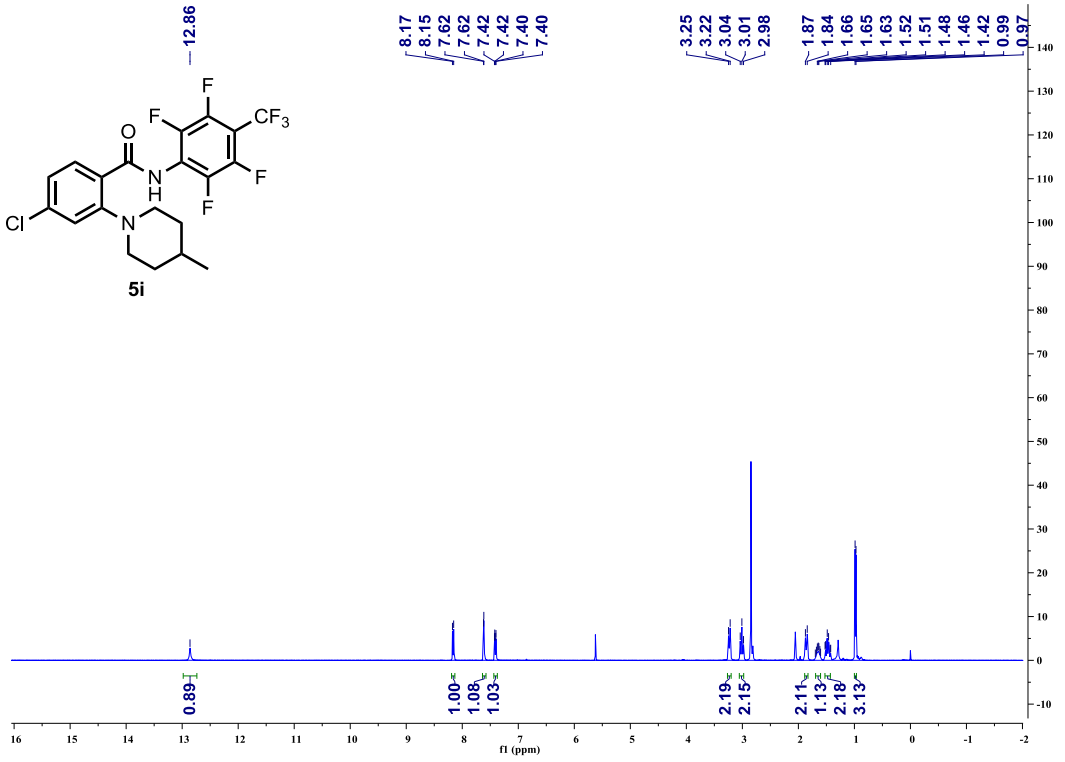
154.80
139.22
133.27
126.24
125.83
123.74
55.14
26.51
23.67
F
F
CF3
O
N
H
F
F
Cl
N
5h
fl (ppm)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8.17
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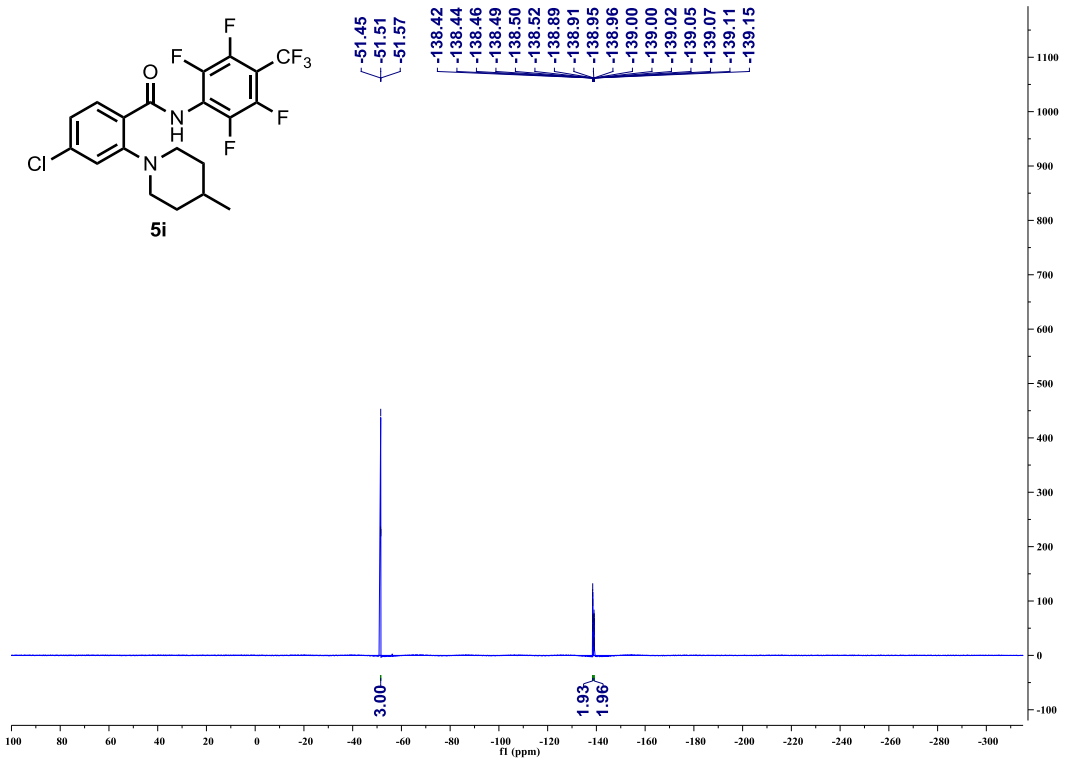
7.62
7.62
7.42
7.42
7.40
7.40
3.25
3.22
3.04
3.01
2.98
1.87
1.84
1.66
1.65
1.63
1.52
1.51
1.48
1.46
1.42
0.99
0.97
F
F
CF3
O
N
H
F
F
Cl
N
5i
0.89
1.00
1.08
1.03
2.19
2.15
2.11
1.13
2.18
3.13
fl (ppm)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-51.51
-51.57
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-138.52
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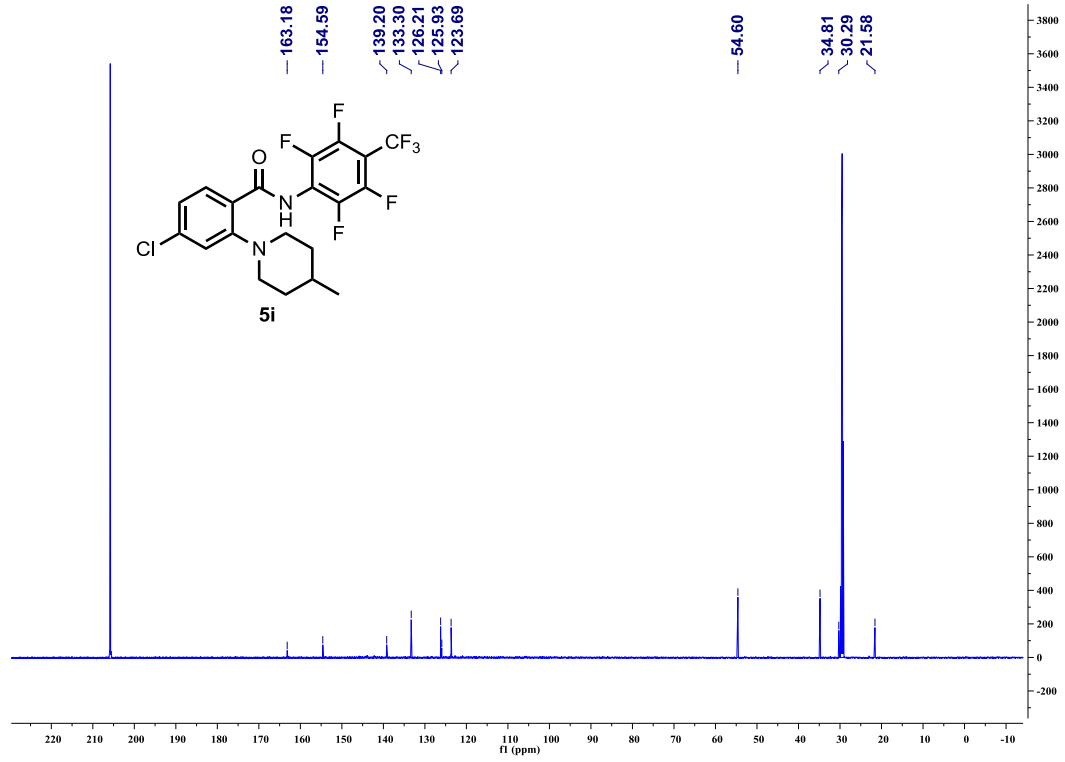
3.00
1.93
1.96
f1 (ppm)

5i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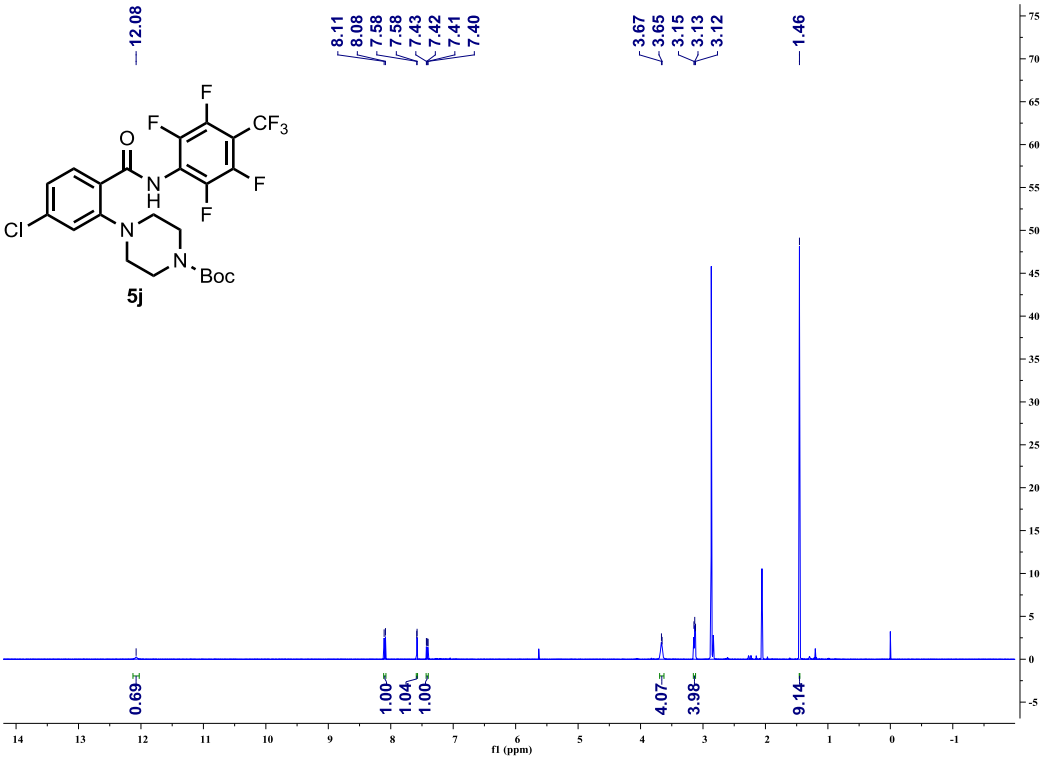
133.30
126.21
125.93
123.69
54.60
34.81
30.29
21.58
f1 (ppm)

5i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8.11
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7.58
7.58
7.43
7.42
7.41
7.40
3.67
3.65
3.15
3.13
3.12
1.46
F
F
CF3
O
N
H
F
Cl
N
N
Boc
5j
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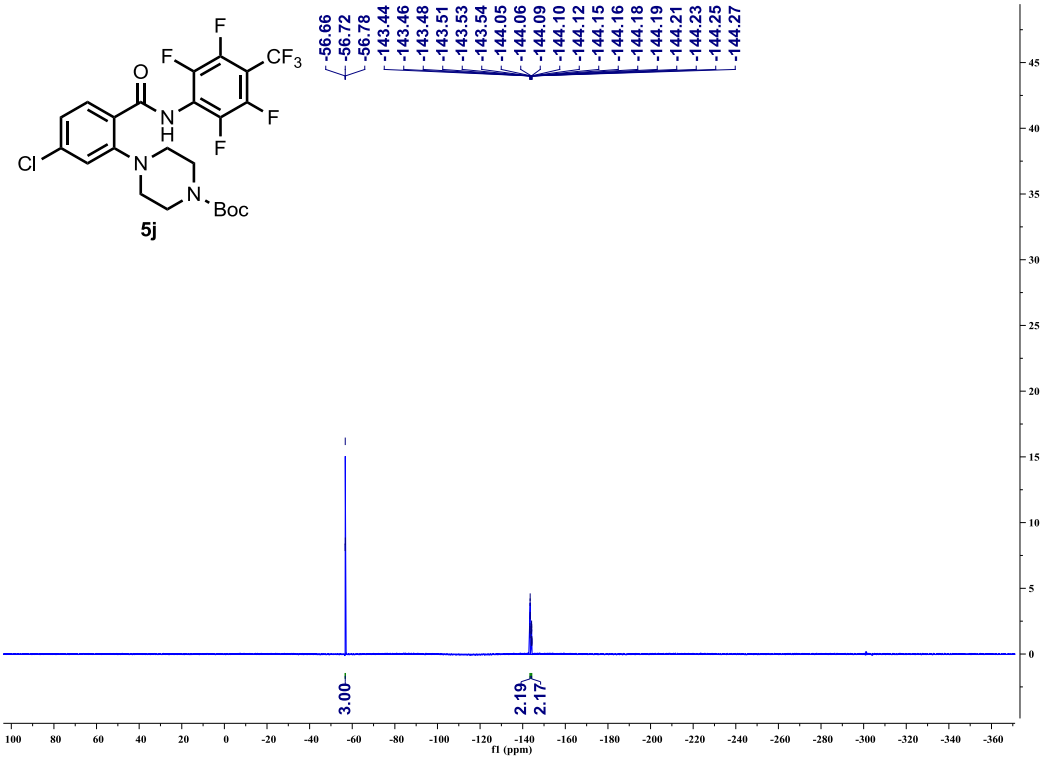
1.00
1.04
1.00
4.07
3.98
9.14
fl (ppm)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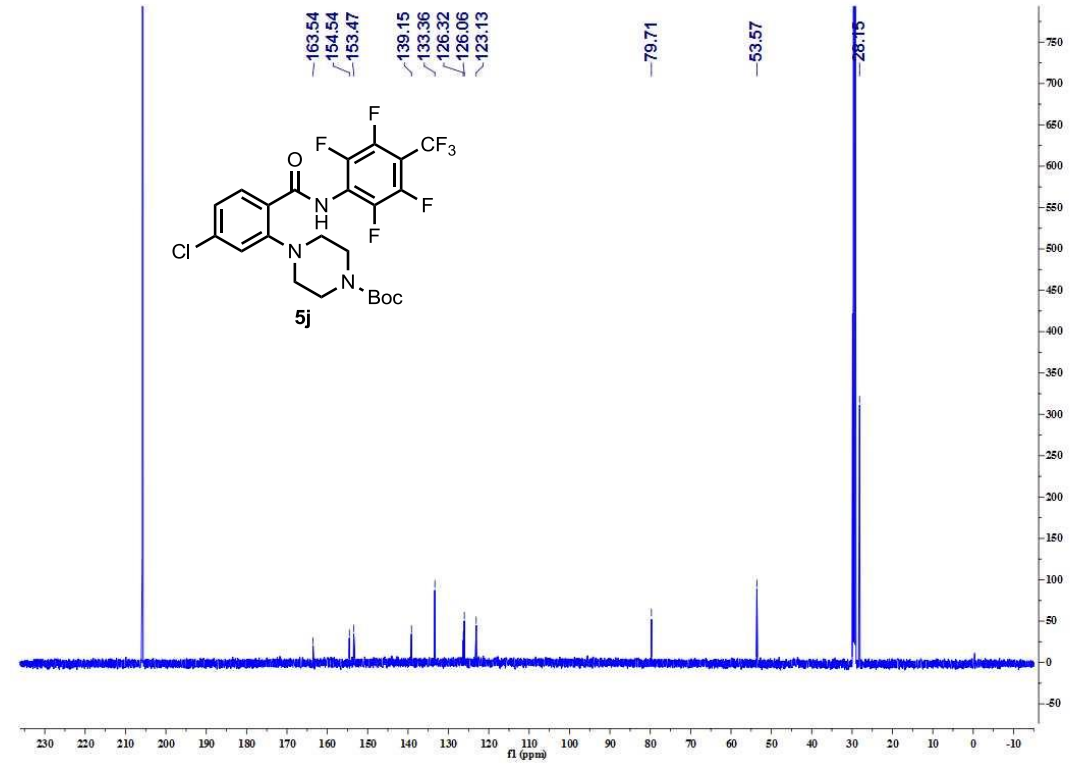
-144.09
-144.10
-144.12
-144.15
-144.16
-144.18
-144.19
-144.21
-144.23
-144.25
-144.27
F
F
CF3
O
N
H
F
Cl
N
N
Boc
5j
3.00
2.19
2.17
fl (ppm)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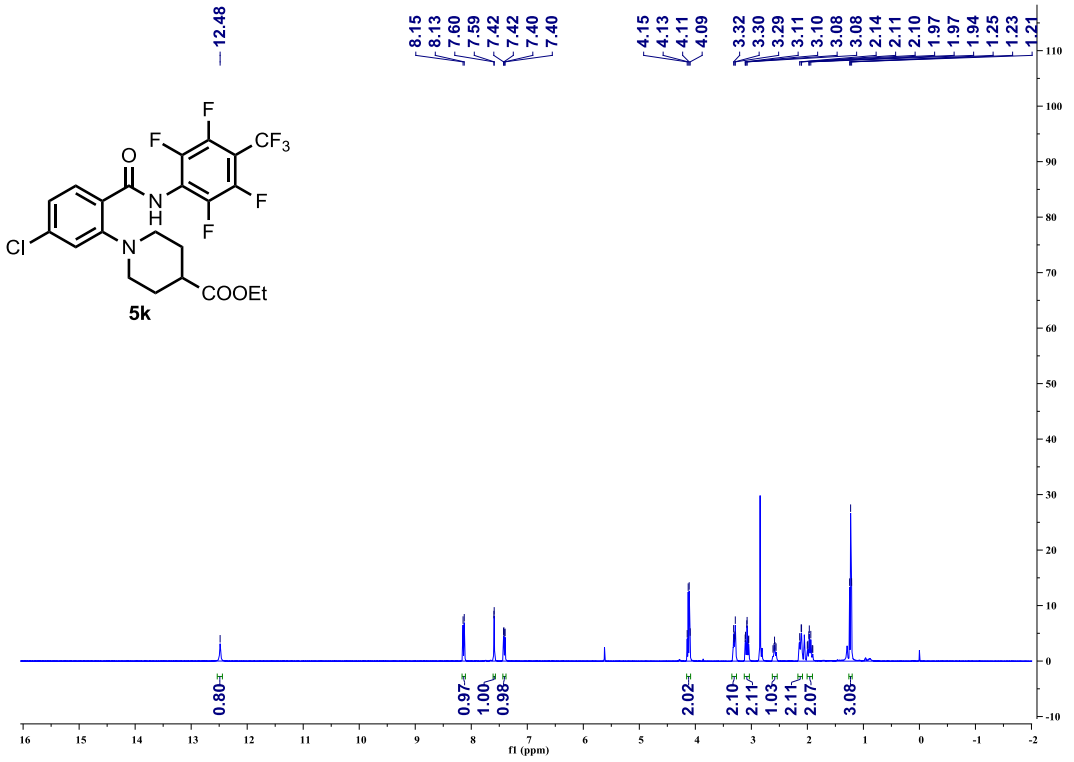
139.15
133.36
126.32
126.06
123.13
79.71
53.57
28.15
F
F
CF3
O
N
H
F
F
Cl
N
N
Boc
5j
f1 (ppm)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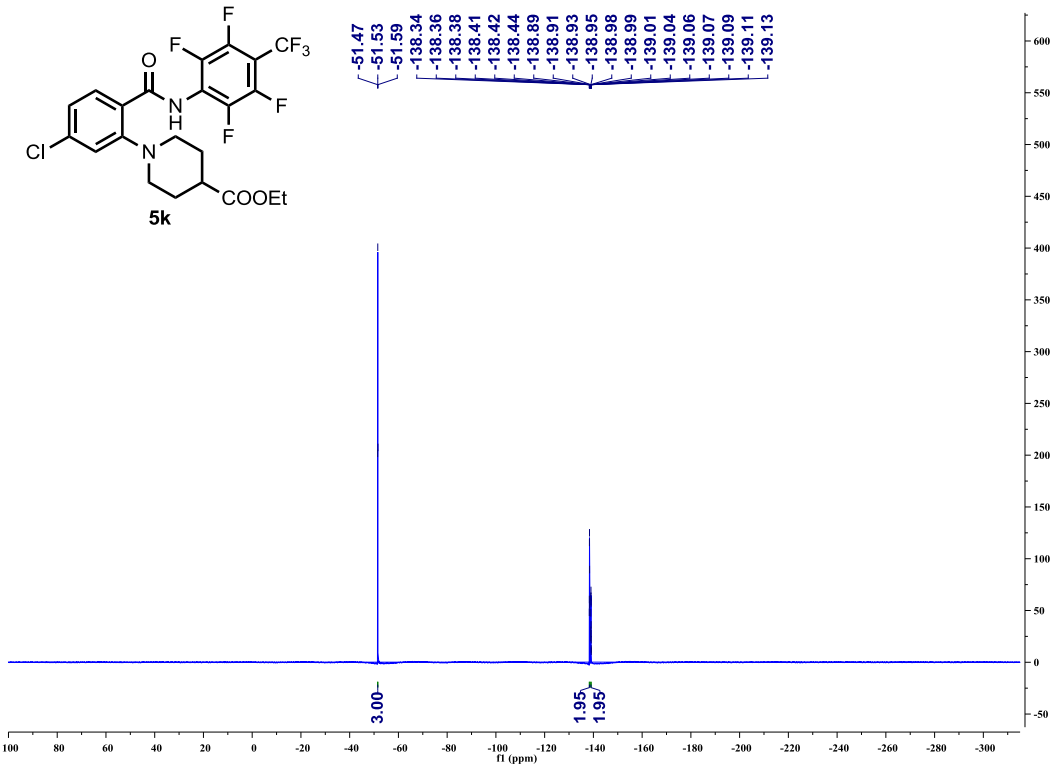
7.42
7.40
7.40
4.15
4.13
4.11
4.09
3.32
3.30
3.29
3.11
3.10
3.08
2.14
2.11
2.10
1.97
1.94
1.25
1.23
1.21
F
F
CF3
O
N
H
F
F
Cl
N
COOEt
5k
0.80
0.97
1.00
0.98
2.02
2.10
2.11
1.03
2.11
2.07
3.08
f1 (ppm)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-138.93
-138.95
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-139.01
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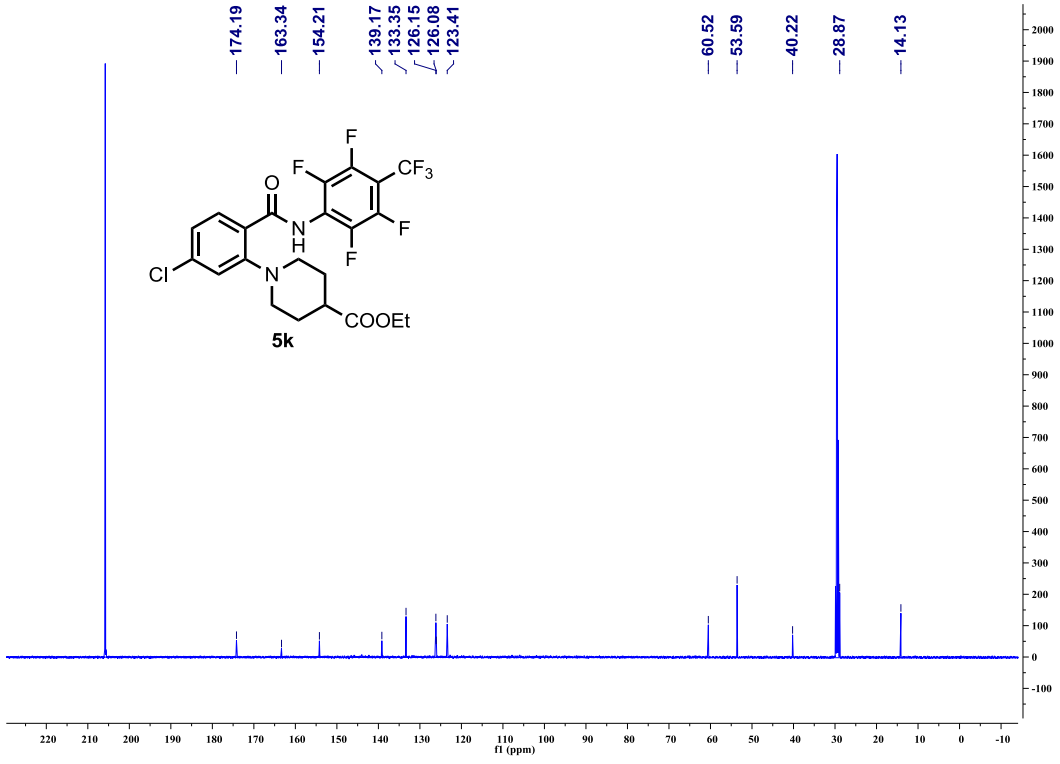
-139.06
-139.07
-139.09
-139.11
-139.13
3.00
1.95
1.95
f1 (ppm)
5k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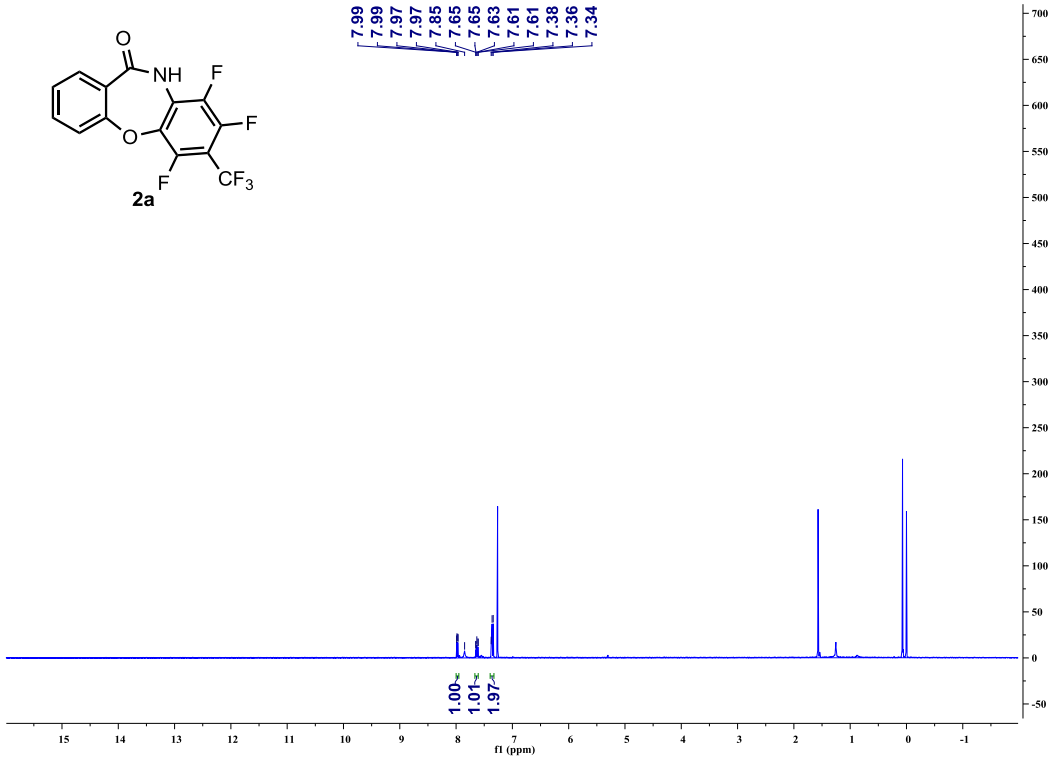
154.21
139.17
133.35
126.15
126.08
123.41
60.52
53.59
40.22
28.87
14.13
f1 (ppm)
5k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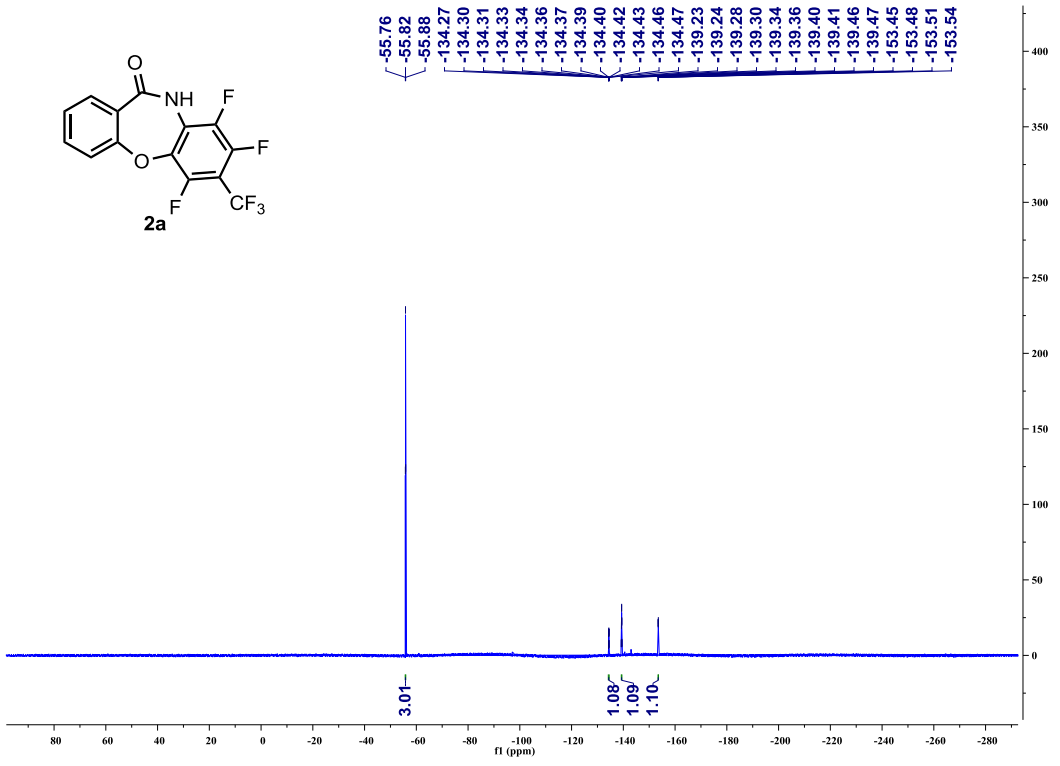
7.99
7.97
7.97
7.85
7.65
7.65
7.63
7.61
7.61
7.38
7.36
7.34
O
NH
F
F
O
F
CF3
2a
1.00
1.01
1.97
f1 (ppm)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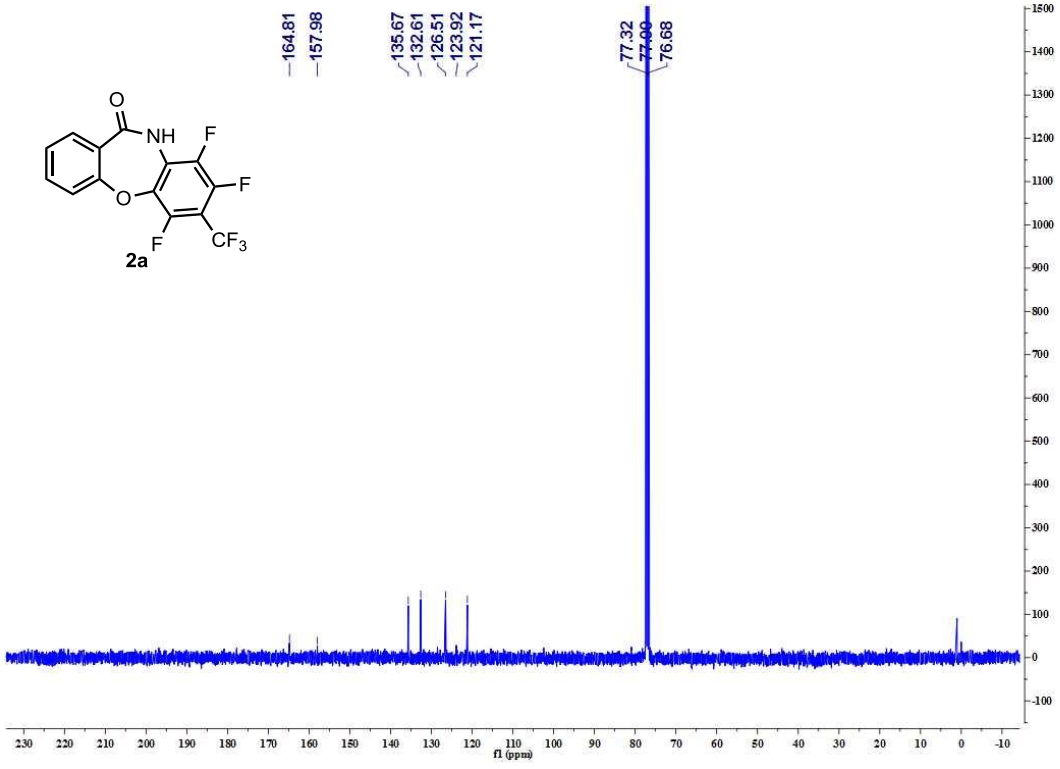
F
F
O
F
CF3
2a
3.01
1.08
1.09
1.10
f1 (ppm)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126.51
123.92
121.17
77.32
77.00
76.68
O
NH
F
F
O
F
CF3
2a
f1 (ppm)