Supplementary Information

Visible-Light-Induced Selective Defluoroalkylations of Polyfluoroarenes with Alcohols

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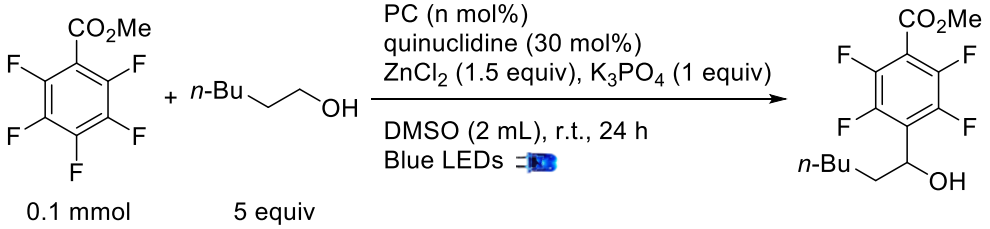
1. General Information

Chemicals and solvents were purchased from commercial suppliers and used as received. ^{1}H NMR, ^{13}C NMR, ^{19}F NMR spectra were recorded on a Bruker AV-III400 (400 MHZ) spectrometer. Chemical shifts were calibrated using residual undeuterated solvent as an internal reference ($CDCl_3$: 7.26 ppm ^{1}H NMR, 77.0 ppm ^{13}C NMR; CD_3OD: 4.87 ppm ^{1}H NMR, 49.0 ppm ^{13}C NMR). Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), p (pentet). High-resolution mass spectra (HRMS) were obtained on Agilent 7200 GC-QTOF spectrometer (EI). Cyclic voltammetry was performed using Vertex. C. EIS Chenhua (China). The high-pressure syringe pump was purchased from Longer (China) for continuous flow setup. The L-cube dual syringe high pressure constant flow pump was purchased from Ou Shi Sheng (Beijing) Technology Co., Ltd (China). The needle valves, and PFA micro tubings were purchased from IDEX Health & Science (USA). The back pressure regulator was purchased from Zaiput (USA). Stern-Volmer fluorescence quenching was performed using an Spectrofluorophotometer RF-6000 Shimadzu Corporation.

2. Complementary Reaction Optimization Data

Table S1. Screening of photocatalysts

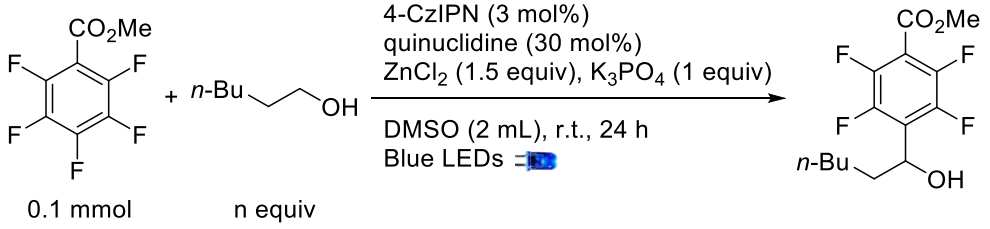


0.1 mmol 5 equiv

entry	PC	yield%[a]
1	4-CzIPN (3 mol%)	83
2	$Ir(ppy)_3$ (2 mol%)	0
3	$Ir(ppy)_2(dtbbpy)PF_6$ (1 mol%)	6
4	$[Ir[dF(CF_3)ppy]_2(dtbbpy)PF_6$ (1 mol%)	70

[a] The yields were obtained with ^{1}H-NMR using trimethoxybenzene as the internal standard.

Table S2. Screening of the amount of hexanol

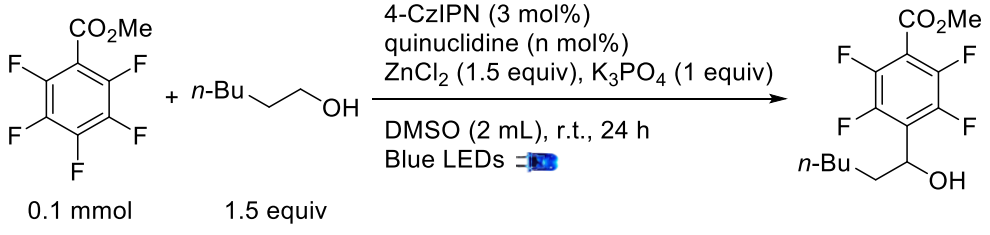


0.1 mmol n equiv

entry	n	yield%[a]
1	5	83
2	3.5	85
3	2.5	89
4	1.5	87

[a] The yields were obtained with ^{19}F-NMR using trifluorotoluene as the internal standard.

Table S3. Screening of the amount of quinuclidine

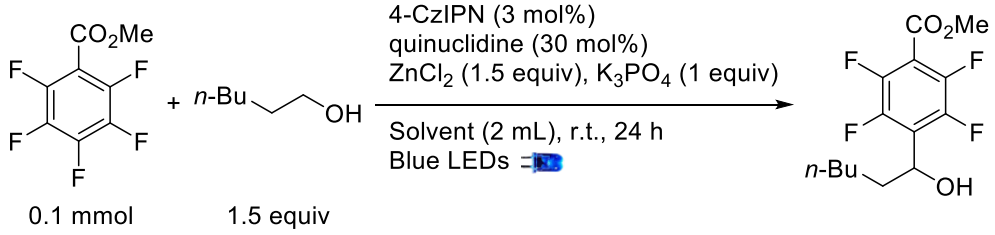


0.1 mmol 1.5 equiv

entry	n	yield%[a]
1	30	87
2	10	39
3	5	24

[a] The yields were obtained with ^{19}F-NMR using trifluorotoluene as the internal standard.

Table S4. Screening of solvents

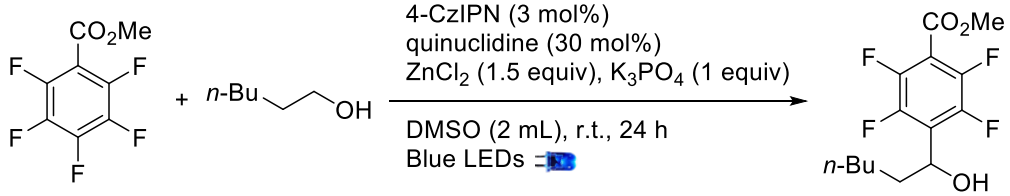


0.1 mmol 1.5 equiv

entry	solvent	yield% [a]
1	DMSO	87
2	DMF	0
3	DMA	0
4	MeCN	13
5	EA	0
6	MeTHF	8

[a] The yields were obtained with ^{19}F-NMR using trifluorotoluene as the internal standard.

Table S5. Control experiments

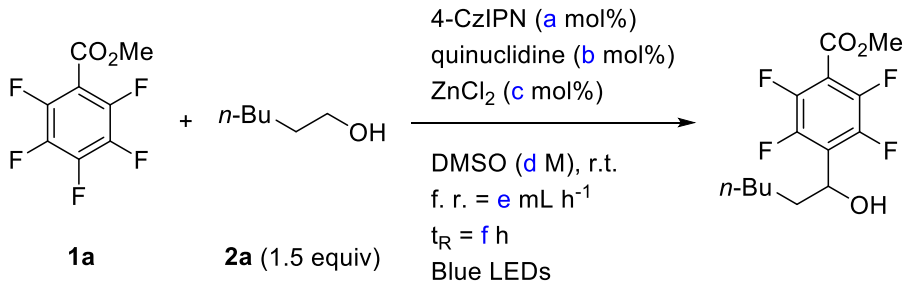


1a (0.1 mmol) **2a** (1.5 equiv) **3aa**

entry	deviation	yield% (**3aa**)[a]
1	no	87[b]
2	no light, 4-CzIPN, or quinuclidine	0
3	w/o $ZnCl_2$	28
4	w/o K_3PO_4	86
5	w/o K_3PO_4 and using $ZnCl_2$ (50 mol%)	70

[a] The yields were obtained with ^{19}F-NMR using trifluorotoluene as the internal standard.
[b] Isolated yield.

Table S6. Optimization in continuous flow reactors



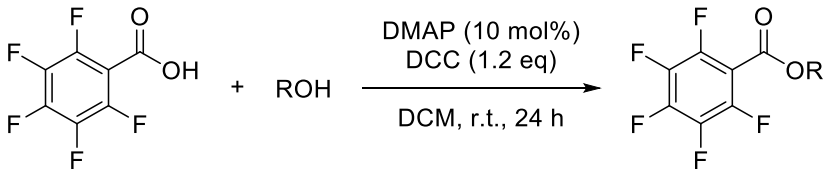
1a **2a** (1.5 equiv)

entry	a	b	c	d	e	f	conv.%[a]	yield%[a]
1	2	30	150	0.05	2	0.5	80	33
2	2	30	150	0.05	1	1	98	43
3	2	20	50	0.05	1	1	81	40
4	1	20	50	0.05	1	1	74	45
5	1	20	50	0.05	1	2	82	60
6	1	20	50	0.05	0.5	2	83	67
7	1	20	50	0.1	0.5	2	81	73
8	1	20	50	0.1	0.5	8	86	85[b]

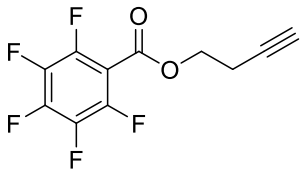
[a] The conversions and yields were obtained with ^{19}F-NMR using trifluorotoluene as the internal standard.
[b] Isolated yield.

3. Starting Material Preparation

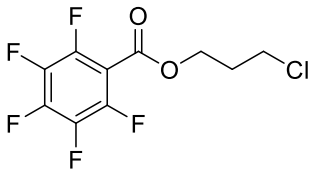
3.1 Preparation of 1k, 1l, 1m



To a solution of pentafluorobenzoic acid (1.06 g, 5 mmol) in DCM (15 mL) was added DCC (1.24g, 6 mmol), DMAP (61.0 mg, 0.5 mmol), and alcohol (6 mmol). The mixture was stirred for 24 h at room temperature. After filtration, the mixture was concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel, eluting with petroleum ether/EtOAc = 9/1 (v/v) to afford the products as colorless oil.

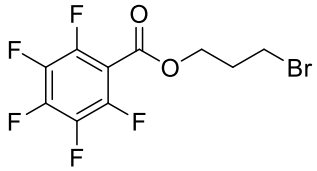


But-3-yn-1-yl 2,3,4,5,6-pentafluorobenzoate (1k): colorless oil (0.95 g, 72%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.50 – 4.45 (m, 2H), 2.68 – 2.63 (m, 2H), 2.04 – 2.02 (m, 1H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -137.85 – -138.07 (m, 2F), -148.25 – -148.56 (m, 1F), -160.30 – -160.59 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.73, 146.90 – 144.02 (m), 144.79 – 141.85 (m), 139.21 – 136.24 (m), 108.15 – 107.74 (m), 79.06, 70.33 (d, J = 1.8 Hz), 64.21, 18.84; HRMS (EI): Calcd for $C_{11}H_6F_5O_2$ $[M+H]^+$ 264.1510, found 264.1512.



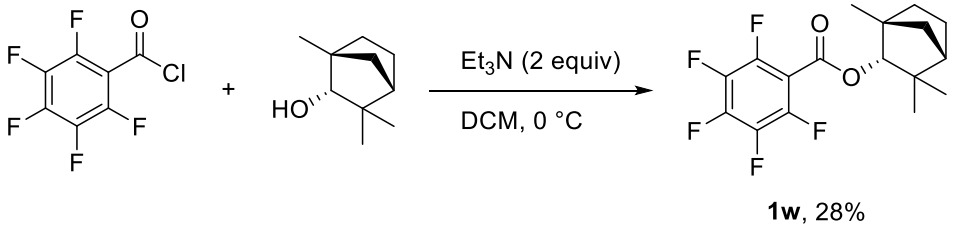
3-Chloropropyl 2,3,4,5,6-pentafluorobenzoate (1l): colorless oil (0.82 g, 57%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.54 (t, J = 6.0 Hz, 2H), 3.68 (t, J = 6.3 Hz, 2H), 2.22 (p, J = 6.2 Hz, 2H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -138.07 – -138.20 (m, 2F), -148.10 –

-148.26 (m, 1F), -160.15 – -160.32 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.82 (d, *J* = 1.4 Hz), 146.91 – 144.04 (m), 144.78 – 141.83 (m), 139.22 – 136.24 (m), 108.17 – 107.78 (m), 63.34, 40.69, 31.28; HRMS (EI): Calcd for $C_{10}H_7ClF_5O_2$ $[M+H]^+$ 289.5980, found 289.5984.



3-Bromopropyl 2,3,4,5,6-pentafluorobenzoate (1m): colorless oil (1.09 g, 65%).^{1}H NMR (400 MHz, $CDCl_3$): δ 4.52 (t, *J* = 5.9 Hz, 2H), 3.51 (t, *J* = 6.4 Hz, 2H), 2.29 (p, *J* = 6.2 Hz, 2H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -138.15 – -138.26 (m, 2F), -148.26 – -148.40 (m, 1F), -160.29 – -160.47 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.78, 146.90 – 144.02 (m), 144.77 – 141.83 (m), 139.19 – 136.25 (m), 108.14 – 107.74 (m), 64.33, 31.32, 28.72; HRMS (EI): Calcd for $C_{10}H_7BrF_5O_2$ $[M+H]^+$ 334.0520, found 334.0525.

3.2 Preparation of 1w

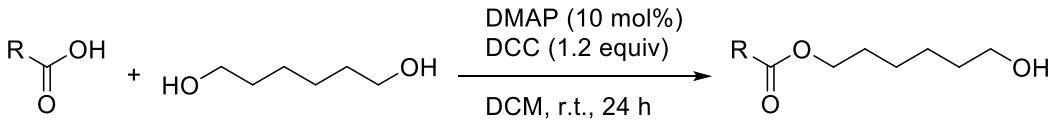


To a 50 mL round-bottom flask charged with (+)-Fenchol (0.77 g, 5.0 mmol) was added Et_3N (1.01 g, 10 mmol) and DCM (10 mL). The resulting mixture was stirred at 0 °C in an ice-water bath for 5 min. Then, pentafluorobenzoyl chloride (1.15 g, 5.0 mmol) was added dropwise. After stirring at 0 °C for 6 hours, the reaction mixture was filtered through celite, and the filtrate was concentrated under vacuum. The residue was purified by flash column chromatography on silica gel, eluting with petroleum ether/EtOAc = 9/1 (v/v) to afford 0.49 g (28%) of **1w** as a colorless oil.

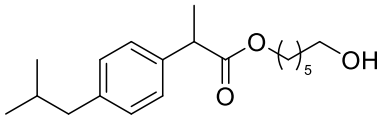
(1R,2R,4S)-1,3,3-trimethylbicyclo[2.2.1]heptan-2-yl 2,3,4,5,6-pentafluorobenzoate (1w): colorless oil (0.49 g, 28%). ^{1}H NMR (400 MHz, $CDCl_3$):

δ 4.64 (d, *J* = 2.0 Hz, 1H), 1.80 – 1.62 (m, 4H), 1.55 – 1.45 (m, 1H), 1.26 (dd, *J* = 10.4, 1.6 Hz, 1H), 1.19 (s, 3H), 1.16 (dt, *J* = 12.3, 2.4 Hz, 1H), 1.12 (s, 3H), 0.87 (s, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -138.24 – -138.40 (m, 2F), -149.25 – -149.46 (m, 1F), -160.49 – -160.72 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.45 (d, *J* = 1.2 Hz), 146.80 – 143.91 (m), 144.52 – 141.58 (m), 139.20 – 136.26 (m), 108.86 – 108.48 (m), 89.87, 48.48, 48.38, 41.36, 39.63, 29.64, 26.64, 25.71, 20.13, 19.18; HRMS (EI): Calcd for $C_{17}H_{18}F_5O_2$ $[M+H]^+$ 349.3130, found 349.3134.

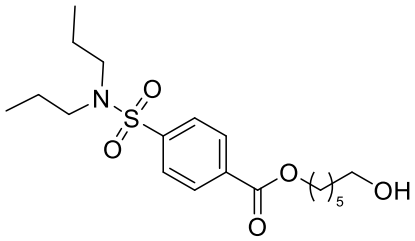
3.3 Preparation of S1, S2, S3



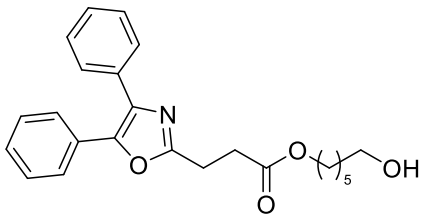
To a solution of acid (5 mmol) in DCM (15 mL) was added DCC (1.24g, 6 mmol), DMAP (61.0 mg, 0.5 mmol), and 1,6-hexanediol (0.71 g, 6 mmol). The mixture was stirred for 24 h at room temperature. After filtration, the mixture was concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel, eluting with petroleum ether/EtOAc = 2/1 (v/v) to afford compound as a colorless oil.



6-Hydroxyhexyl 2-(4-isobutylphenyl)propanoate (S1): colorless oil (0.63 g, 41%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.19 (d, *J* = 8.1 Hz, 2H), 7.08 (d, *J* = 8.1 Hz, 2H), 4.06 (td, *J* = 7.6, 6.7, 1.1 Hz, 2H), 3.68 (q, *J* = 7.2 Hz, 1H), 3.60 (t, *J* = 6.5 Hz, 2H), 2.44 (d, *J* = 7.2 Hz, 2H), 1.89 – 1.79 (m, 1H), 1.62 – 1.50 (m, 5H), 1.48 (d, *J* = 7.2 Hz, 3H), 1.36 – 1.23 (m, 4H), 0.89 (d, *J* = 6.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.84, 140.45, 137.85, 129.24, 127.13, 64.55, 62.77, 45.18, 45.00, 32.53, 30.16, 28.47, 25.52, 25.22, 22.35, 18.42; HRMS (EI): Calcd for $C_{19}H_{31}O_3$ $[M+H]^+$ 307.4460, found 307.4457.



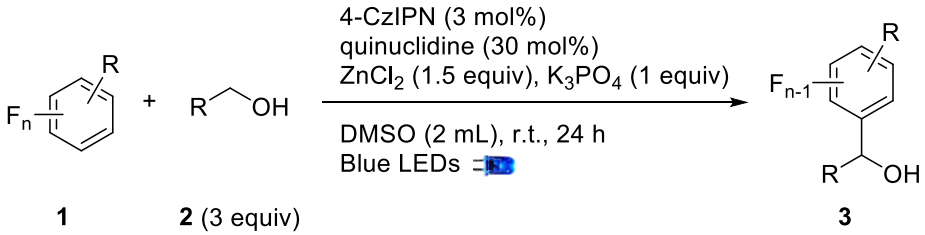
6-Hydroxyhexyl 4-(N,N-dipropylsulfamoyl)benzoate (S2): colorless oil (0.39 g, 20%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14 (d, *J* = 8.5 Hz, 2H), 7.86 (d, *J* = 8.5 Hz, 2H), 4.35 (t, *J* = 6.6 Hz, 2H), 3.65 (t, *J* = 6.5 Hz, 2H), 3.11 – 3.07 (m, 4H), 1.79 (p, *J* = 6.6 Hz, 2H), 1.66 (s, 1H), 1.64 – 1.42 (m, 10H), 0.86 (t, *J* = 7.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.31, 144.22, 133.74, 130.14, 126.98, 65.59, 62.76, 49.93, 32.56, 28.63, 25.80, 25.40, 21.92, 11.12; HRMS (EI): Calcd for $C_{19}H_{32}NO_5S$ $[M+H]^+$ 386.5190, found 386.5187.



6-Hydroxyhexyl 3-(4,5-diphenyloxazol-2-yl)propanoate (S3): colorless oil (0.70 g, 36%).^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63 (dd, *J* = 8.4, 1.7 Hz, 2H), 7.57 (dd, *J* = 8.1, 1.7 Hz, 2H), 7.39 – 7.29 (m, 6H), 4.13 (t, *J* = 6.7 Hz, 2H), 3.60 (t, *J* = 6.5 Hz, 2H), 3.18 (t, *J* = 7.5 Hz, 2H), 2.91 (t, *J* = 7.5 Hz, 2H), 1.68 – 1.49 (m, 5H), 1.36 (p, *J* = 3.5 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.09, 161.79, 145.37, 135.06, 132.39, 128.92, 128.62, 128.53, 128.44, 128.05, 127.87, 126.42, 64.80, 62.77, 32.51, 31.15, 28.52, 25.66, 25.31, 23.55; HRMS (EI): Calcd for $C_{24}H_{28}NO_4$ $[M+H]^+$ 394.4830, found 394.4836.

4. General Procedures for Defluoroalkylation of Polyfluoroarenes

4.1 General Procedures in Batch



1 **2** (3 equiv) **3**

In a 10 mL Schlenk tube with a magnetic stir bar were placed 4-CzIPN (**PC**, 4.8 mg, 0.006 mmol), quinuclidine (6.6 mg, 0.06 mmol), K_3PO_4 (42.4 mg, 0.2 mmol) and $ZnCl_2$ (41.0 mg, 0.3 mmol). Under nitrogen atmosphere, fluoroarenes (**1**, 0.2 mmol), alcohols (**2**, 0.6 mmol), DMSO (4 mL) were added, subsequently. The mixture was degassed *via* freeze-pump-thaw for three times, and irradiated under a blue LED (2-meter strips, 18 W, 456 nm) for 24 hrs at rt. The resulting mixture was quenched with H_2O (2 mL) and extracted with Et_2O (5 mL × 3). The combined organic layer was washed with saturated brine, dried over $MgSO_4$ and concentrated in vacuo. Silica gel chromatography (eluent: petroleum ether/EtOAc = 5/1) of the crude product afforded the desired compound.

4.2 General Procedures in Continuos-Flow

a) Reaction set up

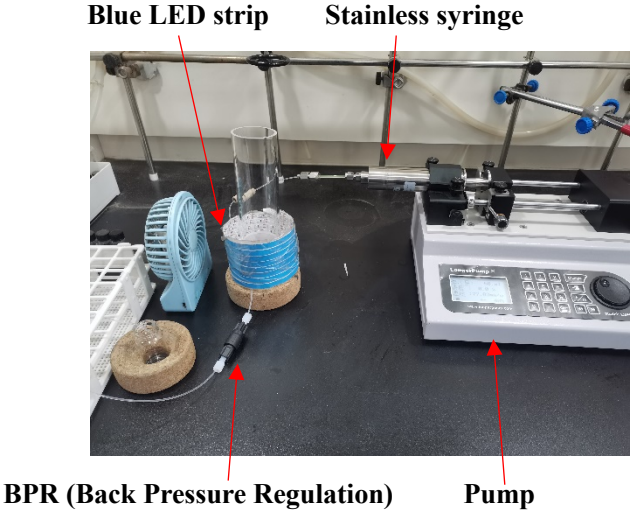
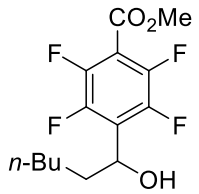


Figure S1. Continuous-flow setup

b) General procedures

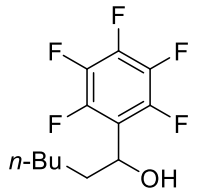
Under nitrogen atmosphere, a round bottom flask was equipped with a rubber septum and magnetic stir bar and charged with 4-CzIPN (PC, 7.9 mg, 0.01mmol), quinuclidine (22.2 mg, 0.2 mmol), $ZnCl_2$ (68.15 mg, 0.5 mmol), pentafluorobenzoate (**1a**, 226.1 mg, 1 mmol) and hexanol (**2a**, 153.3 mg, 1.5 mmol). The resulting mixture was sealed and degassed *via* vacuum evacuation and back-filled with nitrogen for three times. Then anhydrous DMSO (10 mL) was added, and bubbled with a nitrogen balloon for 10-15 min. As shown in Figure S1, a syringe pump was filled with the reaction mixture and attached to the flow apparatus with 5 psi back-pressure regulator (BPR). The tubing (PFA, O.D. = 1/16", I.D. 0.03", 877 cm, volume = 4.0 mL) was placed at rt. The flow apparatus itself was set up with t_R = 8 h, flow rate = 0.5 mL/h. After approximately 9 h of equilibration, the reacted solution was collected for 4 h. The resulting mixture was quenched with H_2O (2 mL) and extracted with Et_2O (5 mL × 3). The combined organic layer was washed with saturated brine, dried over $MgSO_4$ and concentrated in vacuo. Silica gel chromatography (eluent: petroleum ether/EtOAc = 5/1) of the crude product afforded the desired compound.

5. Analytical Data of the Products

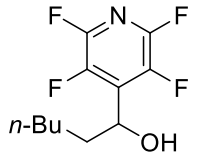


Methyl 2,3,5,6-tetrafluoro-4-(1-hydroxyhexyl)benzoate (3aa): The reaction was performed using 0.2 mmol of fluoroarenes and 0.3 mmol of alcohols; colorless oil (54 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.07 (q, *J* = 7.5 Hz, 1H), 3.97 (s, 3H), 2.33 (d, *J* = 8.1 Hz, 1H), 2.05 – 1.96 (m, 1H), 1.89 – 1.77 (m, 1H), 1.49 – 1.41 (m, 1H), 1.33 – 1.30 (m, 5H), 0.88 (t, *J* = 8.0 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.34 – -139.50 (m, 2F), -143.18 – -143.40 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.09 – 160.19 (m), 145.97 – 143.18 (m), 145.67 – 142.99 (m), 125.70 (t, *J* = 14.9 Hz), 111.38 (t, *J* = 16.0 Hz), 66.81, 53.30, 36.78, 31.30, 25.35, 22.44, 13.92; HRMS (EI): Calcd for

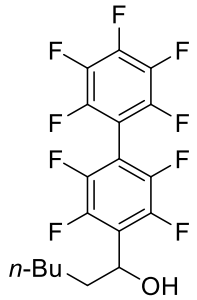
$C_{14}H_{17}O_3F_4$ $[M+H]^+$ 309.1114, found 309.1109.



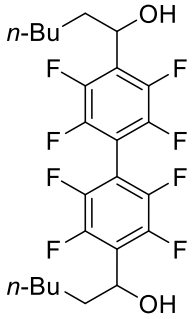
1-(Perfluorophenyl)hexan-1-ol (3ba): The reaction was performed using 0.2 mmol of fluoroarenes and 1 mmol of alcohols; white solid (49 mg, 91%); Mp. 48 – 49 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.03 (t, J = 7.3 Hz, 1H), 2.23 (s, 1H), 2.05 – 1.95 (m, 1H), 1.86 – 1.77 (m, 1H), 1.50 – 1.39 (m, 1H), 1.35 – 1.27 (m, 5H), 0.88 (t, J = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -144.05 (dd, J = 22.4, 8.1 Hz, 2F), -155.51 (td, J = 20.7, 4.2 Hz, 1F), -161.94 (tt, J = 18.5, 5.0 Hz, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.09 – 143.35 (m), 141.87 – 138.96 (m), 138.96 – 136.09 (m), 117.47 – 117.08 (m), 66.54 (q, J = 1.5 Hz), 36.97 (t, J = 1.8 Hz), 31.33, 25.49, 22.45, 13.90; HRMS (EI): Calcd for $C_{12}H_{14}OF_5$ $[M+H]^+$ 269.0965, found 269.0963.



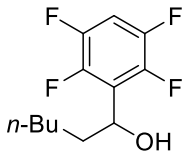
1-(Perfluoropyridin-4-yl)hexan-1-ol (3ca): The reaction was performed using 0.2 mmol of fluoroarenes and 1 mmol of alcohols; colorless oil (39 mg, 77%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.10 (t, J = 8.8 Hz, 1H), 2.31 (s, 1H), 2.06 – 1.96 (m, 1H), 1.89 – 1.76 (m, 1H), 1.54 – 1.41 (m, 1H), 1.37 – 1.27 (m, 5H), 0.89 (t, J = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -90.53 – -90.74 (m, 2F), -145.01 – -145.20 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.89 – 142.05 (m), 141.22 – 138.25 (m), 136.49 – 136.11 (m), 66.96, 36.53 (t, J = 1.4 Hz), 31.25, 25.19, 22.41, 13.91; HRMS (EI): Calcd for $C_{11}H_{13}NOF_4Na$ $[M+Na]^+$ 274.0831, found 274.0833.



1-(Perfluoro-[1,1'-biphenyl]-4-yl)hexan-1-ol (3da): The reaction was performed using 0.2 mmol of fluoroarenes and 0.3 mmol of alcohols; white solid (47 mg, 57%); Mp. 59 – 60 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.14 (q, *J* = 8.1 Hz, 1H), 2.26 (d, *J* = 8.2 Hz, 1H), 2.11 – 2.02 (m, 1H), 1.94 – 1.85 (m, 1H), 1.57 – 1.46 (m, 1H), 1.37 – 1.31 (m, 5H), 0.90 (t, *J* = 6.9 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -137.26 - -137.41 (m, 2F), -138.31 – -138.49 (m, 2F), -143.22 – -143.35 (m, 2F), -150.22 - -150.35 (m, 1F), -160.49 – -160.66 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.91 – 143.06 (m), 145.38 – 142.63 (m), 143.82 – 140.89 (m), 139.30 – 136.60 (m), 139.09 – 136.37 (m), 124.78 (t, *J* = 15.0 Hz), 105.36 – 104.75 (m), 102.59 – 102.05 (m), 66.96 (t, *J* = 1.8 Hz), 36.91 (t, *J* = 1.4 Hz), 31.35, 25.49, 22.47, 13.96; HRMS (EI): Calcd for $C_{18}H_{13}OF_9Na$ $[M+Na]^+$ 439.0720, found 439.0711.

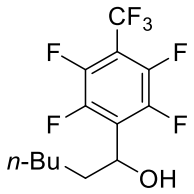


1,1'-(Perfluoro-[1,1'-biphenyl]-4,4'-diyl)bis(hexan-1-ol) (3ea): white solid (73 mg, 73%); Mp. 119 – 120 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.14 (q, *J* = 7.2 Hz, 1H), 2.26 (d, *J* = 7.9 Hz, 1H), 2.12 – 2.00 (m, 1H), 1.94 – 1.85 (m, 1H), 1.56 – 1.50 (m, 1H), 1.38 – 1.30 (m, 5H), 0.91 (t, *J* = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -138.26 – -138.41 (m, 4F), -143.50 – -143.66 (m, 4F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.86 – 143.01 (m), 145.43 – 142.56 (m), 124.46 (t, *J* = 15.0 Hz), 106.33 – 105.76 (m), 66.96, 36.92, 31.35, 25.49, 22.48, 13.97; HRMS (EI): Calcd for $C_{24}H_{27}O_2F_8$ $[M+H]^+$ 499.1883, found 499.1891.

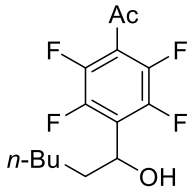


1-(2,3,5,6-Tetrafluorophenyl)hexan-1-ol (3fa): colorless oil (29 mg, 57%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.03 - 6.95 (m, 1H), 5.06 (q, *J* = 7.8 Hz, 1H), 2.18 (d, *J* = 8.6 Hz,

1H), 2.06 – 1.97 (m, 1H), 1.89 – 1.78 (m, 1H), 1.52 – 1.40 (m, 1H), 1.34 – 1.28 (m, 5H), 0.87 (t, J = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -138.92 - -139.03 (m, 2F), -144.68 - -144.80 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.32 – 144.18 (m), 145.87 – 142.74 (m), 123.12 (t, J = 14.7 Hz), 104.93 (t, J = 22.6 Hz), 66.92 (t, J = 1.9 Hz), 37.00 (t, J = 1.7 Hz), 31.35, 25.45, 22.47, 13.96; HRMS (EI): Calcd for $C_{12}H_{15}OF_4$ $[M+H]^+$ 251.1059, found 251.1064.

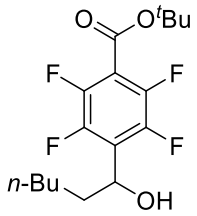


1-(2,3,5,6-Tetrafluoro-4-(trifluoromethyl)phenyl)hexan-1-ol (3ga): The reaction was performed using 0.2 mmol of fluoroarenes and 1 mmol of alcohols; white solid (50 mg, 78%); Mp. 51 – 52 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.09 (t, J = 7.3 Hz, 1H), 2.28 (s, 1H), 2.06 – 1.97 (m, 1H), 1.91 – 1.78 (m, 1H), 1.52 – 1.43 (m, 1H), 1.37 – 1.28 (m, 5H), 0.89 (t, J = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -56.40 (t, J = 21.7 Hz, 3F), -140.32 – -140.62 (m, 2F), -142.19 - -142.30 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.99 – 143.19 (m), 145.46 – 142.55 (m), 126.84 (t, J = 15.0 Hz), 120.71 (q, J = 274.6 Hz), 108.74 (q, J = 11.3 Hz), 66.81 (t, J = 1.8 Hz), 36.74 (t, J = 1.5 Hz), 31.29, 25.35, 22.44, 13.92; HRMS (EI): Calcd for $C_{13}H_{14}OF_7$ $[M+H]^+$ 319.0933, found 319.0926.

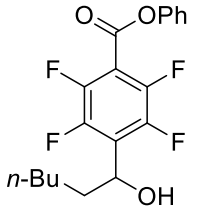


1-(2,3,5,6-Tetrafluoro-4-(1-hydroxyhexyl)phenyl)ethan-1-one (3ha): The reaction was performed using 0.2 mmol of fluoroarenes and 0.3 mmol of alcohols; colorless liquid (38 mg, 65%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.07 (q, J = 7.1 Hz, 1H), 2.62 (t, J = 1.8 Hz, 3H), 2.24 (d, J = 7.8 Hz, 1H), 2.06 – 1.96 (m, 1H), 1.89 – 1.76 (m, 1H), 1.50 – 1.42 (m, 1H), 1.37 – 1.28 (m, 5H), 0.89 (t, J = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -141.67 – -141.79 (m, 2F), -143.07 – -143.19 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.13 (t, J = 1.6 Hz), 145.80 – 143.00 (m), 145.21 – 142.35 (m), 125.30 (t,

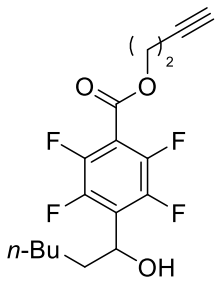
J = 15.1 Hz), 118.44 (t, J = 16.7 Hz), 66.81 (t, J = 1.7 Hz), 36.81 (t, J = 1.6 Hz), 32.42 (t, J = 2.4 Hz), 31.31, 25.37, 22.44, 13.93; HRMS (EI): Calcd for $C_{14}H_{17}O_2F_4$ $[M+H]^+$ 293.1165, found 293.1166.



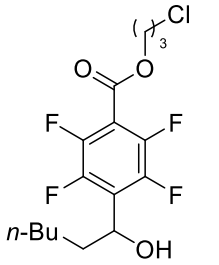
Tert-butyl 2,3,5,6-tetrafluoro-4-(1-hydroxyhexyl)benzoate (3ia): white solid (65 mg, 93%); Mp. 46 – 47 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.06 (t, J = 7.2 Hz, 1H), 2.24 (s, 1H), 2.05 – 1.94 (m, 1H), 1.86 -1.77 (m, 1H), 1.59 (s, 9H), 1.49 – 1.40 (m, 1H), 1.35 – 1.28 (m, 5H), 0.88 (t, J = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -140.95 – -141.06 (m, 2F), -143.66 – -143.82 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.58 – 158.45 (m), 145.70 – 142.99 (m), 145.48 – 142.71 (m), 124.62 (t, J = 15.0 Hz), 113.56 (t, J = 17.0 Hz), 84.69, 66.84 (t, J = 1.9 Hz), 36.91 (t, J = 1.4 Hz), 31.34, 28.06, 25.37, 22.45, 13.94; HRMS (EI): Calcd for $C_{17}H_{23}O_3F_4$ $[M+H]^+$ 351.1583, found 351.1581.



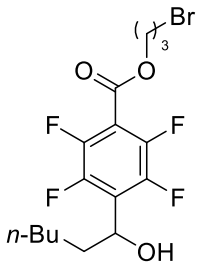
Phenyl 2,3,5,6-tetrafluoro-4-(1-hydroxyhexyl)benzoate (3ja): white solid (62 mg, 84%); Mp. 72 – 73 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48 – 7.42 (m, 2H), 7.34 – 7.29 (m, 1H), 7.27 – 7.23 (m, 2H), 5.12 (q, J = 7.7 Hz, 1H), 2.25 (d, J = 8.4 Hz, 1H), 2.08 – 1.99 (m, 1H), 1.91 – 1.82 (m, 1H), 1.53 – 1.42 (m, 1H), 1.39 – 1.28 (m, 5H), 0.90 (t, J = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -138.46 – -138.58 (m, 2F), -142.80 – -142.93 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.17 – 157.97 (m), 150.07, 146.29 – 143.42 (m), 145.88 – 143.11 (m), 129.68, 126.66, 126.38 (t, J = 15.0 Hz), 121.31, 111.07 (t, J = 15.3 Hz), 66.93 (t, J = 1.7 Hz), 36.88 (t, J = 1.5 Hz), 31.33, 25.38, 22.46, 13.94; HRMS (EI): Calcd for $C_{19}H_{18}O_3F_4Na$ $[M+Na]^+$ 393.1090, found 393.1095.



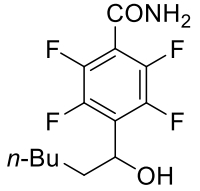
But-3-yn-1-yl 2,3,5,6-tetrafluoro-4-(1-hydroxyhexyl)benzoate (3ka): colorless oil (47 mg, 68%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.07 (q, *J* = 7.6 Hz, 1H), 4.49 (t, *J* = 6.8 Hz, 2H), 2.67 (td, *J* = 6.8, 2.7 Hz, 2H), 2.25 (d, *J* = 8.3 Hz, 1H), 2.05 (t, *J* = 2.6 Hz, 1H), 2.03 – 1.95 (m, 1H), 1.87 – 1.77 (m, 1H), 1.51 – 1.41 (m, 1H), 1.37 – 1.27 (m, 5H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -138.98 – -139.11 (m, 2F), -143.11 – -143.25 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.44 – 159.28 (m), 146.30 – 143.19 (m), 145.76 – 142.92 (m), 125.84 (t, *J* = 15.1 Hz), 111.26 (t, *J* = 15.6 Hz), 79.18, 70.38, 66.86 (t, *J* = 1.8 Hz), 64.04, 36.85 (t, *J* = 1.8 Hz), 31.31, 25.36, 22.45, 18.86, 13.94; HRMS (EI): Calcd for $C_{17}H_{19}O_3F_4$ $[M+H]^+$ 347.1270, found 347.1272.



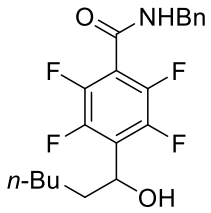
3-Chloropropyl 2,3,5,6-tetrafluoro-4-(1-hydroxyhexyl)benzoate (3la): colorless oil (62 mg, 84%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.08 (q, *J* = 7.5 Hz, 1H), 4.55 (t, *J* = 5.9 Hz, 2H), 3.69 (t, *J* = 6.3 Hz, 2H), 2.26 – 2.18 (m, 3H), 2.06 – 1.96 (m, 1H), 1.88 – 1.76 (m, 1H), 1.52 – 1.40 (m, 1H), 1.36 – 1.29 (m, 5H), 0.88 (t, *J* = 6.9 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.20 – -139.33 (m, 2F), -143.05 – -143.17 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.52 – 159.35 (m), 146.15 – 143.26 (m), 145.78 – 142.96 (m), 125.87 (t, *J* = 15.1 Hz), 111.29 (t, *J* = 15.5 Hz), 66.86 (t, *J* = 1.9 Hz), 63.10, 40.78, 36.84 (t, *J* = 1.7 Hz), 31.31, 31.25, 25.36, 22.45, 13.94; HRMS (EI): Calcd for $C_{16}H_{20}O_3F_4Cl$ $[M+H]^+$ 371.1037, found 371.1028.



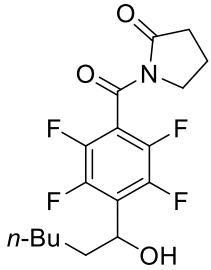
3-Bromopropyl 2,3,5,6-tetrafluoro-4-(1-hydroxyhexyl)benzoate (3ma): colorless oil (61 mg, 74%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.08 (q, *J* = 7.7 Hz, 1H), 4.56 – 4.52 (m, 2H), 3.69 (t, *J* = 6.3 Hz, 1H), 3.54 (t, *J* = 6.4 Hz, 1H), 2.33 – 2.27 (m, 1H), 2.26 – 2.19 (m, 2H), 2.06 – 1.96 (m, 1H), 1.89 – 1.76 (m, 1H), 1.51 – 1.40 (m, 1H), 1.37 – 1.28 (m, 5H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.16 – -139.32 (m, 2F), -143.03 – -143.19 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.49 – 159.36 (m), 146.16 – 143.26 (m), 145.88 – 143.03 (m), 125.80 (t, *J* = 15.0 Hz), 111.26 (t, *J* = 15.0 Hz), 66.88 (t, *J* = 1.9 Hz), 64.11, 40.79, 36.86 (t, *J* = 1.8 Hz), 31.31, 28.93, 25.36, 22.45, 13.95; HRMS (EI): Calcd for $C_{16}H_{20}O_3F_4Br$ $[M+H]^+$ 415.0532, found 415.0522.



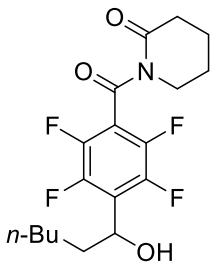
2,3,5,6-Tetrafluoro-4-(1-hydroxyhexyl)benzamide (3na): white solid (42 mg, 72%); Mp. 98 – 99 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 5.04 (t, *J* = 7.3 Hz, 1H), 2.04 – 1.95 (m, 1H), 1.87 – 1.77 (m, 1H), 1.49 – 1.39 (m, 1H), 1.36 – 1.26 (m, 5H), 0.89 (t, *J* = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, CD_3OD): δ -144.88 – -145.15 (m, 4F); ^{13}C NMR (100 MHz, CD_3OD): δ 162.78 (t, *J* = 2.6 Hz), 147.25 – 144.29 (m), 145.90 – 142.90 (m), 125.65 (t, *J* = 15.2 Hz), 117.31 – 116.73 (m), 66.72 (t, *J* = 1.8 Hz), 36.96 (t, *J* = 2.0 Hz), 32.62, 26.72, 23.59, 14.31; HRMS (EI): Calcd for $C_{13}H_{16}NO_2F_4$ $[M+H]^+$ 294.1117, found 294.1124.



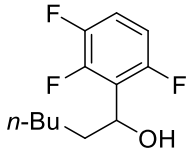
N-benzyl-2,3,5,6-tetrafluoro-4-(1-hydroxyhexyl)benzamide (3oa): yellow solid (73 mg, 95%); Mp. 76 – 77 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39 – 7.28 (m, 5H), 6.38 (s, 1H), 5.04 (t, *J* = 7.3 Hz, 1H), 4.64 (d, *J* = 5.7 Hz, 2H), 2.39 (s, 1H), 2.06 – 1.93 (m, 1H), 1.86 – 1.74 (m, 1H), 1.48 – 1.38 (m, 1H), 1.35 – 1.27 (m, 5H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -141.21 - -141.32 (m, 2F), -142.84 – -142.96 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.10 (t, *J* = 2.6 Hz), 145.79 – 142.96 (m), 144.97 – 142.21 (m), 136.87, 128.87, 127.89, 127.75, 124.48 (t, *J* = 15.1 Hz), 114.88 (t, *J* = 18.4 Hz), 66.74 (t, *J* = 1.6 Hz), 44.26, 36.79 (t, *J* = 1.5 Hz), 31.32, 25.36, 22.43, 13.91; HRMS (EI): Calcd for $C_{20}H_{22}NO_2F_4$ $[M+H]^+$ 384.1587, found 384.1586.



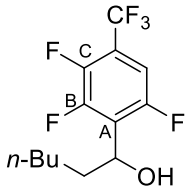
1-(2,3,5,6-Tetrafluoro-4-(1-hydroxyhexyl)benzoyl)pyrrolidin-2-one (3pa): colorless oil (67 mg, 93%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.07 (q, *J* = 7.5 Hz, 1H), 4.01 (t, *J* = 7.3 Hz, 2H), 2.64 (t, *J* = 8.1 Hz, 2H), 2.21 – 2.14 (m, 3H), 2.05 – 1.96 (m, 1H), 1.88 – 1.79 (m, 1H), 1.51 – 1.42 (m, 1H), 1.37 – 1.27 (m, 5H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -142.61 – -142.74 (m, 2F), -143.86 – -144.00 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.11, 158.07 – 157.97 (m), 145.55 – 142.62 (m), 144.30 – 141.51 (m), 124.20 (t, *J* = 15.0 Hz), 115.10 (t, *J* = 18.2 Hz), 66.87 (t, *J* = 1.8 Hz), 45.39, 36.85 (t, *J* = 1.6 Hz), 32.77, 31.35, 25.42, 22.45, 17.22, 13.94; HRMS (EI): Calcd for $C_{17}H_{20}NO_3F_4$ $[M+H]^+$ 362.1379, found 362.1382.



1-(2,3,5,6-Tetrafluoro-4-(1-hydroxyhexyl)benzoyl)piperidin-2-one (3qa): colorless oil (73 mg, 98%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.05 (q, *J* = 7.3 Hz, 1H), 3.90 (t, *J* = 5.9 Hz, 2H), 2.57 (t, *J* = 6.4 Hz, 2H), 2.18 (d, *J* = 8.2 Hz, 1H), 2.03 – 1.89 (m, 5H), 1.86 – 1.77 (m, 1H), 1.52 – 1.41 (m, 1H), 1.36 – 1.27 (m, 5H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -144.00 – -144.26 (m, 4F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.68, 161.04 – 160.95 (m), 145.63 – 142.72 (m), 143.86 – 140.91 (m), 123.46 – 123.13 (m), 117.52 – 117.18 (m), 66.81 (t, *J* = 1.8 Hz), 45.01, 36.86 (t, *J* = 1.5 Hz), 34.21, 31.36, 25.44, 22.45, 22.31, 20.47, 13.96; HRMS (EI): Calcd for $C_{18}H_{21}NO_3F_4Na$ $[M+Na]^+$ 398.1355, found 398.1345.

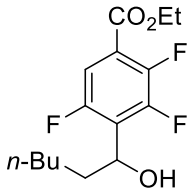


1-(2,3,6-Trifluorophenyl)hexan-1-ol (3ra): white solid (10 mg, 22%); Mp. 79 – 80 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.09 – 7.01 (m, 1H), 6.85 – 6.78 (m, 1H), 5.03 (q, *J* = 7.6 Hz, 1H), 2.18 (d, *J* = 8.3 Hz, 1H), 2.04 – 1.95 (m, 1H), 1.88 – 1.78 (m, 1H), 1.50 – 1.41 (m, 1H), 1.34 – 1.28 (m, 5H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -120.55 – -120.64 (m, 1F), -138.79 (dd, *J* = 21.1, 8.6 Hz, 1F), -142.07 – -142.20 (m, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.21 (dd, *J* = 6.3, 2.5 Hz), 154.78 (dd, *J* = 7.0, 2.7 Hz), 149.82 – 147.00 (m), 148.47 – 145.86 (m), 115.73 (ddd, *J* = 19.5, 10.6, 1.5 Hz), 111.02 (ddd, *J* = 25.2, 6.3, 4.3 Hz), 66.81 (q, *J* = 1.8 Hz), 37.12 (t, *J* = 1.4 Hz), 31.40, 25.50, 22.49, 13.97; HRMS (EI): Calcd for $C_{12}H_{16}OF_3$ $[M+H]^+$ 233.1153, found 233.1148.

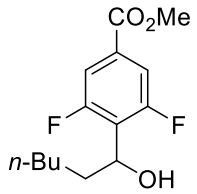


91% (A:B:C = 78:21:1)

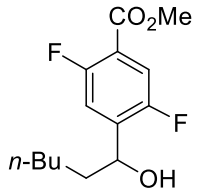
1-(2,3,6-trifluoro-4-(trifluoromethyl)phenyl)hexan-1-ol (3sa): colorless oil (55 mg, 91%). Major component: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.12 (ddd, *J* = 9.7, 5.0, 2.2 Hz, 1H), 5.06 (t, *J* = 7.6 Hz, 1H), 2.30 (s, 1H), 2.07 – 1.96 (m, 1H), 1.88 – 1.77 (m, 1H), 1.52 – 1.39 (m, 1H), 1.36 – 1.28 (m, 5H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -61.38 (d, *J* = 12.9 Hz, 3F), -117.73 (ddd, *J* = 14.5, 9.4, 4.1 Hz, 1F), -135.40 (d, *J* = 20.4 Hz, 1F), -142.77 – -143.00 (m, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.16 (ddd, *J* = 247.0, 7.2, 3.6 Hz), 149.11 (ddd, *J* = 252.5, 13.5, 9.0 Hz), 146.38 – 143.54 (m), 126.06 (dd, *J* = 18.4, 13.5 Hz), 121.34 (qt, *J* = 271.2, 3.3 Hz), 119.53 (qt, *J* = 50.4, 2.8 Hz), 109.00 (dp, *J* = 28.7, 4.3 Hz), 66.69 (d, *J* = 1.5 Hz), 36.84 (t, *J* = 1.5 Hz), 31.34, 25.40, 22.45, 13.91; HRMS (EI): Calcd for $C_{13}H_{15}OF_6$ $[M+H]^+$ 301.2444, found 301.2446.



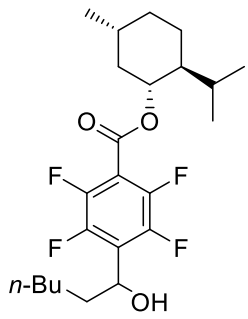
Ethyl 2,3,5-trifluoro-4-(1-hydroxyhexyl)benzoate (3ta): colorless oil (57 mg, 93%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42 (ddd, *J* = 10.4, 5.1, 2.3 Hz, 1H), 5.04 (q, *J* = 7.6 Hz, 1H), 4.40 (q, *J* = 7.2 Hz, 2H), 2.24 (d, *J* = 8.6 Hz, 1H), 2.04 – 1.95 (m, 1H), 1.87 – 1.76 (m, 1H), 1.51 – 1.43 (m, 1H), 1.40 (t, *J* = 7.1 Hz, 3H), 1.34 – 1.27 (m, 5H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -119.71 (ddd, *J* = 15.1, 10.3, 3.3 Hz, 1F), -136.83 (dt, *J* = 19.9, 2.9 Hz, 1F), -138.82 (ddd, *J* = 20.5, 15.9, 5.1 Hz, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.50 – 162.37 (m), 156.29 – 153.61 (m), 150.55 – 147.66 (m), 148.61 – 145.74 (m), 126.18 (dd, *J* = 18.7, 13.9 Hz), 119.36 (t, *J* = 9.2 Hz), 112.83 (dd, *J* = 26.9, 3.8 Hz), 66.83 – 66.75 (m), 62.06, 36.92(t, *J* = 1.5 Hz), 31.35, 25.39, 22.46, 14.14, 13.94; HRMS (EI): Calcd for $C_{15}H_{20}O_3F_3$ $[M+H]^+$ 305.1365, found 305.1361.



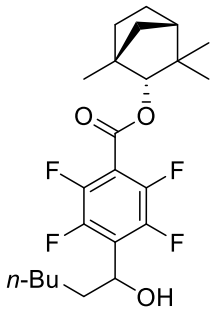
Methyl 3,5-difluoro-4-(1-hydroxyhexyl)benzoate (3ua): colorless oil (52 mg, 95%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 – 7.50 (m, 2H), 5.05 (t, *J* = 7.3 Hz, 1H), 3.92 (s, 3H), 2.27 (s, 1H), 2.03 – 1.94 (m, 1H), 1.86 – 1.77 (m, 1H), 1.49 – 1.41 (m, 1H), 1.35 – 1.27 (m, 5H), 0.87 (t, *J* = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -113.75 (d, *J* = 8.2 Hz, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.78 (t, *J* = 3.3 Hz), 160.55 (dd, *J* = 248.7, 8.8 Hz), 131.29 (t, *J* = 10.0 Hz), 124.68 (t, *J* = 16.9 Hz), 113.17 – 112.80 (m), 66.65 (t, *J* = 2.3 Hz), 52.65, 37.10 (t, *J* = 1.4 Hz), 31.39, 25.45, 22.47, 13.93; HRMS (EI): Calcd for $C_{14}H_{18}O_3F_2Na$ $[M+Na]^+$ 295.1122, found 295.1120.



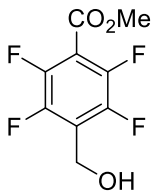
Methyl 2,5-difluoro-4-(1-hydroxyhexyl)benzoate (3va): colorless oil (24 mg, 44%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 – 7.55 (m, 1H), 7.33 – 7.28 (m, 1H), 5.01 (t, *J* = 8.4 Hz, 1H), 3.93 (s, 3H), 2.03 (s, 1H), 1.78 – 1.70 (m, 2H), 1.50 – 1.40 (m, 1H), 1.38 – 1.27 (m, 5H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -114.14 – -114.24 (m, 1F), -124.29 – -124.43 (m, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.80 (dd, *J* = 4.2, 2.1 Hz), 158.18 (dd, *J* = 256.9, 2.2 Hz), 154.62 (dd, *J* = 242.7, 2.5 Hz), 139.39 (dd, *J* = 16.3, 7.8 Hz), 118.09 (dd, *J* = 26.5, 1.7 Hz), 117.93 (t, *J* = 10.1 Hz), 115.64 (dd, *J* = 26.2, 4.9 Hz), 67.81 (t, *J* = 1.1 Hz), 52.52, 37.88, 31.48, 25.01, 22.49, 13.95; HRMS (EI): Calcd for $C_{14}H_{19}O_3F_2$ $[M+H]^+$ 273.1302, found 273.1302.



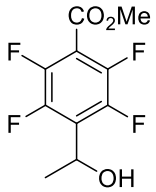
(1R,2S,5R)-2-isopropyl-5-methylcyclohexyl 2,3,5,6-tetrafluoro-4-(1-hydroxyhexyl)benzoate (3wa): colorless oil (43 mg, 50%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.07 (q, *J* = 7.7 Hz, 1H), 4.98 (td, *J* = 10.9, 4.4 Hz, 1H), 2.25 (d, *J* = 8.4 Hz, 1H), 2.19 – 2.12 (m, 1H), 2.05 – 1.94 (m, 2H), 1.87 – 1.77 (m, 1H), 1.76 – 1.69 (m, 2H), 1.59 – 1.40 (m, 4H), 1.37 – 1.27 (m, 6H), 1.17 – 1.04 (m, 3H), 0.94 (d, *J* = 6.5 Hz, 3H), 0.91 (d, *J* = 7.0 Hz, 4H), 0.80 (d, *J* = 7.0 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -140.00 – -140.13 (m, 2F), -143.39 – -143.52 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.33 – 159.23 (m), 145.76 – 142.96 (m), 145.47 – 142.80 (m), 125.01 (t, *J* = 15.0 Hz), 112.54 (t, *J* = 16.8 Hz), 66.85 (t, *J* = 1.8 Hz), 46.82, 40.57, 36.89 (t, *J* = 1.5 Hz), 34.03, 31.47, 31.33, 25.85, 25.37, 23.02, 22.46, 21.95, 20.80, 15.85, 13.96; HRMS (EI): Calcd for $C_{23}H_{33}O_3F_4$ $[M+H]^+$ 433.2366, found 433.2357.



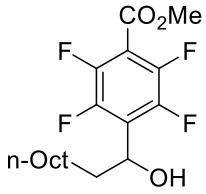
(1R,2R,4S)-1,3,3-trimethylbicyclo[2.2.1]heptan-2-yl 2,3,5,6-tetrafluoro-4-(1-hydroxyhexyl)benzoate (3xa): colorless oil (77 mg, 89%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.08 (q, *J* = 8.0 Hz, 1H), 4.63 (d, *J* = 2.0 Hz, 1H), 2.25 (d, *J* = 8.2 Hz, 1H), 2.06 – 1.97 (m, 1H), 1.88 – 1.82 (m, 1H), 1.81 – 1.59 (m, 5H), 1.53 – 1.42 (m, 2H), 1.38 – 1.23 (m, 8H), 1.19 (s, 3H), 1.11 (s, 3H), 0.89 (s, 1H), 0.87 (s, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.28 – -139.40 (m, 2F), -143.37 – -143.49 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.11 – 159.98 (m), 146.01 – 143.24 (m), 145.72 – 143.00 (m), 125.33 (t, *J* = 15.2 Hz), 112.06 (t, *J* = 16.1 Hz), 89.56, 66.89, 48.45, 48.34, 41.34, 39.59, 36.89, 31.34, 29.64, 26.61, 25.71, 25.40, 22.45, 20.13, 19.20, 13.94; HRMS (EI): Calcd for $C_{23}H_{30}O_3F_4Na$ $[M+Na]^+$ 453.2029, found 453.2036.



Methyl 2,3,5,6-tetrafluoro-4-(hydroxymethyl)benzoate (3ab): The reaction was performed using 0.2 mmol of fluoroarenes and 1 mmol of alcohols; colorless oil (23 mg, 49%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.84 (s, 2H), 3.99 (s, 3H), 2.12 (s, 1H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.24 – -139.34 (m, 2F), -143.40 – -143.51 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.09 – 160.03 (m), 146.31 – 143.59 (m), 145.88 – 143.08 (m), 121.63 (t, J = 17.6 Hz), 112.45 (t, J = 16.2 Hz), 53.34, 53.00 – 52.90 (m); HRMS (EI): Calcd for $C_9H_7O_3F_4$ $[M+H]^+$ 239.0331, found 239.0332.

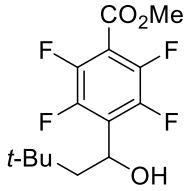


Methyl 2,3,5,6-tetrafluoro-4-(1-hydroxyethyl)benzoate (3ac): The reaction was performed using 0.2 mmol of fluoroarenes and 1 mmol of alcohols; colorless oil (46 mg, 92%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.29 (p, J = 6.9 Hz, 1H), 3.98 (s, 3H), 2.31 (d, J = 7.8 Hz, 1H), 1.66 (d, J = 6.7 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.27 – -139.43 (m, 2F), -143.81 – -143.95 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.14 – 160.04 (m), 146.04 – 143.17 (m), 145.64 – 142.92 (m), 126.26 (t, J = 14.8 Hz), 111.50 (t, J = 15.8 Hz), 62.66 (t, J = 1.5 Hz), 53.28, 23.02 (t, J = 1.0 Hz); HRMS (EI): Calcd for $C_{10}H_8O_3F_4Na$ $[M+Na]^+$ 275.0307, found 275.0316.

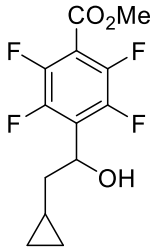


Methyl 2,3,5,6-tetrafluoro-4-(1-hydroxydecyl)benzoate (3ad): The reaction was performed using 0.2 mmol of fluoroarenes and 0.3 mmol of alcohols; colorless oil (64 mg, 88%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.07 (t, J = 7.3 Hz, 1H), 3.98 (s, 3H), 2.24 (s, 1H), 2.05 – 1.96 (m, 1H), 1.87 – 1.77 (m, 1H), 1.49 – 1.40 (m, 1H), 1.34 – 1.21 (m, 13H), 0.87 (t, J = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.31 – -139.47 (m, 2F), -143.18 – -143.33 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.17 – 160.08 (m), 146.00 – 143.19 (m), 145.69 – 143.03 (m), 125.70 (t, J = 15.0 Hz), 111.47 (t, J = 16.0 Hz), 66.88, 53.28, 36.89, 31.82, 29.44, 29.39, 29.23, 29.15, 25.69, 22.64, 14.07; HRMS

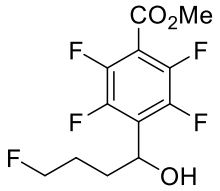
(EI): Calcd for $C_{18}H_{24}O_3F_4Na$ $[M+Na]^+$ 387.1559, found 387.1562.



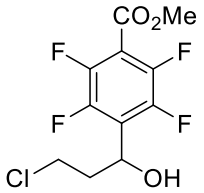
Methyl 2,3,5,6-tetrafluoro-4-(1-hydroxy-3,3-dimethylbutyl)benzoate (3ae): colorless oil (52 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.25 (td, *J* = 8.3, 4.0 Hz, 1H), 3.97 (s, 3H), 2.14 (d, *J* = 8.5 Hz, 1H), 1.99 (ddt, *J* = 14.6, 8.3, 1.4 Hz, 1H), 1.71 (dd, *J* = 14.6, 4.1 Hz, 1H), 1.00 (s, 9H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.20 – -139.33 (m, 2F), -143.45 – -143.57 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.14 – 160.09 (m), 146.08 – 143.27 (m), 145.51 – 142.80 (m), 126.99 (t, *J* = 15.1 Hz), 111.35 (t, *J* = 15.8 Hz), 64.39 (t, *J* = 1.5 Hz), 53.25, 50.75, 30.64, 29.75; HRMS (EI): Calcd for $C_{14}H_{16}O_3F_4Na$ $[M+Na]^+$ 331.0933, found 331.0933.



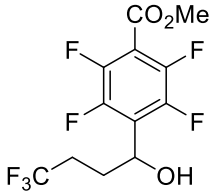
Methyl 4-(2-cyclopropyl-1-hydroxyethyl)-2,3,5,6-tetrafluorobenzoate (3af): The reaction was performed using 0.2 mmol of fluoroarenes and 0.3 mmol of alcohols; colorless oil (46 mg, 78%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.21 (q, *J* = 7.0 Hz, 1H), 3.98 (s, 3H), 2.39 (d, *J* = 7.8 Hz, 1H), 2.00 (dt, *J* = 13.9, 7.0 Hz, 1H), 1.70 (dt, *J* = 14.2, 7.2 Hz, 1H), 0.74 – 0.64 (m, 1H), 0.57 – 0.48 (m, 1H), 0.47 – 0.38 (m, 1H), 0.18 – 0.12 (m, 1H), 0.03 – -0.03 (m, 1H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.43 – -139.56 (m, 2F), -142.99 – -143.13 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.24 – 160.02 (m), 145.98 – 143.32 (m), 145.79 – 143.13 (m), 125.59 (t, *J* = 15.0 Hz), 111.51 (t, *J* = 15.9 Hz), 67.22 (t, *J* = 1.5 Hz), 53.27, 41.60, 7.21, 4.14, 3.98; HRMS (EI): Calcd for $C_{13}H_{13}O_3F_4$ $[M+H]^+$ 293.0801, found 293.0796.



Methyl 2,3,5,6-tetrafluoro-4-(4-fluoro-1-hydroxybutyl)benzoate (3ag): colorless oil (36 mg, 60%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.13 (q, *J* = 7.9 Hz, 1H), 4.60 – 4.54 (m, 1H), 4.48 – 4.42 (m, 1H), 3.98 (s, 3H), 2.36 (d, *J* = 8.1 Hz, 1H), 2.20 – 2.12 (m, 1H), 2.01 – 1.91 (m, 2H), 1.80 – 1.68 (m, 1H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -140.02 – -140.13 (m, 2F), -142.59 – -142.69 (m, 2F), -217.52 – -217.90 (m, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.01 – 159.96 (m), 146.06 – 143.24 (m), 145.73 – 143.01 (m), 125.10 (t, *J* = 15.0 Hz), 111.85 (t, *J* = 16.1 Hz), 83.27 (d, *J* = 165.7 Hz), 66.41 (t, *J* = 1.5 Hz), 53.31, 32.77 (d, *J* = 4.4 Hz), 26.91 (d, *J* = 20.1 Hz); HRMS (EI): Calcd for $C_{12}H_{11}O_3F_5Na$ $[M+Na]^+$ 321.0526, found 321.0534.

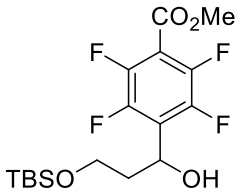


Methyl 4-(3-chloro-1-hydroxypropyl)-2,3,5,6-tetrafluorobenzoate (3ah): colorless oil (26 mg, 44%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.43 – 5.38 (m, 1H), 3.98 (s, 3H), 3.82 – 3.76 (m, 1H), 3.68 – 3.63 (m, 1H), 2.58 – 2.49 (m, 1H), 2.41 (d, *J* = 6.8 Hz, 1H), 2.23 – 2.13 (m, 1H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -138.76 – -138.91 (m, 2F), -142.58 – -142.74 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.96 – 159.92 (m), 146.06 – 143.29 (m), 145.79 – 143.12 (m), 124.28 (t, *J* = 14.9 Hz), 112.13 (t, *J* = 15.7 Hz), 63.44 (t, *J* = 1.9 Hz), 53.37, 40.76, 38.60 (t, *J* = 2.0 Hz); HRMS (EI): Calcd for $C_{11}H_{10}O_3F_4Cl$ $[M+H]^+$ 301.0255, found 301.0249.

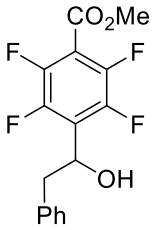


Methyl 2,3,5,6-tetrafluoro-4-(4,4,4-trifluoro-1-hydroxybutyl)benzoate (3ai): colorless oil (47 mg, 70%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.13 (td, *J* = 8.4, 4.7 Hz,

1H), 3.99 (s, 3H), 2.45 – 2.36 (m, 2H), 2.34 – 2.14 (m, 2H), 2.09 – 2.00 (m, 1H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -66.23 (t, *J* = 10.3 Hz, 3F), -138.49 – -138.62 (m, 2F), -142.89 – -143.05 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.87 – 159.77 (m), 146.11 – 143.26 (m), 145.70 – 142.91 (m), 126.69 (q, *J* = 274.4 Hz), 124.10 (t, *J* = 14.8 Hz), 112.33 (t, *J* = 15.9 Hz), 65.29 (t, *J* = 2.1 Hz), 53.40, 30.49 (q, *J* = 29.6 Hz), 29.10 (q, *J* = 2.2 Hz); HRMS (EI): Calcd for $C_{12}H_{10}O_3F_7$ $[M+H]^+$ 335.0518, found 335.0516.

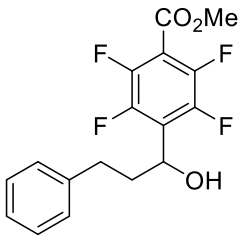


Methyl 4-(3-((tert-butyldimethylsilyl)oxy)-1-hydroxypropyl)-2,3,5,6-tetrafluorobenzoate (3aj): The reaction was performed using 0.2 mmol of fluoroarenes and 0.3 mmol of alcohols; colorless oil (59 mg, 75%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.38 (dt, *J* = 8.7, 4.2 Hz, 1H), 3.97 (s, 3H), 3.95 – 3.89 (m, 1H), 3.87 – 3.81 (m, 1H), 3.68 (d, *J* = 5.0 Hz, 1H), 2.32 – 2.23 (m, 1H), 1.98 – 1.91 (m, 1H), 0.90 (s, 9H), 0.09 (d, *J* = 2.1 Hz, 6H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.65 – -139.86 (m, 2F), -142.56 – -142.82 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.20 – 160.12 (m), 146.02 – 143.35 (m), 145.85 – 143.21 (m), 125.32 (t, *J* = 14.6 Hz), 111.48 (t, *J* = 15.8 Hz), 66.05, 61.36, 53.21, 37.84, 25.74, 18.07, -5.63 (d, *J* = 0.6 Hz); HRMS (EI): Calcd for $C_{17}H_{24}O_4F_4NaSi$ $[M+Na]^+$ 419.1278, found 419.1280.

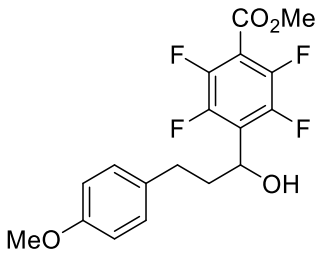


Methyl 2,3,5,6-tetrafluoro-4-(1-hydroxy-2-phenylethyl)benzoate (3ak): The reaction was performed using 0.2 mmol of fluoroarenes and 0.3 mmol of alcohols; white solid (33 mg, 51%); Mp. 85 – 86 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33 – 7.29 (m, 2H), 7.27 – 7.25 (m, 1H), 7.17 (d, *J* = 6.7 Hz, 2H), 5.33 (q, *J* = 7.2 Hz, 1H), 3.97 (s, 3H), 3.32 (dd, *J* = 13.5, 8.0 Hz, 1H), 3.12 (dd, *J* = 13.5, 6.4 Hz, 1H), 2.39 (d, *J* = 7.2 Hz, 1H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.19 – -139.42 (m, 2F), -142.61 – -142.80

(m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.11 – 159.99 (m), 145.97 – 143.20 (m), 145.72 – 143.05 (m), 135.97, 129.16, 128.79, 127.25, 124.57 (t, *J* = 14.8 Hz), 111.71 (t, *J* = 15.8 Hz), 67.70 (t, *J* = 1.5 Hz), 53.28, 42.97 (t, *J* = 1.5 Hz); HRMS (EI): Calcd for $C_{16}H_{12}O_3F_4Na$ $[M+Na]^+$ 351.0620, found 351.0629.

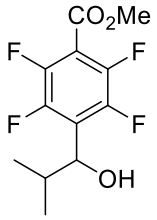


Methyl 2,3,5,6-tetrafluoro-4-(1-hydroxy-3-phenylpropyl)benzoate (3al): The reaction was performed using 0.2 mmol of fluoroarenes and 0.3 mmol of alcohols; white solid (39 mg, 57%); Mp. 63 – 64 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29 (t, *J* = 7.2 Hz, 2H), 7.22 – 7.16 (m, 3H), 5.10 (q, *J* = 7.1 Hz, 1H), 3.98 (s, 3H), 2.88 – 2.81 (m, 1H), 2.71 – 2.63 (m, 1H), 2.41 – 2.33 (m, 1H), 2.31 (d, *J* = 10.3 Hz, 1H), 2.21 – 2.11 (m, 1H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.12 – -139.36 (m, 2F), -142.88 – -143.06 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.09 – 159.99 (m), 146.00 – 143.20 (m), 145.74 – 142.99 (m), 140.30, 128.53, 128.28, 126.26, 125.28 (t, *J* = 15.0 Hz), 111.67 (t, *J* = 15.8 Hz), 66.16 (t, *J* = 1.8 Hz), 53.30, 38.05 (t, *J* = 1.8 Hz), 31.94; HRMS (EI): Calcd for $C_{17}H_{14}O_3F_4Na$ $[M+Na]^+$ 365.0777, found 365.0777.

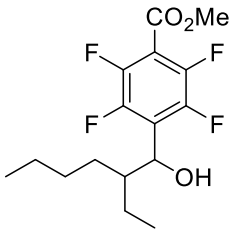


Methyl 2,3,5,6-tetrafluoro-4-(1-hydroxy-3-(4-methoxyphenyl)propyl)benzoate (3am): The reaction was performed using 0.2 mmol of fluoroarenes and 0.3 mmol of alcohols; colorless oil (31 mg, 41%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.09 (d, *J* = 8.6 Hz, 2H), 6.82 (d, *J* = 8.6 Hz, 2H), 5.09 (t, *J* = 7.2 Hz, 1H), 3.98 (s, 3H), 3.78 (s, 3H), 2.82 – 2.74 (m, 1H), 2.67 – 2.55 (m, 1H), 2.39 – 2.07 (m, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.21 – -139.33 (m, 2F), -142.88 – -143.05 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.08 – 160.02 (m), 158.07, 146.00 – 143.19 (m), 145.68 – 143.01 (m),

132.30, 129.20, 125.36 (t, J = 15.0 Hz), 113.94, 111.62 (t, J = 16.1 Hz), 66.13 (t, J = 1.9 Hz), 55.25, 53.28, 38.26, 31.03; HRMS (EI): Calcd for $C_{18}H_{17}F_4O_4$ $[M+H]^+$ 373.3156, found 373.3158.

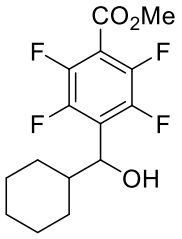


Methyl 2,3,5,6-tetrafluoro-4-(1-hydroxy-2-methylpropyl)benzoate (3an): colorless oil (49 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.68 (d, J = 9.0 Hz, 1H), 3.98 (s, 3H), 2.26 (s, 1H), 2.22 – 2.10 (m, 1H), 1.15 (d, J = 6.6 Hz, 3H), 0.81 (d, J = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.37 – -139.49 (m, 2F), -142.06 – -142.18 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.15 – 160.10 (m), 145.96 – 143.24 (m), 145.71 – 143.08 (m), 125.11 (t, J = 15.2 Hz), 111.51 (t, J = 16.1 Hz), 72.75, 53.29, 34.27 (t, J = 1.6 Hz), 19.11, 18.66; HRMS (EI): Calcd for $C_{12}H_{12}O_3F_4Na$ $[M+Na]^+$ 303.0620, found 303.0622.

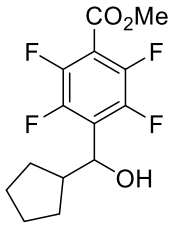


Methyl 4-(2-ethyl-1-hydroxyhexyl)-2,3,5,6-tetrafluorobenzoate (dr = 1:1) (3ao): The reaction was performed using 0.2 mmol of fluoroarenes and 0.3 mmol of alcohols; colorless oil (33 mg, 49%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.93 (t, J = 8.6 Hz, 1H), 3.98 (s, 3H), 2.24 (d, J = 8.8 Hz, 1H), 1.92 – 1.84 (m, 1H), 1.67 – 1.59 (m, 2H), 1.39 – 1.31 (m, 2H), 1.22 – 1.13 (m, 4H), 0.93 (q, J = 7.3 Hz, 3H), 0.82 (t, J = 7.5 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.32 – -139.48 (m, 2F), -142.14 – -142.30 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.21 – 160.04 (m), 146.00 – 143.31 (m), 145.79 – 143.19 (m), 125.64 (td, J = 15.0, 3.0 Hz), 111.45 (td, J = 15.7, 15.3, 2.2 Hz), 69.63, 69.38, 53.26, 44.75, 44.33, 28.44, 28.31, 28.07, 28.06, 23.11, 22.78, 22.06, 21.17, 14.02,

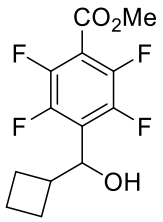
13.86, 10.44, 9.69; HRMS (EI): Calcd for $C_{16}H_{20}O_3F_4Na$ $[M+Na]^+$ 359.1246, found 359.1248.



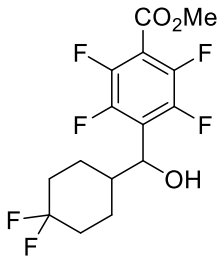
Methyl 4-(cyclohexyl(hydroxy)methyl)-2,3,5,6-tetrafluorobenzoate (3ap): colorless oil (53 mg, 83%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.74 (t, *J* = 8.5 Hz, 1H), 3.98 (s, 3H), 2.23 (d, *J* = 8.5 Hz, 1H), 2.19 – 2.15 (m, 1H), 1.86 – 1.79 (m, 2H), 1.72 – 1.65 (m, 2H), 1.22 – 0.82 (m, 6H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.41 – -139.53 (m, 2F), -141.97 – -142.09 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.18 – 160.03 (m), 145.96 – 143.23 (m), 145.71 – 143.11 (m), 125.03 (t, *J* = 15.3 Hz), 111.48 (t, *J* = 15.6 Hz), 71.75, 53.25, 43.47 (t, *J* = 1.2 Hz), 29.58, 28.89, 26.08, 25.63, 25.52; HRMS (EI): Calcd for $C_{15}H_{16}O_3F_4Na$ $[M+Na]^+$ 343.0933, found 343.0933.



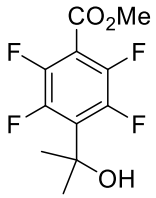
Methyl 4-(cyclopentyl(hydroxy)methyl)-2,3,5,6-tetrafluorobenzoate (3aq): colorless oil (61 mg, 99%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.77 (dd, *J* = 9.4, 5.3 Hz, 1H), 3.98 (s, 3H), 2.50 – 2.42 (m, 1H), 2.27 (d, *J* = 8.0 Hz, 1H), 2.04 – 1.95 (m, 1H), 1.78 – 1.51 (m, 5H), 1.48 – 1.38 (m, 1H), 1.14 – 1.05 (m, 1H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.31 – -139.45 (m, 2F), -142.31 – -142.44 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.18 – 160.08 (m), 145.99 – 143.23 (m), 145.74 – 143.09 (m), 125.58 (t, *J* = 15.3 Hz), 111.50 (t, *J* = 15.8 Hz), 71.08, 53.26, 45.91 (t, *J* = 1.5 Hz), 30.27, 28.96, 25.24, 25.21; HRMS (EI): Calcd for $C_{14}H_{14}O_3F_4Na$ $[M+Na]^+$ 329.0777, found 329.0780.



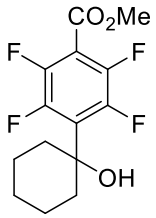
Methyl 4-(cyclobutyl(hydroxy)methyl)-2,3,5,6-tetrafluorobenzoate (3ar): colorless oil (46 mg, 78%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.01 (dd, *J* = 7.8, 6.3 Hz, 1H), 3.97 (s, 3H), 2.88 – 2.78 (m, 1H), 2.25 – 2.17 (m, 2H), 2.07 – 1.96 (m, 1H), 1.95 – 1.79 (m, 3H), 1.71 (q, *J* = 9.6, 9.2 Hz, 1H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.35 – -139.47 (m, 2F), -142.53 – -142.67 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.18 – 160.06 (m), 145.95 – 143.22 (m), 145.75 – 143.10 (m), 124.30 (t, *J* = 15.4 Hz), 111.54 (t, *J* = 15.9 Hz), 71.07, 53.27, 40.44 (t, *J* = 1.4 Hz), 25.58, 23.72, 17.67; HRMS (EI): Calcd for $C_{13}H_{13}O_3F_4$ $[M+H]^+$ 293.0801, found 293.0796.



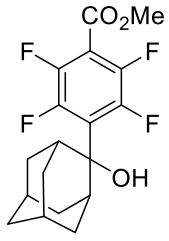
Methyl 4-((4,4-difluorocyclohexyl)(hydroxy)methyl)-2,3,5,6-tetrafluorobenzoate (3as): colorless oil (64 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.81 (t, *J* = 8.6 Hz, 1H), 3.99 (s, 3H), 2.35 (d, *J* = 8.2 Hz, 1H), 2.28 (d, *J* = 13.4 Hz, 1H), 2.24 – 2.14 (m, 1H), 2.12 – 2.05 (m, 1H), 1.96 (s, 1H), 1.83 – 1.62 (m, 2H), 1.52 – 1.41 (m, 1H), 1.39 – 1.32 (m, 2H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -92.60 (d, *J* = 236.6 Hz, 1F), -102.41 (dt, *J* = 242.2, 36.6 Hz, 1F), -138.76 – -138.89 (m, 2F), -141.81 – -141.94 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.06 – 159.85 (m), 146.00 – 143.19 (m), 145.76 – 142.97 (m), 124.15 (t, *J* = 15.1 Hz), 123.00 (t, *J* = 240.8 Hz) 112.04 (t, *J* = 16.0 Hz), 70.35, 53.38, 41.36 (d, *J* = 1.0 Hz), 32.87 (ddd, *J* = 25.6, 23.3, 4.8 Hz), 25.45 (dd, *J* = 60.0, 9.8 Hz); HRMS (EI): Calcd for $C_{15}H_{15}O_3F_6$ $[M+H]^+$ 357.0925, found 357.0926.



Methyl 2,3,5,6-tetrafluoro-4-(2-hydroxypropan-2-yl)benzoate (3at): colorless oil (41 mg, 78%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.97 (s, 3H), 2.75 (t, *J* = 3.9 Hz, 1H), 1.74 (t, *J* = 2.0 Hz, 6H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.33 – -139.45 (m, 2F), -139.63 – -139.77 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.11 – 160.01 (m), 146.57 – 143.68 (m), 145.90 – 142.94 (m), 129.33 (t, *J* = 12.3 Hz), 110.92 (t, *J* = 15.9 Hz), 73.52 (t, *J* = 2.1 Hz), 53.27, 30.55 (t, *J* = 4.0 Hz); HRMS (EI): Calcd for $C_{11}H_{10}O_3F_4Na$ $[M+Na]^+$ 289.0464, found 289.0473.

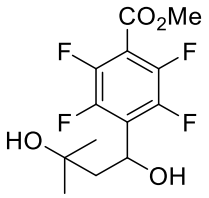


Methyl 2,3,5,6-tetrafluoro-4-(1-hydroxycyclohexyl)benzoate (3au): colorless oil (45 mg, 73%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.97 (s, 3H), 2.42 (t, *J* = 3.6 Hz, 1H), 2.06 (d, *J* = 5.0 Hz, 4H), 1.89 – 1.68 (m, 4H), 1.32 (tt, *J* = 13.1, 4.0 Hz, 2H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.18 – -139.26 (m, 2F), -139.36 – -139.49 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.17 – 160.03 (m), 146.63 – 143.70 (m), 146.16 – 143.37 (m), 129.79 (t, *J* = 11.3 Hz), 110.78 (t, *J* = 15.7 Hz), 75.62 – 75.51 (m), 53.21, 36.93 (t, *J* = 4.2 Hz), 25.10, 21.35; HRMS (EI): Calcd for $C_{14}H_{14}O_3F_4Na$ $[M+Na]^+$ 329.0777, found 329.0780.

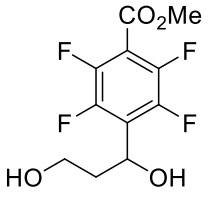


Methyl 2,3,5,6-tetrafluoro-4-((1r,3r,5r,7r)-2-hydroxyadamantan-2-yl)benzoate (3av): colorless oil (39 mg, 55%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.97 (s, 3H), 2.78 (s, 2H), 2.48 (s, 1H), 2.34 (d, *J* = 12.5 Hz, 2H), 1.92 (d, *J* = 12.2 Hz, 2H), 1.81 (q, *J* = 3.3

Hz, 2H), 1.76 (s, 2H), 1.70 – 1.65 (m, 4H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -136.45 (q, *J* = 9.4 Hz, 2F), -139.12 – -139.24 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.14 – 160.01 (m), 147.34 – 144.57 (m), 146.77 – 143.94 (m), 127.58 (t, *J* = 12.0 Hz), 111.06 (t, *J* = 16.3 Hz), 80.67 – 80.62 (m), 53.20, 46.96, 39.25, 37.19, 36.23 (t, *J* = 6.4 Hz), 35.61 (t, *J* = 2.1 Hz), 32.93, 27.45, 26.30, 26.16; HRMS (EI): Calcd for $C_{18}H_{18}O_3F_4Na$ $[M+Na]^+$ 381.1090, found 381.1093.

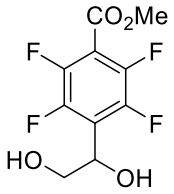


Methyl 4-(1,3-dihydroxy-3-methylbutyl)-2,3,5,6-tetrafluorobenzoate (3aw): The reaction was performed using 0.2 mmol of fluoroarenes and 0.3 mmol of alcohols; colorless oil (54 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.53 (dd, *J* = 11.1, 2.7 Hz, 1H), 4.05 (s, 1H), 3.97 (s, 3H), 2.37 (dd, *J* = 14.6, 11.0 Hz, 1H), 2.08 (s, 1H), 1.69 (dd, *J* = 14.6, 2.5 Hz, 1H), 1.44 (s, 3H), 1.35 (s, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.47 – -139.59 (m, 2F), -142.55 – -142.67 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.21 – 160.10 (m), 146.11 – 143.26 (m), 145.80 – 143.17 (m), 125.26 (t, *J* = 14.2 Hz), 111.55 (t, *J* = 15.9 Hz), 72.11, 64.10 (t, *J* = 2.0 Hz), 53.26, 46.69, 31.93, 27.59; HRMS (EI): Calcd for $C_{13}H_{14}O_4F_4Na$ $[M+Na]^+$ 333.0726, found 333.0731.

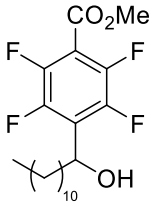


Methyl 4-(1,3-dihydroxypropyl)-2,3,5,6-tetrafluorobenzoate (3ax): The reaction was performed using 0.2 mmol of fluoroarenes and 0.3 mmol of alcohols; colorless oil (37 mg, 65%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.38 (dd, *J* = 9.4, 3.9 Hz, 1H), 3.97 (s, 3H), 3.96 – 3.84 (m, 2H), 3.46 (s, 1H), 2.36 – 2.25 (m, 1H), 2.01 – 1.93 (m, 1H), 1.80 (s, 1H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.31 – -139.43 (m, 2F), -142.79 – -142.91 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.21 – 160.09 (m), 146.02 – 143.23 (m), 145.77 – 143.09 (m), 125.05 (t, *J* = 14.8 Hz), 111.61 (t, *J* = 15.9 Hz), 65.42 (t, *J* = 1.9

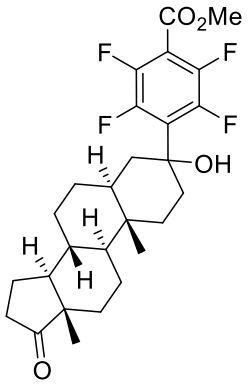
Hz), 60.58, 53.30, 37.73 (t, J = 1.6 Hz); HRMS (EI): Calcd for $C_{11}H_{11}O_4F_4$ $[M+H]^+$ 283.0593, found 283.0592.



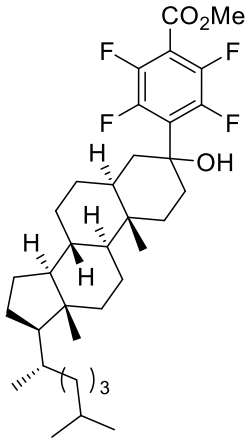
Methyl 4-(1,2-dihydroxyethyl)-2,3,5,6-tetrafluorobenzoate (3ay): white solid (28 mg, 53%); Mp. 85 – 86 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 5.10 (t, J = 6.8 Hz, 1H), 3.93 (s, 3H), 3.88 (dd, J = 11.1, 7.0 Hz, 1H), 3.75 (dd, J = 11.0, 6.9 Hz, 1H); ^{19}F NMR (377 MHz, CD_3OD): δ -142.84 – -142.96 (m, 2F), -144.00 – -144.12 (m, 2F); ^{13}C NMR (100 MHz, CD_3OD): δ 161.35 – 161.25 (m), 147.79 – 145.07 (m), 147.16 – 144.38 (m), 125.38 (t, J = 15.5 Hz), 112.96 (t, J = 16.4 Hz), 67.96 (t, J = 1.8 Hz), 65.17 (t, J = 2.5 Hz), 53.76; HRMS (EI): Calcd for $C_{10}H_8O_4F_4Na$ $[M+Na]^+$ 291.0256, found 291.0249.



Methyl 2,3,5,6-tetrafluoro-4-(1-hydroxydodecyl)benzoate (3az): The reaction was performed using 0.2 mmol of fluoroarenes and 0.3 mmol of alcohols; colorless oil (78 mg, 99%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.07 (q, J = 7.3 Hz, 1H), 3.98 (s, 3H), 2.23 (d, J = 8.1 Hz, 1H), 2.06 – 1.95 (m, 1H), 1.88 – 1.78 (m, 1H), 1.49 – 1.40 (m, 1H), 1.37 – 1.18 (m, 17H), 0.87 (t, J = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.28 – -139.40 (m, 2F), -143.18 – -143.32 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.17 – 160.06 (m), 146.00 – 143.19 (m), 145.75 – 143.02 (m), 125.71 (t, J = 15.0 Hz), 111.48 (t, J = 15.8 Hz), 66.88 (t, J = 1.6 Hz), 53.27, 36.90, 31.88, 29.57, 29.48, 29.39, 29.31, 29.16, 25.69, 22.66, 14.08; HRMS (EI): Calcd for $C_{20}H_{28}O_3F_4Na$ $[M+Na]^+$ 415.1872, found 415.1873.

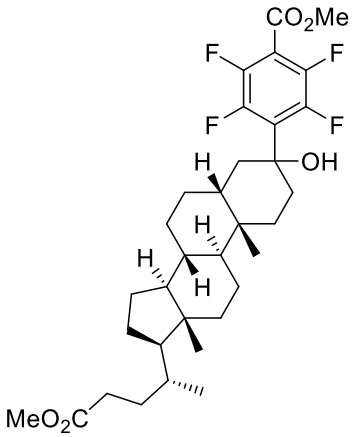


Methyl 2,3,5,6-tetrafluoro-4-((5S,8R,9S,10S,13S,14S)-3-hydroxy-10,13-dimethyl-17-oxohexadecahydro-1H-cyclopenta[a]phenanthren-3-yl)benzoate (4): white solid (92 mg, 93%); Mp. 152 – 153 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.96 (s, 3H), 2.47 – 2.39 (m, 2H), 2.38 – 2.30 (m, 1H), 2.28 – 2.20 (m, 1H), 2.13 – 2.00 (m, 2H), 1.97 – 1.89 (m, 2H), 1.86 – 1.75 (m, 4H), 1.74 – 1.65 (m, 2H), 1.63 – 1.47 (m, 4H), 1.34 – 1.27 (m, 3H), 1.10 – 0.95 (m, 2H), 0.90 (s, 3H), 0.86 (s, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.27 – -139.40 (m, 2F), -139.55 – -139.69 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 211.70, 160.10 – 159.97 (m), 146.59 – 143.70 (m), 146.10 – 143.14 (m), 129.64 (t, J = 11.2 Hz), 110.70 (t, J = 15.6 Hz), 75.84, 54.05, 53.22, 51.39, 47.78, 40.30, 39.38 (t, J = 4.0 Hz), 35.79, 35.62, 34.99, 33.36, 32.89 (t, J = 4.0 Hz), 31.48, 30.74, 27.83, 21.70, 20.15, 13.79, 11.42; HRMS (EI): Calcd for $C_{27}H_{32}O_4F_4Na$ $[M+Na]^+$ 519.2134, found 519.2138.



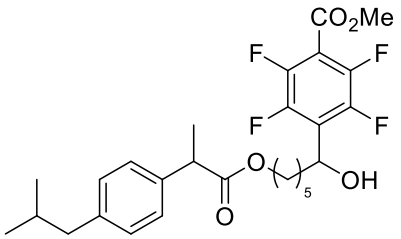
Methyl 2,3,5,6-tetrafluoro-4-((5S,8R,9S,10S,13R,14S,17R)-3-hydroxy-10,13-dimethyl-17-((S)-6-methylheptan-2-yl)hexadecahydro-1H-cyclopenta[a]phenanthren-3-yl)benzoate (5): white solid (63 mg, 53%); Mp. 129 –

130 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.97 (s, 3H), 2.35 (s, 1H), 2.23 (dd, *J* = 13.9, 4.5 Hz, 1H), 2.12 – 1.88 (m, 4H), 1.85 – 1.65 (m, 4H), 1.63 – 1.47 (m, 6H), 1.40 – 1.29 (m, 6H), 1.17 – 1.06 (m, 6H), 1.05 – 0.96 (m, 4H), 0.90 (d, *J* = 6.5 Hz, 3H), 0.87 (s, 3H), 0.87 (s, 3H), 0.85 (d, *J* = 1.9 Hz, 3H), 0.66 (s, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.34 – -139.46 (m, 2F), -139.56 – -139.64 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.15 – 160.04 (m), 146.61 – 143.74 (m), 146.09 – 143.28 (m), 129.81 (t, *J* = 11.0 Hz), 110.65 (t, *J* = 15.5 Hz), 76.07 (m), 56.47, 56.24, 53.97, 53.22, 42.60, 40.37, 39.97, 39.58 (t, *J* = 3.9 Hz), 39.50, 36.16, 35.79, 35.47, 33.43, 32.95 (t, *J* = 4.0 Hz), 31.94, 28.22, 28.20, 28.00, 24.16, 23.82, 22.81, 22.68 (t, *J* = 3.1 Hz), 22.55, 20.91, 18.66, 12.08, 11.45; HRMS (EI): Calcd for $C_{35}H_{50}O_3F_4Na$ $[M+Na]^+$ 617.3594, found 617.3602.

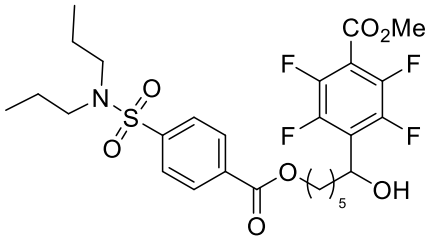


Methyl 2,3,5,6-tetrafluoro-4-((5R,8R,9S,10S,13R,14S,17R)-3-hydroxy-17-((R)-5-methoxy-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1H-cyclopenta[a]phenanthren-3-yl)benzoate (6): The reaction was performed using 0.6 mmol of fluoroarenes and 0.2 mmol of alcohols; white solid (88 mg, 74%); Mp. 99 – 100 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.95 (s, 3H), 3.64 (s, 3H), 2.54 (s, 1H), 2.46 (t, *J* = 13.3 Hz, 1H), 2.37 – 2.29 (m, 1H), 2.24 – 2.10 (m, 2H), 2.03 – 1.72 (m, 7H), 1.68 – 1.51 (m, 4H), 1.46 – 1.35 (m, 5H), 1.35 – 1.27 (m, 2H), 1.22 – 1.14 (m, 3H), 1.12 – 1.02 (m, 3H), 0.98 (s, 3H), 0.90 (d, *J* = 6.4 Hz, 3H), 0.64 (s, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.22 – -139.53 (m, 4F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.73, 160.09 – 159.97 (m), 146.57 – 143.69 (m), 146.08 – 143.30 (m), 129.90 (t, *J* = 10.7 Hz), 110.60 (t, *J* = 15.5 Hz), 76.42, 56.48, 55.83, 53.15, 51.40, 42.69, 40.09, 39.94, 37.89, 37.44 (t,

J = 3.6 Hz), 35.56, 35.28, 34.40, 31.62 (t, *J* = 4.3 Hz), 31.08, 30.96, 30.93, 28.09, 26.46, 26.31, 24.08, 23.44, 21.04, 18.20, 12.01; HRMS (EI): Calcd for $C_{33}H_{45}O_5F_4$ $[M+H]^+$ 597.3203, found 597.3199.

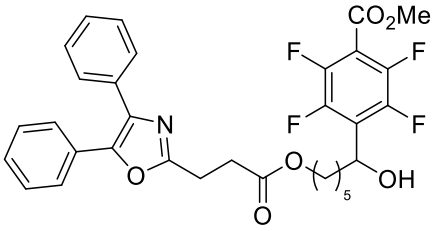


Methyl 2,3,5,6-tetrafluoro-4-(1-hydroxy-6-((2-(4-isobutylphenyl)propanoyl)oxy)hexyl)benzoate (7): The reaction was performed using 0.6 mmol of fluoroarenes and 0.2 mmol of alcohols; colorless oil (73 mg, 71%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.18 (d, *J* = 8.1 Hz, 2H), 7.08 (d, *J* = 8.1 Hz, 2H), 5.03 (t, *J* = 7.3 Hz, 1H), 4.04 (t, *J* = 6.3 Hz, 2H), 3.98 (s, 3H), 3.67 (q, *J* = 7.2 Hz, 1H), 2.43 (d, *J* = 7.2 Hz, 2H), 2.01 – 1.90 (m, 1H), 1.88 – 1.71 (m, 2H), 1.68 (s, 1H), 1.57 (p, *J* = 6.7 Hz, 2H), 1.47 (d, *J* = 7.2 Hz, 3H), 1.33 – 1.17 (m, 4H), 0.88 (d, *J* = 6.6 Hz, 6H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.24 – -139.36 (m, 2F), -143.12 – -143.24 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.84, 160.13 – 160.01 (m), 146.00 – 143.19 (m), 145.71 – 142.97 (m), 140.47, 137.78, 129.23, 127.10, 125.57 (t, *J* = 15.0 Hz), 111.51 (t, *J* = 15.9 Hz), 66.55, 64.33, 53.27, 45.14, 44.96, 36.57, 30.13, 28.31, 25.33 (d, *J* = 1.5 Hz), 25.25, 22.30, 18.35; HRMS (EI): Calcd for $C_{27}H_{33}O_5F_4$ $[M+H]^+$ 513.5416, found 513.5420.



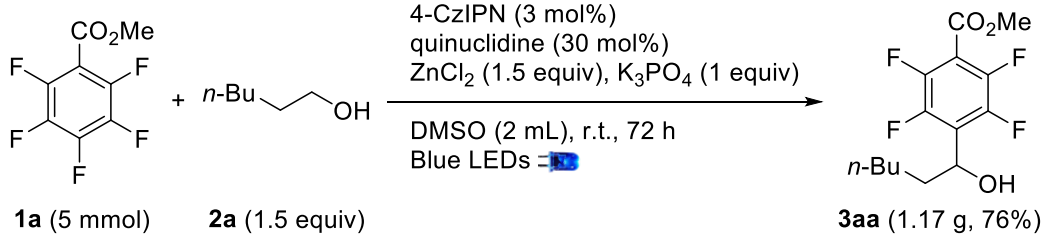
Methyl 4-(6-((4-(N,N-dipropylsulfamoyl)benzoyl)oxy)-1-hydroxyhexyl)-2,3,5,6-tetrafluorobenzoate (8): The reaction was performed using 0.6 mmol of fluoroarenes and 0.2 mmol of alcohols; colorless oil (73 mg, 62%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 (d, *J* = 8.5 Hz, 2H), 7.86 (d, *J* = 8.5 Hz, 2H), 5.09 (t, *J* = 7.2 Hz, 1H), 4.34 (t, *J* = 6.5 Hz, 2H), 3.97 (s, 3H), 3.09 (t, *J* = 7.6 Hz, 4H), 2.45 (s, 1H), 2.10 – 2.01 (m, 1H),

1.91 – 1.83 (m, 1H), 1.79 (p, *J* = 6.8 Hz, 2H), 1.59 – 1.46 (m, 7H), 1.41 – 1.32 (m, 1H), 0.86 (t, *J* = 7.4 Hz, 6H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.20 – -139.32 (m, 2F), -143.14 – -143.26 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.28, 160.10 – 159.97 (m), 146.01 – 143.20 (m), 144.22, 145.70 – 142.99 (m), 133.62, 130.13, 126.97, 125.48 (t, *J* = 15.0 Hz), 111.61 (t, *J* = 15.9 Hz), 66.56 (t, *J* = 1.7 Hz), 65.38, 53.28, 49.92, 36.60 (t, *J* = 1.6 Hz), 28.49, 25.64, 25.41, 21.90, 11.10; HRMS (EI): Calcd for $C_{27}H_{34}F_4NO_7S$ $[M+H]^+$ 592.6146, found 592.6150.



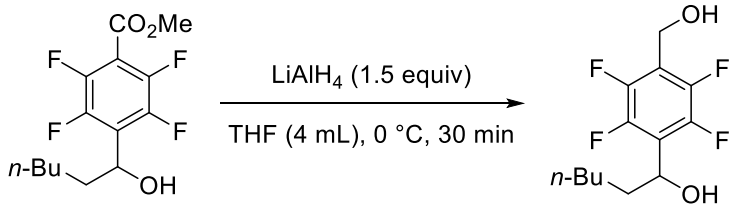
Methyl 4-(6-((3-(4,5-diphenyloxazol-2-yl)propanoyl)oxy)-1-hydroxyhexyl)-2,3,5,6-tetrafluorobenzoate (9): The reaction was performed using 0.6 mmol of fluoroarenes and 0.2 mmol of alcohols; colorless oil (85 mg, 71%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61 (dd, *J* = 8.0, 1.7 Hz, 2H), 7.56 (dd, *J* = 8.0, 1.7 Hz, 2H), 7.37 – 7.28 (m, 6H), 5.02 (dd, *J* = 8.1, 6.3 Hz, 1H), 4.12 (t, *J* = 6.5 Hz, 2H), 3.97 (s, 3H), 3.18 (t, *J* = 7.4 Hz, 2H), 2.91 (t, *J* = 7.4 Hz, 2H), 2.40 (s, 1H), 2.01 – 1.92 (m, 1H), 1.80 – 1.71 (m, 1H), 1.63 (p, *J* = 6.6 Hz, 2H), 1.53 – 1.43 (m, 1H), 1.39 (p, *J* = 7.2 Hz, 2H), 1.34 – 1.28 (m, 1H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.26 – -139.38 (m, 2F), -143.10 – -143.23 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.00, 161.81, 160.13 – 160.02 (m), 145.43, 146.02 – 143.16 (m), 145.74 – 142.89 (m), 135.07, 132.36, 128.93, 128.62, 128.51, 128.46, 128.07, 127.88, 126.44, 125.58 (t, *J* = 15.1 Hz), 111.62 (t, *J* = 15.8 Hz), 66.52 (t, *J* = 1.5 Hz), 64.60, 53.26, 36.60 (t, *J* = 1.5 Hz), 31.15, 28.39, 25.52, 25.37, 23.56; HRMS (EI): Calcd for $C_{32}H_{29}F_4NO_6$ $[M+H]^+$ 600.5786, found 600.5791.

6. Gram-Scale Preparation of 3aa and Transformations of the Products



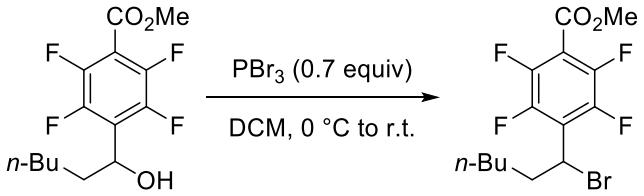
1a (5 mmol) **2a** (1.5 equiv) **3aa** (1.17 g, 76%)

In a 100 mL Schlenk tube with a magnetic stir bar were placed 4-CzIPN (**PC**, 118.3 mg, 0.15 mmol), quinuclidine (166.8 mg, 1.5 mmol), K_3PO_4 (1.06 g, 5 mmol) and $ZnCl_2$ (1.02 g, 7.5 mmol). Under nitrogen atmosphere, methyl pentafluorobenzoate (**1a**, 1.13 g, 5 mmol), hexanol (**2a**, 0.77g, 7.5 mmol), DMSO (40 mL) were added, subsequently. The resulting mixture was sealed and degassed *via* freeze-pump-thaw for three times. Then, the reaction was placed under a blue LED (2-meter strips, 18 W, 456 nm) and irradiated for 72 hrs at rt. The resulting mixture was quenched with H_2O and and extracted with ether (20 mL × 3). The combined organic layer was washed with brine, dried over $MgSO_4$ and concentrated in vacuo. The residue was purified by column chromatography. Silica gel chromatography (eluent: petroleum ether/EtOAc = 5/1) of the crude product afforded the desired compound as a colorless oil (1.17 g).



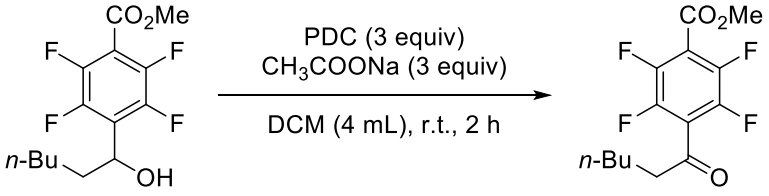
3aa **10**, 99%

1-(2,3,5,6-Tetrafluoro-4-(hydroxymethyl)phenyl)hexan-1-ol (10): Under nitrogen atmosphere, **3aa** (44 μL, 0.2 mmol), THF (4 mL) and lithium aluminum hydride solution (0.3 mL, 1 M in THF) were added in a 10 mL Schlenk tube with a magnetic stir bar at 0 ℃. Subsequently. The resulting mixture was sealed and cooled to 0 ˚C for 30 mins. The solvent was removed under vacuum. Silica gel chromatography (eluent: petroleum ether/EtOAc = 2/1) of the crude product afforded the desired compounds as a colorless oil (55 mg, 99%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.03 (t, J = 7.4 Hz, 1H), 4.77 (s, 2H), 2.62 (s, 2H), 2.04 – 1.92 (m, 1H), 1.88 – 1.76 (m, 1H), 1.48 – 1.37 (m, 1H), 1.34 – 1.26 (m, 5H), 0.88 (t, J = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -144.73 (dd, J = 22.1, 13.0 Hz, 2F), -145.23 (dd, J = 22.0, 13.0 Hz, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.21 – 143.46 (m), 145.52 – 142.87 (m), 122.28 (t, J = 15.0 Hz), 117.51 (t, J = 17.7 Hz), 66.71 (t, J = 2.1 Hz), 52.68 – 52.59 (m), 36.78, 31.34, 25.41, 22.43, 13.89; HRMS (EI): Calcd for $C_{13}H_{17}F_4O_2$ $[M+H]^+$ 281.2626, found 281.2629.



3aa **11**, 77%

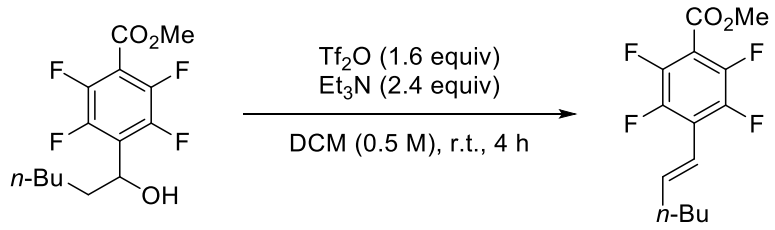
Methyl 4-(1-bromohexyl)-2,3,5,6-tetrafluorobenzoate (11): In a 10 mL Schlenk tube with a magnetic stir bar were placed **3aa** (44 μL, 0.2 mmol) and CH_2Cl_2 (1 mL). Under nitrogen atmosphere, added PBr_3(14 μL, 0.14 mmol) at 0 °C. After completion of reaction (monitored by TLC), the mixture was quenched by water and extracted with CH_2Cl_2 three times. The combined organic layer was washed by brine, dried over $MgSO_4$ and concentrated in vacuo. Silica gel chromatography (eluent: petroleum ether/EtOAc = 5/1) of the crude product afforded the desired compounds as a colorless oil (57 mg, 77%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.19 (t, *J* = 7.9 Hz, 1H), 3.99 (s, 3H), 2.42 – 2.32 (m, 1H), 2.28 – 2.19 (m, 1H), 1.51 – 1.44 (m, 1H), 1.36 – 1.28 (m, 5H), 0.88 (t, *J* = 6.9 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -138.82 – -138.96 (m, 2F), -139.91 (s, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.92 – 159.82 (m), 146.05 – 143.25 (m), 145.79 – 143.06 (m), 123.73 (t, *J* = 14.2 Hz), 112.27 (t, *J* = 16.0 Hz), 53.37, 38.85 (t, *J* = 1.7 Hz), 36.93 (t, *J* = 2.8 Hz), 30.81, 27.93, 22.33, 13.87; HRMS (EI): Calcd for $C_{14}H_{16}O_2F_4Br$ $[M+H]^+$ 371.0270, found 371.0261.



3aa **12**, 88%

Methyl 2,3,5,6-tetrafluoro-4-hexanoylbenzoate (12): In a 10 mL Schlenk tube with a magnetic stir bar were placed sodium acetate (49.2 mg, 0.6 mmol), pyridinium dichromate (225.7 mg, 0.6 mmol). Under nitrogen atmosphere, CH_2Cl_2 (4 mL) and **3aa** (44 μL, 0.2 mmol) were added at room temperature. After stirred for 2 hrs, the mixture was quenched by water and extracted with CH_2Cl_2 (5 mL × 3). The combined organic layer was washed by brine, dried over $MgSO_4$ and concentrated in vacuo. Silica gel chromatography (eluent: petroleum ether/EtOAc = 5/1) of the crude product afforded

the desired compounds as a colorless oil (54 mg, 88%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.99 (s, 3H), 2.85 (t, *J* = 7.3 Hz, 2H), 1.74 – 1.67 (m, 2H), 1.37 – 1.29 (m, 4H), 0.89 (t, *J* = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -137.72 – -137.85 (m, 2F), -141.13 – -141.27 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 194.68 – 194.59 (m), 159.57 – 159.45 (m), 145.93 – 143.03 (m), 144.55 – 141.70 (m), 122.47 (t, *J* = 19.3 Hz), 114.15 (t, *J* = 16.4 Hz), 53.50, 44.98, 31.01, 23.03, 22.30, 13.78; HRMS (EI): Calcd for $C_{14}H_{14}O_3F_4Na$ $[M+Na]^+$ 329.0777, found 329.0776.

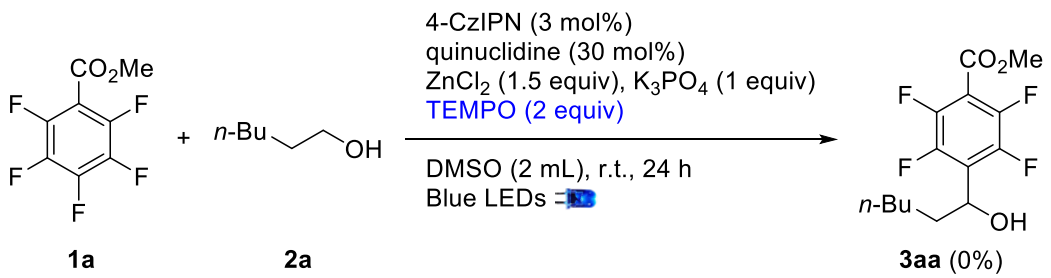


3aa **13**, 62%

Methyl (*E*)-2,3,5,6-tetrafluoro-4-(hex-1-en-1-yl)benzoate (13): In a 10 mL Schlenk tube with a magnetic stir bar were placed **3aa** (44 μL, 0.2 mmol), Et_3N (67 μL, 0.48 mmol) and CH_2Cl_2 (2 mL). Then, dropwise added trifluoromethanesulfonic anhydride (54 μL, 0.32 mmol) at 0 °C. After stirring for 4 h, the reaction was quenched by adding water, and the mixture was extracted with CH_2Cl_2 three times. The combined organic layer were washed with brine, dried ($MgSO_4$), and concentrated in vacuo. Silica gel chromatography (eluent: petroleum ether/EtOAc = 10/1) of the crude product afforded the desired compounds as a colorless oil (36 mg, 62%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.72 (dt, *J* = 16.2, 7.0 Hz, 1H), 6.36 (dt, *J* = 16.4, 1.6 Hz, 1H), 3.96 (s, 3H), 2.30 (q, *J* = 7.9 Hz, 2H), 1.52 – 1.45 (m, 2H), 1.43 – 1.33 (m, 2H), 0.93 (t, *J* = 7.2 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -140.76 – -140.88 (m, 2F), -143.25 – -143.37 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.47 – 160.35 (m), 146.32 – 143.46 (m), 143.86 (t, *J* = 7.8 Hz), 145.60 – 142.80 (m), 120.35 (t, *J* = 13.6 Hz), 114.79 (t, *J* = 2.9 Hz), 109.21 (t, *J* = 15.6 Hz), 53.06, 34.15, 30.84, 22.22, 13.83; HRMS (EI): Calcd for $C_{14}H_{14}O_2F_4Na$ $[M+Na]^+$ 313.0828, found 313.0834.

7. Additional Experiments to Elucidate the Mechanism

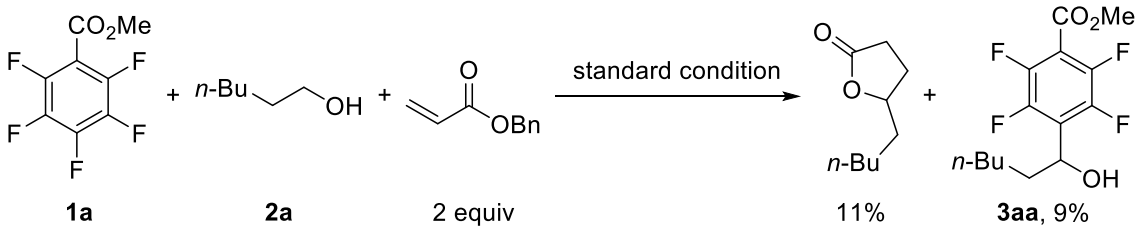
7.1 Radical Inhibition Experiments



1a **2a** **3aa** (0%)

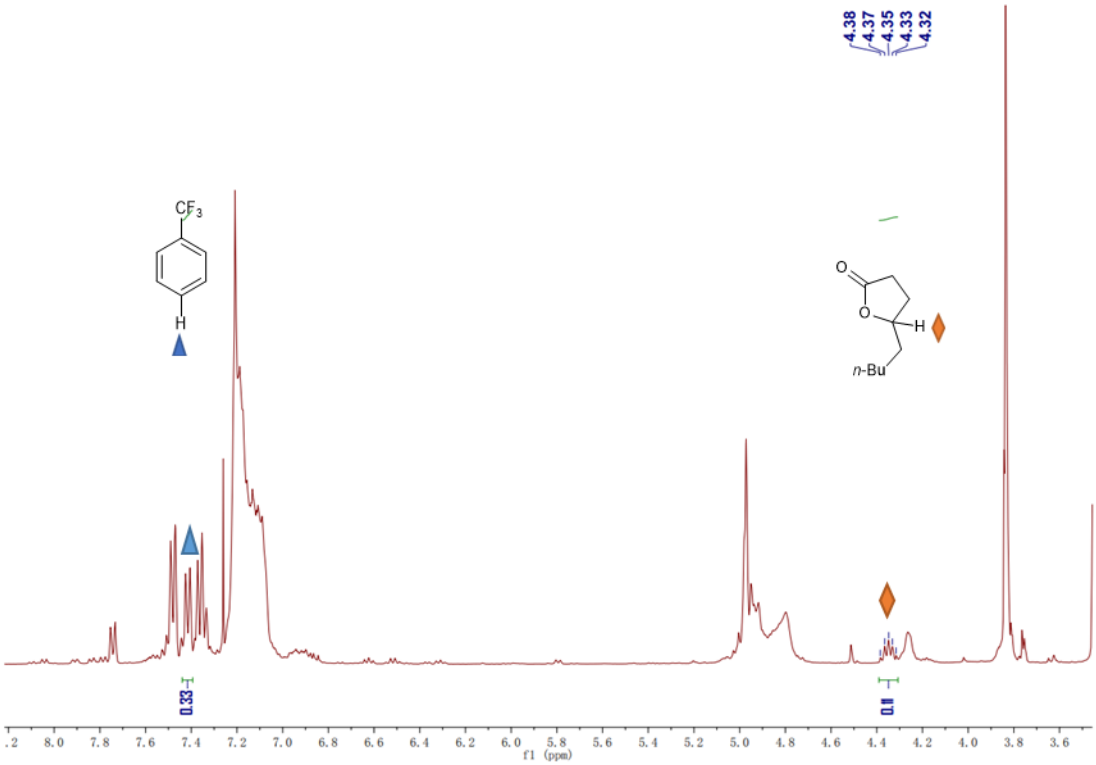
The radical initiator, TEMPO, can totally inhibit the formation of product, **3aa**, thus supporting a radical-based mechanism.

7.2 Evidence for the Presence of Carbon Radical

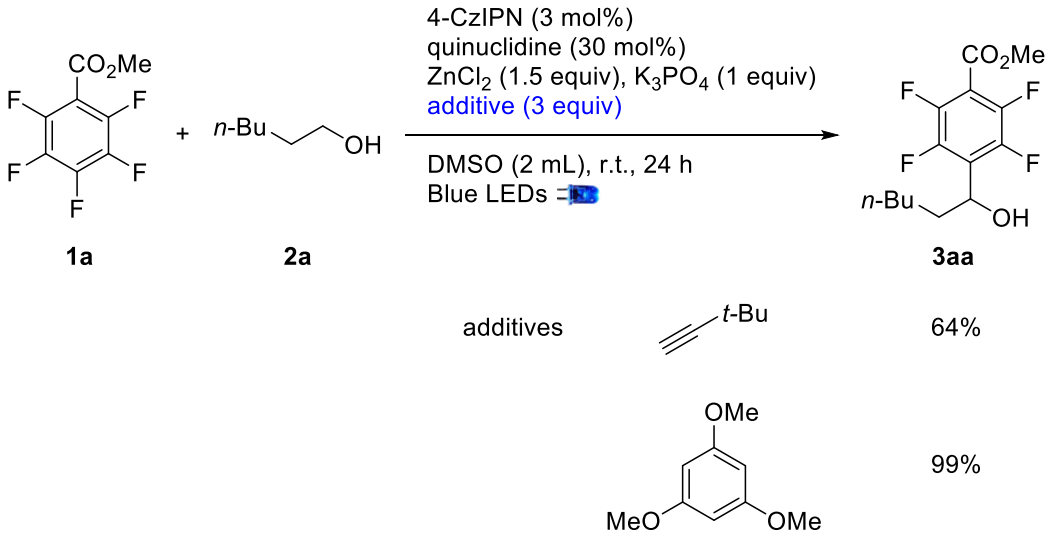


1a **2a** 2 equiv 11% **3aa**, 9%

In a 10 mL Schlenk tube with a magnetic stir bar were placed 4-CzIPN (**PC**, 2.4 mg, 0.003 mmol), quinuclidine (3.3 mg, 0.03 mmol), K_3PO_4 (21.2 mg, 0.1 mmol) and $ZnCl_2$ (20.5 mg, 0.15 mmol). Under nitrogen atmosphere, methyl pentafluorobenzoate (**1a**, 0.1 mmol), hexanol (**2a**, 0.15 mmol), benzyl acrylate (0.2 mmol), DMSO (2 mL) were added, subsequently. The mixture was degassed *via* freeze-pump-thaw for three times, and irradiated under a blue LED (2-meter strips, 18 W, 456 nm) for 24 hrs at rt. The resulting mixture was quenched with H_2O (2 mL) and extracted with Et_2O (2 mL × 3). The combined organic layer was washed with saturated brine, dried over $MgSO_4$ and concentrated in vacuo. The yields of **3aa** and 5-pentyldihydrofuran-2(3*H*)-one were determined by ^1H NMR and ^{19}F NMR of the crude products using trifluorotoluene (0.033 mmol) as an internal standard.[1]



7.3 Evidence for the Presence of Polyfluorophenyl Radical

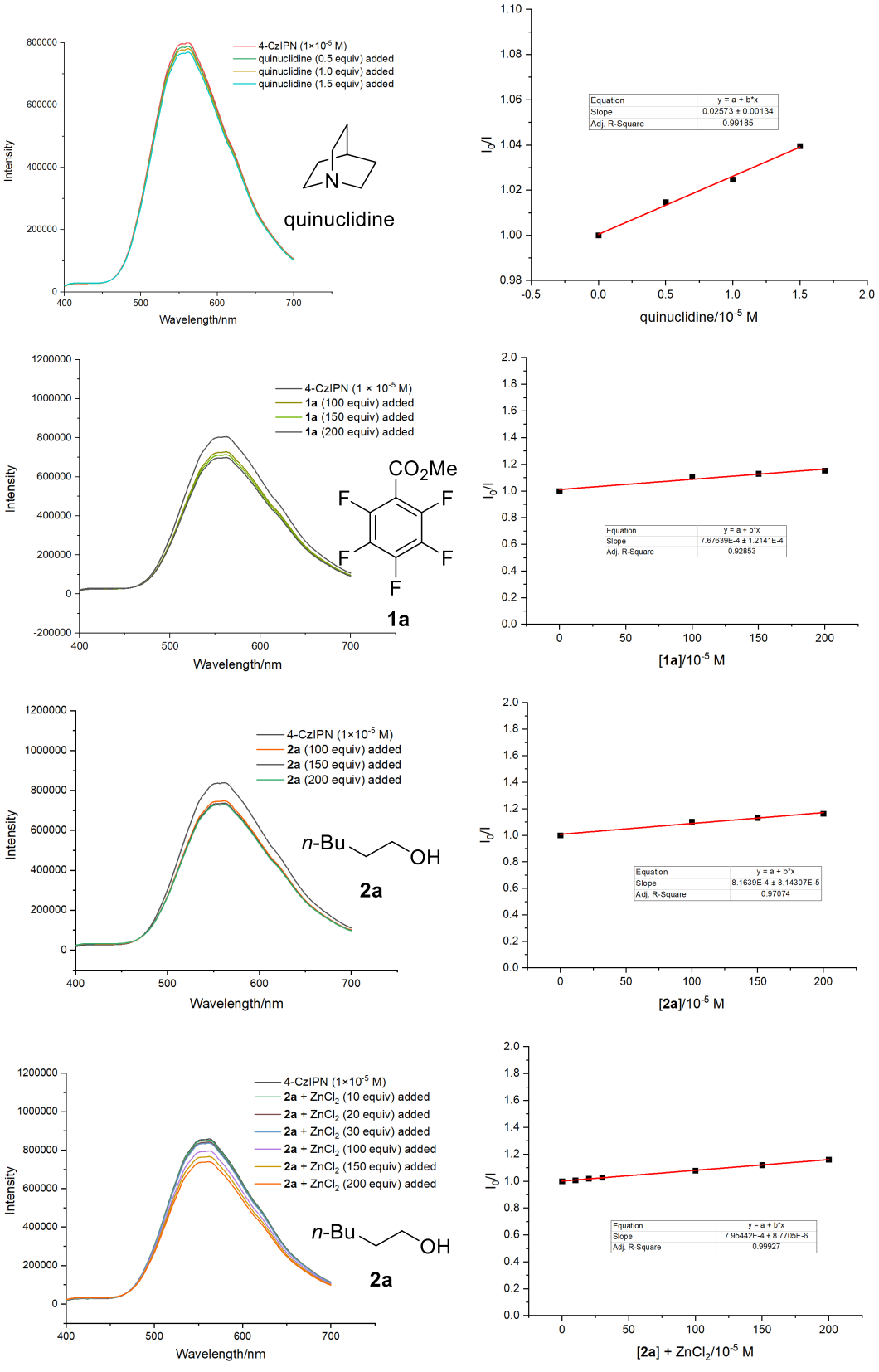


When adding the radical trappers for polyfluoroaryl radicals, such as alkynes and trimethoxybenzene, no radical addition products was observed with no significant influence on the yields of alkylpolyfluoroarenes.

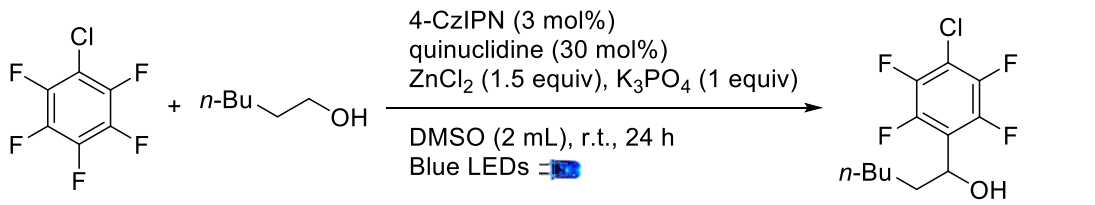
7.4 Stern-Volmer Quenching Experiments

In a typical experiment, a solution of 4-CzIPN in anhydrous reaction solvent (DMSO)

(1.0×10^{-5} M) was added with an appropriate amount of quencher in a quartz cuvette. Then the emission of the sample was collected. The emission intensity was collected with excited wavelength of photocatalysts, respectively.

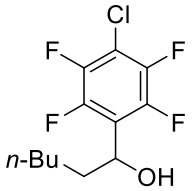


7.5 Defluoroalkylation of Pentafluorochlorobenzene



1y **2a** **3ya**, 45% (p:m:o = 67:20:13)

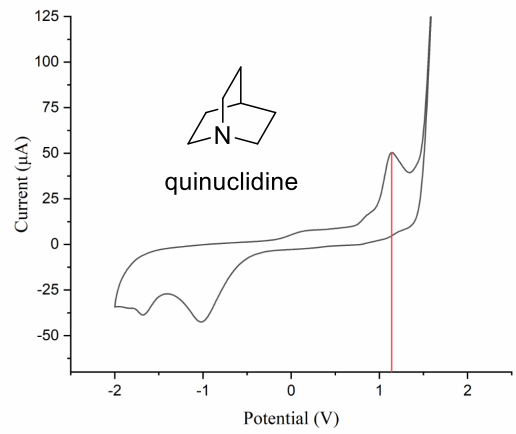
In a 10 mL Schlenk tube with a magnetic stir bar were placed 4-CzIPN (**PC**, 4.8 mg, 0.006 mmol), quinuclidine (6.6 mg, 0.06 mmol), K_3PO_4 (42.4 mg, 0.2 mmol) and $ZnCl_2$ (41.0 mg, 0.3 mmol). Under nitrogen atmosphere, pentafluorochlorobenzene (**1y**, 0.2 mmol), hexanol (**2a**, 0.6 mmol,), DMSO (4 mL) were added, subsequently. The mixture was degassed *via* freeze-pump-thaw for three times, and irradiated under a blue LED (2-meter strips, 18 W, 456 nm) for 24 hrs at rt. The resulting mixture was quenched with H_2O (2 mL) and extracted with Et_2O (5 mL × 3). The combined organic layer was washed with saturated brine, dried over $MgSO_4$ and concentrated in vacuo. Silica gel chromatography (eluent: petroleum ether/EtOAc = 5/1) of the crude product afforded the desired compound.



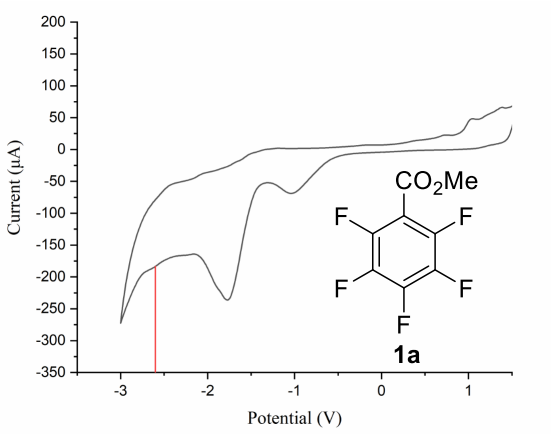
1-(4-Chloro-2,3,5,6-tetrafluorophenyl)hexan-1-ol (3ya): colorless oil (26 mg, 45%). Major component: ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.05 (t, J = 7.4 Hz, 1H), 2.16 (s, 1H), 2.05 – 1.95 (m, 1H), 1.88 – 1.77 (m, 1H), 1.52 – 1.39 (m, 1H), 1.36 – 1.28 (m, 5H), 0.88 (t, J = 6.8 Hz, 3H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -140.91 – -141.03 (m, 2F), -143.31 – -143.42 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.04 – 143.18 (m), 145.47 – 142.62 (m), 126.10 (t, J = 5.2 Hz), 121.13 (t, J = 15.3 Hz), 66.79 (t, J = 1.6 Hz), 36.96 (t, J = 1.7 Hz), 31.34, 25.45, 22.46, 13.93; HRMS (EI): Calcd for $C_{12}H_{14}OF_4Cl$ $[M+H]^+$ 285.0669, found 285.0665.

7.6 Cyclic Voltammetry Experiments

Cyclic Voltammograms were collected using Vertex. C. EIS Chenhua (China) with a typical three-electrode cell which contained 0.5 M sodium sulfate (Na_2SO_4) aqueous solution (pH = ~ 7) as electrolyte. The KCl-saturated Ag/AgCl and Pt net were used as the reference electrode and counter electrode, respectively. Sample (0.01 M) and tetrabutylammonium tetrafluoroborate (0.1 M) in DMSO were used for tests. Measurements were performed using glassy carbon working electrode, platinum wire counter electrode, and KCl-saturated Ag/AgCl reference electrode in a scan rate of 0.1 V/s.

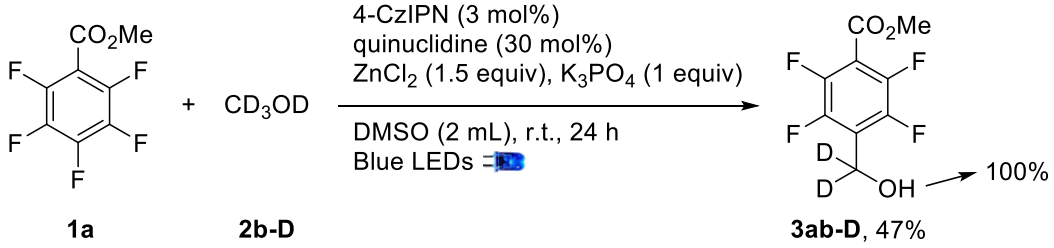


E_p^{ox} = +1.14 V vs Ag/AgCl in DMSO

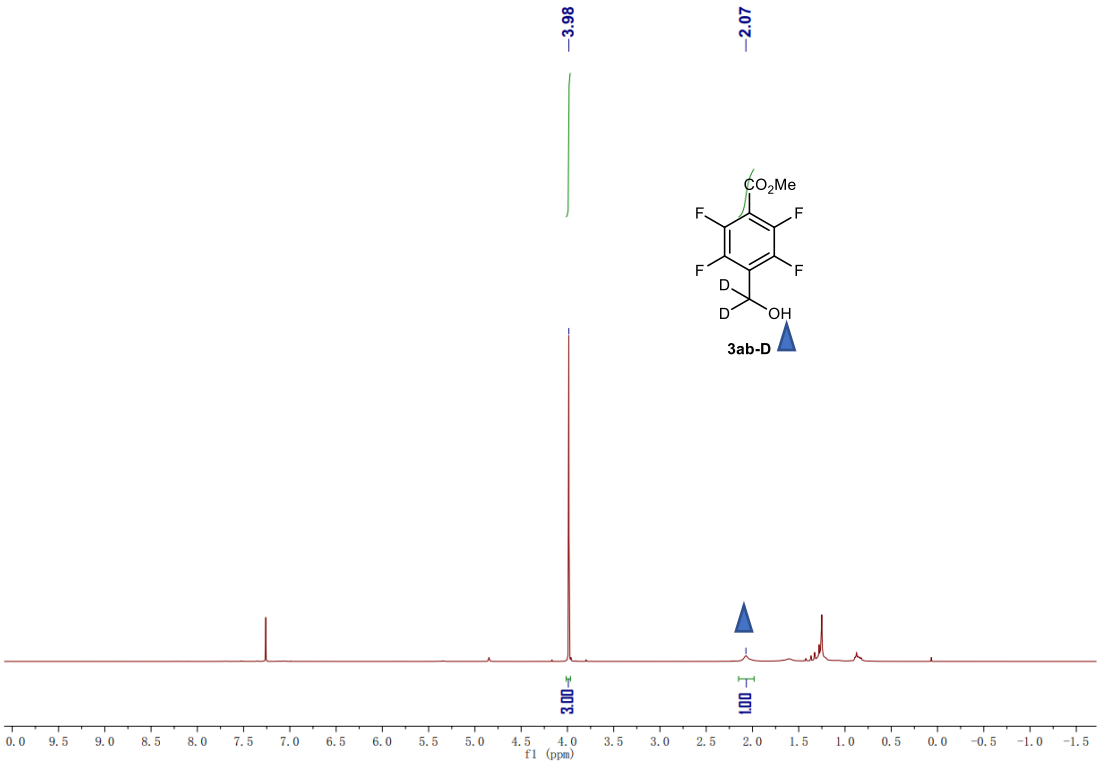


E_p^{red} = -2.67 V vs Ag/AgCl in DMSO

7.7 Deuterium-Labeling Experiments and KIE Determination

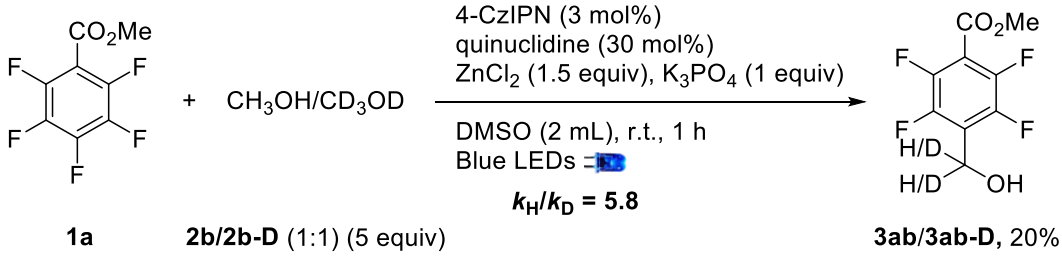


Deuterium-labeling experiments: 2b-D (21 μL, 0.5 mmol) was used to perform the defluoroalkylation reaction under the standard conditions. Silica gel chromatography (eluent: petroleum ether/EtOAc = 2/1) of the crude product mixture afforded compound **3ab-D** as a colorless liquid. The product was analyzed by ^1H NMR to determine the ratio of H-D exchange.



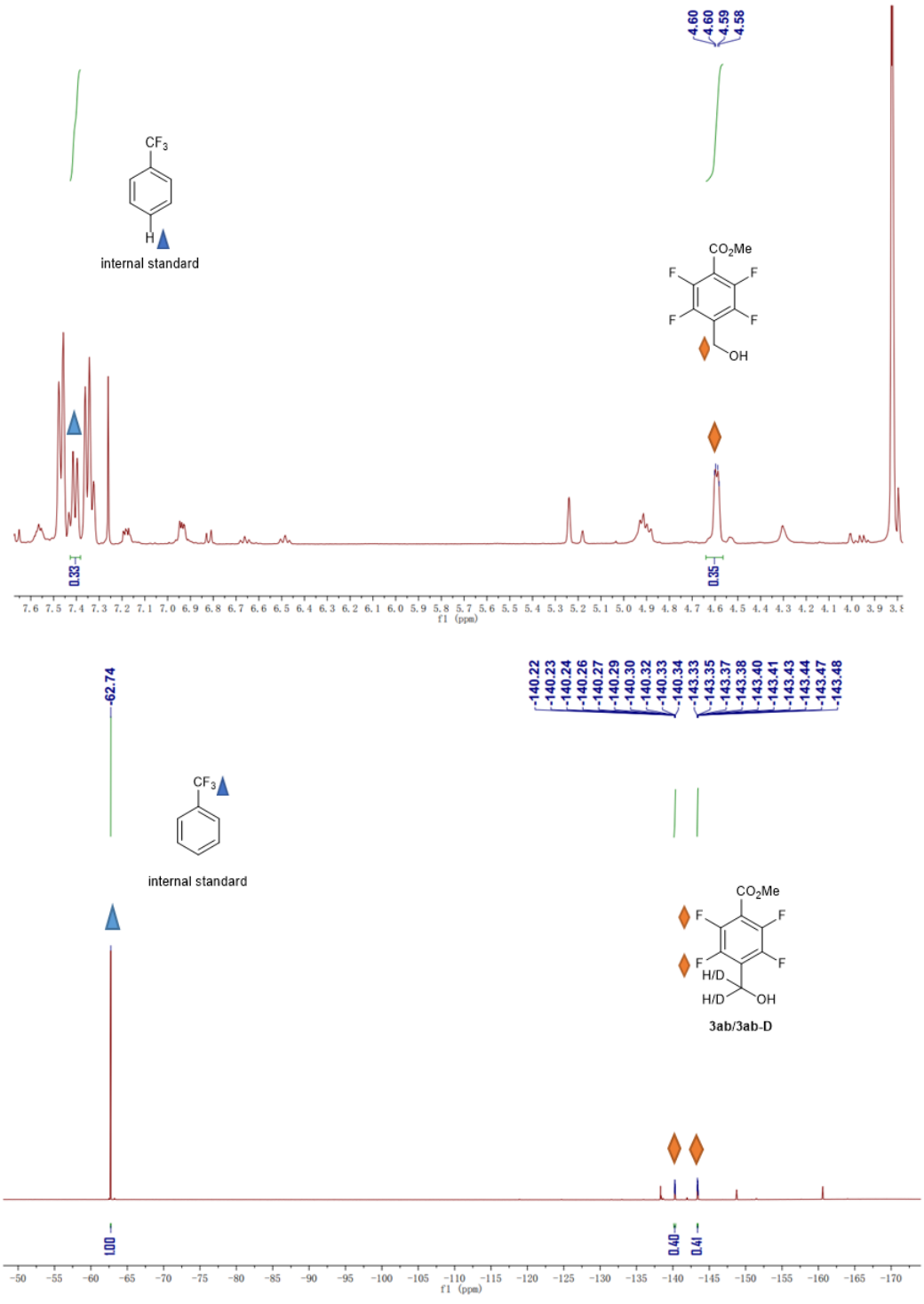
Methyl 2,3,5,6-tetrafluoro-4-(hydroxymethyl-d2)benzoate (**3ab-D**): colorless oil (23 mg, 47%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.98 (s, 3H), 2.07 (s, 1H); ^{19}F NMR (377 MHz, $CDCl_3$): δ -139.22 – -139.34 (m, 2F), -143.44 – -143.56 (m, 2F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.11 – 160.01 (m), 146.38 – 143.57 (m), 145.89 - 143.08 (m), 121.54 (t, J = 17.4 Hz), 112.48 (t, J = 16.1 Hz), 53.33; HRMS (EI): Calcd for $C_9H_5D_2O_3F_4$ $[M+H]^+$ 241.0457, found 241.0451.

Determination of the KIE value



1a **2b/2b-D** (1:1) (5 equiv) **3ab/3ab-D**, 20%

The KIE value (5.8) was determined by the measurement of initial rates of the reaction by ^{1}H NMR and ^{19}F NMR using trifluorotoluene (0.033 mmol) as an internal standard.



7.8 Quantum Yield Measurement

Determination of the light intensity at 470 nm: Following Yoon's protocol,[2] the photon flux of the spectrophotometer was determined by standard ferrioxalate actinometry. A 0.15 M solution of ferrioxalate was prepared by dissolving 2.21 g of potassium

ferrioxalate hydrate in 30 mL of 0.05 M H_2SO_4. A buffered solution of phenanthroline was prepared by dissolving 50 mg of phenanthroline and 11.25 g of sodium acetate in 50 mL of 0.5 M H_2SO_4. Both solutions were stored in the dark. To determine the photon flux of the spectrophotometer, 2.0 mL of the ferrioxalate solution was placed in a cuvette and irradiated for 90.0 seconds at λ = 470 nm with an emission slit width at 10.0 nm. After irradiation, 0.35 mL of the phenanthroline solution was added to the cuvette. The solution was then allowed to rest for 1 h to allow the ferrous ions to completely coordinate to the phenanthroline. The absorbance of the solution was measured at 510 nm. A non-irradiated sample was also prepared and the absorbance at 510 nm measured. Conversion was calculated using eq (1).

$$\text{mol } Fe^{2+} = \frac{V \cdot \Delta A}{1 \cdot \varepsilon} \quad (1)$$

Where V is the total volume (0.00235 L) of the solution after addition of phenanthroline, ΔA is the difference in absorbance at 510 nm between the irradiated and non-irradiated solutions, l is the path length (1.000 cm), and ε is the molar absorptivity at 510 nm (11,100 L mol^{-1} cm^{-1}). The photon flux can be calculated using eq (2).

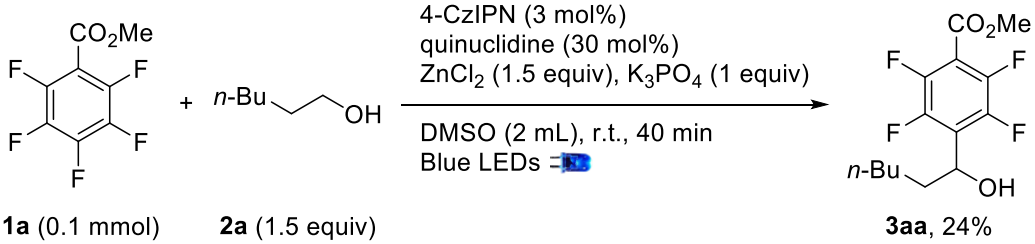
$$Photon\ flux = \frac{\text{mol } Fe^{2+}}{\Phi \cdot t \cdot f} \quad (2)$$

Where Φ is the quantum yield for the ferrioxalate actinometer (0.92 for a 0.15 M solution at λ = 468 nm),[3] t is the time (90.0 s), and f is the fraction of light absorbed at λ = 470 nm (0.14, vide infra).[4] The photon flux was calculated (average of three experiments) to be 3.22 × 10^{-8} einstein s^{-1}.

$$\text{mol } Fe^{2+} = \frac{0.00235\ \text{L} \cdot\ 1.76}{1.000\ \text{cm} \cdot 11100\ \text{L mol}^{-1}\text{cm}^{-1}} = 3.73\ \times\ 10^{-7}\ \text{mol}$$

$$Photon\ flux = \frac{3.73\ \times\ 10^{-7}\ \text{mol}}{0.92 \cdot 90.0\ \text{s} \cdot 0.14} = 3.22\ \times\ 10^{-8}\ \text{mol}$$

Determination of quantum yield:



1a (0.1 mmol) **2a** (1.5 equiv) **3aa**, 24%

A cuvette was charged with **1a** (15 μL, 0.1 mmol), **2a** (19 μL, 0.15mmol), 4-CzIPN (**PC**, 2.4 mg, 0.003 mmol), quinuclidine (3.3 mg, 0.03 mmol), K_3PO_4 (21.2 mg, 0.1 mmol) and $ZnCl_2$ (20.5 mg, 0.15 mmol).and DMSO (2 mL). The cuvette was then capped with a PTFE stopper. The sample was stirred and irradiated (λ = 470 nm, slit width = 10.0 nm) for 2400 s (40 min). After irradiation, the solvent was removed. The yield of product formed was determined as 24% by crude ^{19}F NMR using trifluorotoluene as the internal standard. The quantum yield was determined using eq (3). Essentially all incident light (f > 0.999, vide infra) is absorbed by the 4-CzIPN at the reaction conditions described above. Φ (24%) = 0.31.

$$\Phi = \frac{mol\ product}{flux \cdot t \cdot f} \quad (3)$$

$$\Phi = \frac{0.24 \times 0.1 \times 10^{-3}\ mol}{3.21 \times 10^{-8}\ \text{mol} \cdot 2400\ \text{s} \cdot 1.00} = 0.31$$

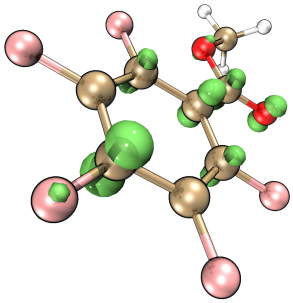
8. DFT Calculation

1. Computational details

All density functional theory (DFT) calculations were conducted with the Gaussian 16C program,[5] using the popular functionals of M06-2X.[6] Geometry optimizations were carried out with the Def2-TZVP basis set for all atoms,[7] using Truhlar's S56 SMD method (Solvation Model based on the Quantum Mechanical Charge Density),[8] with DMSO as the solvent. Cartesian coordinates (in Å) of related structures which optimized at the M06-2X/Def2-TZVP level of theory. The grid data of orbital Weighted Fukui function f_w^+ (OW_f^+, delta:0.066) were calculated *via* Multiwfn developed by Tian Lu,[9-10] which were further illustrated by VMD 1.9.3 program.[11]

2. Condensed Orbital Weighted (OW) Fukui function and dual descriptors

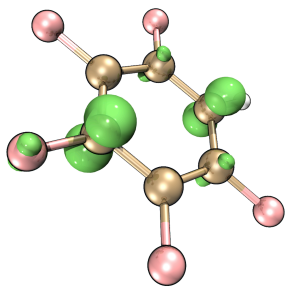
1a



Radial points: 30 Angular points: 302 Total: 9060 per center

Atom index	OW f+	OW f-	OW f0	OW DD
1(C)	0.15419	0.08005	0.11712	0.07414
2(C)	0.06089	0.15429	0.10759	-0.09340
3(C)	0.10444	0.14246	0.12345	-0.03802
4(C)	0.14709	0.08574	0.11641	0.06135
5(C)	0.10357	0.14437	0.12397	-0.04079
6(C)	0.06122	0.15191	0.10656	-0.09069
7(F)	0.01898	0.04554	0.03226	-0.02656
8(F)	0.00695	0.04728	0.02711	-0.04033
9(F)	0.01927	0.04691	0.03309	-0.02764
10(F)	0.00705	0.04637	0.02671	-0.03933
11(F)	0.03529	0.01893	0.02711	0.01636
12(C)	0.13368	0.00938	0.07153	0.12430
13(O)	0.09554	0.01782	0.05668	0.07772
14(O)	0.04227	0.00564	0.02396	0.03663
15(C)	0.00477	0.00159	0.00318	0.00318
16(H)	0.00037	0.00013	0.00025	0.00024
17(H)	0.00217	0.00076	0.00146	0.00140
18(H)	0.00217	0.00076	0.00146	0.00140

1f



Radial points: 30 Angular points: 302 Total: 9060 per center

Atom index	OW f+	OW f-	OW f0	OW

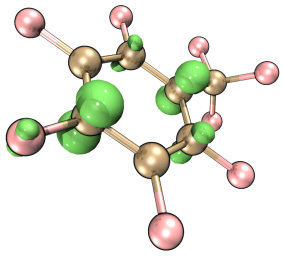
DD

1(C)	0.17330	0.09109	0.13220	0.08221
2(C)	0.11877	0.15508	0.13692	-0.03631
3(C)	0.12721	0.14563	0.13642	-0.01843
4(C)	0.17238	0.09695	0.13466	0.07544
5(C)	0.12721	0.14563	0.13642	-0.01843
6(C)	0.11877	0.15508	0.13692	-0.03631
7(H)	0.02944	0.00657	0.01801	0.02287
8(F)	0.02345	0.04441	0.03393	-0.02095
9(F)	0.02316	0.04647	0.03481	-0.02331
10(F)	0.02345	0.04441	0.03393	-0.02095
11(F)	0.02316	0.04647	0.03481	-0.02331
12(F)	0.03973	0.02224	0.03099	0.01750

Sum of orbital weighted f+ 1.000033

Sum of orbital weighted f- 1.000016

1g

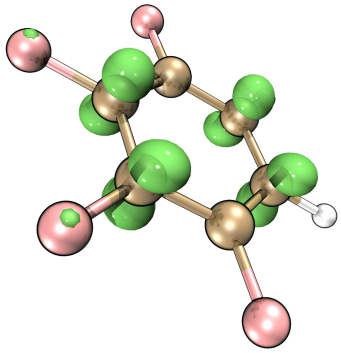


Radial points: 30 Angular points: 302 Total: 9060 per center

Atom index	OW f+	OW f-	OW f0	OW DD
1(C)	0.15114	0.11492	0.13303	0.03621
2(C)	0.10480	0.16791	0.13636	-0.06311
3(C)	0.16995	0.12371	0.14683	0.04624
4(C)	0.16993	0.12369	0.14681	0.04624
5(C)	0.10480	0.16791	0.13635	-0.06311
6(C)	0.15116	0.11494	0.13305	0.03622

7(F)	0.01626	0.05303	0.03465	-0.03678
8(F)	0.01626	0.05303	0.03464	-0.03678
9(F)	0.03091	0.03131	0.03111	-0.00040
10(F)	0.03090	0.03130	0.03110	-0.00040
11(H)	0.02690	0.00908	0.01799	0.01783
12(H)	0.02691	0.00908	0.01799	0.01783

1r

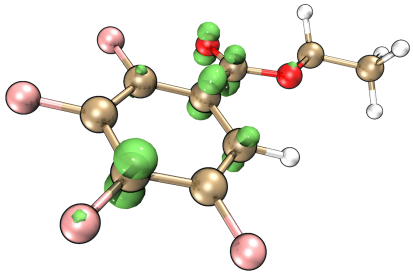


Radial points: 30 Angular points: 302 Total: 9060 per center

Atom index	OW f+	OW f-	OW f0	OW DD
1(C)	0.18438	0.07932	0.13185	0.10506
2(C)	0.09161	0.15416	0.12288	-0.06255
3(C)	0.12701	0.15350	0.14025	-0.02649
4(C)	0.17436	0.08052	0.12744	0.09384
5(C)	0.11930	0.14642	0.13286	-0.02712
6(C)	0.10073	0.16166	0.13119	-0.06092
7(F)	0.02327	0.04783	0.03555	-0.02456
8(F)	0.01400	0.04799	0.03099	-0.03399
9(F)	0.02072	0.04641	0.03357	-0.02568
10(F)	0.01655	0.05100	0.03377	-0.03445
11(F)	0.04180	0.01878	0.03029	0.02301
12(C)	0.04559	0.00617	0.02588	0.03942
13(F)	0.01701	0.00284	0.00992	0.01417

14(F)	0.01697	0.00283	0.00990	0.01414
15(F)	0.00675	0.00062	0.00369	0.00613

1t



Radial points: 30 Angular points: 302 Total: 9060 per center

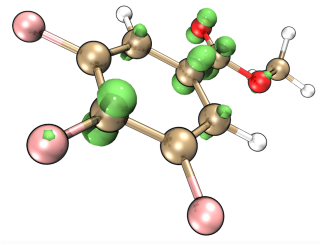
Atom index	OW f+	OW f-	OW f0	OW DD
1(C)	0.07250	0.11563	0.09406	-0.04313
2(C)	0.09171	0.15504	0.12337	-0.06334
3(C)	0.15162	0.11265	0.13213	0.03897
4(C)	0.12261	0.12615	0.12438	-0.00354
5(C)	0.05693	0.15787	0.10740	-0.10094
6(C)	0.14542	0.10298	0.12420	0.04244
7(F)	0.01547	0.05068	0.03307	-0.03522
8(F)	0.00590	0.05093	0.02841	-0.04503
9(F)	0.03241	0.02831	0.03036	0.00410
10(F)	0.01040	0.03309	0.02174	-0.02269
11(H)	0.01633	0.00920	0.01277	0.00713
12(C)	0.13391	0.01365	0.07378	0.12026
13(O)	0.09690	0.02735	0.06212	0.06955
14(O)	0.03834	0.00907	0.02370	0.02927
15(C)	0.00433	0.00292	0.00363	0.00141
16(H)	0.00184	0.00151	0.00168	0.00034
17(H)	0.00183	0.00143	0.00163	0.00040
18(C)	0.00079	0.00076	0.00078	0.00003
19(H)	0.00033	0.00030	0.00032	0.00003

20(H)	0.00016	0.00017	0.00017	-0.00001
21(H)	0.00032	0.00030	0.00031	0.00002

Sum of orbital weighted f+ 1.000030

Sum of orbital weighted f- 1.000001

1u



Radial points: 30 Angular points: 302 Total: 9060 per center

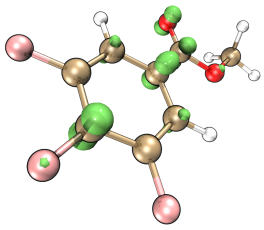
Atom index	OW f+	OW f-	OW f0	OW DD
1(C)	0.06161	0.12632	0.09397	-0.06471
2(C)	0.10919	0.13944	0.12431	-0.03025
3(C)	0.15602	0.13034	0.14318	0.02567
4(C)	0.10851	0.13612	0.12232	-0.02761
5(C)	0.06224	0.12982	0.09603	-0.06757
6(C)	0.13483	0.13693	0.13588	-0.00209
7(F)	0.00797	0.03960	0.02379	-0.03163
8(F)	0.02979	0.04111	0.03545	-0.01132
9(F)	0.00779	0.03826	0.02303	-0.03047
10(H)	0.01429	0.01004	0.01216	0.00425
11(C)	0.14333	0.01658	0.07996	0.12675
12(O)	0.09765	0.02921	0.06343	0.06844
13(O)	0.04222	0.01047	0.02634	0.03175
14(H)	0.01485	0.01033	0.01259	0.00452
15(C)	0.00482	0.00262	0.00372	0.00221
16(H)	0.00220	0.00127	0.00174	0.00093
17(H)	0.00041	0.00021	0.00031	0.00020

18(H)	0.00220	0.00127	0.00174	0.00093

Sum of orbital weighted f+ 0.999926

Sum of orbital weighted f- 0.999930

1v



Radial points: 30 Angular points: 302 Total: 9060 per center

Atom index	OW f+	OW f-	OW f0	OW DD
1(C)	0.08282	0.08623	0.08452	-0.00341
2(C)	0.07847	0.15937	0.11892	-0.08089
3(C)	0.13914	0.13765	0.13839	0.00149
4(C)	0.14273	0.09454	0.11864	0.04819
5(C)	0.05736	0.18545	0.12140	-0.12809
6(C)	0.15090	0.11609	0.13350	0.03481
7(F)	0.00510	0.06029	0.03270	-0.05519
8(F)	0.03216	0.03314	0.03265	-0.00098
9(H)	0.01973	0.00626	0.01300	0.01347
10(C)	0.13014	0.01722	0.07368	0.11292
11(O)	0.09522	0.03067	0.06294	0.06455
12(O)	0.03521	0.00831	0.02176	0.02690
13(C)	0.00407	0.00222	0.00315	0.00185
14(H)	0.00183	0.00106	0.00145	0.00077
15(H)	0.00183	0.00106	0.00145	0.00077
16(F)	0.01279	0.05446	0.03363	-0.04167
17(H)	0.01008	0.00571	0.00790	0.00437
18(H)	0.00036	0.00018	0.00027	0.00017

Sum of orbital weighted f+ 0.999951

Sum of orbital weighted f- 0.999919

3. Current orbital weights (delta=0.066 a.u.) used in orbital-weighted (OW) calculation

1a

HOMO energy: -0.319925 a.u. -8.706 eV

LUMO energy: -0.031879 a.u. -0.867 eV

Chemical potential: -0.175902 a.u. -4.787 eV

Delta parameter: 0.066000 a.u. 1.796 eV

The "E_diff" in below output denotes difference between orbital energy with respect to chemical potential

10 Highest weights in orbital-weighted f+

Orbital	57 (LUMO)	Weight:	96.54 %	E_diff:	3.919 eV
Orbital	58 (LUMO+1)	Weight:	2.90 %	E_diff:	5.164 eV
Orbital	59 (LUMO+2)	Weight:	0.56 %	E_diff:	5.655 eV
Orbital	60 (LUMO+3)	Weight:	0.00 %	E_diff:	7.114 eV
Orbital	61 (LUMO+4)	Weight:	0.00 %	E_diff:	7.222 eV
Orbital	62 (LUMO+5)	Weight:	0.00 %	E_diff:	7.610 eV
Orbital	63 (LUMO+6)	Weight:	0.00 %	E_diff:	8.130 eV
Orbital	64 (LUMO+7)	Weight:	0.00 %	E_diff:	8.526 eV
Orbital	65 (LUMO+8)	Weight:	0.00 %	E_diff:	8.835 eV

Total weight of above listed orbitals: 100.00 %

10 Highest weights in orbital-weighted f-

Orbital	56 (HOMO)	Weight:	73.77 %	E_diff:	-3.919 eV
Orbital	55 (HOMO-1)	Weight:	24.85 %	E_diff:	-4.344 eV
Orbital	54 (HOMO-2)	Weight:	1.03 %	E_diff:	-5.399 eV
Orbital	53 (HOMO-3)	Weight:	0.35 %	E_diff:	-5.715 eV
Orbital	52 (HOMO-4)	Weight:	0.00 %	E_diff:	-6.969 eV
Orbital	51 (HOMO-5)	Weight:	0.00 %	E_diff:	-7.174 eV

Orbital 50 (HOMO-6) Weight: 0.00 % E_diff: -8.233 eV

Orbital 49 (HOMO-7) Weight: 0.00 % E_diff: -8.315 eV

Orbital 48 (HOMO-8) Weight: 0.00 % E_diff: -8.334 eV

Orbital 47 (HOMO-9) Weight: 0.00 % E_diff: -9.145 eV

Total weight of above listed orbitals: 100.00 %

1f

HOMO energy: -0.315474 a.u. -8.584 eV

LUMO energy: 0.007142 a.u. 0.194 eV

Chemical potential: -0.154166 a.u. -4.195 eV

Delta parameter: 0.066000 a.u. 1.796 eV

The "E_diff" in below output denotes difference between orbital energy with respect to chemical potential

10 Highest weights in orbital-weighted f+

Orbital 42 (LUMO) Weight: 68.26 % E_diff: 4.389 eV

Orbital 43 (LUMO+1) Weight: 25.63 % E_diff: 4.736 eV

Orbital 44 (LUMO+2) Weight: 6.10 % E_diff: 5.201 eV

Orbital 45 (LUMO+3) Weight: 0.01 % E_diff: 7.028 eV

Orbital 46 (LUMO+4) Weight: 0.00 % E_diff: 7.391 eV

Orbital 47 (LUMO+5) Weight: 0.00 % E_diff: 8.108 eV

Orbital 48 (LUMO+6) Weight: 0.00 % E_diff: 8.857 eV

Orbital 49 (LUMO+7) Weight: 0.00 % E_diff: 9.548 eV

Orbital 50 (LUMO+8) Weight: 0.00 % E_diff: 9.643 eV

Total weight of above listed orbitals: 100.00 %

10 Highest weights in orbital-weighted f-

Orbital 41 (HOMO) Weight: 71.98 % E_diff: -4.389 eV

Orbital 40 (HOMO-1) Weight: 28.02 % E_diff: -4.723 eV

Orbital 39 (HOMO-2) Weight: 0.00 % E_diff: -7.773 eV

Orbital 38 (HOMO-3) Weight: 0.00 % E_diff: -8.661 eV

Orbital 37 (HOMO-4) Weight: 0.00 % E_diff: -8.781 eV

Orbital 36 (HOMO-5) Weight: 0.00 % E_diff: -9.585 eV

Orbital 35 (HOMO-6) Weight: 0.00 % E_diff: -10.861 eV

Orbital 34 (HOMO-7) Weight: 0.00 % E_diff: -10.877 eV

Orbital 33 (HOMO-8) Weight: 0.00 % E_diff: -11.102 eV

Orbital 32 (HOMO-9) Weight: 0.00 % E_diff: -11.493 eV

Total weight of above listed orbitals: 100.00 %

1g

HOMO energy: -0.313335 a.u. -8.526 eV

LUMO energy: 0.008771 a.u. 0.239 eV

Chemical potential: -0.152282 a.u. -4.144 eV

Delta parameter: 0.066000 a.u. 1.796 eV

The "E_diff" in below output denotes difference between orbital energy with respect to chemical potential

10 Highest weights in orbital-weighted f+

Orbital 38 (LUMO) Weight: 72.63 % E_diff: 4.382 eV

Orbital 39 (LUMO+1) Weight: 25.08 % E_diff: 4.758 eV

Orbital 40 (LUMO+2) Weight: 2.28 % E_diff: 5.511 eV

Orbital 41 (LUMO+3) Weight: 0.00 % E_diff: 7.134 eV

Orbital 42 (LUMO+4) Weight: 0.00 % E_diff: 7.329 eV

Orbital 43 (LUMO+5) Weight: 0.00 % E_diff: 8.103 eV

Orbital 44 (LUMO+6) Weight: 0.00 % E_diff: 8.787 eV

Orbital 45 (LUMO+7) Weight: 0.00 % E_diff: 9.154 eV

Orbital 46 (LUMO+8) Weight: 0.00 % E_diff: 9.638 eV

Total weight of above listed orbitals: 100.00 %

10 Highest weights in orbital-weighted f-

Orbital 37 (HOMO) Weight: 70.44 % E_diff: -4.382 eV

Orbital 36 (HOMO-1) Weight: 29.56 % E_diff: -4.691 eV

Orbital 35 (HOMO-2) Weight: 0.00 % E_diff: -7.855 eV

Orbital 34 (HOMO-3) Weight: 0.00 % E_diff: -8.158 eV

Orbital 33 (HOMO-4) Weight: 0.00 % E_diff: -8.673 eV

Orbital 32 (HOMO-5) Weight: 0.00 % E_diff: -9.268 eV

Orbital 31 (HOMO-6) Weight: 0.00 % E_diff: -10.661 eV

Orbital 30 (HOMO-7) Weight: 0.00 % E_diff: -10.905 eV

Orbital 29 (HOMO-8) Weight: 0.00 % E_diff: -10.961 eV

Orbital 28 (HOMO-9) Weight: 0.00 % E_diff: -11.434 eV

Total weight of above listed orbitals: 100.00 %

1r

HOMO energy: -0.326010 a.u. -8.871 eV

LUMO energy: -0.016123 a.u. -0.439 eV

Chemical potential: -0.171067 a.u. -4.655 eV

Delta parameter: 0.066000 a.u. 1.796 eV

The "E_diff" in below output denotes difference between orbital energy with respect to chemical potential

10 Highest weights in orbital-weighted f+

Orbital 58 (LUMO) Weight: 84.48 % E_diff: 4.216 eV

Orbital 59 (LUMO+1) Weight: 12.84 % E_diff: 4.884 eV

Orbital 60 (LUMO+2) Weight: 2.67 % E_diff: 5.377 eV

Orbital 61 (LUMO+3) Weight: 0.00 % E_diff: 7.284 eV

Orbital 62 (LUMO+4) Weight: 0.00 % E_diff: 7.951 eV

Orbital 63 (LUMO+5) Weight: 0.00 % E_diff: 8.774 eV

Orbital 64 (LUMO+6) Weight: 0.00 % E_diff: 9.082 eV

Orbital 65 (LUMO+7) Weight: 0.00 % E_diff: 9.328 eV

Orbital 66 (LUMO+8) Weight: 0.00 % E_diff: 9.465 eV

Total weight of above listed orbitals: 100.00 %

10 Highest weights in orbital-weighted f-

Orbital 57 (HOMO) Weight: 77.80 % E_diff: -4.216 eV

Orbital 56 (HOMO-1) Weight: 22.20 % E_diff: -4.671 eV

Orbital 55 (HOMO-2) Weight: 0.00 % E_diff: -7.624 eV

Orbital 54 (HOMO-3) Weight: 0.00 % E_diff: -8.273 eV

Orbital 53 (HOMO-4) Weight: 0.00 % E_diff: -8.511 eV

Orbital 52 (HOMO-5) Weight: 0.00 % E_diff: -9.499 eV

Orbital 51 (HOMO-6) Weight: 0.00 % E_diff: -9.730 eV

Orbital 50 (HOMO-7) Weight: 0.00 % E_diff: -10.037 eV

Orbital 49 (HOMO-8) Weight: 0.00 % E_diff: -10.139 eV

Orbital 48 (HOMO-9) Weight: 0.00 % E_diff: -10.240 eV

Total weight of above listed orbitals: 100.00 %

1t

HOMO energy: -0.319853 a.u. -8.704 eV

LUMO energy: -0.027371 a.u. -0.745 eV

Chemical potential: -0.173612 a.u. -4.724 eV

Delta parameter: 0.066000 a.u. 1.796 eV

The "E_diff" in below output denotes difference between orbital energy with respect to chemical potential

10 Highest weights in orbital-weighted f+

Orbital 57 (LUMO) Weight: 95.49 % E_diff: 3.979 eV

Orbital 58 (LUMO+1) Weight: 4.34 % E_diff: 5.080 eV

Orbital 59 (LUMO+2) Weight: 0.16 % E_diff: 6.033 eV

Orbital 60 (LUMO+3) Weight: 0.01 % E_diff: 6.810 eV

Orbital 61 (LUMO+4) Weight: 0.00 % E_diff: 7.135 eV

Orbital 62 (LUMO+5) Weight: 0.00 % E_diff: 7.625 eV

Orbital 63 (LUMO+6) Weight: 0.00 % E_diff: 8.043 eV

Orbital 64 (LUMO+7) Weight: 0.00 % E_diff: 8.080 eV

Orbital 65 (LUMO+8) Weight: 0.00 % E_diff: 8.524 eV

Total weight of above listed orbitals: 100.00 %

10 Highest weights in orbital-weighted f-

Orbital 56 (HOMO) Weight: 67.46 % E_diff: -3.979 eV

Orbital 55 (HOMO-1) Weight: 30.33 % E_diff: -4.291 eV

Orbital 54 (HOMO-2) Weight: 1.61 % E_diff: -5.280 eV

Orbital 53 (HOMO-3) Weight: 0.59 % E_diff: -5.580 eV

Orbital 52 (HOMO-4) Weight: 0.01 % E_diff: -6.721 eV

Orbital 51 (HOMO-5) Weight: 0.00 % E_diff: -6.839 eV

Orbital 50 (HOMO-6) Weight: 0.00 % E_diff: -7.391 eV

Orbital 49 (HOMO-7) Weight: 0.00 % E_diff: -7.585 eV

Orbital 48 (HOMO-8) Weight: 0.00 % E_diff: -8.096 eV

Orbital 47 (HOMO-9) Weight: 0.00 % E_diff: -8.150 eV

Total weight of above listed orbitals: 100.00 %

1u

HOMO energy: -0.323670 a.u. -8.807 eV

LUMO energy: -0.025742 a.u. -0.700 eV

Chemical potential: -0.174706 a.u. -4.754 eV

Delta parameter: 0.066000 a.u. 1.796 eV

The "E_diff" in below output denotes difference between orbital energy with respect to chemical potential

10 Highest weights in orbital-weighted f+

Orbital 49 (LUMO) Weight: 94.88 % E_diff: 4.054 eV

Orbital 50 (LUMO+1) Weight: 5.08 % E_diff: 5.086 eV

Orbital 51 (LUMO+2) Weight: 0.03 % E_diff: 6.492 eV

Orbital 52 (LUMO+3) Weight: 0.00 % E_diff: 7.136 eV

Orbital 53 (LUMO+4) Weight: 0.00 % E_diff: 7.358 eV

Orbital 54 (LUMO+5) Weight: 0.00 % E_diff: 7.828 eV

Orbital 55 (LUMO+6) Weight: 0.00 % E_diff: 8.164 eV

Orbital 56 (LUMO+7) Weight: 0.00 % E_diff: 8.391 eV

Orbital 57 (LUMO+8) Weight: 0.00 % E_diff: 8.798 eV

Total weight of above listed orbitals: 100.00 %

10 Highest weights in orbital-weighted f-

Orbital 48 (HOMO) Weight: 51.14 % E_diff: -4.054 eV

Orbital	47 (HOMO-1)	Weight:	47.20 %	E_diff:	-4.085 eV
Orbital	46 (HOMO-2)	Weight:	1.30 %	E_diff:	-5.319 eV
Orbital	45 (HOMO-3)	Weight:	0.36 %	E_diff:	-5.694 eV
Orbital	44 (HOMO-4)	Weight:	0.00 %	E_diff:	-6.997 eV
Orbital	43 (HOMO-5)	Weight:	0.00 %	E_diff:	-7.217 eV
Orbital	42 (HOMO-6)	Weight:	0.00 %	E_diff:	-7.669 eV
Orbital	41 (HOMO-7)	Weight:	0.00 %	E_diff:	-8.008 eV
Orbital	40 (HOMO-8)	Weight:	0.00 %	E_diff:	-8.376 eV
Orbital	39 (HOMO-9)	Weight:	0.00 %	E_diff:	-8.544 eV

Total weight of above listed orbitals: 100.00 %

1v

HOMO energy: -0.313889 a.u. -8.541 eV

LUMO energy: -0.025042 a.u. -0.681 eV

Chemical potential: -0.169465 a.u. -4.611 eV

Delta parameter: 0.066000 a.u. 1.796 eV

The "E_diff" in below output denotes difference between orbital energy with respect to chemical potential

10 Highest weights in orbital-weighted f+

Orbital	49 (LUMO)	Weight:	94.37 %	E_diff:	3.930 eV
Orbital	50 (LUMO+1)	Weight:	5.62 %	E_diff:	4.954 eV
Orbital	51 (LUMO+2)	Weight:	0.01 %	E_diff:	6.824 eV
Orbital	52 (LUMO+3)	Weight:	0.00 %	E_diff:	7.022 eV
Orbital	53 (LUMO+4)	Weight:	0.00 %	E_diff:	7.140 eV
Orbital	54 (LUMO+5)	Weight:	0.00 %	E_diff:	7.630 eV
Orbital	55 (LUMO+6)	Weight:	0.00 %	E_diff:	7.809 eV
Orbital	56 (LUMO+7)	Weight:	0.00 %	E_diff:	8.029 eV
Orbital	57 (LUMO+8)	Weight:	0.00 %	E_diff:	8.490 eV

Total weight of above listed orbitals: 100.00 %

10 Highest weights in orbital-weighted f-

Orbital	48 (HOMO)	Weight:	80.06 %	E_diff:	-3.930 eV
Orbital	47 (HOMO-1)	Weight:	18.23 %	E_diff:	-4.496 eV
Orbital	46 (HOMO-2)	Weight:	1.42 %	E_diff:	-5.334 eV
Orbital	45 (HOMO-3)	Weight:	0.29 %	E_diff:	-5.798 eV
Orbital	44 (HOMO-4)	Weight:	0.00 %	E_diff:	-7.146 eV
Orbital	43 (HOMO-5)	Weight:	0.00 %	E_diff:	-7.346 eV
Orbital	42 (HOMO-6)	Weight:	0.00 %	E_diff:	-7.766 eV
Orbital	41 (HOMO-7)	Weight:	0.00 %	E_diff:	-8.316 eV
Orbital	40 (HOMO-8)	Weight:	0.00 %	E_diff:	-8.416 eV
Orbital	39 (HOMO-9)	Weight:	0.00 %	E_diff:	-8.742 eV

Total weight of above listed orbitals: 100.00 %

4. Cartesian coordinates (in Å) of related structures

1a

C	0.44192400	-2.17775900	0.00000000
C	-0.84465500	-1.67806600	0.00000000
C	-1.05790800	-0.31258200	0.00000000
C	0.00000000	0.59855500	0.00000000
C	1.28755400	0.05750000	0.00000000
C	1.51152100	-1.30535700	0.00000000
F	-2.32631600	0.07178400	0.00000000
F	-1.87633400	-2.51385500	0.00000000
F	2.36700400	0.82482400	0.00000000
F	2.75158900	-1.77848700	0.00000000
F	0.64844500	-3.48283200	0.00000000
C	-0.17475000	2.08581900	0.00000000
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C	-1.68724000	3.86368100	0.00000000
H	-2.76691200	3.97852700	0.00000000

H	-1.25650500	4.31847600	0.89068300
H	-1.25650500	4.31847600	-0.89068300

1f

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C	0.00000000	1.19810300	0.41972800
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C	0.00000000	-1.18261100	-0.96291800
C	0.00000000	-1.19810300	0.41972800
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F	0.00000000	-2.35144400	-1.60386600
F	0.00000000	-2.34755200	1.08783200
F	0.00000000	0.00000000	2.43711500

1g

C	0.69073826	0.67916883	0.00000169
C	1.37125386	-0.52609775	0.00000658
C	0.69430112	-1.72606836	0.00000179
C	-0.69429152	-1.72604169	0.00000187
C	-1.37125717	-0.52609969	0.00000371
C	-0.69072835	0.67916546	-0.00000244
F	2.70766002	-0.49029634	-0.00000114
F	-2.70767253	-0.49028942	-0.00000235
F	-1.35131623	1.83338009	-0.00000502
F	1.35132101	1.83339332	-0.00000026
H	-1.25639535	-2.64989702	0.00000005
H	1.25636770	-2.64995262	-0.00000038

1r

C	-2.12150615	-0.05876700	-0.00006100
C	-1.38041110	-1.22738409	0.00001900
C	-0.00427000	-1.15253808	0.00004000
C	0.66307705	0.06538900	-0.00010600
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C	-1.48120410	1.16434508	-0.00007700
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F	-2.19229116	2.28339516	-0.00007100
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F	2.63918019	-0.60047205	1.07519008
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F	2.70615119	1.25706309	-0.00213200

1t

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C	2.42212075	0.58853011	0.01739663
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H	1.37725988	4.32876297	0.89063019
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H	1.37725988	4.32876297	-0.89063019

1v

C	1.81561675	-1.15455115	0.00000000

C	1.35516142	0.14929429	0.00000000
C	0.00000000	0.46457980	0.00000000
C	-0.91495927	-0.59124700	0.00000000
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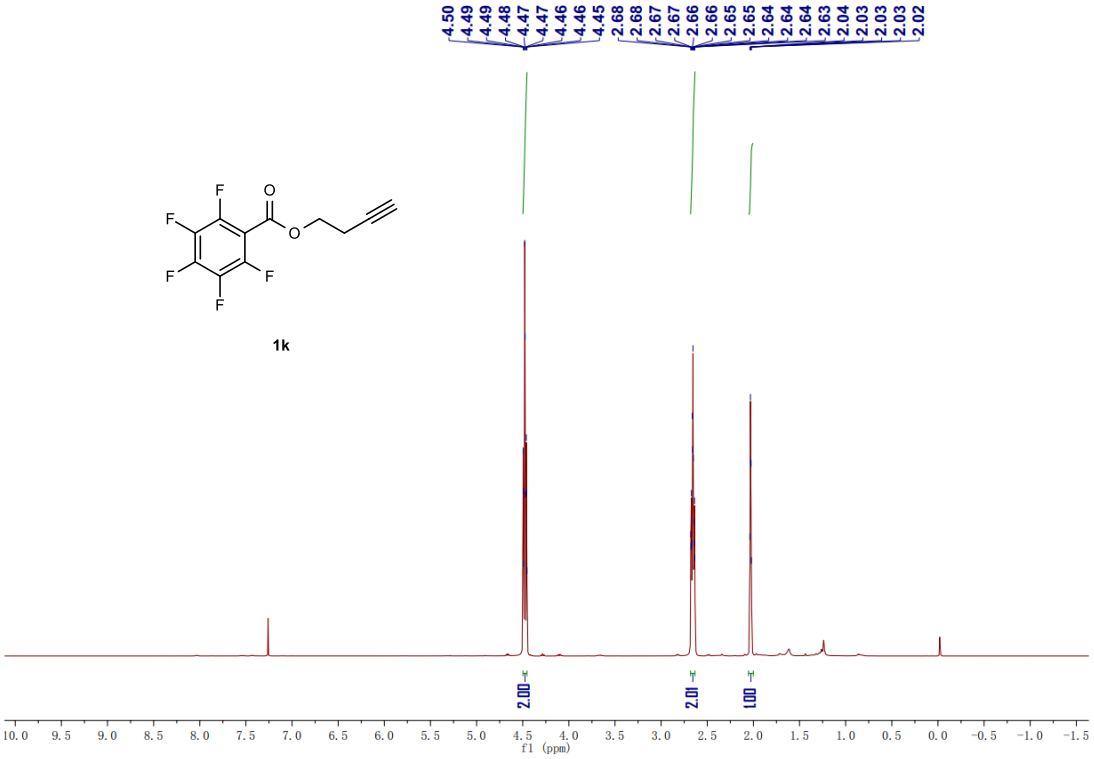
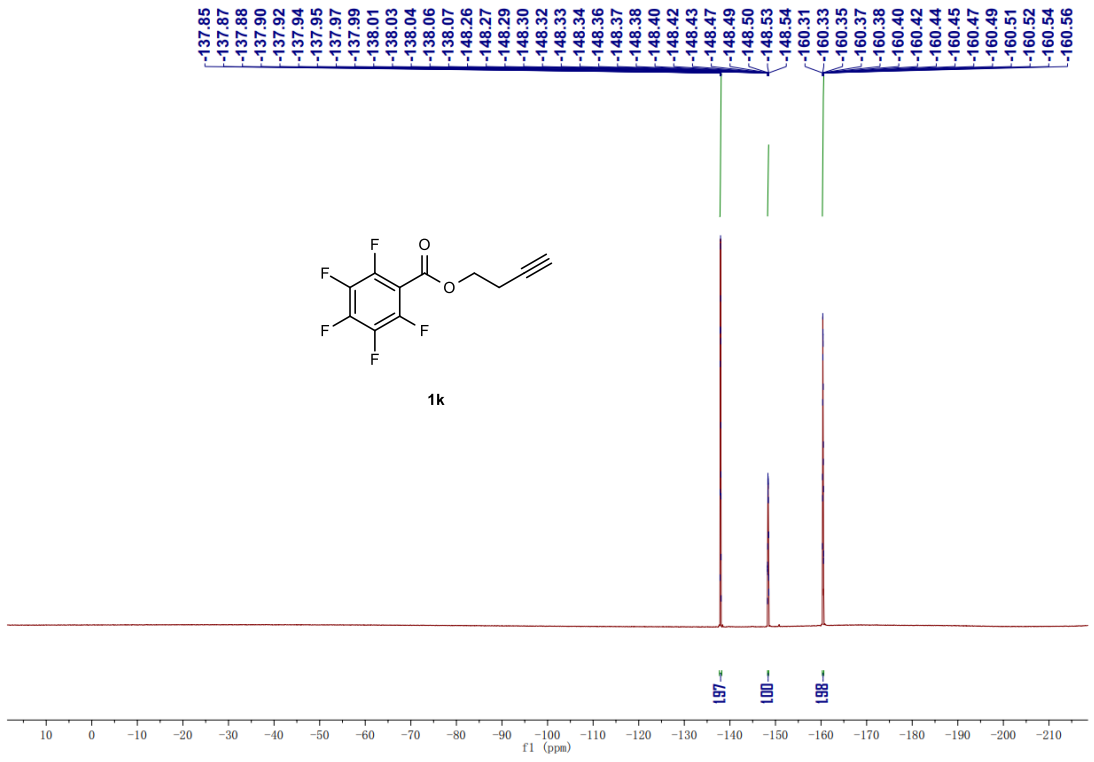
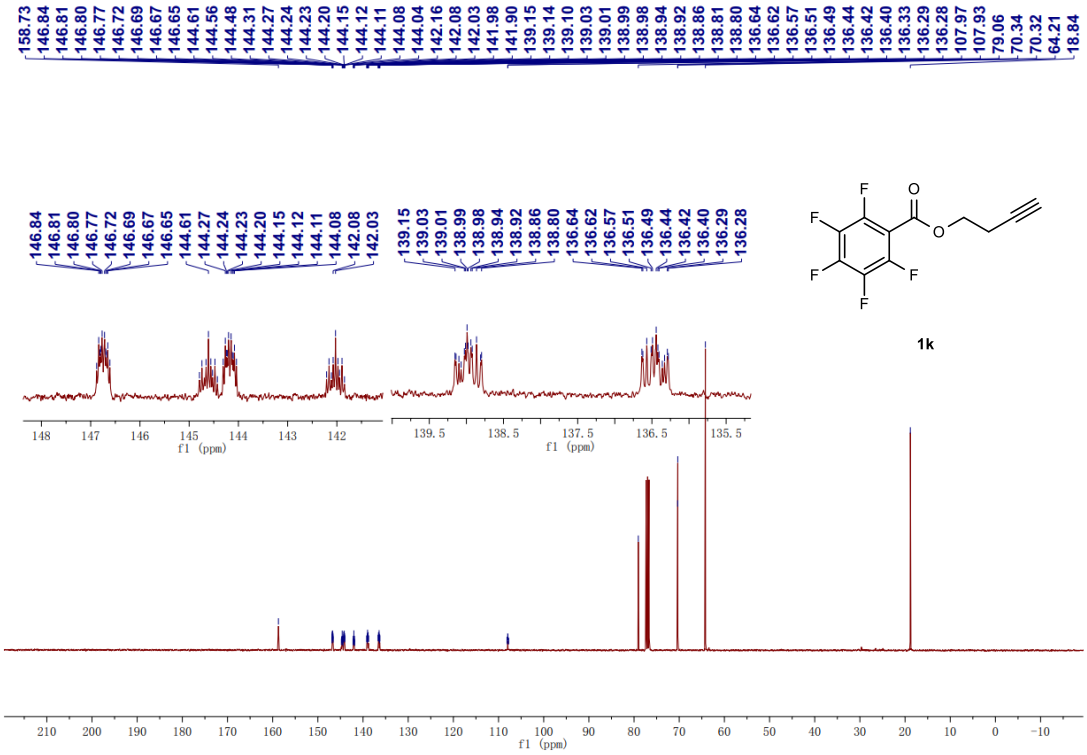
^{1}H, ^{19}F, ^{13}C-NMR Spectra



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144.27
144.24
144.23
144.20
144.15
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142.08
142.03
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139.03
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136.33
136.29
136.28
107.97
107.93
79.06
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70.32
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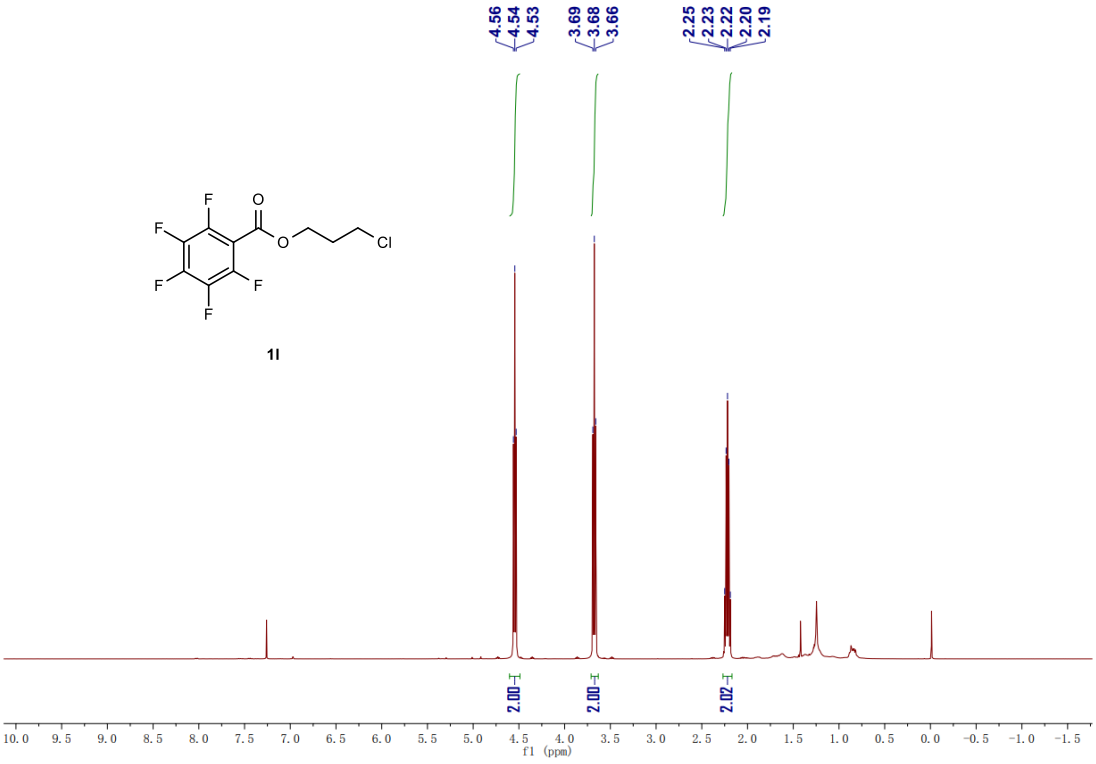
18.84
F
O
O
F
F
F
F
1k
f1 (ppm)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O
O
Cl
F
F
F
F
1l
2.00
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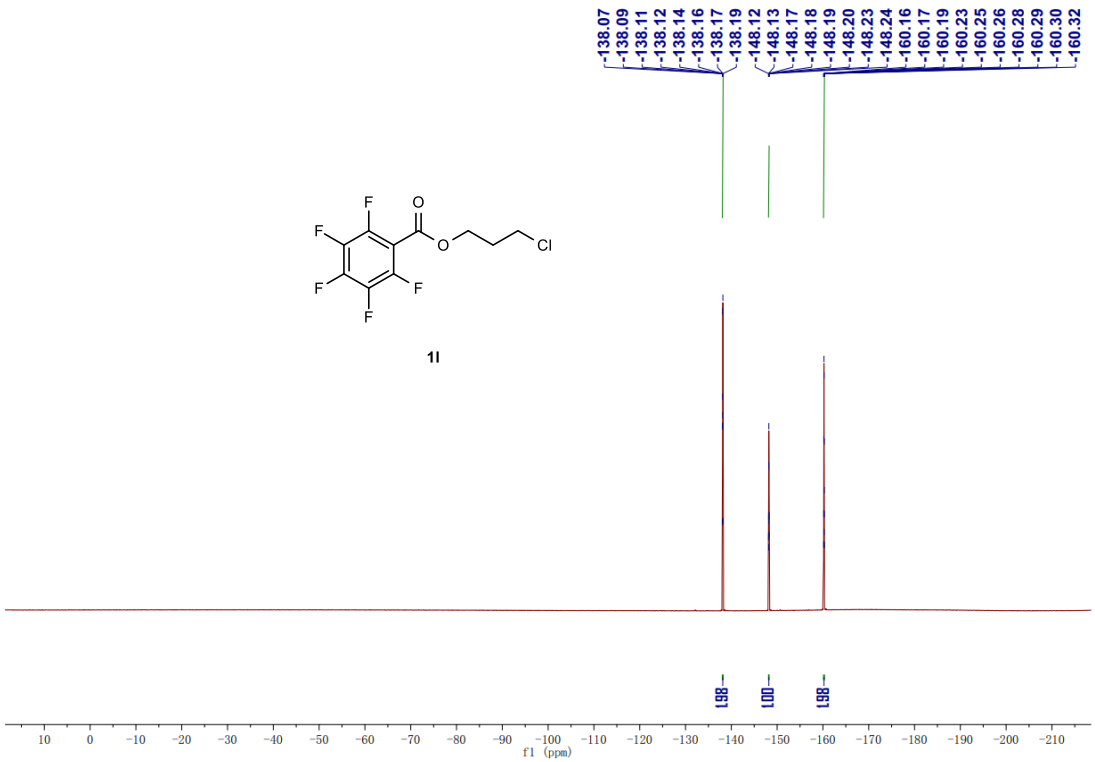
2.02
f1 (ppm)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-148.24
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-160.19
-160.23
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-160.26
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-160.29
-160.30
-160.32
F
O
F
O
Cl
F
F
F
1.98
1.00
1.98
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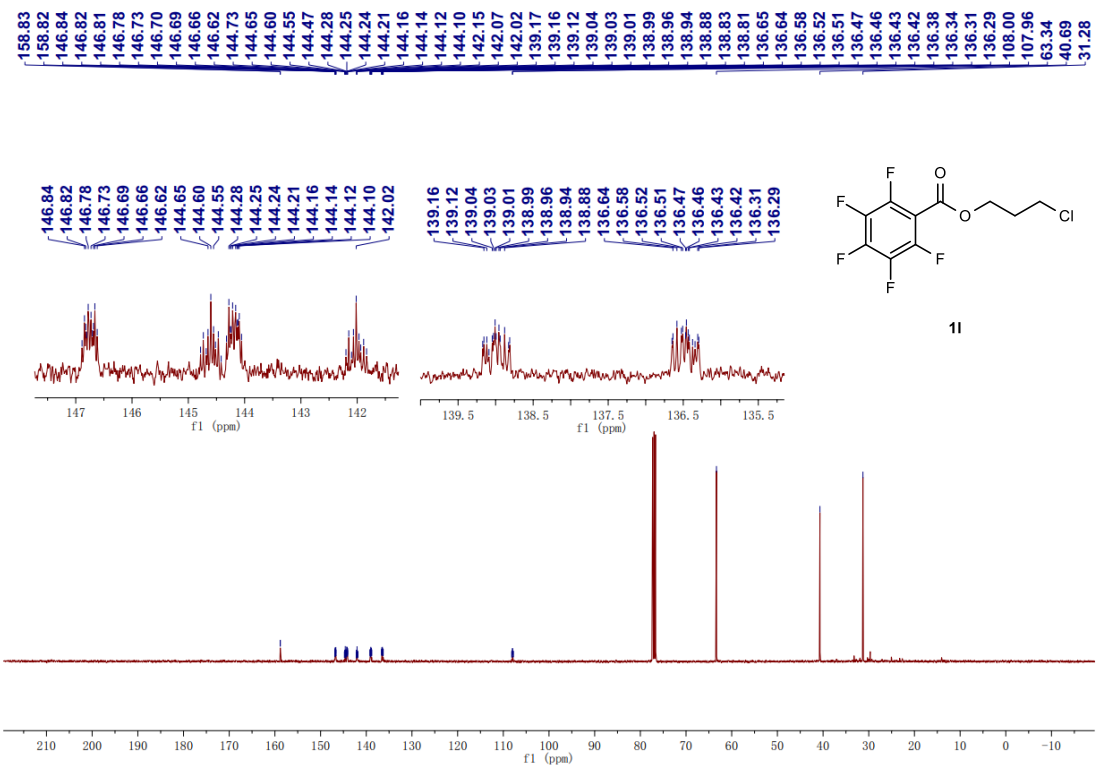
f1 (ppm)

1l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136.51
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136.46
136.43
136.42
136.31
136.29
147 146 145 144 143 142
f1 (ppm)
139.5 138.5 137.5 136.5 135.5
f1 (ppm)
F
O
F
O
Cl
F
F
F
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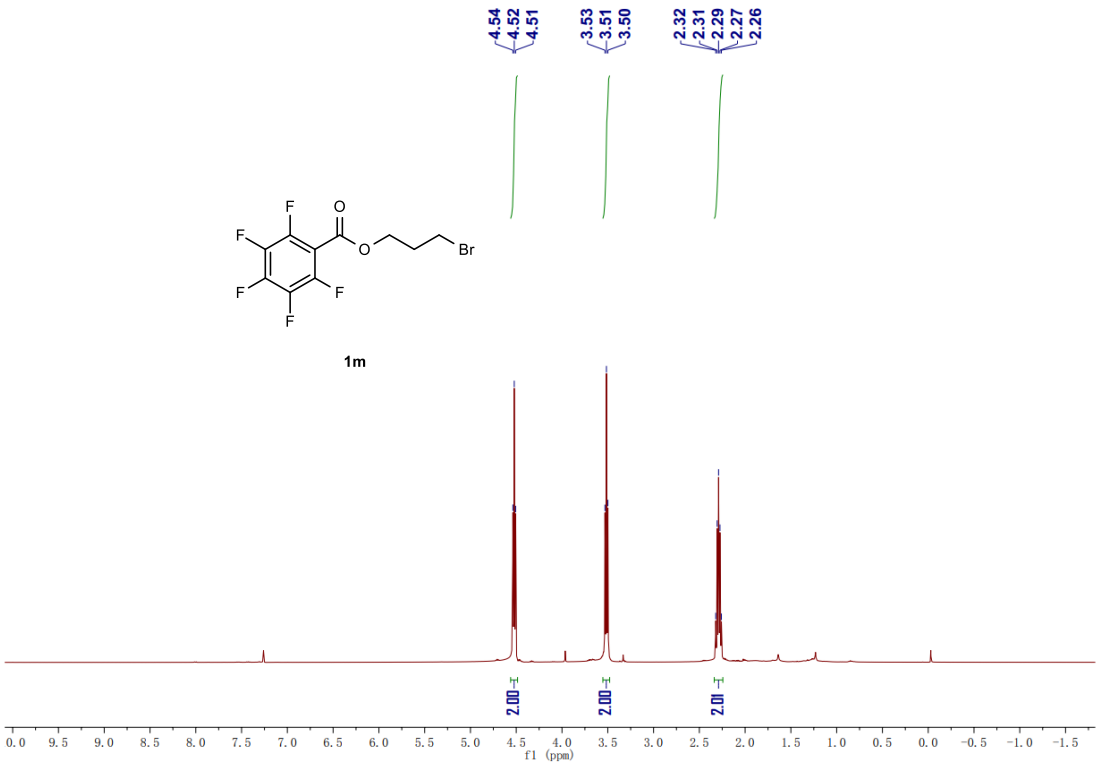
f1 (ppm)

1l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F
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Br
F
F
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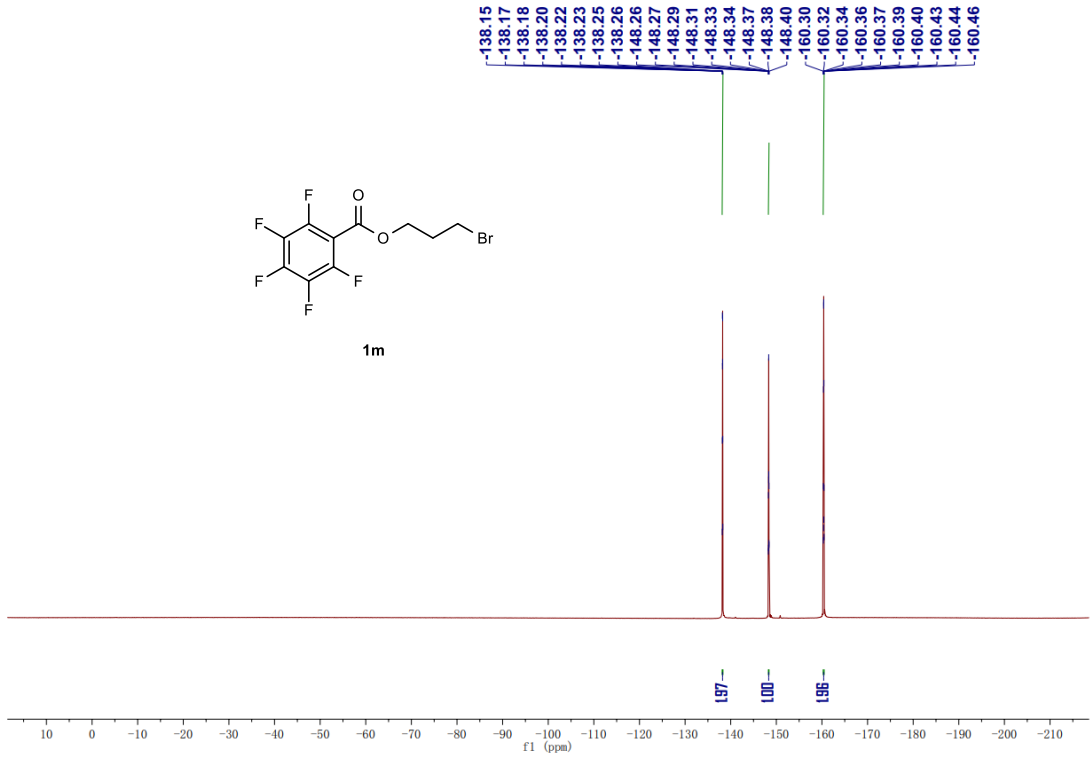
2.00
2.01
f1 (ppm)

1m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F
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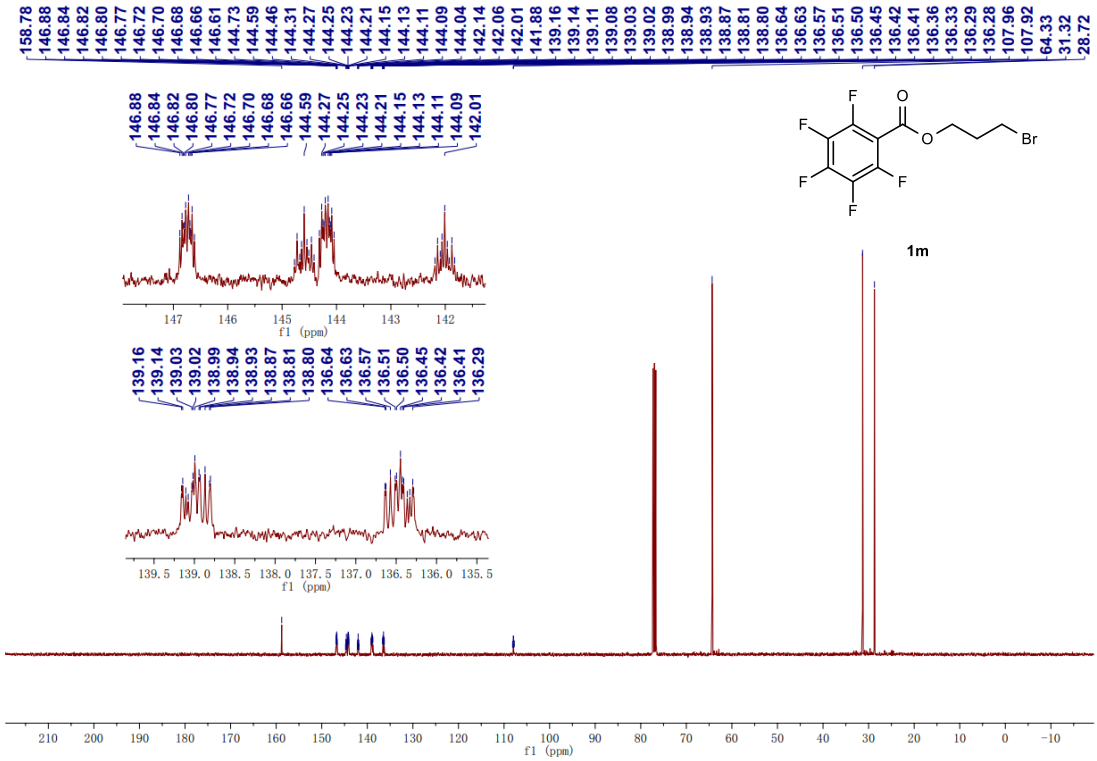
f1 (ppm)

1m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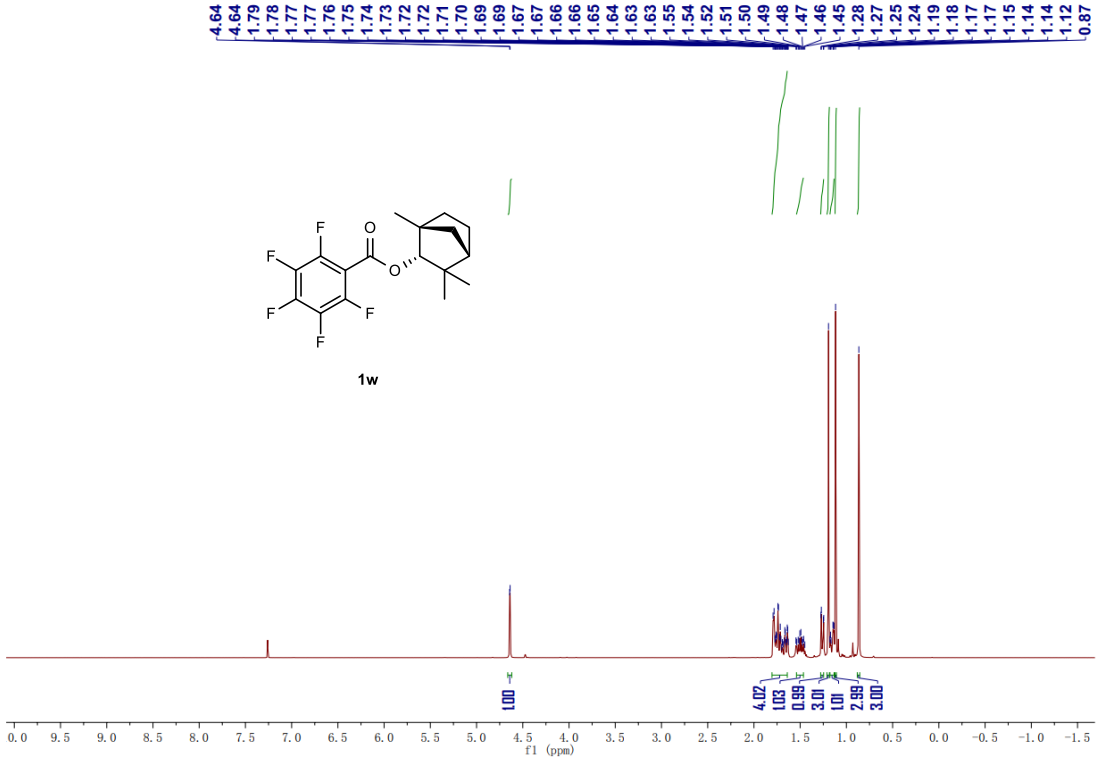
O
F
O
Br
F
F
F
1m
f1 (ppm)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O
F
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F
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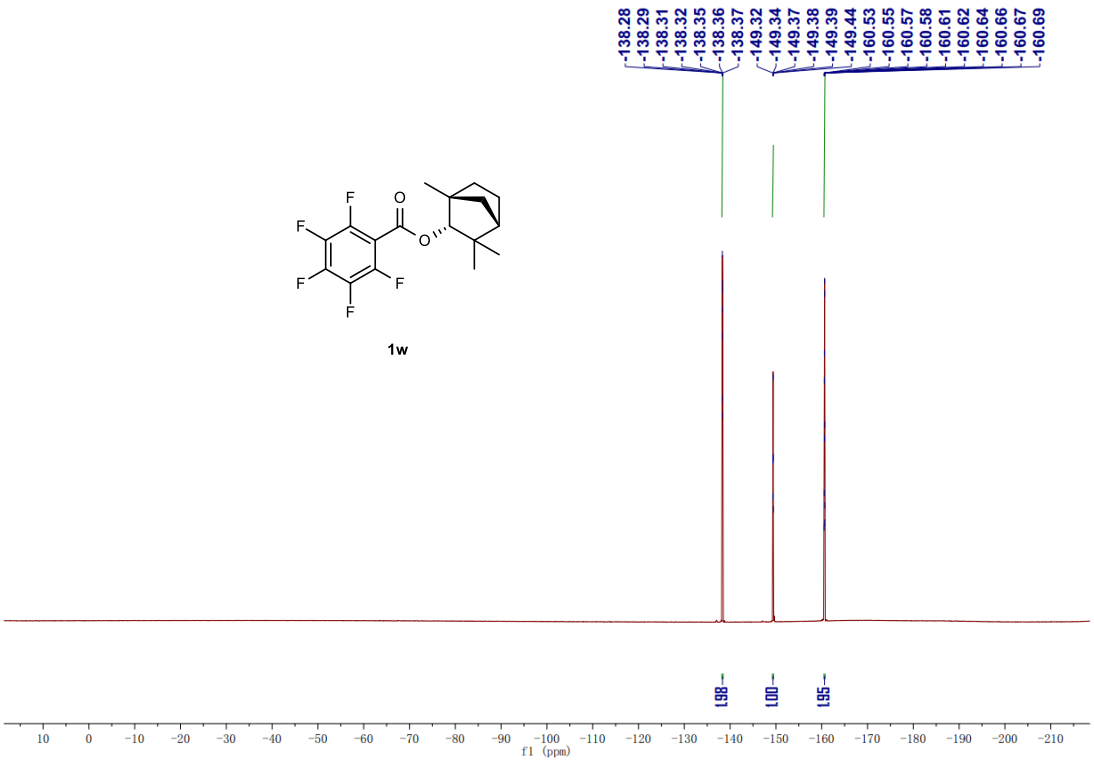
3.00
f1 (ppm)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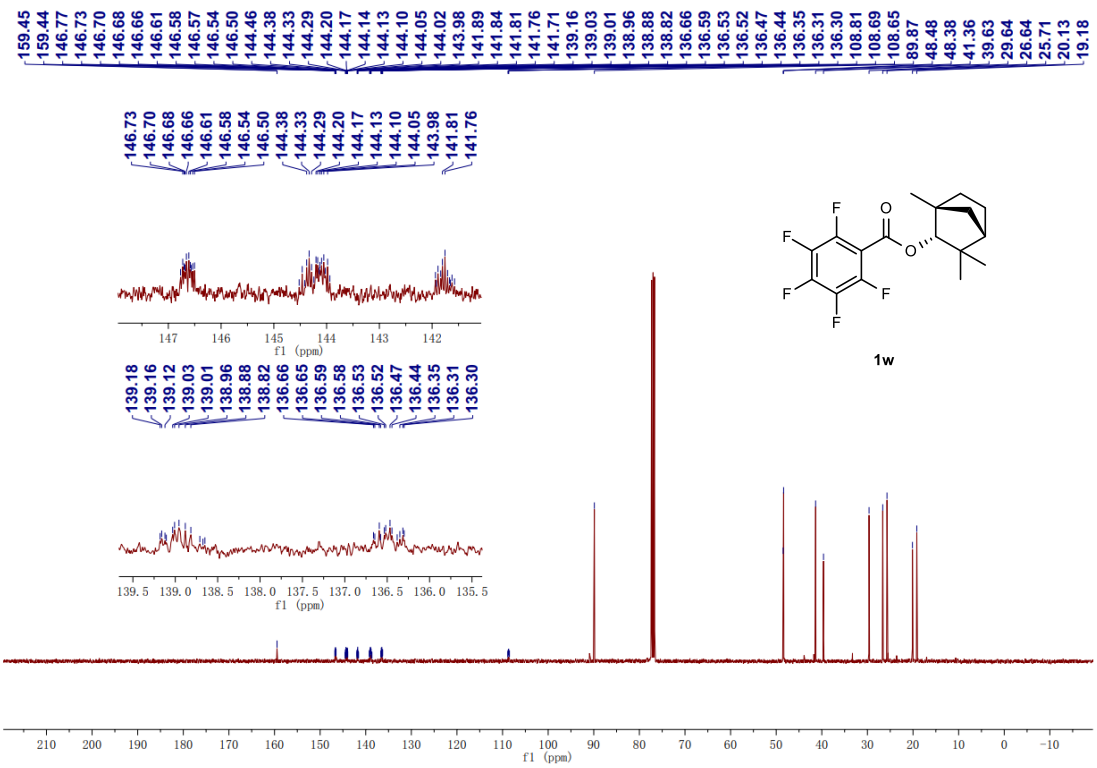
1.95
f1 (ppm)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146.58
146.57
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144.33
144.29
144.20
144.17
144.14
144.13
144.10
144.05
144.02
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141.81
141.76
141.71
139.16
139.03
139.01
138.96
138.88
138.82
136.66
136.59
136.53
136.52
136.47
136.44
136.35
136.31
136.30
108.81
108.69
108.65
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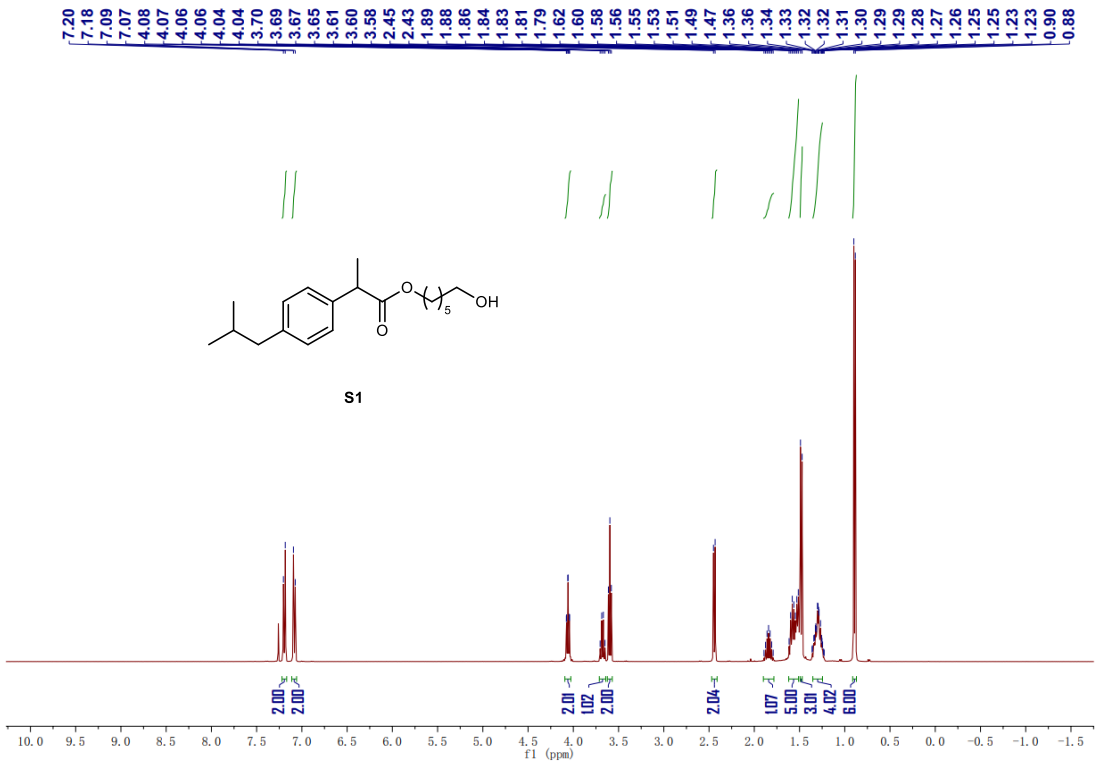
29.64
26.64
25.71
20.13
19.18
1w
f1 (ppm)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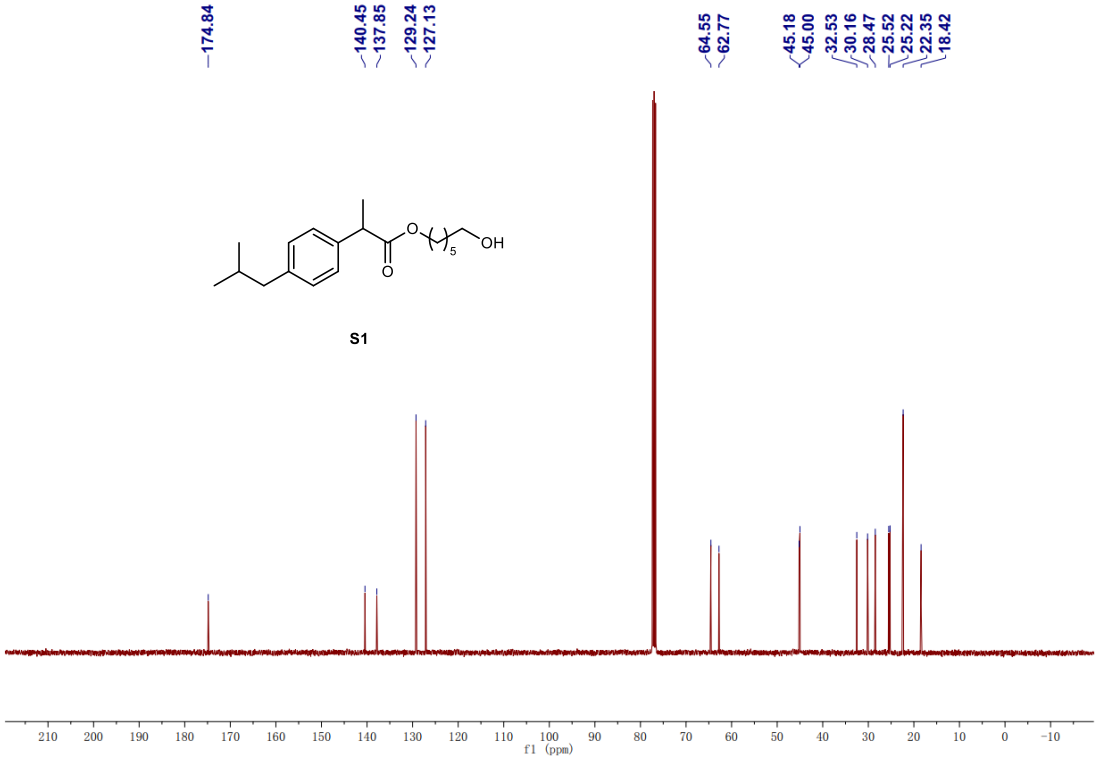
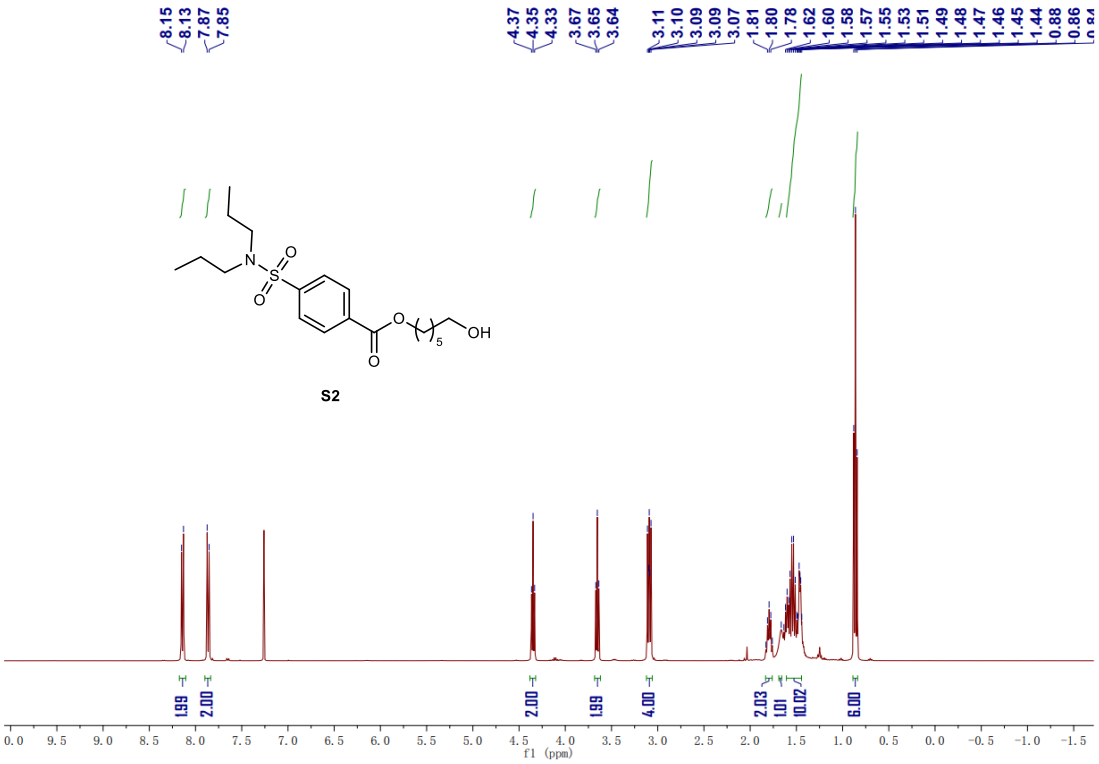
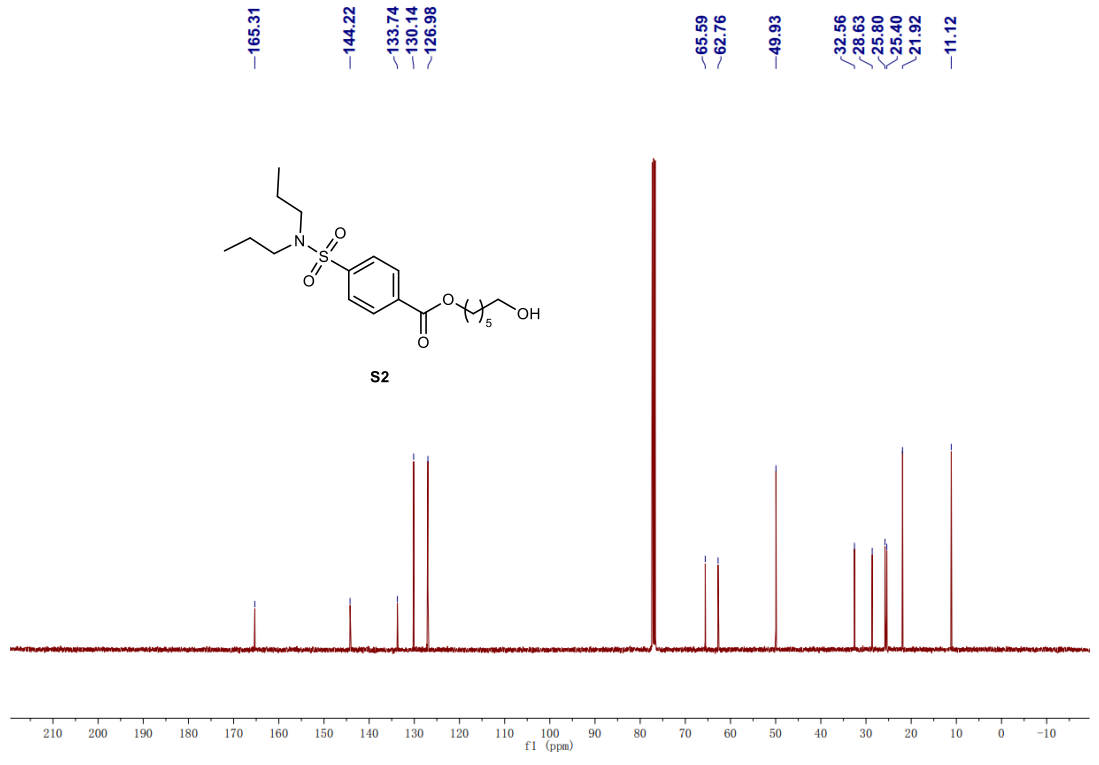
OH
O
5
S1
2.00 2.00 2.01 1.02 2.00 2.04 1.07 5.00 3.01 4.02 6.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0 −1.5
f1 (ppm)


174.84
140.45 137.85 129.24 127.13
64.55 62.77
45.18 45.00 32.53 30.16 28.47 25.52 25.22 22.35 18.42
OH
O
5
S1
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


8.15
8.13
7.87
7.85
4.37
4.35
4.33
3.67
3.65
3.64
3.11
3.10
3.09
3.09
3.07
1.81
1.80
1.78
1.62
1.60
1.58
1.57
1.55
1.53
1.51
1.49
1.48
1.47
1.46
1.45
1.44
0.88
0.86
S2
1.99
2.00
2.00
1.99
4.00
2.03
1.01
10.02
6.00
f1 (ppm)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133.74
130.14
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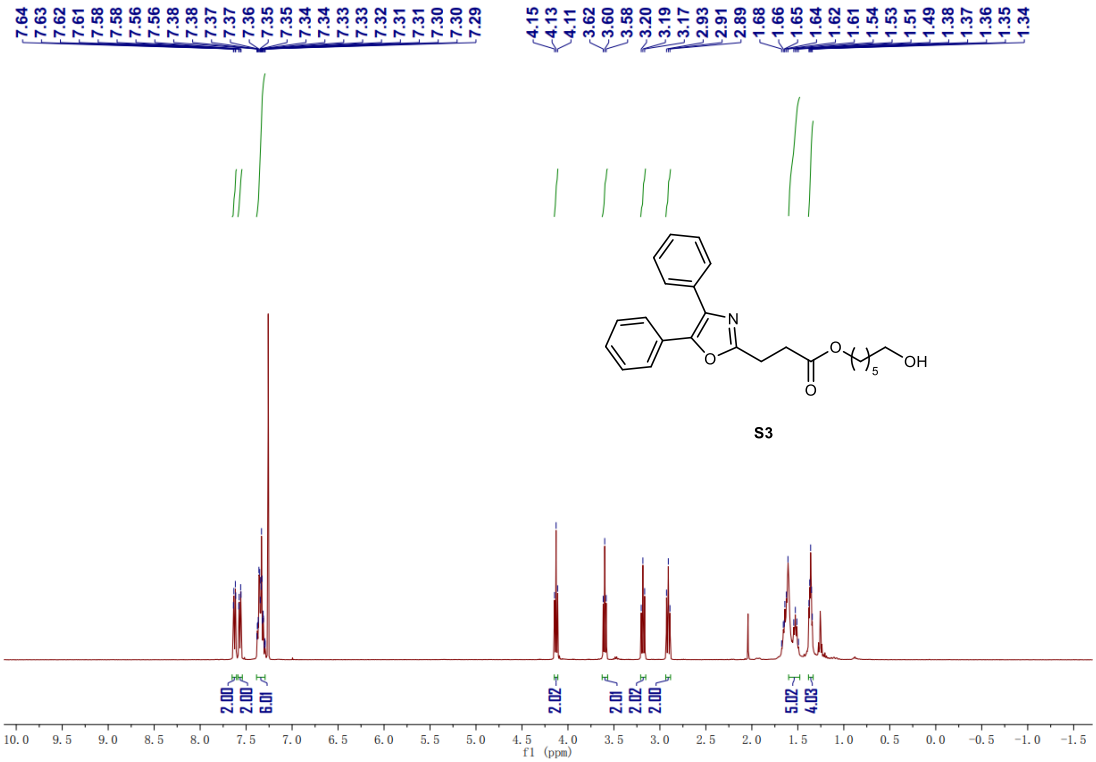
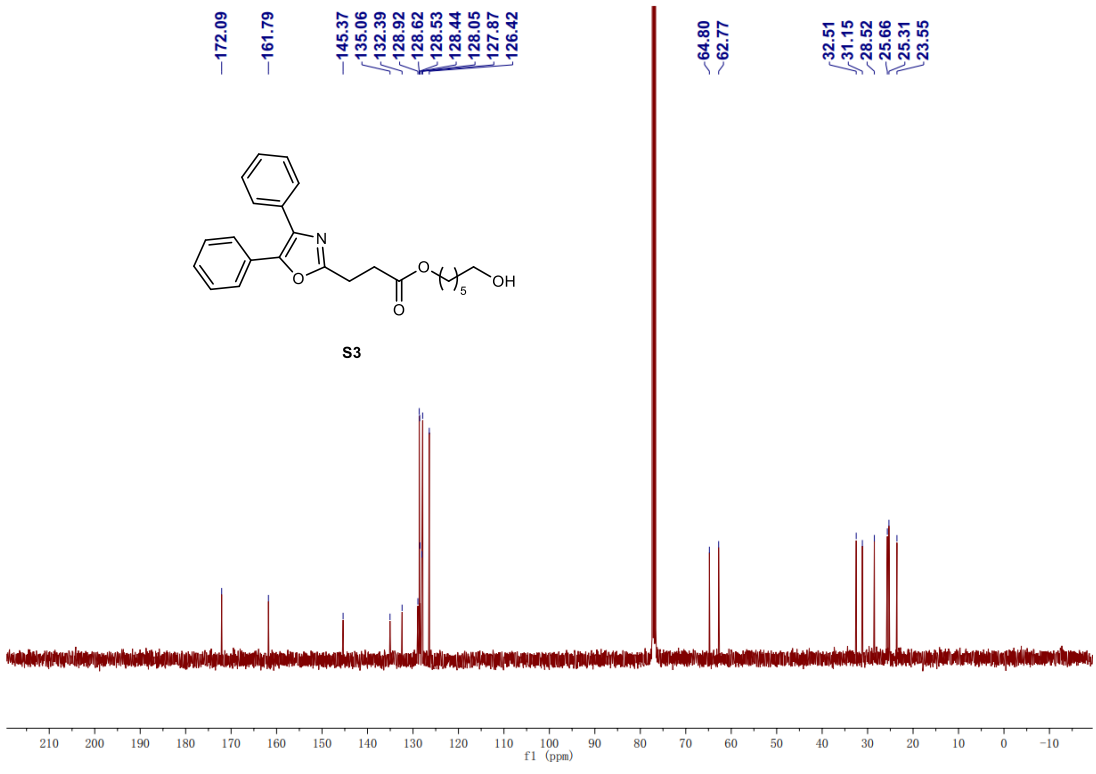
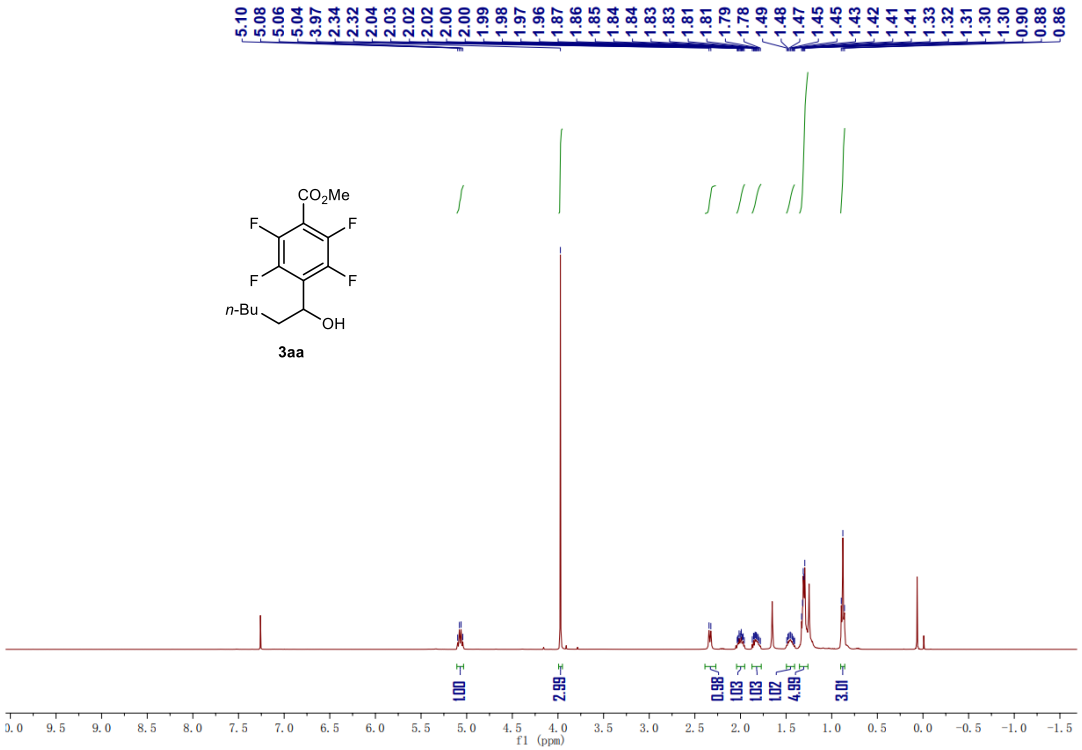
62.76
49.93
32.56
28.63
25.80
25.40
21.92
11.12
S2
f1 (ppm)


7.64 7.63 7.62 7.61 7.58 7.58 7.56 7.56 7.38 7.38 7.37 7.37 7.36 7.35 7.35 7.34 7.34 7.33 7.33 7.32 7.31 7.31 7.30 7.30 7.29
4.15 4.13 4.11 3.62 3.60 3.58 3.20 3.19 3.17 2.93 2.91 2.89 1.68 1.66 1.65 1.64 1.62 1.61 1.54 1.53 1.51 1.49 1.38 1.37 1.36 1.35 1.34
N
O
O
O
5
OH
O
S3
2.00 2.00 6.01 2.02 2.01 2.02 2.00 5.02 4.03
f1 (ppm)


172.09 161.79 145.37 135.06 132.39 128.92 128.62 128.53 128.44 128.05 127.87 126.42
64.80 62.77
32.51 31.15 28.52 25.66 25.31 23.55
N
O
O
O
5
OH
O
S3
f1 (ppm)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5.06
5.04
3.97
2.34
2.32
2.04
2.03
2.02
2.02
2.00
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1.99
1.98
1.97
1.96
1.87
1.86
1.85
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1.84
1.83
1.83
1.81
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1.79
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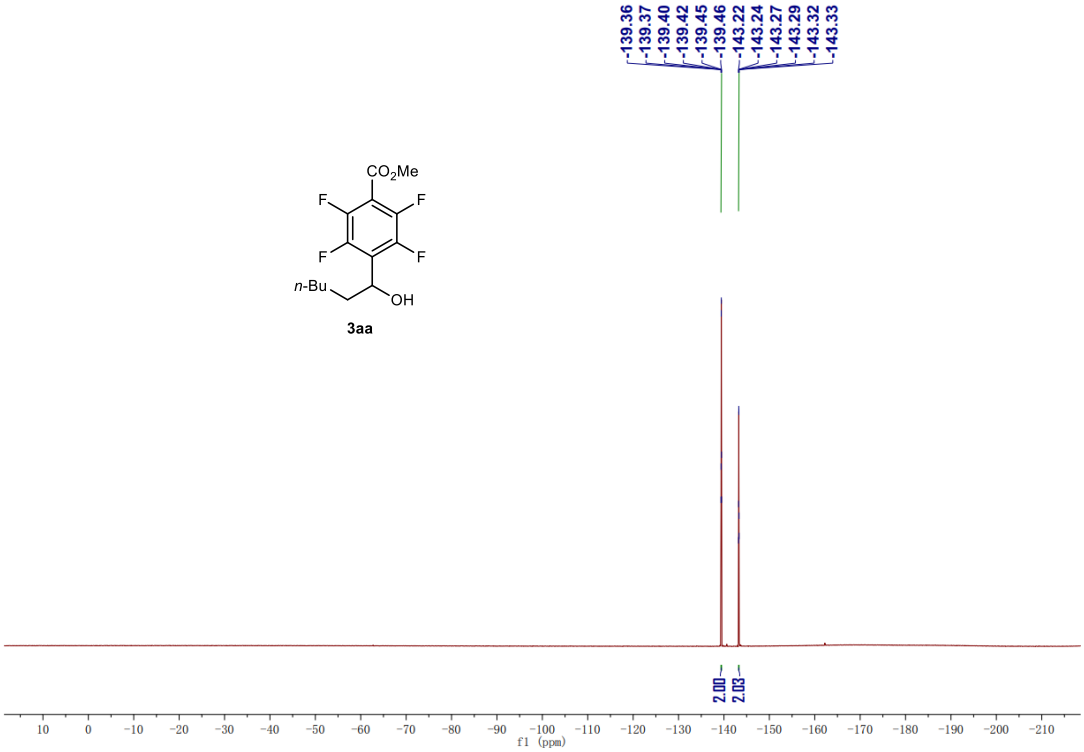
1.47
1.45
1.45
1.43
1.42
1.41
1.41
1.33
1.32
1.31
1.30
1.30
0.90
0.88
0.86
CO2Me
F
F
F
F
n-Bu
OH
3aa
1.00
2.99
0.98
1.03
1.03
1.02
4.99
3.01
f1 (ppm)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-139.37
-139.40
-139.42
-139.45
-139.46
-143.22
-143.24
-143.27
-143.29
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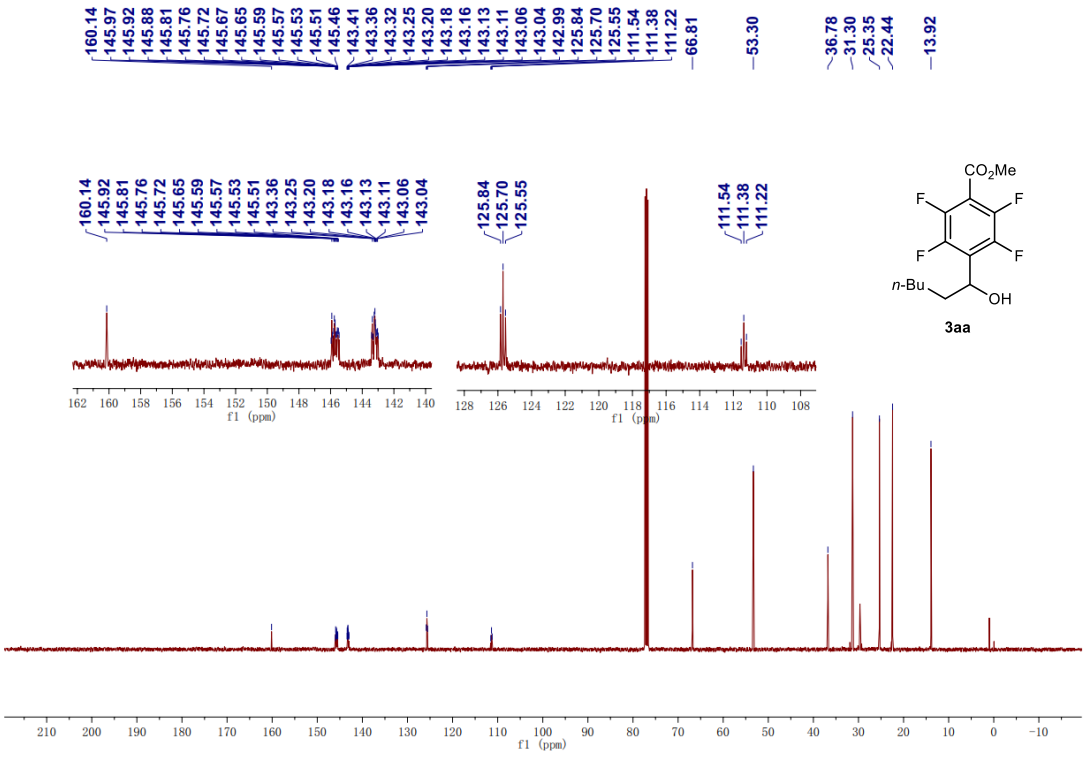
-143.33
CO2Me
F
F
F
F
n-Bu
OH
3aa
2.00
2.03
f1 (ppm)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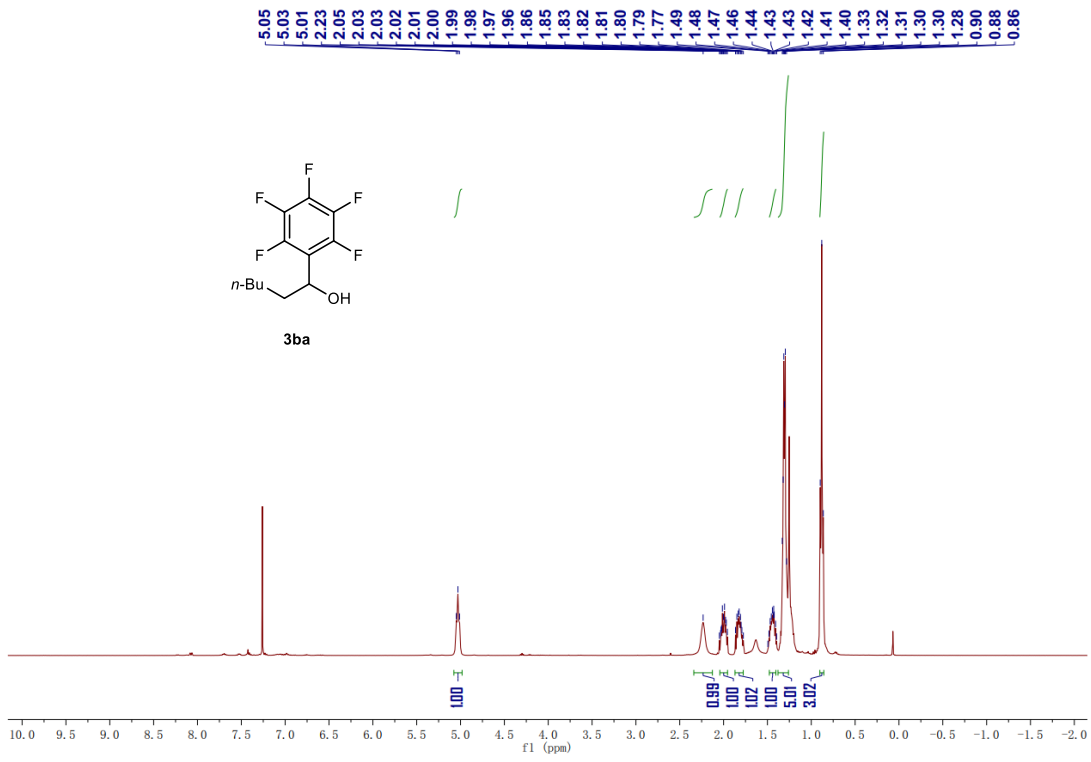
145.97
145.92
145.88
145.81
145.76
145.72
145.67
145.65
145.59
145.57
145.53
145.51
145.46
143.41
143.36
143.32
143.25
143.20
143.18
143.16
143.13
143.11
143.06
143.04
142.99
125.84
125.70
125.55
111.54
111.38
111.22
66.81
53.30
36.78
31.30
25.35
22.44
13.92
CO2Me
F
F
F
F
n-Bu
OH
3aa
f1 (ppm)


5.05
5.03
5.01
2.23
2.05
2.03
2.03
2.02
2.01
2.00
1.99
1.98
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1.96
1.86
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1.82
1.81
1.80
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1.77
1.49
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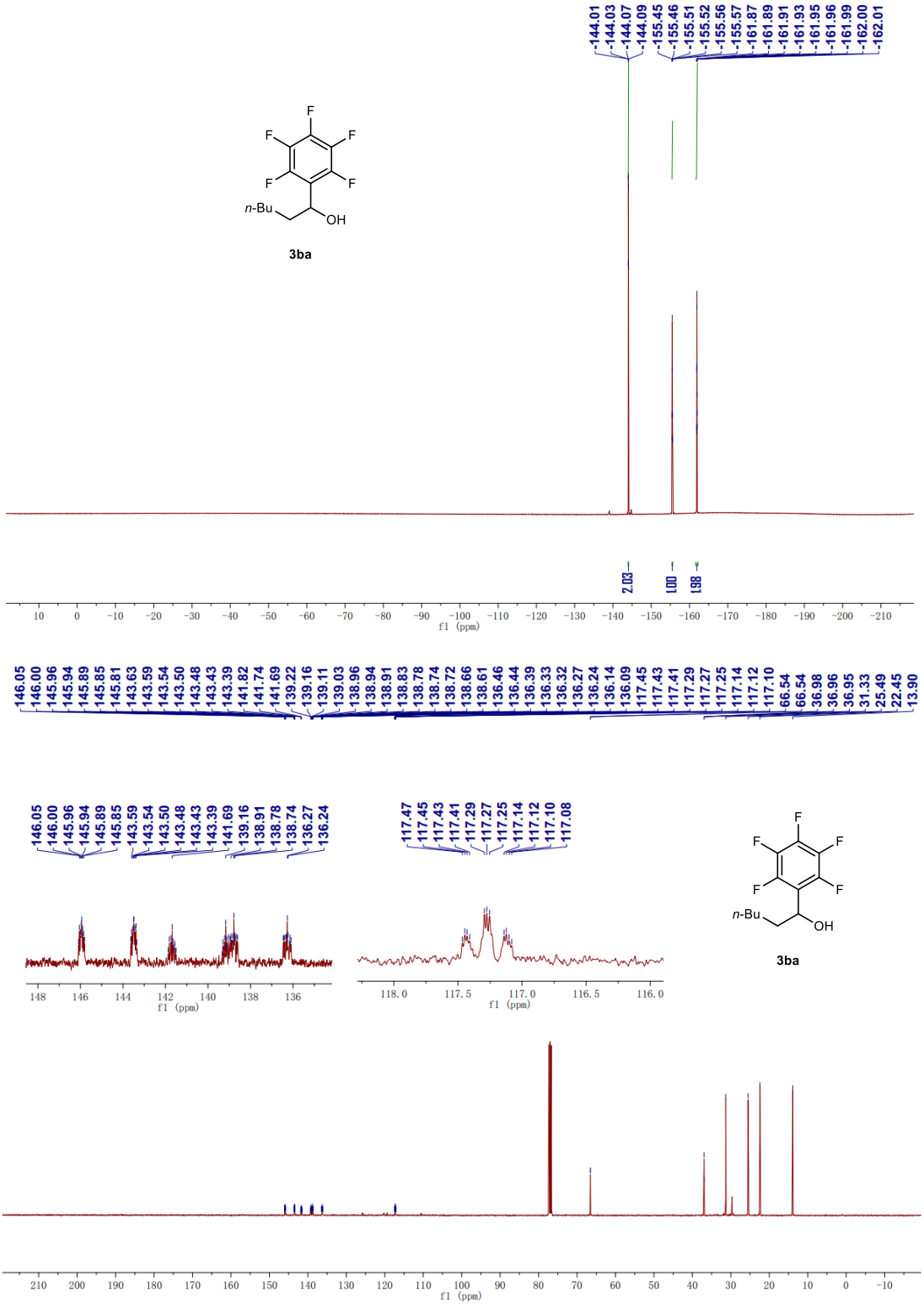
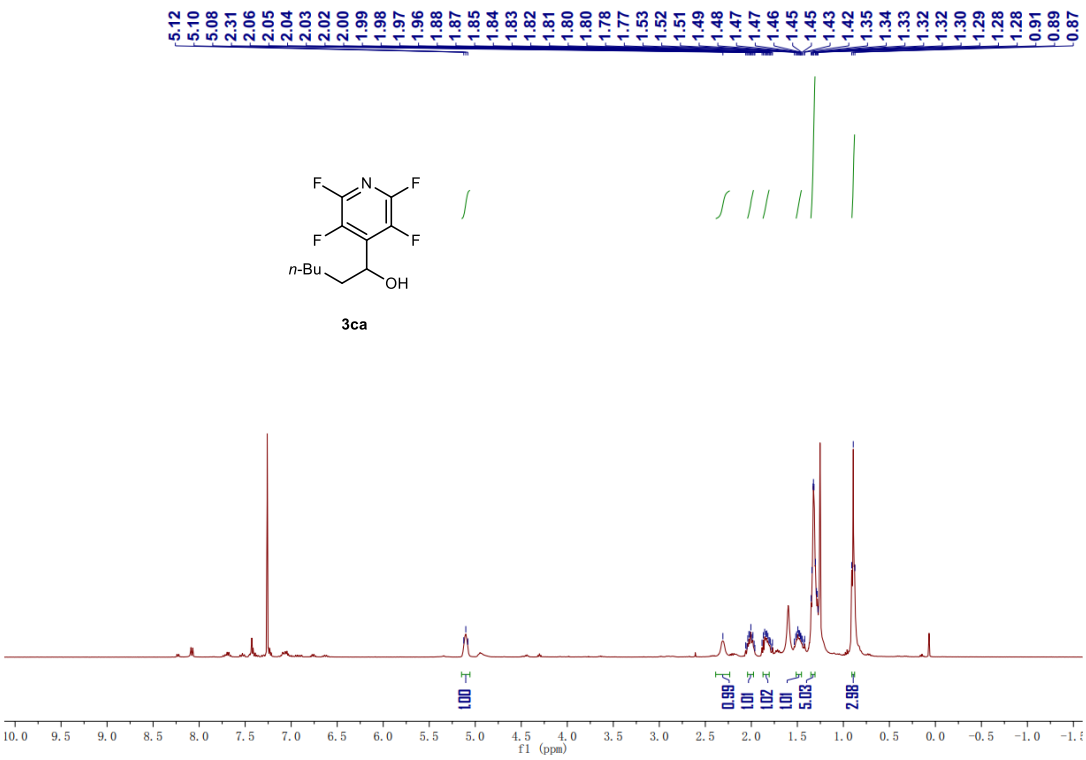
1.46
1.44
1.43
1.42
1.41
1.40
1.33
1.32
1.31
1.30
1.30
1.28
0.90
0.88
0.86
F
F
F
F
F
n-Bu
OH
3ba
1.00
0.99
1.00
1.02
1.00
5.01
3.02
f1 (ppm)


3ba
3ba


5.12
5.10
5.08
2.31
2.06
2.05
2.04
2.03
2.02
2.00
1.99
1.98
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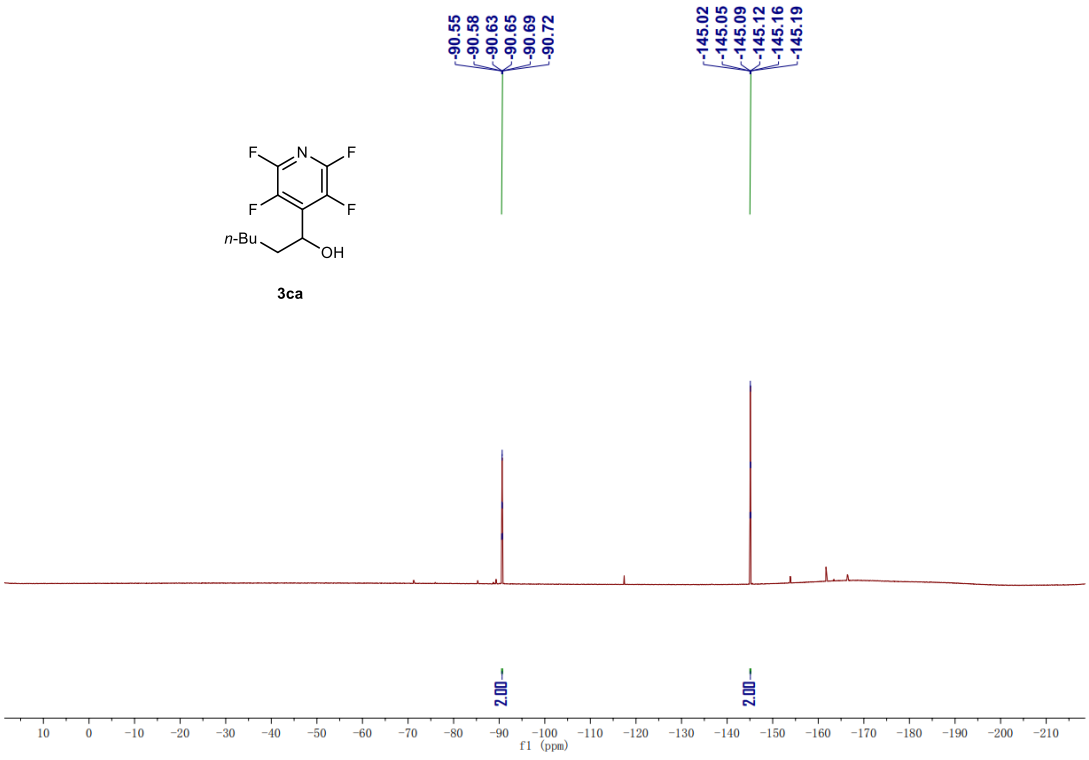
1.43
1.42
1.35
1.34
1.33
1.32
1.32
1.30
1.29
1.28
1.28
0.91
0.89
0.87
F
N
F
F
F
n-Bu
OH
3ca
1.00
0.99
1.01
1.02
1.01
5.03
2.98
f1 (ppm)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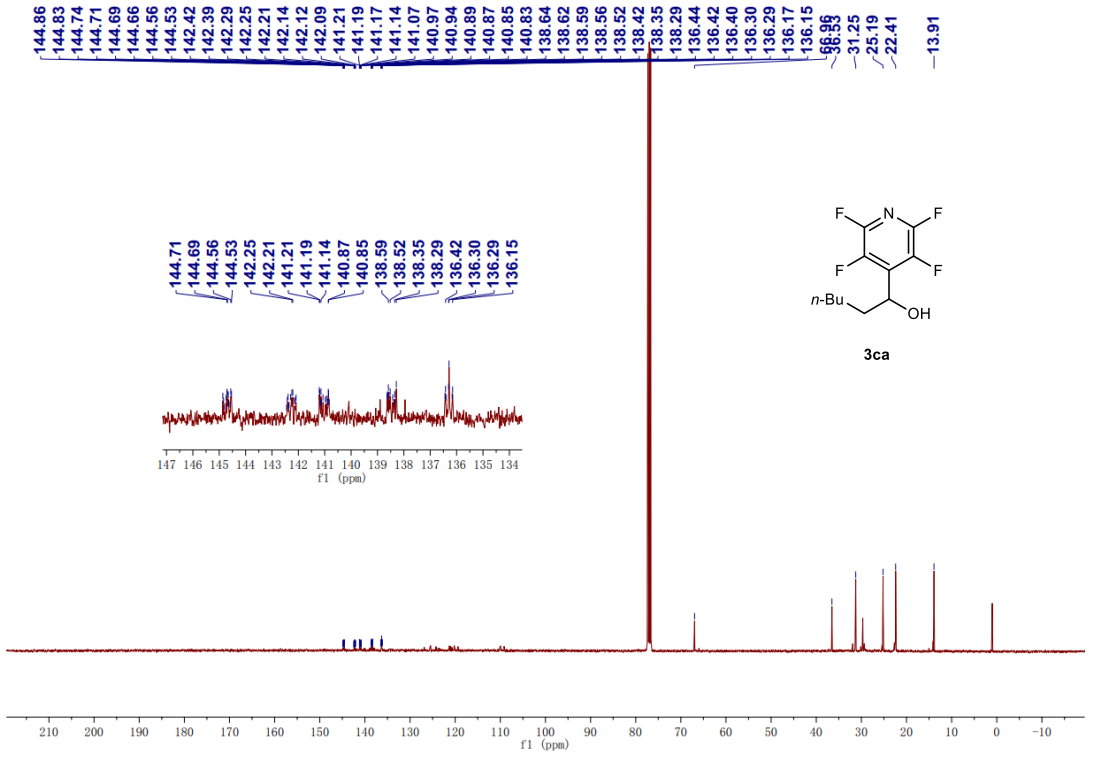
-145.05
-145.09
-145.12
-145.16
-145.19
F
N
F
F
F
n-Bu
OH
3ca
2.00
2.00
f1 (ppm)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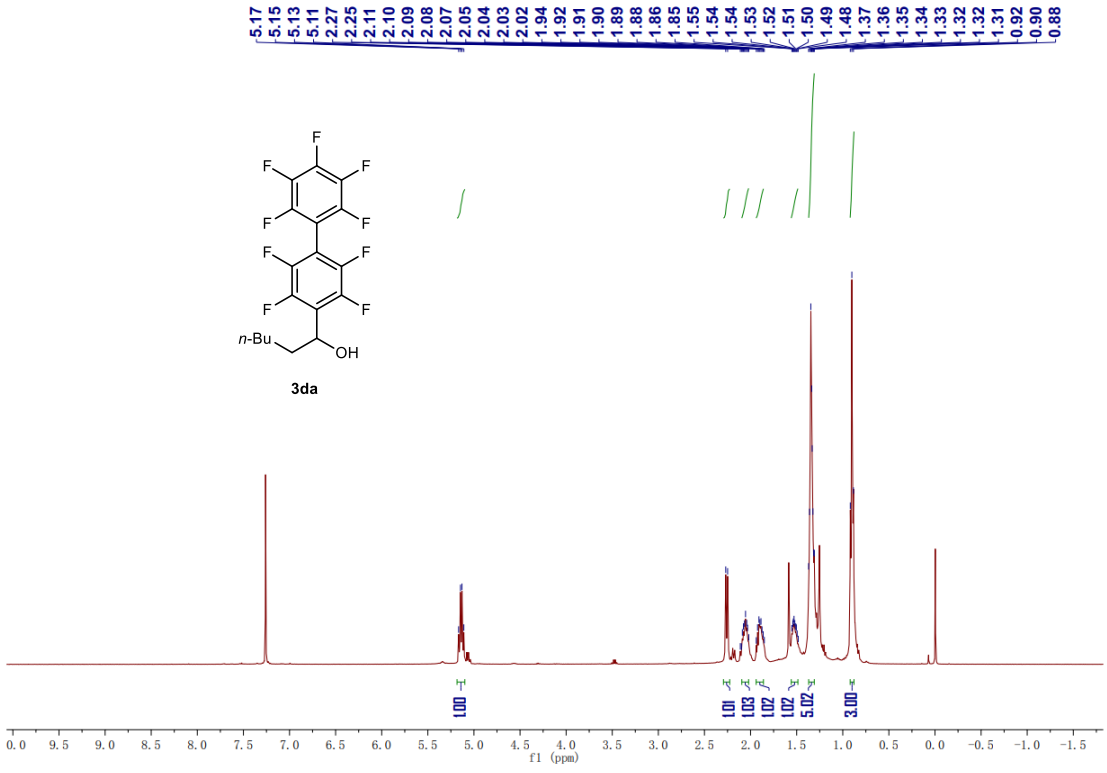
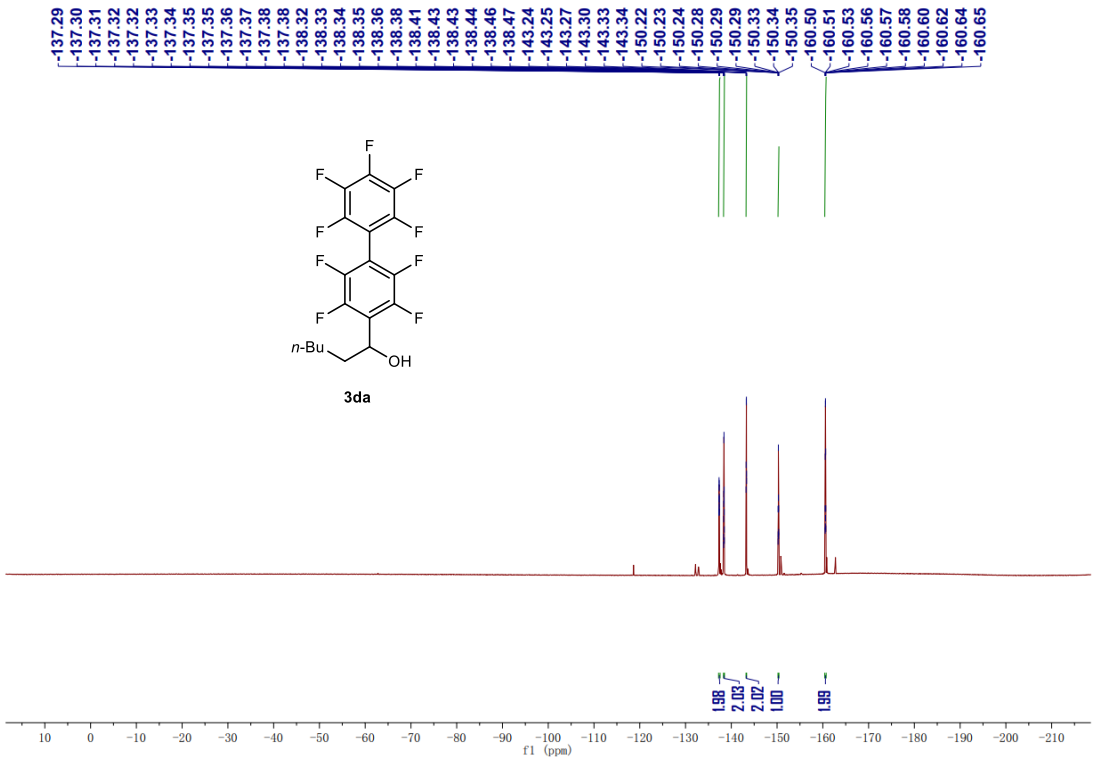
144.71 144.69 144.56 144.53 142.25 142.21 141.21 141.19 141.14 140.87 140.85 138.59 138.52 138.35 138.29 136.42 136.30 136.29 136.15
147 146 145 144 143 142 141 140 139 138 137 136 135 134
f1 (ppm)
F N F F F n-Bu OH
3ca
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


5.17 5.15 5.13 5.11 2.27 2.25 2.11 2.10 2.09 2.08 2.07 2.05 2.04 2.03 2.02 1.94 1.92 1.91 1.90 1.89 1.88 1.86 1.85 1.55 1.54 1.54 1.53 1.52 1.51 1.50 1.49 1.48 1.37 1.36 1.35 1.34 1.33 1.32 1.32 1.31 0.92 0.90 0.88
F F F F F F F F F F n-Bu OH
3da
1.00 1.01 1.03 1.02 1.02 5.02 3.00
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0 −1.5
f1 (ppm)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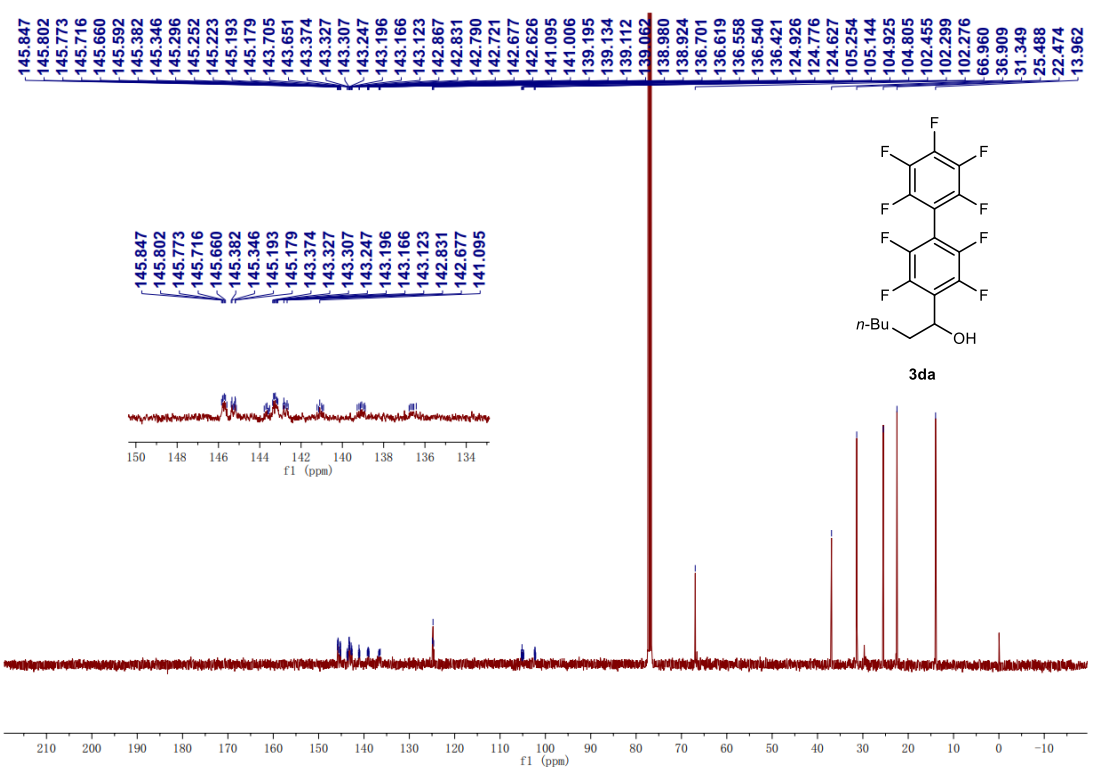
-160.51
-160.53
-160.56
-160.57
-160.58
-160.60
-160.62
-160.64
-160.65
F
F
F
F
F
F
F
F
n-Bu
OH
3da
1.98
2.03
2.02
1.00
1.99
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)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143.651
143.374
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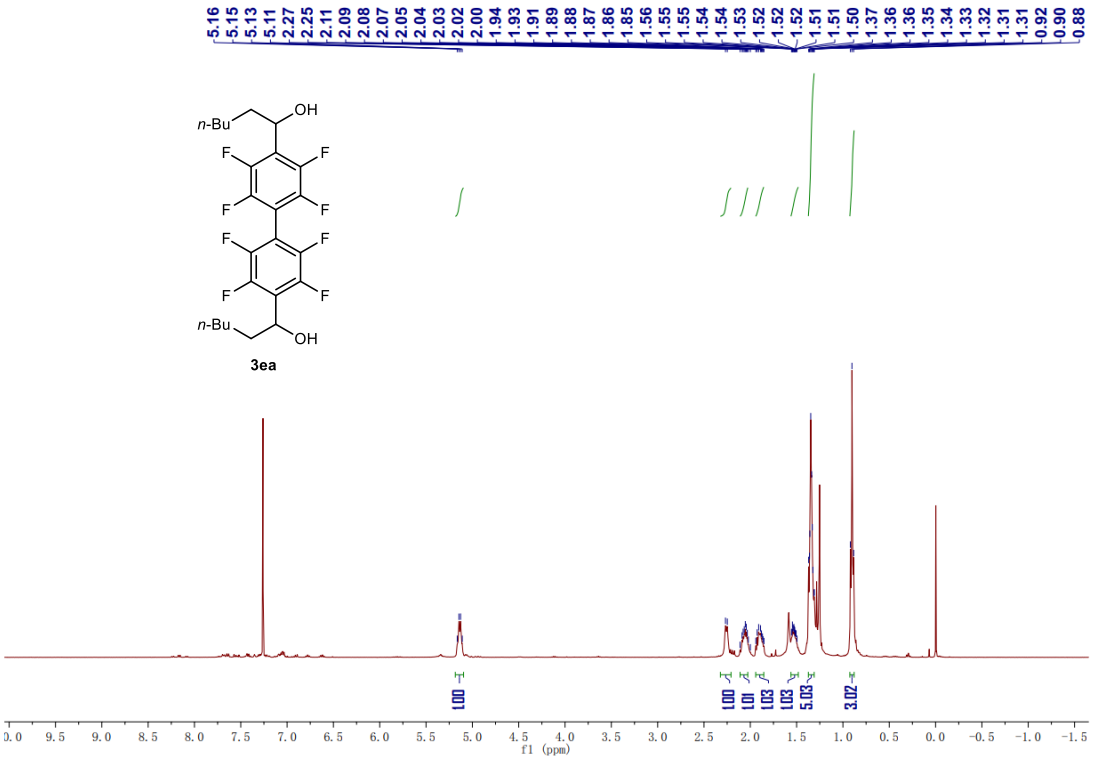
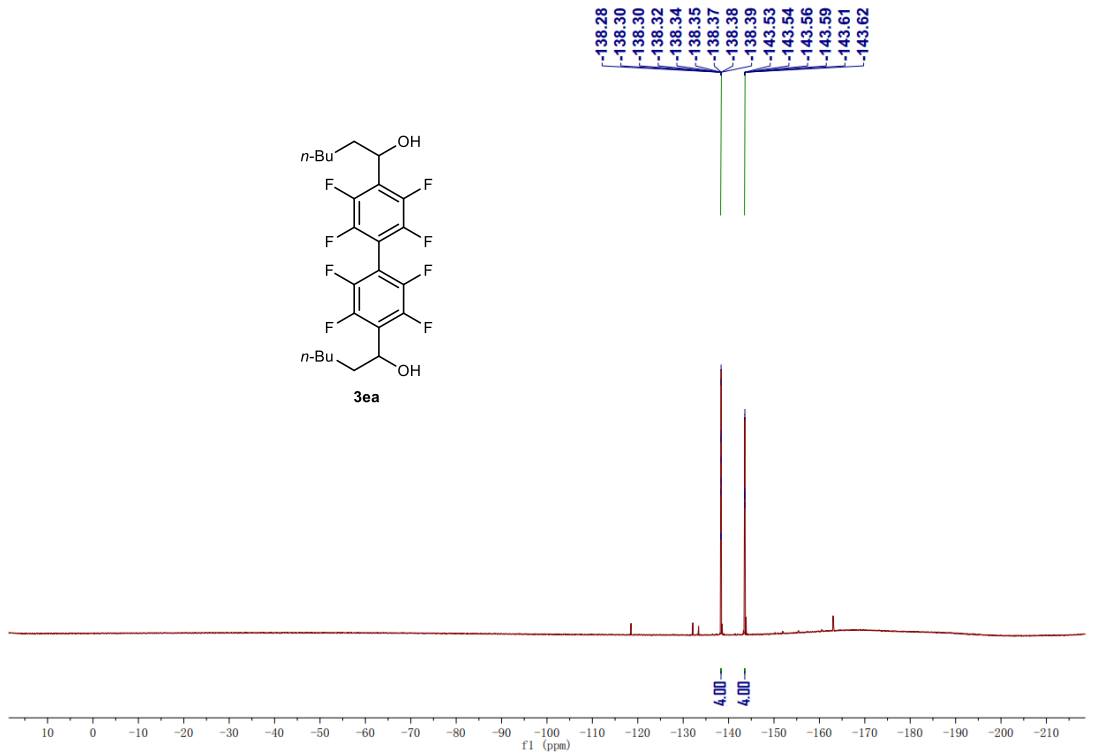
143.307
143.247
143.196
143.166
143.123
142.867
142.831
142.790
142.721
142.677
142.626
141.095
141.006
139.195
139.134
139.112
139.062
138.980
138.924
136.701
136.619
136.558
136.540
136.421
124.926
124.776
124.627
105.254
105.144
104.925
104.805
102.455
102.299
102.276
66.960
36.909
31.349
25.488
22.474
13.962
F
F
F
F
F
F
F
F
n-Bu
OH
3da
150 148 146 144 142 140 138 136 134
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


5.16 5.15 5.13 5.11 2.27 2.25 2.11 2.09 2.08 2.07 2.05 2.04 2.03 2.02 2.00 1.94 1.93 1.91 1.89 1.88 1.87 1.86 1.85 1.56 1.55 1.55 1.54 1.54 1.53 1.52 1.52 1.52 1.51 1.51 1.50 1.37 1.36 1.36 1.35 1.34 1.33 1.32 1.31 1.31 0.92 0.90 0.88
n-Bu
OH
F
n-Bu
OH
3ea
1.00 1.00 1.01 1.03 1.03 5.03 3.02
f1 (ppm)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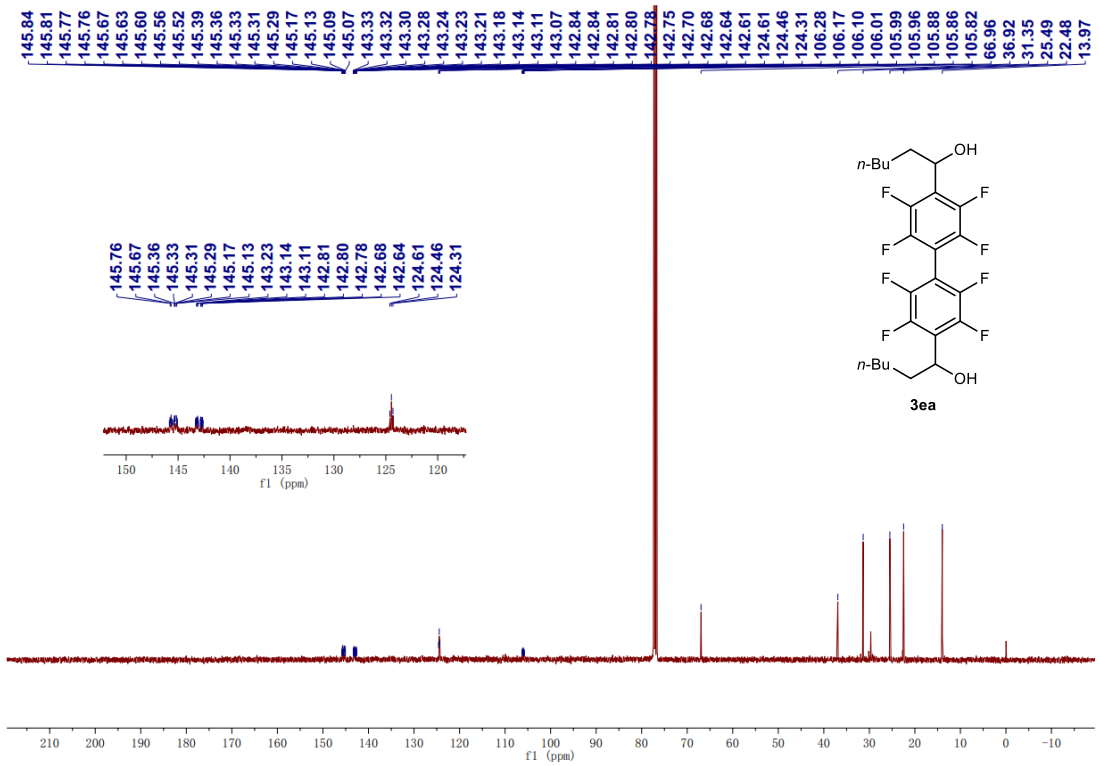
F
n-Bu
OH
3ea
4.00 4.00
f1 (ppm)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n-Bu
OH
F
F
F
F
F
F
F
F
n-Bu
OH
3ea
145.76 145.67 145.36 145.33 145.31 145.29 145.17 145.13 143.23 143.14 143.11 142.81 142.80 142.78 142.68 142.64 124.61 124.46 124.31
150 145 140 135 130 125 120
f1 (ppm)
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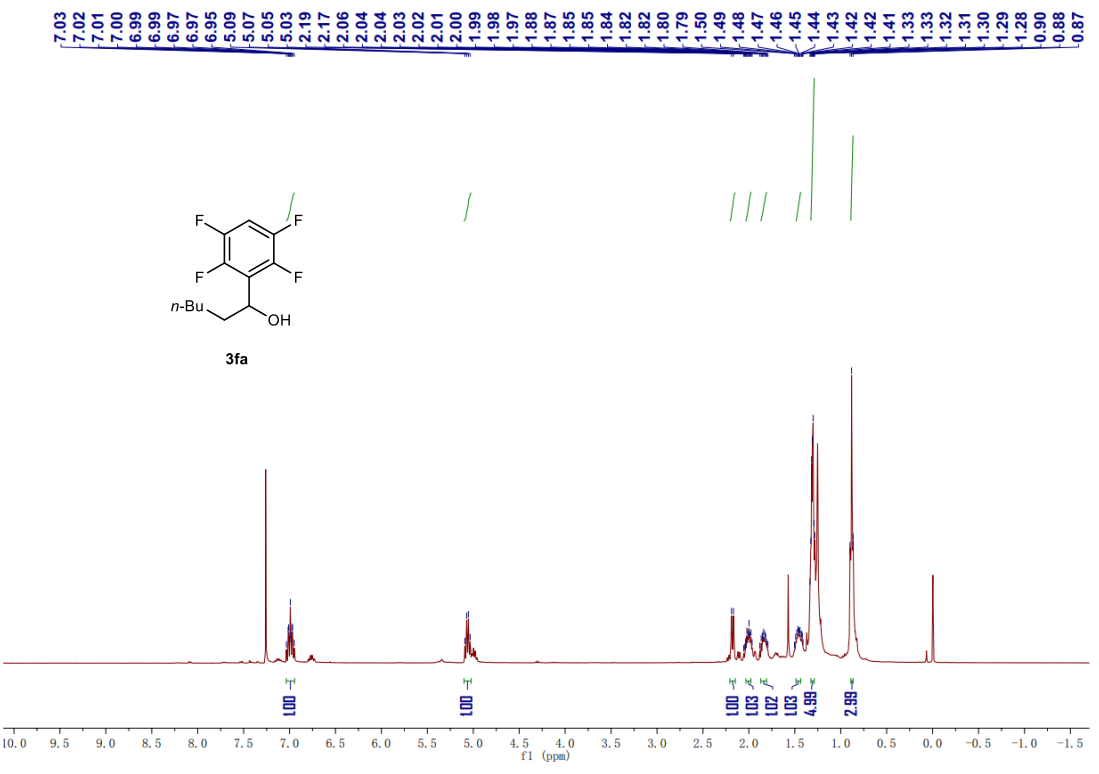
f1 (ppm)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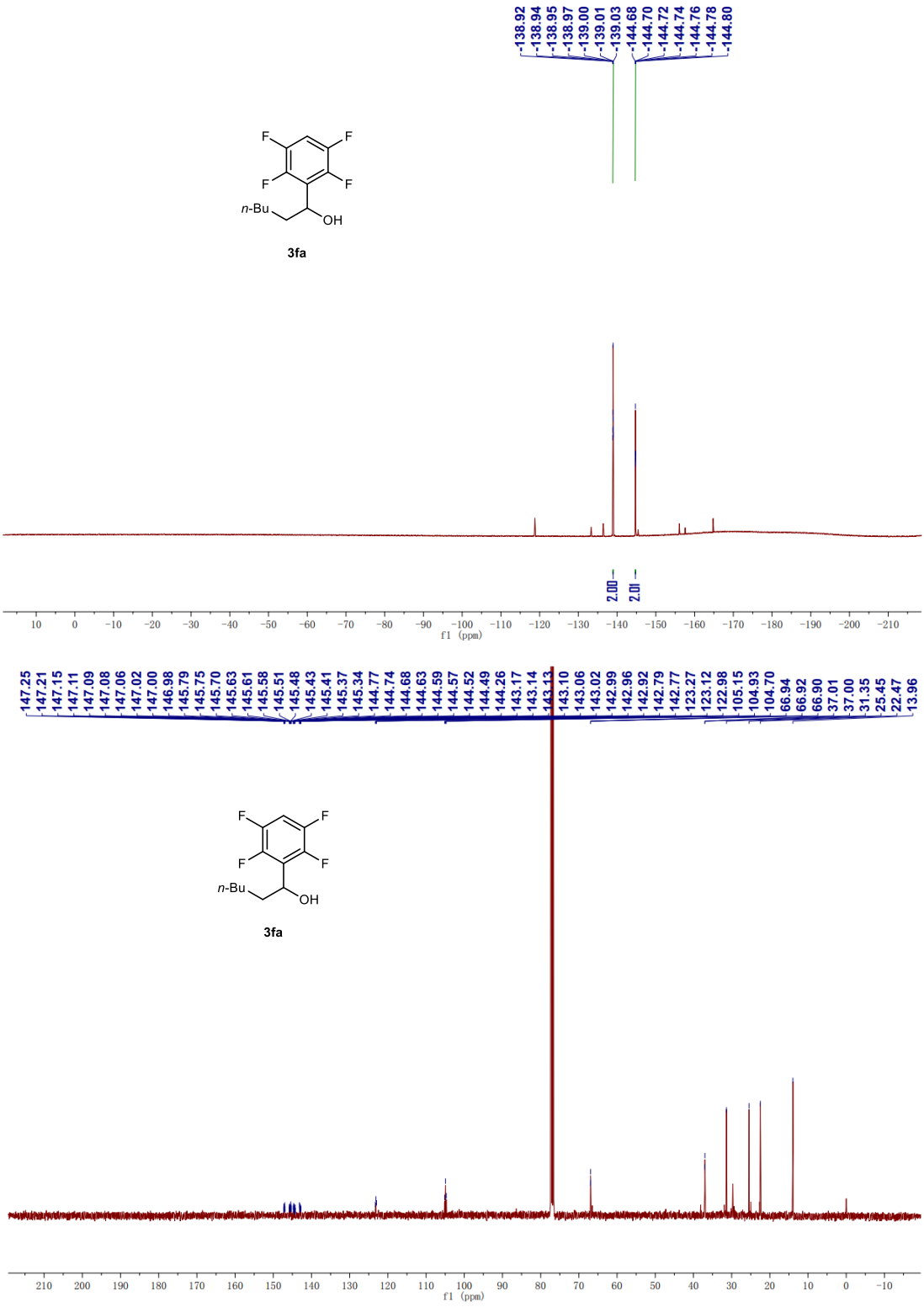
F
F
F
F
n-Bu
OH
3fa
1.00 1.00 1.00 1.03 1.02 1.03 4.99 2.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0 −1.5
f1 (ppm)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-139.00
-139.01
-139.03
-144.68
-144.70
-144.72
-144.74
-144.76
-144.78
-144.80
F
F
F
F
n-Bu
OH
3fa
2.00
2.01
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)
147.25
147.21
147.15
147.11
147.09
147.08
147.06
147.02
147.00
146.98
145.79
145.75
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123.12
122.98
105.15
104.93
104.70
66.94
66.92
66.90
37.01
37.00
31.35
25.45
22.47
13.96
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F
F
n-Bu
OH
3fa
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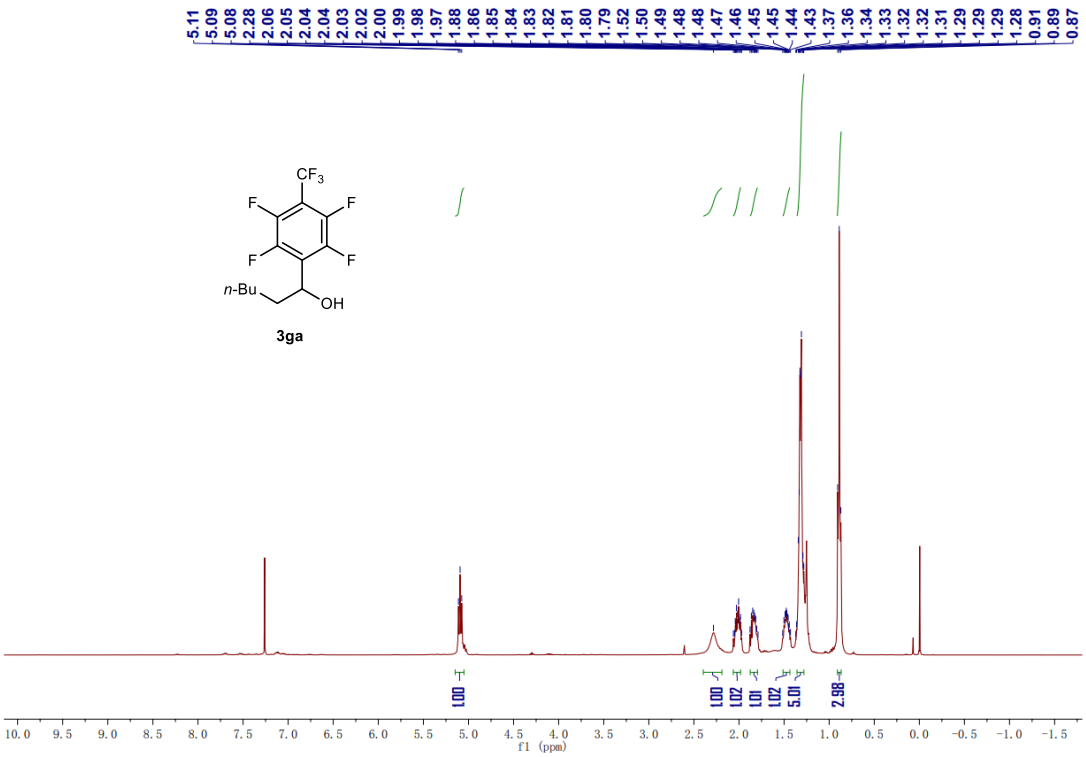
f1 (ppm)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F
F
F
n-Bu
OH
3ga
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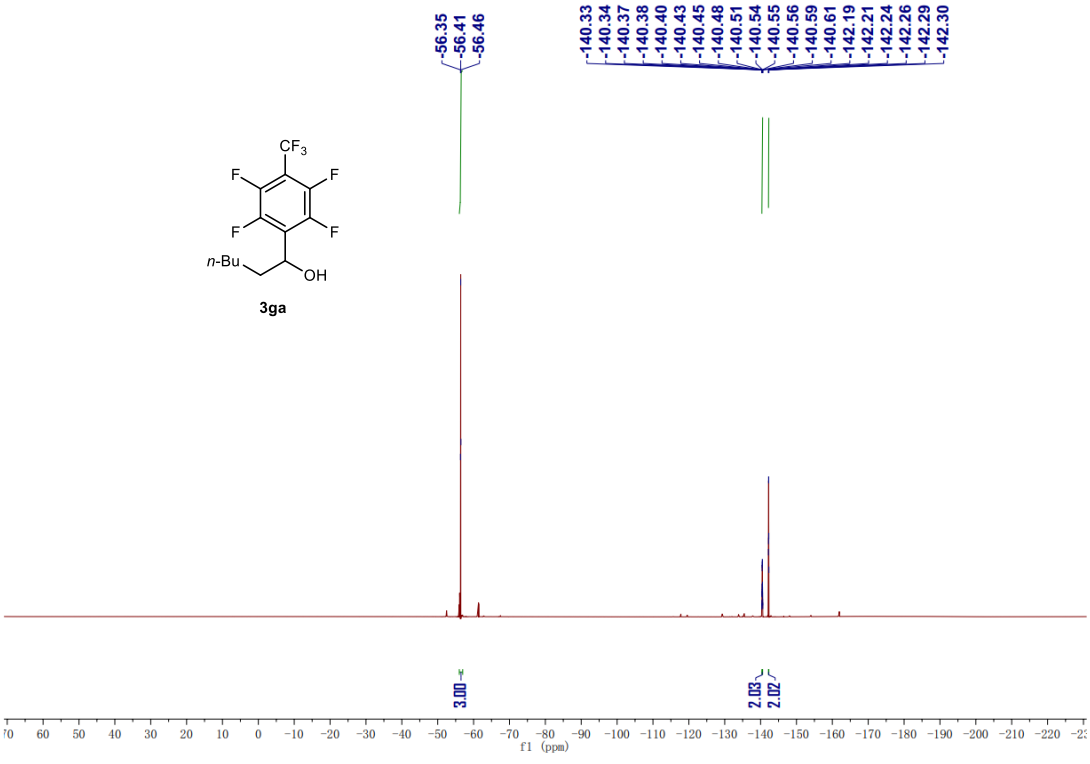
f1 (ppm)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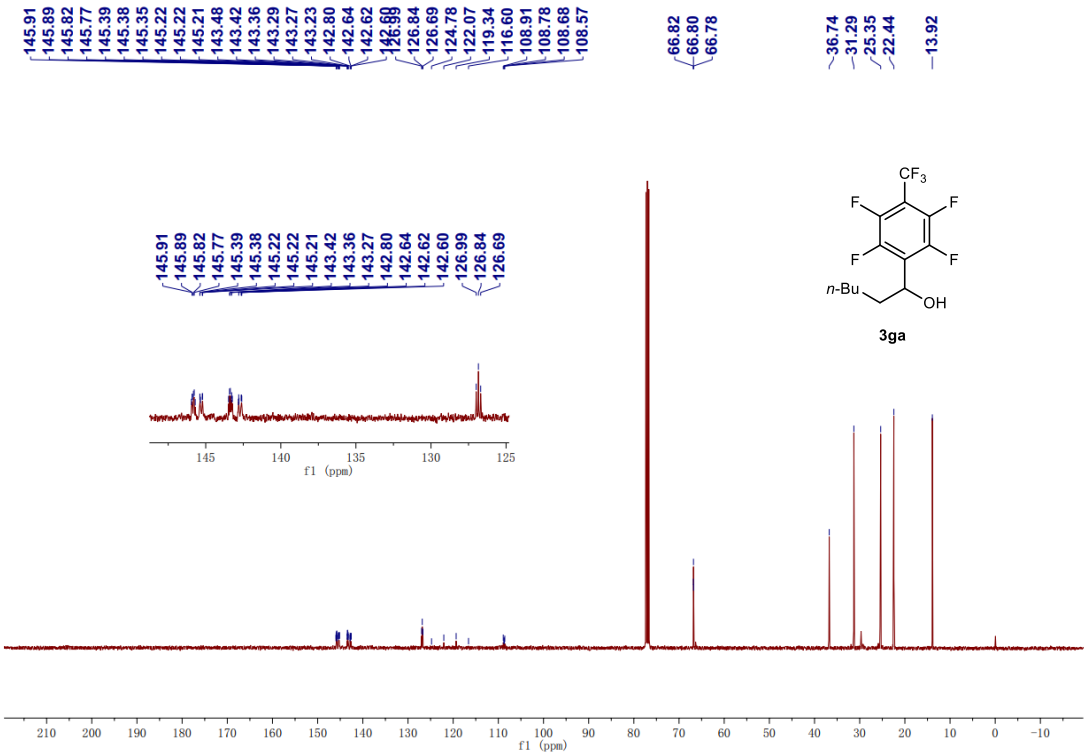
CF3
F
F
F
F
n-Bu
OH
3ga
3.00 2.03 2.02
f1 (ppm)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126.69
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122.07
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108.68
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66.78
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22.44
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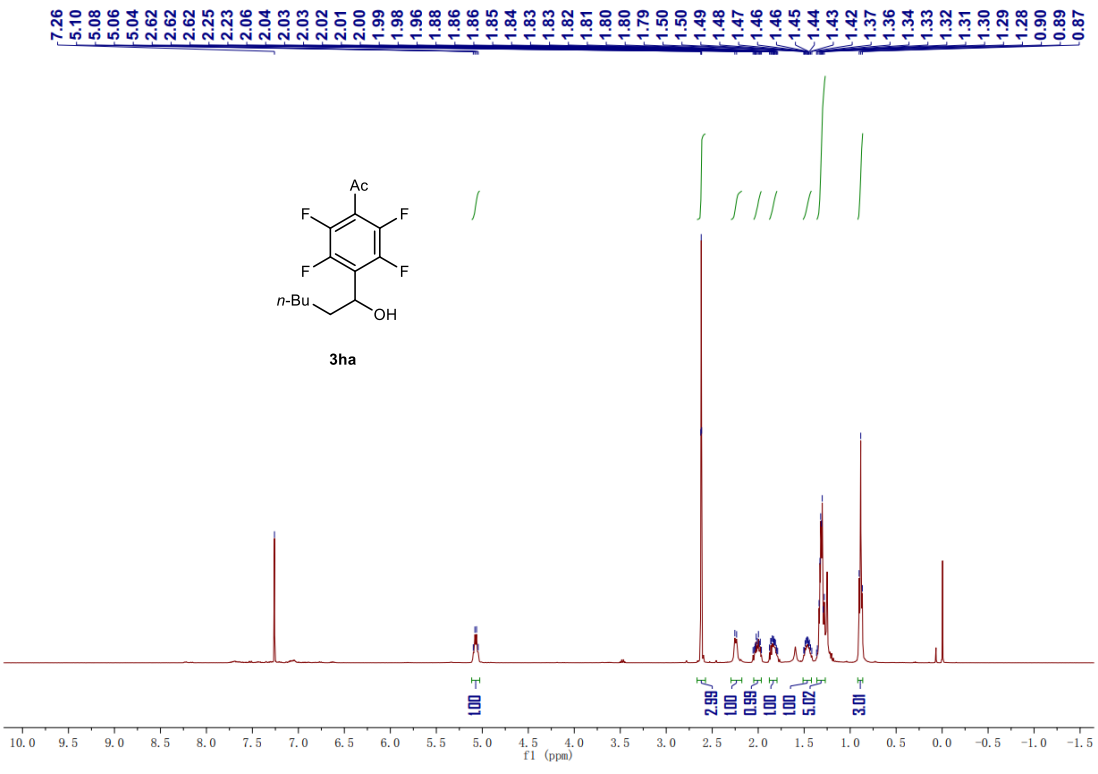
CF3
F
F
F
F
n-Bu
OH
3ga
f1 (ppm)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2.04
2.03
2.03
2.02
2.01
2.00
1.99
1.98
1.96
1.88
1.86
1.86
1.85
1.84
1.83
1.83
1.82
1.81
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1.80
1.79
1.50
1.50
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1.48
1.47
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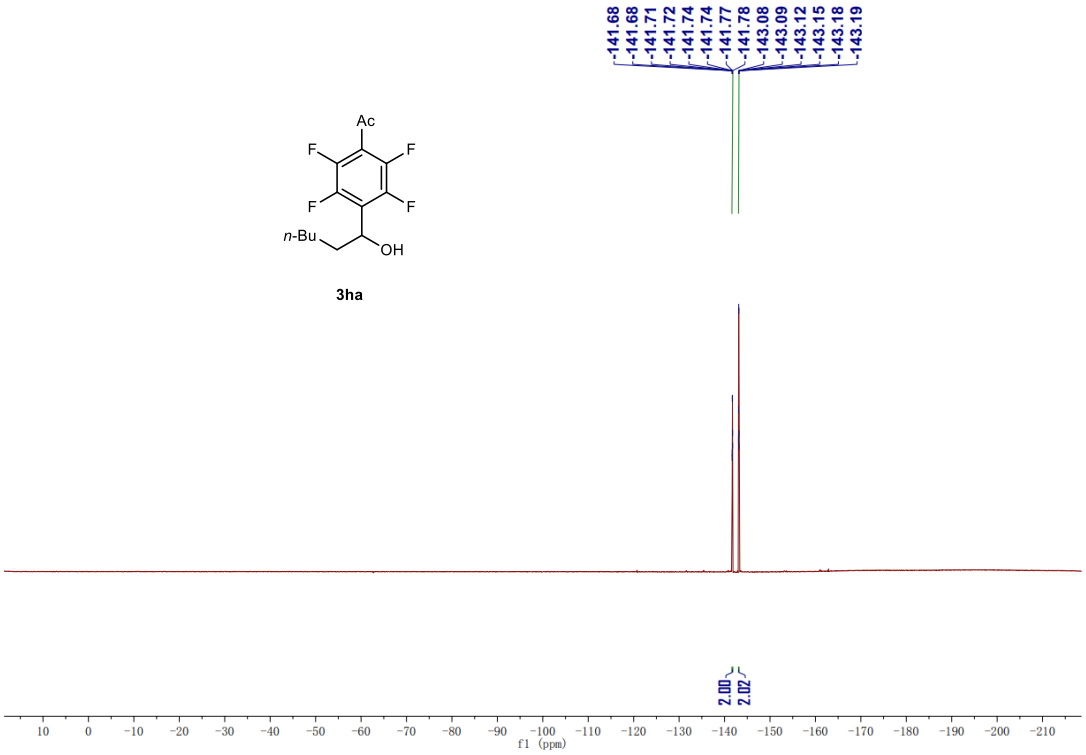
1.46
1.45
1.44
1.43
1.42
1.37
1.36
1.34
1.33
1.32
1.31
1.30
1.29
1.28
0.90
0.89
0.87
Ac
F
F
F
F
n-Bu
OH
3ha
1.00
2.99
1.00
0.99
1.00
1.00
5.02
3.01
f1 (ppm)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-141.74
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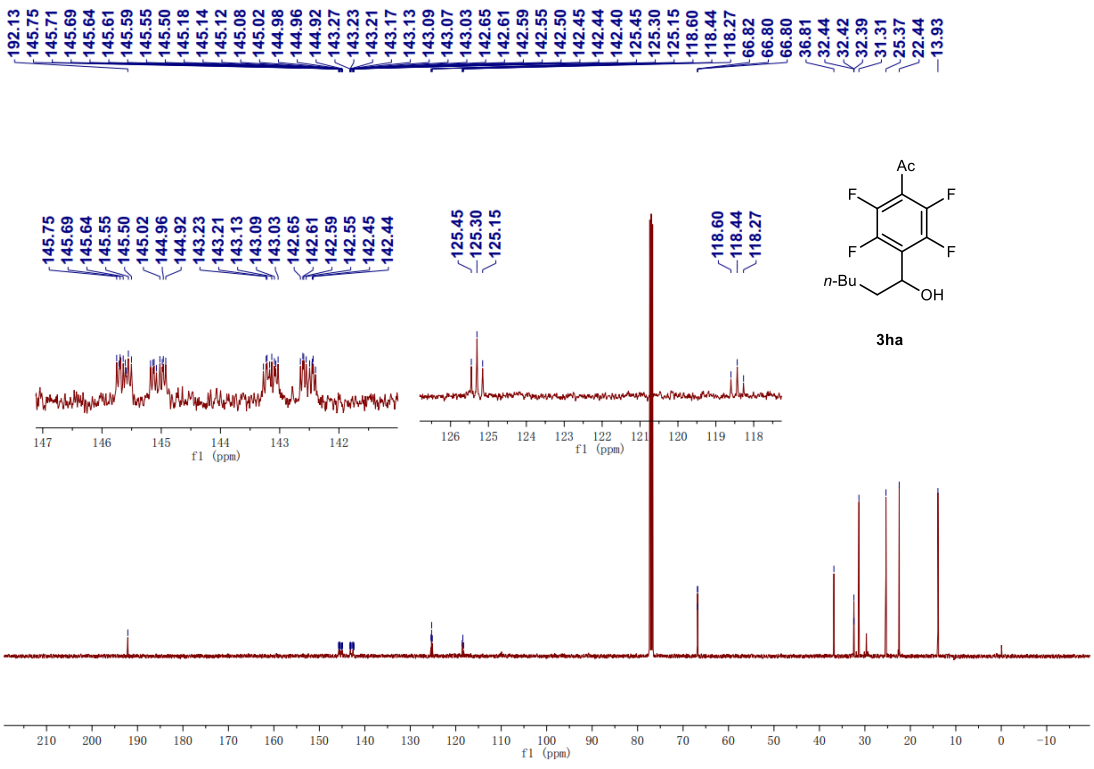
-143.08
-143.09
-143.12
-143.15
-143.18
-143.19
Ac
F
F
F
F
n-Bu
OH
3ha
2.00
2.02
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)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31.31
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22.44
13.93
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145.69
145.64
145.55
145.50
145.02
144.96
144.92
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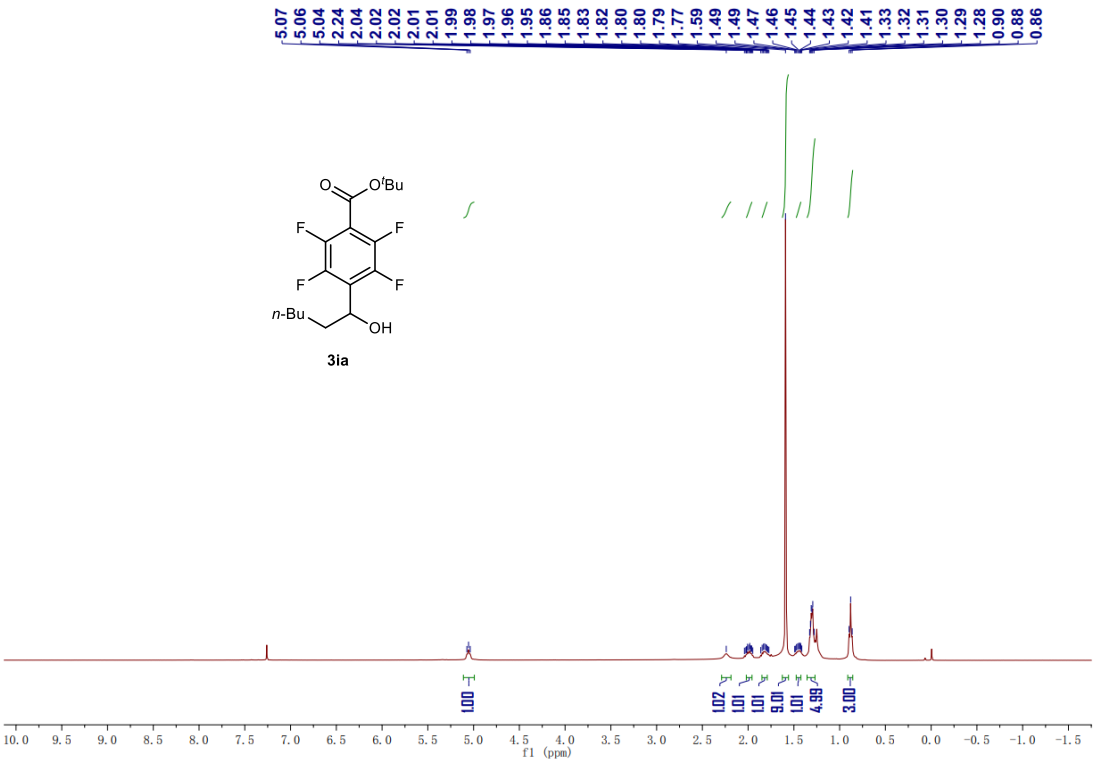
143.09
143.03
142.65
142.61
142.59
142.55
142.45
142.44
125.45
125.30
125.15
118.60
118.44
118.27
Ac
F
F
F
F
n-Bu
OH
3ha
147 146 145 144 143 142
f1 (ppm)
126 125 124 123 122 121 120 119 118
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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2.02
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1.85
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1.82
1.80
1.80
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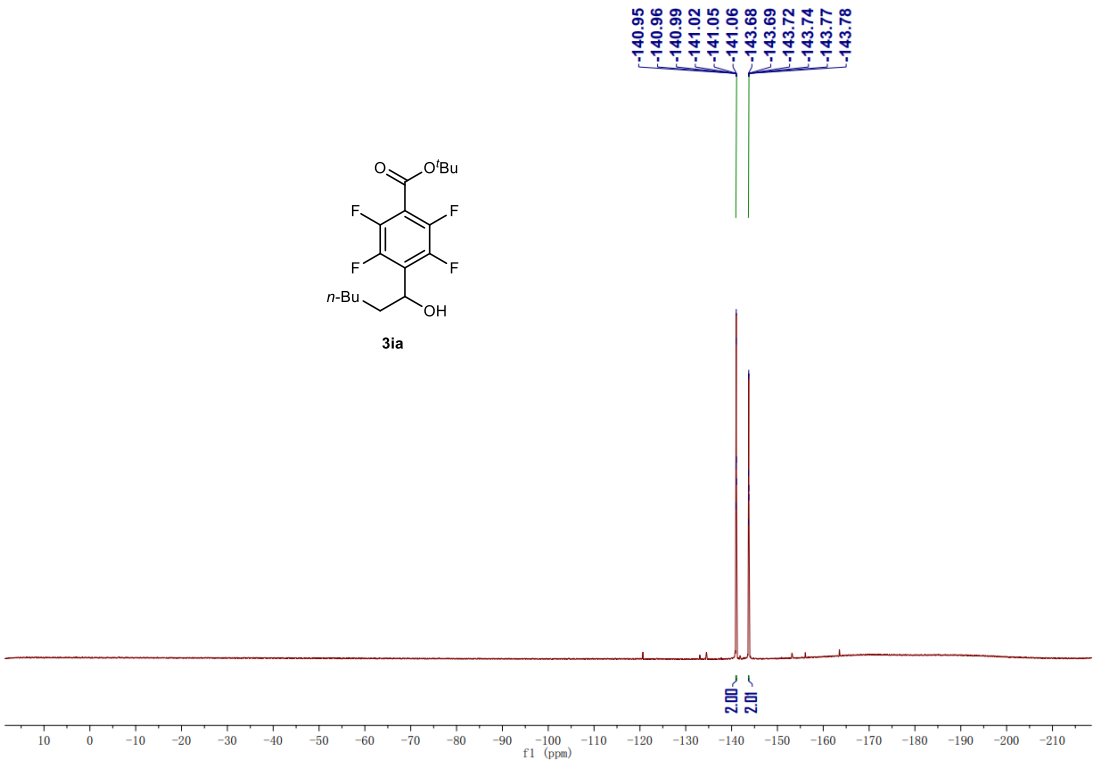
1.46
1.45
1.44
1.43
1.42
1.41
1.33
1.32
1.31
1.30
1.29
1.28
0.90
0.88
0.86
O
O^{t}Bu
F
F
F
F
n-Bu
OH
3ia
1.00
1.02
1.01
1.01
9.01
1.01
4.98
3.00
f1 (ppm)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-140.99
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-143.68
-143.69
-143.72
-143.74
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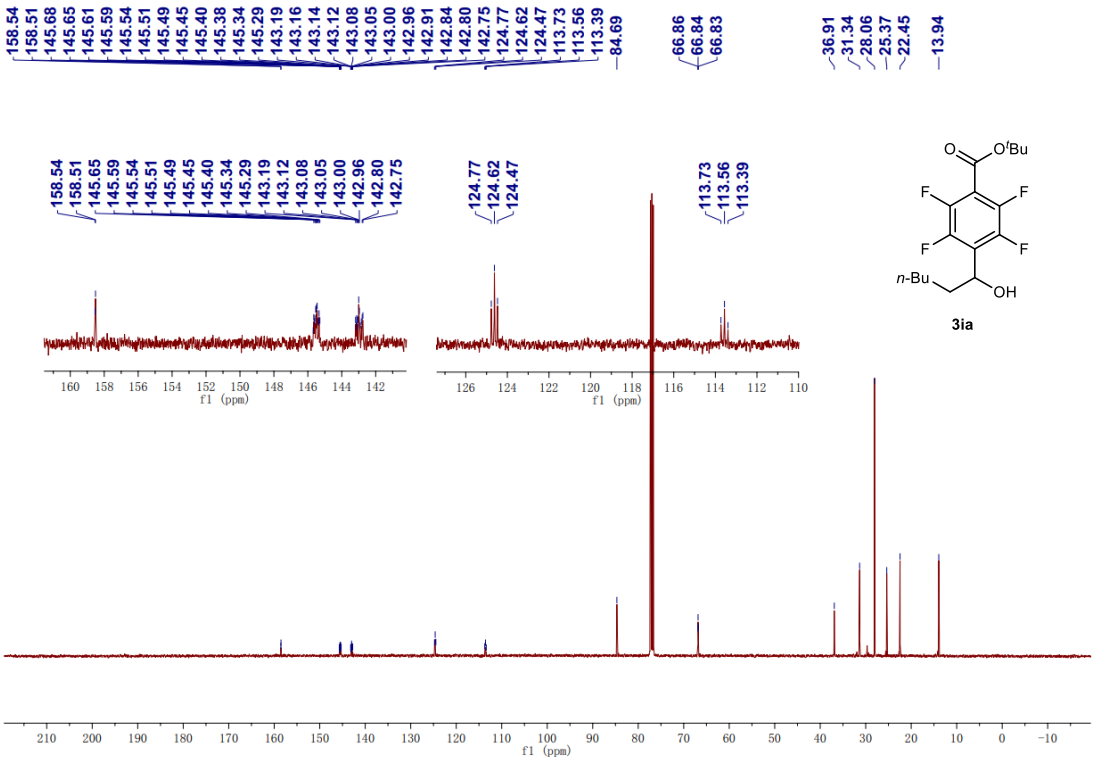
-143.78
O
O^{t}Bu
F
F
F
F
n-Bu
OH
3ia
2.00
2.01
f1 (ppm)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145.40
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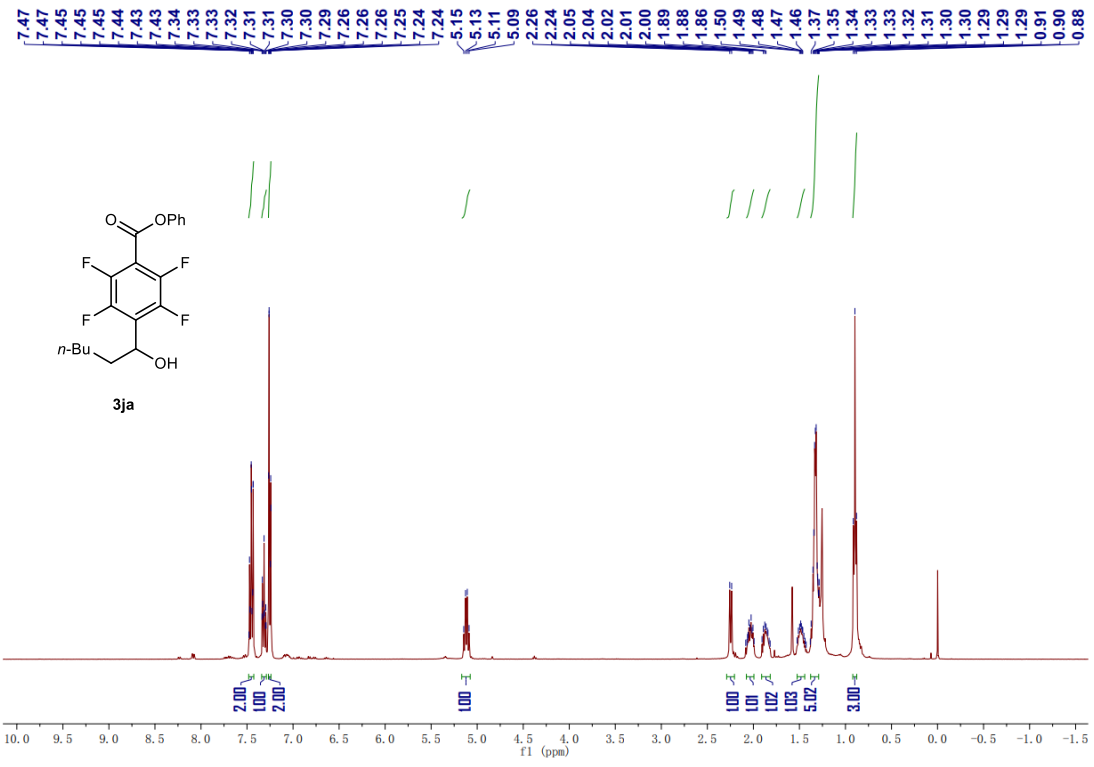
145.29
143.19
143.16
143.14
143.12
143.08
143.05
143.00
142.96
142.91
142.84
142.80
142.75
124.77
124.62
124.47
113.73
113.56
113.39
84.69
66.86
66.84
66.83
36.91
31.34
28.06
25.37
22.45
13.94
f1 (ppm)
O
O^{t}Bu
F
F
F
F
n-Bu
OH
3ia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7.26
7.25
7.24
5.15
5.13
5.11
5.09
2.26
2.24
2.05
2.04
2.02
2.01
2.00
1.89
1.88
1.86
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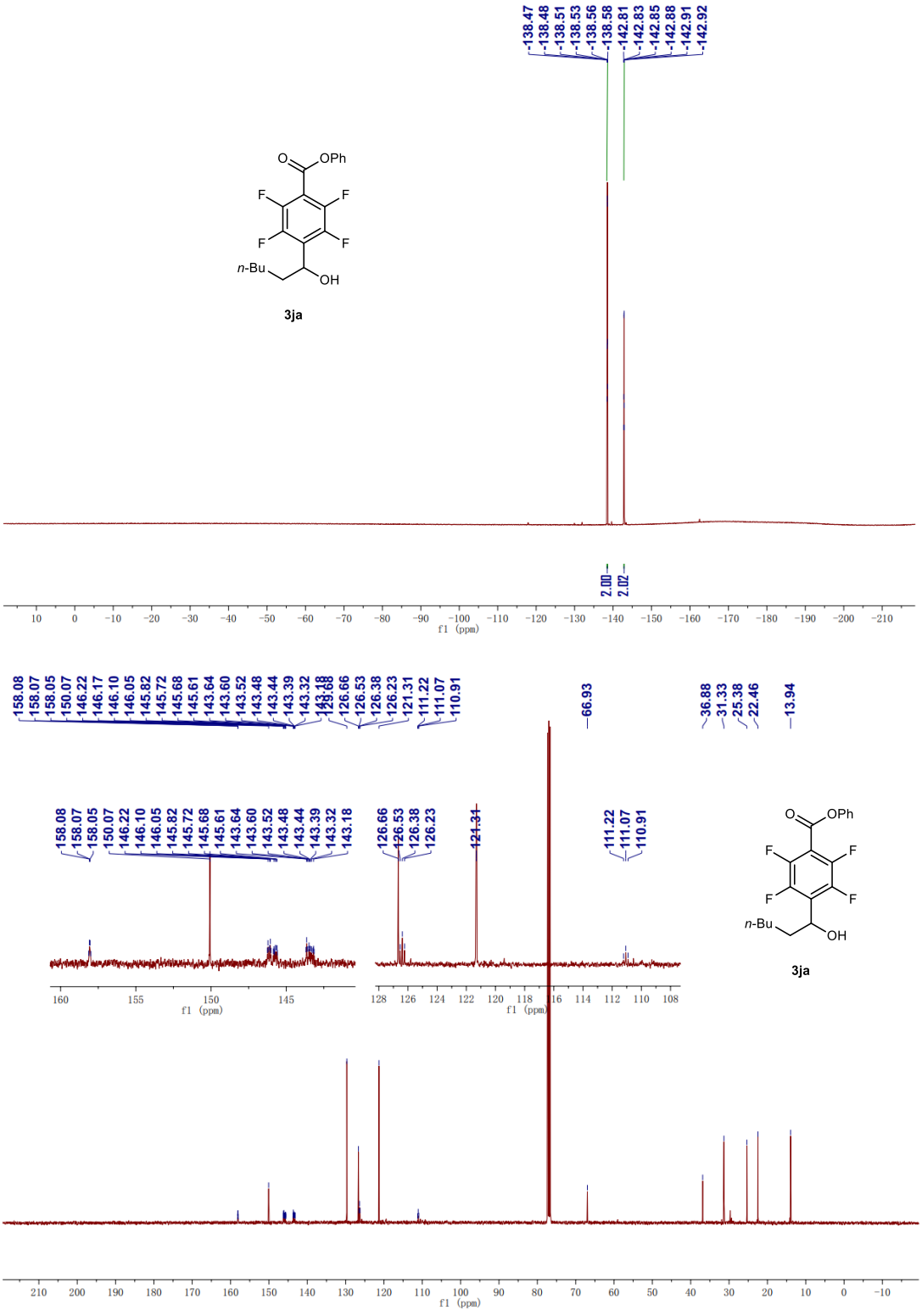
1.48
1.47
1.46
1.37
1.35
1.34
1.33
1.32
1.31
1.30
1.29
0.91
0.90
0.88
2.00
1.00
2.00
1.00
1.00
1.01
1.02
1.03
5.02
3.00
f1 (ppm)
O
OPh
F
F
F
F
n-Bu
OH
3ja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-142.81
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-142.85
-142.88
-142.91
-142.92
O
OPh
F
F
F
F
n-Bu
OH
3ja
2.00
2.02
f1 (ppm)
158.08
158.07
158.05
150.07
146.22
146.17
146.10
146.05
145.82
145.72
145.68
145.61
143.64
143.60
143.52
143.48
143.44
143.39
143.32
126.66
126.53
126.38
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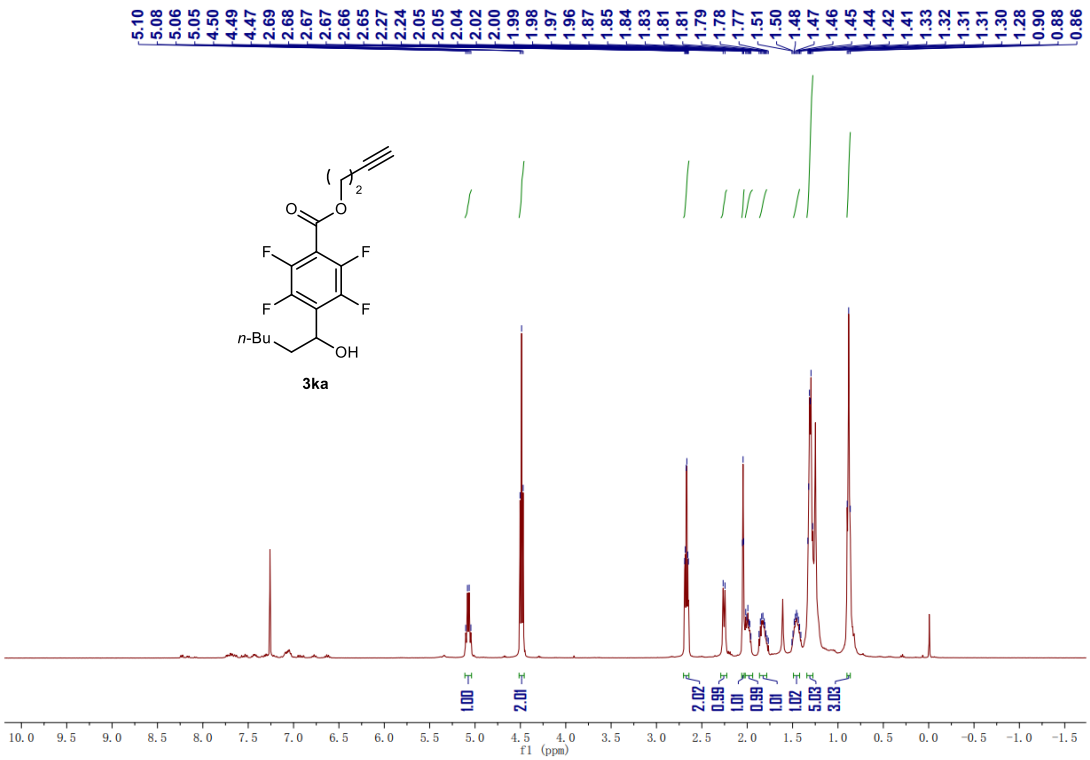
66.93
36.88
31.33
25.38
22.46
13.94
3ja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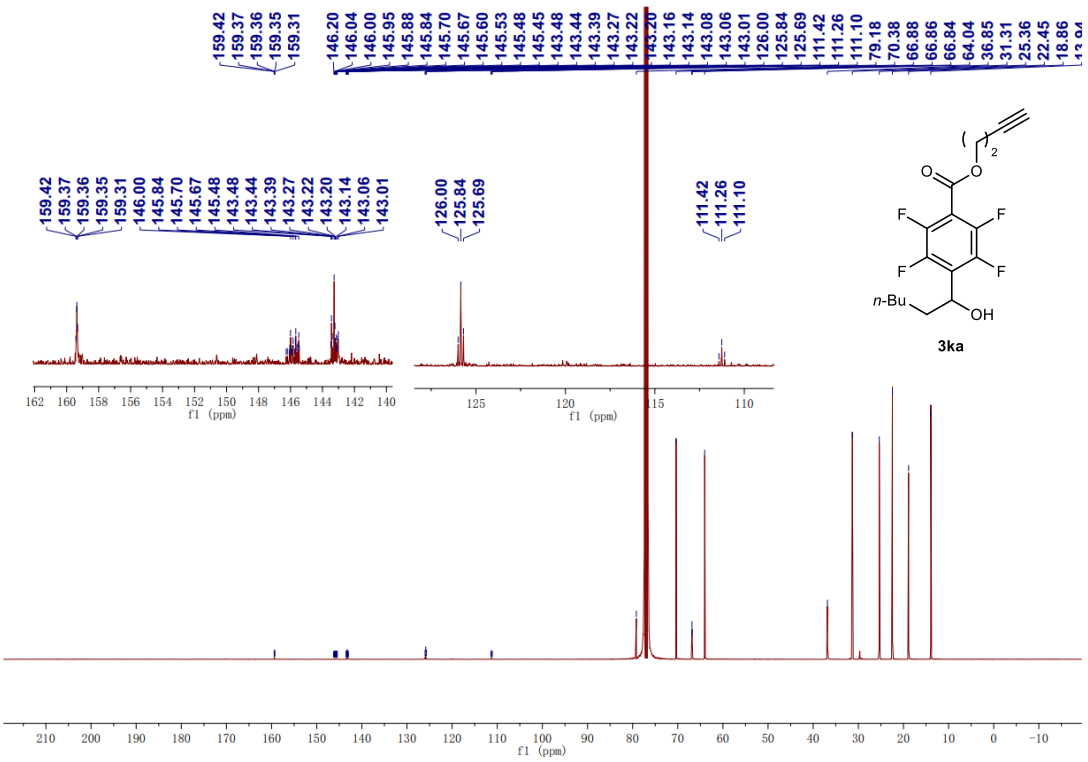
n-Bu
OH
3ka
1.00 2.01 2.02 0.99 1.01 0.99 1.01 1.02 5.03 3.03
f1 (ppm)


-138.99 -139.00 -139.03 -139.06 -139.09 -139.10 -143.12 -143.14 -143.17 -143.19 -143.22 -143.23
n-Bu
OH
3ka
2.00 2.02
f1 (ppm)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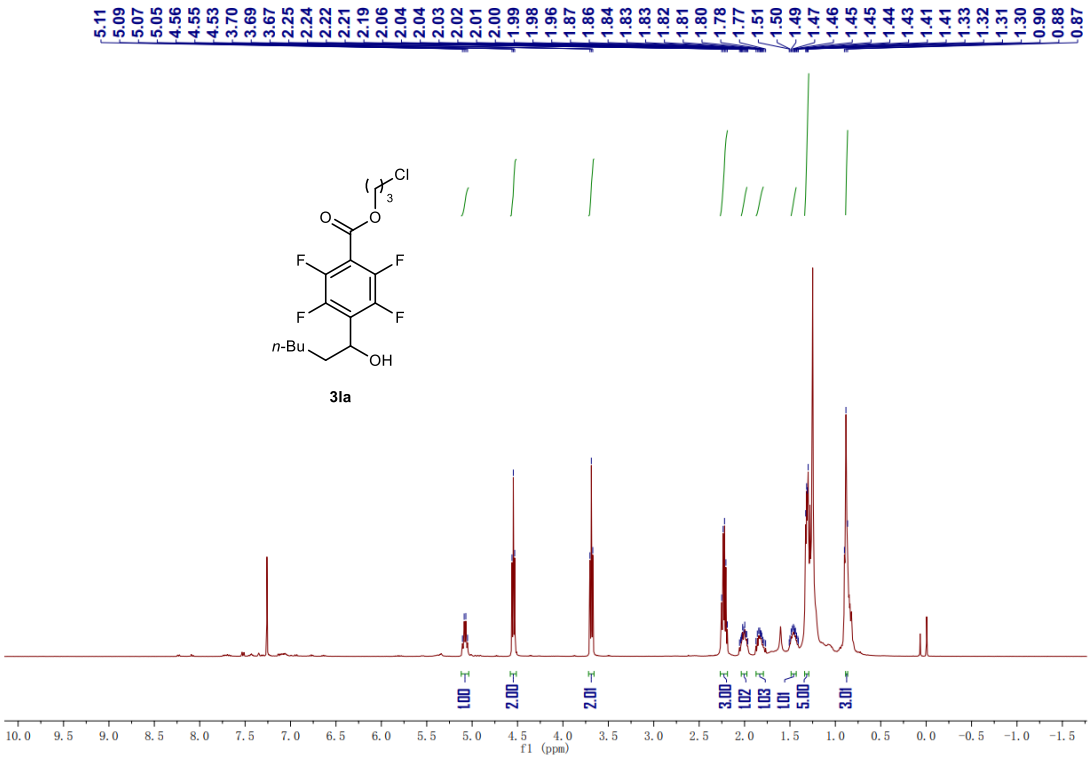
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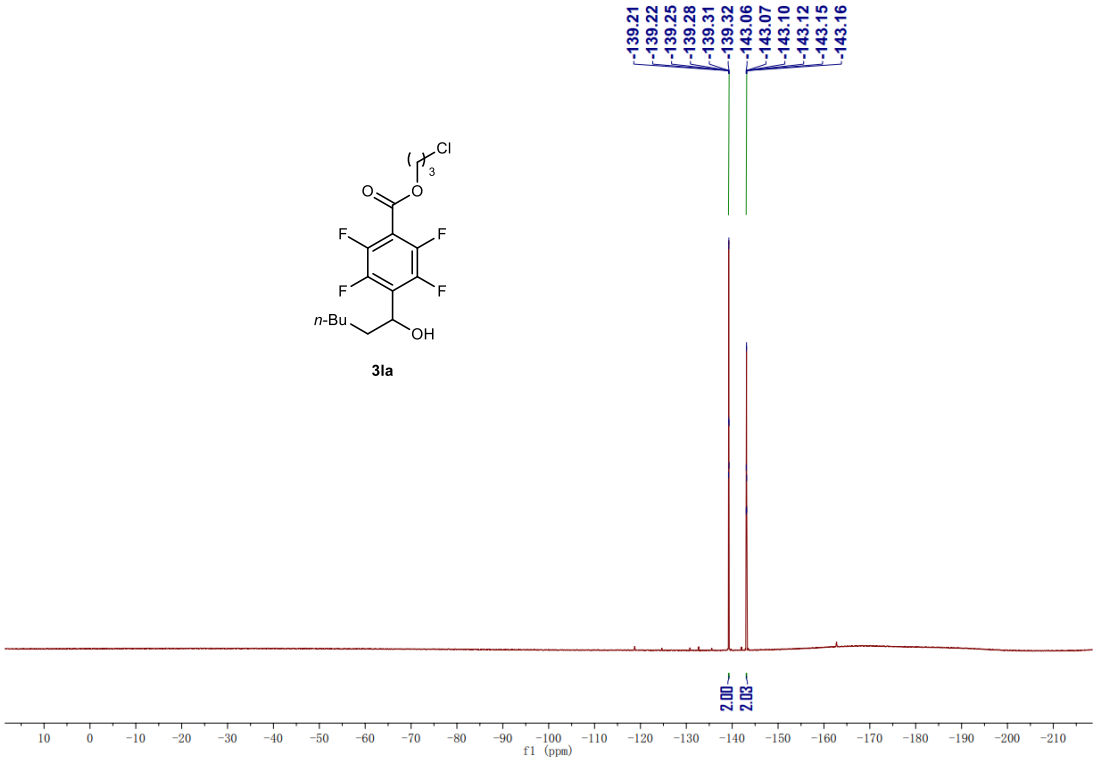
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-139.25
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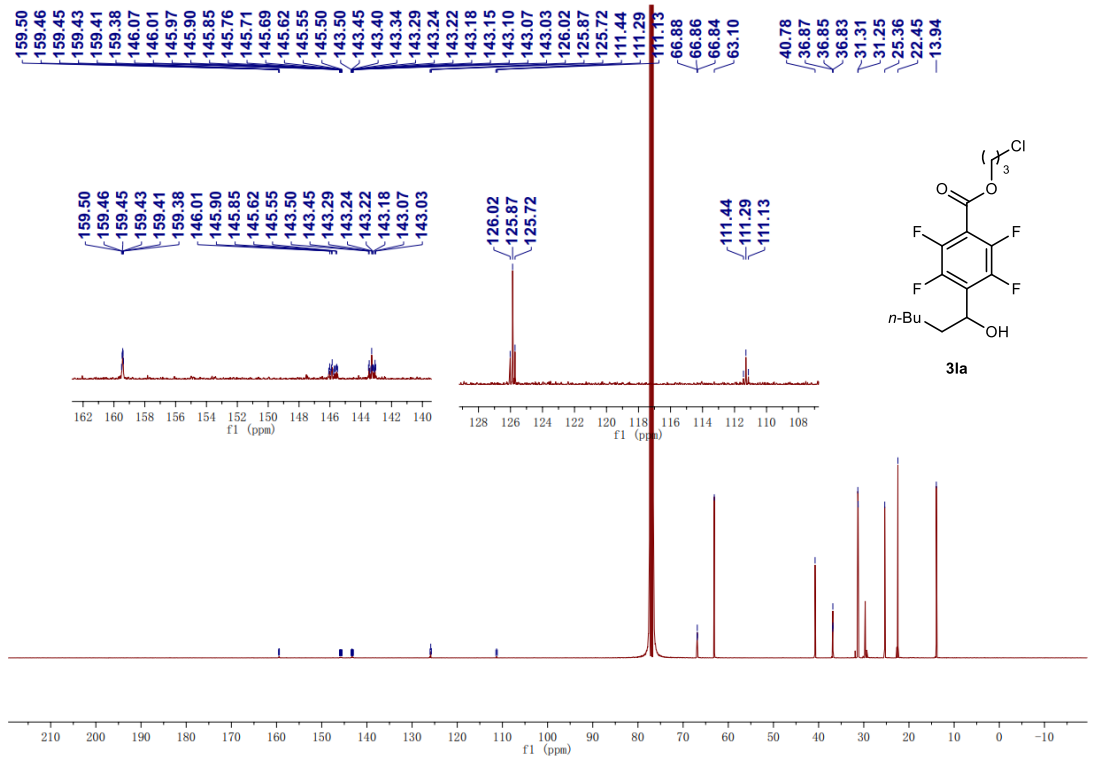
-143.07
-143.10
-143.12
-143.15
-143.16
Cl
3
O
O
F
F
F
F
n-Bu
OH
3la
2.00
2.03
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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145.50
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143.40
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143.18
143.15
143.10
143.07
143.03
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125.87
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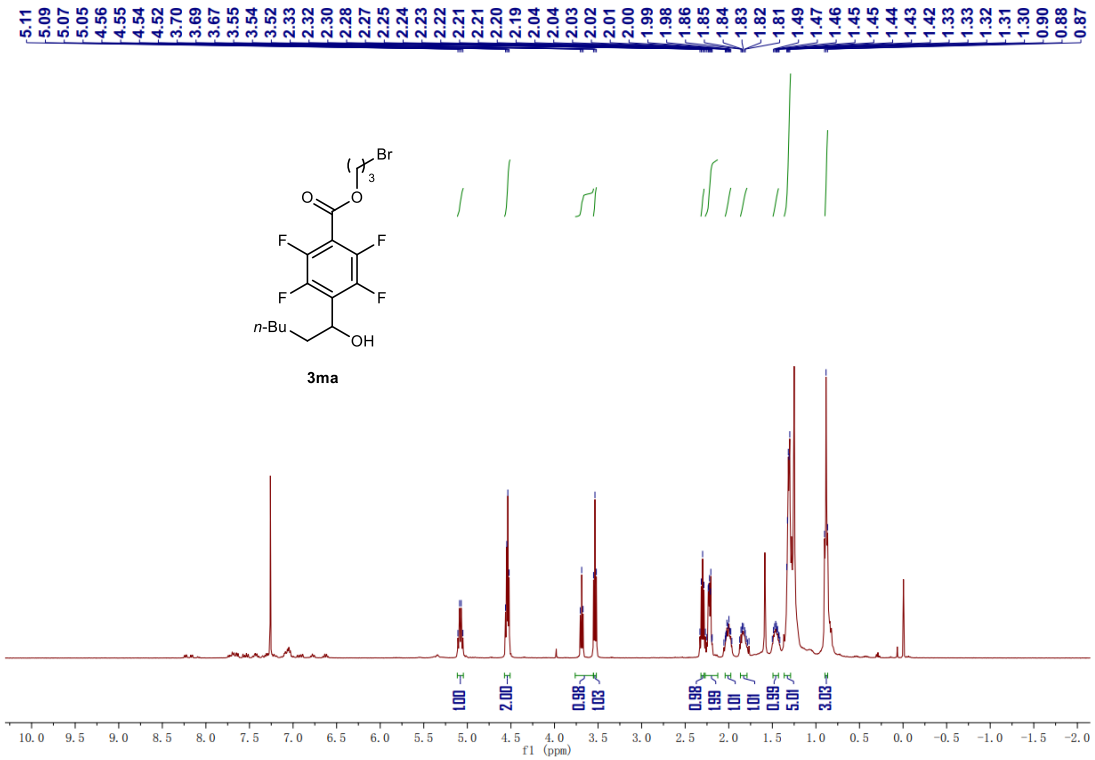
111.29
111.13
66.88
66.86
66.84
63.10
40.78
36.87
36.85
36.83
31.31
31.25
25.36
22.45
13.94
Cl
3
O
O
F
F
F
F
n-Bu
OH
3la
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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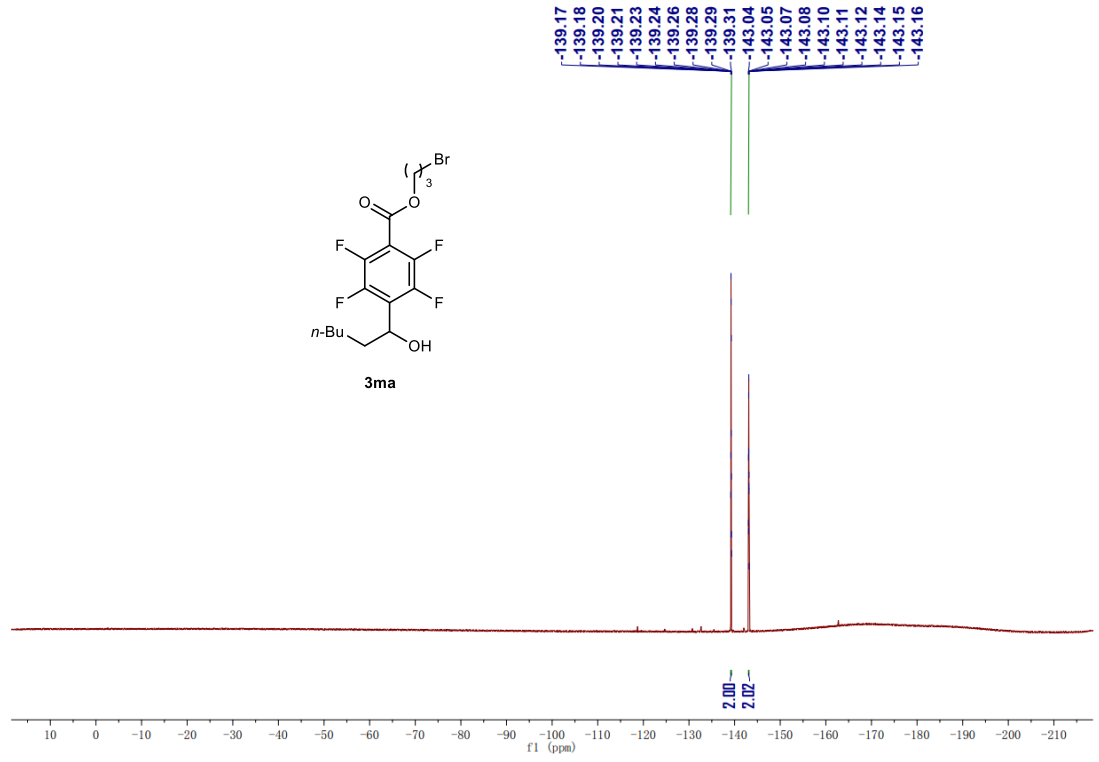
Br
3
O
O
F
F
F
F
n-Bu
OH
3ma
1.00 2.00 0.98 1.03 0.98 1.99 1.01 1.01 0.99 5.01 3.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)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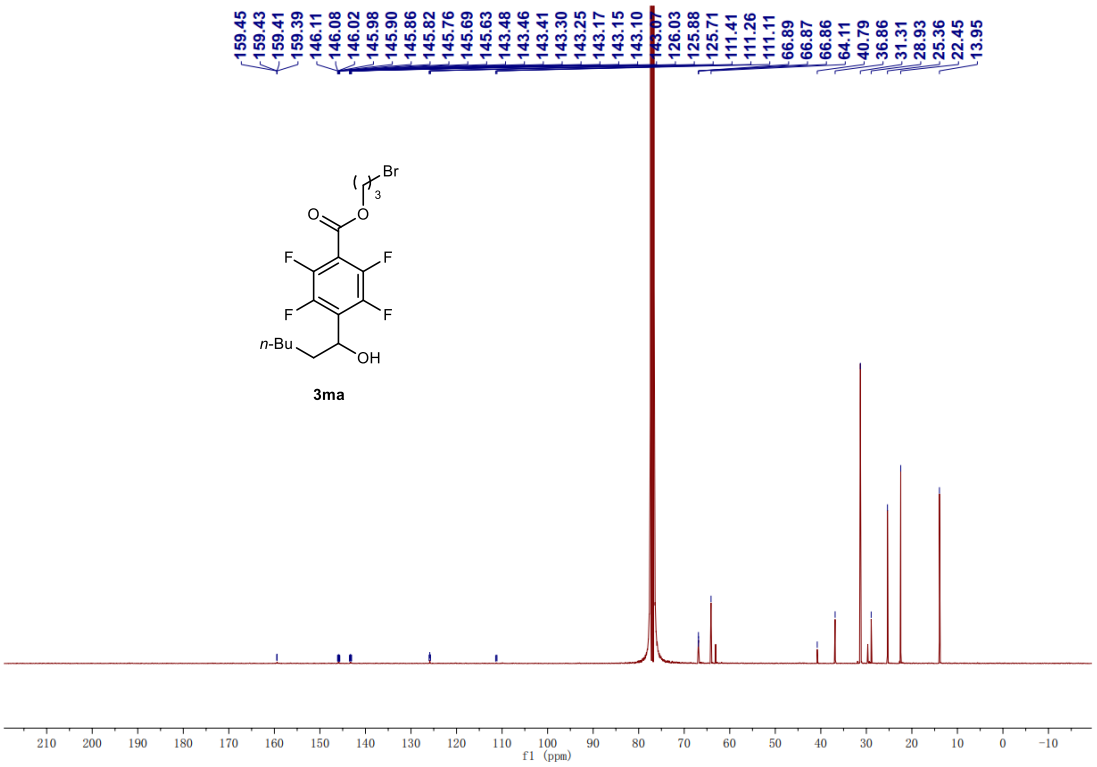
Br
3
O
O
F
F
F
F
n-Bu
OH
3ma
2.00 2.02
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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145.63
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143.10
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Br
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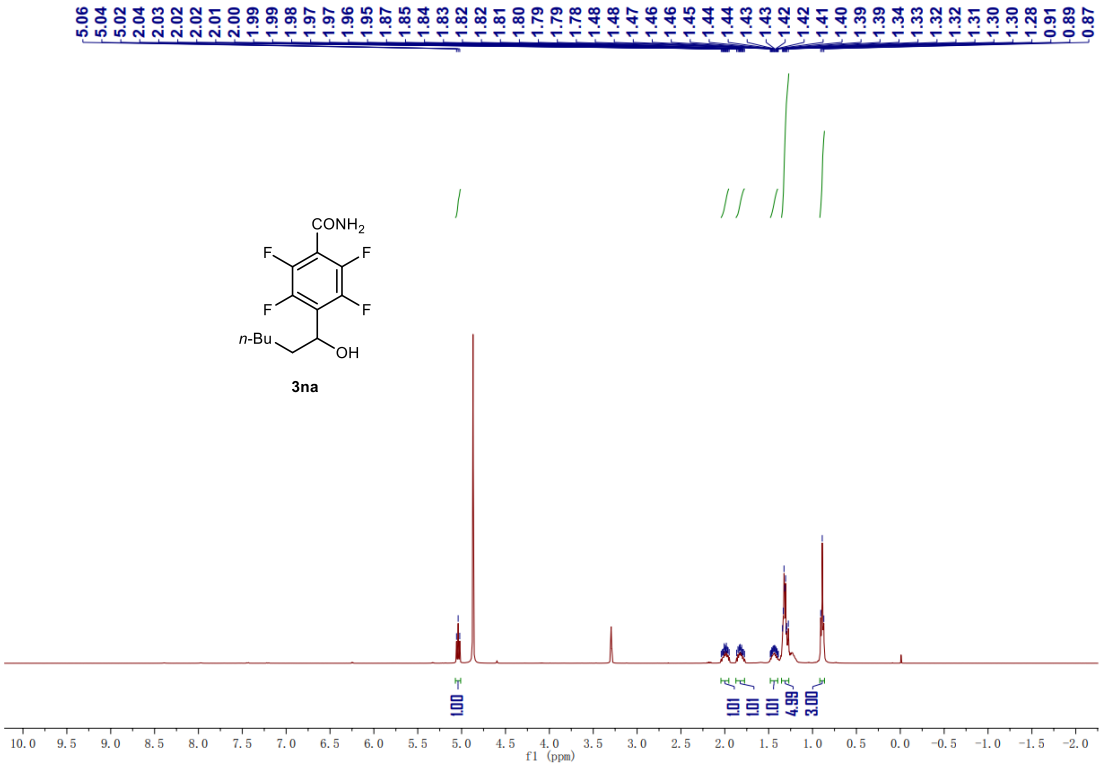
O
O
F
F
F
F
n-Bu
OH
3ma
f1 (ppm)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2.02
2.02
2.01
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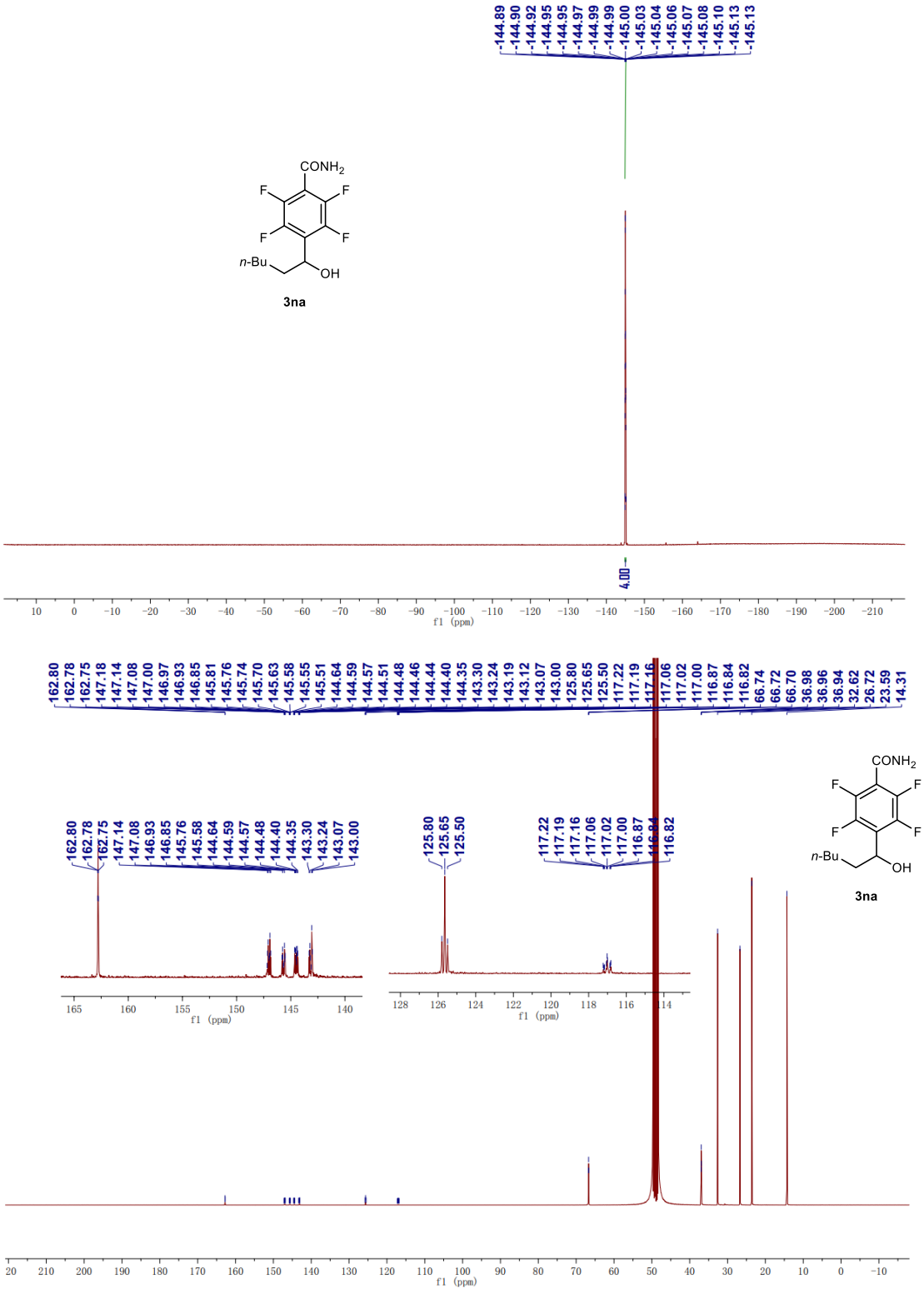
1.39
1.39
1.34
1.33
1.32
1.32
1.31
1.30
1.30
1.28
0.91
0.89
0.87
CONH2
F
F
F
F
n-Bu
OH
3na
1.00
1.01
1.01
1.01
4.99
3.00
f1 (ppm)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-145.06
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-145.08
-145.10
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-145.13
CONH2
F
F
F
F
n-Bu
OH
3na
4.00
f1 (ppm)
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162.75
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147.08
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32.62
26.72
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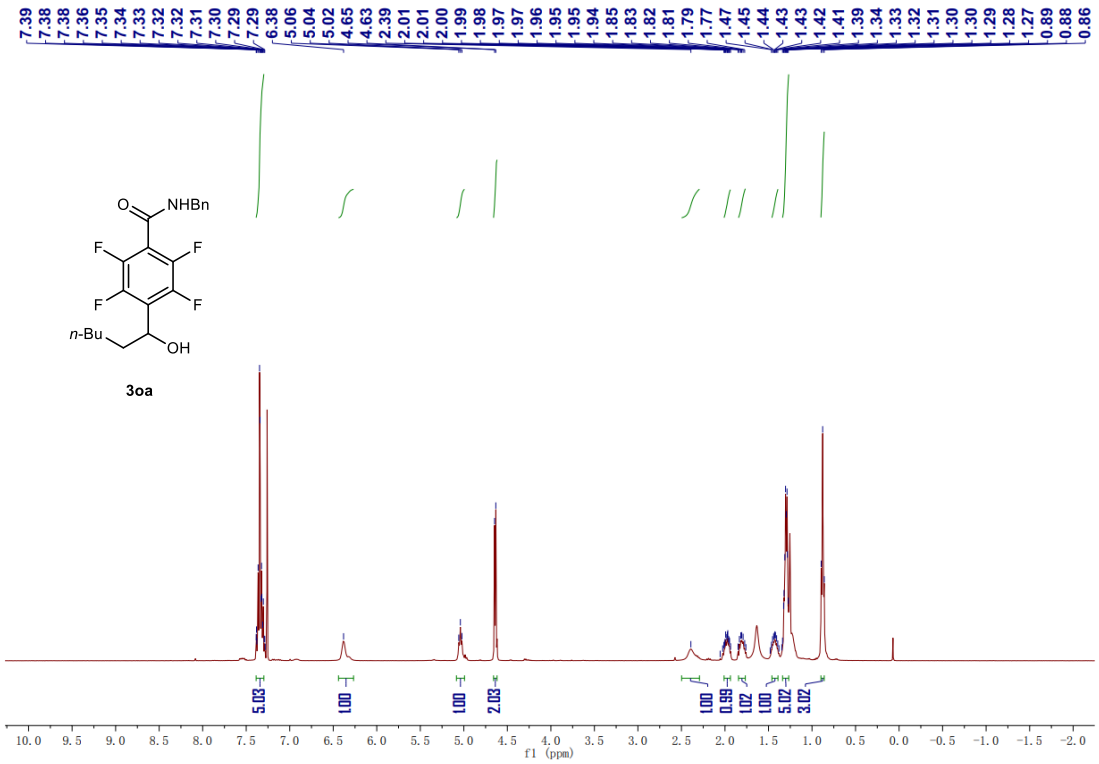
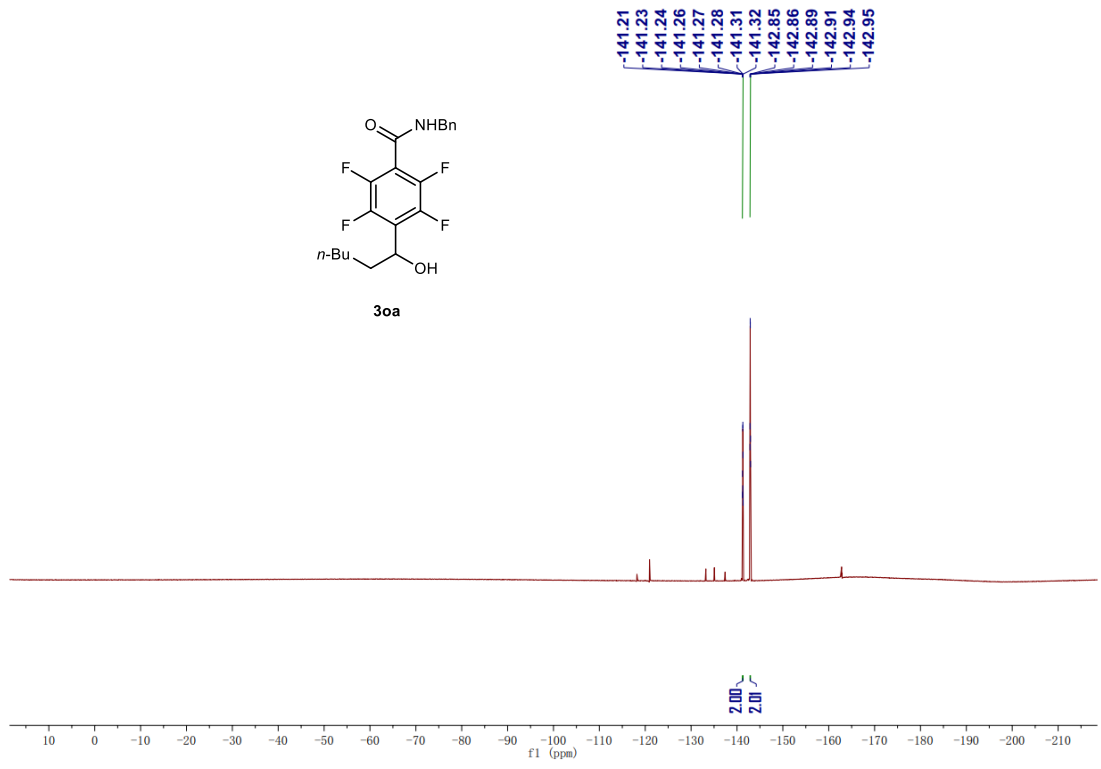
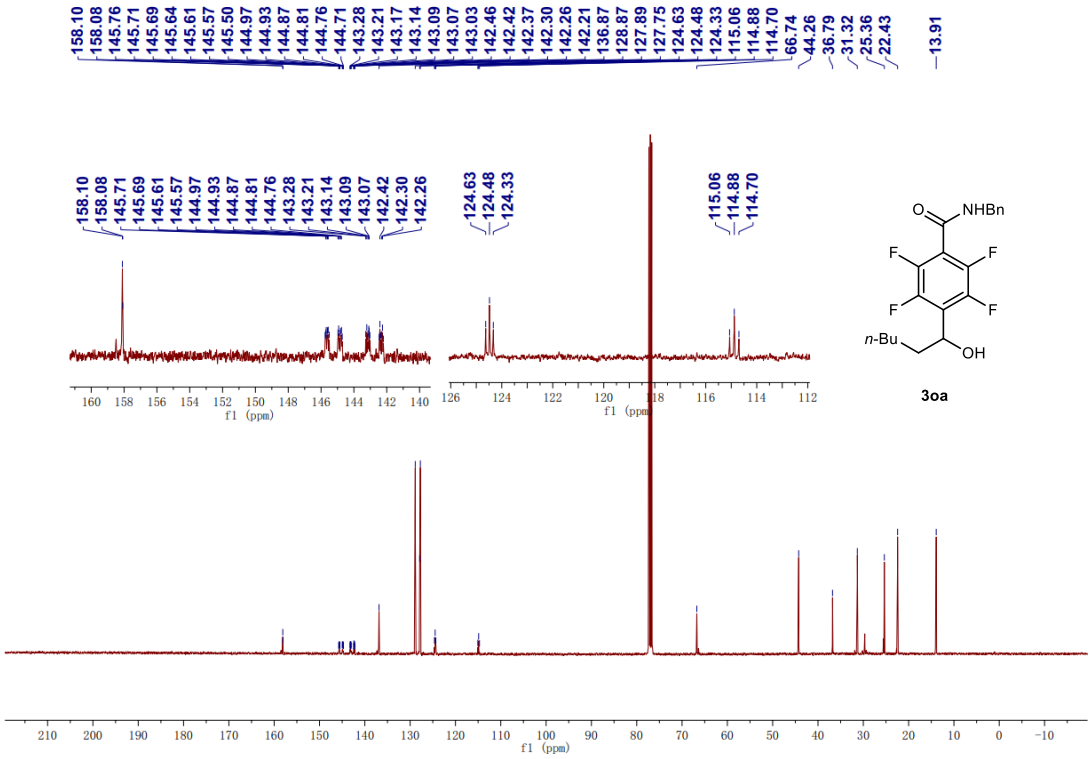
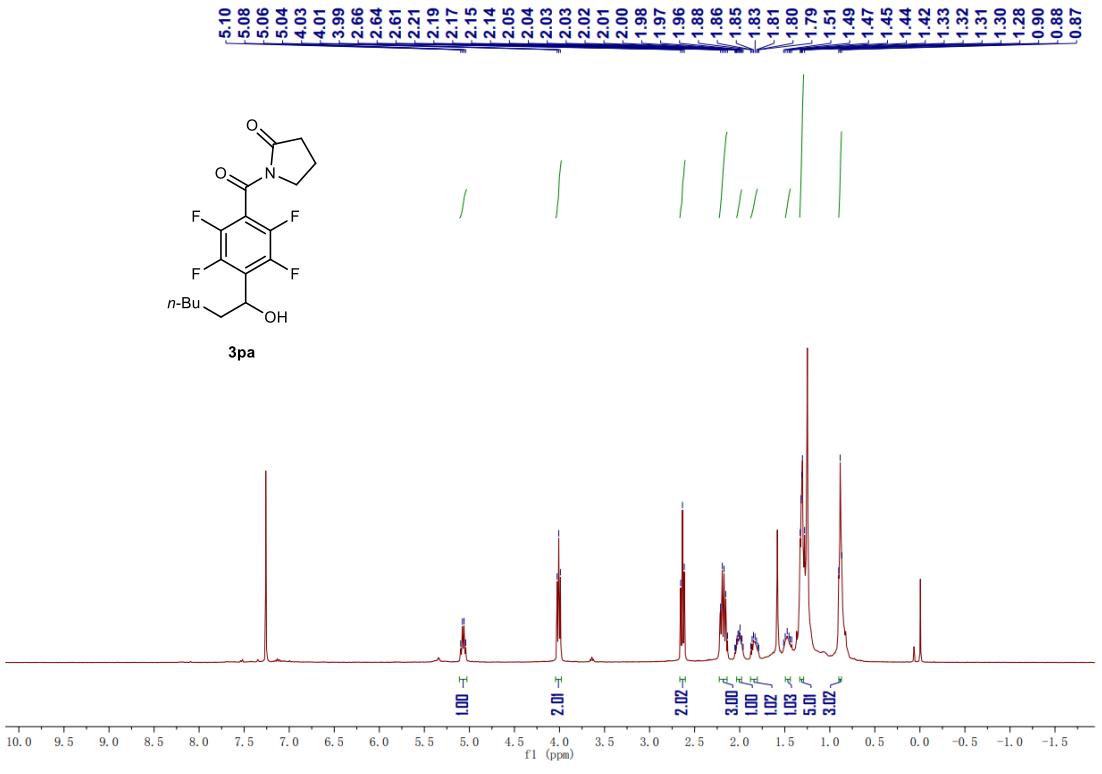
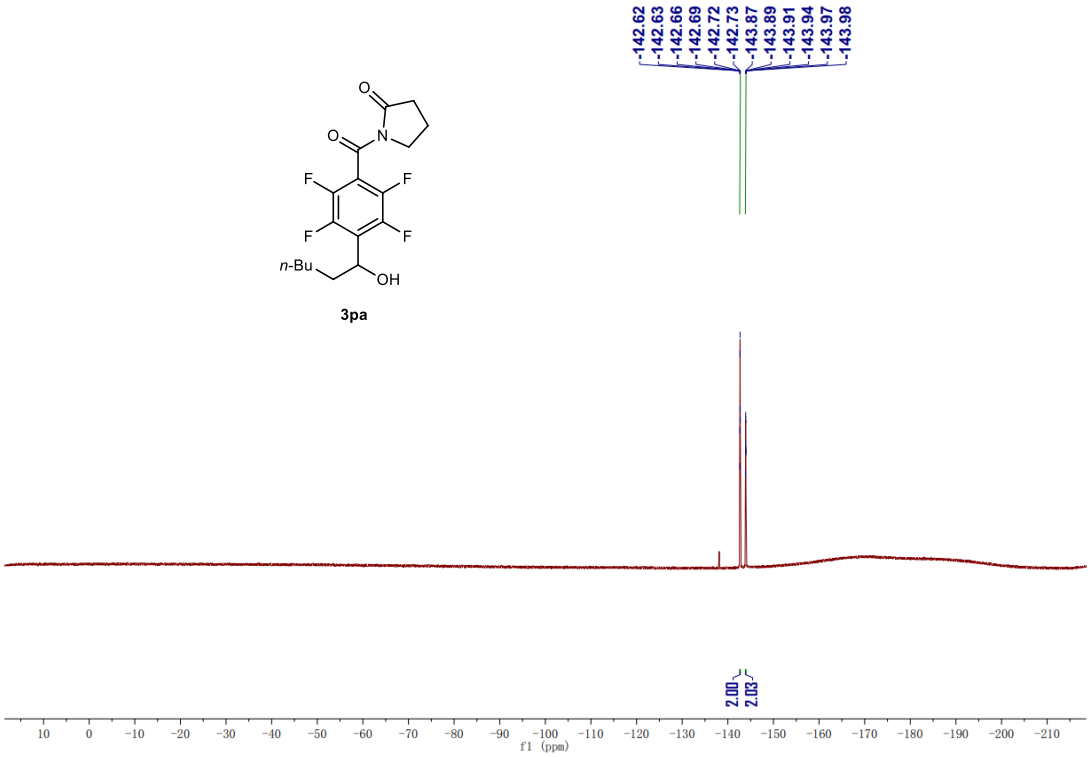
CONH2
F
F
F
F
n-Bu
OH
3na
f1 (ppm)
f1 (ppm)
f1 (ppm)

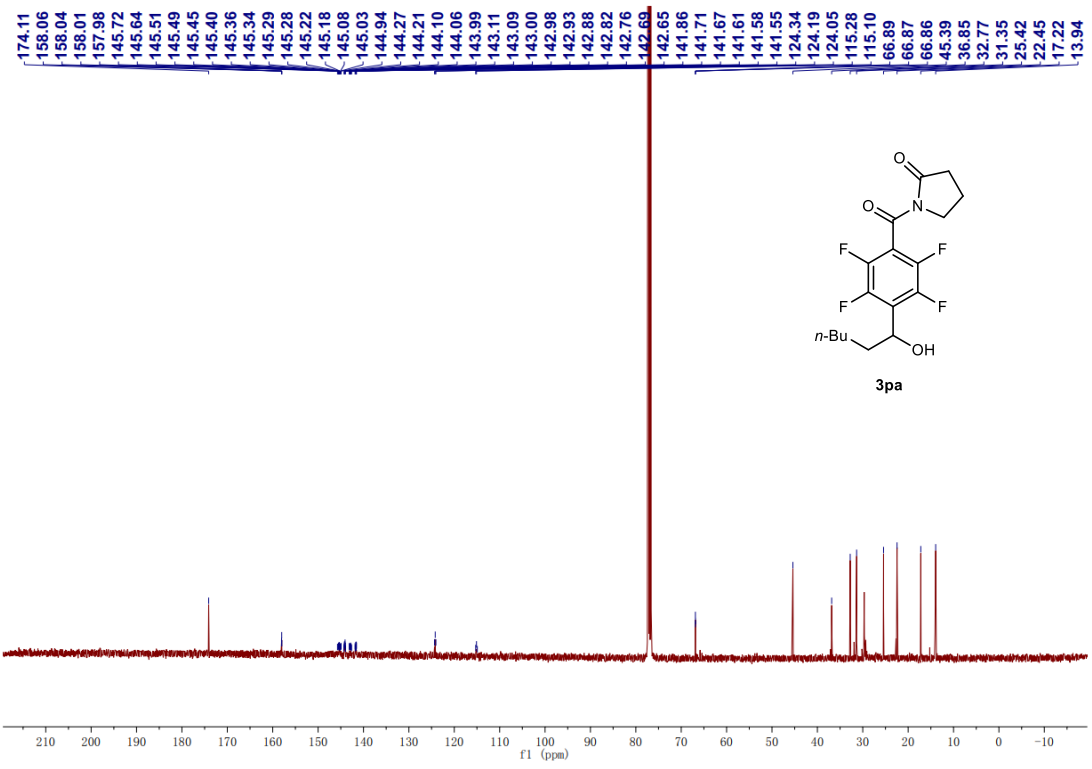

7.39
7.38
7.38
7.36
7.35
7.34
7.33
7.32
7.32
7.31
7.30
7.29
7.29
6.38
5.06
5.04
5.02
4.65
4.63
2.39
2.01
2.01
2.00
1.99
1.98
1.97
1.97
1.96
1.95
1.95
1.94
1.85
1.83
1.82
1.81
1.79
1.77
1.47
1.45
1.44
1.43
1.43
1.42
1.41
1.39
1.34
1.33
1.32
1.31
1.30
1.30
1.29
1.28
1.27
0.89
0.88
0.86
O
NHBn
F
F
F
F
n-Bu
OH
3oa
5.03
1.00
1.00
2.03
1.00
0.99
1.02
1.00
5.02
3.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
f1 (ppm)

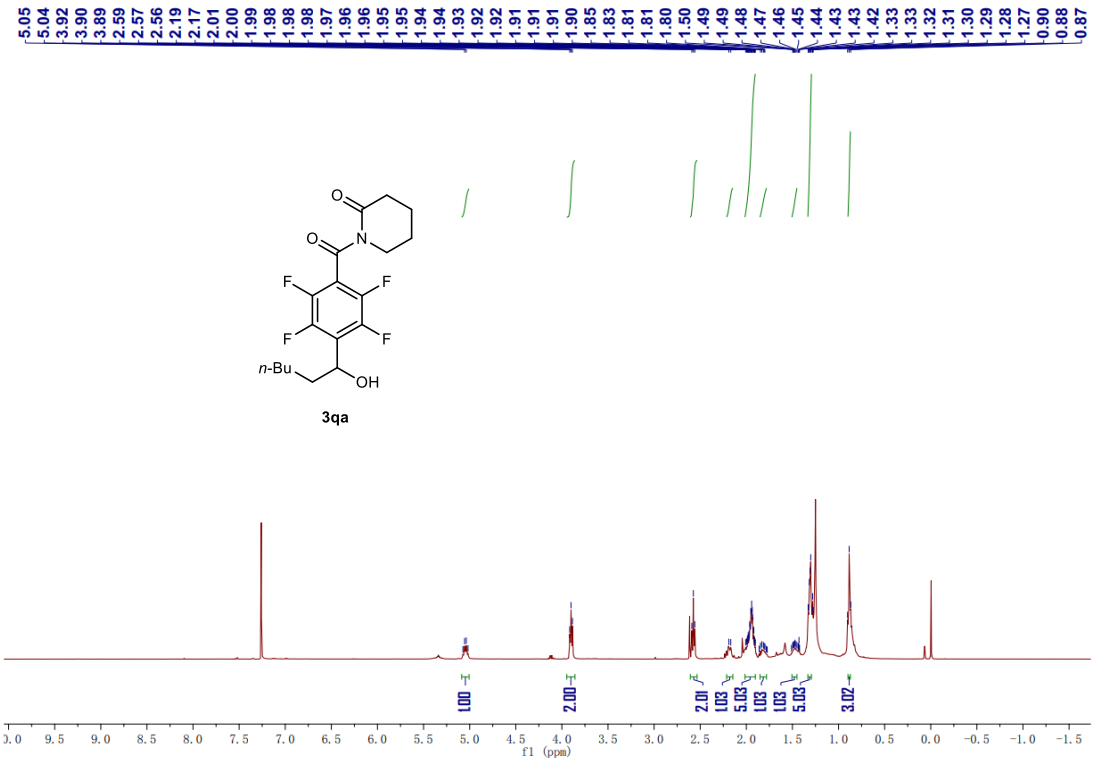

-141.21
-141.23
-141.24
-141.26
-141.27
-141.28
-141.31
-141.32
-142.85
-142.86
-142.89
-142.91
-142.94
-142.95
O
NHBn
F
F
F
F
n-Bu
OH
3oa
2.00
2.01
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

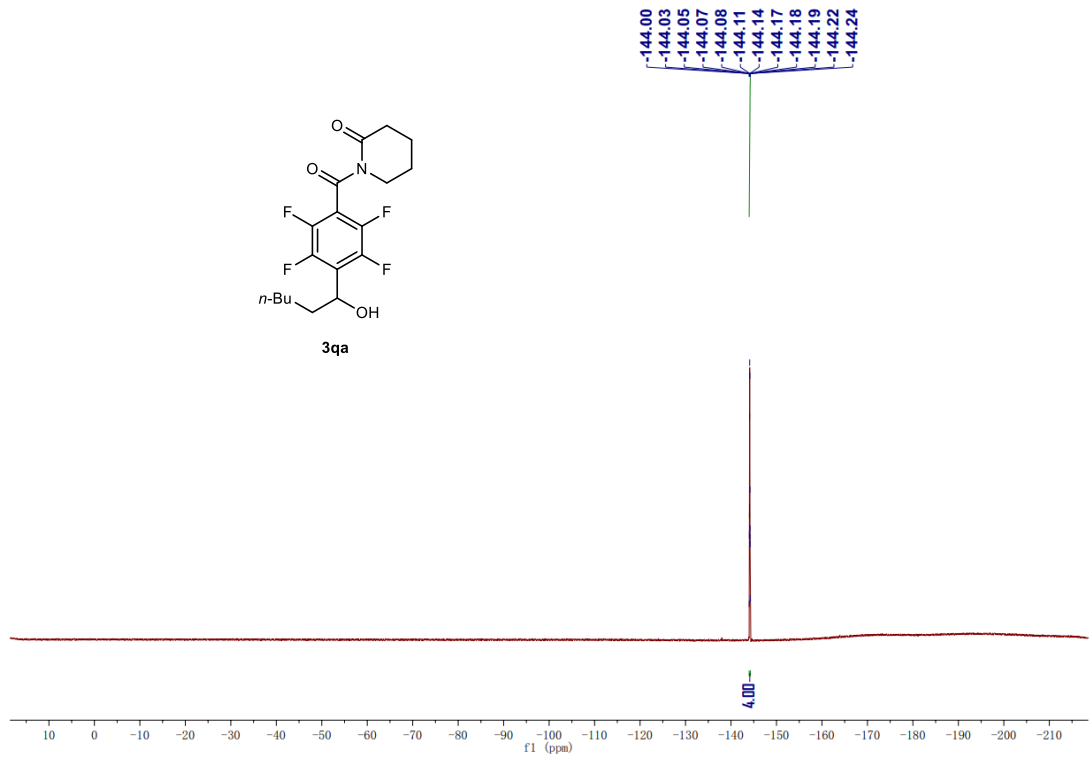

158.10
158.08
145.76
145.71
145.69
145.64
145.61
145.57
145.50
144.97
144.93
144.87
144.81
144.76
144.71
143.28
143.21
143.17
143.14
143.09
143.07
143.03
142.46
142.42
142.37
142.30
142.26
142.21
136.87
128.87
127.89
127.75
124.63
124.48
124.33
115.06
114.88
114.70
66.74
44.26
36.79
31.32
25.36
22.43
13.91
O
NHBn
F
F
F
F
n-Bu
OH
3oa

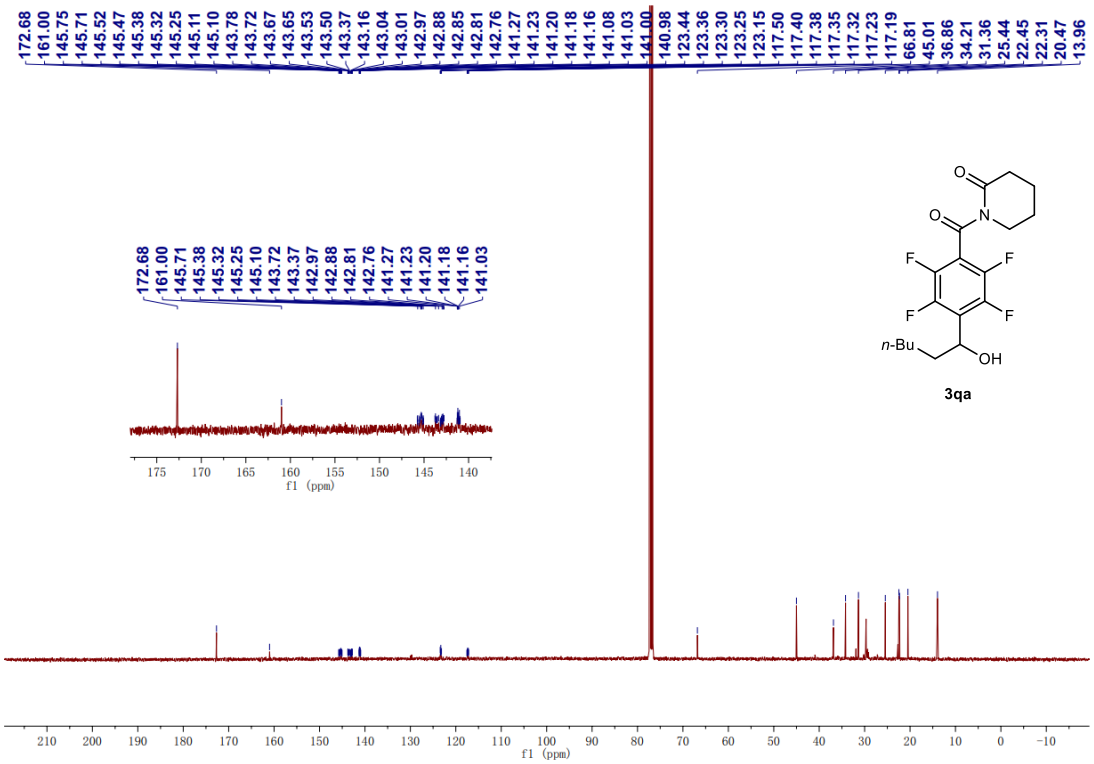

5.10
5.08
5.06
5.04
4.03
4.01
3.99
2.66
2.64
2.61
2.21
2.19
2.17
2.15
2.14
2.05
2.04
2.03
2.03
2.02
2.01
2.00
1.98
1.97
1.96
1.88
1.86
1.85
1.83
1.81
1.80
1.79
1.51
1.49
1.47
1.45
1.44
1.42
1.33
1.32
1.31
1.30
1.28
0.90
0.88
0.87
O
O
N
F
F
F
F
n-Bu
OH
3pa
1.00
2.01
2.02
3.00
1.00
1.02
1.03
5.01
3.02

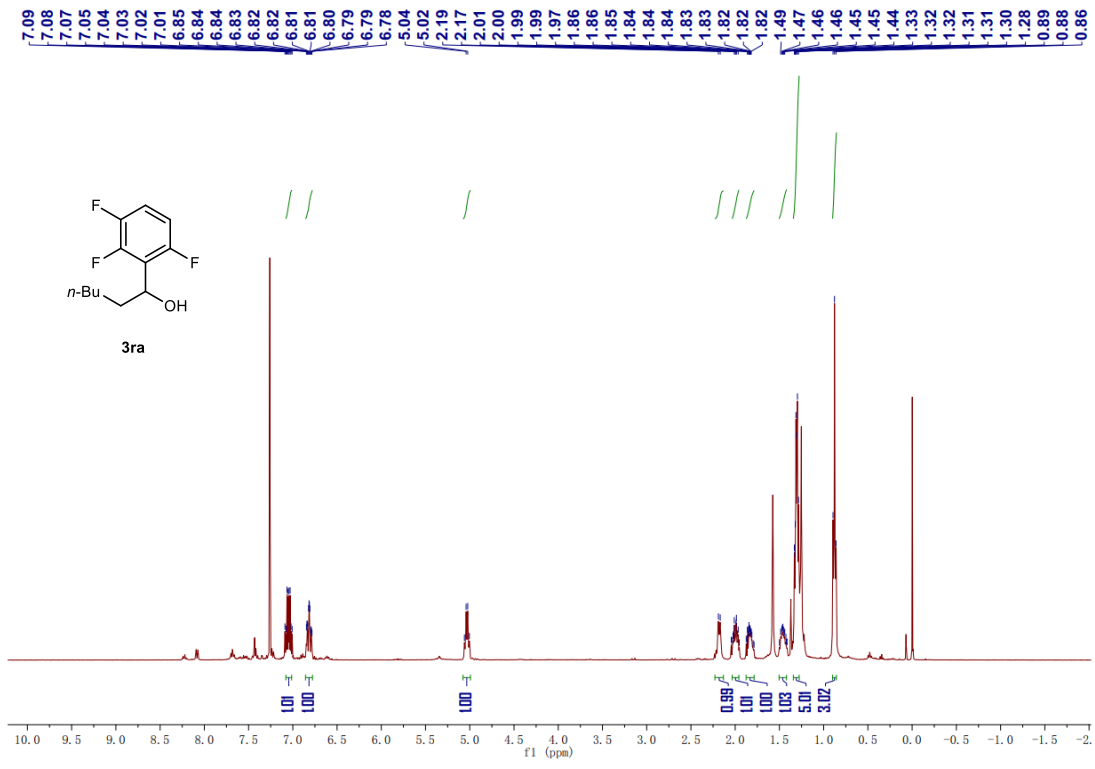

-142.62
-142.63
-142.66
-142.69
-142.72
-142.73
-143.87
-143.89
-143.91
-143.94
-143.97
-143.98
O
O
N
F
F
F
F
n-Bu
OH
3pa
2.00
2.03
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)

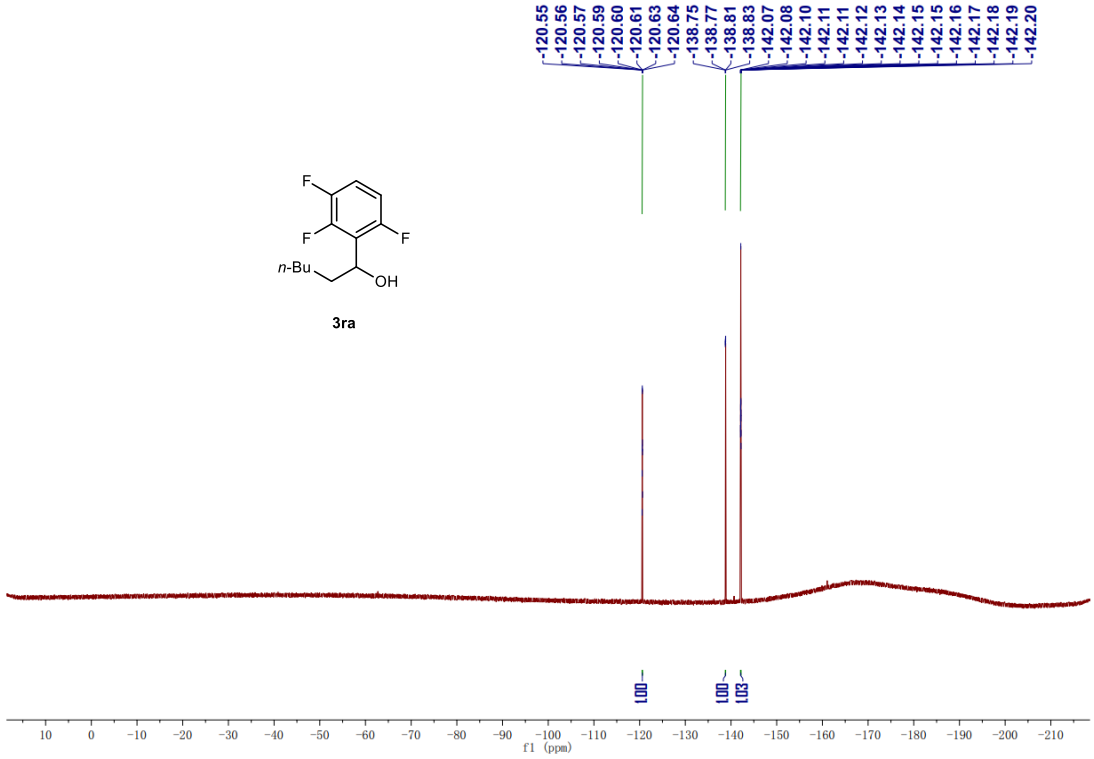

174.11
158.06
158.04
158.01
157.98
145.72
145.64
145.51
145.49
145.45
145.40
145.36
145.34
145.29
145.28
145.22
145.18
145.08
145.03
144.94
144.27
144.21
144.10
144.06
143.99
143.11
143.09
143.00
142.98
142.93
142.88
142.82
142.76
142.69
142.65
141.86
141.71
141.67
141.61
141.58
141.55
124.34
124.19
124.05
115.28
115.10
66.89
66.87
66.86
45.39
36.85
32.77
31.35
25.42
22.45
17.22
13.94
O
O
N
F
F
F
F
n-Bu
OH
3pa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

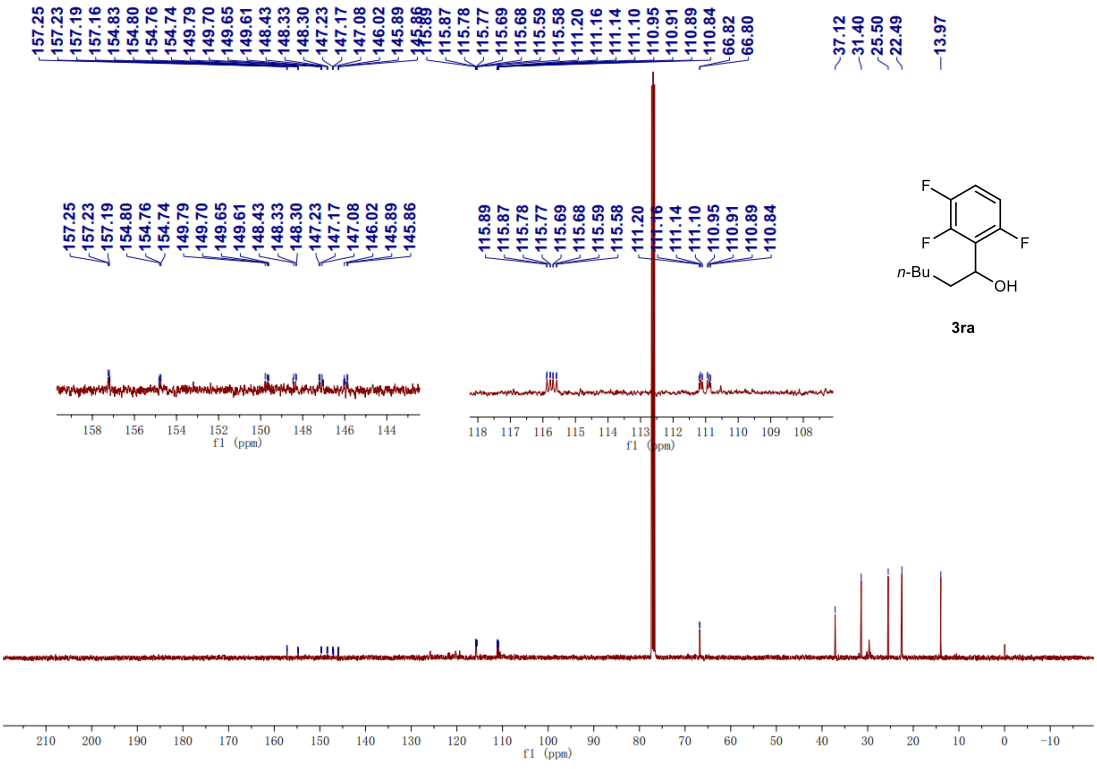

5.05 5.04 3.92 3.90 3.89 2.59 2.57 2.56 2.19 2.17 2.01 2.00 1.99 1.98 1.98 1.98 1.97 1.96 1.96 1.95 1.95 1.94 1.94 1.93 1.92 1.92 1.91 1.91 1.91 1.90 1.85 1.83 1.81 1.81 1.80 1.50 1.49 1.49 1.48 1.47 1.46 1.45 1.44 1.43 1.43 1.42 1.33 1.33 1.32 1.31 1.30 1.29 1.28 1.27 0.90 0.88 0.87
O
O
N
F
F
F
F
n-Bu
OH
3qa
1.00 2.00 2.01 1.03 5.03 1.03 1.03 5.03 3.02
f1 (ppm)

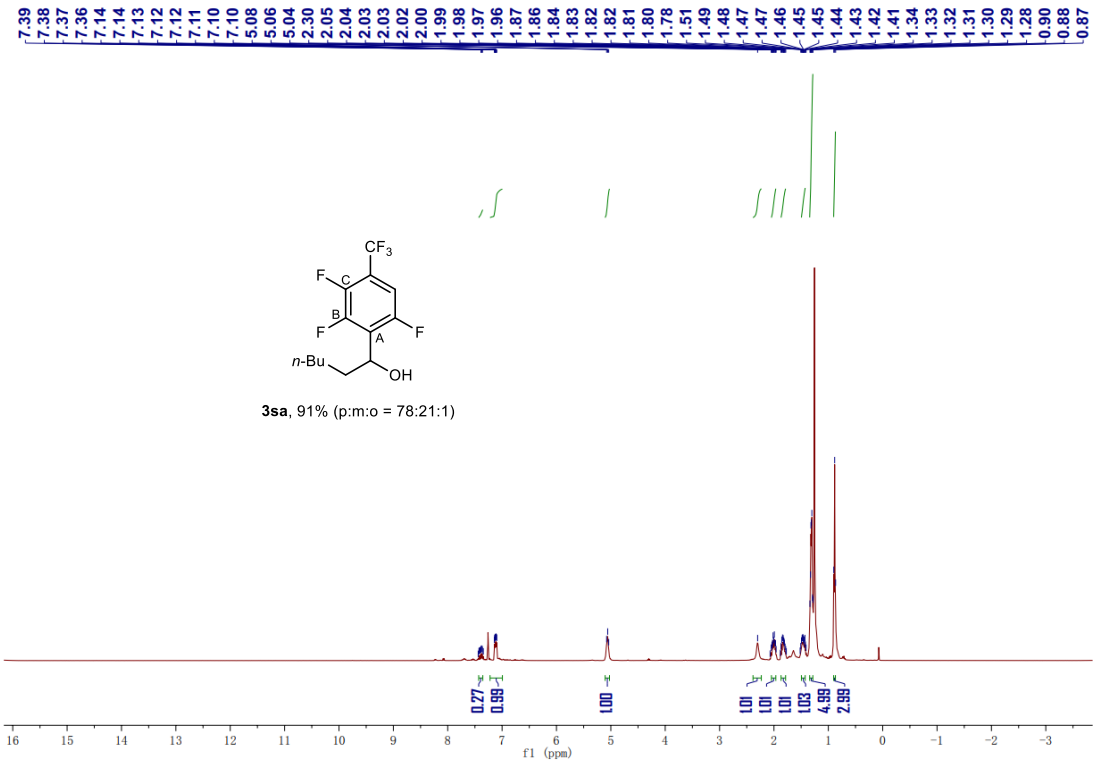

-144.00 -144.03 -144.05 -144.07 -144.08 -144.11 -144.14 -144.17 -144.18 -144.19 -144.22 -144.24
O
O
N
F
F
F
F
n-Bu
OH
3qa
4.00
f1 (ppm)


3qa

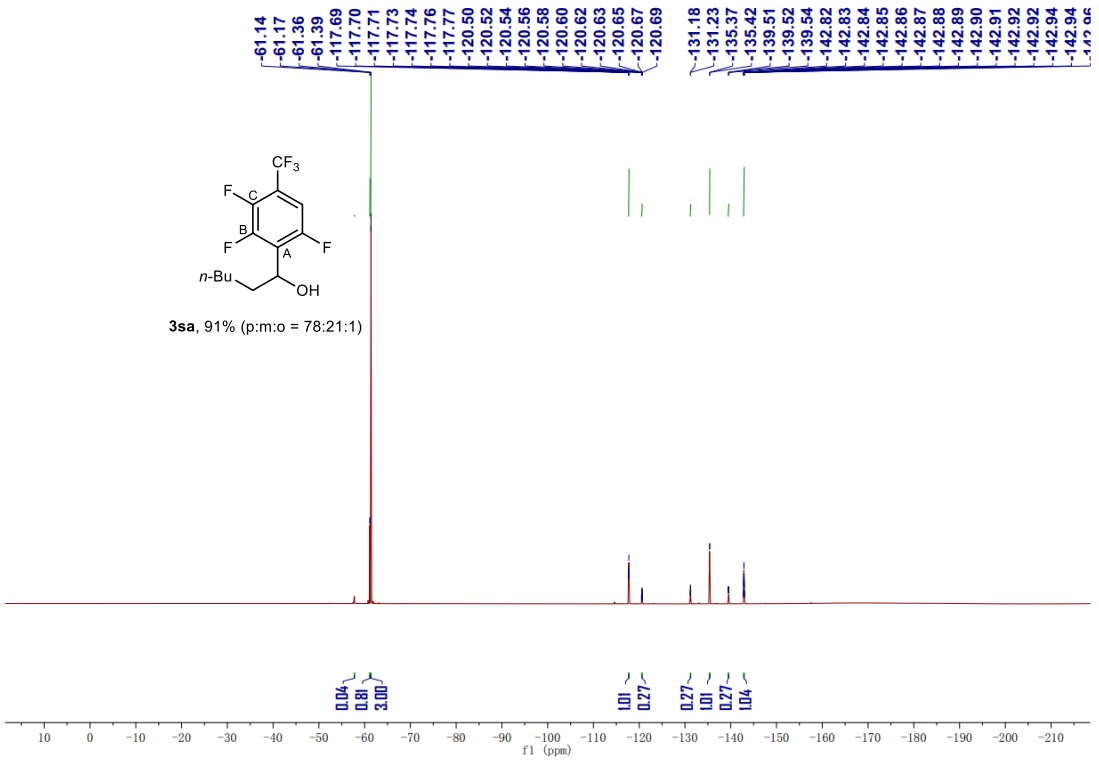

3ra


-120.55
-120.56
-120.57
-120.59
-120.60
-120.61
-120.63
-120.64
-138.75
-138.77
-138.81
-138.83
-142.07
-142.08
-142.10
-142.11
-142.11
-142.12
-142.13
-142.14
-142.15
-142.15
-142.16
-142.17
-142.18
-142.19
-142.20
F
F
F
n-Bu
OH
3ra
1.00
1.00
1.03
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)

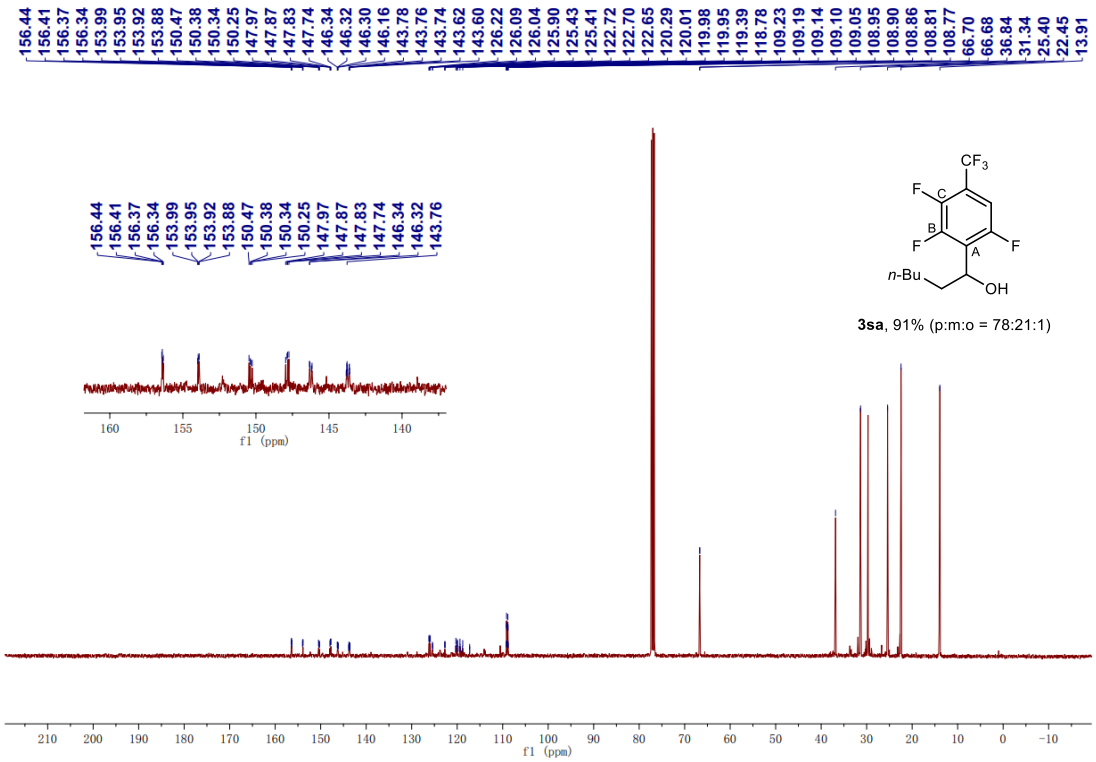

157.25
157.23
157.19
157.16
154.83
154.80
154.76
154.74
149.79
149.70
149.65
149.61
148.43
148.33
148.30
147.23
147.17
147.08
146.02
145.89
115.87
115.78
115.77
115.69
115.68
115.59
115.58
111.20
111.16
111.14
111.10
110.95
110.91
110.89
110.84
66.82
66.80
37.12
31.40
25.50
22.49
13.97
F
F
F
n-Bu
OH
3ra
158 156 154 152 150 148 146 144
f1 (ppm)
118 117 116 115 114 113 112 111 110 109 108
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

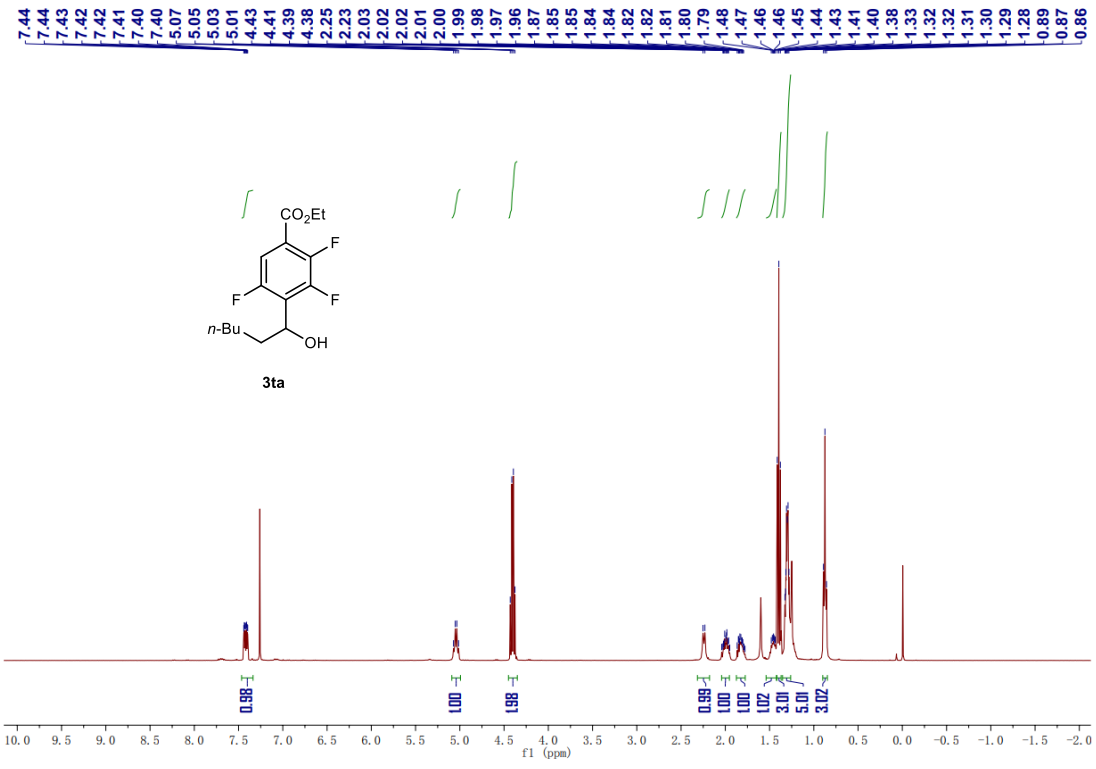


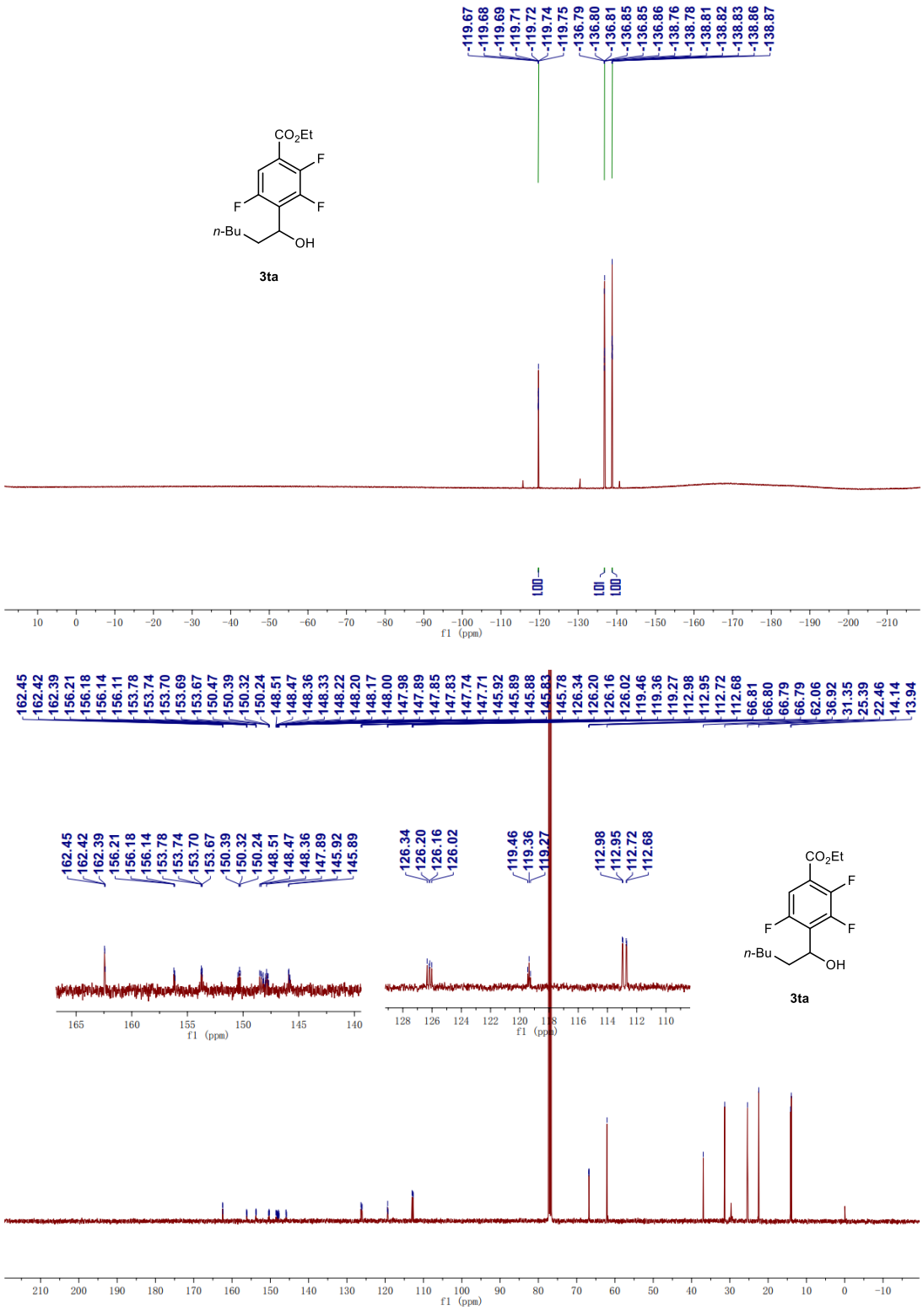
3sa, 91% (p:m:o = 78:21:1)

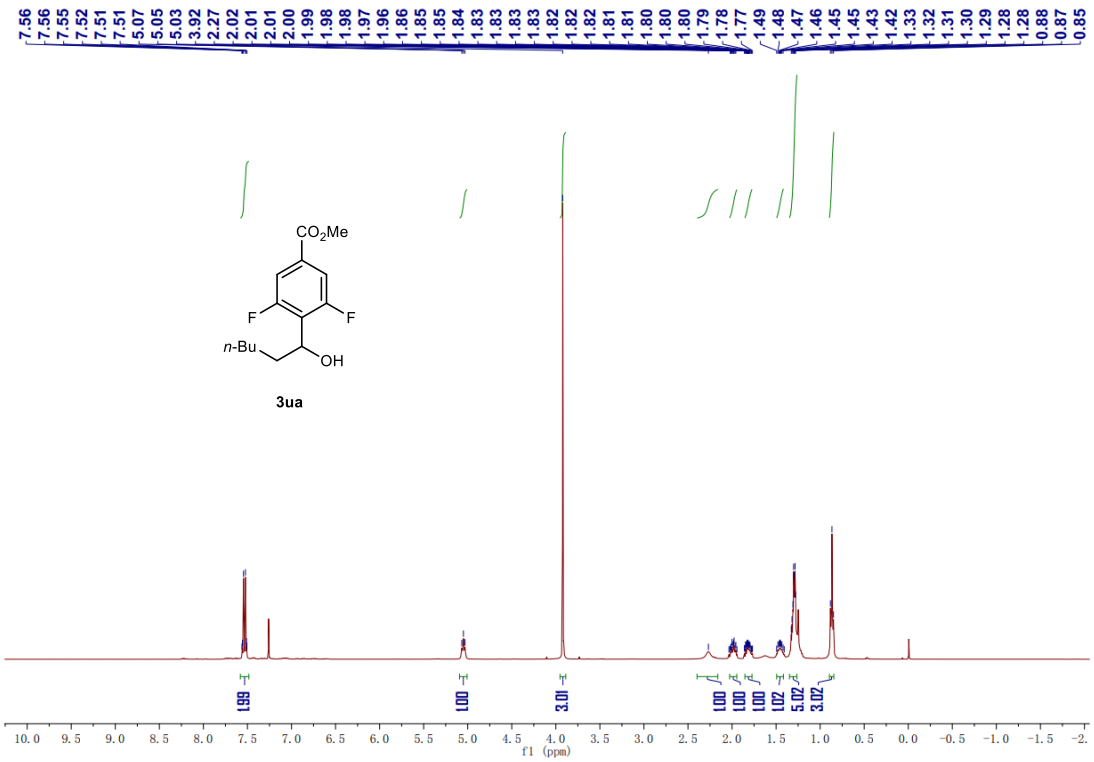


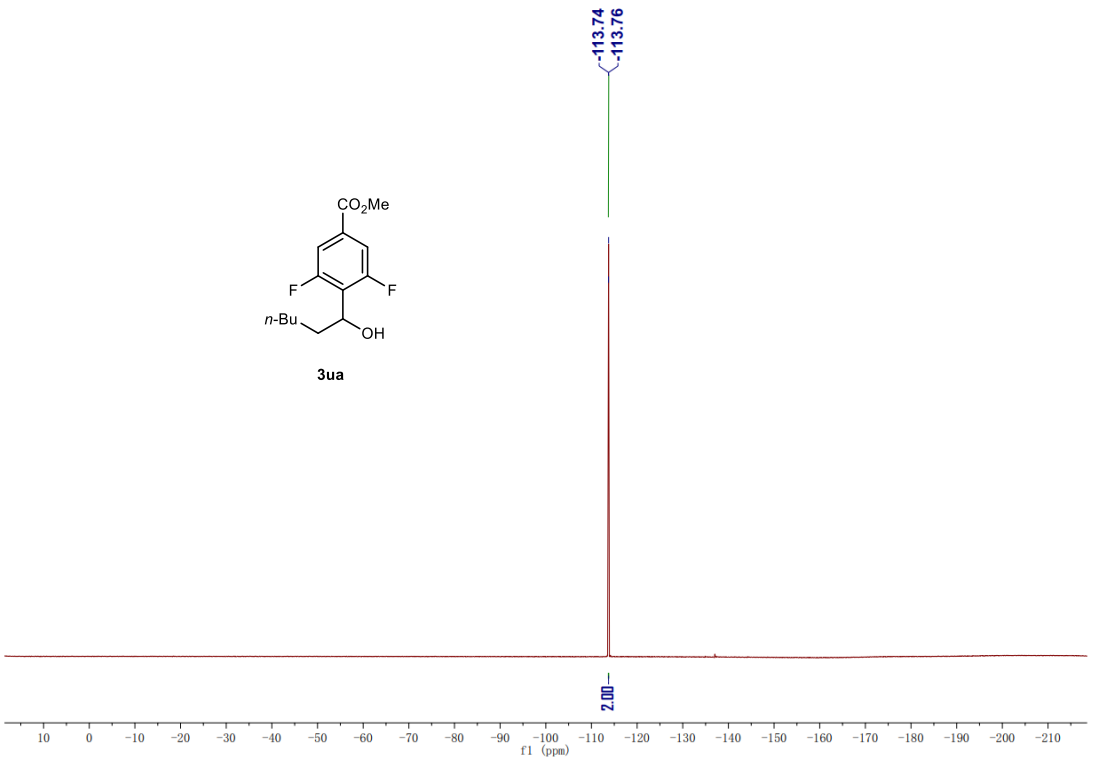
3sa, 91% (p:m:o = 78:21:1)

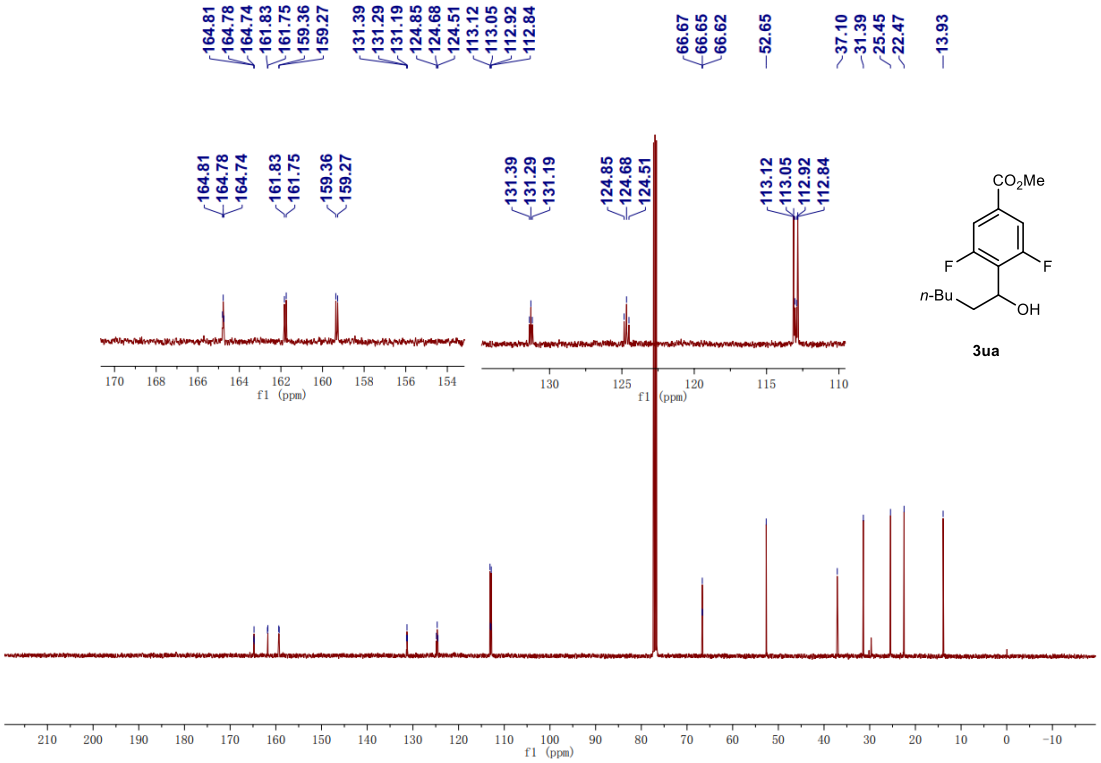

156.44 156.41 156.37 156.34 153.99 153.95 153.92 153.88 150.47 150.38 150.34 150.25 147.97 147.87 147.83 147.74 146.34 146.32 146.30 146.16 143.78 143.76 143.74 143.62 143.60 126.22 126.09 126.04 125.90 125.43 125.41 122.72 122.70 122.65 120.29 120.01 119.98 119.95 119.39 118.78 109.23 109.19 109.14 109.10 109.05 108.95 108.90 108.86 108.81 108.77 66.70 66.68 36.84 31.34 25.40 22.45 13.91
CF3
F
C
B
F
A
F
n-Bu
OH
3sa, 91% (p:m:o = 78:21:1)
f1 (ppm)

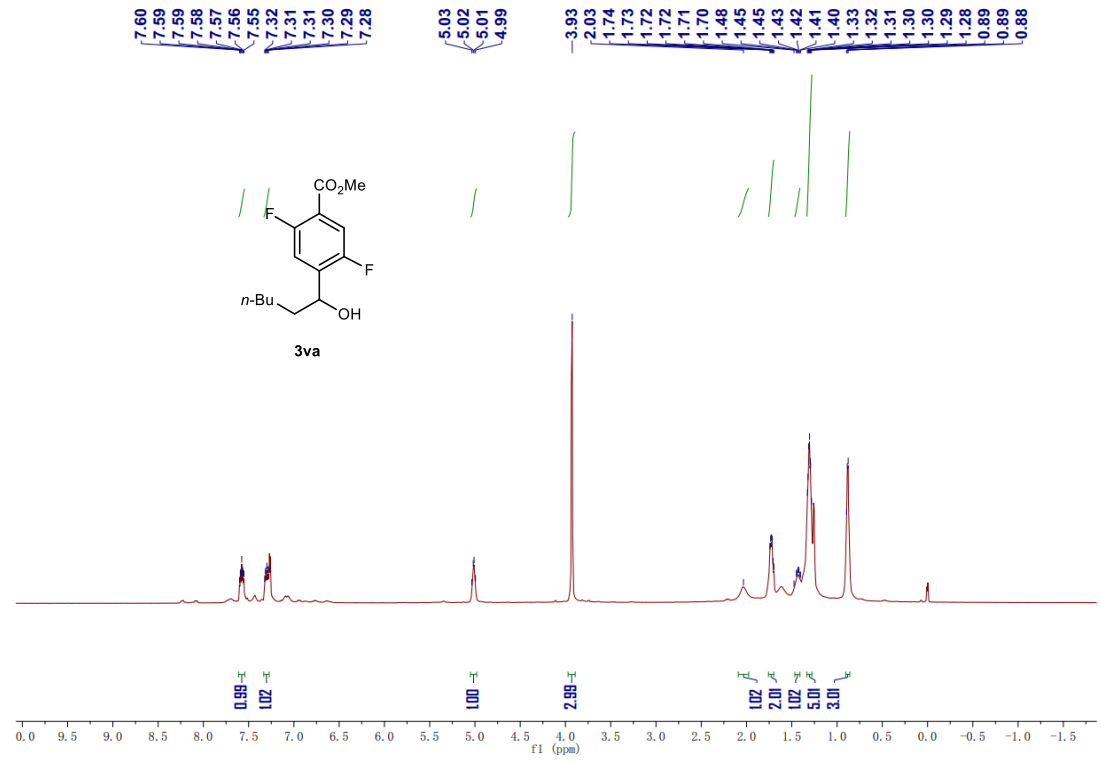

7.44 7.44 7.43 7.42 7.42 7.41 7.40 7.40 5.07 5.05 5.03 5.01 4.43 4.41 4.39 4.38 2.25 2.23 2.03 2.02 2.02 2.01 2.00 1.99 1.98 1.97 1.96 1.87 1.85 1.85 1.84 1.84 1.82 1.82 1.81 1.80 1.79 1.48 1.47 1.46 1.46 1.45 1.44 1.43 1.41 1.40 1.38 1.33 1.32 1.32 1.31 1.30 1.29 1.28 0.89 0.87 0.86
CO2Et
F
F
F
n-Bu
OH
3ta
0.98 1.00 1.98 0.99 1.00 1.00 1.02 3.01 5.01 3.02
f1 (ppm)

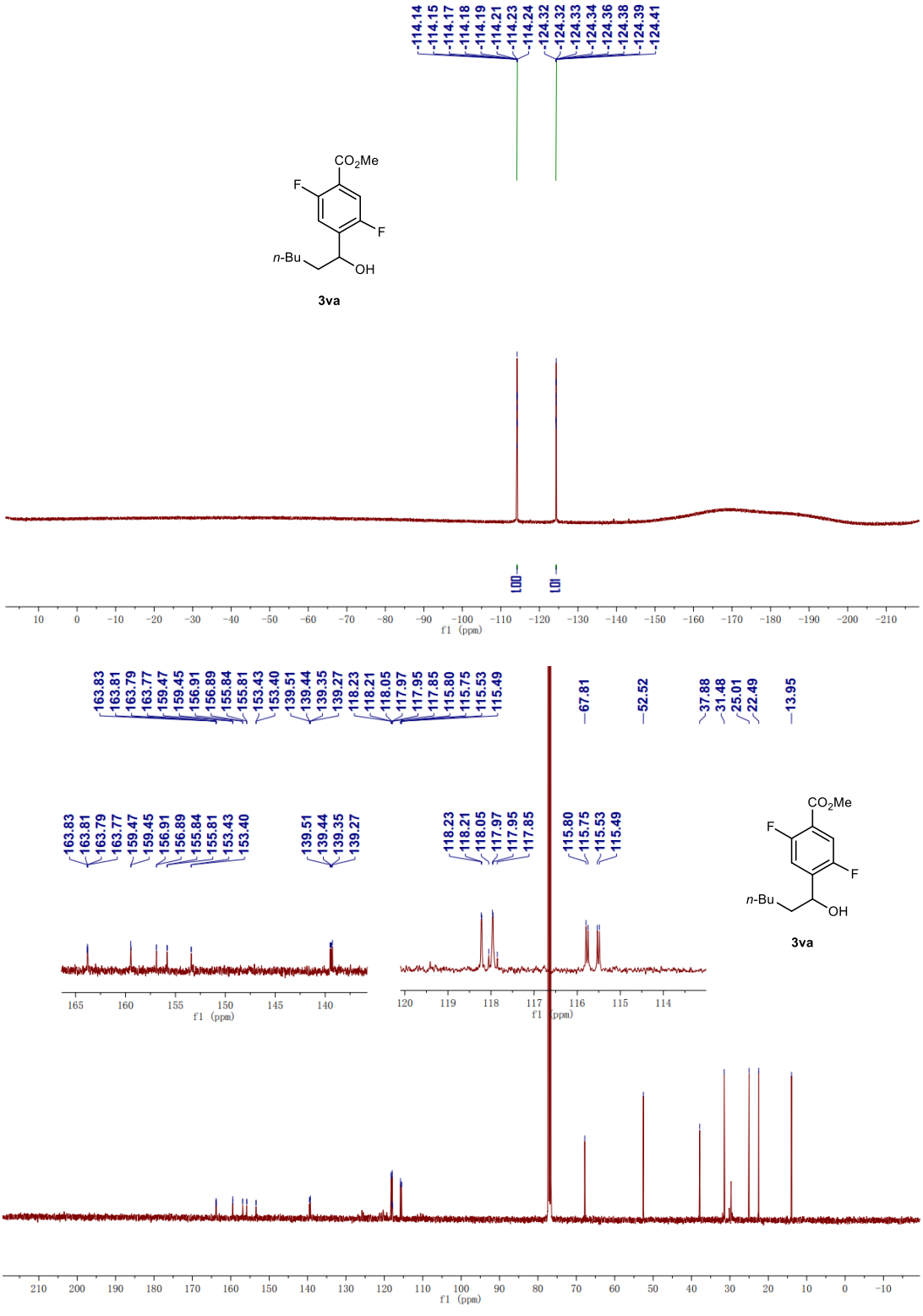

119.67
119.68
119.69
119.71
119.72
119.74
119.75
136.79
136.80
136.81
136.85
136.85
136.86
138.76
138.78
138.81
138.82
138.83
138.86
138.87
CO2Et
F
F
F
n-Bu
OH
3ta
1.00
1.01
1.00
f1 (ppm)
162.45
162.42
162.39
156.21
156.18
156.14
156.11
153.78
153.74
153.70
153.69
153.67
150.47
150.39
150.32
150.24
148.51
148.47
148.36
148.33
148.22
148.20
148.17
148.00
147.98
147.89
147.85
147.83
147.74
147.71
145.92
145.89
145.88
145.83
145.78
126.34
126.20
126.16
126.02
119.46
119.36
119.27
112.98
112.95
112.72
112.68
66.81
66.80
66.79
66.79
62.06
36.92
31.35
25.39
22.46
14.14
13.94
f1 (ppm)

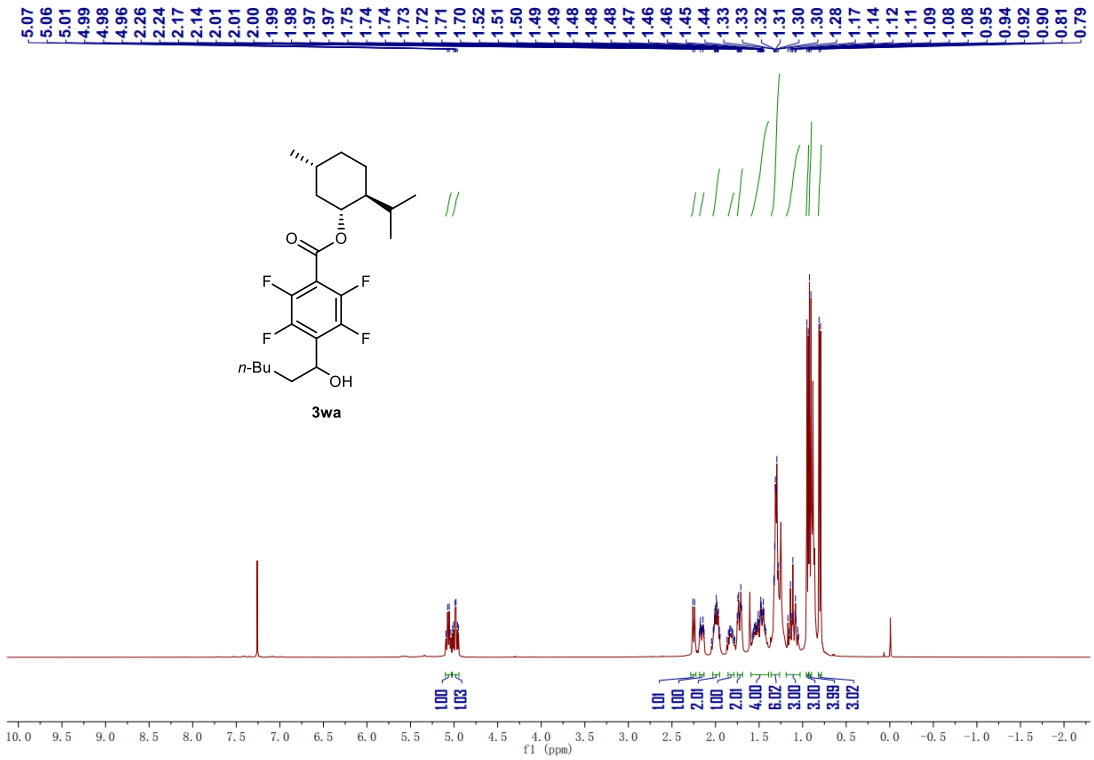

7.56 7.56 7.55 7.52 7.51 7.51 5.07 5.05 5.03 3.92 2.27 2.02 2.01 2.01 2.00 1.99 1.98 1.98 1.97 1.96 1.86 1.85 1.85 1.84 1.83 1.83 1.83 1.82 1.82 1.82 1.81 1.81 1.80 1.80 1.80 1.79 1.78 1.77 1.49 1.48 1.47 1.46 1.45 1.45 1.43 1.42 1.33 1.32 1.31 1.30 1.29 1.28 1.28 0.88 0.87 0.85
CO2Me
F
F
n-Bu
OH
3ua
1.98
1.00
3.01
1.00
1.00
1.00
1.02
5.02
3.02
f1 (ppm)

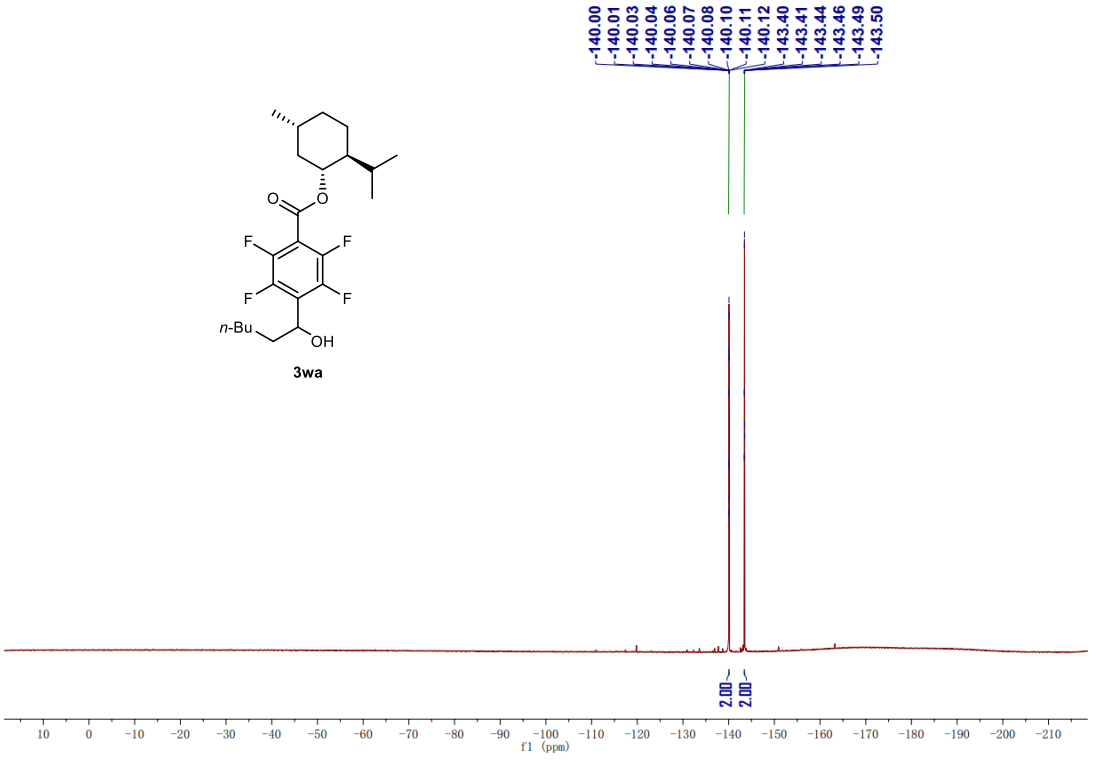

-113.74
-113.76
CO2Me
F
F
n-Bu
OH
3ua
2.00
f1 (ppm)


164.81
164.78
164.74
161.83
161.75
159.36
159.27
131.39
131.29
131.19
124.85
124.68
124.51
113.12
113.05
112.92
112.84
66.67
66.65
66.62
52.65
37.10
31.39
25.45
22.47
13.93
CO2Me
F
F
n-Bu
OH
3ua
f1 (ppm)


7.60
7.59
7.59
7.58
7.57
7.56
7.55
7.32
7.31
7.31
7.30
7.29
7.28
5.03
5.02
5.01
4.99
3.93
2.03
1.74
1.73
1.72
1.72
1.71
1.70
1.48
1.45
1.45
1.43
1.42
1.41
1.40
1.33
1.32
1.31
1.30
1.30
1.29
1.28
0.89
0.89
0.88
CO2Me
F
F
n-Bu
OH
3va
0.99
1.02
1.00
2.99
1.02
2.01
1.02
5.01
3.01
f1 (ppm)


-114.14
-114.15
-114.17
-114.18
-114.19
-114.21
-114.23
-114.24
-124.32
-124.32
-124.33
-124.34
-124.36
-124.38
-124.39
-124.41
CO2Me
F
F
n-Bu
OH
3va
1.00
1.01
f1 (ppm)
163.83
163.81
163.79
163.77
159.47
159.45
156.91
156.89
155.84
155.81
153.43
153.40
139.51
139.44
139.35
139.27
118.23
118.21
118.05
117.97
117.95
117.85
115.80
115.75
115.53
115.49
67.81
52.52
37.88
31.48
25.01
22.49
13.95
f1 (ppm)


5.07 5.06 5.01 4.99 4.98 4.96 2.26 2.24 2.17 2.14 2.01 2.01 2.00 1.99 1.98 1.97 1.97 1.75 1.74 1.74 1.73 1.72 1.71 1.70 1.52 1.51 1.50 1.49 1.49 1.48 1.48 1.48 1.47 1.46 1.46 1.45 1.44 1.33 1.33 1.32 1.31 1.30 1.30 1.28 1.17 1.14 1.12 1.11 1.09 1.08 1.08 0.95 0.94 0.92 0.90 0.81 0.79
O
O
F
F
F
F
n-Bu
OH
3wa
1.00 1.03
1.01 1.00 2.01 1.00 2.01 4.00 6.02 3.00 3.00 3.99 3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)


-140.00 -140.01 -140.03 -140.04 -140.06 -140.07 -140.08 -140.10 -140.11 -140.12 -143.40 -143.41 -143.44 -143.46 -143.49 -143.50
O
O
F
F
F
F
n-Bu
OH
3wa
2.00 2.00
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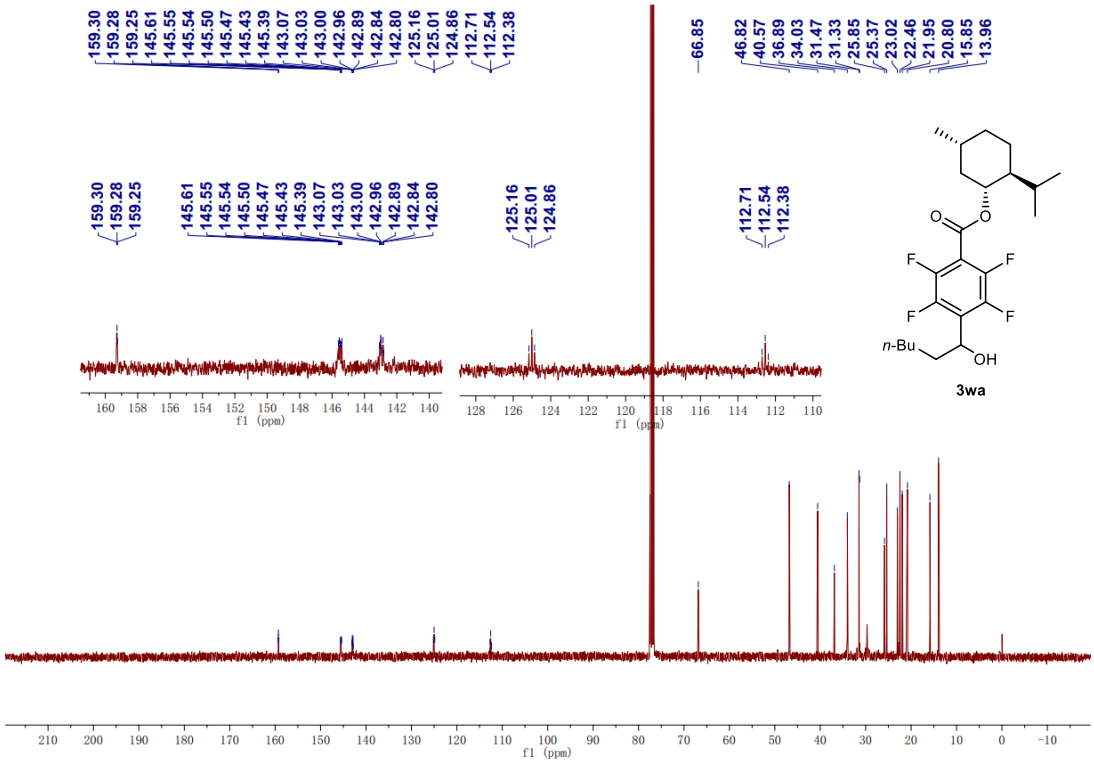
f1 (ppm)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145.39
143.07
143.03
143.00
142.96
142.89
142.84
142.80
125.16
125.01
124.86
112.71
112.54
112.38
66.85
46.82
40.57
36.89
34.03
31.47
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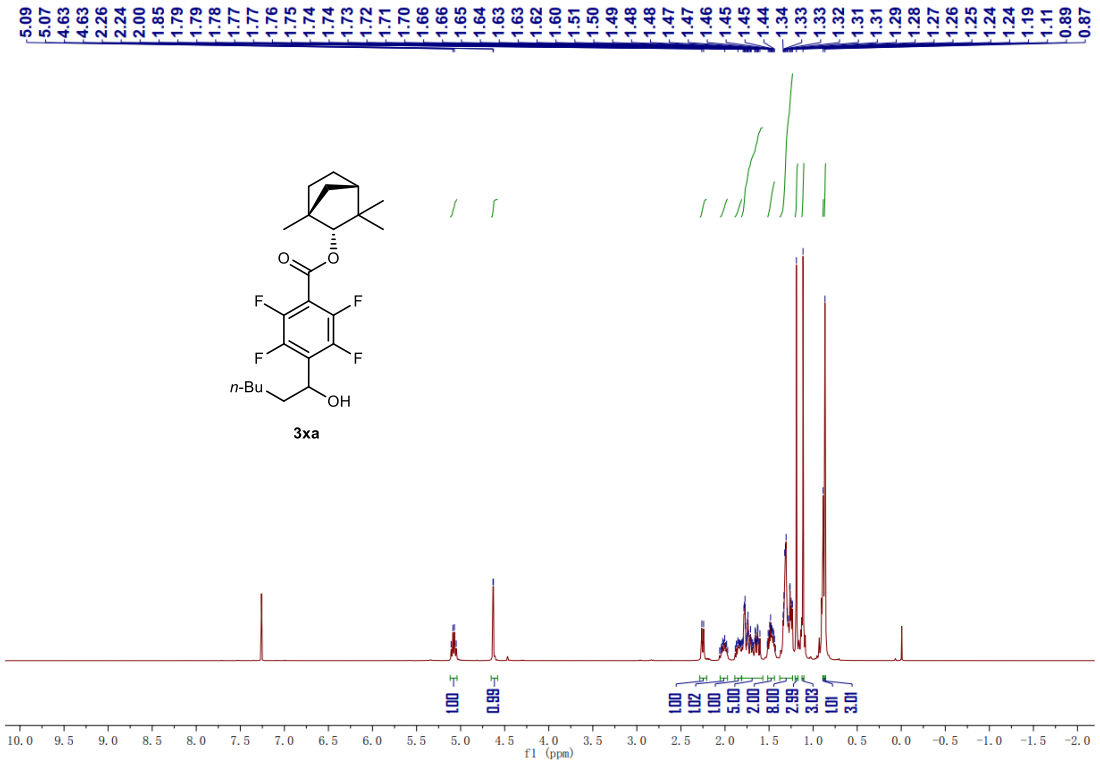
23.02
22.46
21.95
20.80
15.85
13.96
f1 (ppm)
3wa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1.75
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1.74
1.73
1.72
1.71
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1.66
1.65
1.64
1.63
1.63
1.62
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1.51
1.50
1.49
1.48
1.48
1.47
1.47
1.46
1.45
1.45
1.44
1.34
1.33
1.33
1.32
1.31
1.31
1.29
1.28
1.27
1.26
1.25
1.24
1.24
1.19
1.11
0.89
0.87
1.00
0.99
1.00
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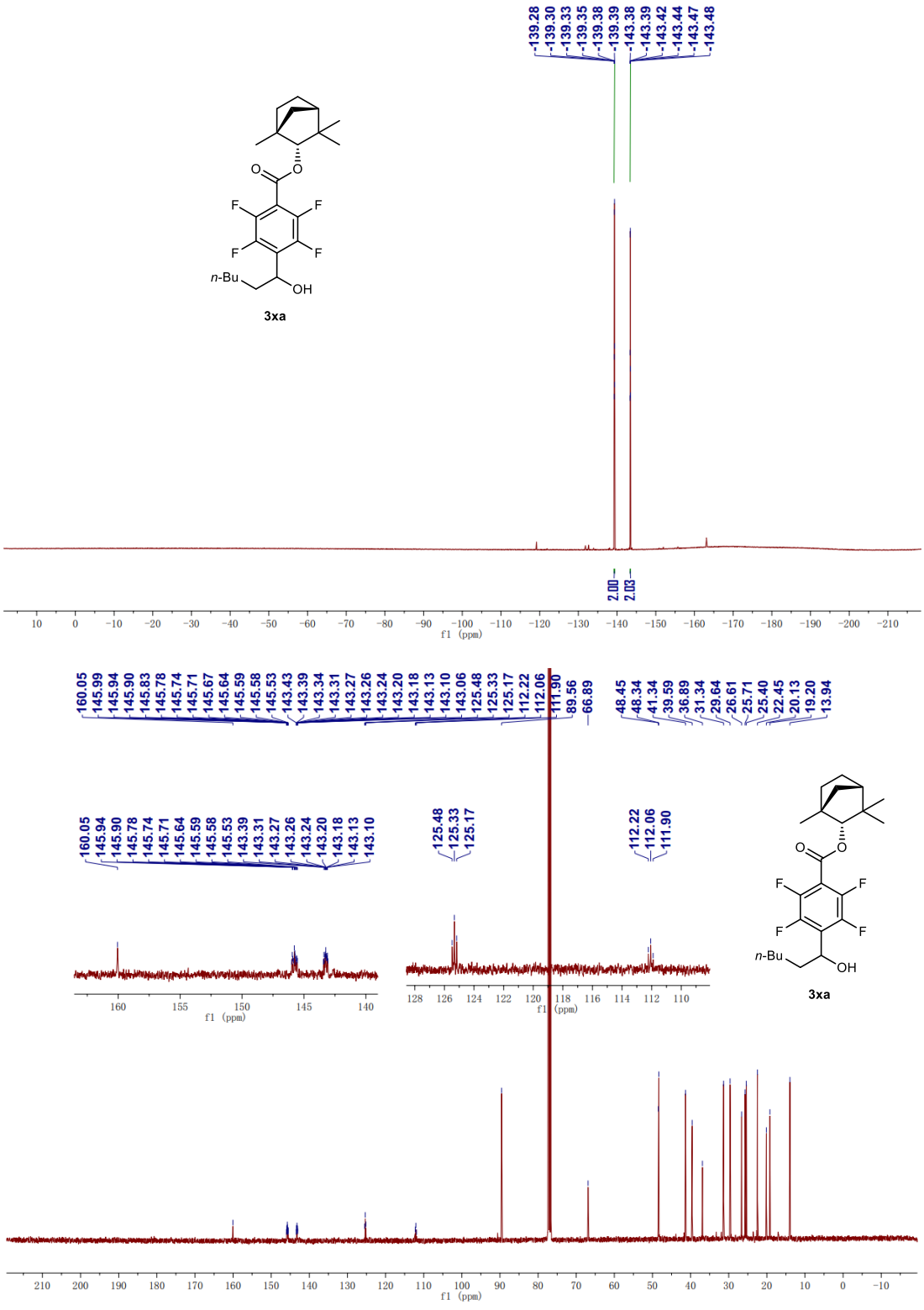
5.00
2.00
8.00
2.99
3.03
1.01
3.01
f1 (ppm)
3xa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-143.42
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-143.47
-143.48
O
O
F
F
F
F
n-Bu
OH
3xa
2.00
2.03
f1 (ppm)
160.05
145.99
145.94
145.90
145.83
145.78
145.74
145.71
145.67
145.64
145.59
145.58
145.53
143.43
143.39
143.34
143.31
143.27
143.26
143.24
143.20
143.18
143.13
143.10
125.48
125.33
125.17
112.22
112.06
111.90
89.56
66.89
48.45
48.34
41.34
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25.40
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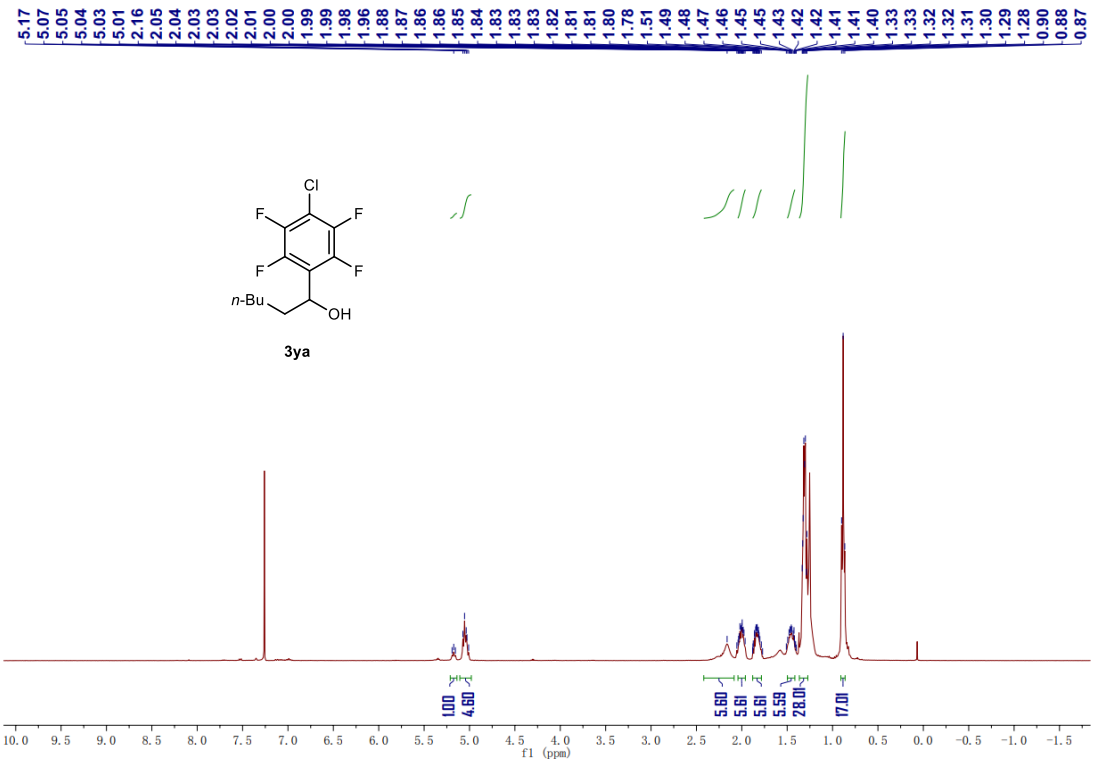
13.94
3xa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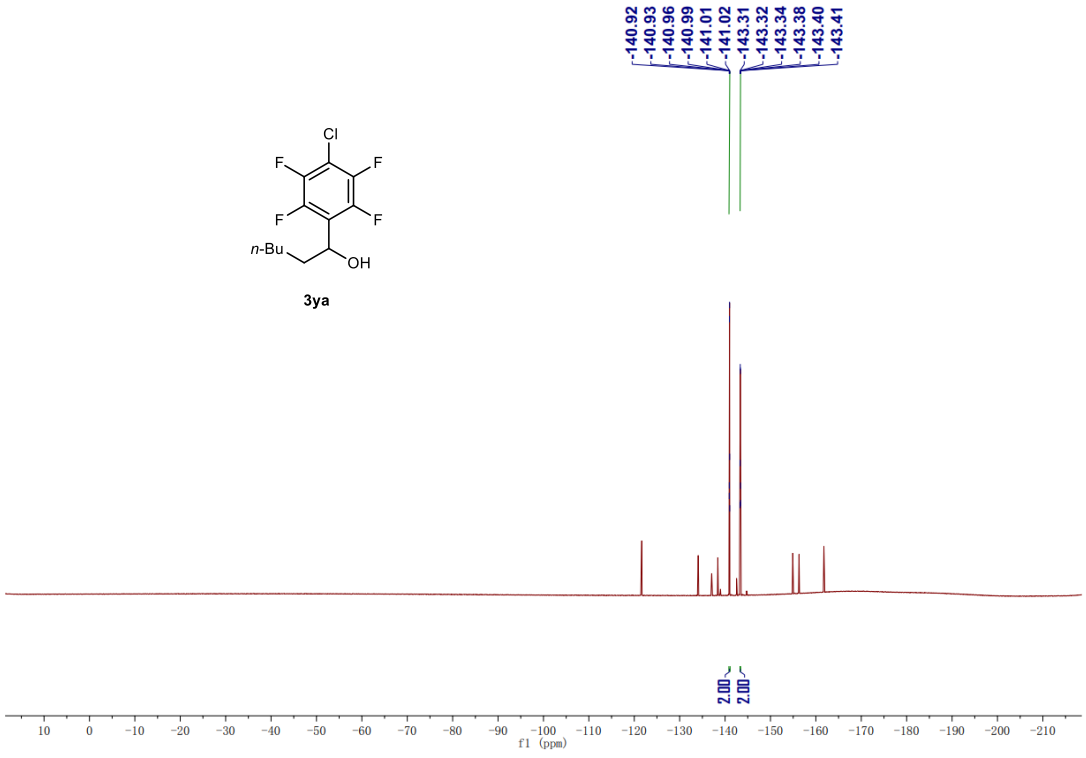
Cl
F
F
F
F
n-Bu
OH
3ya
1.00 4.60 5.60 5.61 5.61 5.58 28.04 17.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)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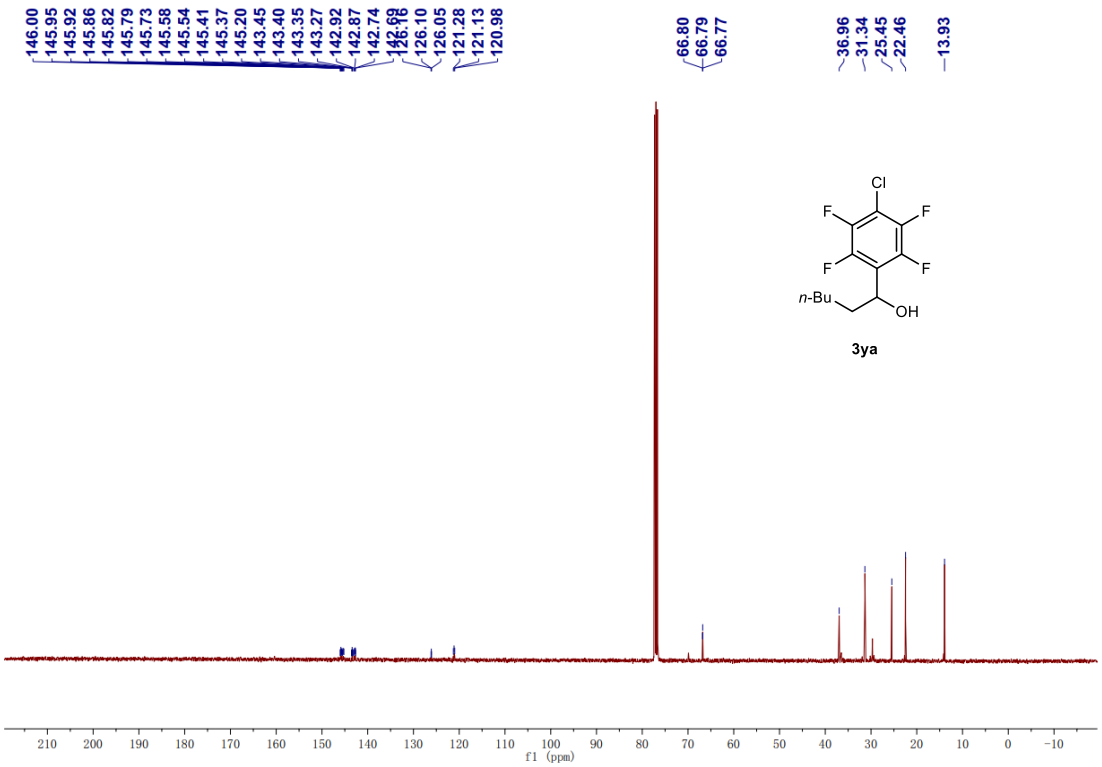
Cl
F
F
F
F
n-Bu
OH
3ya
2.00 2.00
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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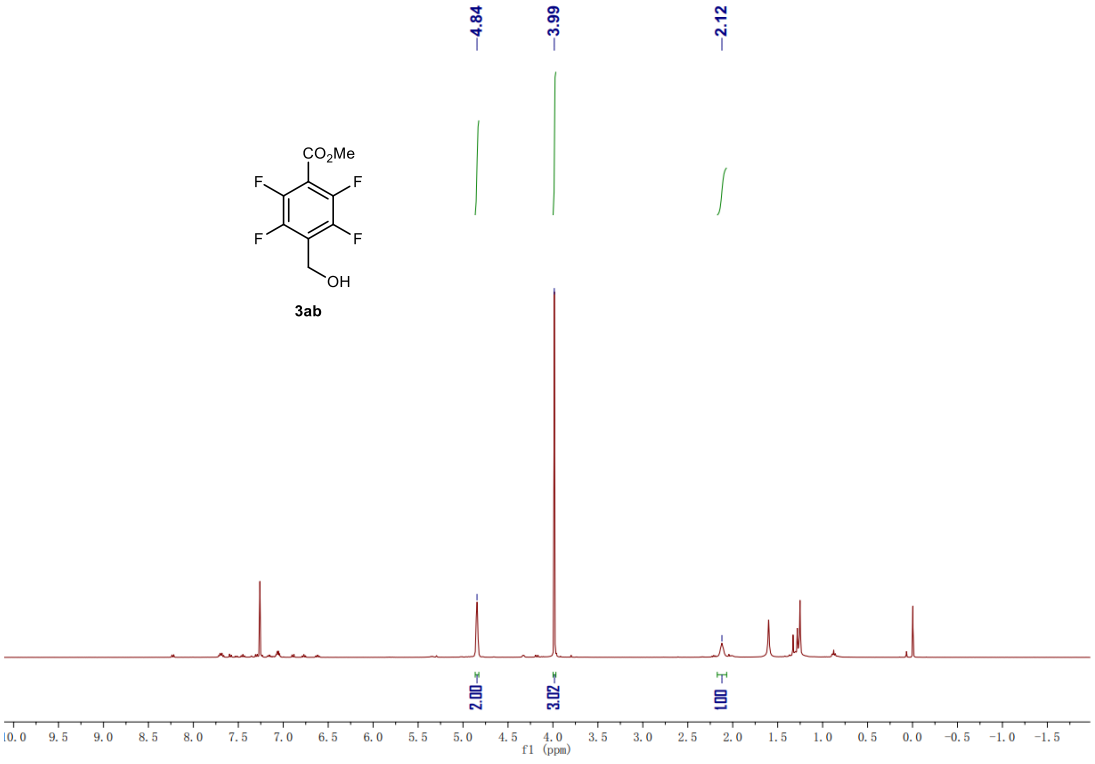
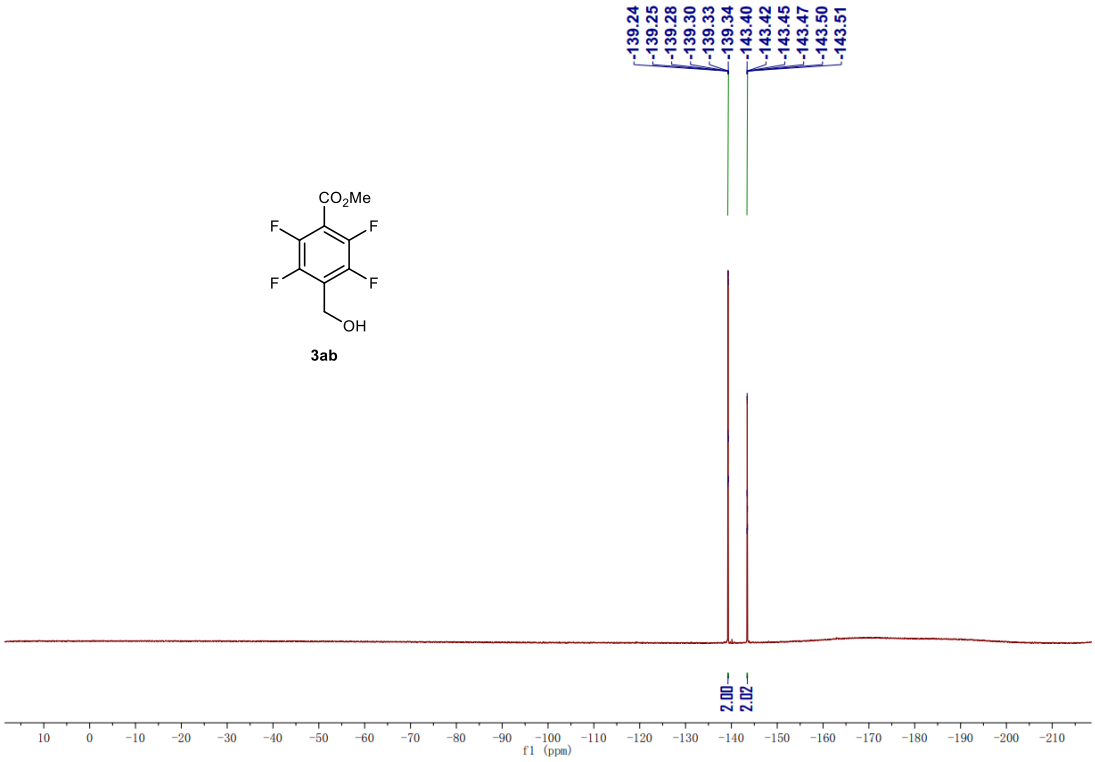
145.79
145.73
145.58
145.54
145.41
145.37
145.20
143.45
143.40
143.35
143.27
142.92
142.87
142.74
126.10
126.05
121.28
121.13
120.98
66.80
66.79
66.77
36.96
31.34
25.45
22.46
13.93
Cl
F
F
F
F
n-Bu
OH
3ya
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


4.84
3.99
2.12
CO2Me
F
F
F
F
OH
3ab
2.00
3.02
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0 −1.5
f1 (ppm)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-143.40
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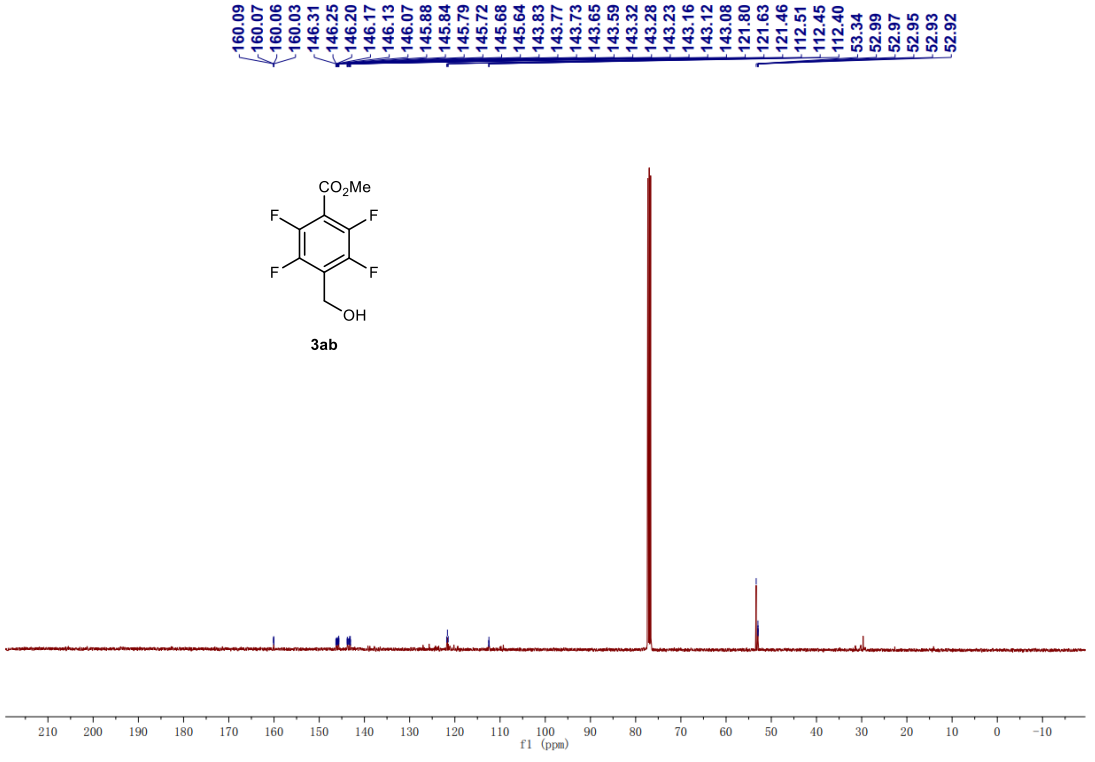
-143.51
CO2Me
F
F
F
F
OH
3ab
2.00
2.02
f1 (ppm)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146.17
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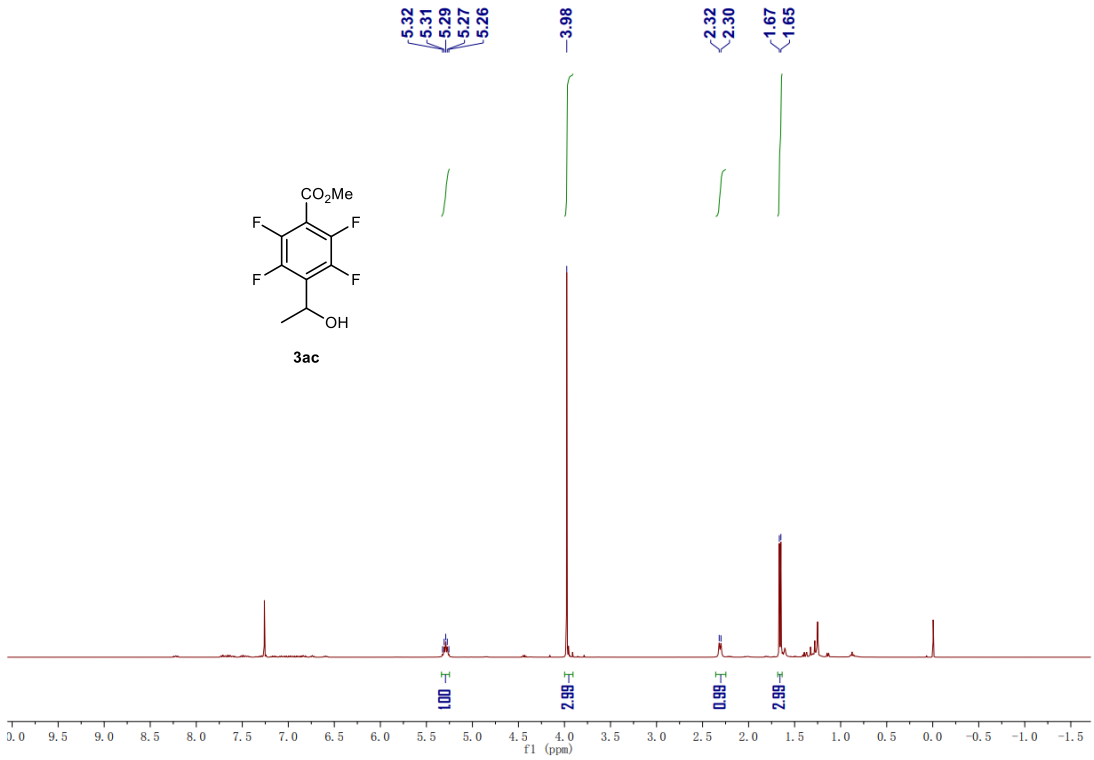
145.79
145.72
145.68
145.64
143.83
143.77
143.73
143.65
143.59
143.32
143.28
143.23
143.16
143.12
143.08
121.80
121.63
121.46
112.51
112.45
112.40
53.34
52.99
52.97
52.95
52.93
52.92
CO2Me
F
F
F
F
OH
3ab
f1 (ppm)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5.31
5.29
5.27
5.26
3.98
2.32
2.30
1.67
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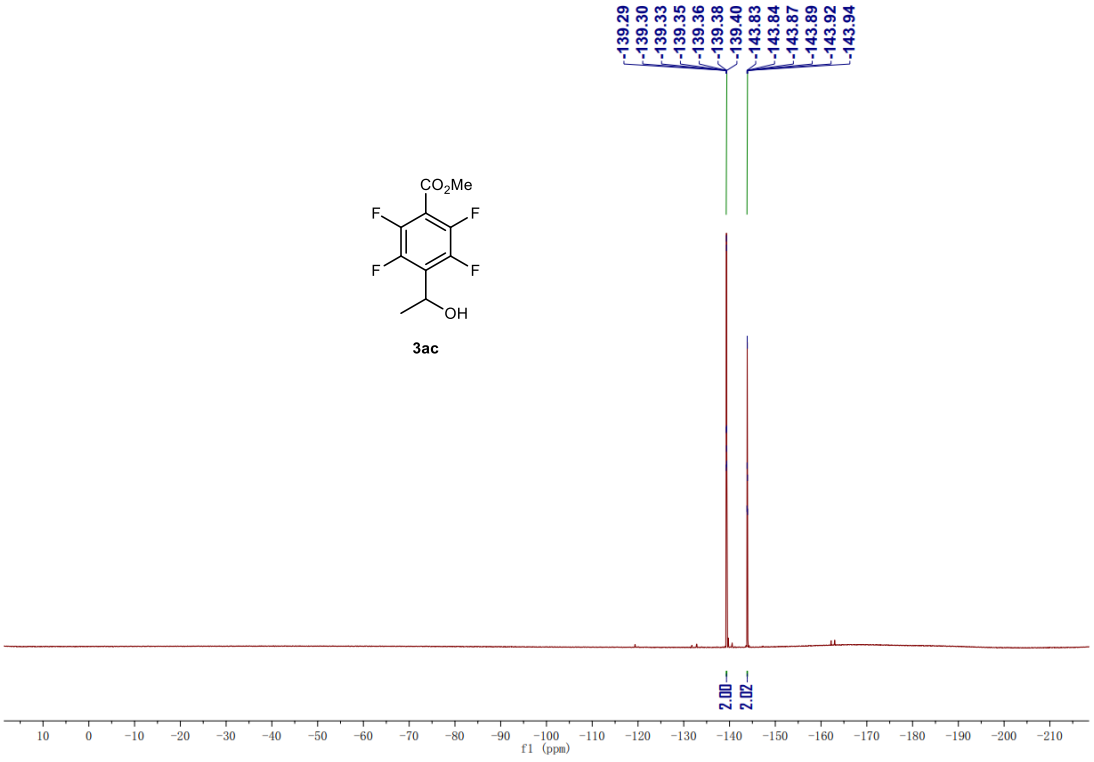
CO2Me
F
F
F
F
OH
3ac
1.00
2.99
0.99
2.99
f1 (ppm)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-139.38
-139.40
-143.83
-143.84
-143.87
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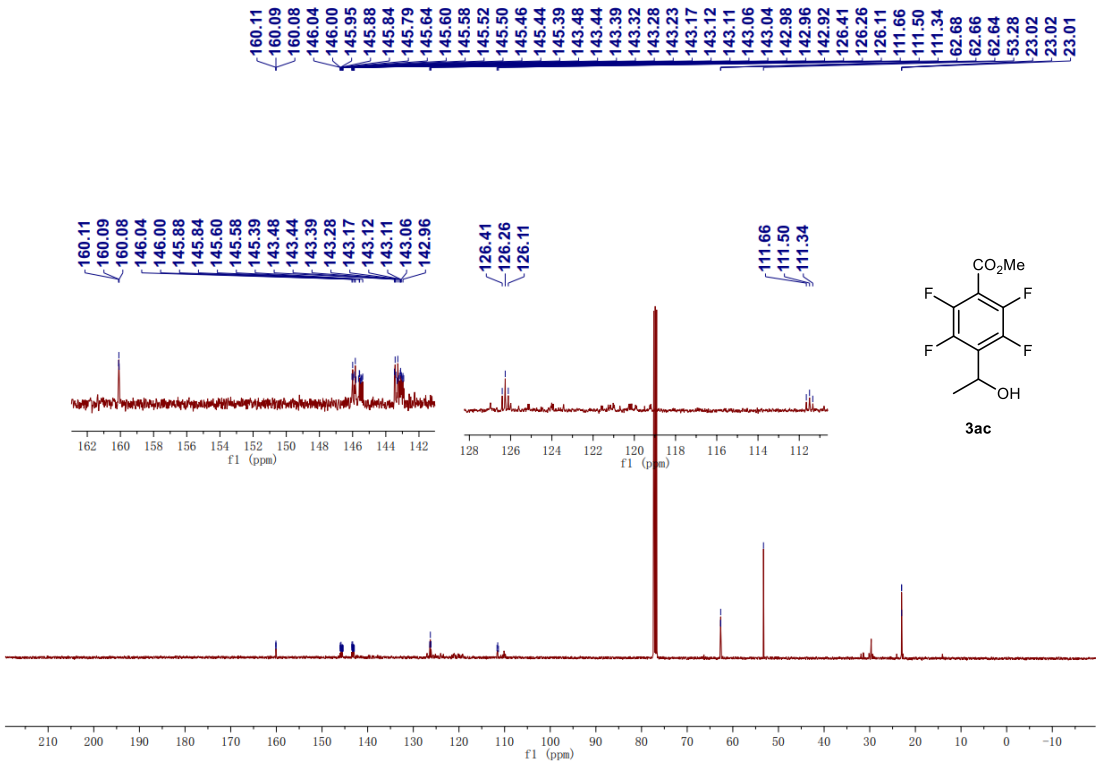
-143.92
-143.94
CO2Me
F
F
F
F
OH
3ac
2.00
2.02
f1 (ppm)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145.60
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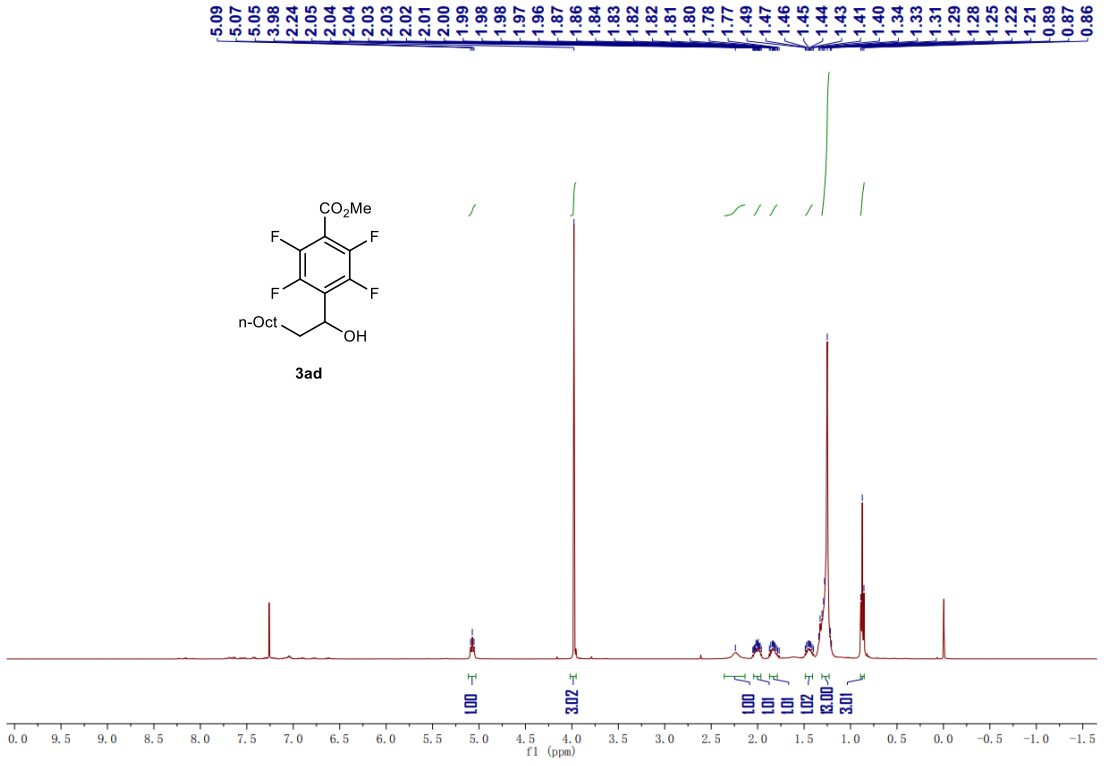
145.52
145.50
145.46
145.44
145.39
143.48
143.44
143.39
143.32
143.28
143.23
143.17
143.12
143.11
143.06
143.04
142.98
142.96
142.92
126.41
126.26
126.11
111.66
111.50
111.34
62.68
62.66
62.64
53.28
23.02
23.02
23.01
CO2Me
F
F
F
F
OH
3ac
f1 (ppm)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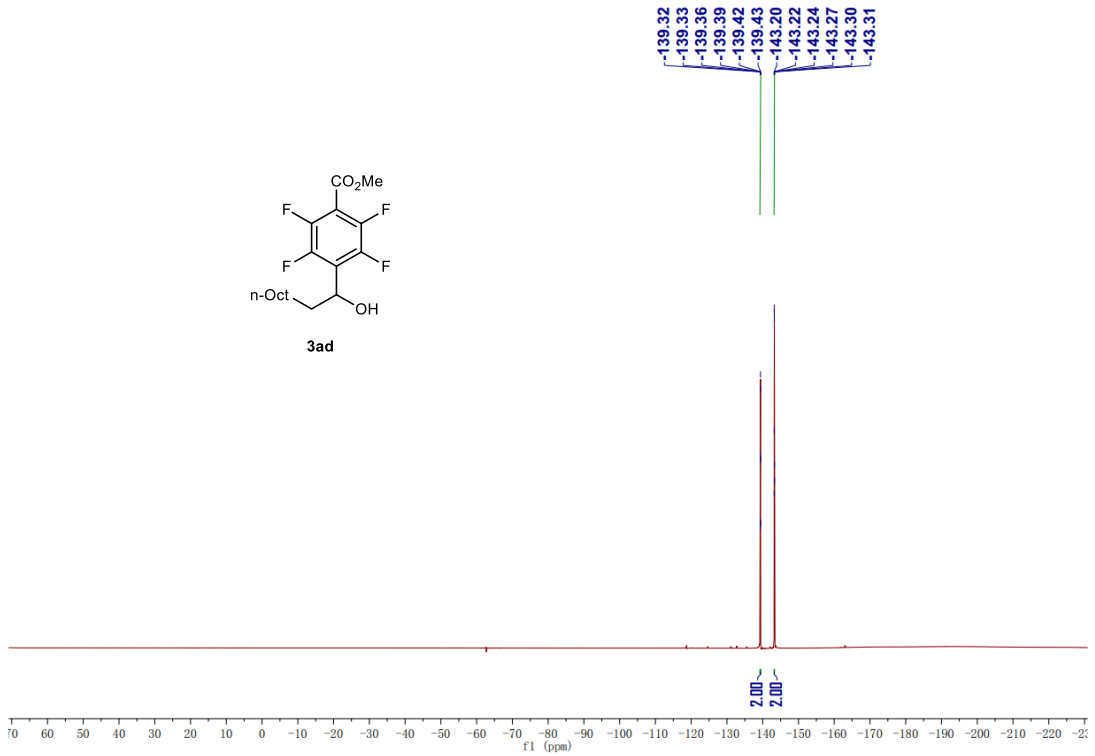
5.07
5.05
3.98
2.24
2.05
2.04
2.04
2.03
2.03
2.02
2.01
2.00
1.99
1.98
1.98
1.97
1.96
1.87
1.86
1.84
1.83
1.82
1.82
1.81
1.80
1.78
1.77
1.49
1.47
1.46
1.45
1.44
1.43
1.41
1.40
1.34
1.33
1.31
1.29
1.28
1.25
1.22
1.21
0.89
0.87
0.86
CO2Me
F
F
F
F
n-Oct
OH
3ad
1.00
3.02
1.00
1.01
1.01
1.02
6.00
3.01
f1 (ppm)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-139.43
-143.20
-143.22
-143.24
-143.27
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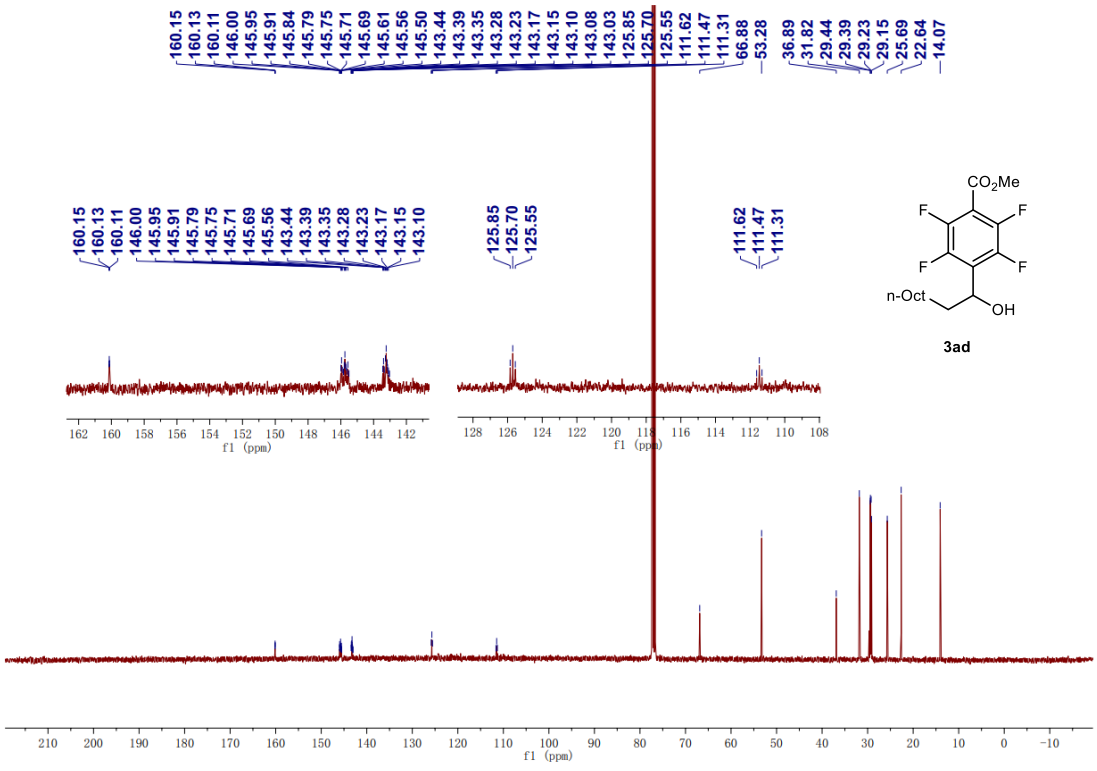
-143.31
CO2Me
F
F
F
F
n-Oct
OH
3ad
2.00
2.00
f1 (ppm)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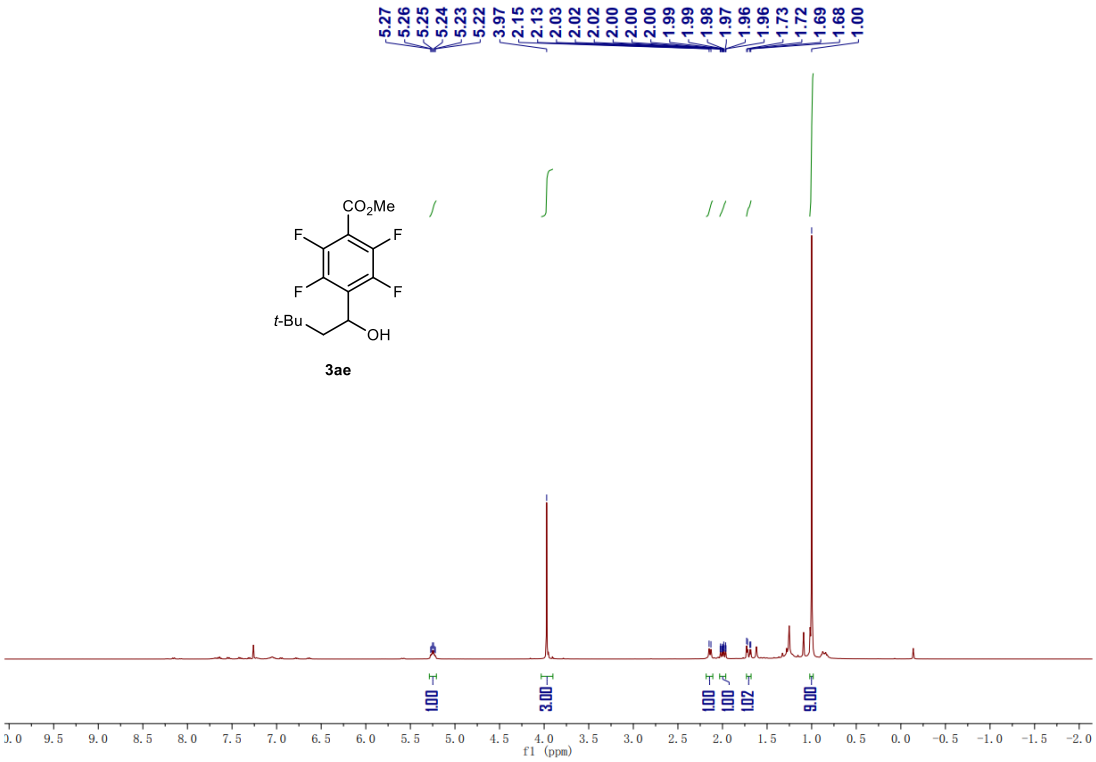
145.50
143.44
143.39
143.35
143.28
143.23
143.17
143.15
143.10
143.08
143.03
125.85
125.70
125.55
111.62
111.47
111.31
66.88
53.28
36.89
31.82
29.44
29.39
29.23
29.15
25.69
22.64
14.07
CO2Me
F
F
F
F
n-Oct
OH
3ad
f1 (ppm)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2.15
2.13
2.03
2.02
2.02
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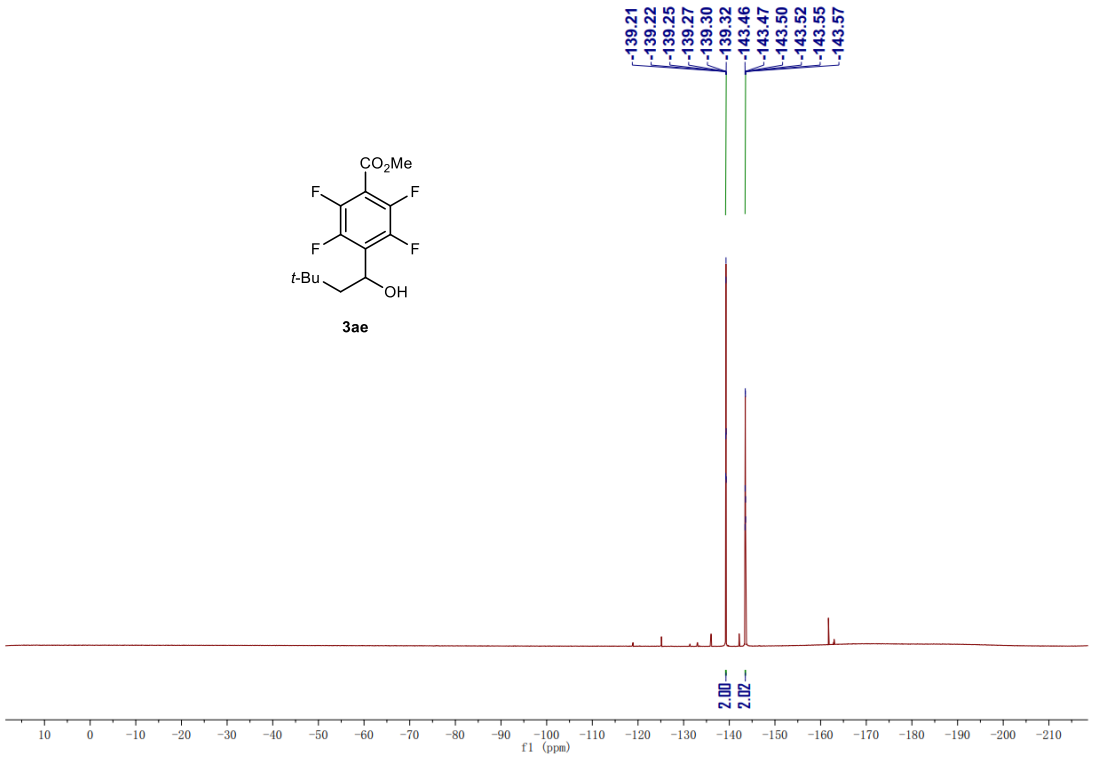
2.00
2.00
1.99
1.99
1.98
1.97
1.96
1.96
1.73
1.72
1.69
1.68
1.00
CO2Me
F
F
F
F
t-Bu
OH
3ae
1.00
3.00
1.00
1.00
1.02
9.00
f1 (ppm)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-143.46
-143.47
-143.50
-143.52
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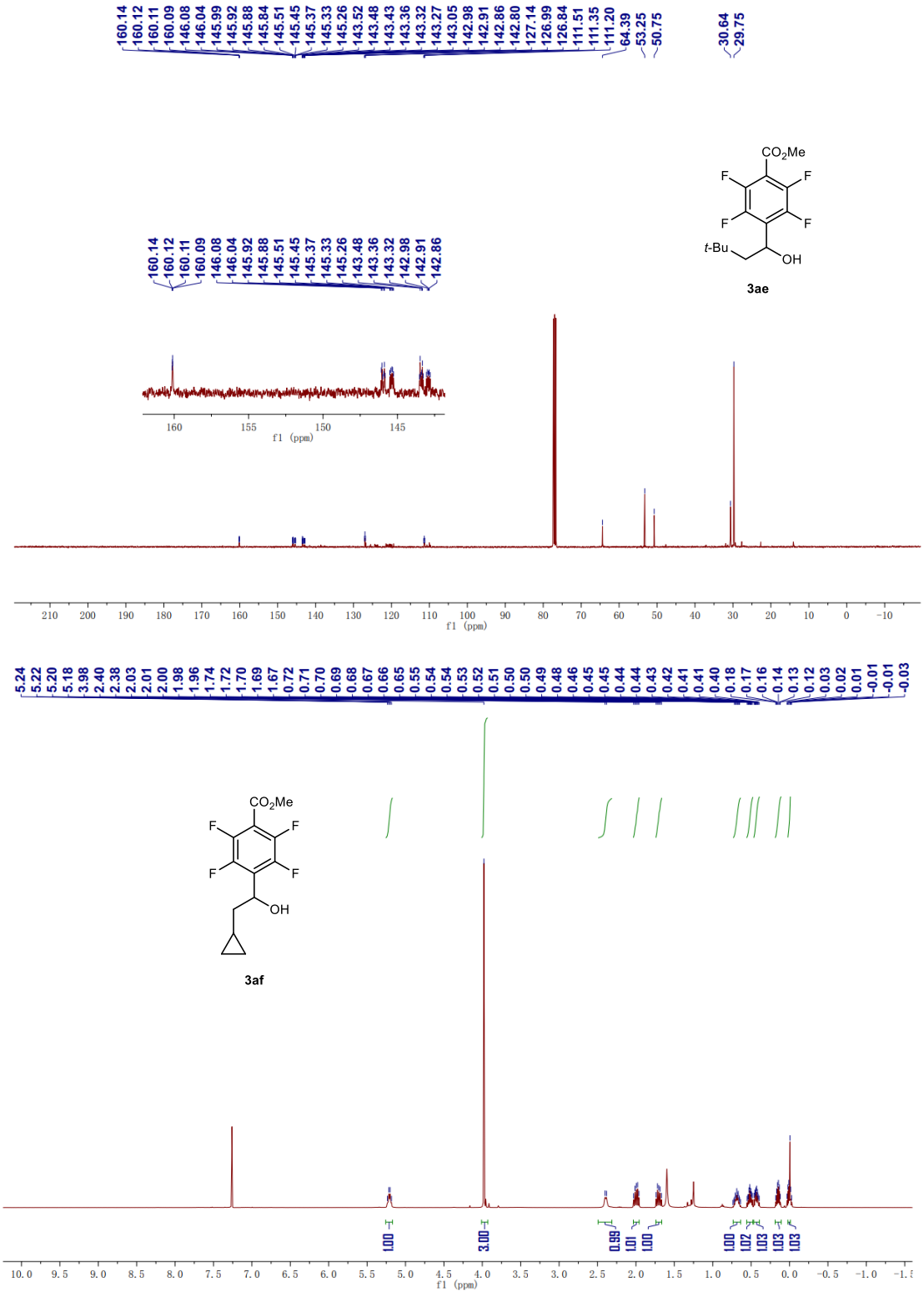
CO2Me
F
F
F
F
t-Bu
OH
3ae
2.00
2.02
f1 (ppm)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145.37
145.33
145.26
143.52
143.48
143.43
143.36
143.32
143.27
143.05
142.98
142.91
142.86
142.80
127.14
126.99
126.84
111.51
111.35
111.20
64.39
53.25
50.75
30.64
29.75
CO2Me
F
F
F
F
t-Bu
OH
3ae
f1 (ppm)
5.24
5.22
5.20
5.18
3.98
2.40
2.38
2.03
2.01
2.00
1.98
1.96
1.74
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1.69
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0.69
0.68
0.67
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0.50
0.50
0.49
0.48
0.46
0.45
0.45
0.44
0.44
0.43
0.42
0.41
0.41
0.40
0.18
0.17
0.16
0.14
0.13
0.12
0.03
0.02
0.01
-0.01
-0.01
-0.03
CO2Me
F
F
F
F
OH
3af
1.00
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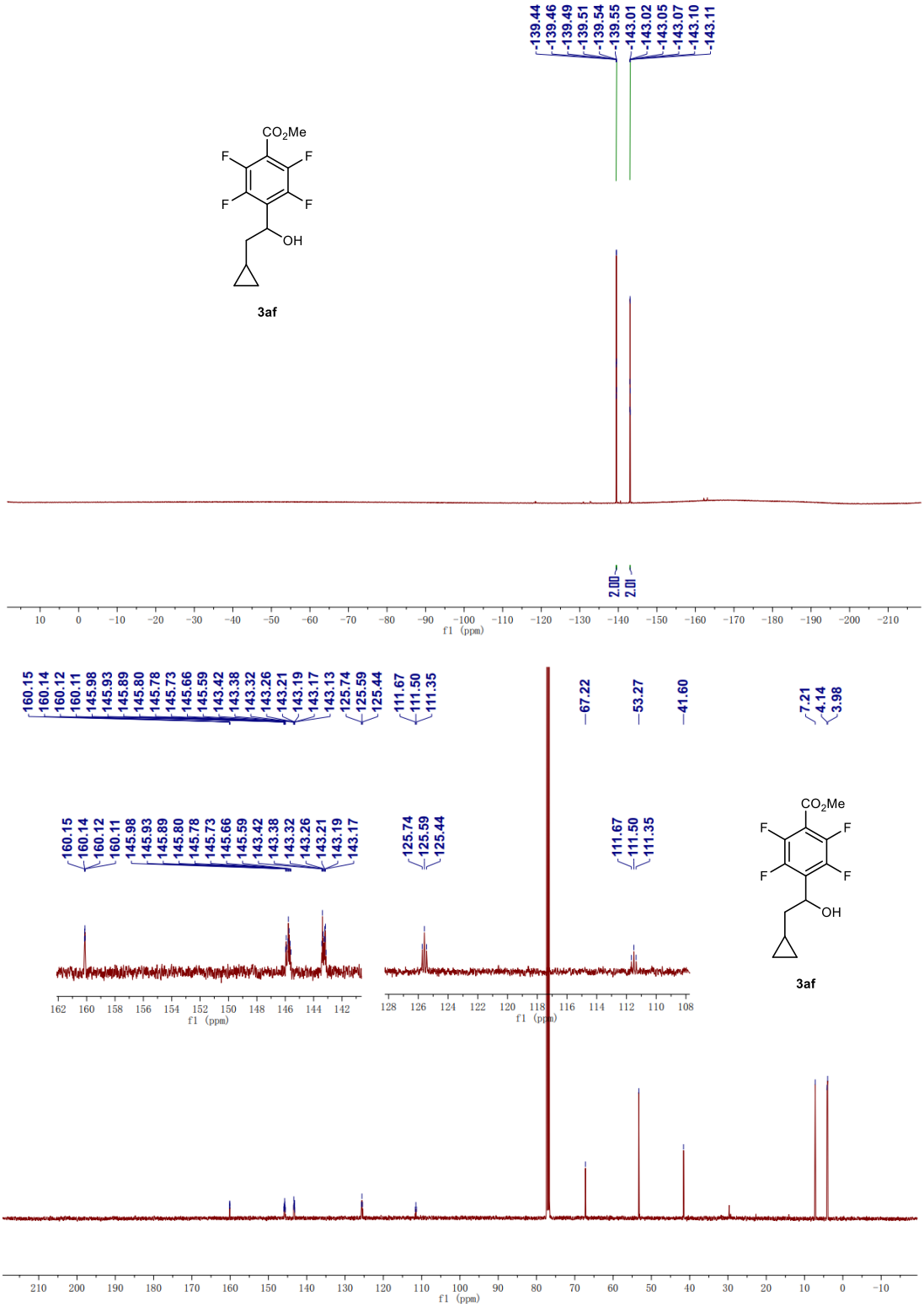
0.99
1.01
1.00
1.00
1.02
1.03
1.03
1.03
f1 (ppm)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-143.01
-143.02
-143.05
-143.07
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-143.11
CO2Me
F
F
F
F
OH
3af
2.00
2.01
f1 (ppm)
160.15
160.14
160.12
160.11
145.98
145.93
145.89
145.80
145.78
145.73
145.66
145.59
145.42
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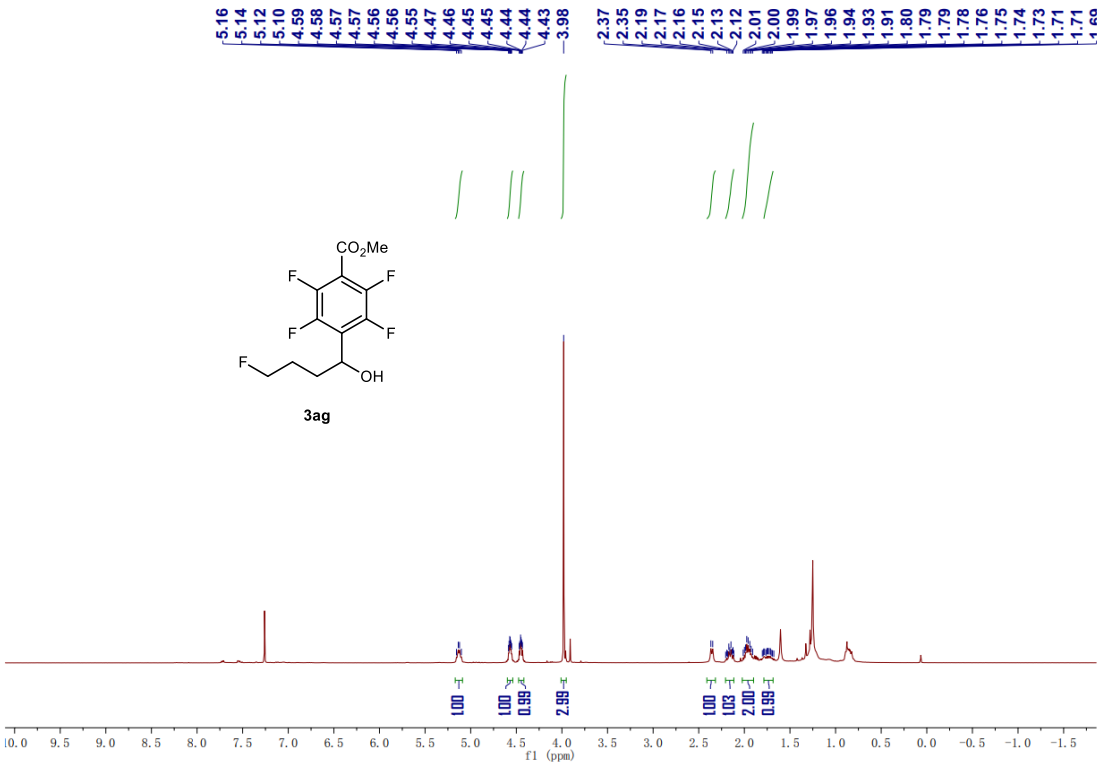
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4.46
4.45
4.45
4.44
4.44
4.43
3.98
2.37
2.35
2.19
2.17
2.16
2.15
2.13
2.12
2.01
2.00
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1.93
1.91
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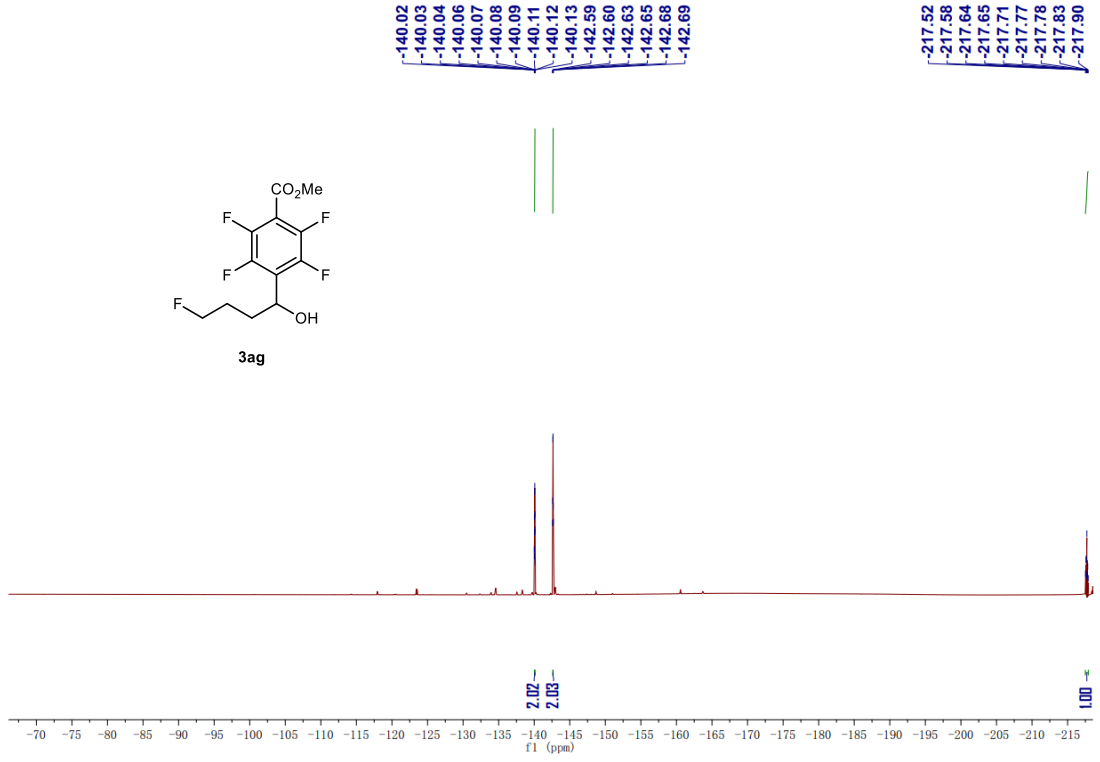
1.79
1.79
1.78
1.76
1.75
1.74
1.73
1.71
1.71
CO2Me
F
F
F
F
F
OH
3ag
1.00
1.00
0.99
2.99
1.00
1.03
2.00
0.99
f1 (ppm)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-142.68
-142.69
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-217.64
-217.65
-217.71
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F
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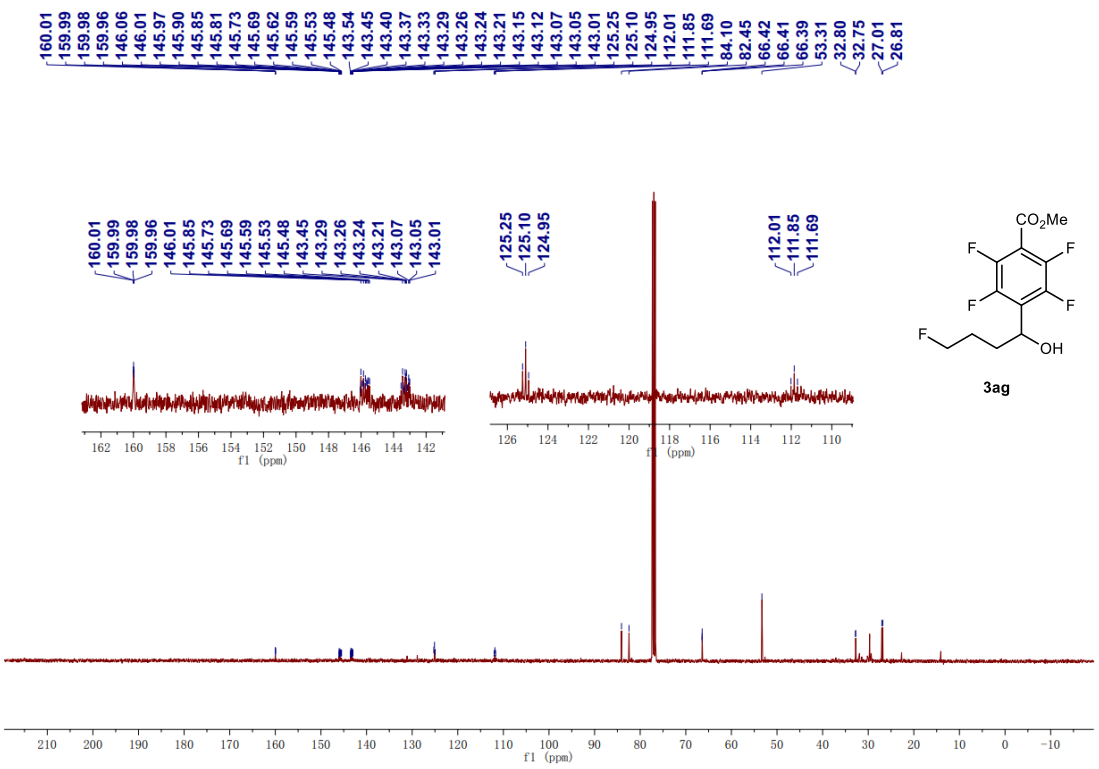
F
OH
3ag
2.02
2.03
1.00
f1 (ppm)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145.53
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143.12
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143.01
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125.10
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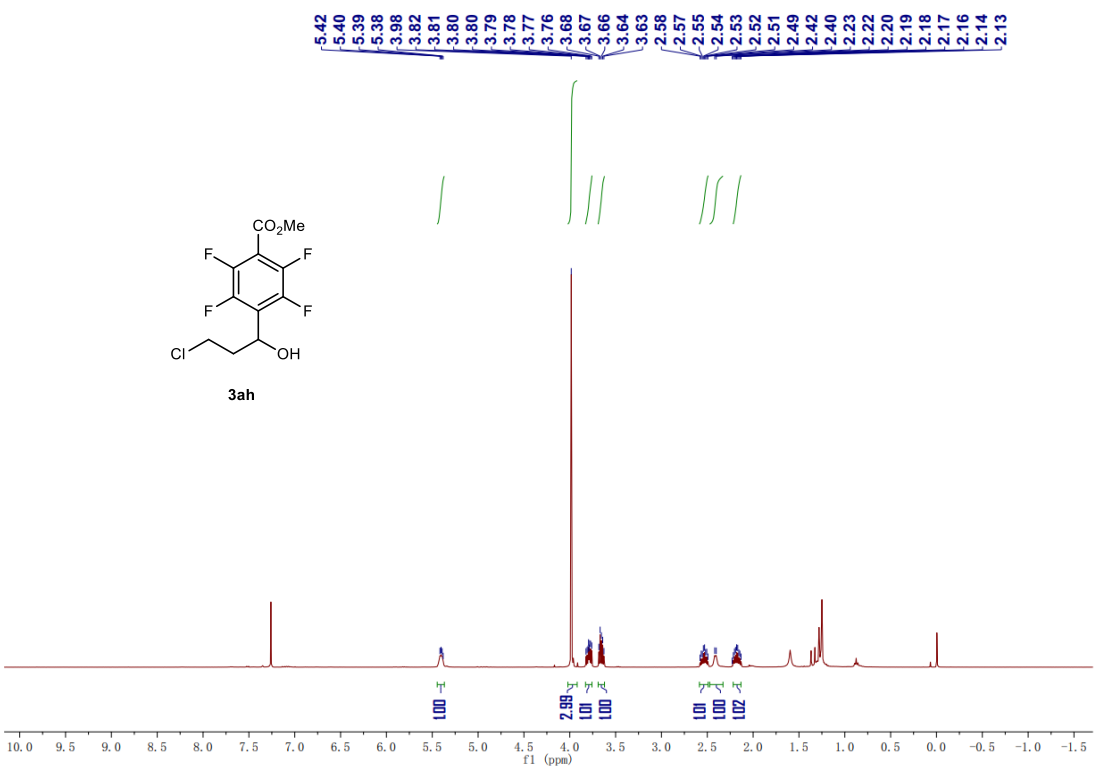
112.01
111.85
111.69
84.10
82.45
66.42
66.41
66.39
53.31
32.80
32.75
27.01
26.81
f1 (ppm)
3ag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3.76
3.68
3.67
3.66
3.64
3.63
2.58
2.57
2.55
2.54
2.53
2.52
2.51
2.49
2.42
2.40
2.23
2.22
2.20
2.19
2.18
2.17
2.16
2.14
2.13
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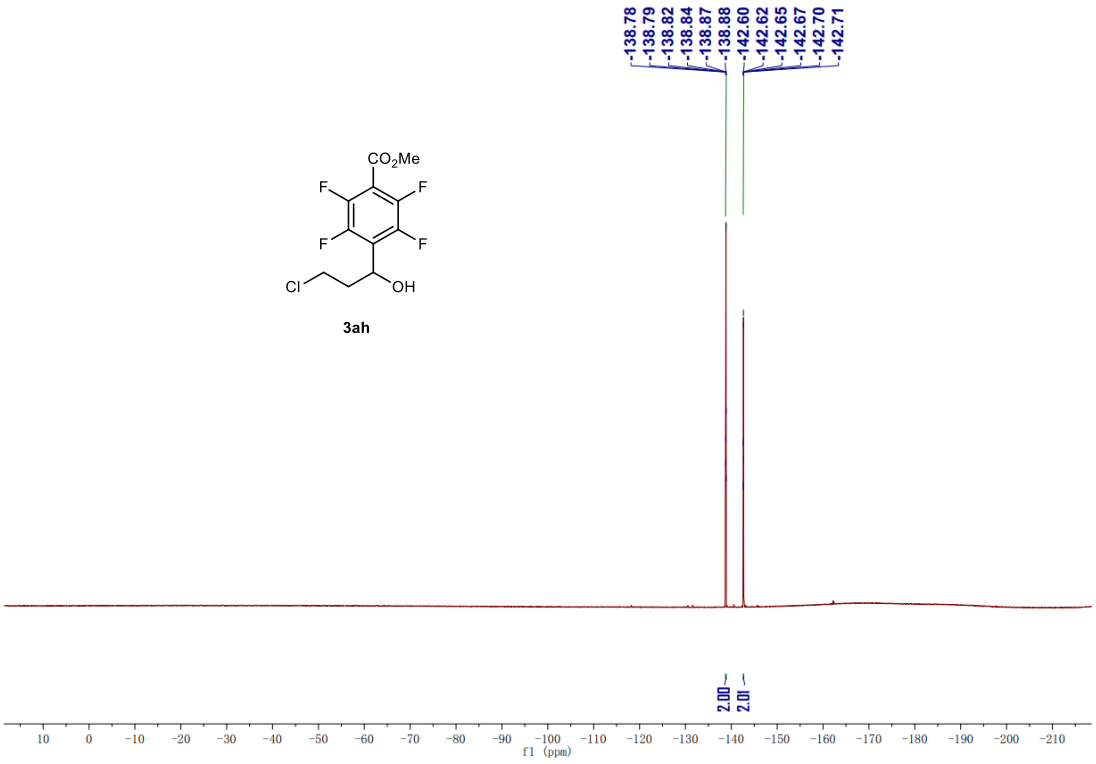
2.99
1.01
1.01
1.00
1.01
1.00
2.02
f1 (ppm)
3ah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-142.62
-142.65
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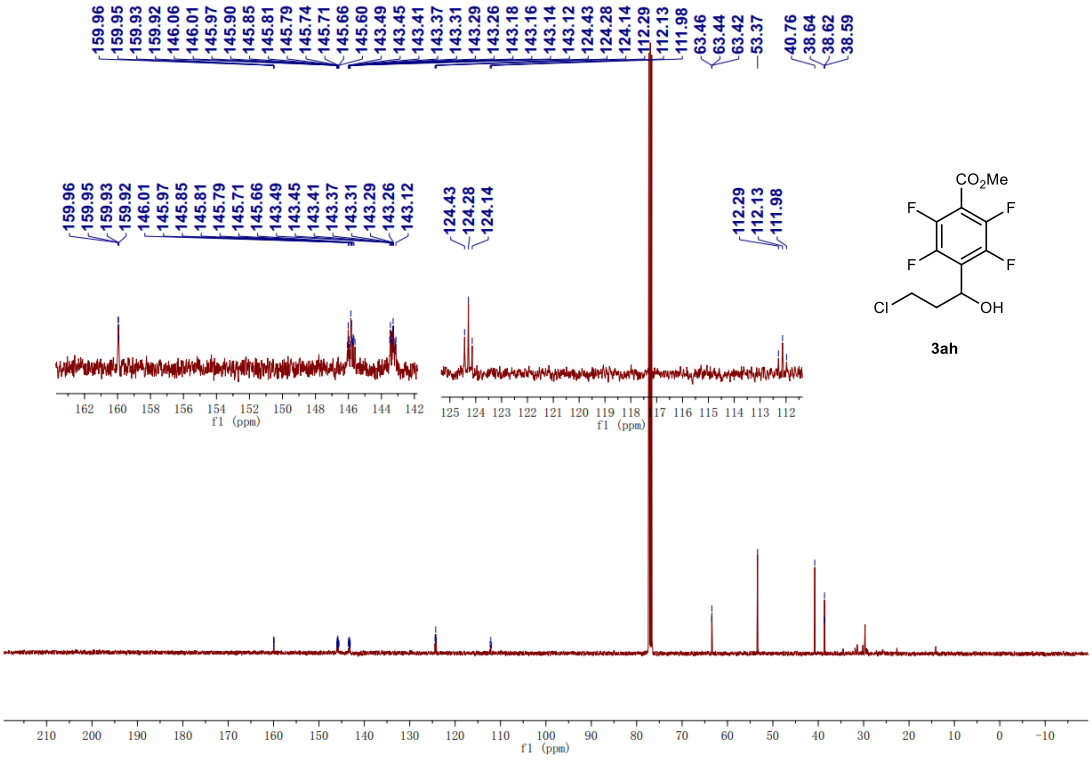
-142.70
-142.71
CO2Me
F
F
F
F
Cl
OH
3ah
2.00
2.01
f1 (ppm)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143.45
143.41
143.37
143.31
143.29
143.26
143.18
143.16
143.14
143.12
124.43
124.28
124.14
112.29
112.13
111.98
63.46
63.44
63.42
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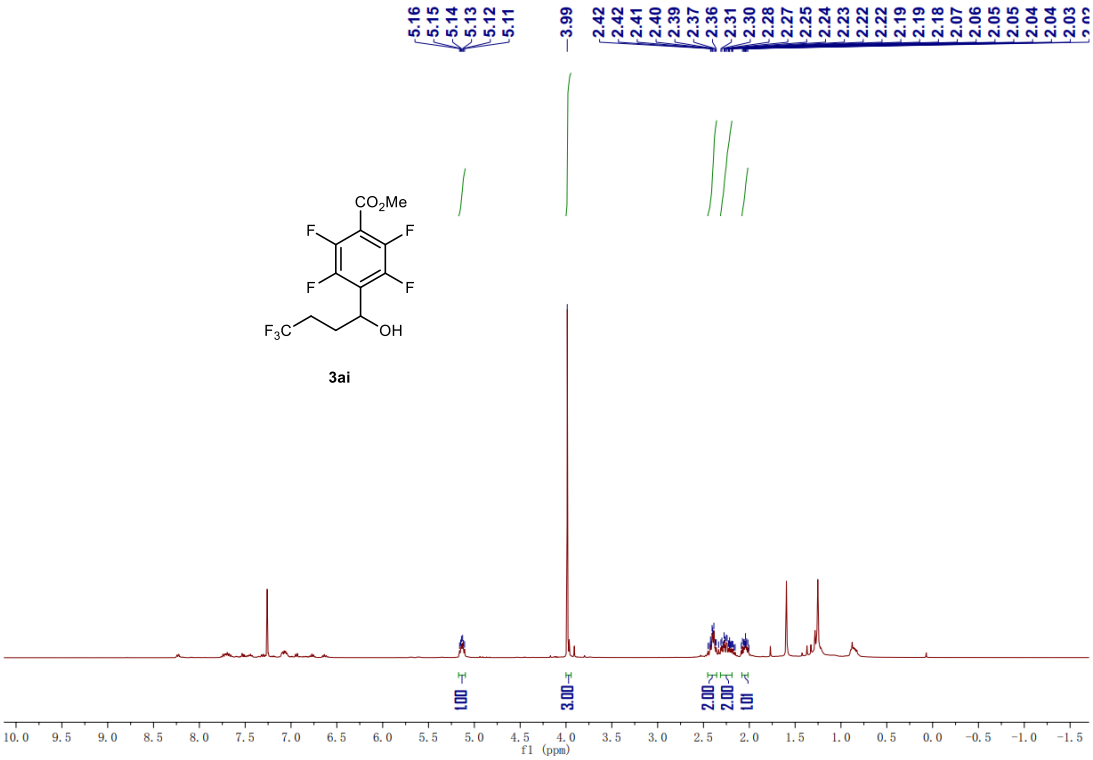
38.64
38.62
38.59
CO2Me
F
F
F
F
Cl
OH
3ah
f1 (ppm)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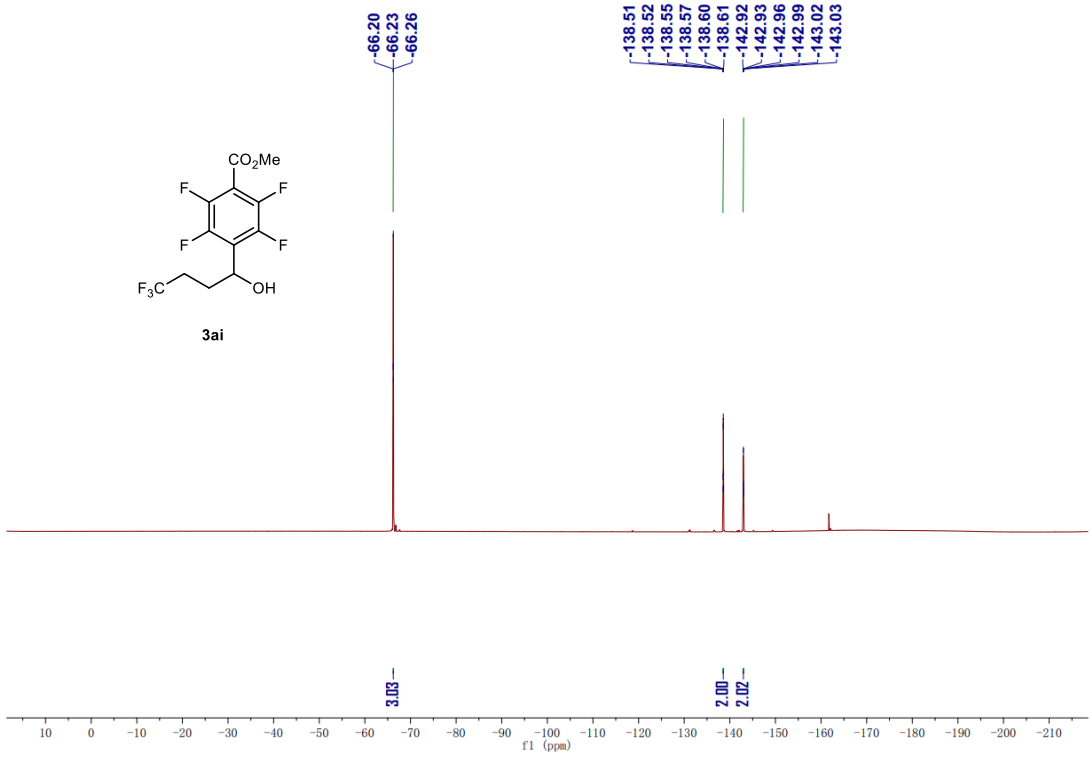
2.37
2.36
2.31
2.30
2.28
2.27
2.25
2.24
2.23
2.22
2.22
2.19
2.19
2.18
2.07
2.06
2.05
2.05
2.04
2.04
2.03
CO2Me
F
F
F
F
F3C
OH
3ai
1.00
3.00
2.00
2.00
1.01
f1 (ppm)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-142.93
-142.96
-142.99
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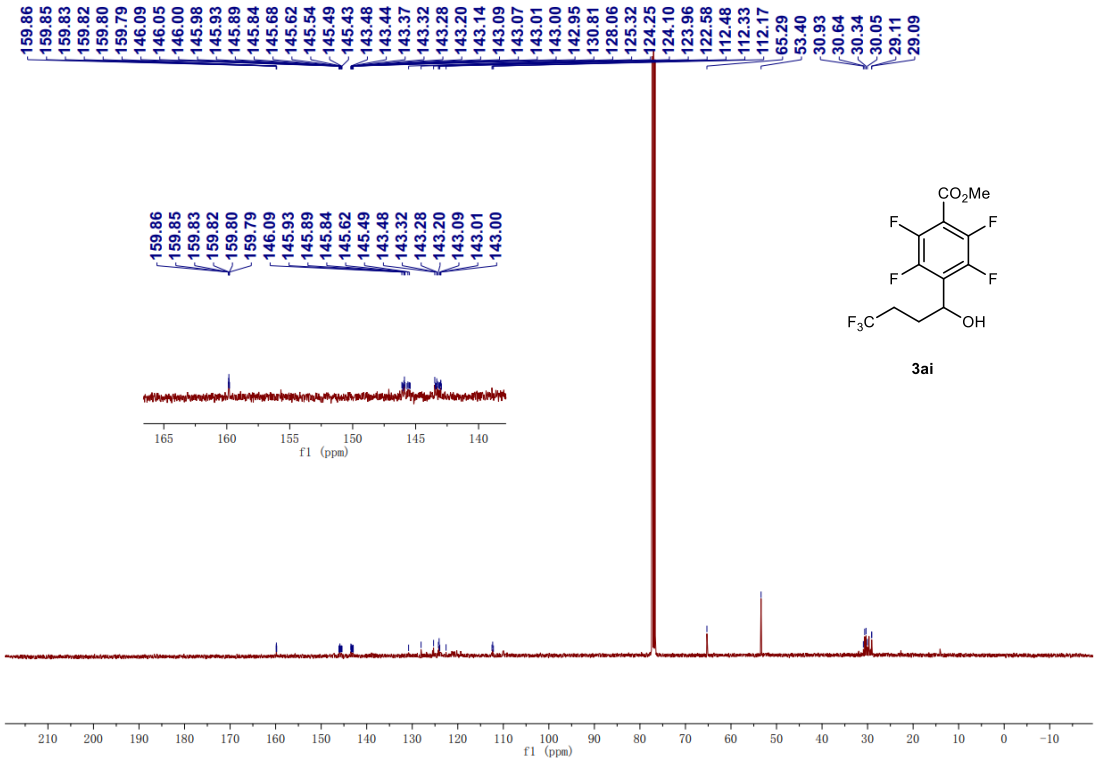
CO2Me
F
F
F
F
F3C
OH
3ai
3.03
2.00
2.02
f1 (ppm)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143.37
143.32
143.28
143.20
143.14
143.09
143.07
143.01
143.00
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130.81
128.06
125.32
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124.10
123.96
122.58
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30.34
30.05
29.11
29.09
159.86
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159.82
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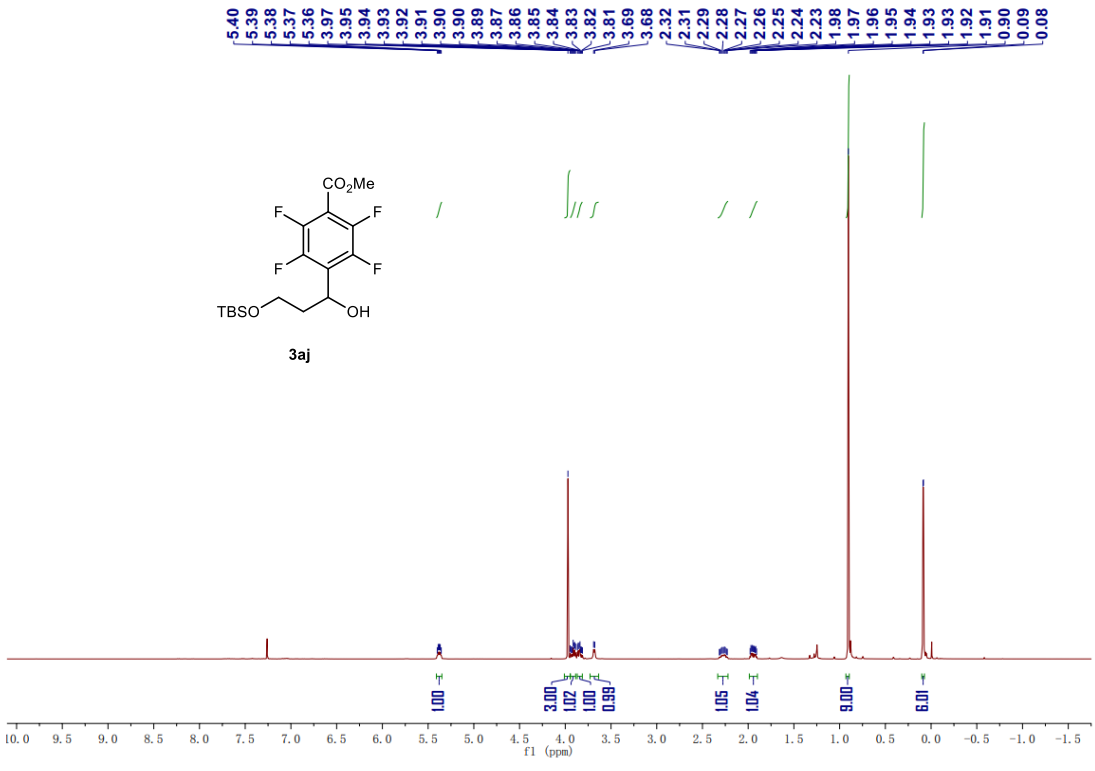
146.09
145.93
145.89
145.84
145.62
145.49
143.48
143.32
143.28
143.20
143.09
143.01
143.00
165
160
155
150
145
140
f1 (ppm)
CO2Me
F
F
F
F
F3C
OH
3ai
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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3.91
3.90
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3.86
3.85
3.84
3.83
3.82
3.81
3.69
3.68
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2.27
2.26
2.25
2.24
2.23
1.98
1.97
1.96
1.95
1.94
1.93
1.93
1.92
1.91
0.90
0.09
0.08
CO2Me
F
F
F
F
TBSO
OH
3aj
1.00
3.00
1.02
1.00
0.99
1.05
1.04
9.00
6.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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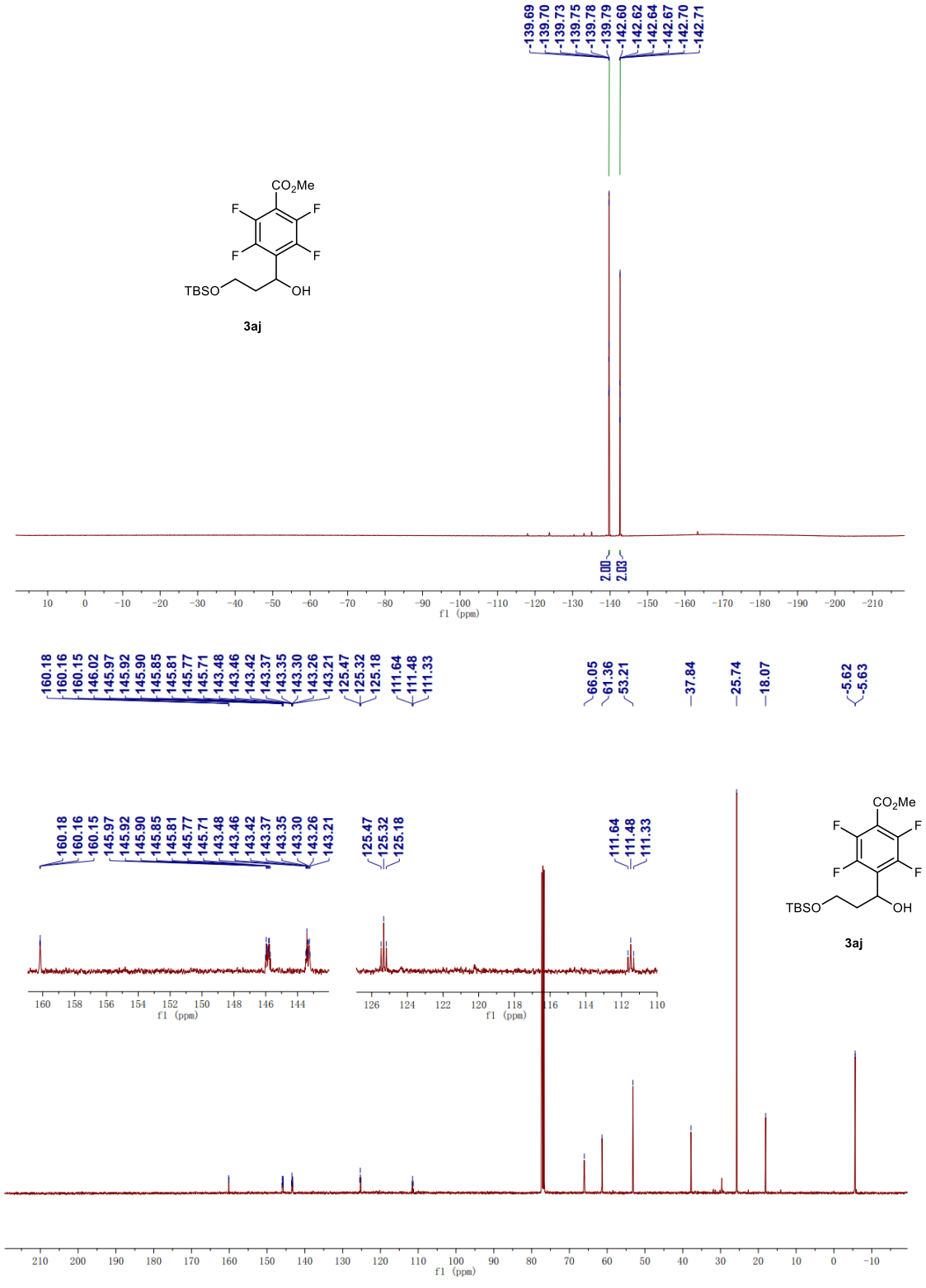
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
f1 (ppm)


CO2Me
F
F
F
F
TBSO
OH
3aj
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-139.70
-139.73
-139.75
-139.78
-139.79
-142.60
-142.62
-142.64
-142.67
-142.70
-142.71
2.00
2.03
f1 (ppm)
160.18
160.16
160.15
146.02
145.97
145.92
145.90
145.85
145.81
145.77
145.71
143.48
143.46
143.42
143.37
143.35
143.30
143.26
143.21
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125.32
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66.05
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53.21
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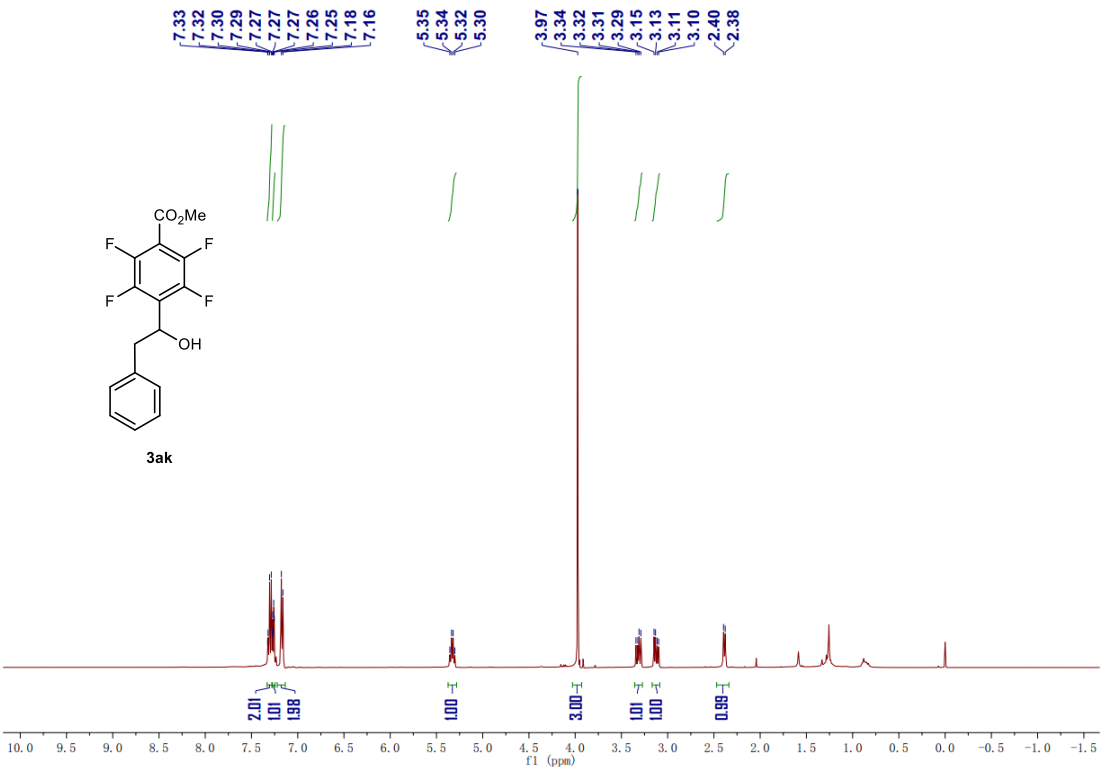
25.74
18.07
-5.62
-5.63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7.18
7.16
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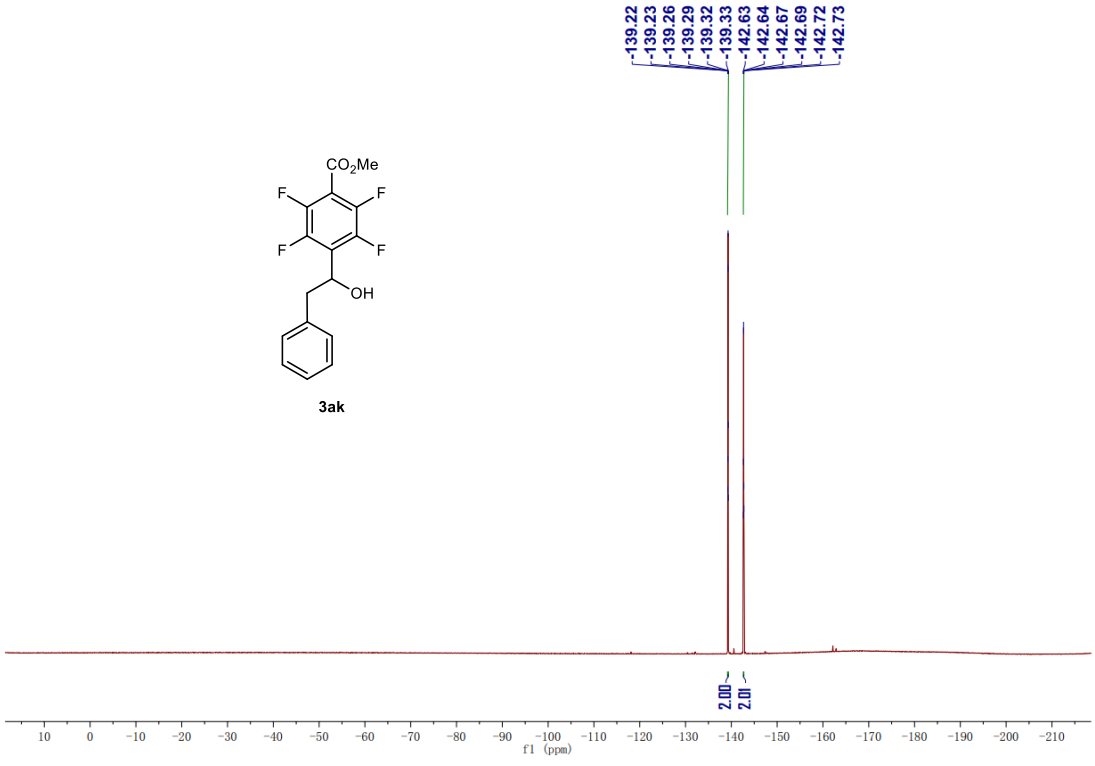
5.34
5.32
5.30
3.97
3.34
3.32
3.31
3.29
3.15
3.13
3.11
3.10
2.40
2.38
CO2Me
F
F
F
F
OH
2.01
1.01
1.98
1.00
3.00
1.01
1.00
0.99
f1 (ppm)

3ak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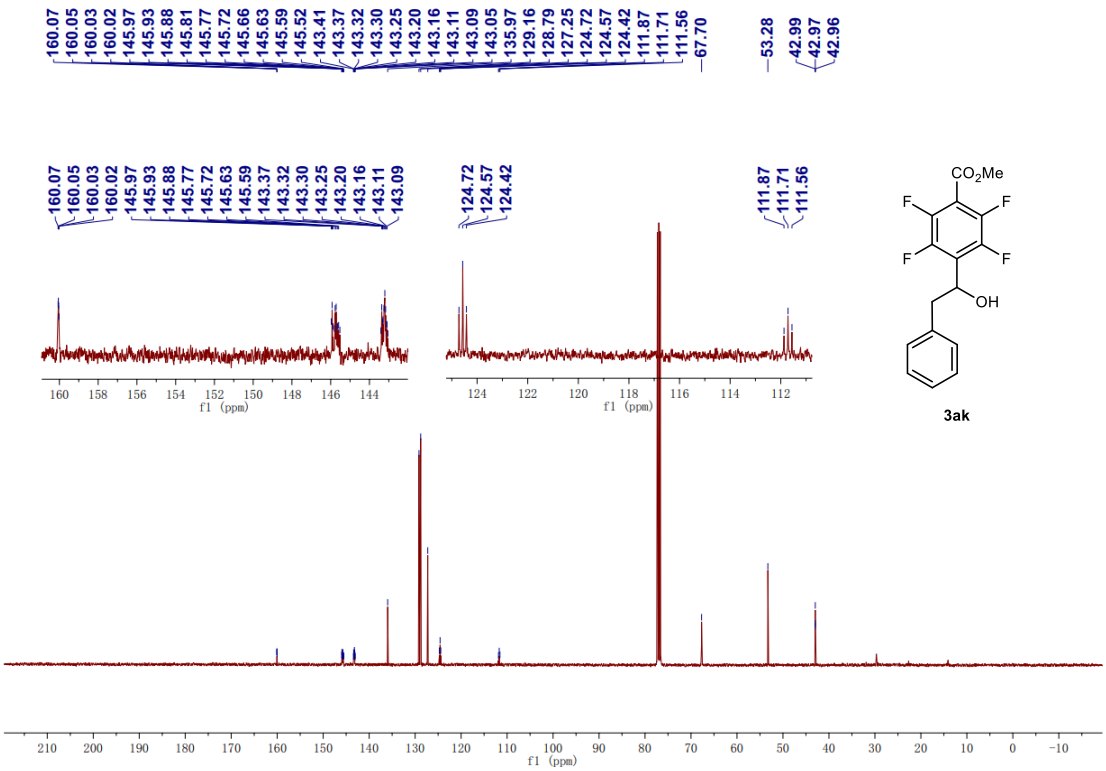
-142.63
-142.64
-142.67
-142.69
-142.72
-142.73
CO2Me
F
F
F
F
OH
2.00
2.01
f1 (ppm)

3ak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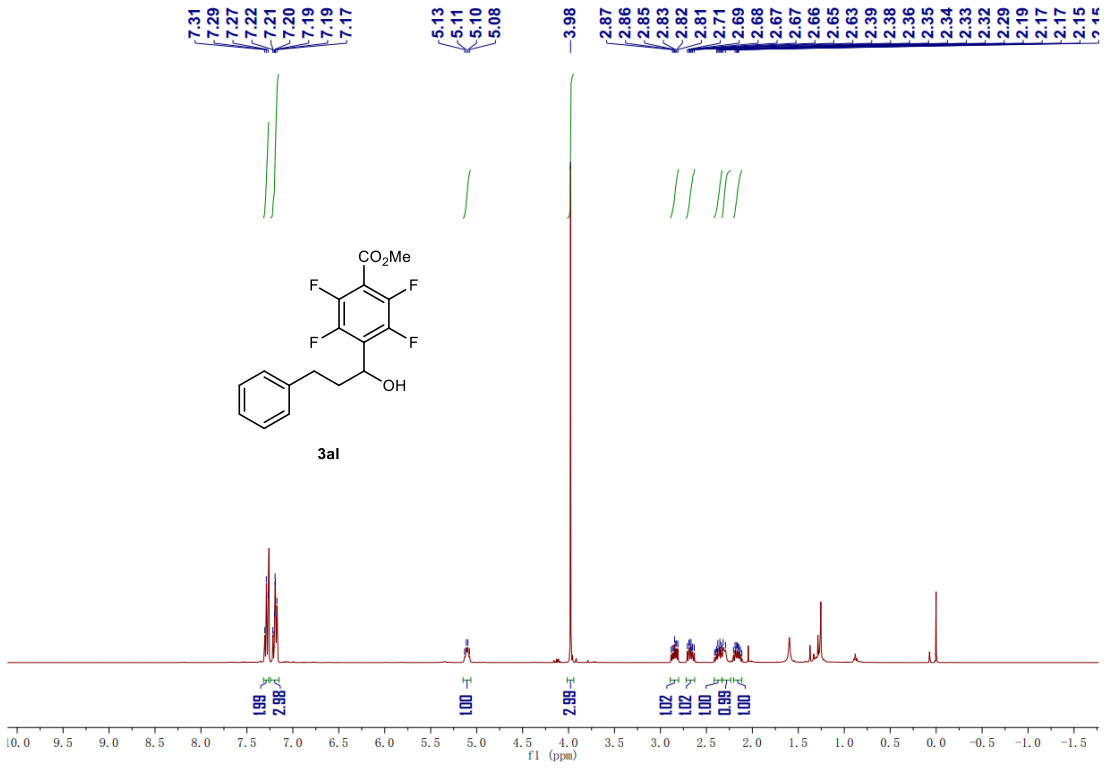
145.52
143.41
143.37
143.32
143.30
143.25
143.20
143.16
143.11
143.09
143.05
135.97
129.16
128.79
127.25
124.72
124.57
124.42
111.87
111.71
111.56
67.70
53.28
42.99
42.97
42.96
f1 (ppm)
CO2Me
F
F
F
F
OH
3ak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7.19
7.17
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5.11
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5.08
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2.87
2.86
2.85
2.83
2.82
2.81
2.71
2.69
2.68
2.67
2.67
2.66
2.65
2.63
2.39
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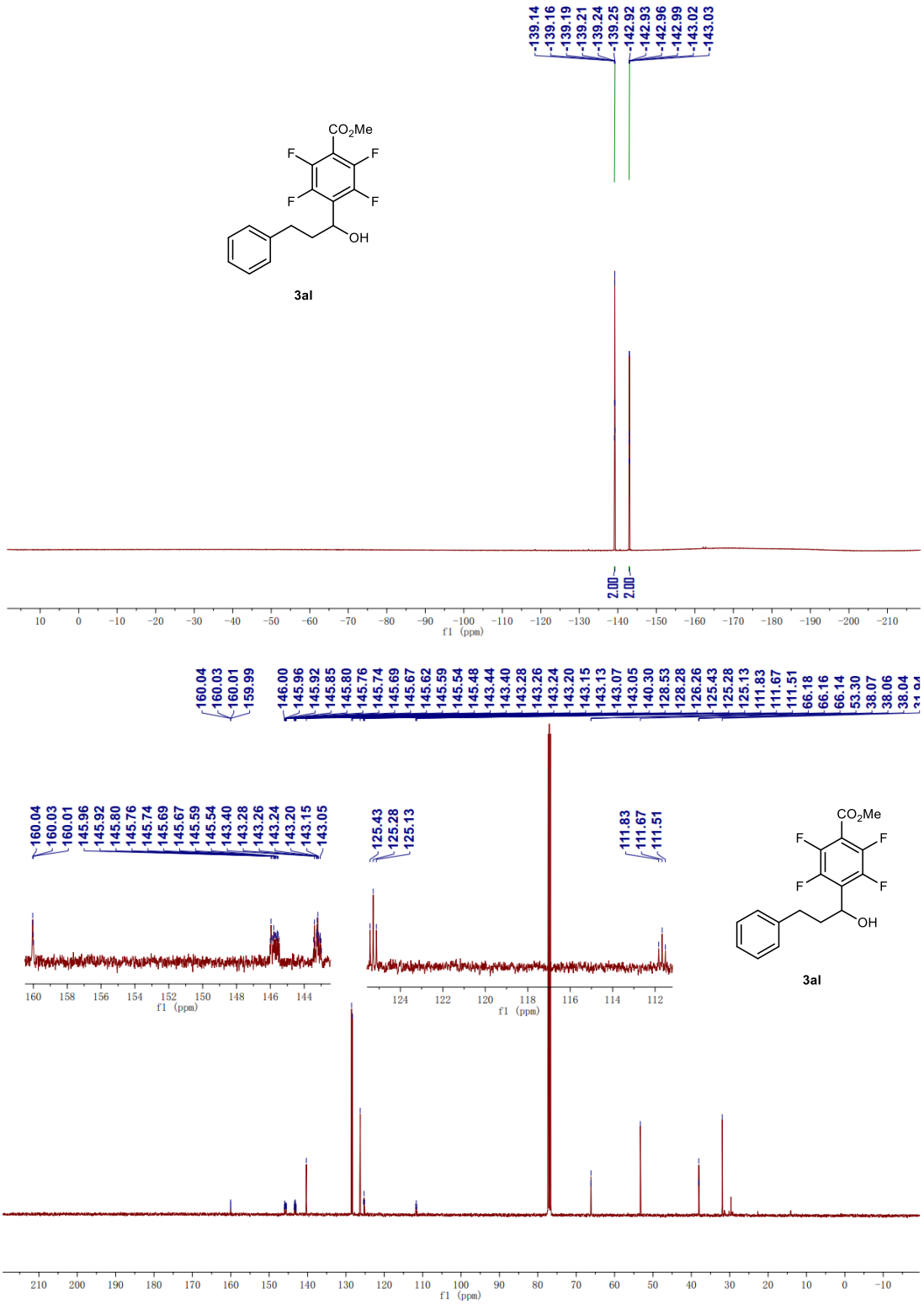
2.36
2.35
2.34
2.33
2.32
2.29
2.19
2.17
2.17
2.15
1.99
2.98
1.00
2.99
1.02
1.02
1.00
0.99
1.00
f1 (ppm)
CO2Me
F
F
F
F
OH
3al


CO2Me
F
F
F
F
OH
3al
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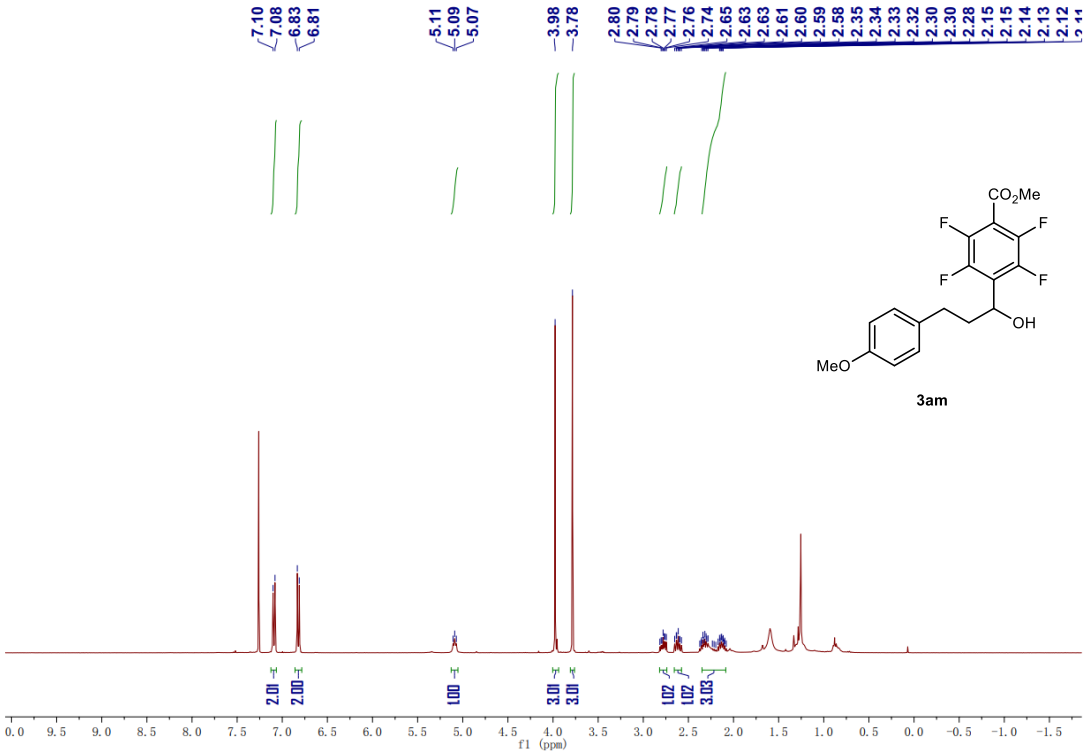
-139.16
-139.19
-139.21
-139.24
-139.25
-142.92
-142.93
-142.96
-142.99
-143.02
-143.03
2.00
2.00
f1 (ppm)
160.04
160.03
160.01
159.99
146.00
145.96
145.92
145.85
145.80
145.76
145.74
145.69
145.67
145.62
145.59
145.54
145.48
143.44
143.40
143.28
143.26
143.24
143.20
143.15
143.13
143.07
143.05
140.30
128.53
128.28
126.26
125.43
125.28
125.13
111.83
111.67
111.51
66.18
66.16
66.14
53.30
38.07
38.06
38.04
125.43
125.28
125.13
111.83
111.67
111.51
CO2Me
F
F
F
F
OH
3al
f1 (ppm)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2.76
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2.63
2.61
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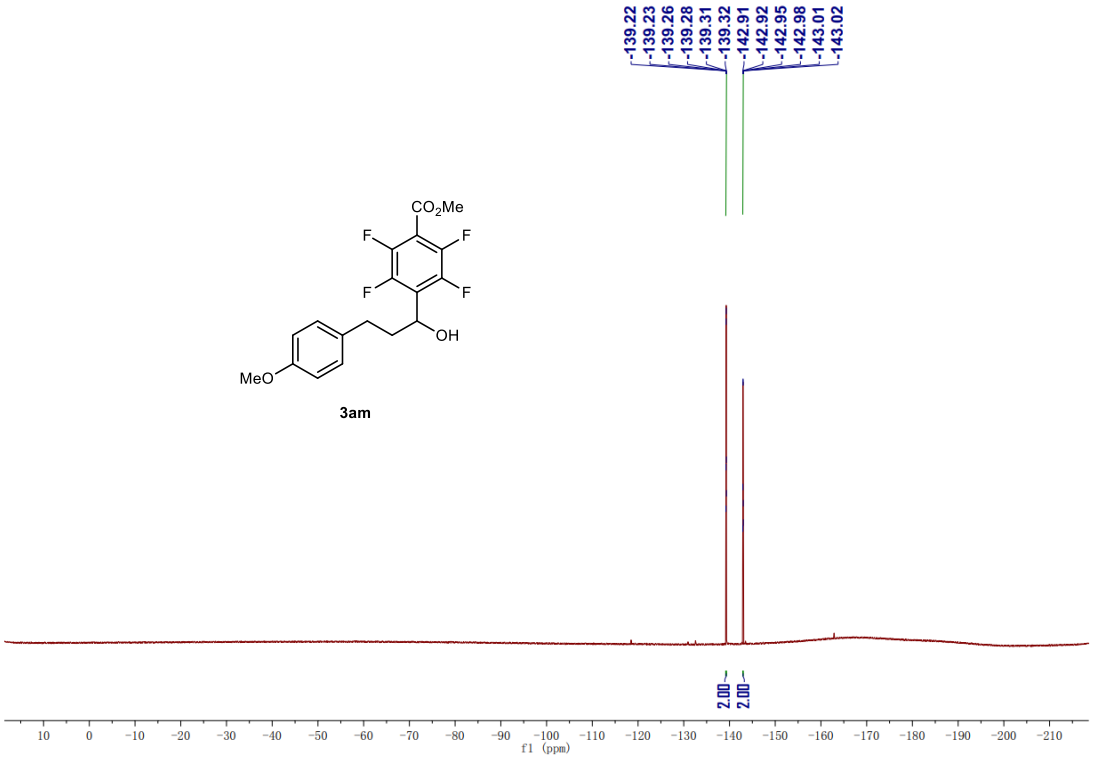
2.59
2.58
2.35
2.34
2.33
2.32
2.30
2.30
2.28
2.15
2.15
2.14
2.13
2.12
CO2Me
F
F
F
F
OH
MeO
3am
2.01
2.00
1.00
3.01
3.01
1.02
1.02
3.03
f1 (ppm)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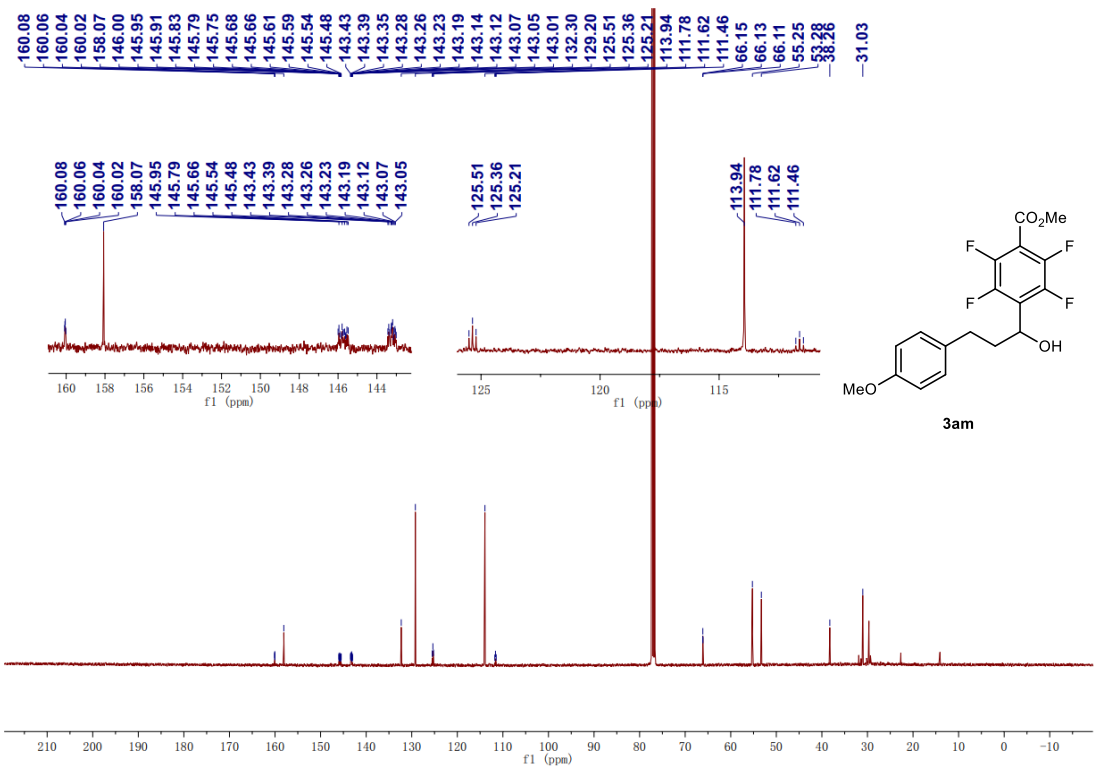
-142.91
-142.92
-142.95
-142.98
-143.01
-143.02
CO2Me
F
F
F
F
OH
MeO
3am
2.00
2.00
f1 (ppm)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145.79
145.75
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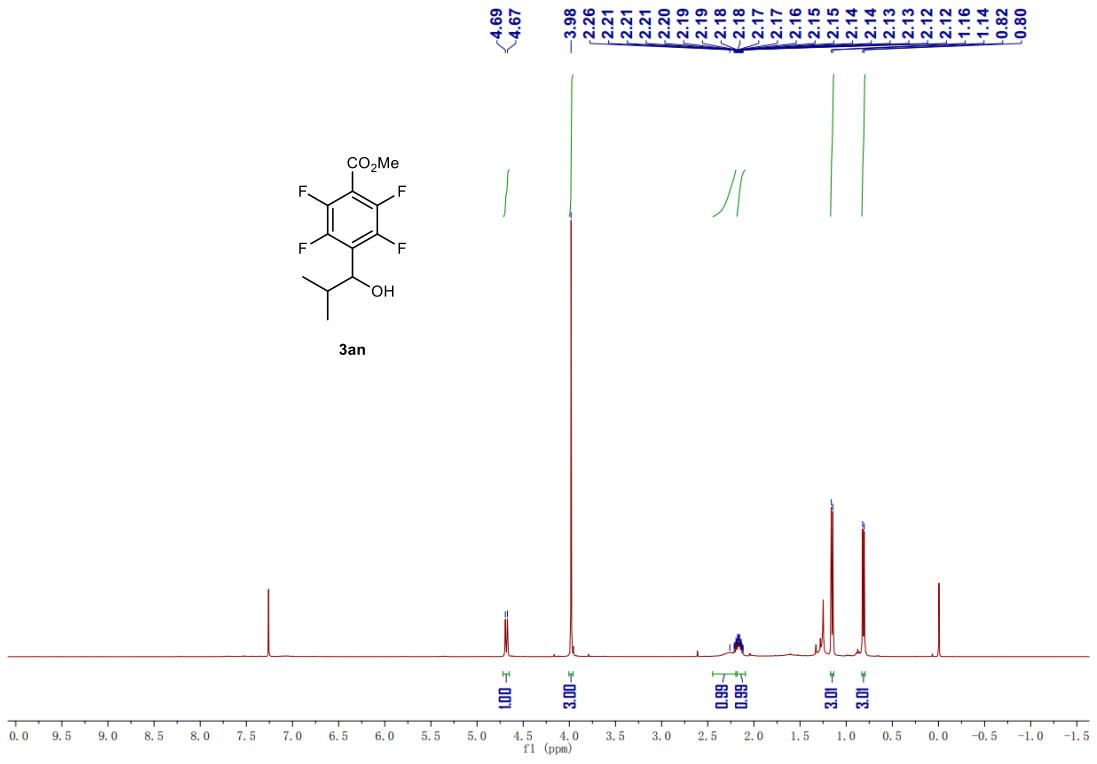
145.61
145.59
145.54
145.48
143.43
143.39
143.35
143.28
143.26
143.23
143.19
143.14
143.12
143.07
143.05
143.01
132.30
129.20
125.51
125.36
125.21
113.94
111.78
111.62
111.46
66.15
66.13
66.11
55.25
53.28
38.26
31.03
f1 (ppm)
CO2Me
F
F
F
F
OH
MeO

3am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2.17
2.16
2.15
2.15
2.14
2.14
2.13
2.12
2.12
1.16
1.14
0.82
0.80
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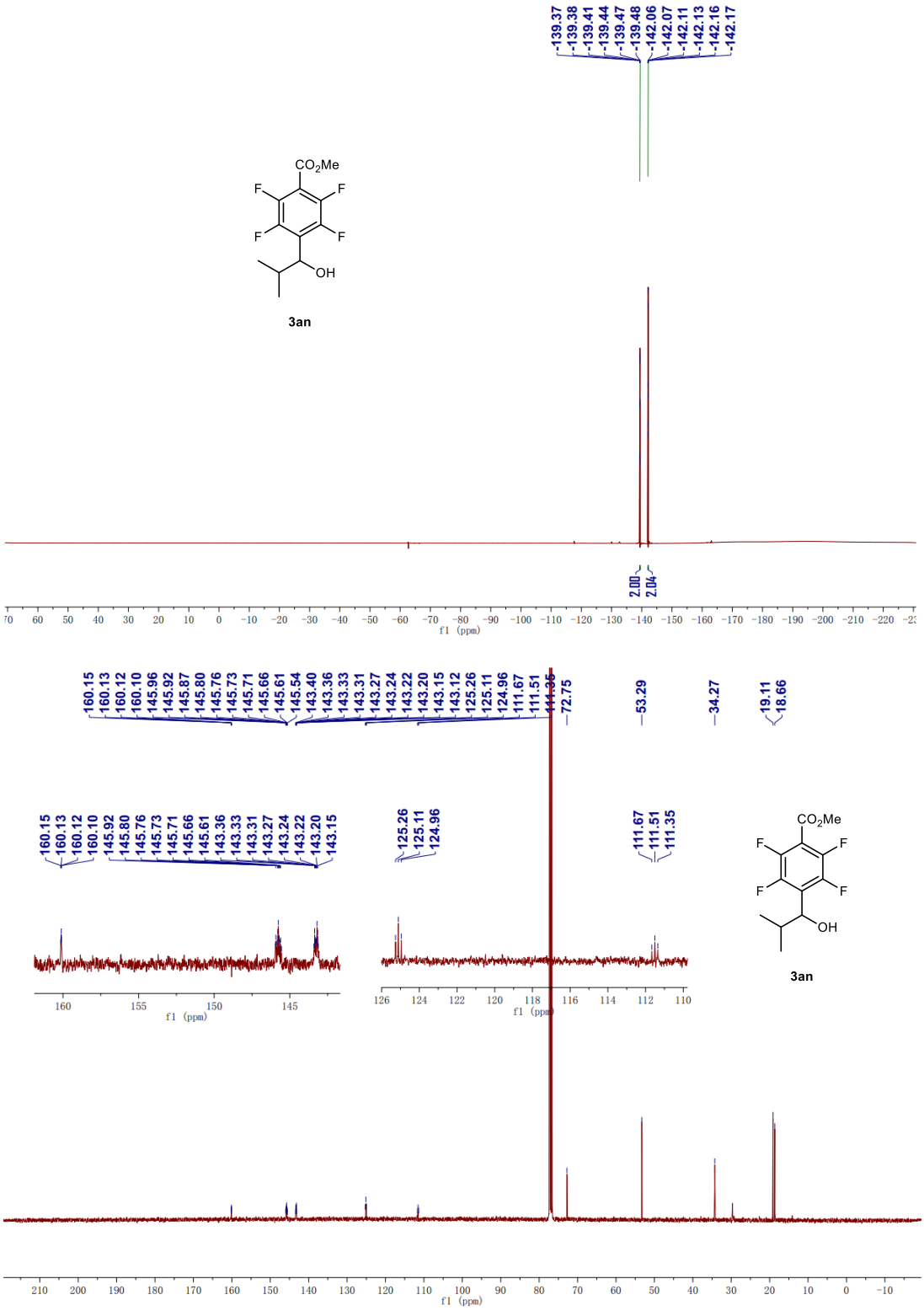
3.00
0.99
0.99
3.01
3.01
f1 (ppm)
CO2Me
F
F
F
F
OH

3an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-142.06
-142.07
-142.11
-142.13
-142.16
-142.17
CO2Me
F
F
F
F
OH
3an
2.00
2.04
f1 (ppm)
160.15
160.13
160.12
160.10
145.96
145.92
145.87
145.80
145.76
145.73
145.71
145.66
145.61
145.54
143.40
143.36
143.33
143.31
143.27
143.24
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143.20
143.15
143.12
125.26
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72.75
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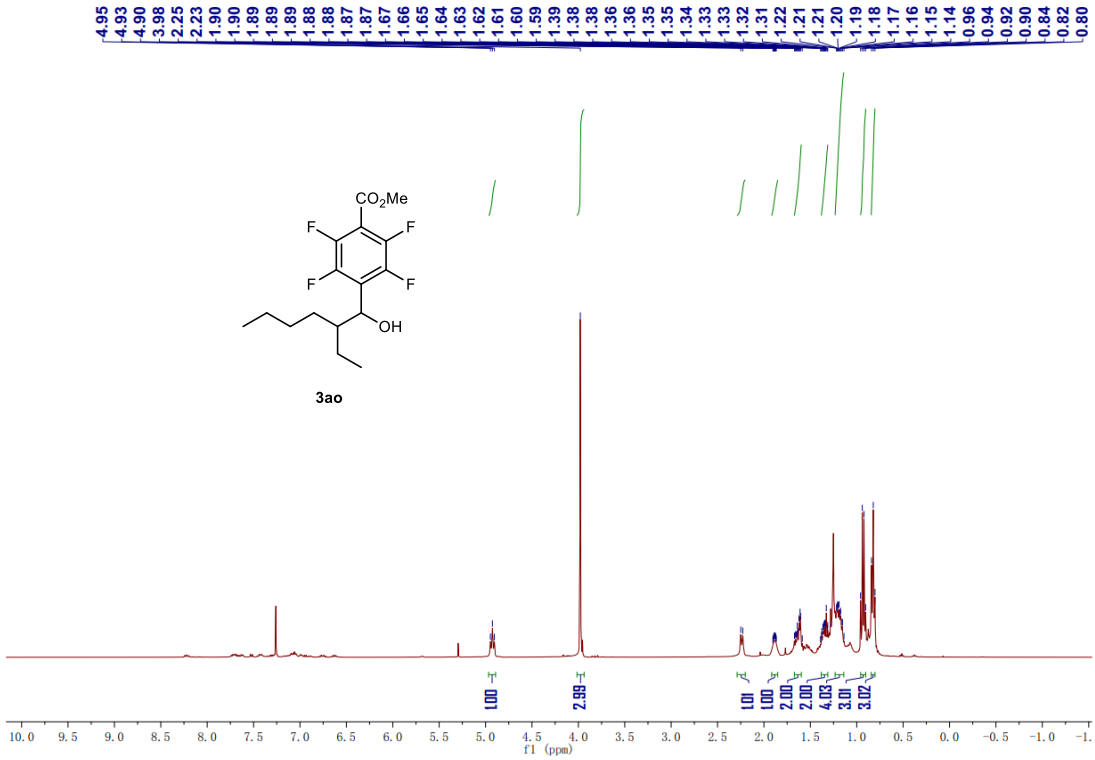
34.27
19.11
18.66
3an
f1 (ppm)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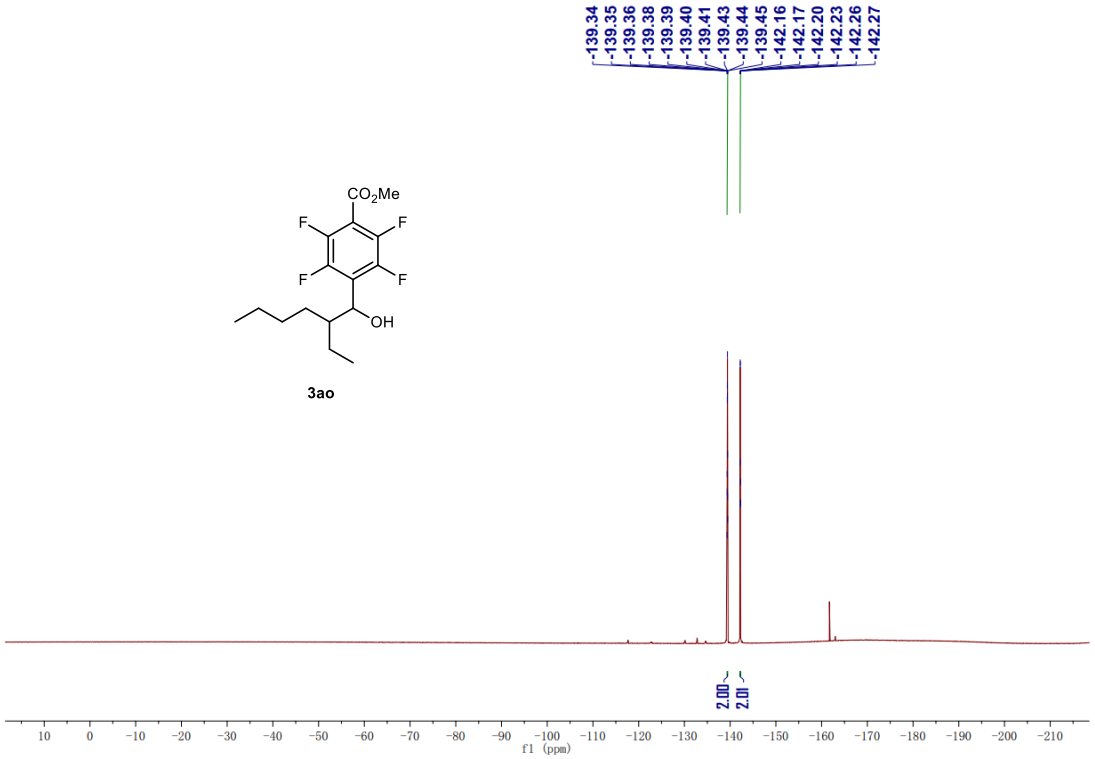
CO2Me
F
F
F
F
OH
3ao
1.00 2.99 1.01 1.00 2.00 2.00 4.03 3.01 3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.
f1 (ppm)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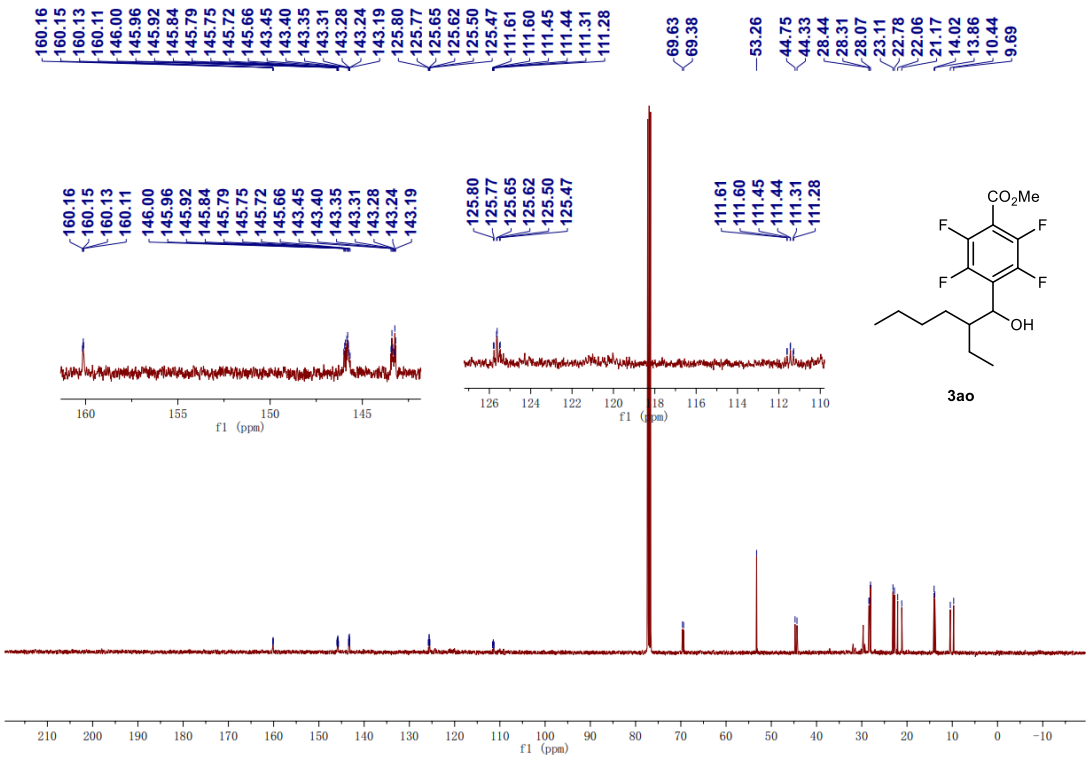
CO2Me
F
F
F
F
OH
3ao
2.00 2.01
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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143.40
143.35
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143.24
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69.38
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28.44
28.31
28.07
23.11
22.78
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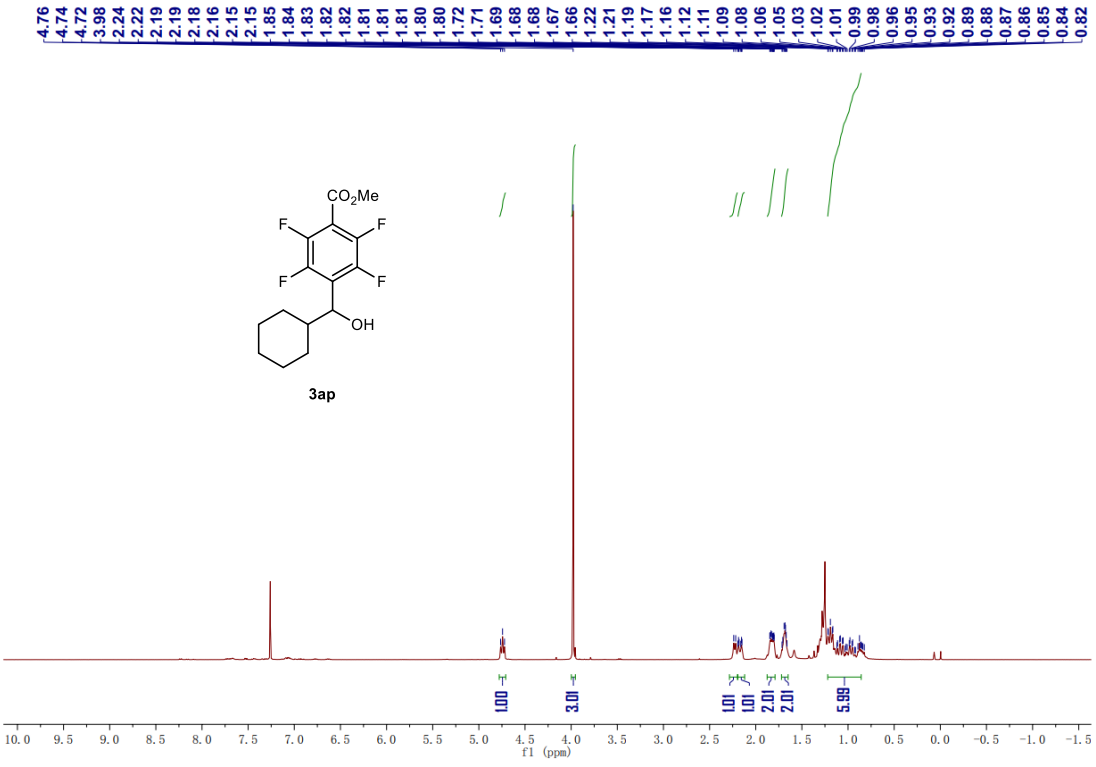
13.86
10.44
9.69
f1 (ppm)
CO2Me
F
F
F
F
OH
3ao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1.85
1.84
1.83
1.82
1.82
1.81
1.81
1.81
1.80
1.80
1.72
1.71
1.69
1.68
1.68
1.67
1.66
1.22
1.21
1.19
1.17
1.16
1.12
1.11
1.09
1.08
1.06
1.05
1.03
1.02
1.01
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0.98
0.96
0.95
0.93
0.92
0.89
0.88
0.87
0.86
0.85
0.84
0.82
CO2Me
F
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F
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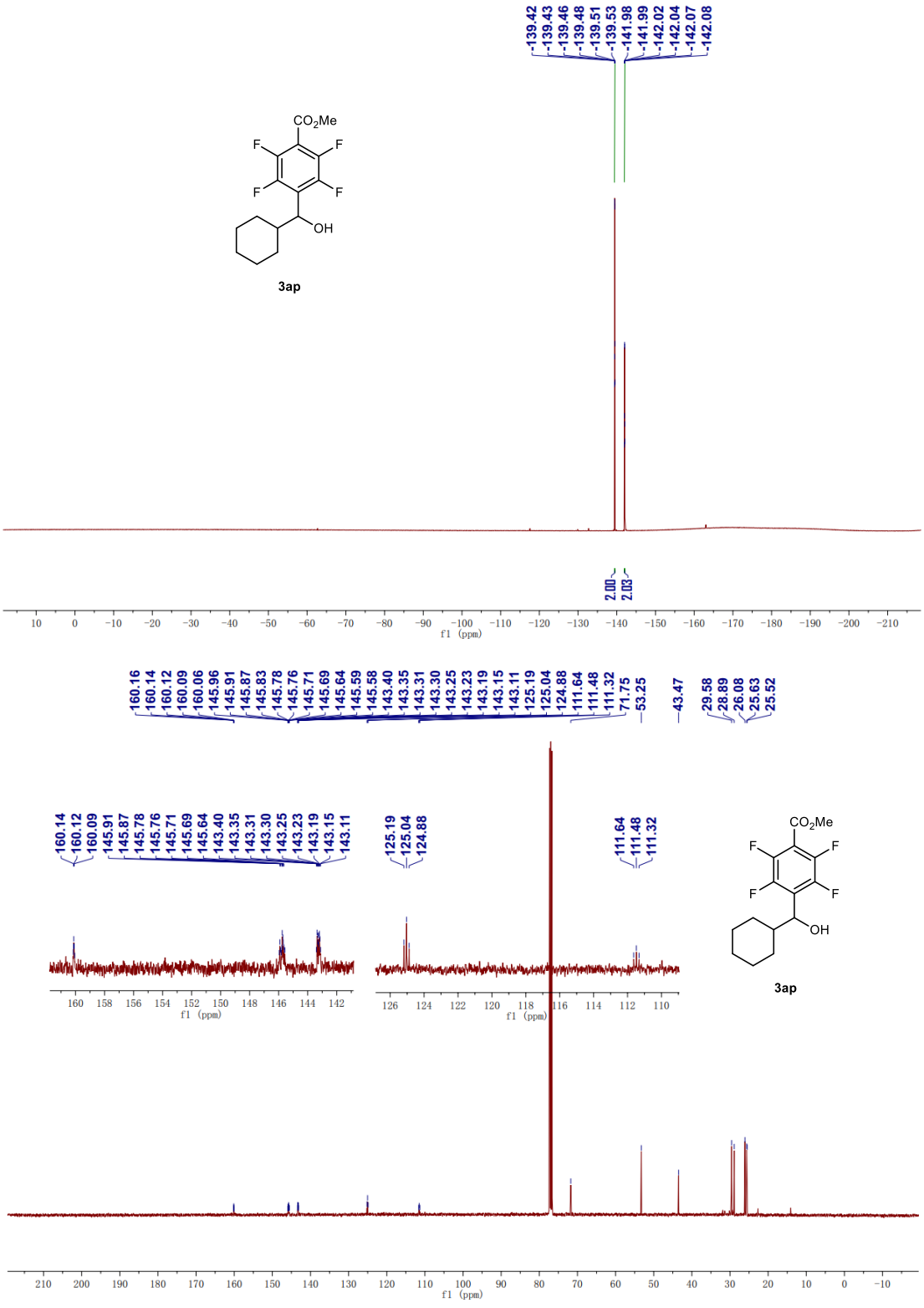
3.01
1.01
1.01
2.01
2.01
5.99
f1 (ppm)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-142.07
-142.08
CO2Me
F
F
F
F
OH
3ap
2.00
2.03
f1 (ppm)
160.16
160.14
160.12
160.09
160.06
145.96
145.91
145.87
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145.76
145.71
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143.15
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125.04
124.88
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25.52
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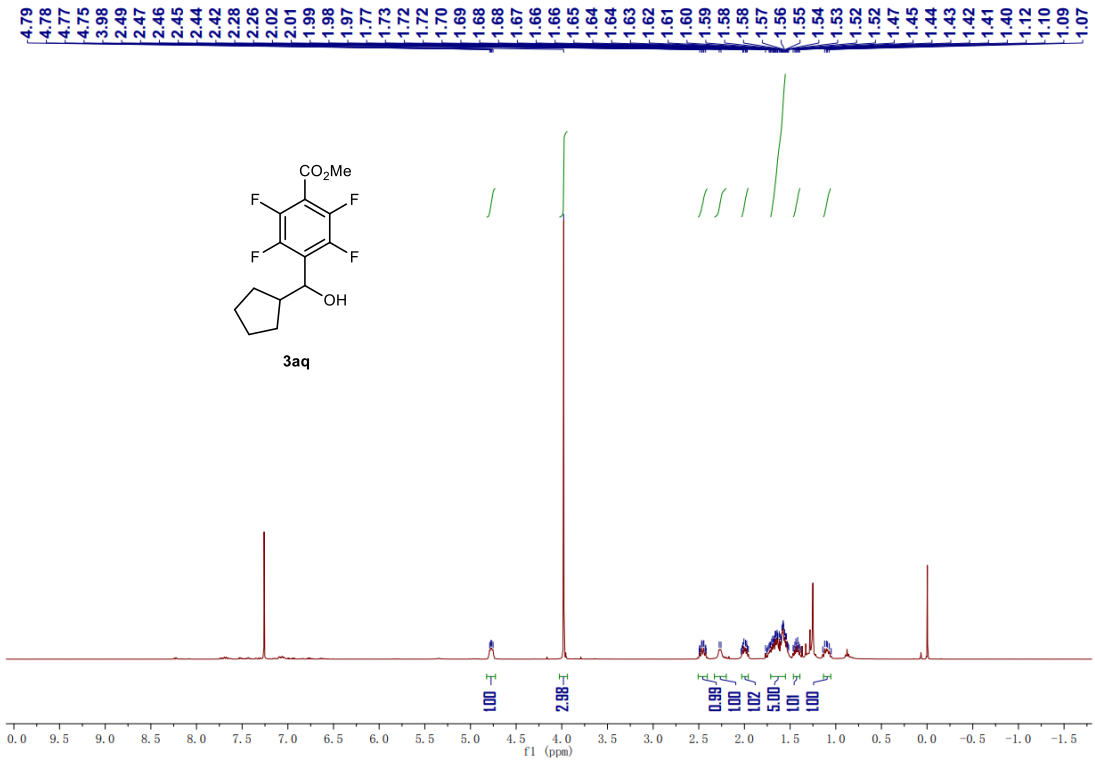
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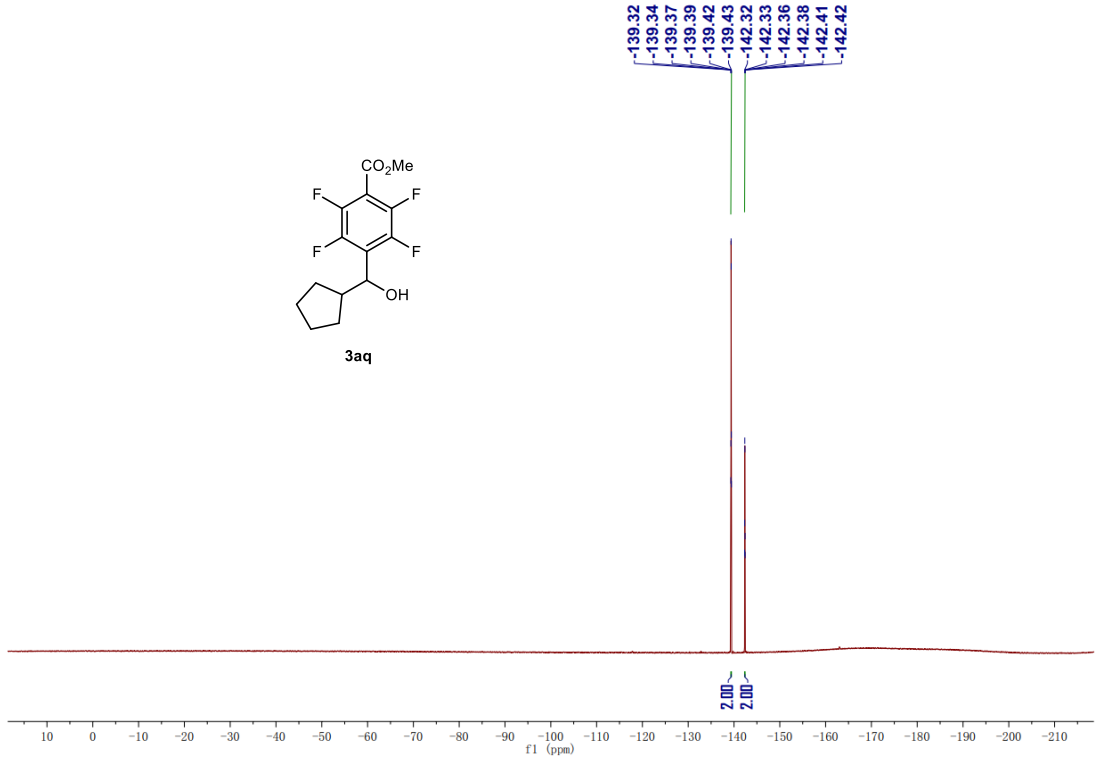
CO2Me
F
F
F
F
OH
3aq
1.00 2.98 0.99 1.00 2.01 5.00 1.01 1.00
f1 (ppm)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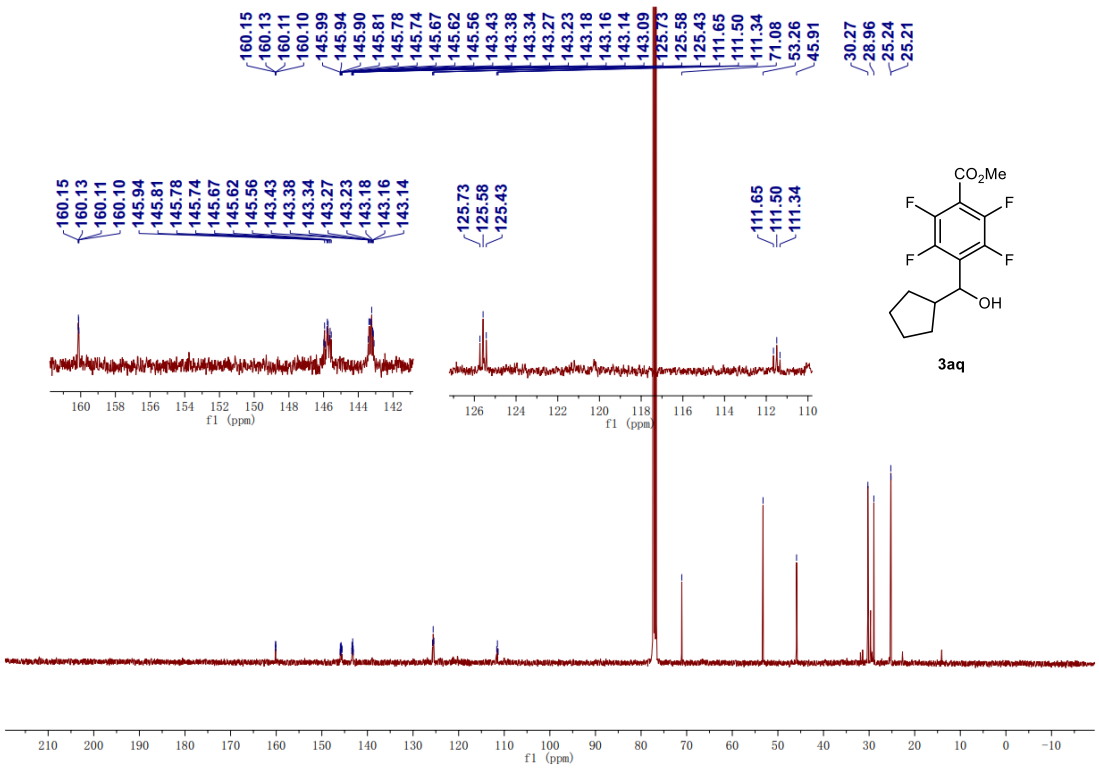
CO2Me
F
F
F
F
OH
3aq
2.00 2.00
f1 (ppm)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143.38
143.34
143.27
143.23
143.18
143.16
143.14
143.09
125.73
125.58
125.43
111.65
111.50
111.34
71.08
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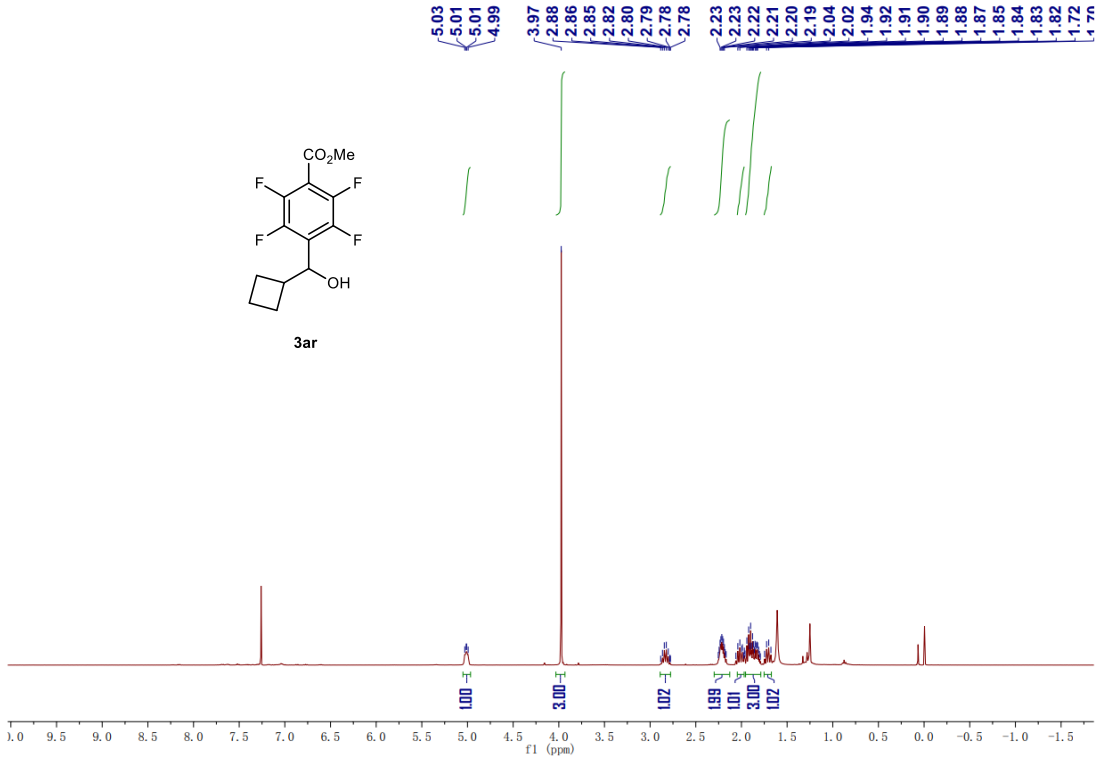
28.96
25.24
25.21
CO2Me
F
F
F
F
OH
3aq
f1 (ppm)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2.78
2.23
2.23
2.22
2.21
2.20
2.19
2.04
2.02
1.94
1.92
1.91
1.90
1.89
1.88
1.87
1.85
1.84
1.83
1.82
1.72
1.00
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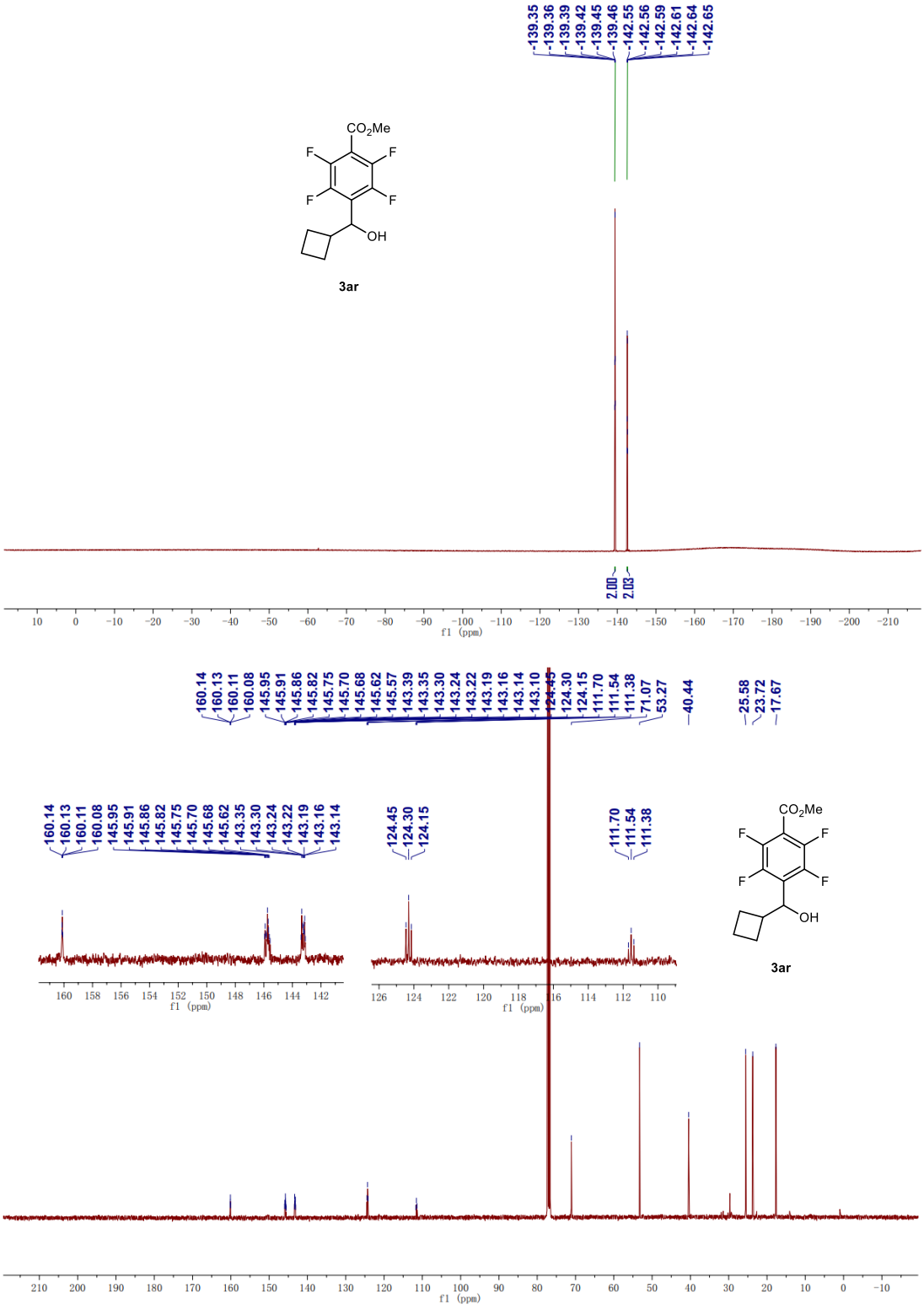
1.01
3.00
1.02
CO2Me
F
F
F
F
OH
3ar
f1 (ppm)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-142.65
CO2Me
F
F
F
F
OH
3ar
2.00
2.03
f1 (ppm)
160.14
160.13
160.11
160.08
145.95
145.91
145.86
145.82
145.75
145.70
145.68
145.62
145.57
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143.30
143.24
143.22
143.19
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143.14
143.10
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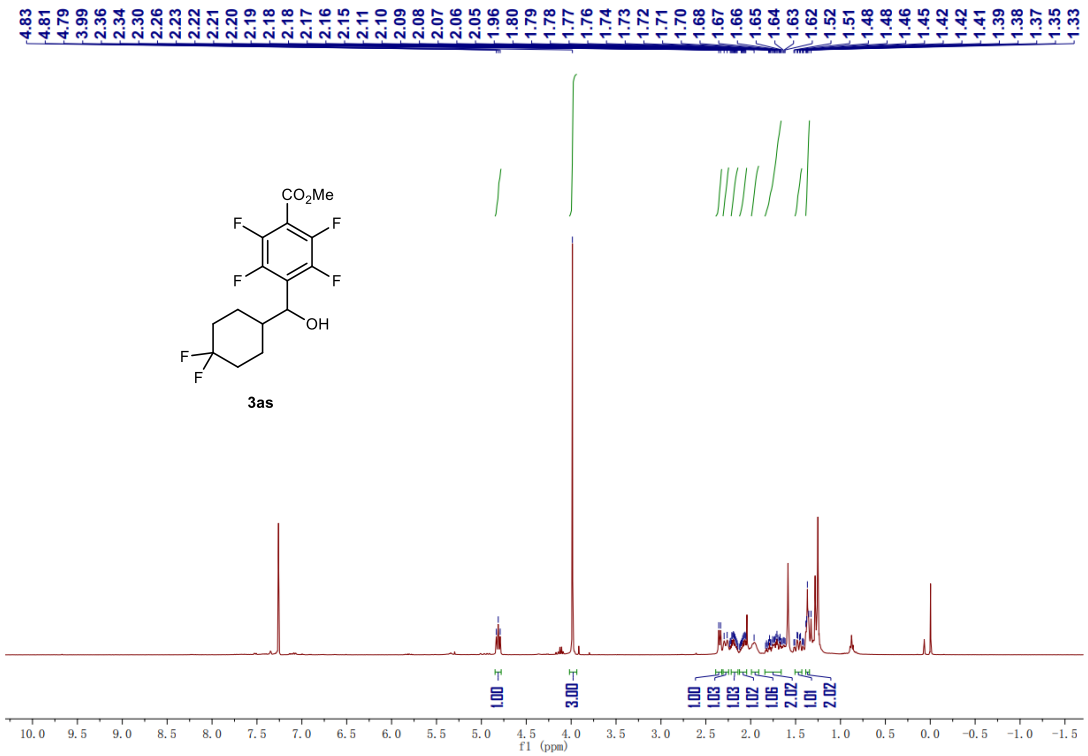
25.58
23.72
17.67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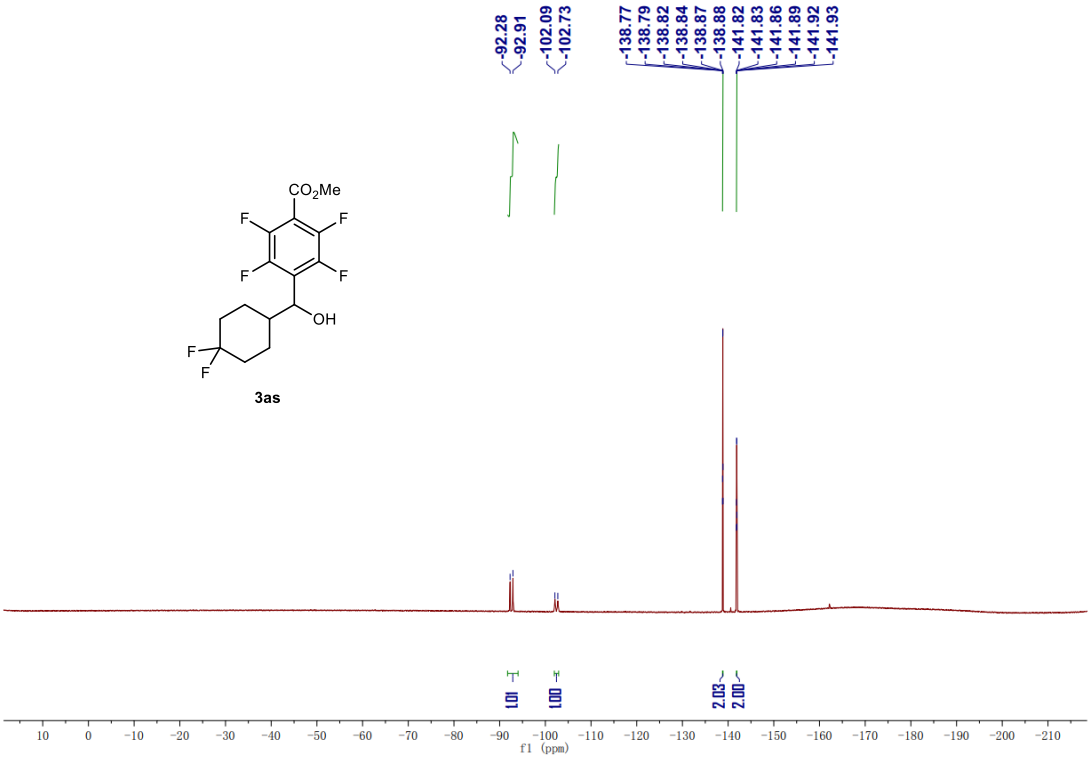
CO2Me
F
F
F
F
OH
F
F
3as
1.00 3.00 1.00 1.03 1.03 1.02 1.06 2.02 1.01 2.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)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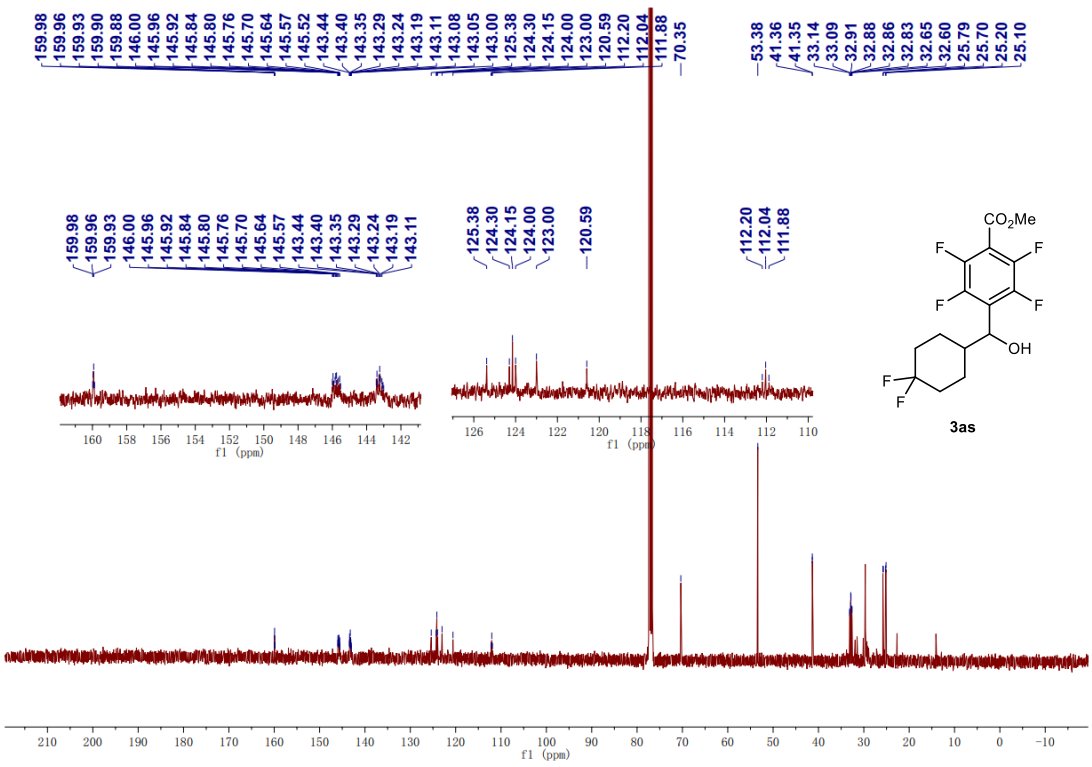
CO2Me
F
F
F
F
OH
F
F
3as
1.01 1.00 2.03 2.00
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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145.57
145.52
143.44
143.40
143.35
143.29
143.24
143.19
143.11
143.08
143.05
143.00
125.38
124.30
124.15
124.00
123.00
120.59
112.20
112.04
111.88
70.35
53.38
41.36
41.35
33.14
33.09
32.91
32.88
32.86
32.83
32.65
32.60
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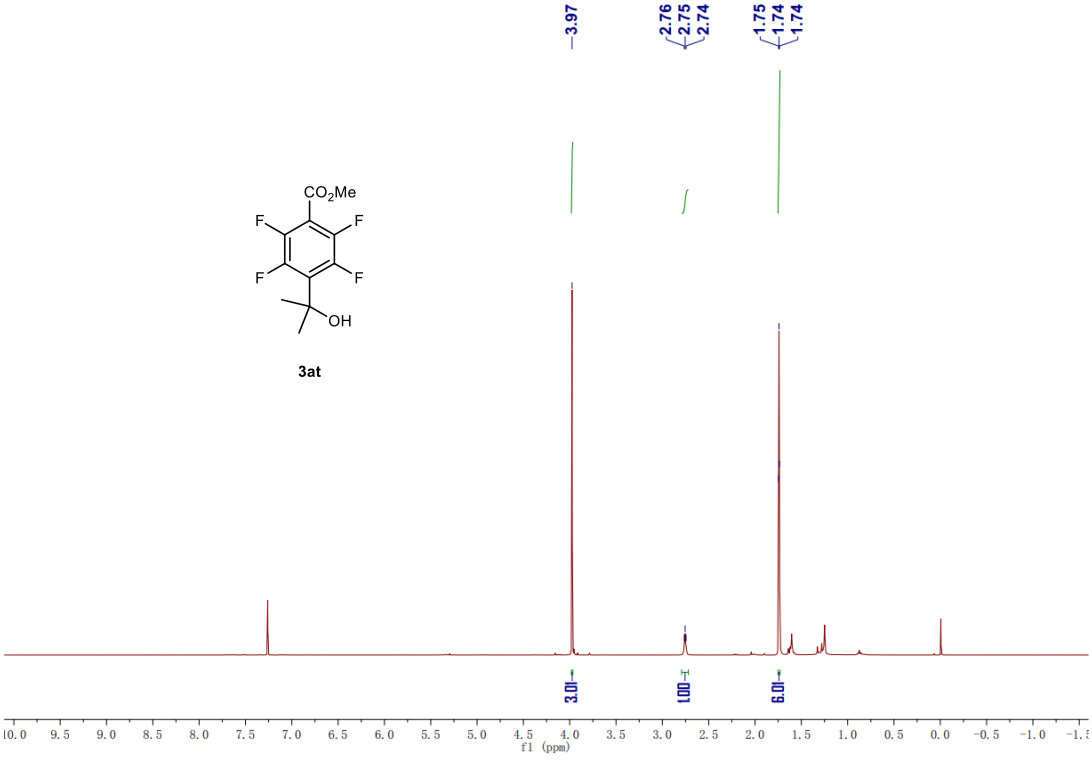
25.70
25.20
25.10
CO2Me
F
F
F
F
OH
F
F
3as
f1 (ppm)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2.74
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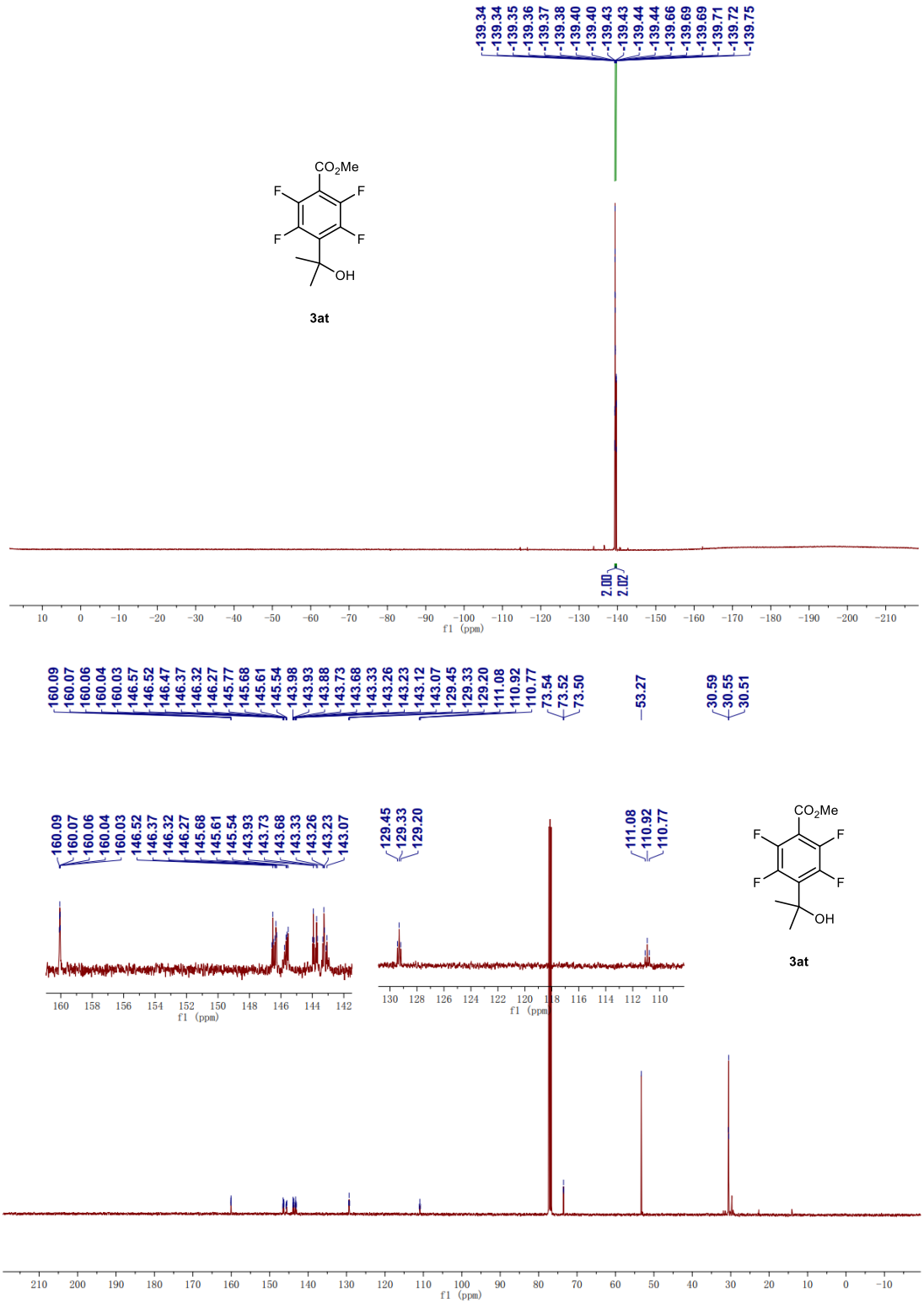
1.74
1.74
CO2Me
F
F
F
F
OH
3at
3.01
1.00
6.01
f1 (ppm)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-139.66
-139.69
-139.69
-139.71
-139.72
-139.75
CO2Me
F
F
F
F
OH
3at
2.00
2.02
f1 (ppm)
160.09
160.07
160.06
160.04
160.03
146.52
146.57
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143.26
143.23
143.12
143.07
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129.33
129.20
111.08
110.92
110.77
73.54
73.52
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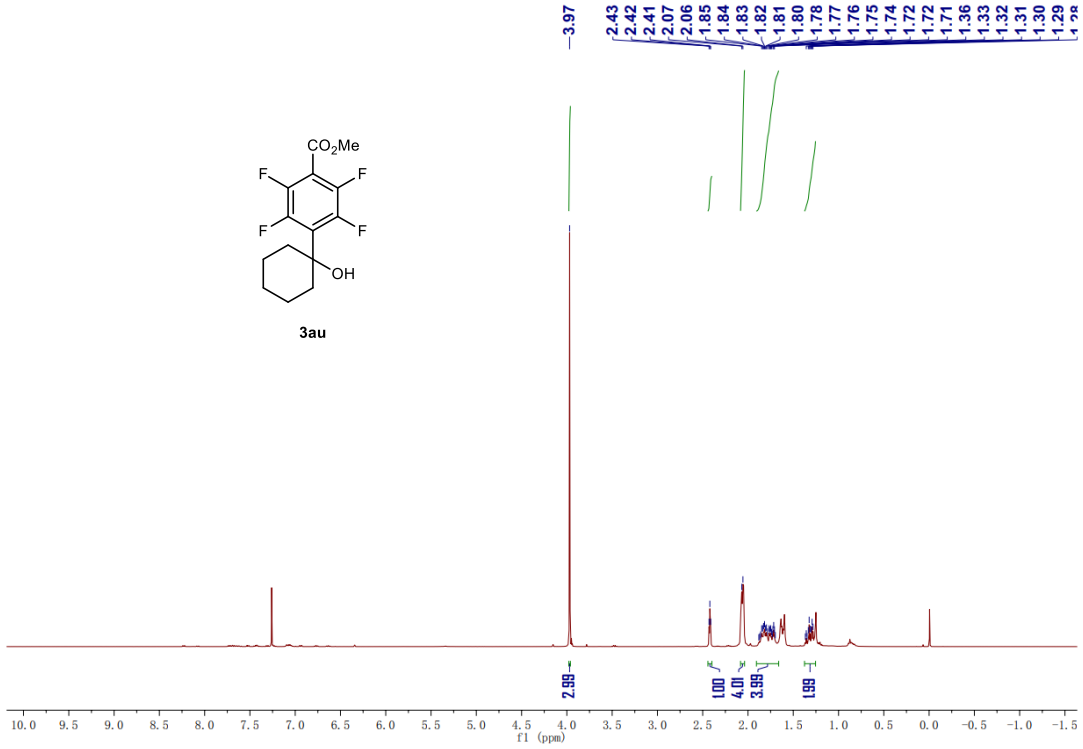
30.59
30.55
30.51
CO2Me
F
F
F
F
OH
3at
f1 (ppm)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1.83
1.82
1.81
1.80
1.78
1.77
1.76
1.75
1.74
1.72
1.72
1.71
1.36
1.33
1.32
1.31
1.30
1.29
CO2Me
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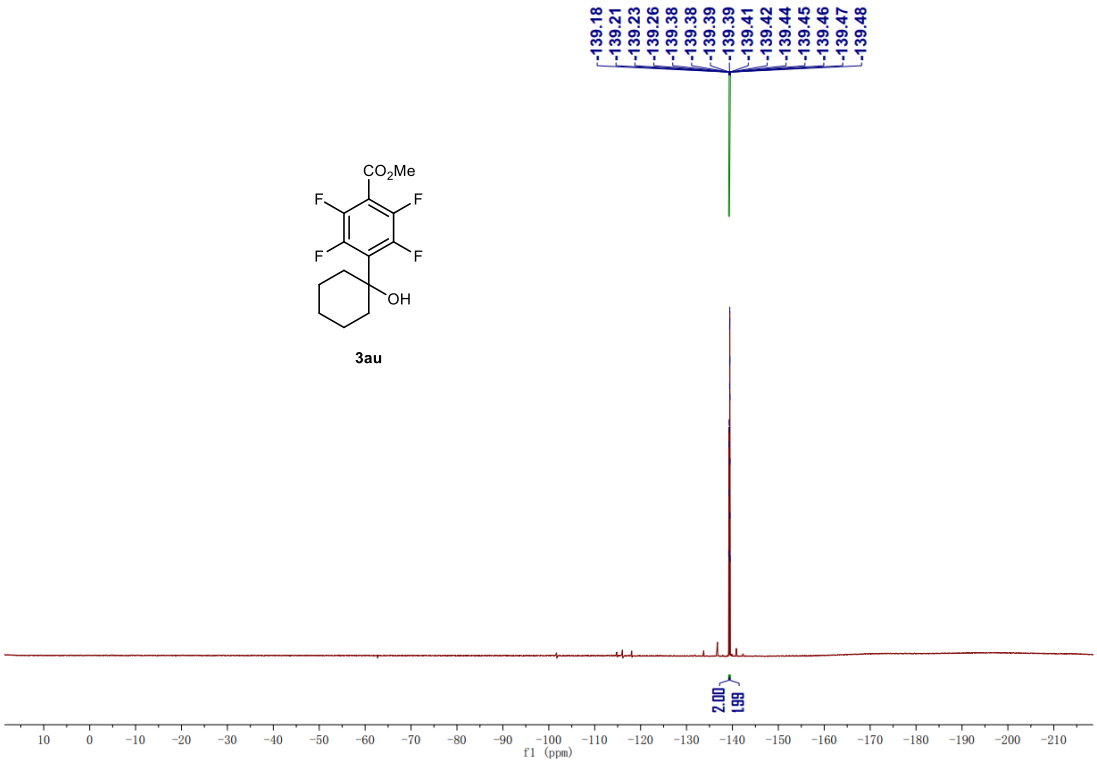
F
F
F
OH
2.99
1.00
4.01
3.99
1.99
f1 (ppm)

3au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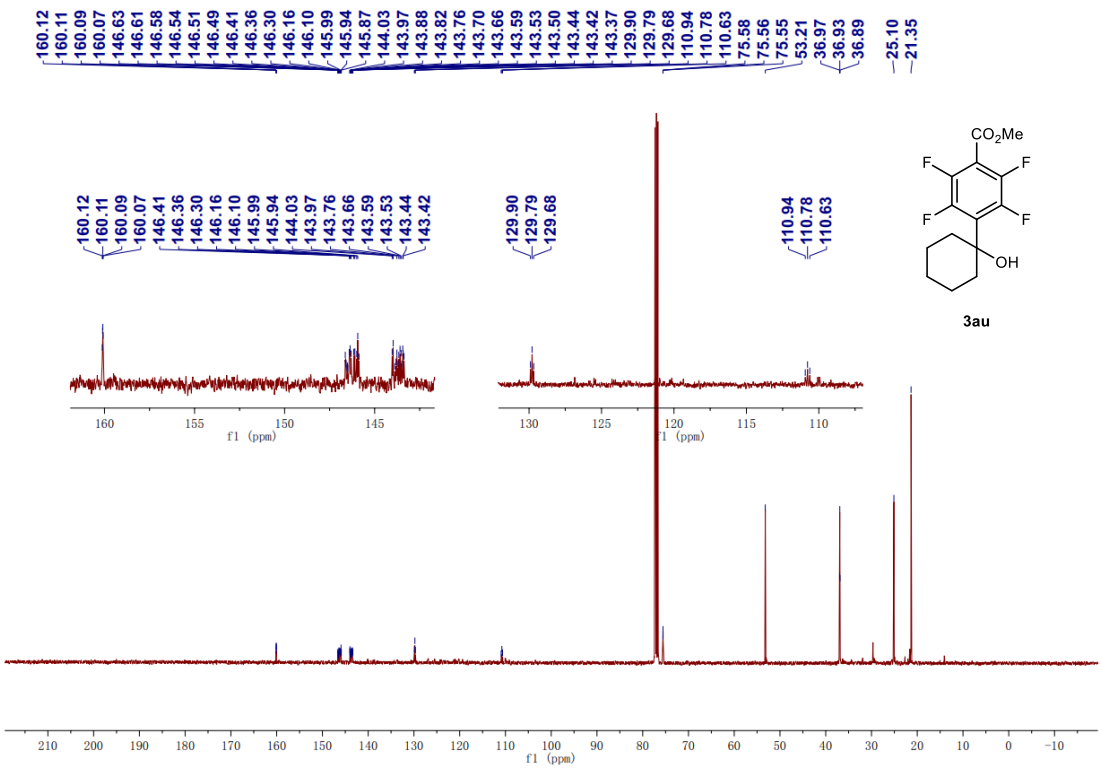
F
F
F
F
OH
2.00
1.99
f1 (ppm)

3au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146.10
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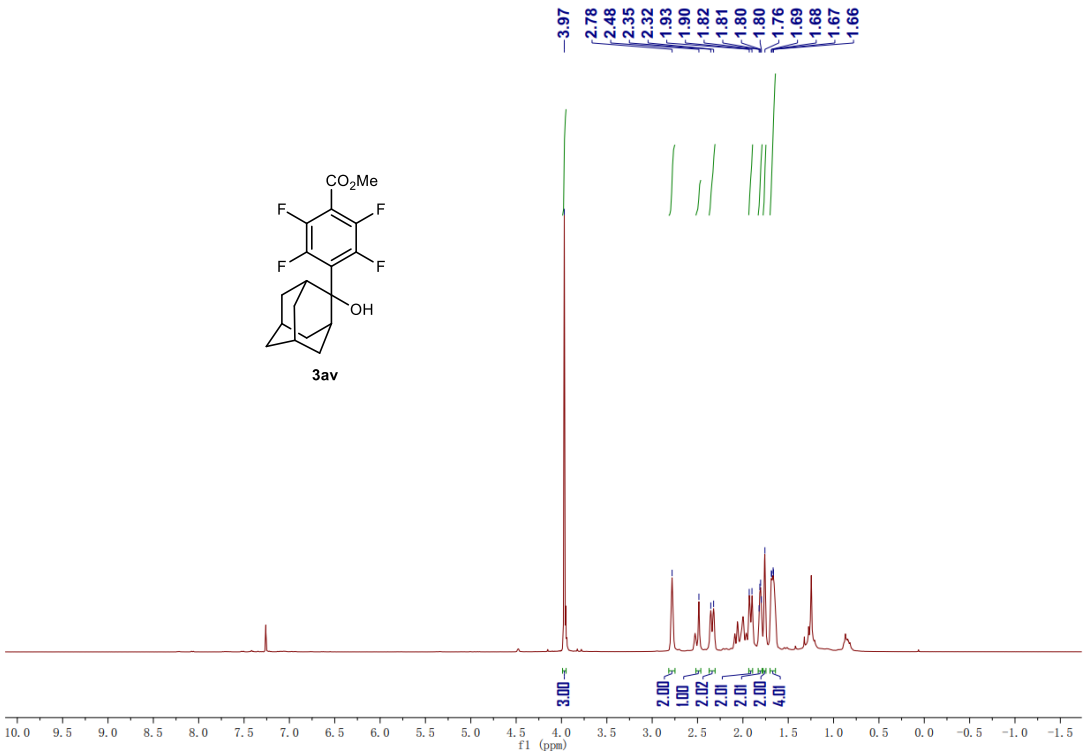
144.03
143.97
143.88
143.82
143.76
143.70
143.66
143.59
143.53
143.50
143.44
143.42
143.37
129.90
129.79
129.68
110.94
110.78
110.63
75.58
75.56
75.55
53.21
36.97
36.93
36.89
25.10
21.35
CO2Me
F
F
F
F
OH
3au
f1 (ppm)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1.80
1.80
1.76
1.69
1.68
1.67
1.66
CO2Me
F
F
F
F
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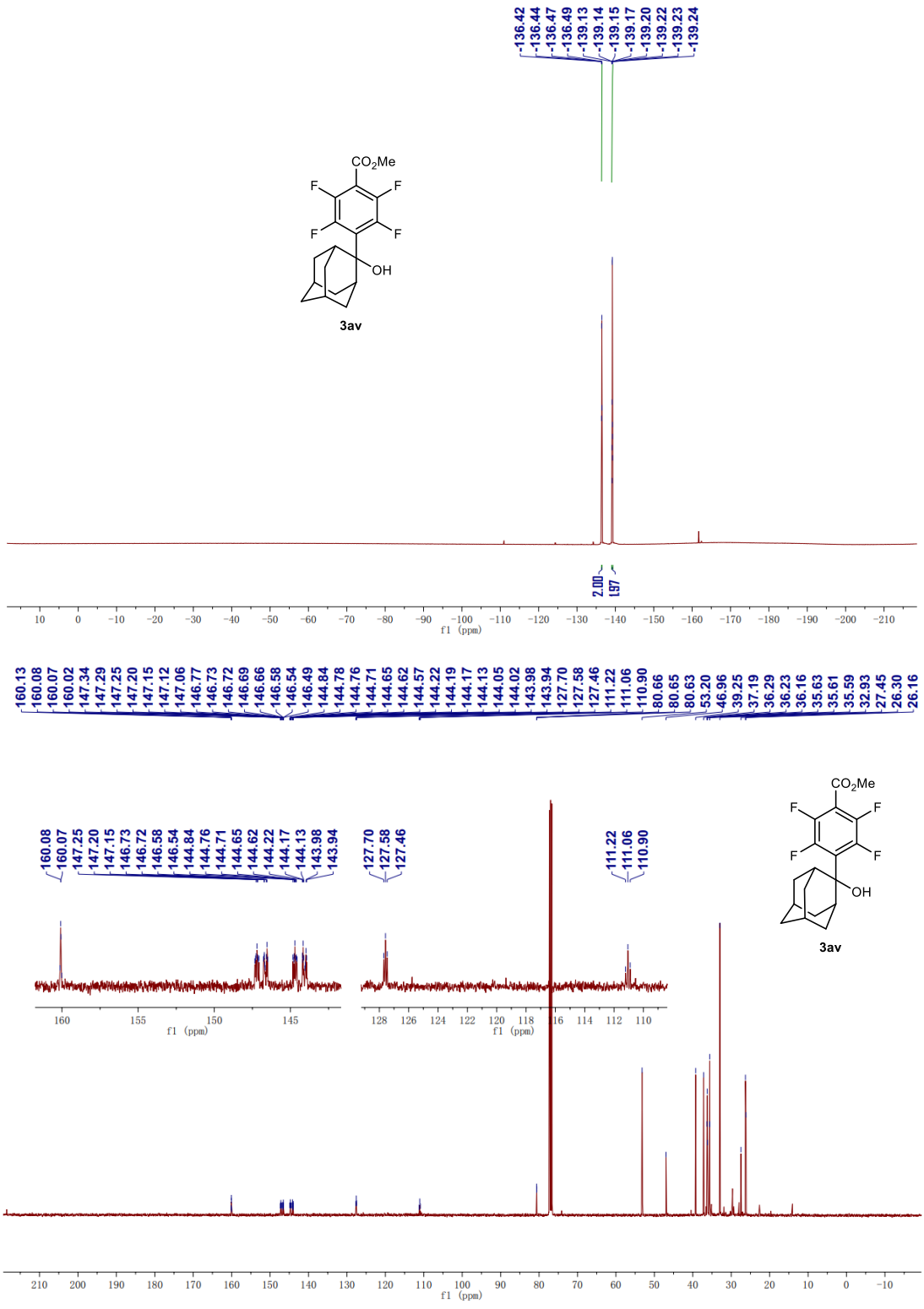
2.00
1.00
2.02
2.01
2.01
2.00
4.01
f1 (ppm)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CO2Me
F
F
F
F
OH
3av
2.00
1.97
f1 (ppm)
160.13
160.08
160.07
160.02
147.34
147.29
147.25
147.20
147.15
147.12
147.06
146.77
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146.66
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146.54
146.49
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144.76
144.71
144.65
144.62
144.22
144.19
144.17
144.13
144.05
144.02
143.98
143.94
127.70
127.58
127.46
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111.06
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80.65
80.63
53.20
46.96
39.25
37.19
36.29
36.23
36.16
35.63
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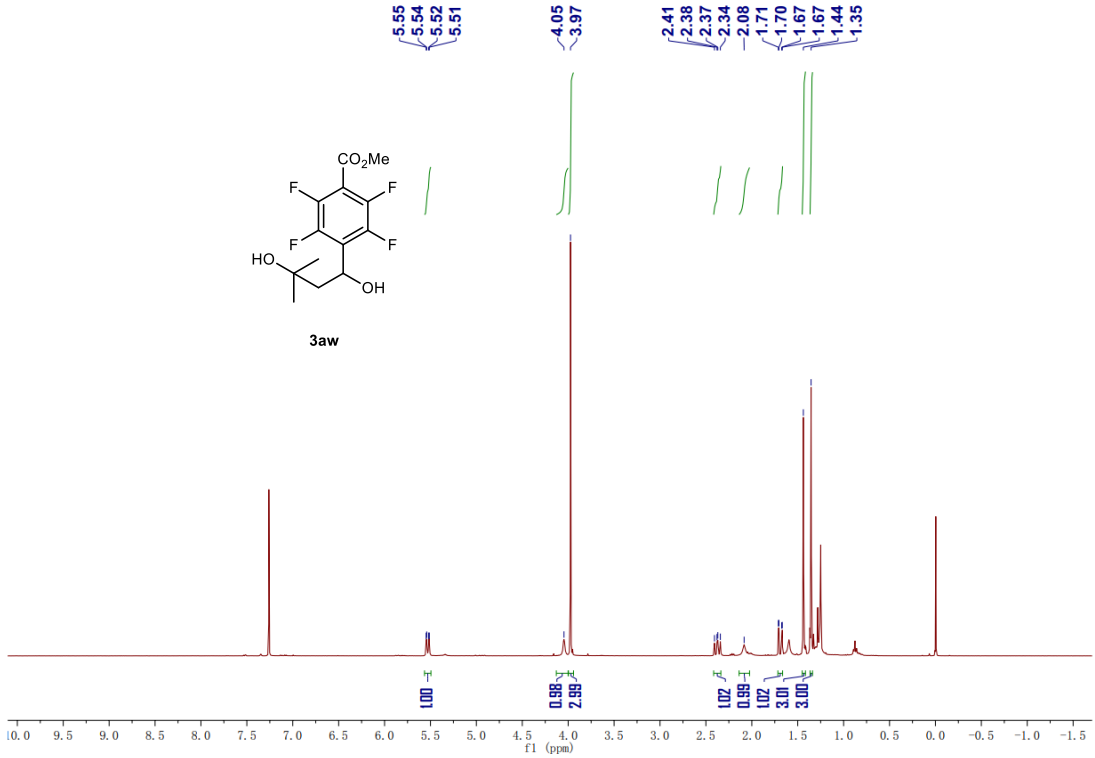
27.45
26.30
26.16
CO2Me
F
F
F
F
OH
3av
f1 (ppm)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2.34
2.08
1.71
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1.67
1.44
1.35
CO2Me
F
F
F
F
HO
OH
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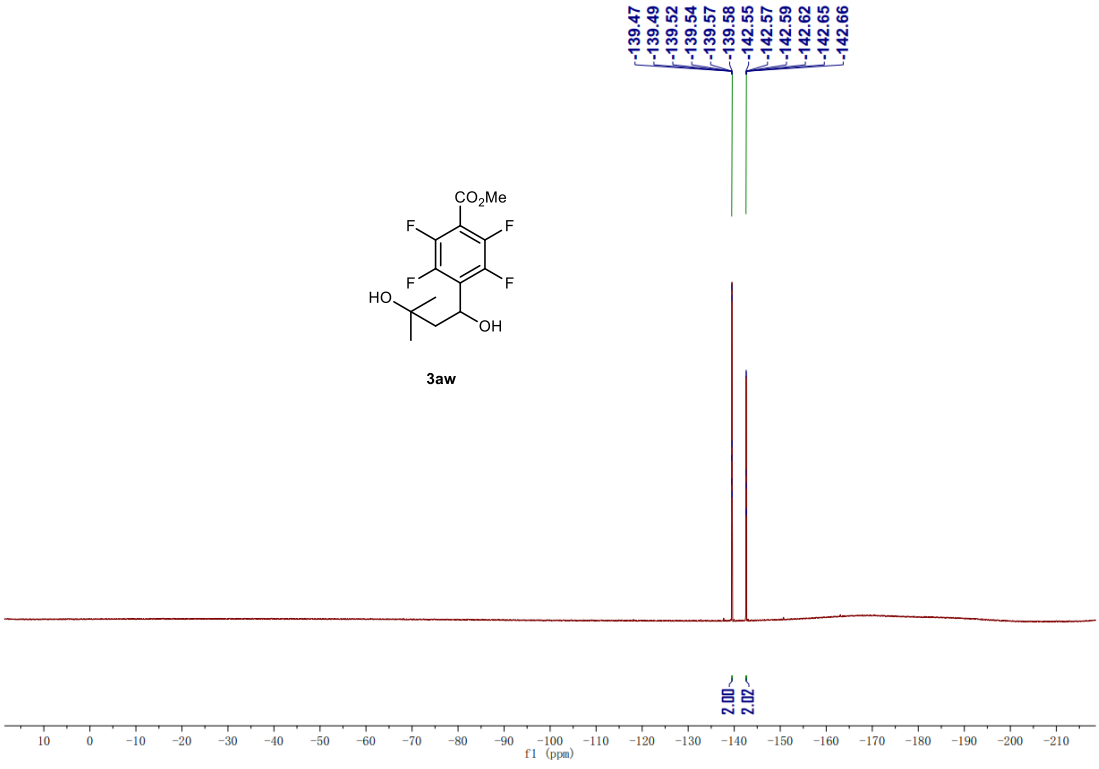
0.98
2.99
1.02
0.99
1.02
3.01
3.00
f1 (ppm)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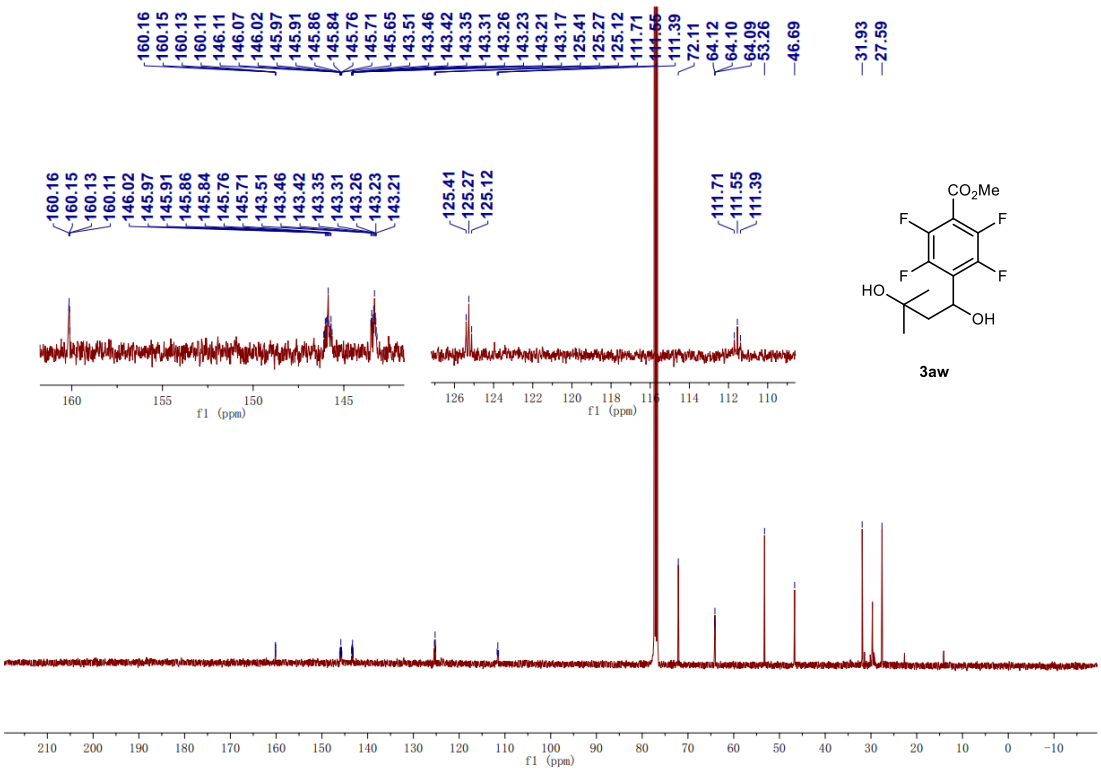
F
HO
OH
3aw
2.00
2.02
f1 (ppm)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72.11
64.12
64.10
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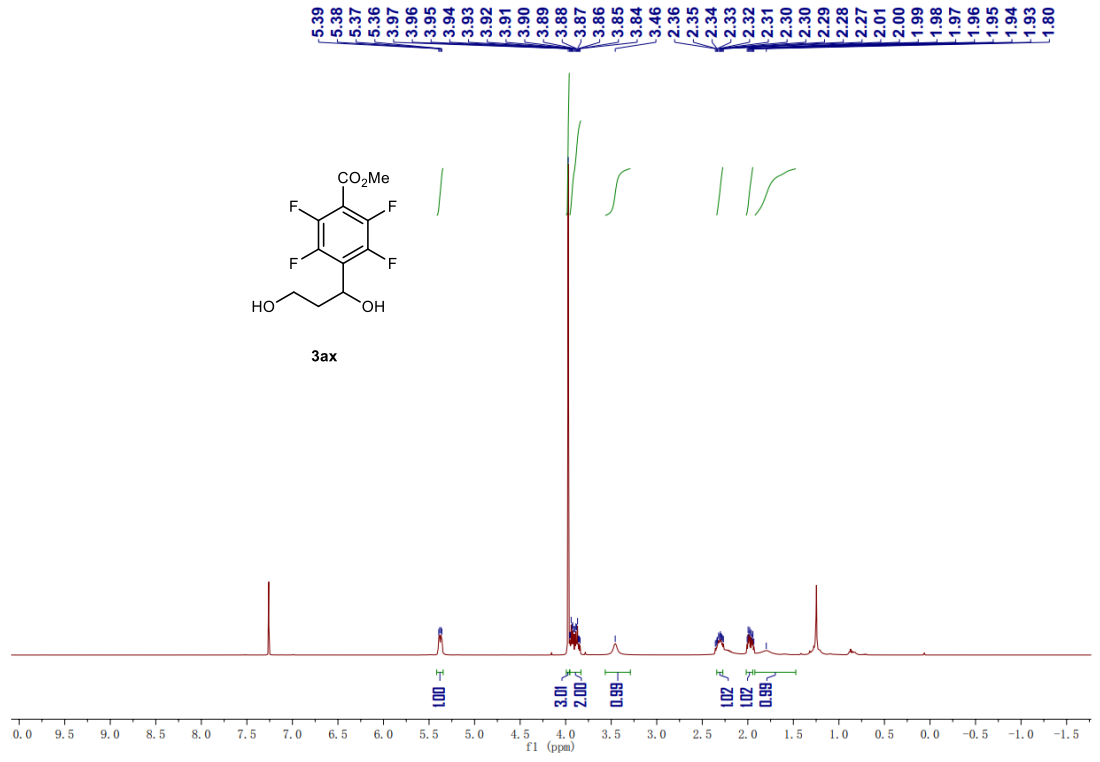
46.69
31.93
27.59
CO2Me
F
F
F
F
HO
OH
3aw
f1 (ppm)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3.89
3.88
3.87
3.86
3.85
3.84
3.46
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2.35
2.34
2.33
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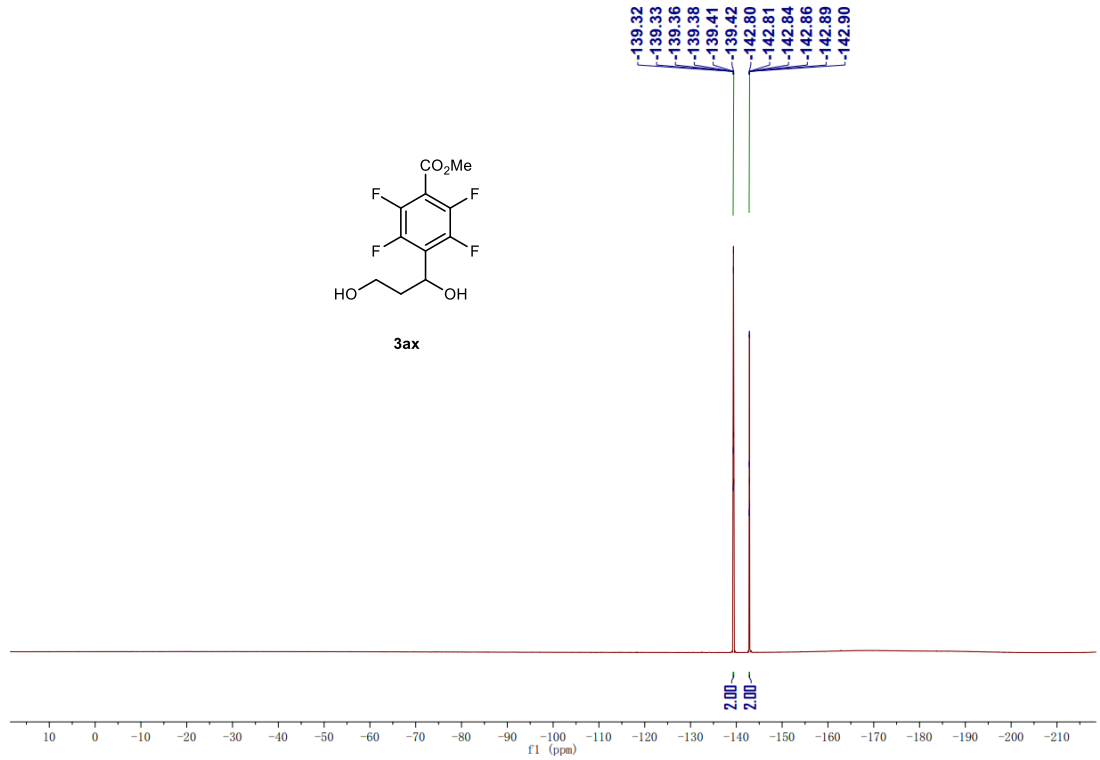
2.30
2.29
2.28
2.27
2.01
2.00
1.99
1.98
1.97
1.96
1.95
1.94
1.93
1.80
CO2Me
F
F
F
F
HO
OH
3ax
1.00
3.01
2.00
0.99
1.02
1.02
0.99
f1 (ppm)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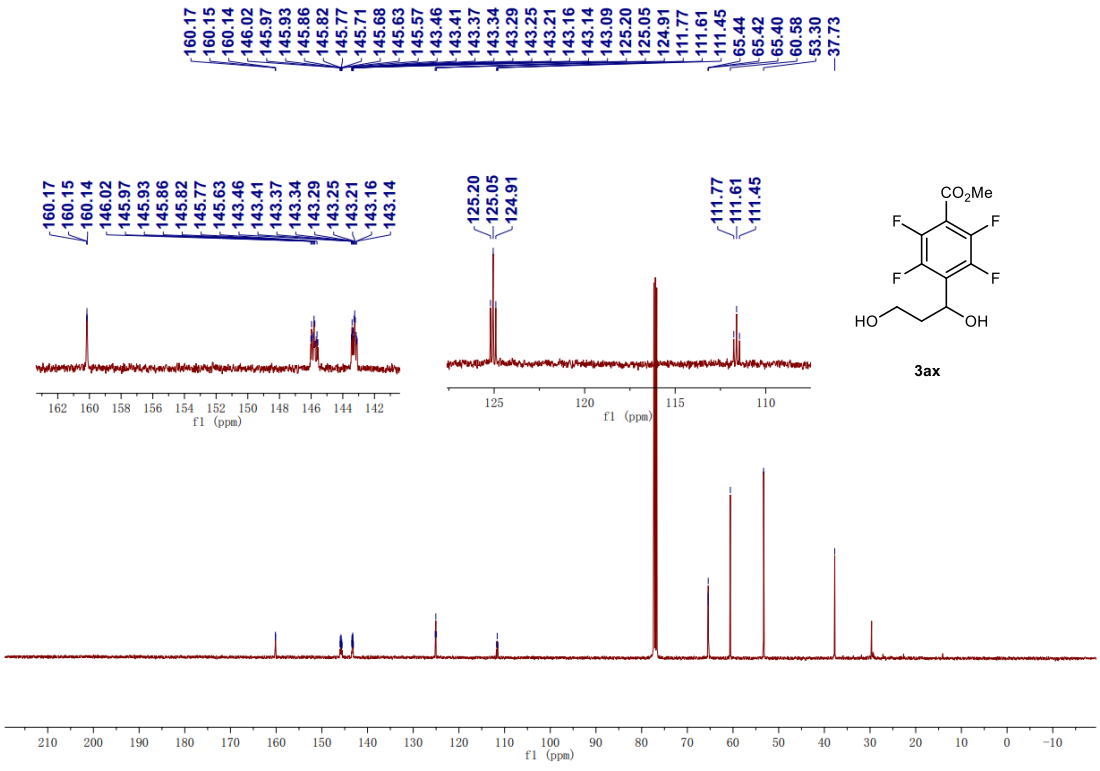
-142.90
CO2Me
F
F
F
F
HO
OH
3ax
2.00
2.00
f1 (ppm)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143.34
143.29
143.25
143.21
143.16
143.14
125.20
125.05
124.91
111.77
111.61
111.45
CO2Me
F
F
F
F
HO
OH
3ax
f1 (ppm)

160.17
160.15
160.14
160.02
145.97
145.93
145.86
145.82
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125.05
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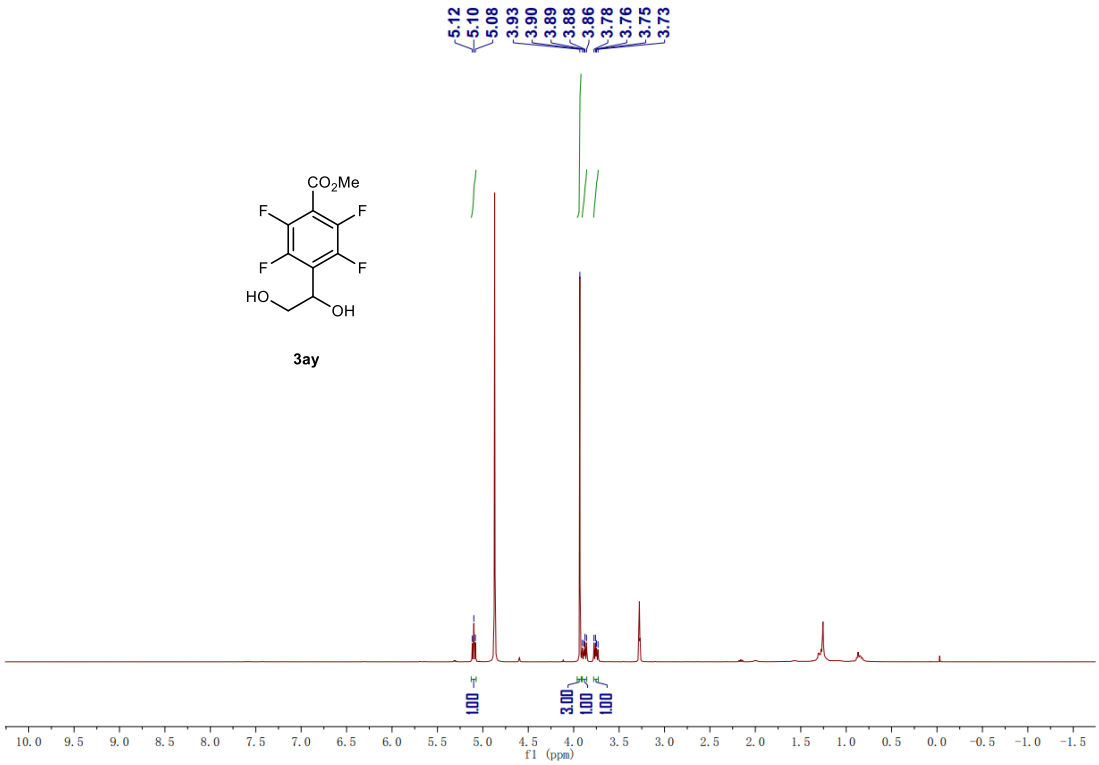
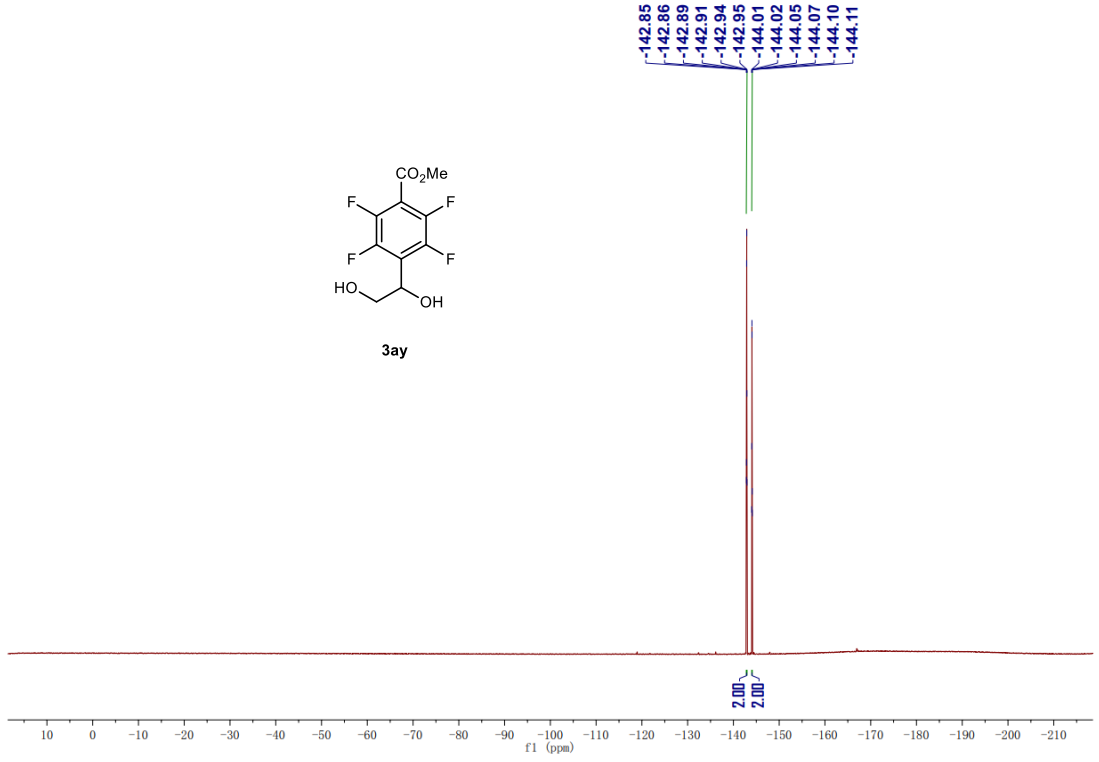
65.42
65.40
60.58
53.30
37.73
f1 (ppm)


5.12
5.10
5.08
3.93
3.90
3.89
3.88
3.86
3.78
3.76
3.75
3.73
CO2Me
F
F
F
F
HO
OH
1.00
3.00
1.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

3ay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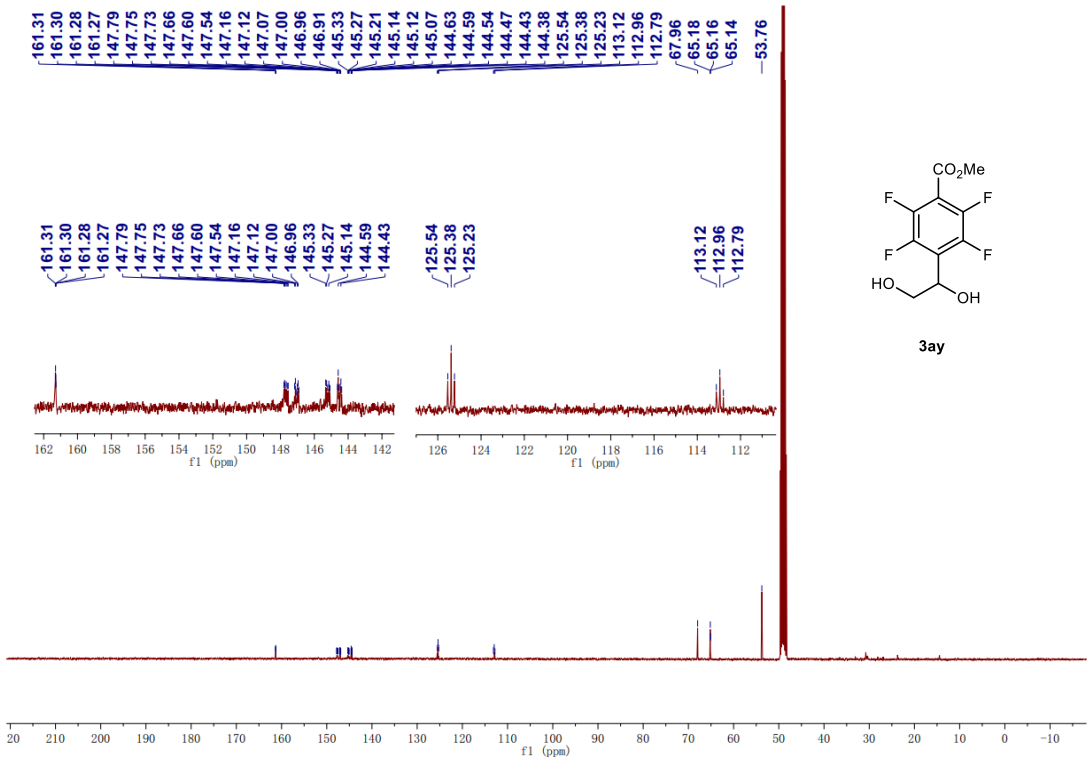
-142.86
-142.89
-142.91
-142.94
-142.95
-144.01
-144.02
-144.05
-144.07
-144.10
-144.11
CO2Me
F
F
F
F
HO
OH
2.00
2.00
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

3ay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161.30
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147.75
147.73
147.66
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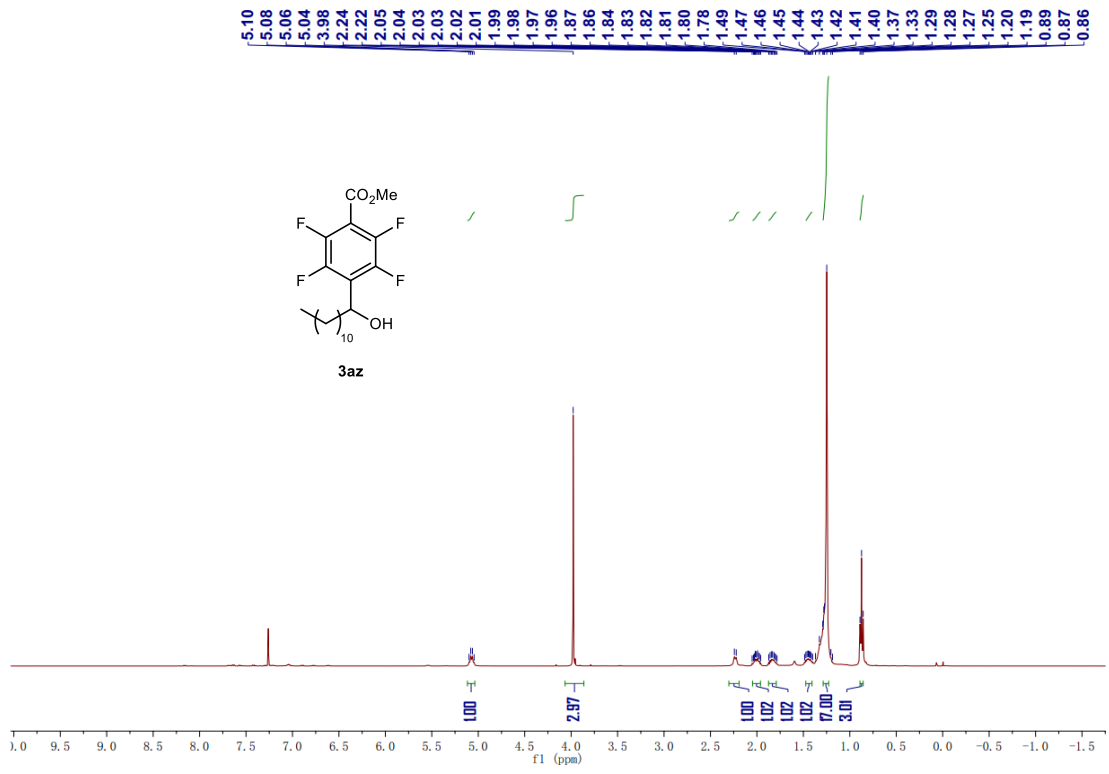
147.54
147.16
147.12
147.07
147.00
146.96
146.91
145.33
145.27
145.21
145.14
145.12
145.07
144.63
144.59
144.54
144.47
144.43
144.38
125.54
125.38
125.23
113.12
112.96
112.79
67.96
65.18
65.16
65.14
53.76
f1 (ppm)

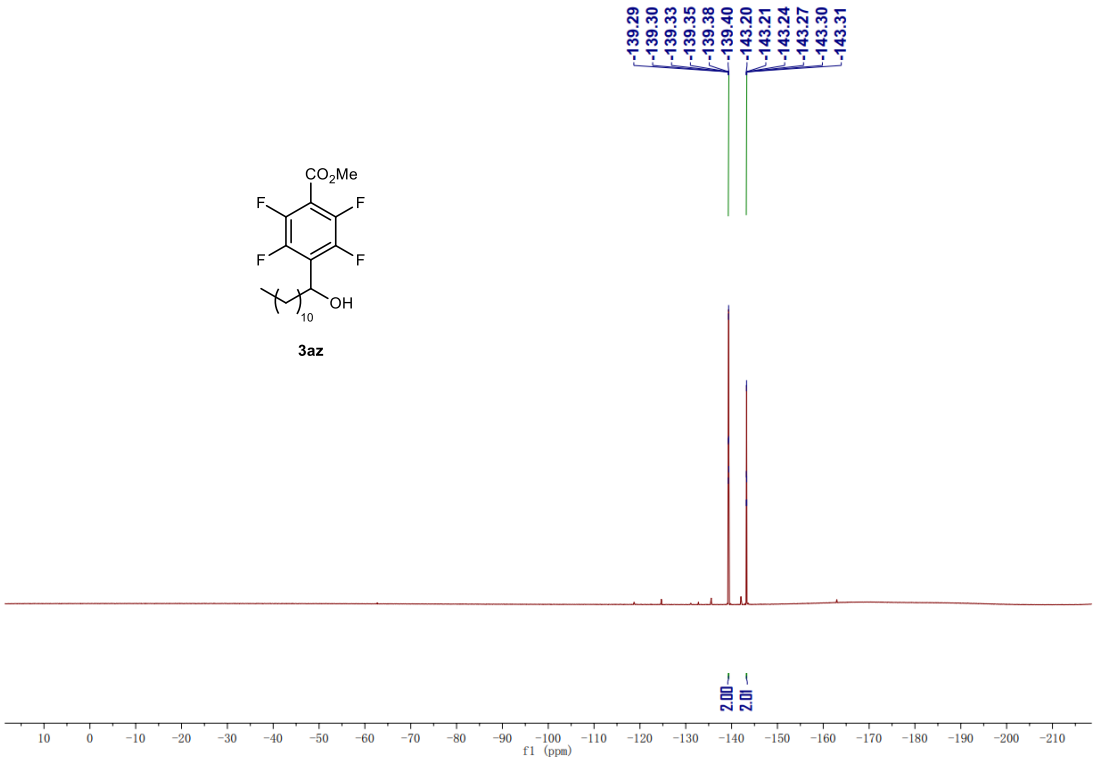
CO2Me
F
F
F
F
HO
OH

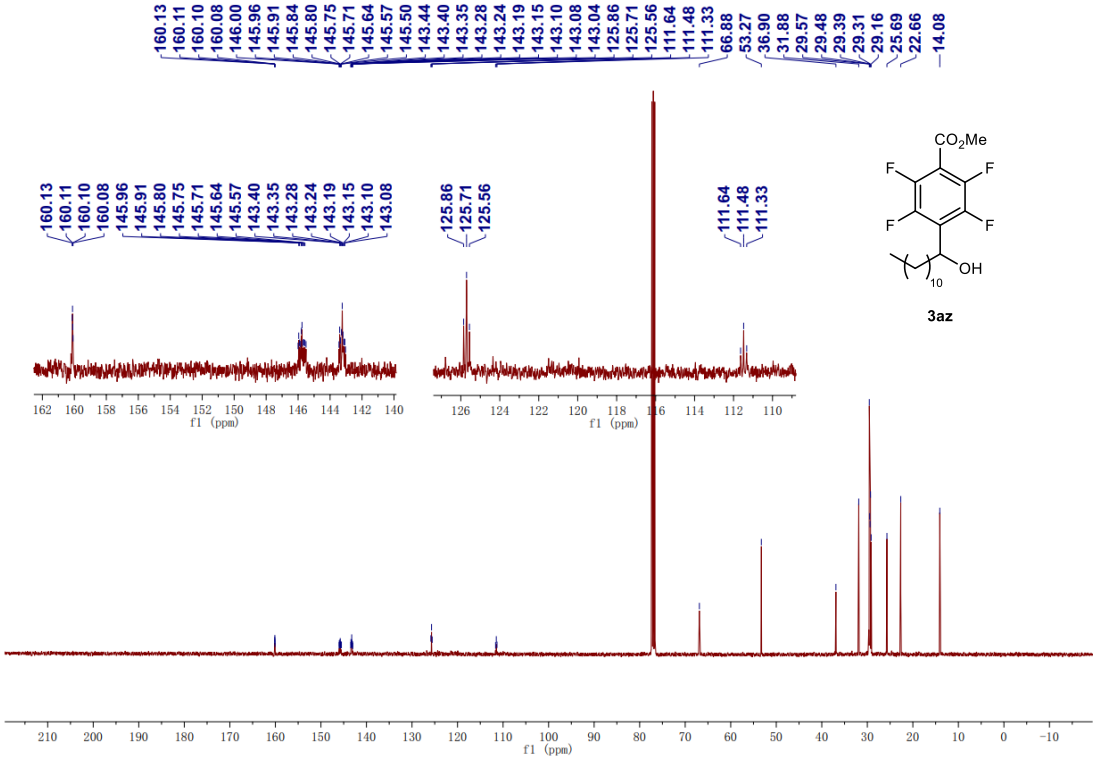
3ay

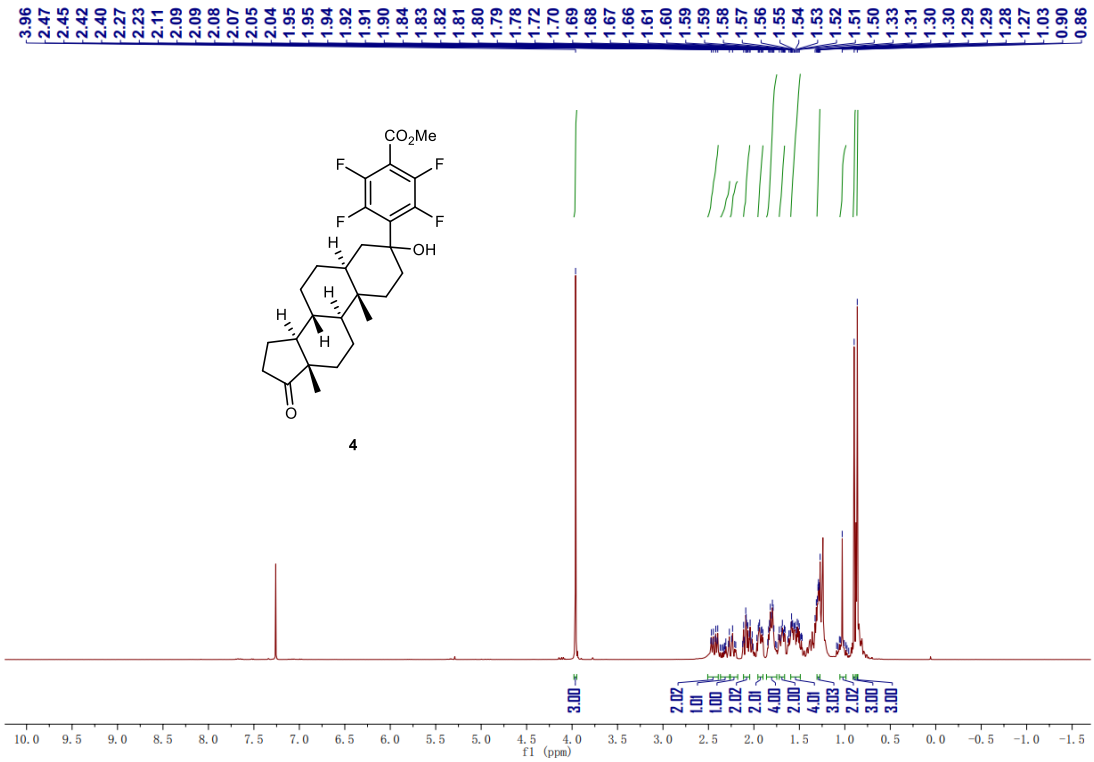

5.10
5.08
5.06
5.04
3.98
2.24
2.22
2.05
2.04
2.03
2.03
2.02
2.01
1.99
1.98
1.97
1.96
1.87
1.86
1.84
1.83
1.82
1.81
1.80
1.78
1.49
1.47
1.46
1.45
1.44
1.43
1.42
1.41
1.40
1.37
1.33
1.29
1.28
1.27
1.25
1.20
1.19
0.89
0.87
0.86
1.00
2.97
1.00
1.02
2.01
2.02
17.00
3.01
f1 (ppm)

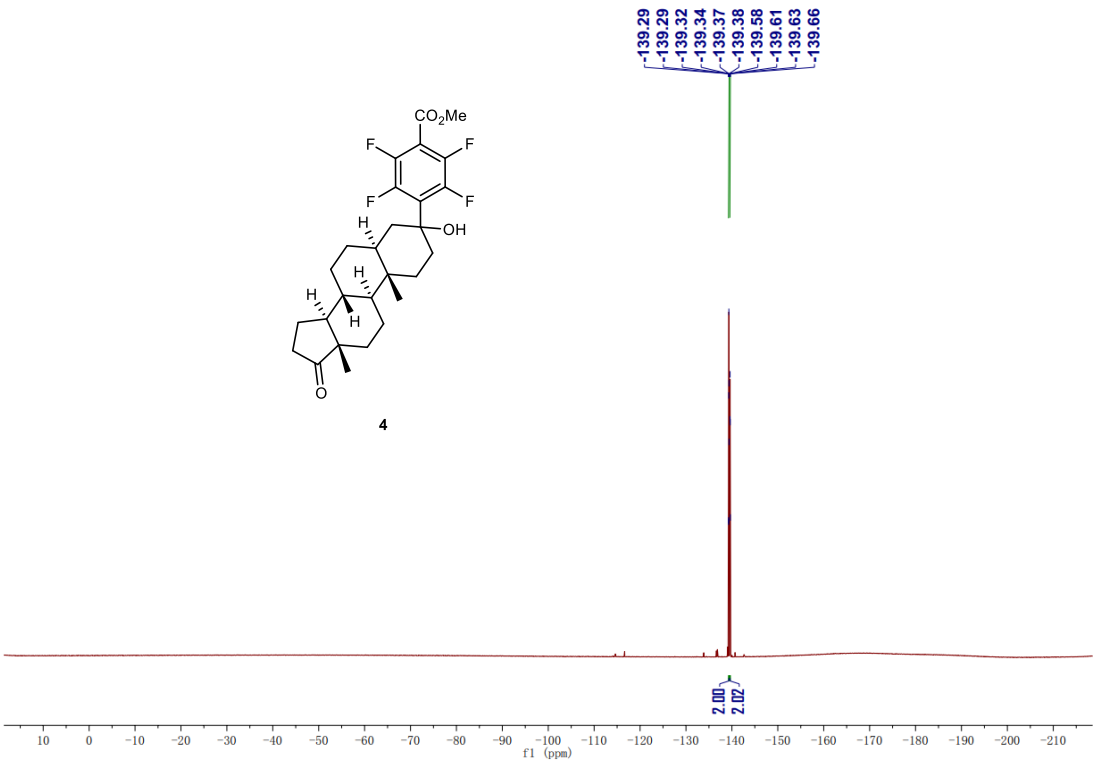
CO2Me
F
F
F
F
OH
10

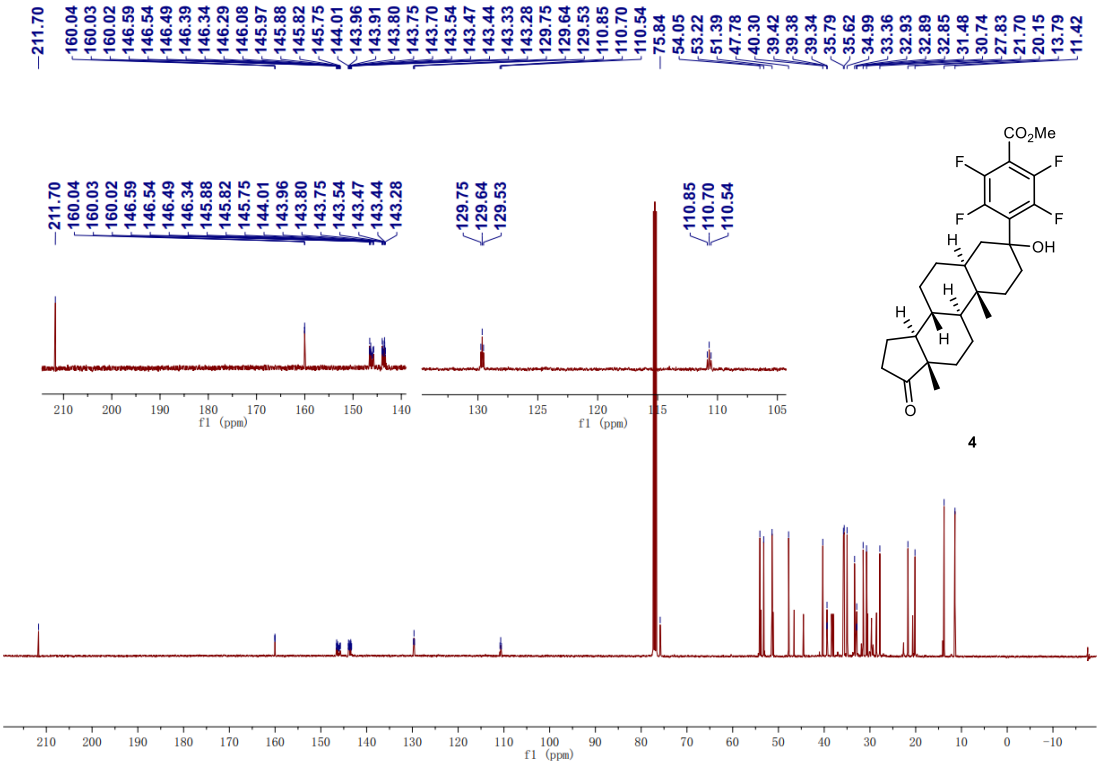
3az

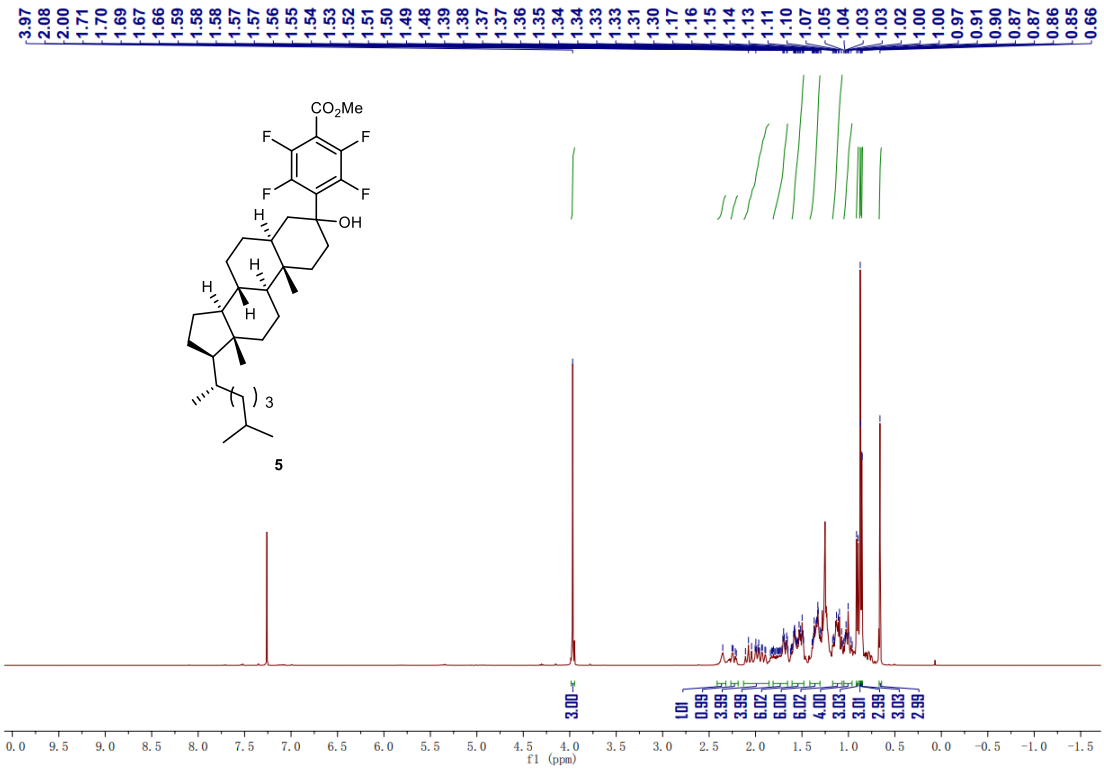

-139.29
-139.30
-139.33
-139.35
-139.38
-139.40
-143.20
-143.21
-143.24
-143.27
-143.30
-143.31
CO2Me
F
F
F
F
OH
10
3az
2.00
2.01
f1 (ppm)

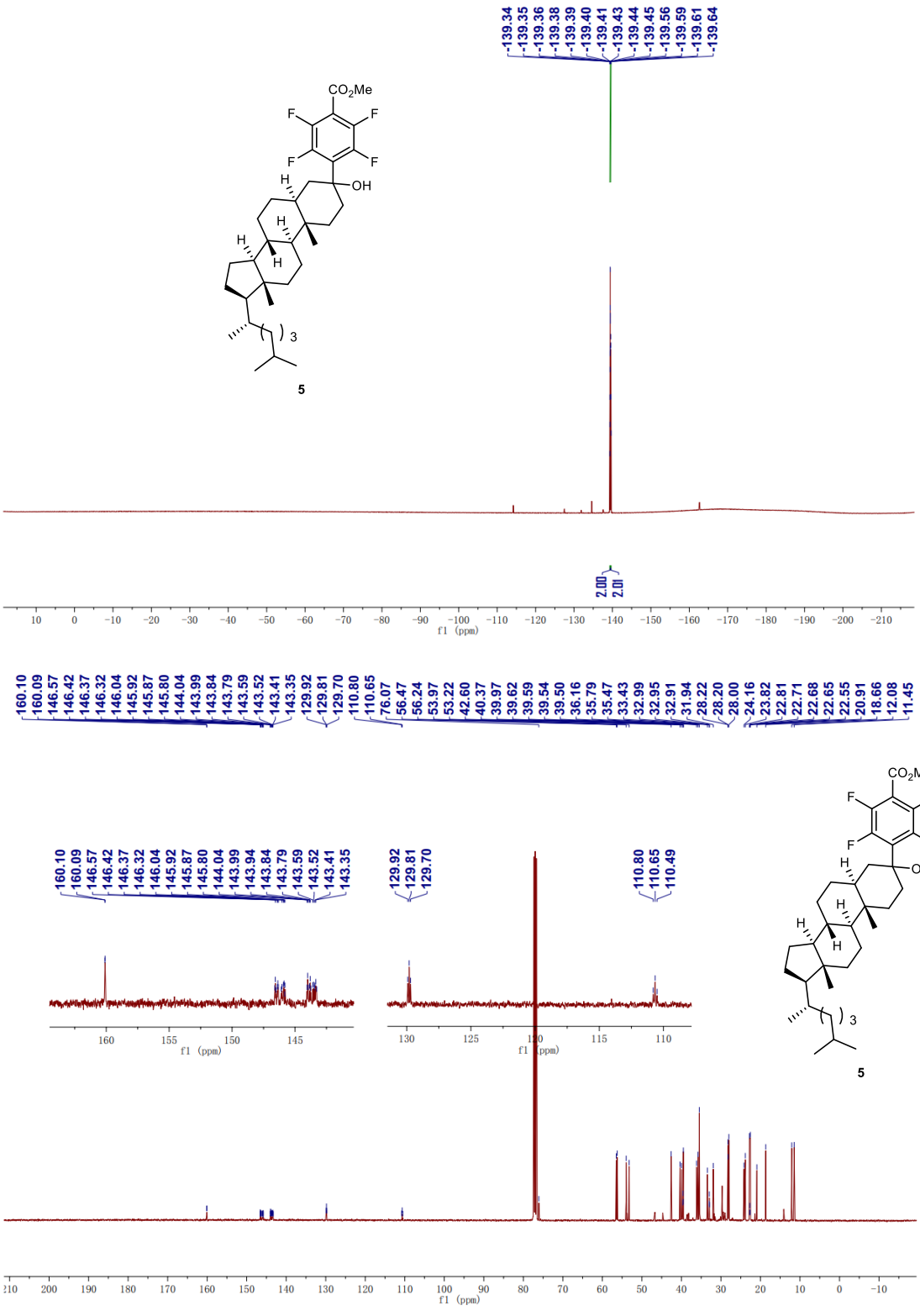

160.13
160.11
160.10
160.08
146.00
145.96
145.91
145.84
145.80
145.75
145.71
145.64
145.57
145.50
143.44
143.40
143.35
143.28
143.24
143.19
143.15
143.10
143.08
143.04
125.86
125.71
125.56
111.64
111.48
111.33
66.88
53.27
36.90
31.88
29.57
29.48
29.39
29.31
29.16
25.69
22.66
14.08
CO2Me
F
F
F
F
OH
10
3az
f1 (ppm)


3.96 2.47 2.45 2.42 2.40 2.27 2.23 2.11 2.09 2.09 2.08 2.07 2.05 2.04 1.95 1.95 1.94 1.92 1.91 1.90 1.84 1.83 1.82 1.81 1.80 1.79 1.78 1.72 1.70 1.69 1.68 1.67 1.66 1.61 1.60 1.59 1.59 1.58 1.57 1.56 1.55 1.54 1.53 1.52 1.51 1.50 1.33 1.31 1.30 1.30 1.29 1.29 1.28 1.27 1.03 0.90 0.86
CO2Me
F
F
F
F
H
OH
H
H
H
O
4
3.00
2.02 1.01 1.00 2.02 2.01 4.00 2.00 4.01 3.03 2.02 3.00 3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)


-139.29 -139.29 -139.32 -139.34 -139.37 -139.38 -139.58 -139.61 -139.63 -139.66
CO2Me
F
F
F
F
H
OH
H
H
H
O
4
2.00 2.02
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


211.70
160.04
160.03
160.02
146.59
146.54
146.49
146.39
146.34
146.29
146.08
145.97
145.88
145.82
145.75
144.01
143.96
143.91
143.80
143.75
143.70
143.54
143.47
143.44
143.33
143.28
129.75
129.64
129.53
110.85
110.70
110.54
75.84
54.05
53.22
51.39
47.78
40.30
39.42
39.38
39.34
35.79
35.62
34.99
33.36
32.93
32.89
32.85
31.48
30.74
27.83
21.70
20.15
13.79
11.42
f1 (ppm)
CO2Me
F
OH
H
O
4


3.97
2.08
2.00
1.71
1.70
1.69
1.67
1.66
1.59
1.58
1.58
1.57
1.57
1.56
1.55
1.54
1.53
1.52
1.51
1.50
1.49
1.48
1.39
1.38
1.37
1.37
1.36
1.35
1.34
1.34
1.33
1.33
1.31
1.30
1.17
1.16
1.15
1.14
1.13
1.11
1.10
1.07
1.05
1.04
1.03
1.03
1.02
1.00
1.00
0.97
0.91
0.90
0.87
0.87
0.86
0.85
0.66
3.00
1.01
0.99
3.99
3.99
6.02
6.00
6.02
4.00
3.03
3.01
2.99
3.03
2.99
f1 (ppm)
CO2Me
F
OH
H
3
5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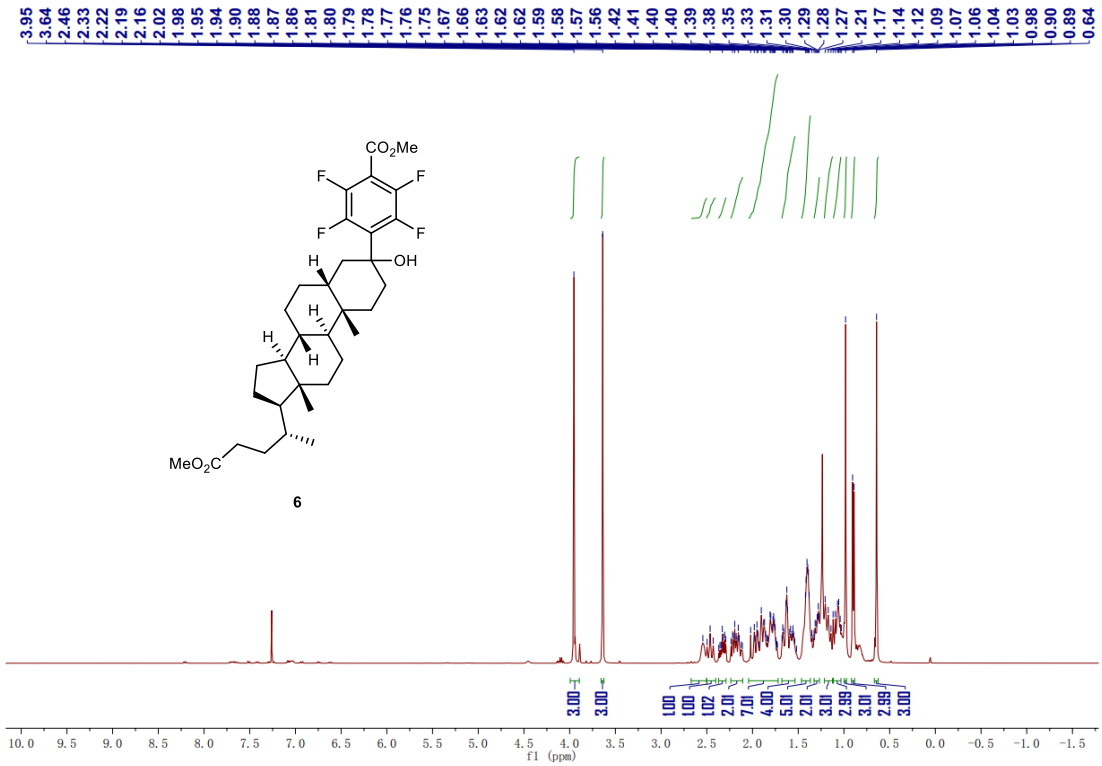
-139.40
-139.41
-139.43
-139.44
-139.45
-139.56
-139.59
-139.61
-139.64
CO2Me
F
F
F
F
H
OH
H
H
H
3
5
2.00
2.01
f1 (ppm)
160.10
160.09
146.57
146.42
146.37
146.32
146.04
145.92
145.87
145.80
144.04
143.99
143.84
143.79
143.59
143.52
143.41
143.35
129.92
129.81
129.70
110.80
110.65
76.07
56.47
56.24
53.97
53.22
42.60
40.37
39.97
39.62
39.59
39.54
39.50
36.16
35.79
35.47
33.43
32.99
32.95
32.91
31.94
28.22
28.20
28.00
24.16
23.82
22.81
22.71
22.68
22.65
22.55
20.91
18.66
12.08
11.45
110.49
f1 (ppm)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-3.64
-2.46
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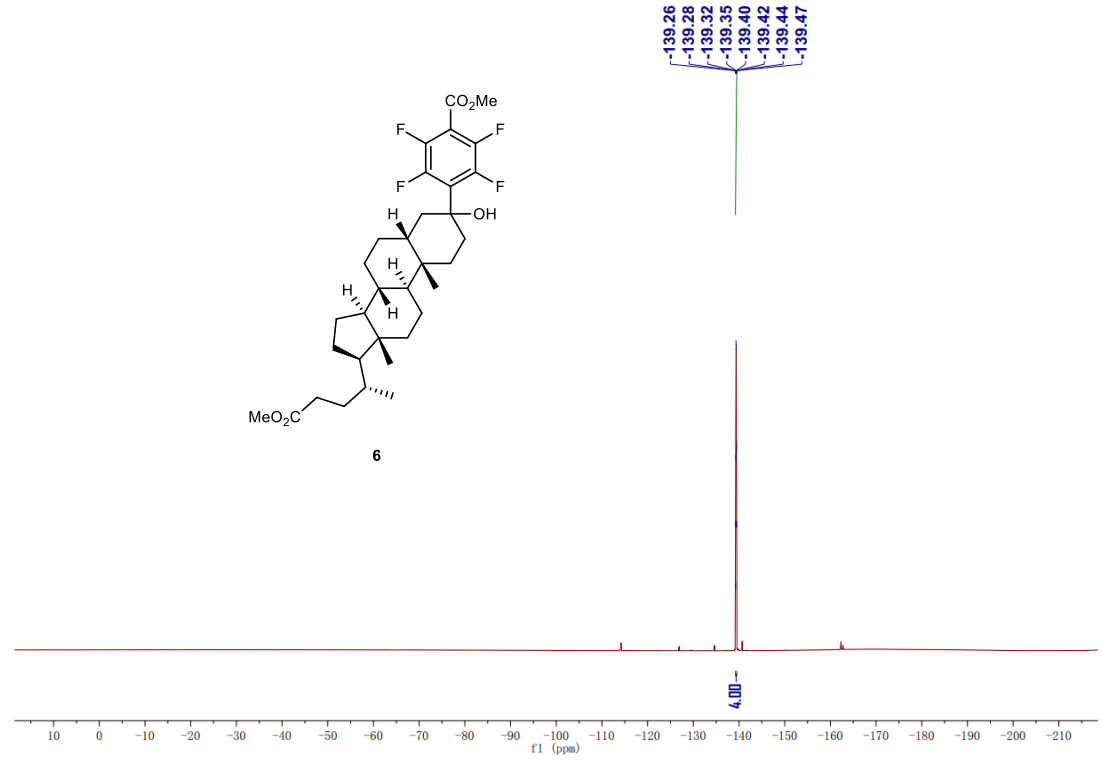
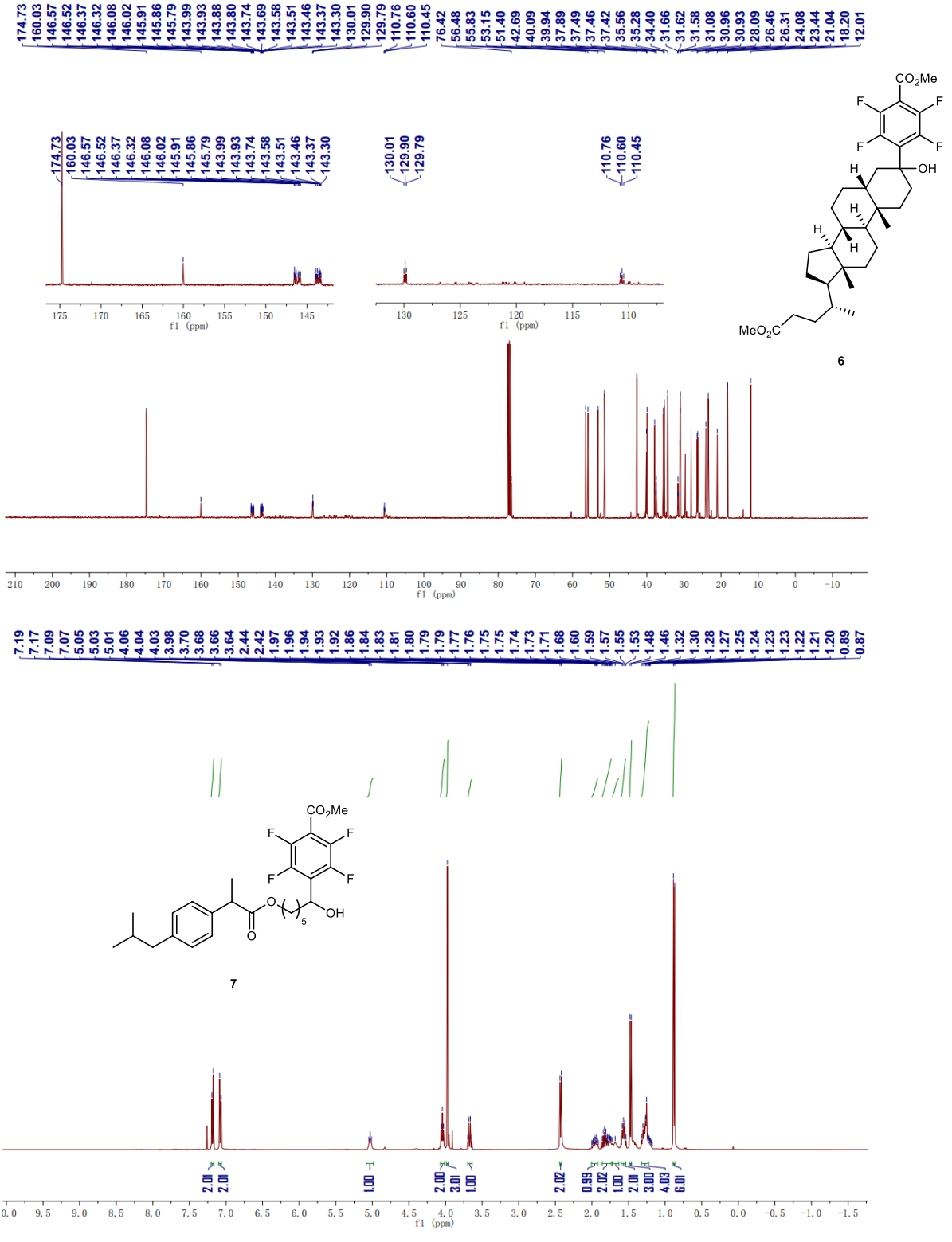
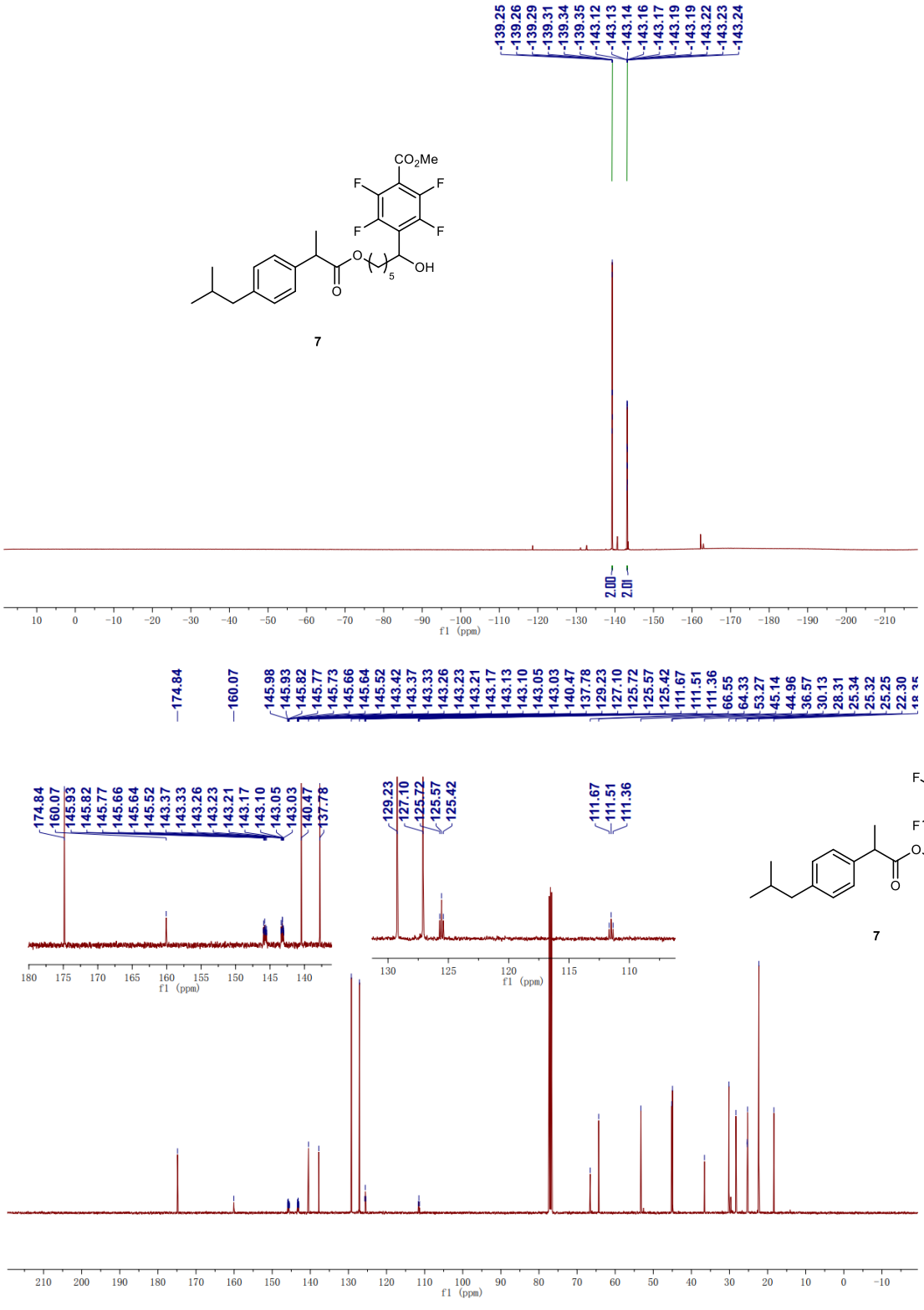
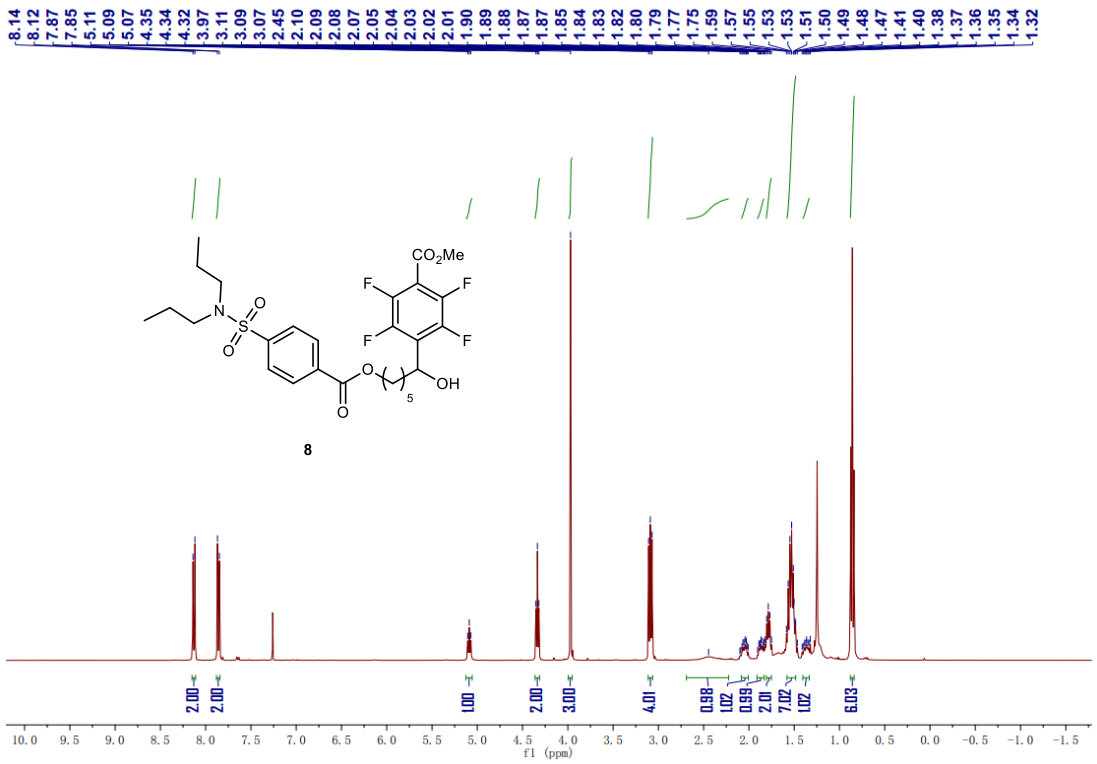
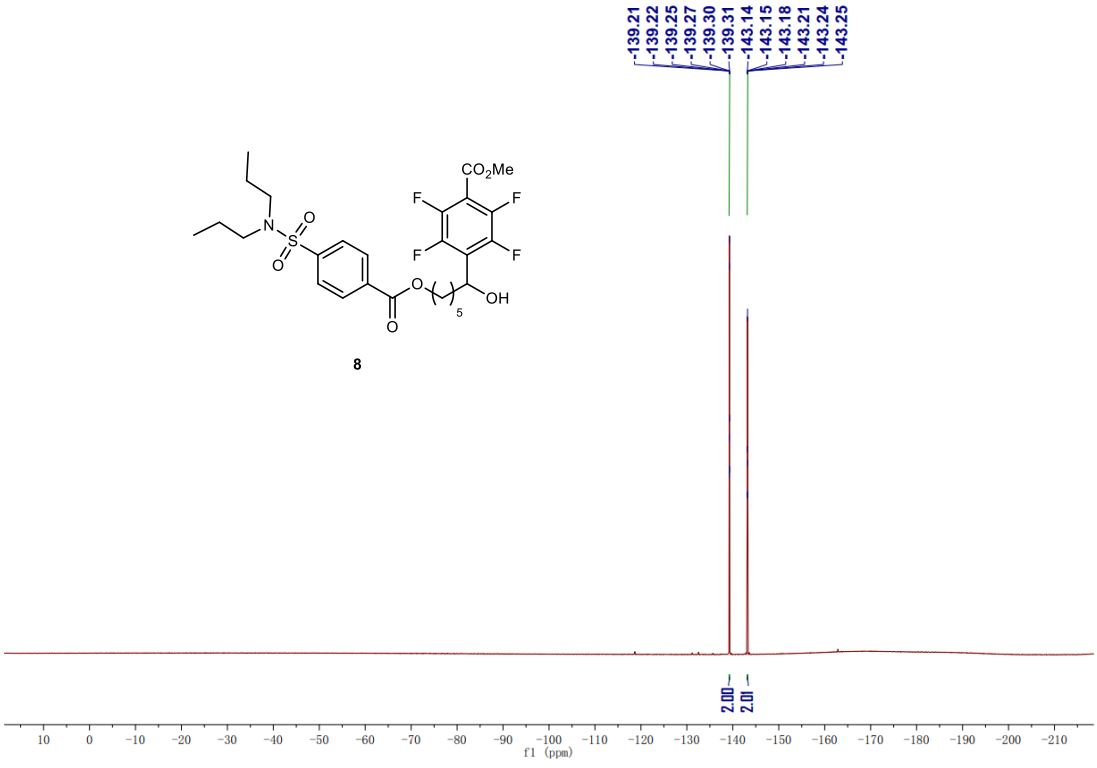
-2.22
-2.19
-2.16
-2.02
-1.98
-1.95
-1.94
-1.90
-1.88
-1.87
-1.86
-1.81
-1.80
-1.79
-1.78
-1.77
-1.76
-1.75
-1.67
-1.66
-1.63
-1.62
-1.62
-1.59
-1.58
-1.57
-1.56
-1.42
-1.41
-1.40
-1.40
-1.39
-1.38
-1.35
-1.33
-1.31
-1.30
-1.29
-1.28
-1.27
-1.21
-1.17
-1.14
-1.12
-1.09
-1.07
-1.06
-1.04
-1.03
-0.98
-0.90
-0.89
-0.64
CO2Me
F
F
F
F
H
OH
H
H
H
MeO2C
6
3.00
3.00
1.00
1.00
1.02
2.01
7.01
4.00
5.01
2.01
3.01
2.99
3.01
2.99
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
f1 (ppm)

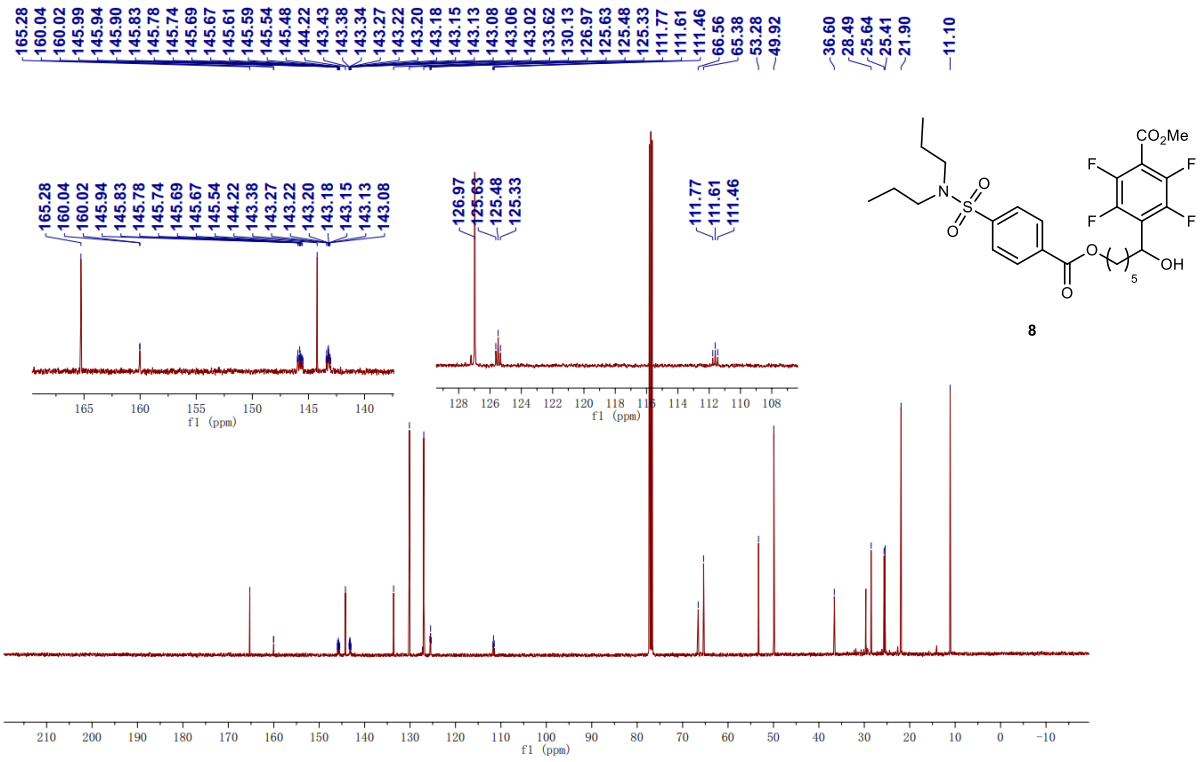

-139.26
-139.28
-139.32
-139.35
-139.40
-139.42
-139.44
-139.47
CO2Me
F
F
F
F
H
OH
H
H
H
MeO2C
6
4.00
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

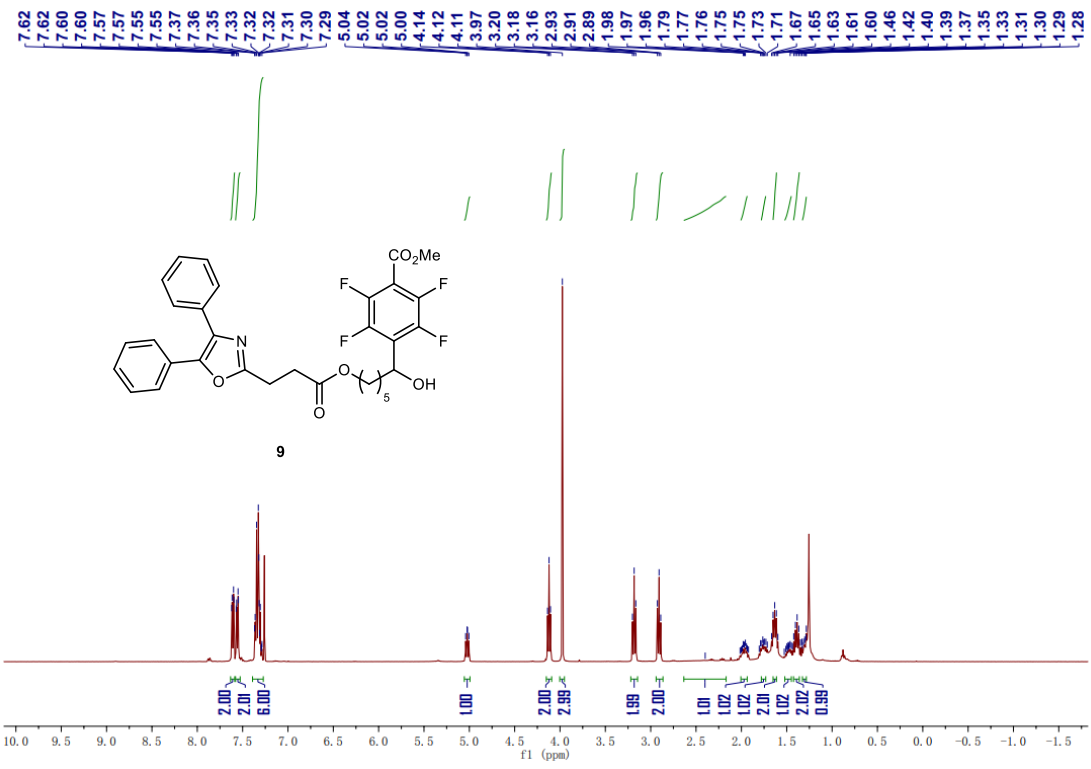

174.73 160.03 146.57 146.52 146.37 146.32 146.08 146.02 145.91 145.86 145.79 143.99 143.93 143.88 143.80 143.74 143.69 143.58 143.51 143.46 143.37 143.30 130.01 129.90 129.79 110.76 110.60 110.45 76.42 56.48 55.83 53.15 51.40 42.69 40.09 39.94 37.89 37.49 37.46 37.42 35.56 35.28 34.40 31.66 31.62 31.58 31.08 30.96 30.93 28.09 26.46 26.31 24.08 23.44 21.04 18.20 12.01
f1 (ppm)
CO2Me
F
F
F
F
H
OH
H
H
H
MeO2C
6
7.19 7.17 7.09 7.07 5.05 5.03 5.01 4.06 4.04 4.03 3.98 3.70 3.68 3.66 3.64 2.44 2.42 1.97 1.96 1.94 1.93 1.92 1.86 1.84 1.83 1.81 1.80 1.79 1.79 1.77 1.76 1.75 1.75 1.74 1.73 1.71 1.68 1.60 1.59 1.57 1.55 1.53 1.48 1.46 1.32 1.30 1.28 1.27 1.25 1.24 1.23 1.23 1.22 1.21 1.20 0.89 0.87
CO2Me
F
F
F
F
O
5
OH
O
7
2.01 2.01 1.00 2.00 3.01 1.00 2.02 0.99 2.02 1.00 2.01 3.00 4.03 6.01
f1 (ppm)

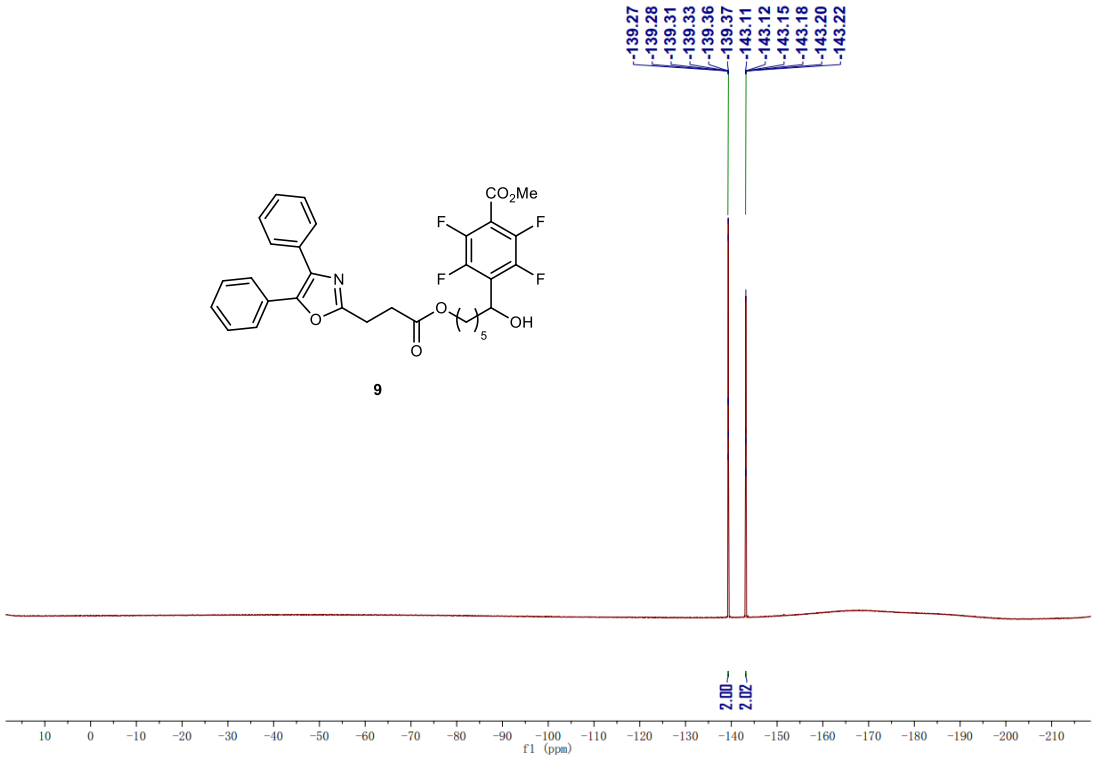

-139.25
-139.26
-139.29
-139.31
-139.34
-139.35
-143.12
-143.13
-143.14
-143.16
-143.17
-143.19
-143.19
-143.22
-143.23
-143.24
CO2Me
F
F
F
F
O
5
OH
O
7
2.00
2.01
f1 (ppm)
174.84
160.07
145.98
145.93
145.82
145.77
145.73
145.66
145.64
145.52
143.42
143.37
143.33
143.26
143.23
143.21
143.17
143.13
143.10
143.05
143.03
140.47
137.78
129.23
127.10
125.72
125.57
125.42
111.67
111.51
111.36
66.55
64.33
53.27
45.14
44.96
36.57
30.13
28.31
25.34
25.32
25.25
22.30
f1 (ppm)


8.14
8.12
7.87
7.85
5.11
5.09
5.07
4.35
4.34
4.32
3.97
3.11
3.09
3.07
2.45
2.10
2.09
2.08
2.07
2.05
2.04
2.03
2.02
2.01
1.90
1.89
1.88
1.87
1.87
1.85
1.84
1.83
1.82
1.80
1.79
1.77
1.75
1.59
1.57
1.55
1.53
1.53
1.51
1.50
1.49
1.48
1.47
1.41
1.40
1.38
1.37
1.36
1.35
1.34
1.32
CO2Me
F
F
F
F
N
S
O
O
O
O
5
OH
8
2.00
2.00
1.00
2.00
3.00
4.01
0.98
1.02
0.99
2.01
7.02
1.02
6.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)

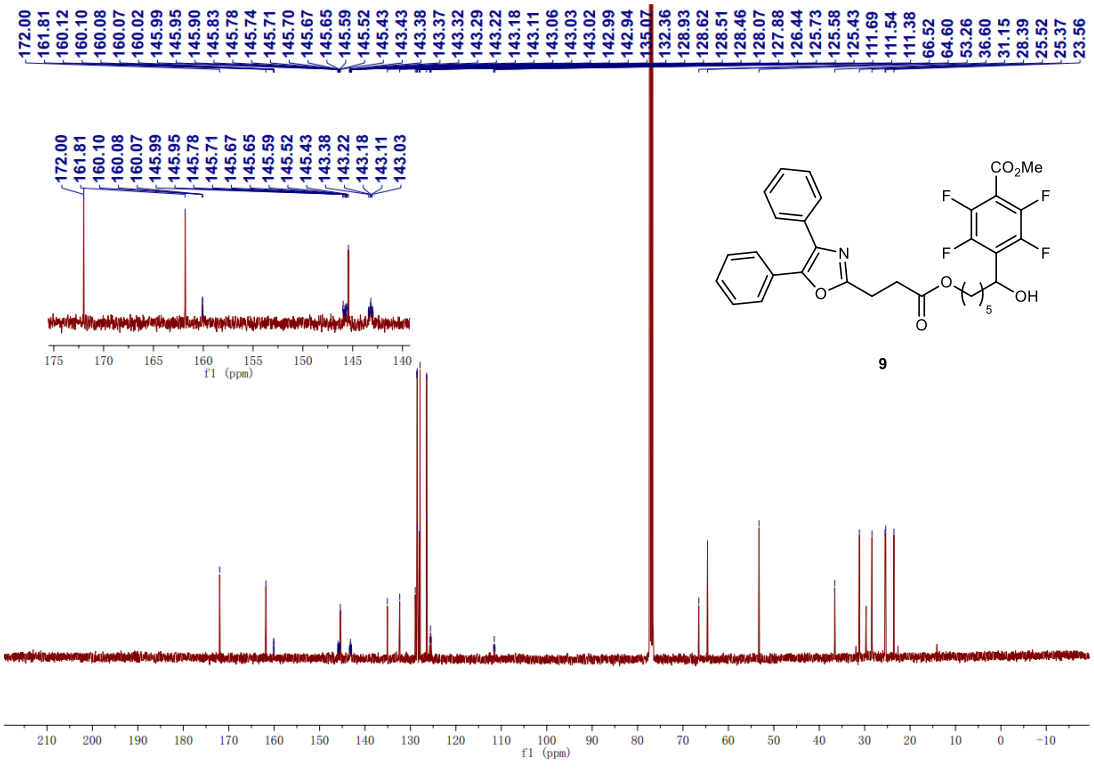

-139.21
-139.22
-139.25
-139.27
-139.30
-139.31
-143.14
-143.15
-143.18
-143.21
-143.24
-143.25
CO2Me
F
F
F
F
N
S
O
O
O
O
5
OH
8
2.00
2.01
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


f1 (ppm)
8

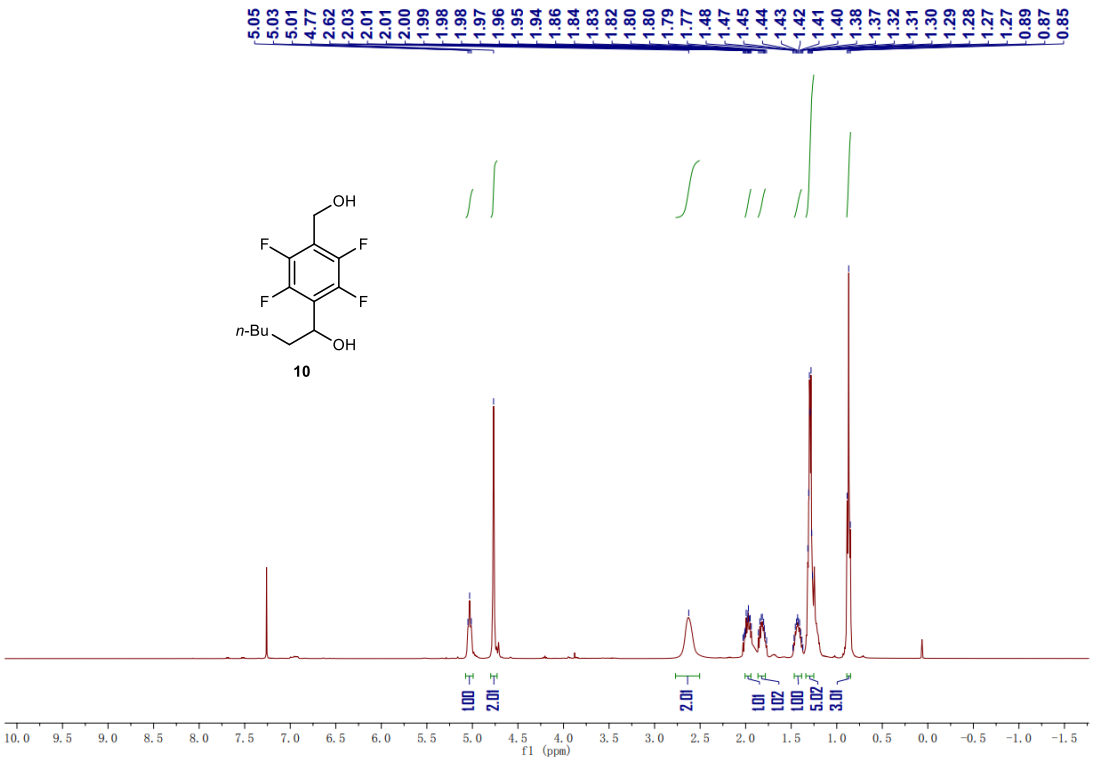

f1 (ppm)
9

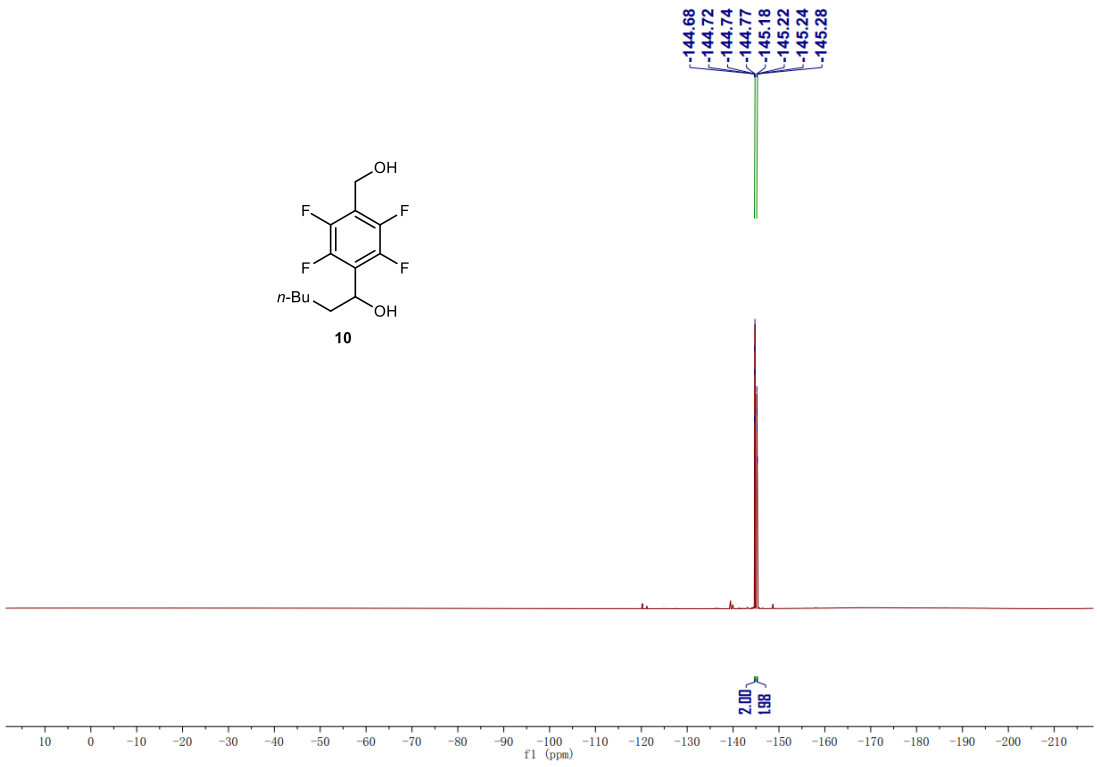

-139.27
-139.28
-139.31
-139.33
-139.36
-139.37
-143.11
-143.12
-143.15
-143.18
-143.20
-143.22
CO2Me
F
F
F
F
N
O
O
O
5
OH
2.00
2.02
f1 (ppm)

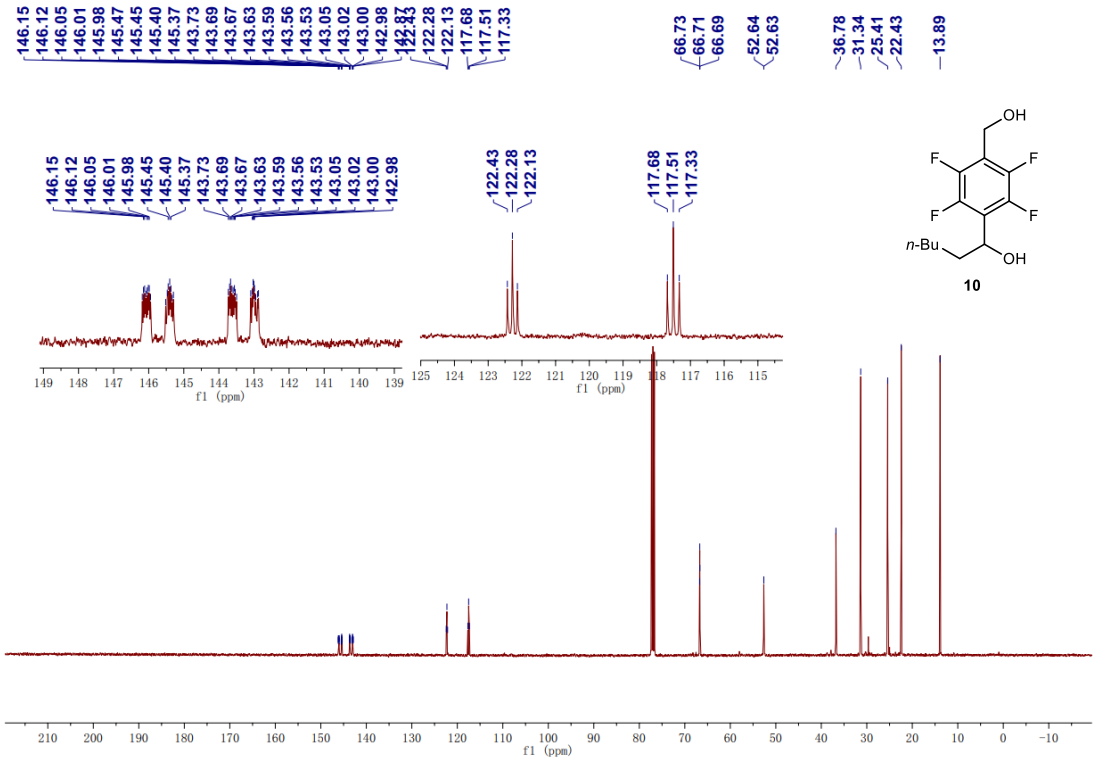
9


172.00
161.81
160.12
160.10
160.08
160.07
160.02
145.99
145.95
145.90
145.83
145.78
145.74
145.71
145.70
145.67
145.65
145.59
145.52
145.43
143.38
143.37
143.32
143.29
143.22
143.18
143.11
143.06
143.03
143.02
142.99
142.94
135.07
132.36
128.93
128.62
128.51
128.46
128.07
127.88
126.44
125.73
125.58
125.43
111.69
111.54
111.38
66.52
64.60
53.26
36.60
31.15
28.39
25.52
25.37
23.56
CO2Me
F
F
F
F
N
O
O
O
5
OH
f1 (ppm)

9


5.05
5.03
5.01
4.77
2.62
2.03
2.01
2.01
2.00
1.99
1.98
1.98
1.97
1.96
1.95
1.94
1.86
1.84
1.83
1.82
1.80
1.80
1.79
1.77
1.48
1.47
1.45
1.44
1.43
1.42
1.41
1.40
1.38
1.37
1.32
1.31
1.30
1.29
1.28
1.27
1.27
0.89
0.87
0.85
OH
F
F
F
F
n-Bu
OH
10
1.00
2.01
2.01
1.01
1.02
1.00
5.02
3.01
f1 (ppm)


-144.68
-144.72
-144.74
-144.77
-145.18
-145.22
-145.24
-145.28
OH
F
F
F
F
n-Bu
OH
10
2.00
1.98
f1 (ppm)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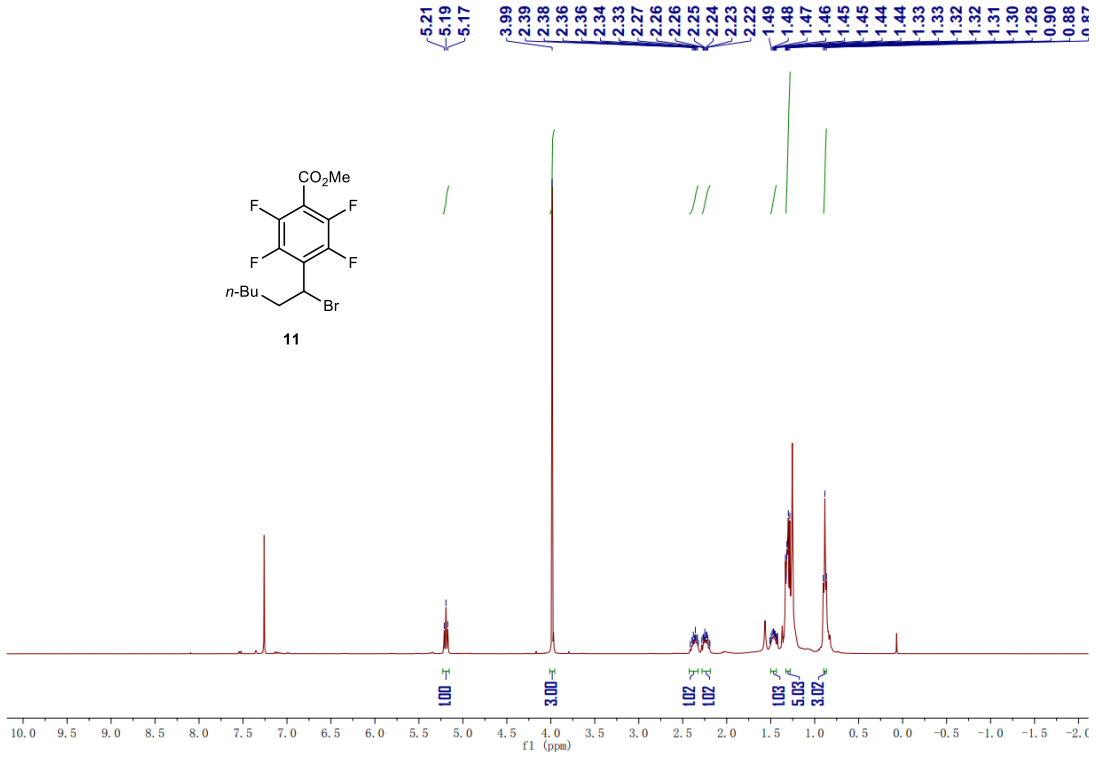
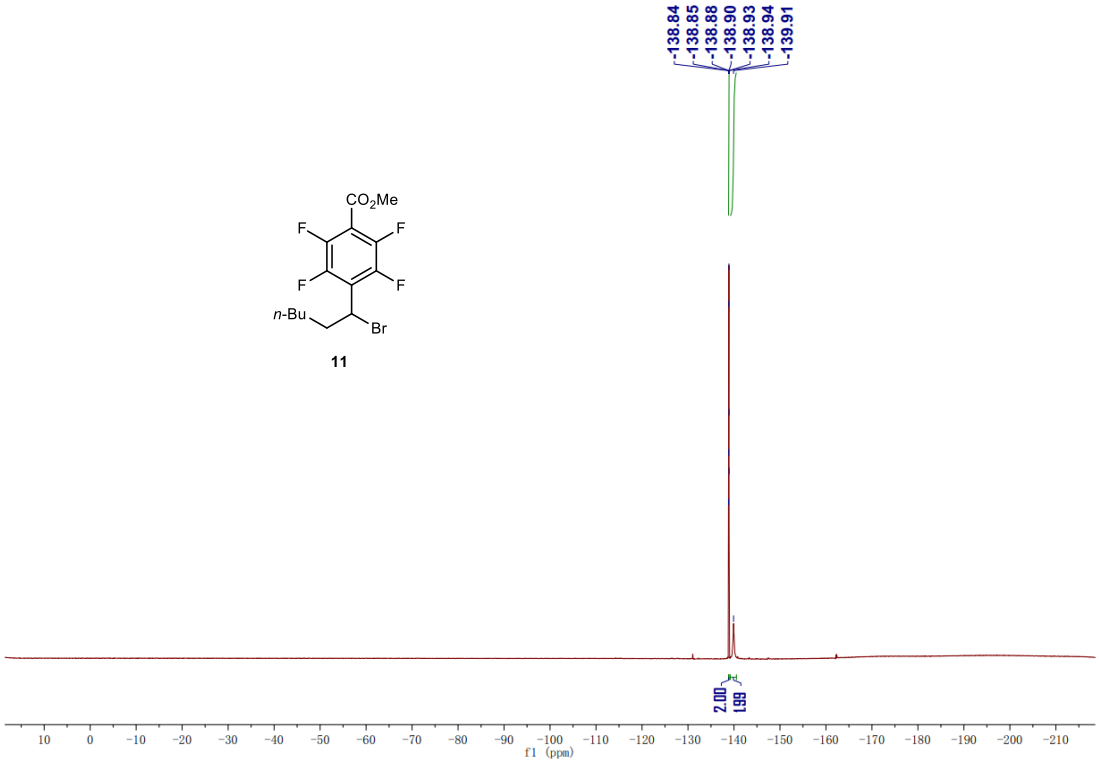
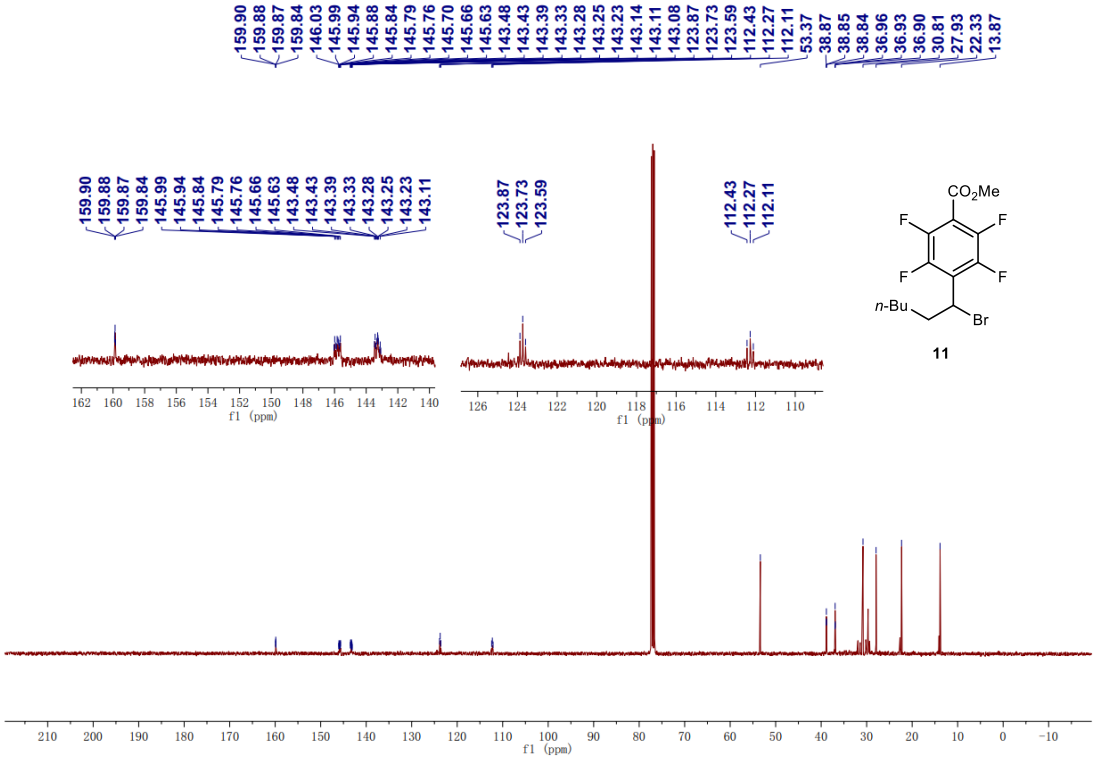
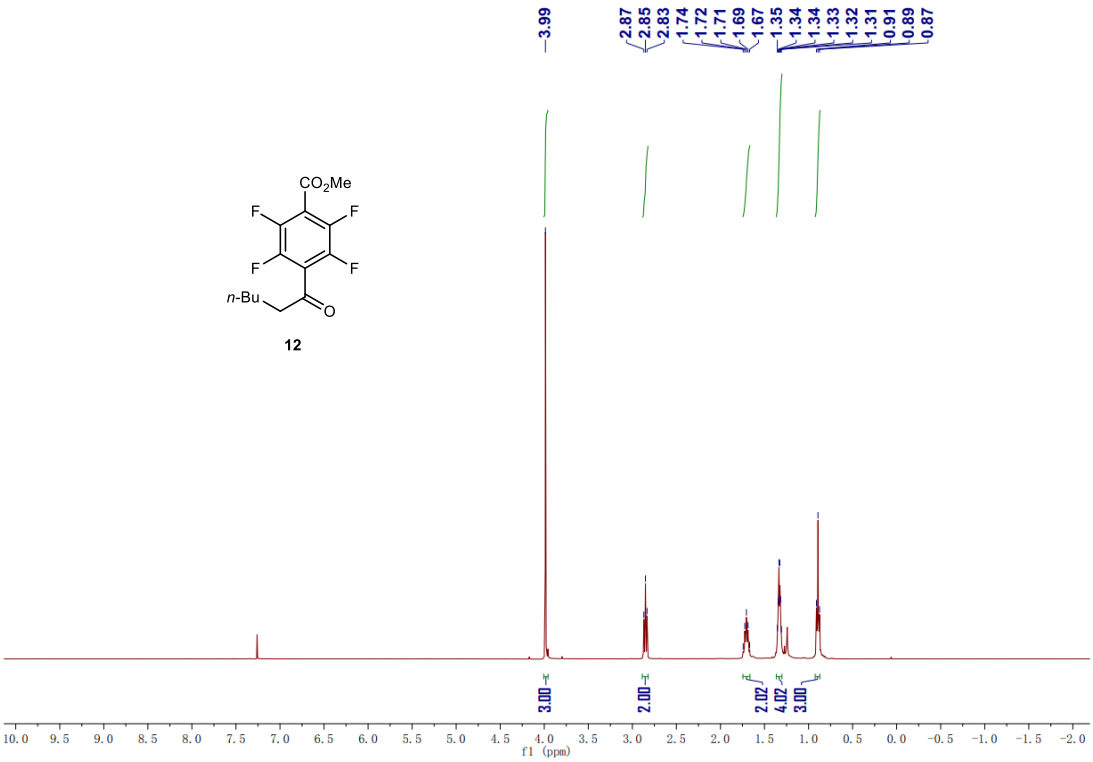
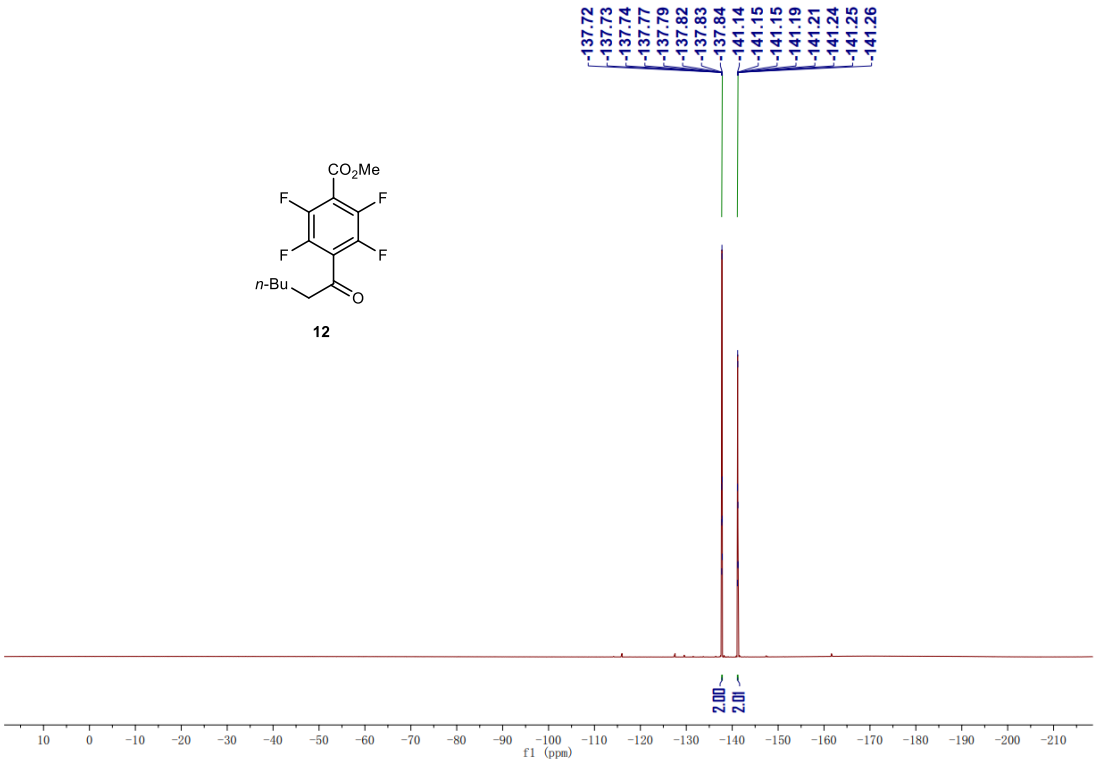
146.12
146.05
146.01
145.98
145.47
145.45
145.40
145.37
143.73
143.69
143.67
143.63
143.59
143.56
143.53
143.05
143.02
143.00
142.98
122.43
122.28
122.13
117.68
117.51
117.33
66.73
66.71
66.69
52.64
52.63
36.78
31.34
25.41
22.43
13.89
OH
F
F
F
F
n-Bu
OH
10
f1 (ppm)

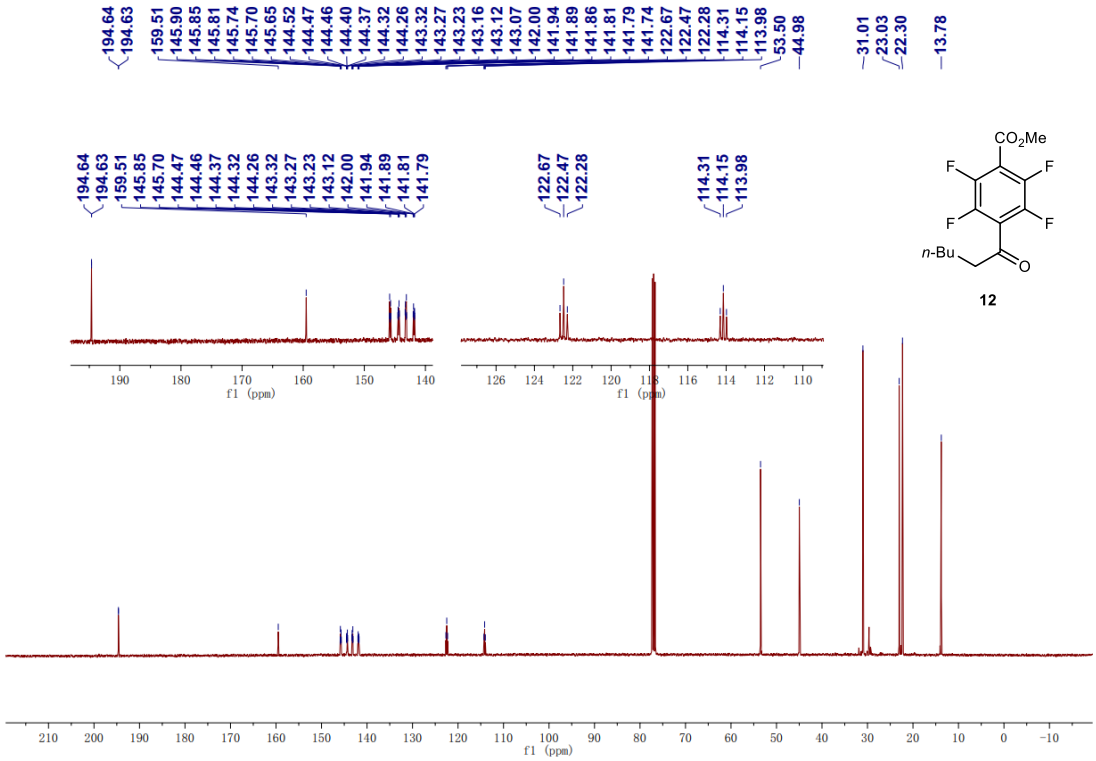

5.21
5.19
5.17
3.99
2.39
2.38
2.36
2.36
2.34
2.33
2.27
2.26
2.26
2.25
2.24
2.23
2.22
1.49
1.48
1.47
1.46
1.45
1.45
1.44
1.44
1.33
1.33
1.32
1.32
1.31
1.30
1.28
0.90
0.88
CO2Me
F
F
F
F
n-Bu
Br
11
1.00
3.00
1.02
1.02
1.03
5.03
3.02
f1 (ppm)

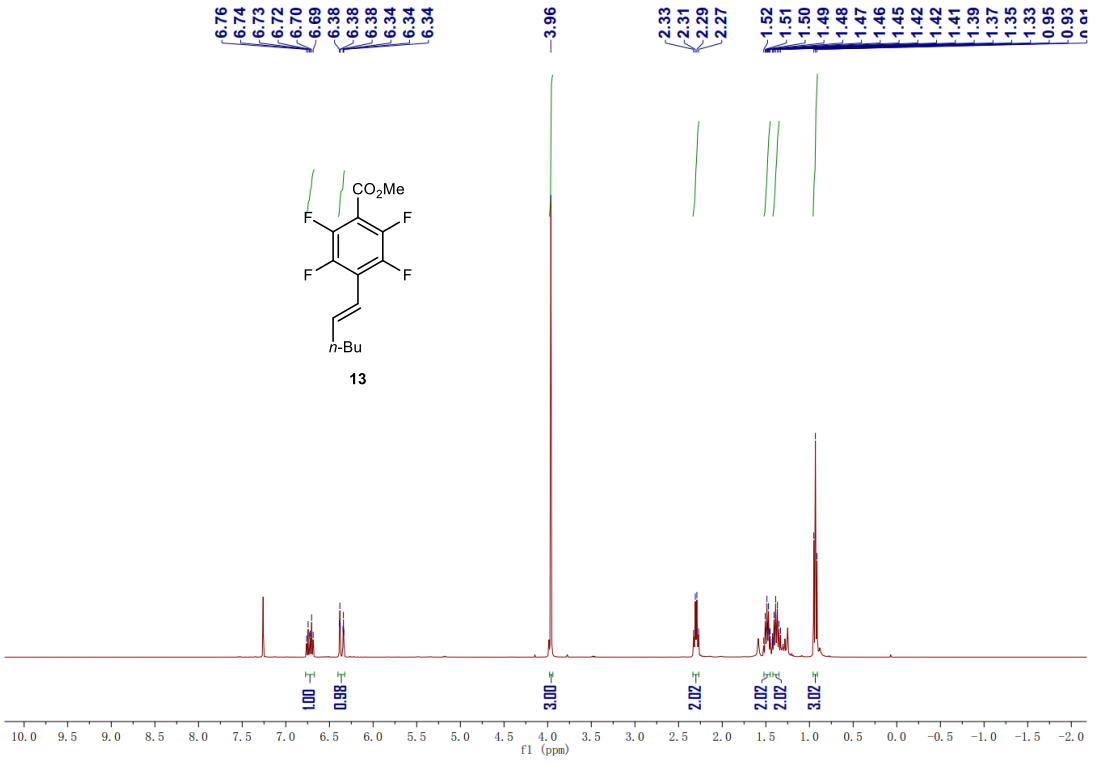

-138.84
-138.85
-138.88
-138.90
-138.93
-138.94
-139.91
CO2Me
F
F
F
F
n-Bu
Br
11
2.00
1.88
f1 (ppm)

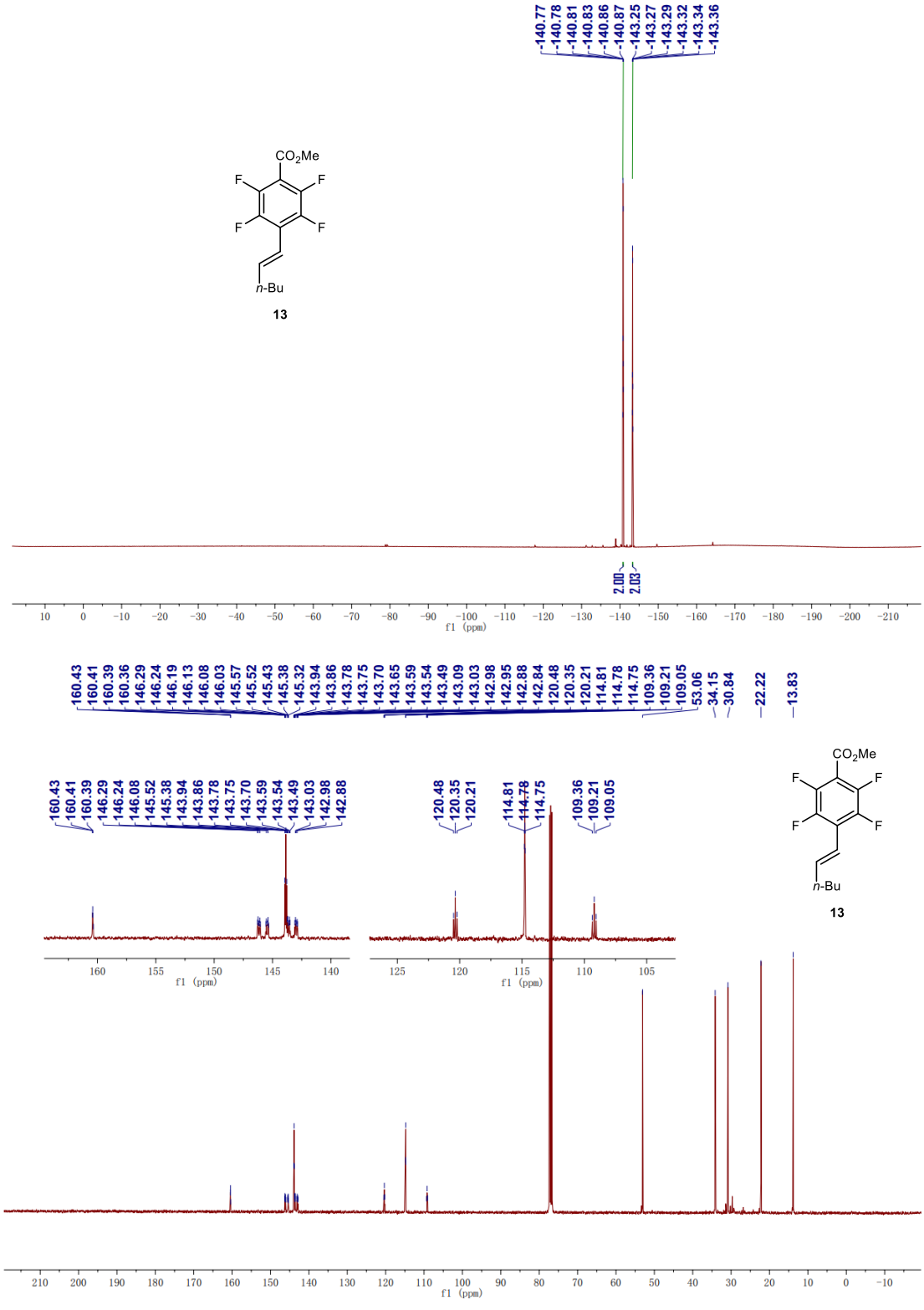

159.90
159.88
159.87
159.84
146.03
145.99
145.94
145.88
145.84
145.79
145.76
145.70
145.66
145.63
143.48
143.43
143.39
143.33
143.28
143.25
143.23
143.14
143.11
143.08
123.87
123.73
123.59
112.43
112.27
112.11
53.37
38.87
38.85
38.84
36.96
36.93
36.90
30.81
27.93
22.33
13.87
CO2Me
F
F
F
F
n-Bu
Br
11
f1 (ppm)

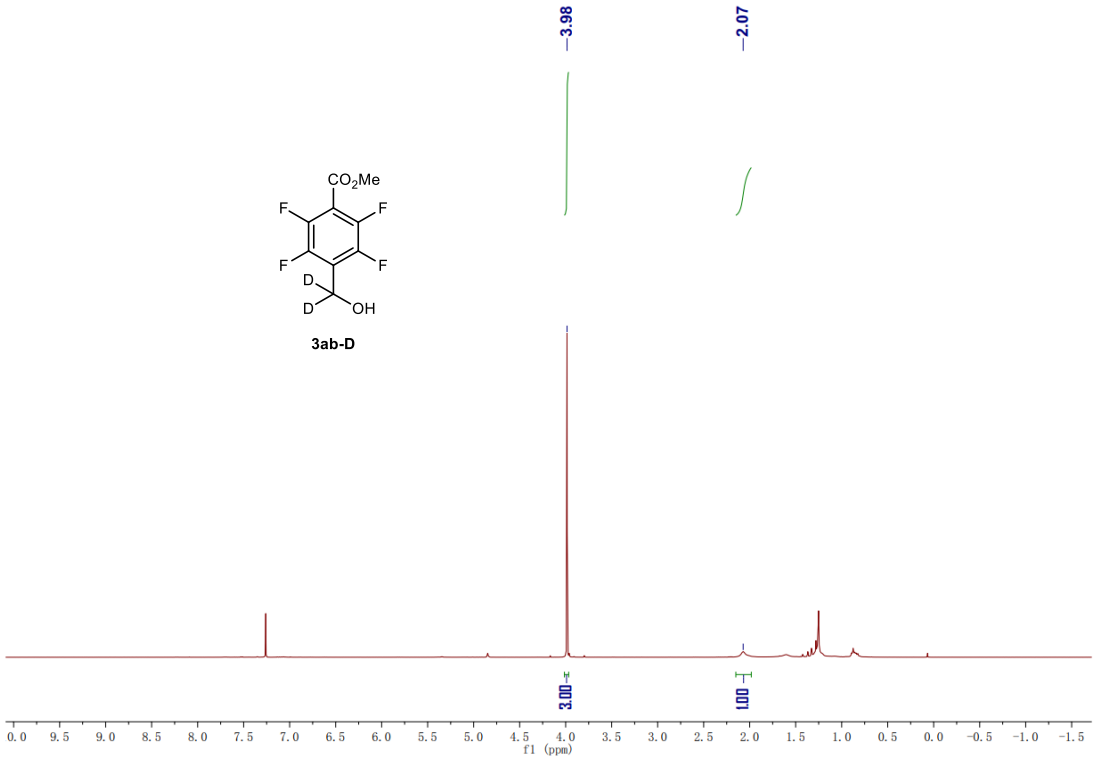

3.99
2.87
2.85
2.83
1.74
1.72
1.71
1.69
1.67
1.35
1.34
1.34
1.33
1.32
1.31
0.91
0.89
0.87
CO2Me
F
F
F
F
n-Bu
O
12
3.00
2.00
2.02
4.02
3.00
f1 (ppm)

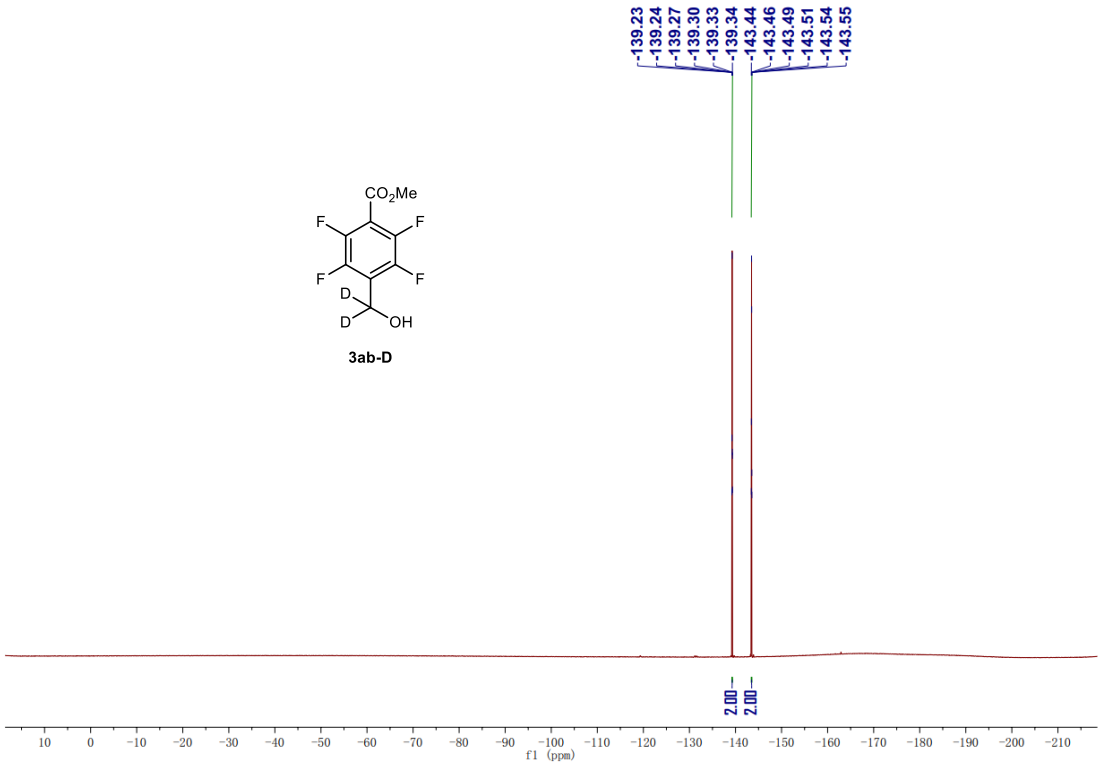

-137.72
-137.73
-137.74
-137.77
-137.79
-137.82
-137.83
-137.84
-141.14
-141.15
-141.15
-141.19
-141.21
-141.24
-141.25
-141.26
CO2Me
F
F
F
F
n-Bu
O
12
2.00
2.01
f1 (ppm)

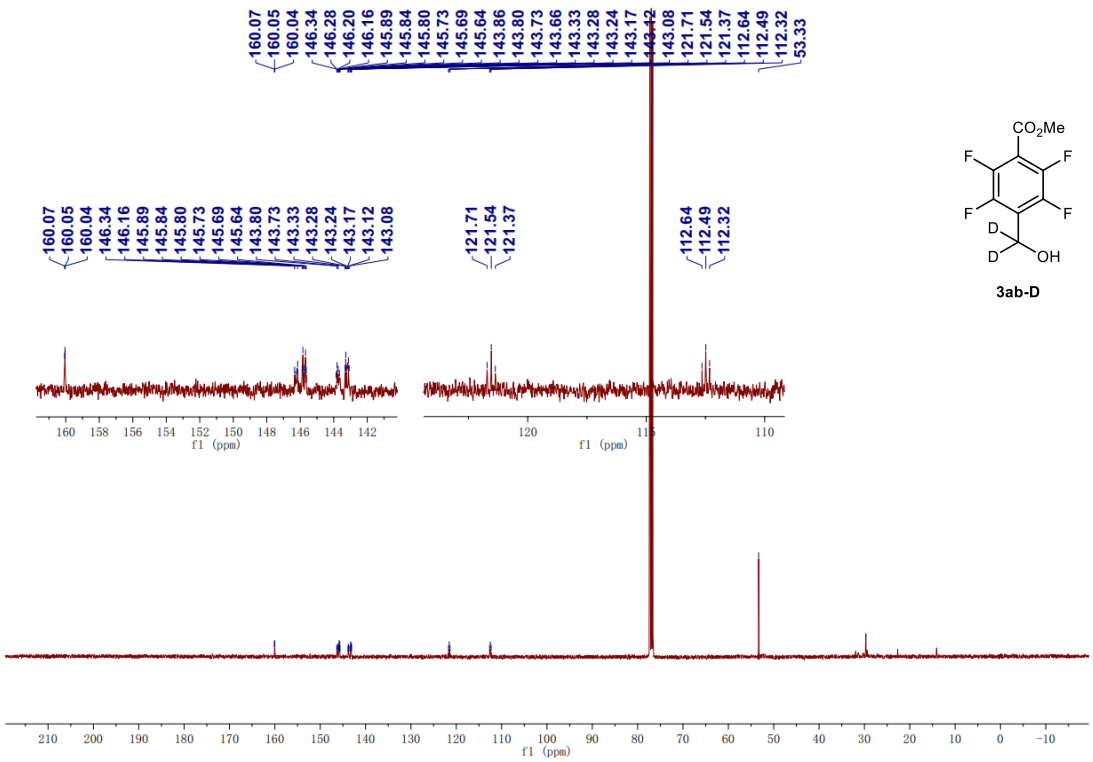

194.64
194.63
159.51
145.90
145.85
145.81
145.74
145.70
145.65
144.52
144.47
144.46
144.40
144.37
144.32
144.26
143.32
143.27
143.23
143.16
143.12
143.07
142.00
141.94
141.89
141.86
141.81
141.79
141.74
122.67
122.47
122.28
114.31
114.15
113.98
53.50
44.98
31.01
23.03
22.30
13.78
f1 (ppm)
CO2Me
F
F
F
F
n-Bu
O
12


6.76
6.74
6.73
6.72
6.70
6.69
6.38
6.38
6.38
6.34
6.34
6.34
3.96
2.33
2.31
2.29
2.27
1.52
1.51
1.50
1.49
1.48
1.47
1.46
1.45
1.42
1.42
1.41
1.39
1.37
1.35
1.33
0.95
0.93
1.00
0.98
3.00
2.02
2.02
2.02
3.02
f1 (ppm)
CO2Me
F
F
F
F
n-Bu
13


-140.77
-140.78
-140.81
-140.83
-140.86
-140.87
-143.25
-143.27
-143.29
-143.32
-143.34
-143.36
CO2Me
F
F
F
F
n-Bu
13
2.00
2.03
f1 (ppm)
160.43
160.41
160.39
160.36
146.29
146.24
146.19
146.13
146.08
146.03
145.57
145.52
145.43
145.38
145.32
143.94
143.86
143.78
143.75
143.70
143.65
143.59
143.54
143.49
143.09
143.03
142.98
142.95
142.88
142.84
120.48
120.35
120.21
114.81
114.78
114.75
109.36
109.21
109.05
53.06
34.15
30.84
22.22
13.83


3.98
2.07
CO2Me
F
F
F
F
D
D
OH
3ab-D
3.00
1.00
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)


139.23
139.24
139.27
139.30
139.33
139.34
143.44
143.46
143.49
143.51
143.54
143.55
CO2Me
F
F
F
F
D
D
OH
3ab-D
2.00
2.00
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


160.07
160.05
160.04
146.34
146.28
146.20
146.16
145.89
145.84
145.80
145.73
145.69
145.64
143.86
143.80
143.73
143.66
143.33
143.28
143.24
143.17
143.12
143.08
121.71
121.54
121.37
112.64
112.49
112.32
53.33
CO2Me
F
F
F
F
D
D
OH
3ab-D
f1 (ppm)