Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

A New Approach to Access Difluoroalkylated Diarylmethanes via Visible-Light Photocatalytic Cross-Coupling Reactions

Yin-Na Zhao, Yong-Chun Luo, Zhu-Yin Wang and Peng-Fei Xu*

Contents

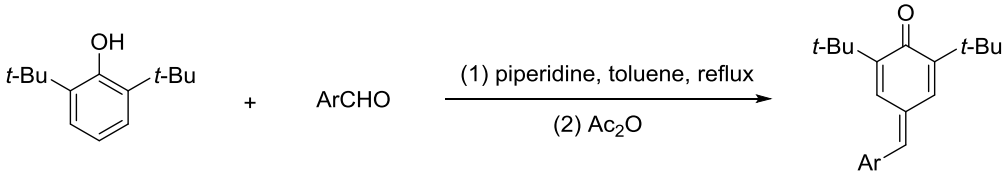
1. General Information

All glassware was thoroughly oven-dried. Chemicals and solvents were either purchased from commercial suppliers or purified by standard techniques. Analytical thin-layer chromatography (TLC) was performed on silicycle silica gel plates with F-254 indicator and compounds were visualized by exposure to ultraviolet light and/or staining with phosphomolybdic acid followed by heating on a hot plate. Flash chromatography was carried out using silica gel (200-300 mesh). ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on a Bruker AM-400 spectrometer (400 MHz ^{1}H, 100 MHz ^{13}C, 376 MHz ^{19}F). The spectra were recorded in $CDCl_3$ as solvent at room temperature, ^{1}H and ^{13}C NMR chemical shifts are reported in ppm relative to the residual solvent peak. The residual solvent signals were used as references and the chemical shifts were converted to the TMS scale ($CDCl_3$: δ_H = 7.26 ppm, δ_C = 77.00 ppm). Data for ^{1}H NMR are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q=quartet, m = multiplet, dd = double doublet), integration, coupling constant (Hz) and assignment. Data for ^{13}C NMR are reported as chemical shift, multiplicity and coupling constant (Hz). Data for ^{19}F NMR are reported in terms of chemical shift, multiplicity and coupling constant (Hz). HRMS were performed on a Bruker Apex II mass instrument (ESI). All luminescence spectra were surveyed on a PE-LS55 fluorescence spectrophotometer and equipped with a 1-cm quartz cell.

2. Preparation of Substrates

2.1 *para*-Quinone Methides (*p*-QMs)

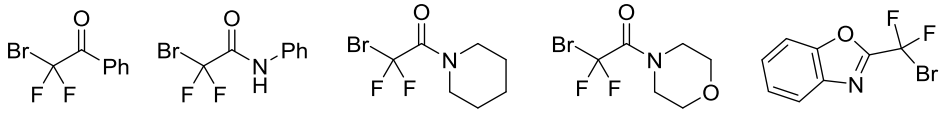
Substrates **1(1a-1p)** were synthesized according to the reported literatures[1-2] with slight modifications:



S1 **S2** **1a-1p**

In a three-necked flask, a solution of 2,6-di-*tert*-butylphenol **S1** (10 mmol) and the corresponding benzaldehyde **S2** (1.2 equiv.) in toluene (60 ml) was heated to reflux. Then piperidine (2.0 equiv.) was added dropwise and the reaction mixture was continued to reflux for 24 h. After cooling the reaction mixture just below the boiling point of toluene, acetic anhydride (2.0 equiv.) was added and the reaction mixture was stirred for another 15 min. Then the reaction mixture was poured on ice-water (200 mL) and extracted with ethyl acetate (3 × 20 mL). The combined organic phases were dried over anhydrous Na_2SO_4, and the solvent of the filtrate was removed under reduced pressure. The crude products were purified by flash column chromatography (petroleum ether/ethyl acetate), affording the desired *p*-QMs (**1a-1q**).

2.2 Preparation of Difluoromethylated Bromides

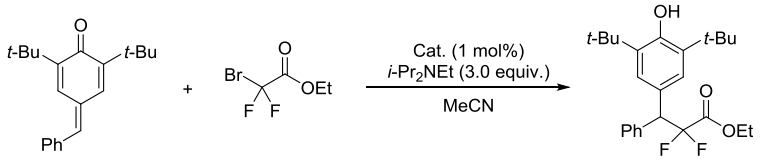


2b **2c** **2d** **2e** **2f**

Difluoromethylated bromides **2b**[3], **2c-e**[4], **2f**[5] was synthesized following the published procedures with slight modifications.

3. Optimization of Reaction Conditions

Table S1. 4. The Optimization of Photocatalysts and Control Experiments

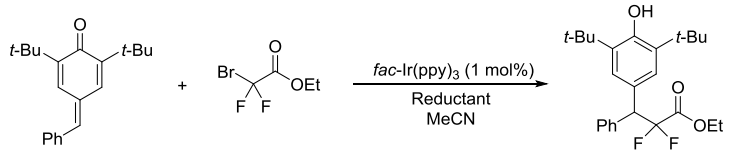


1a **2a** **3aa**

Entry[a]	Catalyst	Yield(%)[b]
1	***fac*-Ir(ppy)$_3$**	**65**
2	$Ru(bpy)_3Cl_2$▪$6H_2O$	32
3[c]	Eosin Y	38
4	$Ir(ppy)_2(dtbbpy)PF_6$	39
5	$Ir[dF(CF_3)(ppy)_2](dtbbpy)PF_6$	40
6[d]	*fac*-Ir(ppy)$_3$	NR[e]
7	-	trace
8[f]	*fac*-Ir(ppy)$_3$	NR

[a]Reaction conditions: **1a** (0.1 mmol), **2a** (1.5 equiv.), photocatalyst (1 mol%), *i*-Pr_2NEt (3.0 equiv.), MeCN (1 mL), and blue LEDs under N_2 at room temperature for 36 h. [b]Isolated yield. [c]Green LEDs. [d]No light. [e]NR (No Reaction). [f]No reductant.

Table S2. The Optimization of Reductants and Control Experiments

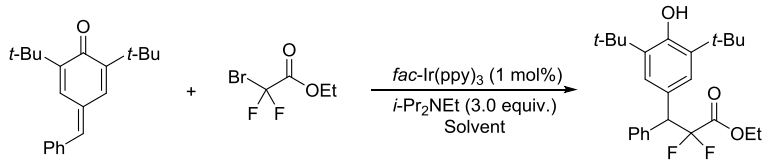


1a **2a** **3aa**

Entry[a]	Reductant	Yield(%)[b]
1	***i*-Pr_2NEt**	**65**
2[c]	Hantzsch Ester	11
3	Et_3N	32
4	*i*-Pr_2NH	38
5	Hantzsch Ester (1.0equiv.)/*i*-Pr_2NEt (2.0equiv)	40
6	DABCO	39
7	K_2CO_3	NR[d]
8[e]	*i*-Pr_2NEt	23
9[f]	*i*-Pr_2NEt	39

[a]Reaction conditions: **1a** (0.1 mmol), **2a** (1.5 equiv.), *fac*-Ir(ppy)$_3$ (1 mol%), reductant (3.0 equiv.), MeCN (1 mL), blue LEDs, under N_2 at room temperature for 36 h. [b]Isolated yield. [c]Reacted for 4 h. [d]NR (No Reaction). [e]*i*-Pr_2NEt (2.0 equiv.). [f]*i*-Pr_2NEt (4.0 equiv.).

Table S3. The Optimization of Solvents and Substrate Concentration

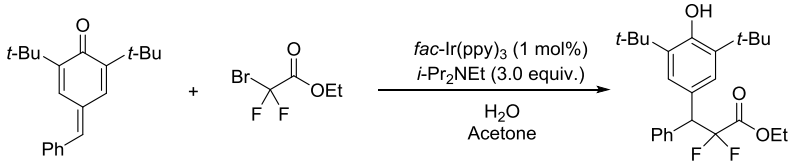


1a **2a** **3aa**

Entry[a]	Solvent	Yield(%)[b]
1	DCM	26
2	MeOH	14
3	DMF	32
4	Toulene	47
5	THF	40
6	DCE	33
7	DMSO	20
8	1,4-dioxane	69
9	**acetone**	**72**
10[c]	**acetone**	**76**
11[d]	acetone	65
12[ce]	acetone	68

[a]Reaction conditions: **1a** (0.1 mmol), **2a** (1.5 equiv.), *fac*-Ir(ppy)$_3$ (1 mol%), *i*-Pr$_2$NEt (3.0 equiv.), solvent (1 mL), and blue LEDs under N_2 at room temperature for 36 h. [b]Isolated yield. [c]**2a** (2.0 equiv.). [d]**2a** (3.0 equiv.). [e]Acetone (2 mL).

Table S4. The Optimization of the Amount of the Additive H_2O



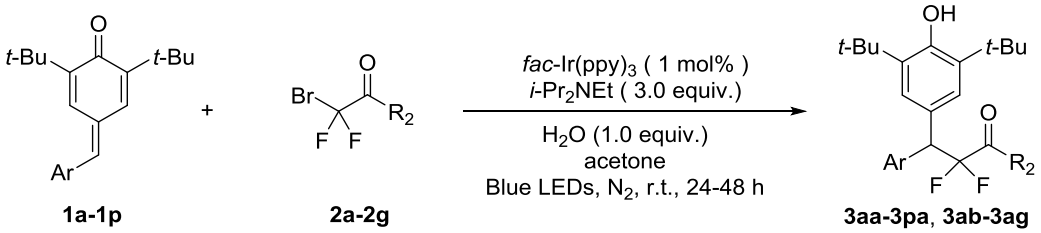
1a **2a** **3aa**

Entry[a]	H_2O (equiv.)	Yield(%)[b]
1	0.5	78
2	**1.0**	**85**
3	1.5	80
4	2.0	79
5	3.0	76

[a]Reaction conditions: **1a** (0.1 mmol), **2a** (2.0 equiv.), *fac*-Ir(ppy)$_3$ (1 mol%), *i*-Pr$_2$NEt (3.0 equiv.), acetone (1 mL), H_2O (additive), and blue LEDs under N_2 at room temperature for 24 h. [b]Isolated yield.

4. General Procedure and Analytical Data of Products 3

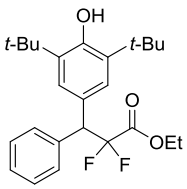
4.1 General Procedure for the Synthesis of Products 3



A mixture of *fac*-Ir(ppy)$_3$ (1 mol%), *p*-QMs **1** (0.1 mmol, 1.0 equiv.), bromodifluoroacetates **2** (0.2 mmol, 2.0 equiv.), *i*-Pr$_2$NEt (50 μL, 3.0 equiv.), H_2O (2 μL, 1.0 equiv.) and acetone (1 mL) was degassed by three cycles of freeze-pump-thaw. The mixture was stirred under nitrogen atmosphere at room temperature while irradiated by blue LEDs for 24-48 h. After completion of the reaction, the crude mixture was purified by flash chromatography (petroleum ether/ethyl acetate) to afford the pure products **3**.

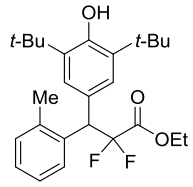
4.2 Analytical Data of Products 3

Ethyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-2,2-difluoro-3-phenyl-propanoate (3aa)



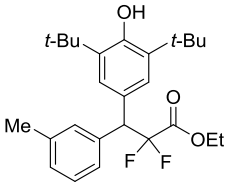
Following the general synthesis procedure, the product **3aa** was obtained as a pale yellow liquid in 85% yield (35.6 mg, PE/EA = 50:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42 (d, J = 7.6 Hz, 2H), 7.34-7.30 (m, 2H), 7.28-7.24 (m, 1H), 7.18 (s, 2H), 5.16 (s, 1H), 4.64 (t, J = 18.4 Hz, 1H), 4.16-4.04 (m, 2H), 1.40 (s, 18H), 1.02 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.0 (t, J = 32 Hz), 153.3, 136.1, 135.7, 129.5, 128.4, 127.5, 126.2, 125.8, 116.1 (t, J = 255 Hz), 62.4, 55.4 (t, J = 21 Hz), 34.3, 30.2, 13.5. ^{19}F NMR (376 MHz, $CDCl_3$): δ -105.68 (d, J = 254.9 Hz, 1F), -107.07 (d, J = 255.3 Hz, 1F). HRMS (ESI): $[M+H]^+$ calcd for $[C_{25}H_{33}F_2O_3]$: 419.2392, found: 419.2400.

Ethyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-2,2-difluoro-3-(o-tolyl)propanoate (3ba)



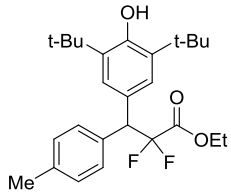
Following the general synthesis procedure, the product **3ba** was obtained as a pale yellow solid in 78% yield (32.4 mg, PE/EA = 50:1). m. p.: 84–86°C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61 (d, J = 7.6 Hz, 1H), 7.25-7.15 (m, 5H), 5.14 (s, 1H), 4.94-4.84 (m, 1H), 4.11 (q, J = 7.2 Hz, 2H), 2.34 (s, 3H) 1.39 (s, 18H), 1.02 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.1 (t, J = 32 Hz), 153.2, 136.7, 135.6, 134.8 (d, J = 5 Hz), 130.7, 128.0, 127.4, 126.7, 126.1, 125.0, 116.3 (t, J = 256 Hz), 62.5, 50.5 (t, J = 22 Hz), 34.2, 30.2, 20.1, 13.5. ^{19}F NMR (376 MHz, $CDCl_3$): δ -101.83 (d, J = 256.1 Hz, 1F), -108.11 (d, J = 256.1 Hz, 1F). HRMS (ESI): $[M+K]^+$ calcd for $[C_{26}H_{34}F_2KO_3]$: 471.2108, found: 471.2096.

Ethyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-2,2-difluoro-3-(m-tolyl)propanoate (3ca)



Following the general synthesis procedure, the product **3ca** was obtained as a pale yellow liquid in 80% yield (34.6 mg, PE/EA = 50:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.23-7.21 (m, 3H), 7.19 (s, 2H), 7.09-7.07 (m, 1H), 5.16 (s, 1H), 4.59 (t, J = 18.4 Hz, 1H), 4.16-4.05 (m, 2H), 2.33 (s, 3H), 1.41 (s,18 H), 1.03 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.0 (t, J = 32 Hz), 153.2, 137.9, 135.9, 135.7, 130.4, 128.2, 128.2, 126.4, 126.2, 125.9, 116.1 (t, J = 254 Hz), 62.4, 55.4 (t, J = 21 Hz), 34.2, 30.2, 21.4, 13.5. ^{19}F NMR (376 MHz, $CDCl_3$): δ -105.77 (d, J = 254.6 Hz, 1F), -106.88 (d, J = 254.6 Hz, 1F). HRMS (ESI): $[M+Na]^+$ calcd for $[C_{26}H_{34}F_2NaO_3]$: 455.2368, found: 455.2358.

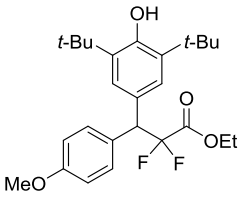
Ethyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-2,2-difluoro-3-(p-tolyl)propanoate (3da)



Following the general synthesis procedure, the product **3da** was obtained as a pale yellow liquid in 77% yield (32.3 mg, PE/EA = 50:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31 (d, J = 7.6 Hz, 2H), 7.18 (s, 2H), 7.13 (d, J = 7.6 Hz, 2H), 5.15 (s, 1H), 4.59 (t, J = 18.4 Hz, 1H), 4.16-4.04 (m, 2H), 2.31 (s, 3H), 1.40 (s,18 H), 1.04 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.1 (t, J = 32 Hz), 153.3, 137.2, 135.7, 133.1 (d, J = 4 Hz), 129.4, 129.1, 126.2, 126.1, 116.2 (t, J = 254 Hz), 62.4, 55.2 (t, J = 21 Hz), 34.3, 30.2, 21.0, 13.6. ^{19}F NMR (376 MHz, $CDCl_3$): δ -105.55 (d, J = 254.6 Hz, 1F), -107.24 (d, J = 254.6 Hz, 1F). HRMS (ESI): $[M+Na]^+$ calcd for $[C_{26}H_{34}F_2NaO_3]$:

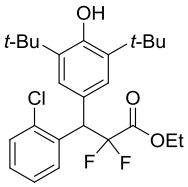
455.2368, found: 455.2355.

Ethyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-2,2-difluoro-3-(4-methoxyphenyl)-propanoate (3ea)



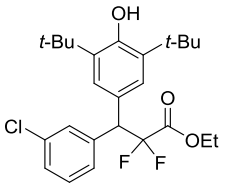
Following the general synthesis procedure, the product **3ea** was obtained as a pale yellow liquid in 84% yield (37.6 mg, PE/EA = 30:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33 (d, J = 8.4 Hz, 2H), 7.17 (s, 2H), 6.86 (d, J = 8.8 Hz, 2H), 5.15 (s, 1H), 4.59 (t, J = 18.4 Hz, 1H), 4.16-4.05 (m, 2H), 3.78 (s, 3H), 1.40 (s,18 H), 1.05 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.9 (t, J = 32 Hz), 158.9, 153.2, 135.7, 130.6, 128.1, 126.2, 126.1, 116.1 (t, J = 254 Hz), 113.8, 62.3, 55.0, 54.6 (t, J = 22 Hz), 34.2, 30.1, 13.5. ^{19}F NMR (376 MHz, $CDCl_3$): δ -105.88 (d, J = 255.3 Hz, 1F), -107.12 (d, J = 254.2 Hz, 1F). HRMS (ESI): $[M+Na]^+$ calcd for $[C_{26}H_{34}F_2NaO_4]$: 471.2317, found: 471.2309.

Ethyl 3-(2-chlorophenyl)-3-(3,5-di-tert-butyl-4-hydroxyphenyl)-2,2-difluoro-propanoate (3fa)



Following the general synthesis procedure, the product **3fa** was obtained as a pale yellow liquid in 83% yield (35.7 mg, PE/EA = 50:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, J = 7.6 Hz, 1H), 7.38-7.36(m, 1H), 7.29-7.28 (m, 1H), 7.22-7.18 (m, 3H), 5.33 (t, J = 18.4 Hz, 1H), 5.16 (s, 1H), 4.14(q, J = 7.2 Hz, 2H), 1.40 (s,18 H), 1.07 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.7 (t, J = 32 Hz), 153.4, 135.7, 134.8, 134.4 (d, J = 5 Hz), 129.9, 129.7, 128.7, 126.9, 126.6, 124.6, 116.0 (t, J = 255 Hz), 62.7, 50.5 (t, J = 23 Hz), 34.3, 30.2, 13.6. ^{19}F NMR (376 MHz, $CDCl_3$): δ -103.91 (d, J = 256.8 Hz, 1F), -107.02 (d, J = 256.8 Hz, 1F). HRMS (ESI): $[M+Na]^+$ calcd for $[C_{25}H_{31}ClF_2NaO_3]$: 475.1822, found: 475.1811.

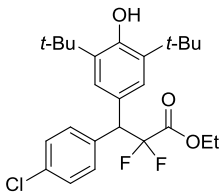
Ethyl 3-(3-chlorophenyl)-3-(3,5-di-tert-butyl-4-hydroxyphenyl)-2,2-difluoro-propanoate (3ga)



Following the general synthesis procedure, the product **3ga** was obtained as a pale yellow liquid in 73% yield (33.0 mg, PE/EA = 50:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40 (s, 1H), 7.34-7.32 (m, 1H), 7.26-7.25 (m, 2H), 7.14 (s, 2H), 5.20 (s, 1H), 4.66-4.57 (m, 1H), 4.19-4.07(m, 2H), 1.41 (s,18 H), 1.06 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.8 (t, J = 32 Hz), 153.5, 138.1 (d, J = 4 Hz), 136.0, 134.2, 129.9, 129.7, 127.8, 127.6, 126.2, 125.2 (d, J = 5 Hz), 115.8 (t, J = 254 Hz), 62.7, 55.1 (t, J = 22

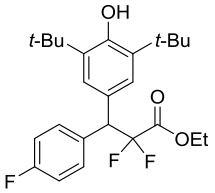
Hz), 34.3, 30.2, 13.6. ^{19}F NMR (376 MHz, $CDCl_3$): δ -104.71 (d, J = 256.1 Hz, 1F), -107.94 (d, J = 256.1 Hz, 1F). HRMS (ESI): $[M+Na]^+$ calcd for $[C_{25}H_{31}ClF_2NaO_3]$: 475.1822, found: 475.1826.

Ethyl 3-(4-chlorophenyl)-3-(3,5-di-tert-butyl-4-hydroxyphenyl)-2,2-difluoro-propanoate (3ha)



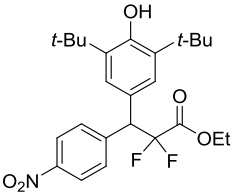
Following the general synthesis procedure, the product **3ha** was obtained as a pale yellow liquid in 82% yield (37.1 mg, PE/EA = 50:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36-7.26 (m, 4H), 7.13 (s, 2H), 5.18 (s, 1H), 4.62 (t, J = 18.4 Hz, 1H), 4.18-4.06 (m, 2H), 1.40 (s,18 H), 1.06 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.8 (t, J = 32 Hz), 153.4, 135.9, 134.7 (d, J = 4 Hz), 133.5, 130.9, 128.6, 126.1, 125.4 (d, J = 5 Hz), 115.9 (t, J = 254 Hz), 62.6, 54.7 (t, J = 22 Hz), 34.3, 30.2, 13.6. ^{19}F NMR (376 MHz, $CDCl_3$): δ -104.65 (d, J = 256 Hz, 1F), -107.99 (d, J = 256.1 Hz, 1F). HRMS (ESI): $[M+Na]^+$ calcd for $[C_{25}H_{31}ClF_2NaO_3]$: 475.1822, found: 475.1814.

Ethyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-2,2-difluoro-3-(4-fluorophenyl)-propanoate (3ia)



Following the general synthesis procedure, the product **3ia** was obtained as a pale yellow liquid in 69% yield (30.1 mg, PE/EA = 50:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40-7.37 (m, 2H), 7.14 (s, 2H), 7.26 (t, 1H), 7.02 (t, J = 8.4 Hz, 2H), 5.18 (s, 1H), 4.63 (t, J = 18.4 Hz, 1H), 4.17-4.06 (m, 2H), 1.41 (s,18 H), 1.05 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.9 (t, J = 32 Hz), 162.2 (d, J = 245 Hz), 153.4, 135.9, 131.9, 131.6 (d, J = 8 Hz), 126.1, 125.7 (d, J = 5 Hz), 115.9 (t, J = 255 Hz), 115.6 (d, J = 21 Hz), 62.6, 54.6 (t, J = 22 Hz), 34.3, 30.2, 13.6. ^{19}F NMR (376 MHz, $CDCl_3$): δ -105.34 (d, J = 255.7 Hz, 1F), -107.73 (d, J = 255.7 Hz, 1F), -114.92 (s, 1F). HRMS (ESI): $[M+Na]^+$ calcd for $[C_{25}H_{31}F_3NaO_3]$: 459.2118, found: 459.2112.

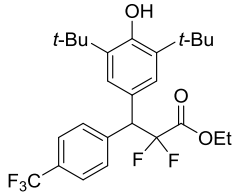
Ethyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-2,2-difluoro-3-(4-nitrophenyl)-propanoate (3ja)



Following the general synthesis procedure, the product **3ja** was obtained as a pale brown liquid in 45% yield (20.8 mg, PE/EA = 30:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.19 (d, J = 8.4 Hz, 2H), 7.59 (d, J = 8.4 Hz, 2H), 7.12 (s, 2H), 5.24 (s, 1H), 4.82-4.73 (m, 1H), 4.20-4.08 (m, 2H), 1.41 (s,18 H), 1.07 (t, J = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.3 (t, J = 32 Hz), 153.7, 147.2, 143.5 (d, J = 3 Hz), 136.2, 130.4, 126.0,

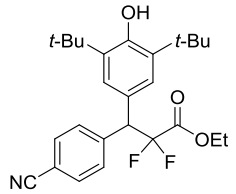
124.4 (d, J = 6 Hz), 123.5, 115.5 (t, J = 254 Hz), 62.8, 54.9 (t, J = 22 Hz), 34.2, 30.1, 13.5. ^{19}F NMR (376 MHz, $CDCl_3$): δ -102.66 (d, J = 257.9 Hz, 1F), -109.24 (d, J = 257.9 Hz, 1F). HRMS (ESI): $[M+H]^+$ calcd for $[C_{25}H_{32}F_2NO_5]$: 464.2243, found: 464.2234.

Ethyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-2,2-difluoro-3-(4-(trifluoromethyl)-phenyl)propanoate (3ka)



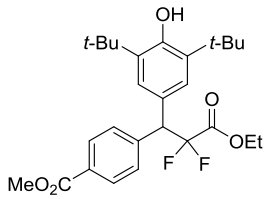
Following the general synthesis procedure, the product **3ka** was obtained as a pale yellow liquid in 68% yield (33.1 mg, PE/EA = 50:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60-7.53 (m, 4H), 7.15 (s, 2H), 5.21 (s, 1H), 4.76-4.67 (m, 1H), 4.19-4.06 (m, 2H), 1.41 (s,18 H), 1.05 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.6 (t, J = 32 Hz), 153.6, 140.3, 136.1, 129.9, 129.6, 126.1, 125.3 (t, J = 4 Hz), 125.0 (d, J = 5 Hz), 124.0 (q, J = 271 Hz), 115.8 (t, J = 254 Hz), 62.7, 55.2 (t, J = 22 Hz), 34.3, 30.1, 13.5. ^{19}F NMR (376 MHz, $CDCl_3$): δ -62.61 (s, 3F), -103.65 (d, J = 256.8 Hz, 1F), -108.67 (d, J = 256.8 Hz, 1F). HRMS (ESI): $[M+Na]^+$ calcd for $[C_{26}H_{31}F_5NaO_3]$: 509.2086, found: 509.2078.

Ethyl 3-(4-cyanophenyl)-3-(3,5-di-tert-butyl-4-hydroxyphenyl)-2,2-difluoropropanoate (3la)



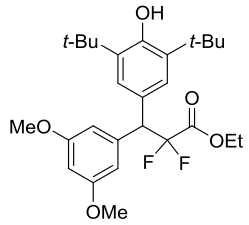
Following the general synthesis procedure, the product **3la** was obtained as a pale yellow liquid in 76% yield (33.7 mg, PE/EA = 15:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63 (d, J = 8.4 Hz, 2H), 7.53 (d, J = 8.0 Hz, 2H), 7.11 (s, 2H), 5.23 (s, 1H), 4.76-4.67 (m, 1H), 4.19-4.07 (m, 2H), 1.40 (s, 18 H), 1.06 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.5 (t, J = 32 Hz), 135.7, 141.6 (d, J = 4 Hz), 136.3, 132.2, 130.3, 126.1, 124.6 (d, J = 6 Hz), 118.6, 115.7 (t, J = 254 Hz), 111.6, 62.8, 55.3 (t, J = 22 Hz), 34.3, 30.2, 13.6. ^{19}F NMR (376 MHz, $CDCl_3$): δ -103.10 (d, J = 257.9 Hz, 1F), -109.02 (d, J = 257.6 Hz, 1F). HRMS (ESI): $[M+Na]^+$ calcd for $[C_{26}H_{31}F_2NNaO_3]$: 466.2164, found: 466.2160.

Methyl 4-(1-(3,5-di-tert-butyl-4-hydroxyphenyl)-3-ethoxy-2,2-difluoro-3-oxopropyl)benzoate (3ma)



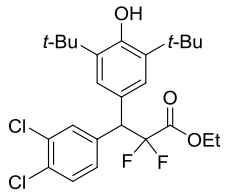
Following the general synthesis procedure, the product **3ma** was obtained as a pale yellow liquid in 80% yield (38.1 mg, PE/EA = 15:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (d, J = 8.0 Hz, 2H), 7.50 (d, J = 8.0 Hz, 2H), 7.14 (s, 2H), 5.20 (s, 1H), 4.71 (t, J = 18.4 Hz, 1H), 4.17-4.06 (m, 2H), 3.90 (s, 1H), 1.40 (s,18 H), 1.05 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.8, 163.8 (t, J = 32 Hz), 153.5, 141.3 (d, J = 4 Hz), 135.9, 129.7, 129.6, 129.4, 126.2, 125.1 (d, J = 5 Hz), 115.8 (t, J = 254 Hz), 62.7, 55.3 (t, J = 22 Hz), 52.1, 34.3, 30.2, 13.6. ^{19}F NMR (376 MHz, $CDCl_3$): δ -104.92 (d, J = 256.8 Hz, 1F), -107.49 (d, J = 256.8 Hz, 1F). HRMS (ESI): $[M+Na]^+$ calcd for $[C_{27}H_{34}F_2NaO_5]$: 499.2267, found: 499.2259.

Ethyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-3-(3,5-dimethoxyphenyl)-2,2-difluoropropanoate (3na)



Following the general synthesis procedure, the product **3na** was obtained as a pale yellow liquid in 55% yield (26.3 mg, PE/EA = 10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.19 (s, 2H), 6.98-6.97 (m, 2H), 6.83-6.81 (m, 1H), 5.17 (s, 1H), 4.58 (t, J = 18.4 Hz, 1H), 4.15-4.08 (m, 2H), 3.87 (s, 3H), 3.85 (s, 3H), 1.41 (s,18 H), 1.06 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.9 (t, J = 32 Hz), 153.2, 148.6, 148.4, 135.7, 128.4, 126.1, 125.9, 121.9, 116.1 (t, J = 254 Hz), 112.8, 110.9, 62.3, 55.6, 54.9 (t, J = 22 Hz), 34.2, 30.1, 13.5. ^{19}F NMR (376 MHz, $CDCl_3$): δ -106.14 (d, J = 254.6 Hz, 1F), -106.89 (d, J = 254.6 Hz, 1F). HRMS (ESI): $[M+H]^+$ calcd for $[C_{27}H_{37}F_2O_5]$: 479.2604, found: 479.2601.

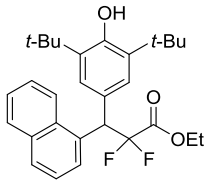
Ethyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-3-(3,5-dichlorophenyl)-2,2-difluoropropanoate (3oa)



Following the general synthesis procedure, the product **3oa** was obtained as a pale yellow liquid in 80% yield (38.9 mg, PE/EA = 50:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.50-7.49 (m, 1H), 7.41-7.40 (m, 1H), 7.28-7.25 (m, 1H), 7.11 (s, 2H), 5.22 (s, 1H), 4.65-4.56 (m, 1H), 4.19-4.07 (m, 2H), 1.41 (s, 18 H), 1.07 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.6 (t, J = 32 Hz), 153.7, 136.4 (d, J = 4 Hz), 136.2, 132.5, 131.8, 131.7, 130.3, 128.8, 126.0, 124.8 (d, J = 5 Hz), 115.7 (t, J = 254 Hz), 62.7, 54.5 (t, J = 22 Hz), 34.3, 30.2, 13.6. ^{19}F NMR (376 MHz, $CDCl_3$): δ -103.70 (d,

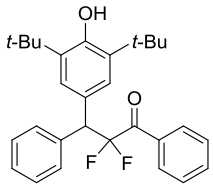
J = 257.2 Hz, 1F), -108.88 (d, J = 256.8 Hz, 1F). HRMS (ESI): $[M+Na]^+$ calcd for $[C_{25}H_{30}Cl_2F_2NaO_3]$: 509.1432, found: 509.1423.

Ethyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-2,2-difluoro-3-(naphthalen-1-yl)-propanoate (3pa)



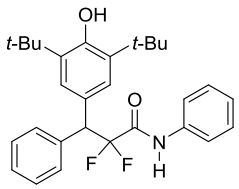
Following the general synthesis procedure, the product **3pa** was obtained as a white solid in 62% yield (29.1 mg, PE/EA = 50:1). m. p.: 126–128°C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.12(d, J = 8.4 Hz, 1H), 7.85-7.77 (m, 3H), 7.54-7.44(m, 3H), 7.25-7.24 (m, 2H), 5.61-5.52 (m, 1H), 5.13 (s, 1H), 4.04 (q, J = 7.2 Hz, 2H), 1.38 (s,18 H), 0.88 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.1 (t, J = 32 Hz), 153.3, 135. , 133.9, 132.1, (d, J = 6 Hz), 131.7, 128.9, 128.2, 126.5, 126.4, 126.1, (d, J = 4 Hz), 125.5, 125.2, (d, J = 3 Hz), 125.1, 123.2, 116.3 (t, J = 254 Hz), 62.5, 49.6 (t, J = 22 Hz), 34.2, 30.1, 13.3. ^{19}F NMR (376 MHz, $CDCl_3$): δ -101.03 (d, J = 256.4 Hz, 1F), -107.58 (d, J = 256.4 Hz, 1F). HRMS (ESI): $[M+Na]^+$ calcd for $[C_{29}H_{34}F_2NaO_3]$: 491.2368, found: 491.2361.

3-(3,5-di-tert-butyl-4-hydroxyphenyl)-2,2-difluoro-1,3-diphenylpropan-1-one (3ab)



Following the general synthesis procedure, the product **3ab** was obtained as a white solid in 52% yield (23.4 mg, PE/EA = 15:1). m. p.: 122–124°C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, J = 7.6 Hz, 2H), 7.53 (t, J = 7.6 Hz, 1H), 7.44(d, J = 7.6 Hz, 2H), 7.37 (t, J = 7.6 Hz, 2H), 7.31 (t, J = 8.0 Hz, 2H), 7.26-7.23 (m, 1H), 7.09 (s, 2H), 5.11 (s, 1H), 4.04-4.81 (m, 1H), 1.33 (s, 18H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.1 (t, J = 29 Hz), 153.2, 136.7 (d, J = 4 Hz), 135.8, 133.5, 129.6, 129.5 (t, J = 4 Hz), 128.4, 128.3, 127.3, 126.6, 126.0 (d, J = 5 Hz), 119.3 (t, J = 258 Hz), 55.4 (t, J = 22 Hz), 34.2, 30.1. ^{19}F NMR (376 MHz, $CDCl_3$): δ -98.80 (d, J = 268.1 Hz, 1F), -103.40 (d, J = 268.1 Hz, 1F). HRMS (ESI): $[M+K]^+$ calcd for $[C_{29}H_{32}F_2KO_2]$: 489.2002, found: 489.1993.

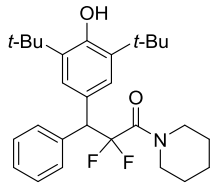
3-(3,5-di-tert-butyl-4-hydroxyphenyl)-2,2-difluoro-N,3-diphenylpropanamide (3ac)



Following the general synthesis procedure, the product **3ac** was obtained as a white solid in 77% yield (35.8 mg, PE/EA = 20:1). m. p.: 140–142°C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (s, 1H), 7.49-7.48 (m, 2H), 7.35-7.32 (m, 2H), 7.29-7.27 (m, 4H), 7.26 (s, 2H), 7.21 (s, 2H), 5.14 (s, 1H), 4.89 (t, J = 18.8 Hz, 1H), 1.36 (s, 18H). ^{13}C NMR

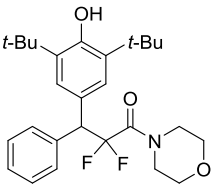
(100 MHz, $CDCl_3$): δ 162.1 (t, J = 28 Hz), 153.2, 136.3, 135.9, 135.7, 129.5, 128.9, 128.5, 127.4, 126.1, 125.4, 120.4, 118.3 (t, J = 258 Hz), 54.3 (t, J = 22 Hz), 34.2, 30.1. ^{19}F NMR (376 MHz, $CDCl_3$): δ -106.72 (d, J = 247.0 Hz, 1F), -108.55 (d, J = 247.0 Hz, 1F). HRMS (ESI): $[M+Na]^+$ calcd for $[C_{29}H_{33}F_2NNaO_2]$: 488.2372, found: 488.2368.

3-(3,5-di-tert-butyl-4-hydroxyphenyl)-2,2-difluoro-3-phenyl-1-(piperidin-1-yl)-propan-1-one (3ad)



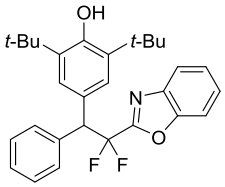
Following the general synthesis procedure, the product **3ad** was obtained as a pale yellow liquid in 78% yield (35.6 mg, PE/EA = 15:1). m. p.: 154–156^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45 (d, J = 7.6 Hz, 2H), 7.30 (t, J = 7.6 Hz, 2H), 7.24-7.19 (m, 3H), 5.13 (s, 1H), 4.85 (t, J = 18.4 Hz, 1H), 3.51-3.41 (m, 4H), 1.60-1.48 (m, 6H), 1.40 (s, 18 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.0 (t, J = 28 Hz), 152.9, 137.8, 135.5, 129.5, 128.3, 127.3, 126.9, 126.5, 119.3 (t, J = 258 Hz), 55.6 (t, J = 22 Hz), 46.8, 44.8, 34.3, 30.2, 26.3, 25.5, 24.3. ^{19}F NMR (376 MHz, $CDCl_3$): δ -98.39 (d, J = 267.7 Hz, 1F), -99.23 (d, J = 267.7 Hz, 1F). HRMS (ESI): $[M+H]^+$ calcd for $[C_{28}H_{38}F_2NO_2]$: 458.2865, found: 458.2857.

3-(3,5-di-tert-butyl-4-hydroxyphenyl)-2,2-difluoro-1-morpholino-3-phenylpropan-1-one (3ae)



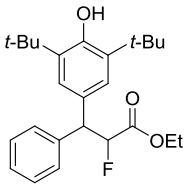
Following the general synthesis procedure, the product **3ae** was obtained as a white solid in 77% yield (35.3 mg, PE/EA = 10:1). m. p.: 134–136^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 (d, J = 7.6 Hz, 2H), 7.24 (t, J = 7.6 Hz, 2H), 7.19-7.16 (m, 1H), 7.12 (s, 2H), 5.09 (s, 1H), 4.75 (t, J = 18.4 Hz, 1H), 3.51-3.35 (m, 7 H), 3.26-3.22 (m, 1 H), 1.32 (s, 18H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.3 (t, J = 29 Hz), 153.1, 137.3 (d, J = 3 Hz), 135.7, 129.3, 128.3, 127.1, 126.7, (d, J = 4 Hz), 126.4, 119.2 (t, J = 258 Hz), 66.4, 55.5 (t, J = 22 Hz), 53.3, 46.4, 43.6, 34.2, 30.1. ^{19}F NMR (376 MHz, $CDCl_3$): δ -98.42 (d, J = 265.8 Hz, 1F), -99.69 (d, J = 265.5 Hz, 1F). HRMS (ESI): $[M+H]^+$ calcd for $[C_{27}H_{36}F_2NO_3]$: 460.2658, found: 460.2650.

Ethyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-2-fluoro-3-phenylpropanoate (3af)



Following the general synthesis procedure, the product **3af** was obtained as a colorless liquid in 70% yield (32.4 mg, PE/EA = 30:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76-7.74 (m, 1H), 7.53-7.49 (m, 3H), 7.41-7.34 (m, 2H), 7.32-7.29 (m, 2H), 7.25-7.22 (m, 1H), 7.16 (s, 2H), 5.10 (s, 1H), 5.03 (t, J = 18.0 Hz, 1H), 1.32 (s, 18 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.4 (t, J = 34 Hz), 153.2, 150.3, 140.1, 136.4, 135.6, 129.5, 128.5, 127.4, 126.4, 126.3, 126.0, 125.1, 121.1, 117.1 (t, J = 247 Hz), 111.1, 57.1 (t, J = 226 Hz), 34.2, 30.1. ^{19}F NMR (376 MHz, $CDCl_3$): δ -98.74 (d, J = 268.0 Hz, 1F), -100.9 (d, J = 267.3 Hz, 1F). HRMS (ESI): $[M+H]^+$ calcd for $[C_{29}H_{31}F_2NO_2]$: 464.2396, found: 464.2390.

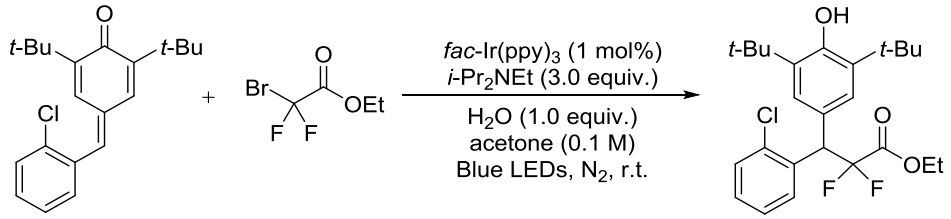
Ethyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-2-fluoro-3-phenylpropanoate (3ag)



Following the general synthesis procedure, the product **3ag** was obtained as a pale yellow liquid in 69% yield (27.6 mg, dr = 1:1, PE/EA = 30:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37-7.21 (m, 5H), 7.12-7.11 (m, 2H), 5.51-5.37 (m, 1H), 5.12-5.10 (m, 1H), 4.52-4.42 (m, 1H), 4.10-4.01 (m, 2H), 1.40 (s, 18 H), 1.05-1.01 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.9, 168.8, 168.7, 168.6, 152.8, 152.8, 140.0, 139.9, 138.9, 135.8, 135.6, 129.9, 129.8, 128.9, 128.8, 128.7, 128.5, 128.4, 128.3, 126.9, 126.8, 125.6, 125.6, 125.1, 92.6, 92.5, 90.7, 90.6, 61.2, 53.5, 53.4, 53.3, 53.2, 34.3, 34.2, 30.2, 30.1, 13.8, 13.7. ^{19}F NMR (376 MHz, $CDCl_3$): δ -192.63 (s, 0.5F), -193.32 (s, 0.5F). HRMS (ESI): $[M+Na]^+$ calcd for $[C_{25}H_{33}FNaO_3]$: 423.2306, found: 423.2297.

5. Applications of the Difluoroalkylation of *p*-QMs

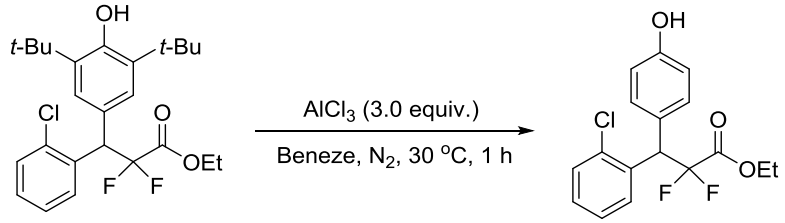
5.1 Gram-Scale Reaction of *p*-QM 1e



1f (3.66 mmol) **2a** (2 equiv) **3fa**, 4 d, 1.361 g, 82%

A mixture of *fac*-Ir(ppy)$_3$ (23.8 mg, 1 mol%), *p*-QM **1f** (3.66 mmol, 1.205 g, 1.0 equiv.), ethyl bromodifluoroacetate **2a** (7.32 mmol, 0.94 mL, 2.0 equiv.), *i*-Pr$_2$NEt (10.98 mmol, 1.80 mL, 3.0 equiv), H_2O (3.66 mmol, 66 μl, 1.0 equiv.) and acetone (37 mL) was degassed by three cycles of freeze-pump-thaw. The mixture was stirred under nitrogen atmosphere at room temperature while irradiated by blue LEDs for 4 days. After completion of the reaction, the crude mixture was purified by flash chromatography (PE/EA = 50:1) to afford the pure product **3fa** (1.361 g, 82%).

5.2 De-*tert*-Butylation of Product 3fa



3fa **4**, 53%

$AlCl_3$ (78.6 mg, 0.6 mmol, 3.0 equiv.) was added to a solution of *p*-QM **1e** (90.6 mg, 0.2 mmol, 1.0 equiv.) in benzene (5 mL) and the mixture was purged with Nitrogen three times. Then the reaction was kept at 30℃ for 1 h. Afterwards, 5 mL water was added to quench the reaction, and the aqueous phase was extracted with 5 mL ethyl acetate for three times. The organic layer was dried over with anhydrous magnesium sulfate, filtered and concentrated. The residue was next purified in flash column chromatography (PE/EA = 5:1) to give the pure product **4** in 53% yield (18.1 mg).

6. Cyclic Voltammetry Experiments

Cyclic voltammetry experients were performed to measure the reduction potentials of $BrCF_2CO_2Et$ **2a** and *p*-QM **1a**. Experiment conditions: **2a**/**1a** [0.01 M] in tetrabutylammonium tetrafluoroborat [0.1 M] in MeCN, scan rates equal to 0.1 V/S, glassy carbon electrode (GCE) as a working electrode, saturated calomel electrode (SCE, KCl saturated) as the reference electrode and Pt wire as the counter electrode. As shown in the results, the reduction potentials of $BrCF_2CO_2Et$ **2a** and *p*-QM **1a** respectively were - 0.89 V and – 0.20 V.

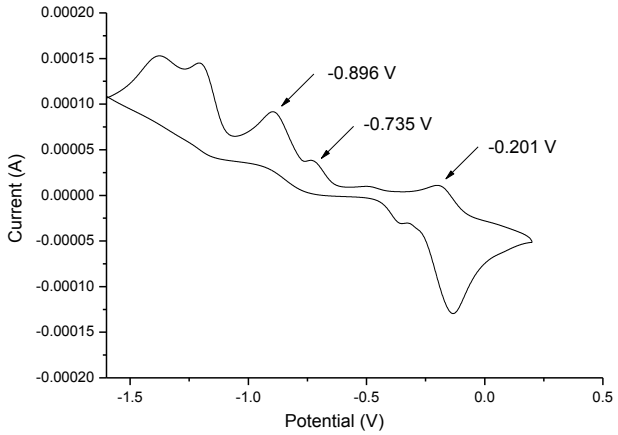


Figure S1. Cyclic Voltammetry of *p*-QM **1a**

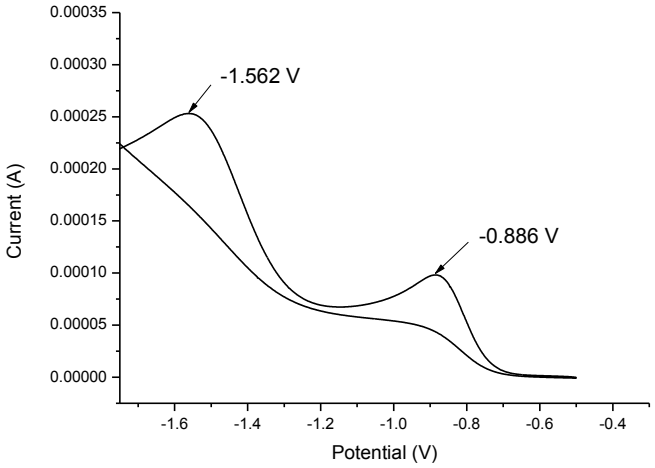


Figure S2. Cyclic Voltammetry of $BrCF_2CO_2Et$ **2a**

7. Stern−Volmer Quenching Experiments

Stern-Volmer fluorescence quenching experiments were run with freshly prepared solutions of 0.1 mM *fac*-Ir(ppy)$_3$, in degassed dry acetone at room temperature. The solutions were irradiated at 395 nm and fluorescence was measured from 450 nm to 650 nm. Control experiments showed that the excited state *fac*-Ir(ppy)$_3^*$ was mainly quenched by *p*-QM **1a**.

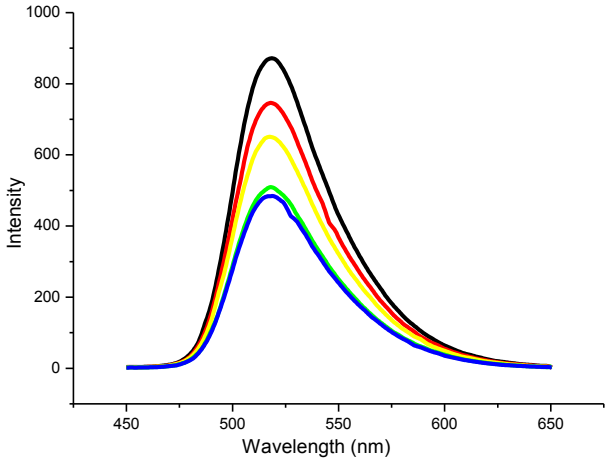


Figure S3. Fluorescence quenching date with *fac*-Ir(ppy)$_3$ and variable *p*-QM **1a** (10^{-5} M)

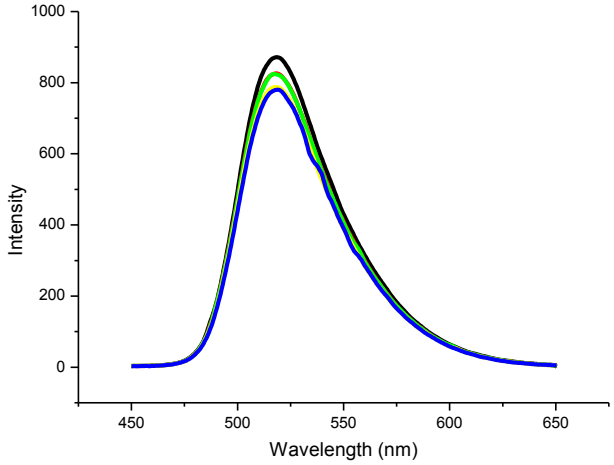


Figure S4. Fluorescence quenching date with *fac*-Ir(ppy)$_3$ and variable $BrCF_2CO_2Et$ **2a** (10^{-5} M)

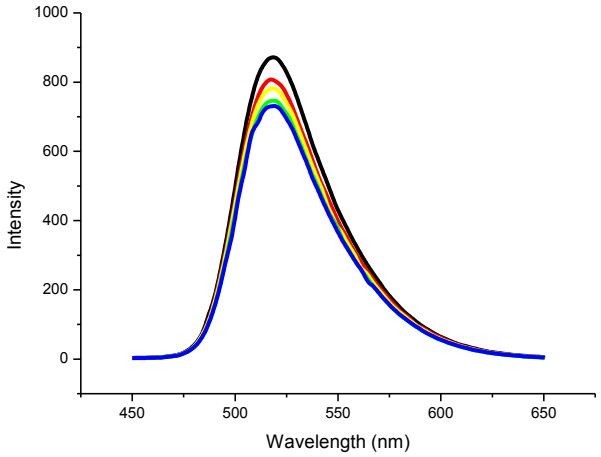


Figure S5. Fluorescence quenching date with *fac*-Ir(ppy)$_3$ and variable *i*-Pr$_2$NEt (10^{-5} M)

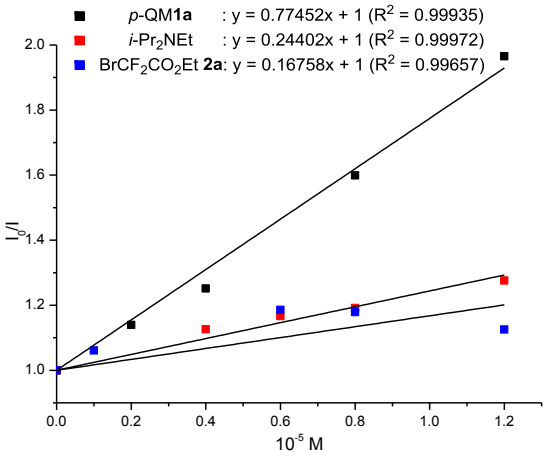


Figure S6. Stern-Volmer plots of *fac*-Ir(ppy)$_3$ and three quenchers. I_0 and I are luminescence intensities in the absence and presence of the indicated concentrations (10^{-5} M) of the corresponding quencher, respectively

8. Radical Trapping Experiments

The radical trapping experiments were conducted with *p*-QM **1a** and BrCF$_2$CO$_2$Et **2a** under the standard conditions with two different trapping agents to capture the radical intermediates expected in our system, and the products were detected by HRMS techniques. **Figure S7** showed that TEMPO, the most common trapping agent, captured diarylmethane radical with TEMPO-trapped compound **6** observed. HRMS (ESI): compound **6**, $[M+H]^+$ calcd for $[C_{30}H_{46}NO_2]$: 452.3523, found: 452.3522.

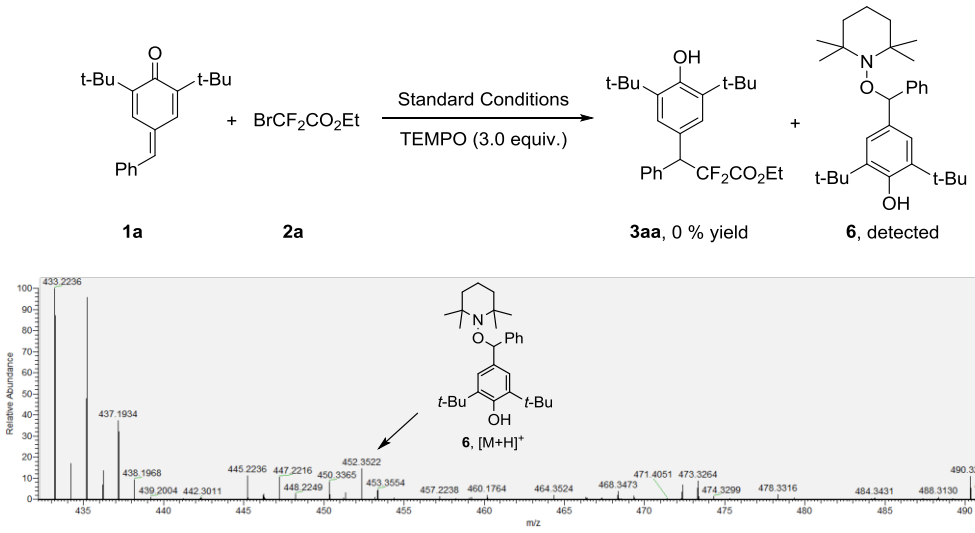


Figure S7. *p*-QM **1a** and $BrCF_2CO_2Et$ **2a** under standard conditions with TEMPO (3.0 equiv.)

Additionally, both compound **7** and product **3aa** were detected in **Figure S8** when the scavenger 1-(phenylsulfonyl)-2-phenyl-2-propene **5** was used, indicating the existence of difluoroacetate radicals. HRMS (ESI): compound **7**, $[M+Na]^+$ calcd for $[C_{13}H_{14}F_2NaO_2]$: 268.0854, found: 268.0856. Product **3aa**, $[M+Na]^+$ calcd for $[C_{25}H_{32}F_2NaO_3]$: 441.2212, found: 441.2214.

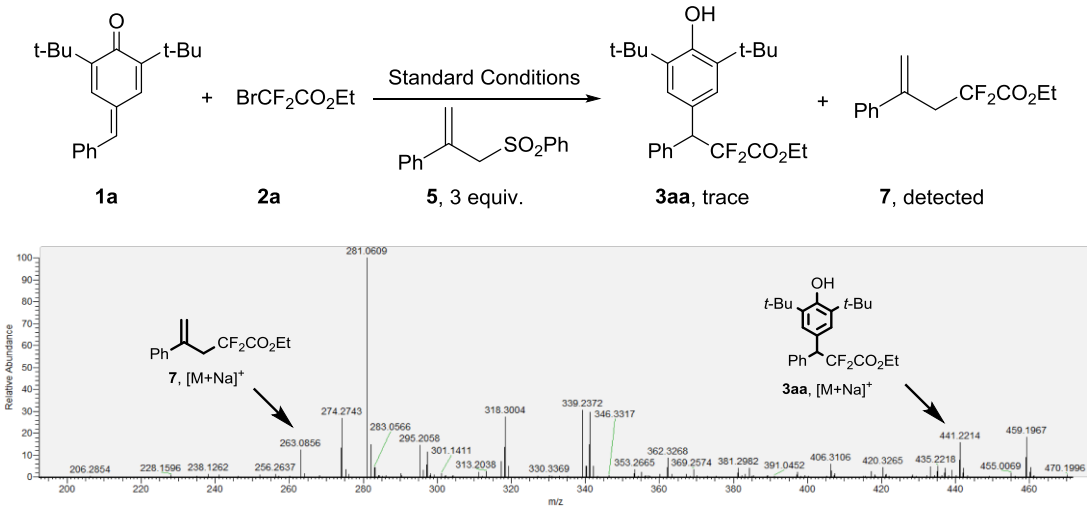
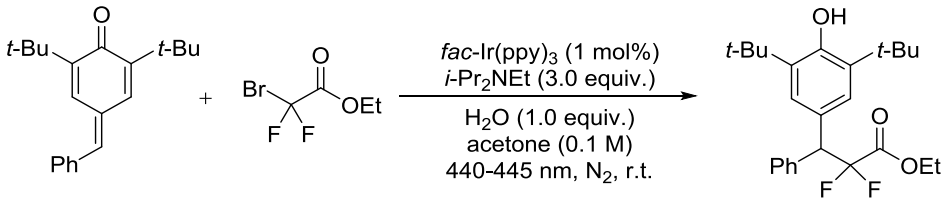


Figure S8. *p*-QM **1a** and $BrCF_2CO_2Et$ **2a** under standard conditions with 1-(phenylsulfonyl)-2-phenyl-2-propene **5 (**3.0 equiv.)

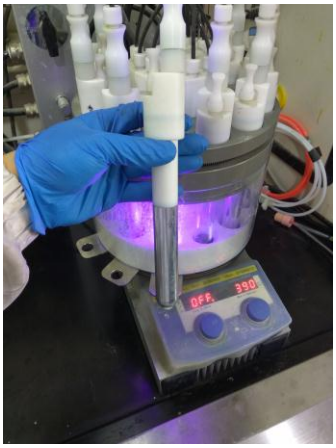
9. Determination of the Quantum Yield

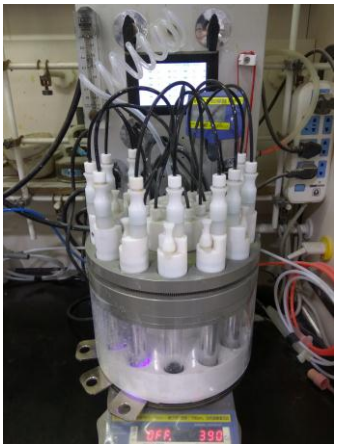


1a (0.1 mmol) **2a** (2 equiv) **3aa**, 125 min, 32% yield

The reaction was conducted under standard conditions in a quartz tube: A mixture of *fac*-Ir(ppy)$_3$ (1 mol%), *p*-QM **1a** (0.1 mmol, 1.0 equiv.), ethyl bromodifluoroacetate **2a** (0.2 mmol, 2.0 equiv.), *i*-Pr$_2$NEt (50 μL, 3.0 equiv.), H_2O (2 μL, 1.0 equiv.) and acetone (1 mL) in an oven-dried 8 mL quartz vial with a magnetic stirring bar was degassed by three cycles of freeze-pump-thaw. The mixture was stirred under nitrogen atmosphere at room temperature while irradiated by blue light (440-445 nm) for 125 minutes (7500 s).

The reaction was irradiated in Parallel Light Reactor (WP-TEC-1020) (the diameter of hole was 16 mm with intensity of 1916.1 mW cm^{-2}). After irradiation, the yield of the product **3aa** was determined by ^{1}H NMR based on a 1,3,5-trimethoxybenzene standard and the final yield was 32%.





Next we determined the absorbance of the catalyst *fac*-Ir(ppy)$_3$ in the reaction. The absorbance of *fac*-Ir(ppy)$_3$ in acetone was measured at the reaction concentration of 1.0×10^{-3} M and at a substantially diluted concentration of 1.0×10^{-4} M. The absorbance of *fac*-Ir(ppy)$_3$ at 443 nm in a 1.0×10^{-3} M solution is 2.271 (A = 2.271).

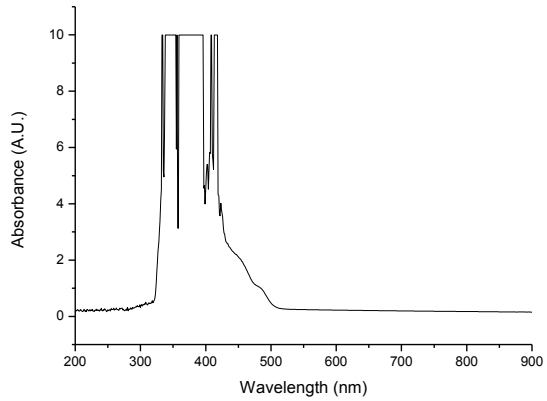


Figure S9. Absorbance of a 1.0 $\times 10^{-3}$ M solution of *fac*-Ir(ppy)$_3$ in acetone

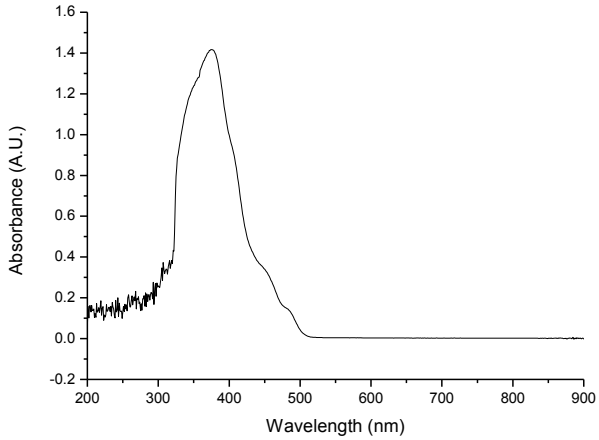


Figure S10. Absorbance of a 1.0 $\times 10^{-4}$ M solution of *fac*-Ir(ppy)$_3$ in acetone

Then we determined the quantum yield as follows.[6]

Φ = **Mole number for product/Mole number for absorption of photons = 3.0 ∗ 10^{-4}**

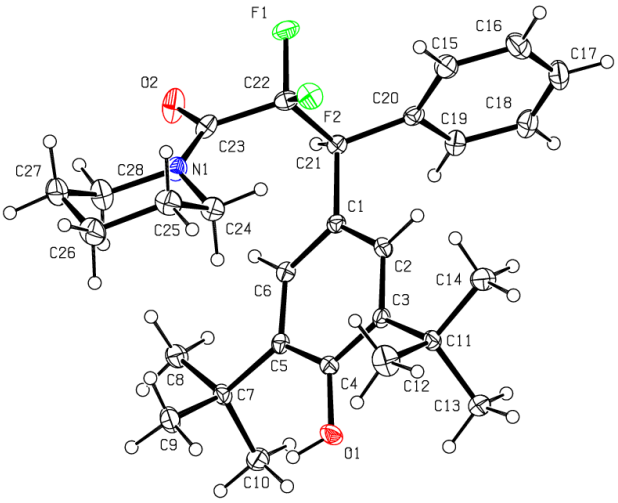
$$\Phi = \frac{n_{3aa}\, N_A/t}{f\, P\, \lambda/hc}$$

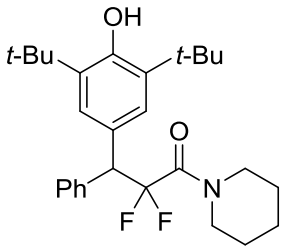
n_{3aa}: the mole number of the product **3aa** (n_{3aa} = 3.2 $\times 10^{-5}$ mol); t: the reaction time (t = 7500 s); N_A: 6.02$\times 10^{23}$/mol; f: 1-10^{-A} (443 nm, A = 2.271, f = 0.998); P: P = E*S (E: illumination intensity, E = 1.9161 W/cm^2; S: the area irradiated S = 2.0 cm^2); λ: wavelength (λ = 4.43 $\times 10^{-7}$ m); h: planck constant (h = 6.626 $\times 10^{-34}$ J*s); c: velocity of light (c = 3 $\times 10^{8}$ m/s).

The result excluded the efficient chain process and the reaction was likely to undergo a photocatalyzed process.

10. X-ray Crystallographic Data

X-ray crystallographic data of product **3ae**.





CCDC 1579852

Bond precision:	C-C = 0.0052 A	Wavelength=0.71073	
Cell:	a=10.6409(9)	b=9.1391(7)	c=12.7748(10)
	alpha=90	beta=91.516(8)	gamma=90
Temperature:	294K		
	Calculated	Reported	
Volume	1241.89(17)	1241.89(17)	
Space group	P n	P 1 n 1	
Hall group	P -2yac	P -2yac	
Moiety formula	C28 H37 F2 N O2	C28 H37 F2 N O2	
Sum formula	C28 H37 F2 N O2	C28 H37 F2 N O2	
Mr	457.59	457.59	
Dx,g cm-3	1.224	1.224	
Z	2	2	
Mu(mm-1)	0.086	0.086	
F000	492.0	492.0	
F000’	492.24		
h, k, lmax	13, 11, 15	13, 11, 15	
Nref	4905[2458]	3189	
Tmin, Tmax	0.983, 0.988	0.811, 1.000	
Tmin’	0.981		

Correction method = # Reported T Limits: Tmin = 0.811 Tmax = 1.000

AbsCorr = MULTI-SCAN

Data completeness = 1.30/0.65 Theta(max) = 26.020

R(reflections) = 0.0494(2694) wR2(reflections) = 0.1499(3189)

S = 0.969 Npar = 308

11. References

(1) Chu, W.-D.; Zhang, L.-F.; Bao, X.; Zhao, X.-H.; Zeng, C.; Du, J.-Y.; Zhang, G.-B.; Wang, F.-X.; Ma, X.-Y.; Fan, C.-A. *Angew. Chem. Int. Ed.* **2013**, *52*, 9229.

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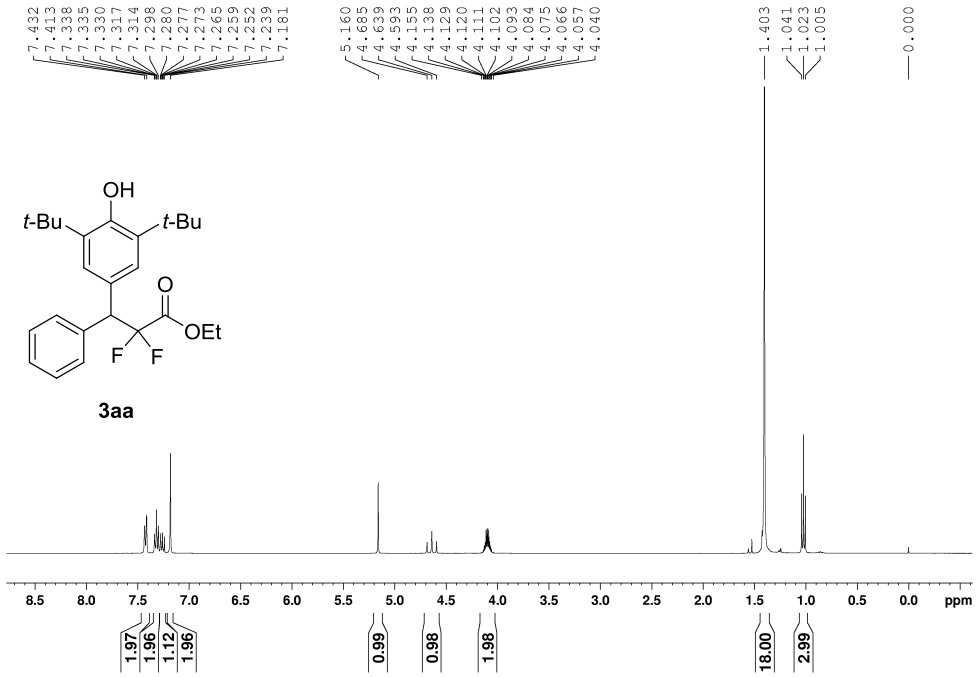
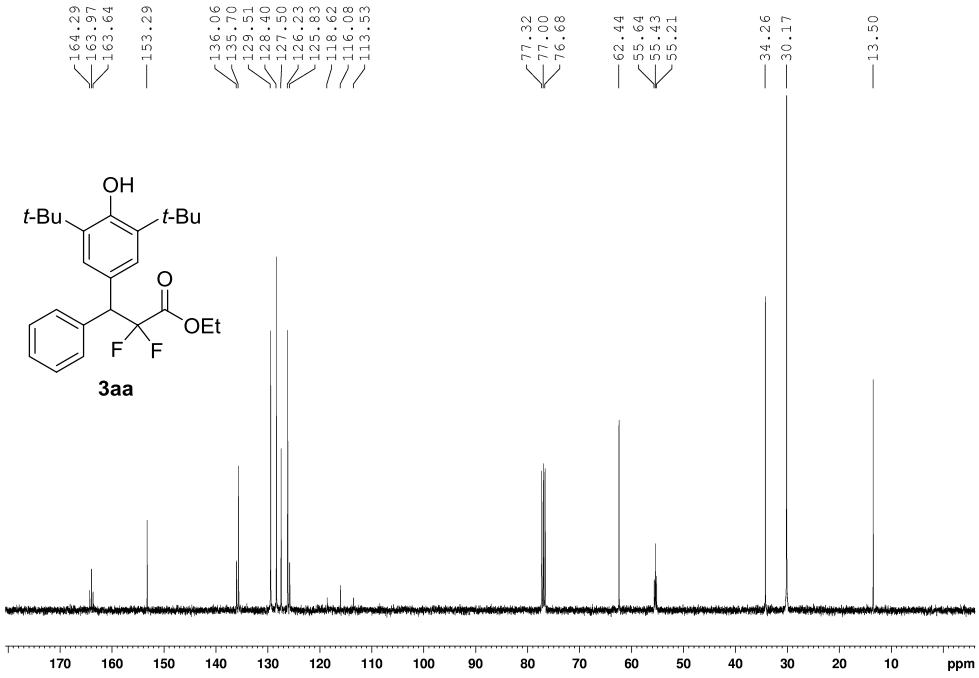
(4) Wang, L.; Wei, X.-J.; Jia, W.-L.; Zhong, J.-J.; Wu, L.-Z.; Liu, Q. *Org. Lett.* **2014**, *16*, 5842.

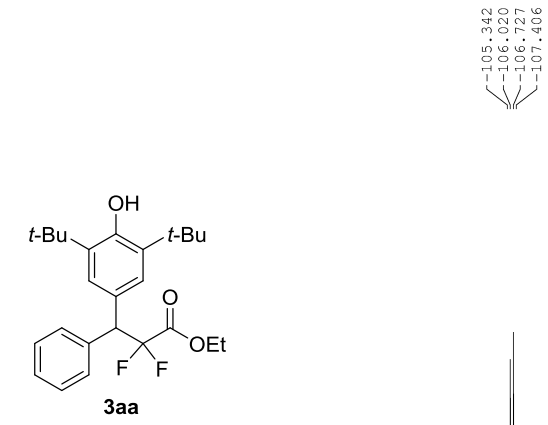
(5) Dolbier Jr., W. R.; Burkholdera, C. R.; Médebielle, M. *J. Fluorine Chem.* **1999**, *95*,127.

(6) Liu, Y.-Y.; Yu, X.-Y.; Chen, J.-R.; Qiao, M.-M.; Qi, X.; Shi, D.-Q.; Xiao, W.-J. *Angew. Chem. Int. Ed.* 2017, 56, 9527.

12. NMR Data of Products 3



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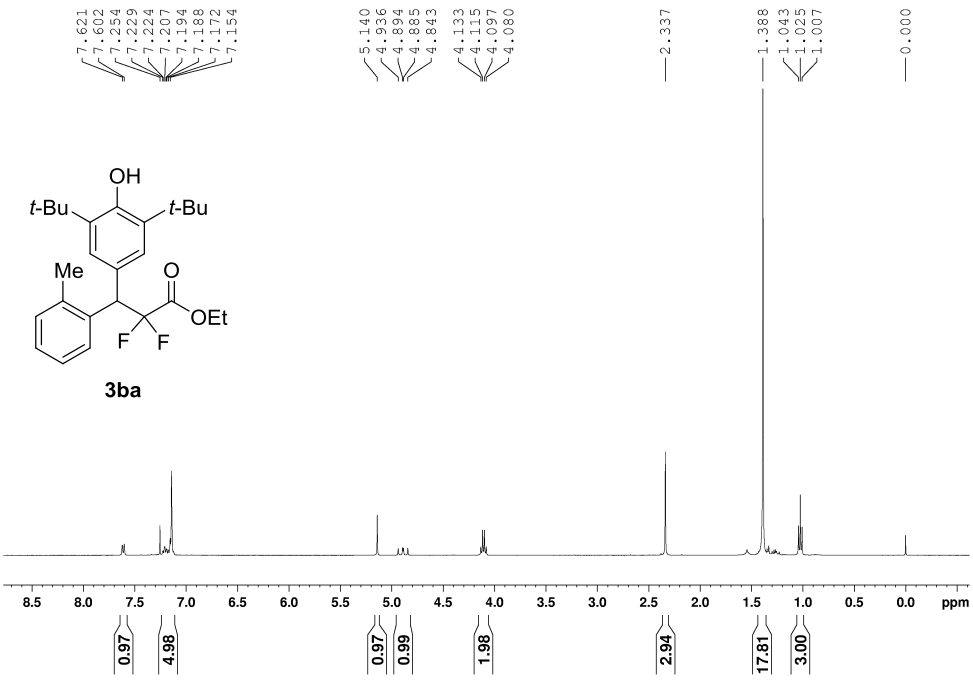
3aa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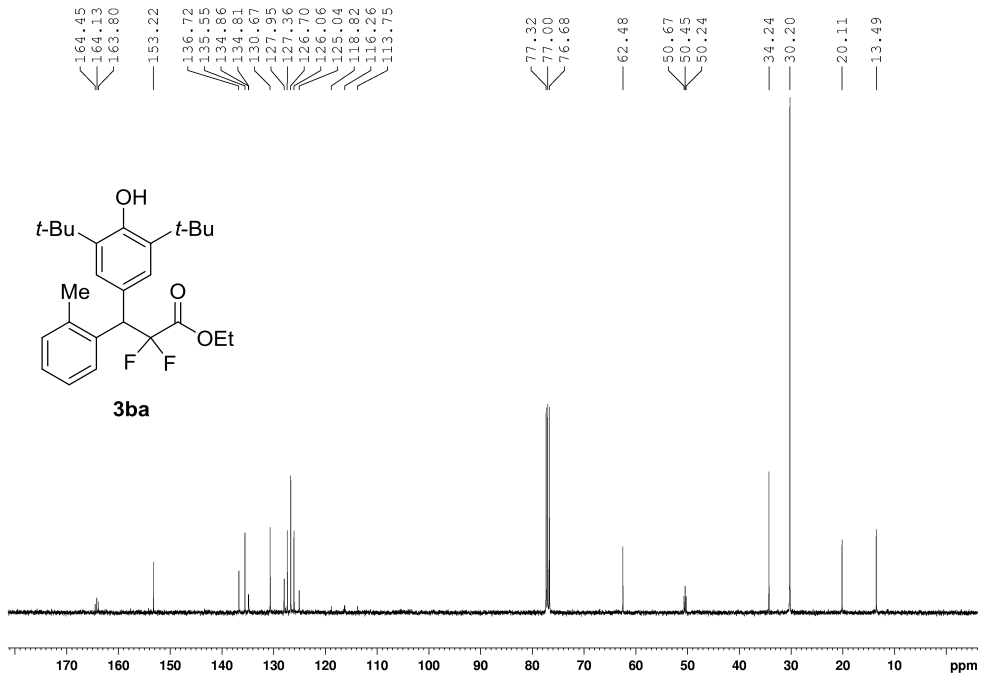
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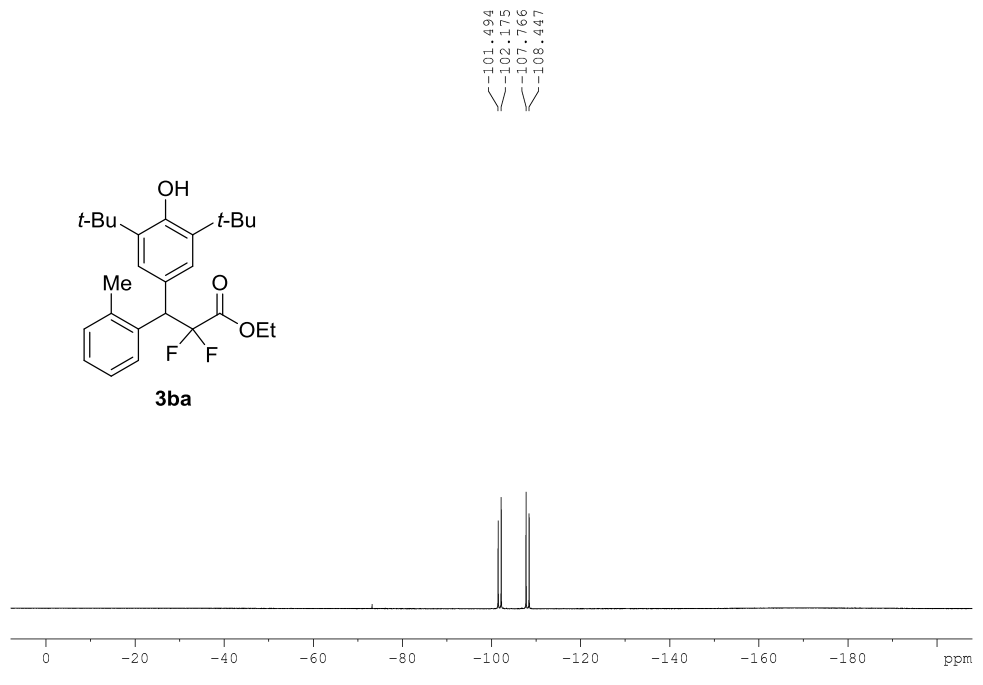
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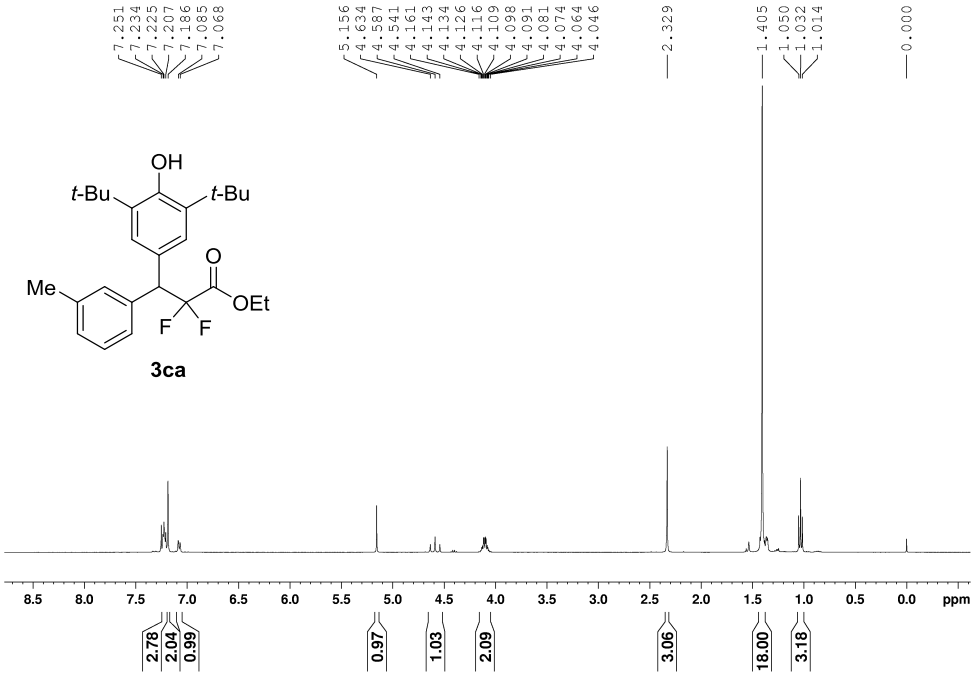
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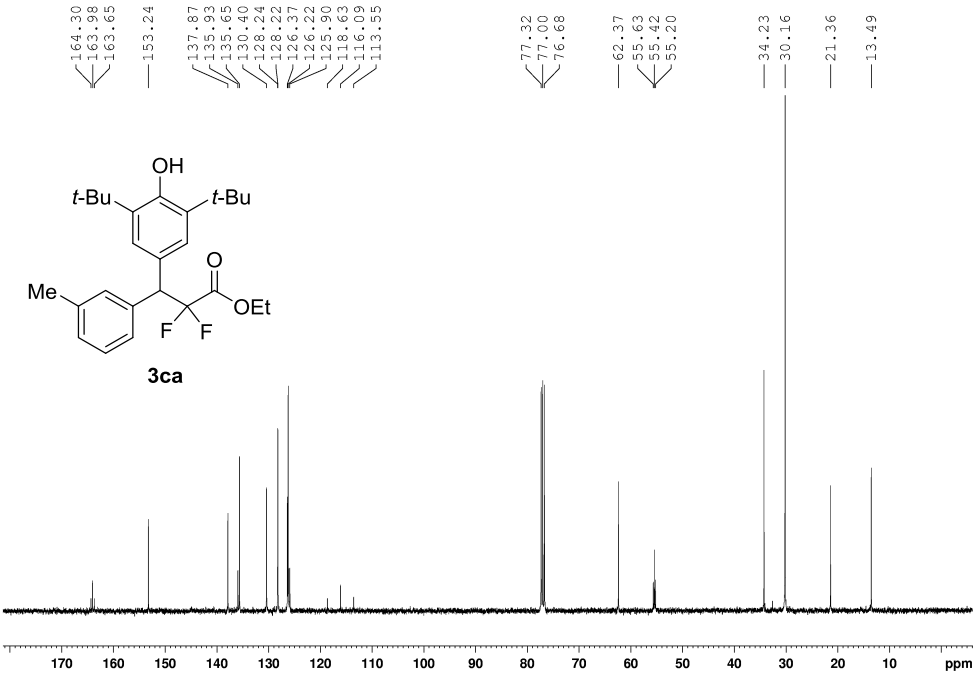
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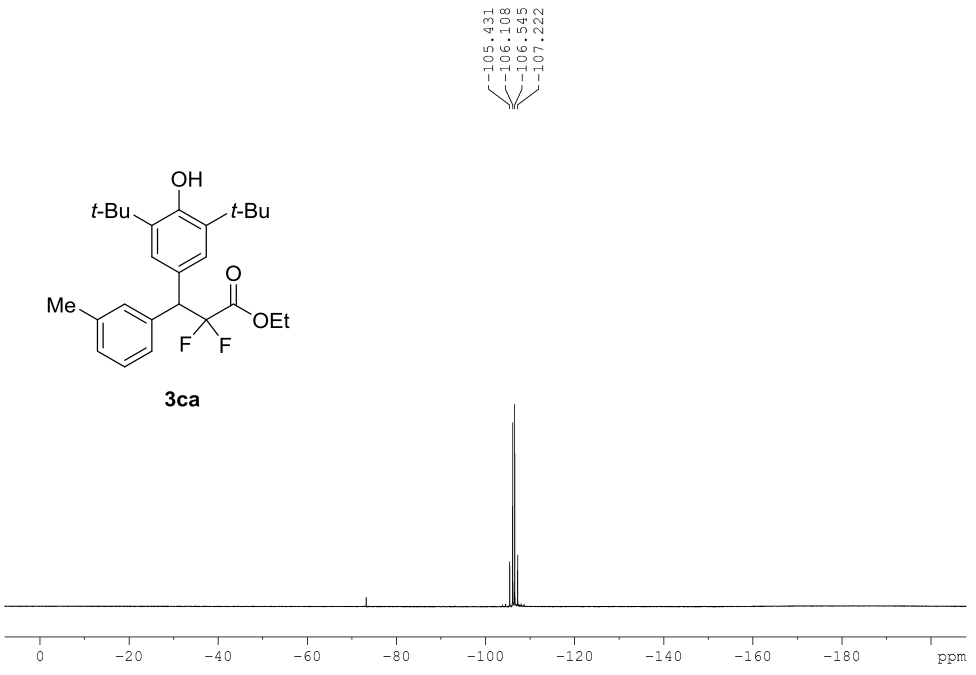
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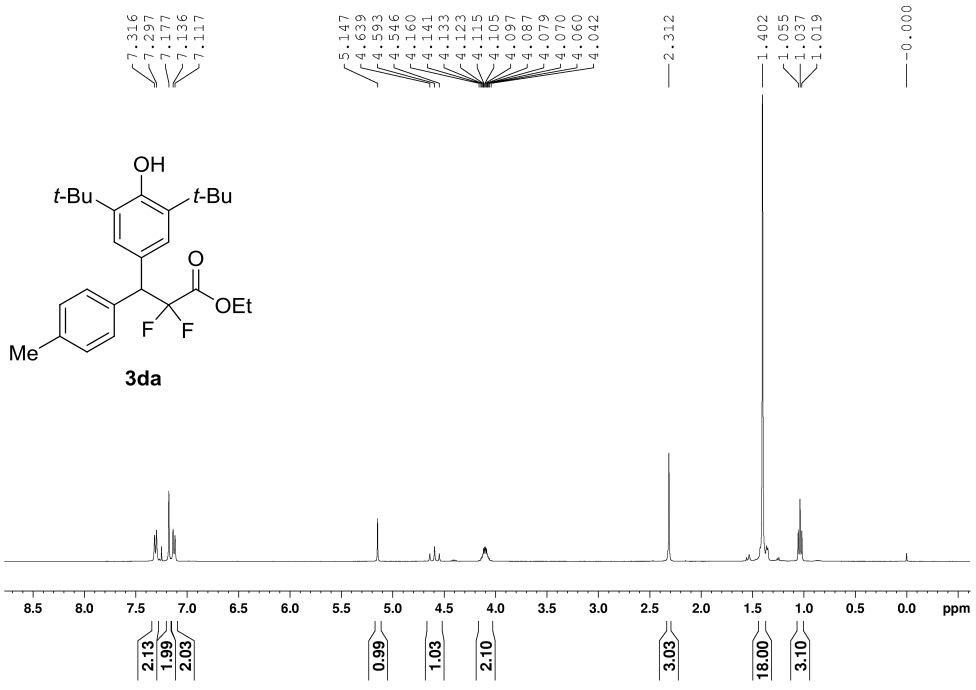
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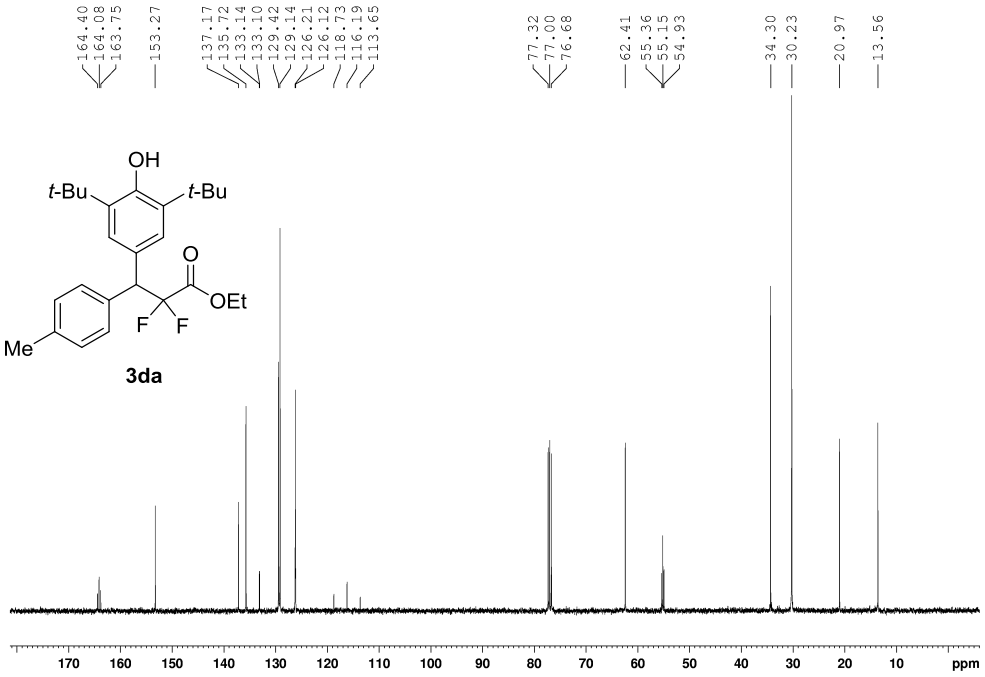
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113.65
77.32
77.00
76.68
62.41
55.36
55.15
54.93
34.30
30.23
20.97
13.56
OH
t-Bu
t-Bu
O
OEt
F
F
Me
3da
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150
140
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110
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90
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70
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30
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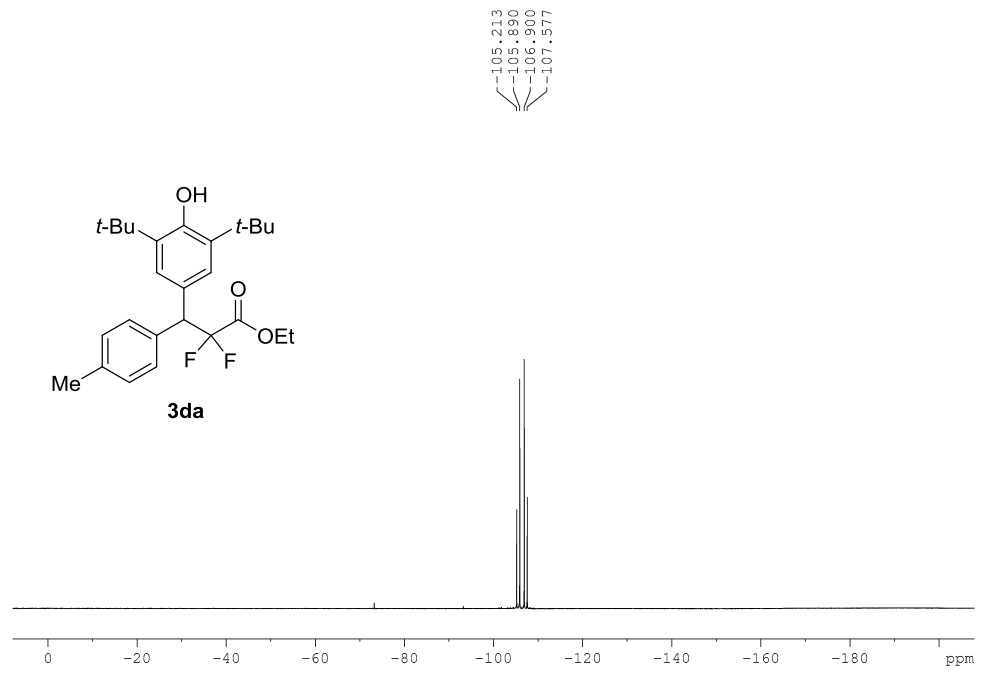
10
ppm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-105.890
-106.900
-107.577
OH
t-Bu
t-Bu
O
OEt
F
F
Me
3da
0
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-40
-60
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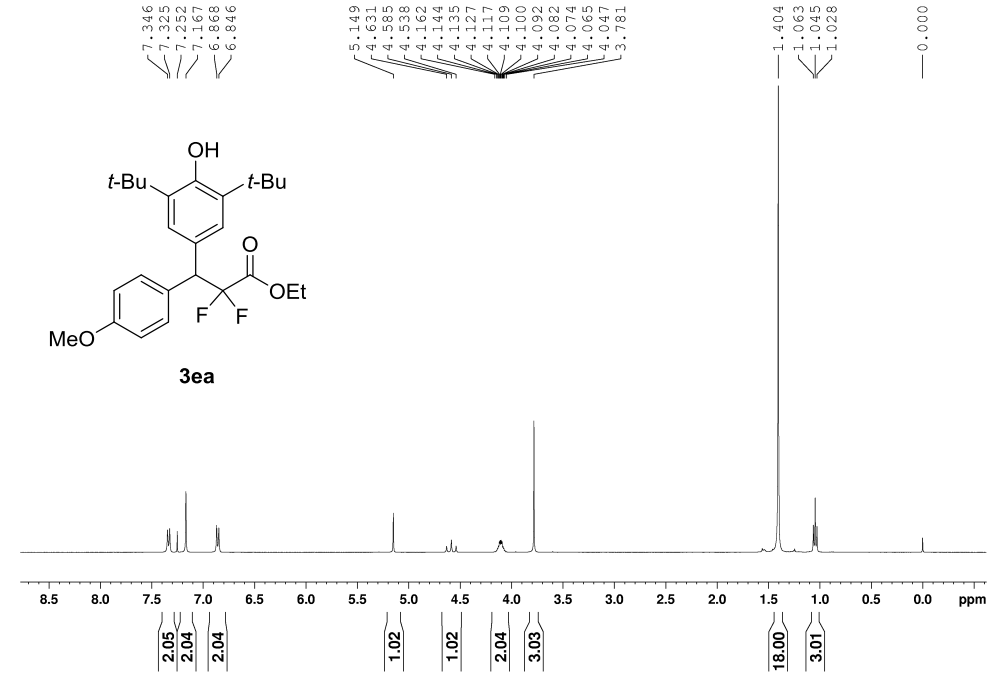
-160
-180
ppm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5.149
4.631
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4.538
4.162
4.144
4.135
4.127
4.117
4.109
4.100
4.092
4.082
4.074
4.065
4.047
3.781
1.404
1.063
1.045
1.028
0.000
OH
t-Bu
t-Bu
O
OEt
F
F
MeO
3ea
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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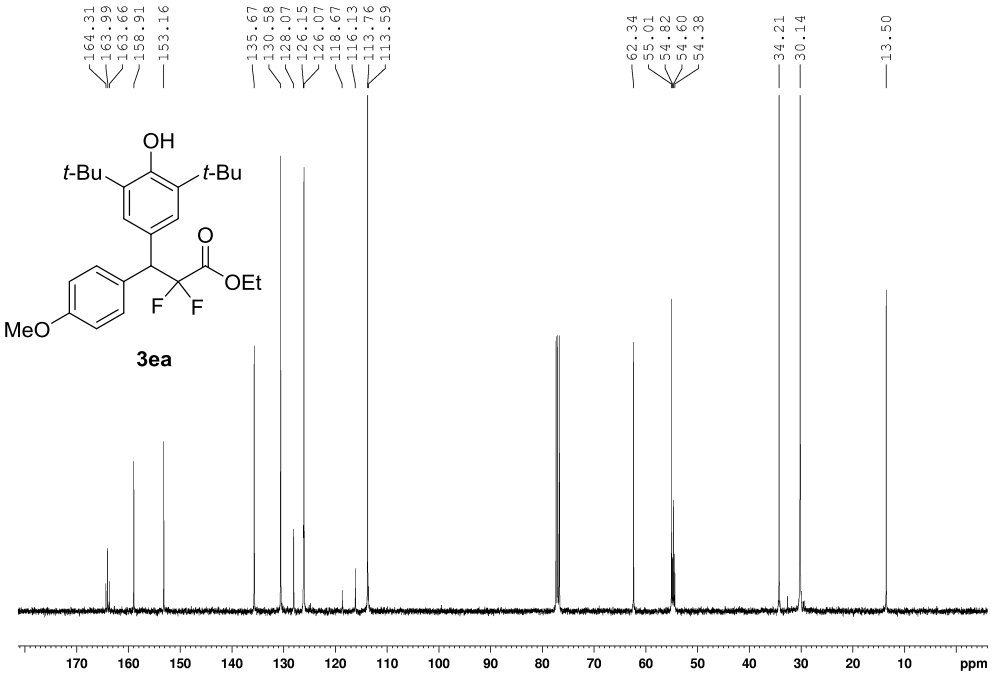
ppm
2.05
2.04
2.04
1.02
1.02
2.04
3.03
18.00
3.01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163.99
163.66
158.91
153.16
135.67
130.58
128.07
126.15
126.07
118.67
116.13
113.76
113.59
62.34
55.01
54.82
54.60
54.38
34.21
30.14
13.50
OH
t-Bu
t-Bu
O
OEt
F
F
MeO
3ea
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150
140
130
120
110
100
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70
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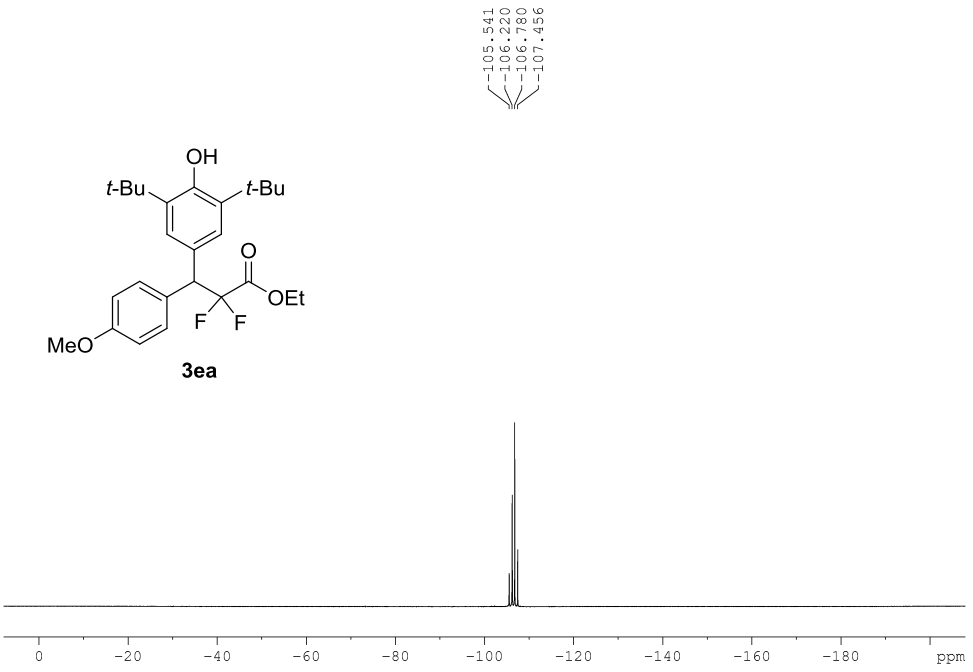
40
30
20
10
ppm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-106.780
-107.456
OH
t-Bu
t-Bu
O
OEt
F
F
MeO
0
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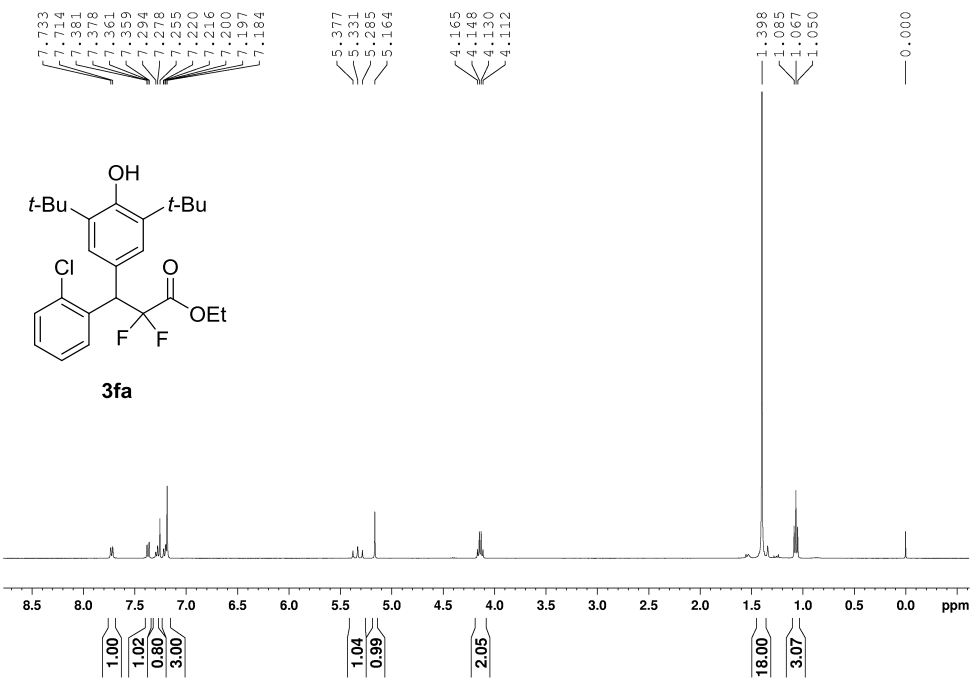
-40
-60
-80
-100
-120
-140
-160
-180
ppm

3ea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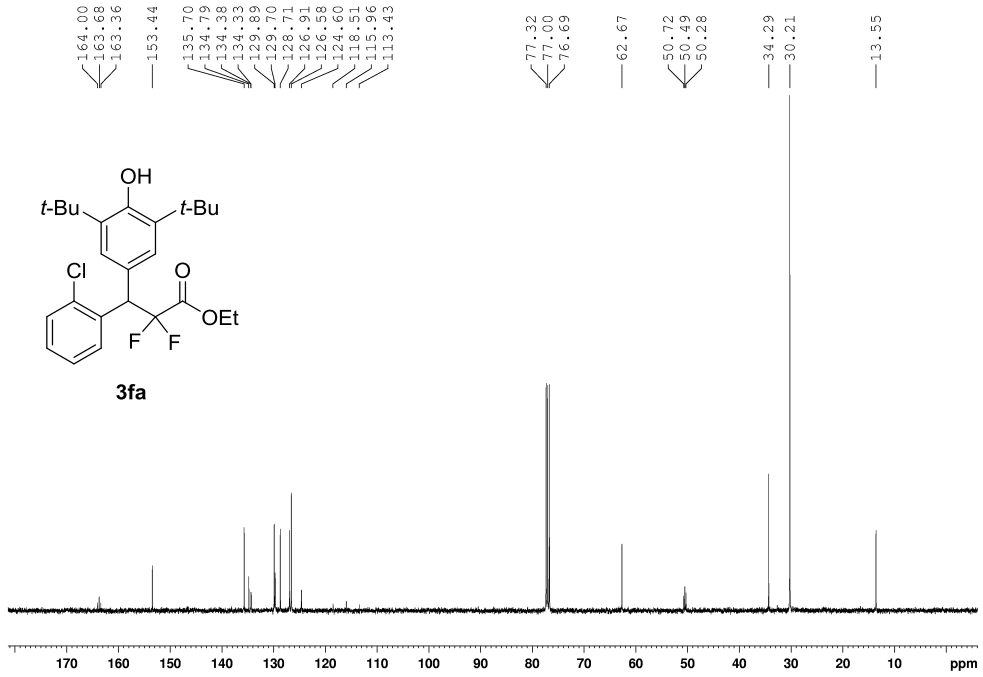
7.714
7.381
7.378
7.361
7.359
7.294
7.278
7.255
7.220
7.216
7.200
7.197
7.184
5.377
5.331
5.285
5.164
4.165
4.148
4.130
4.112
1.398
1.085
1.067
1.050
0.000
OH
t-Bu
t-Bu
Cl
O
OEt
F
F
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.02
0.80
3.00
1.04
0.99
2.05
18.00
3.07

3fa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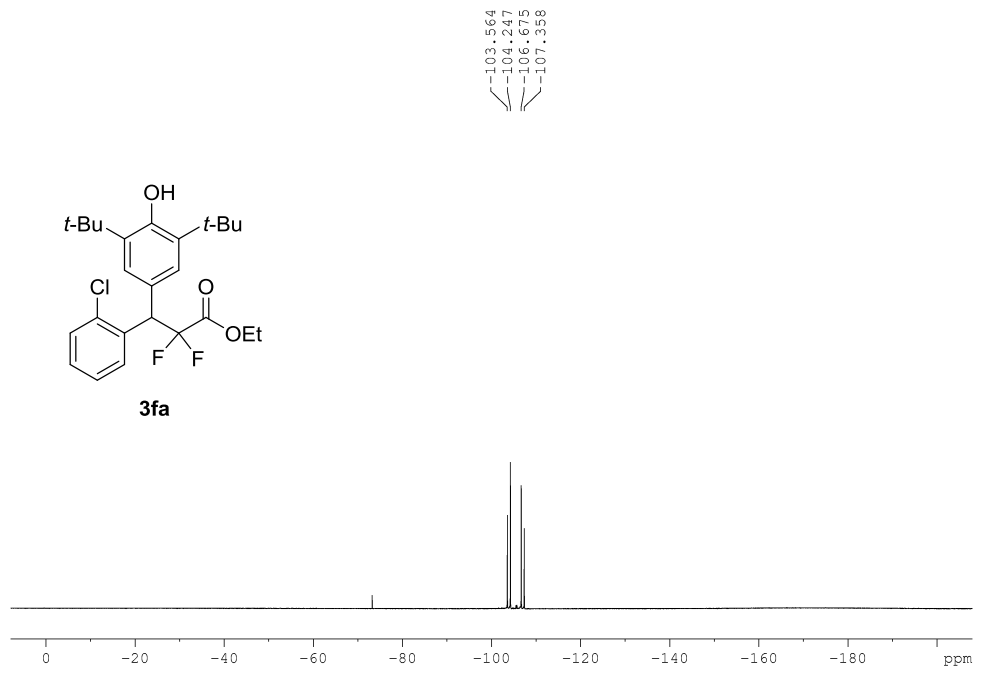
163.36
153.44
135.70
134.79
134.38
134.33
129.89
129.70
128.71
126.91
126.58
124.60
118.51
115.96
113.43
77.32
77.00
76.69
62.67
50.72
50.49
50.28
34.29
30.21
13.55
OH
t-Bu
t-Bu
Cl
O
OEt
F
F
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

3fa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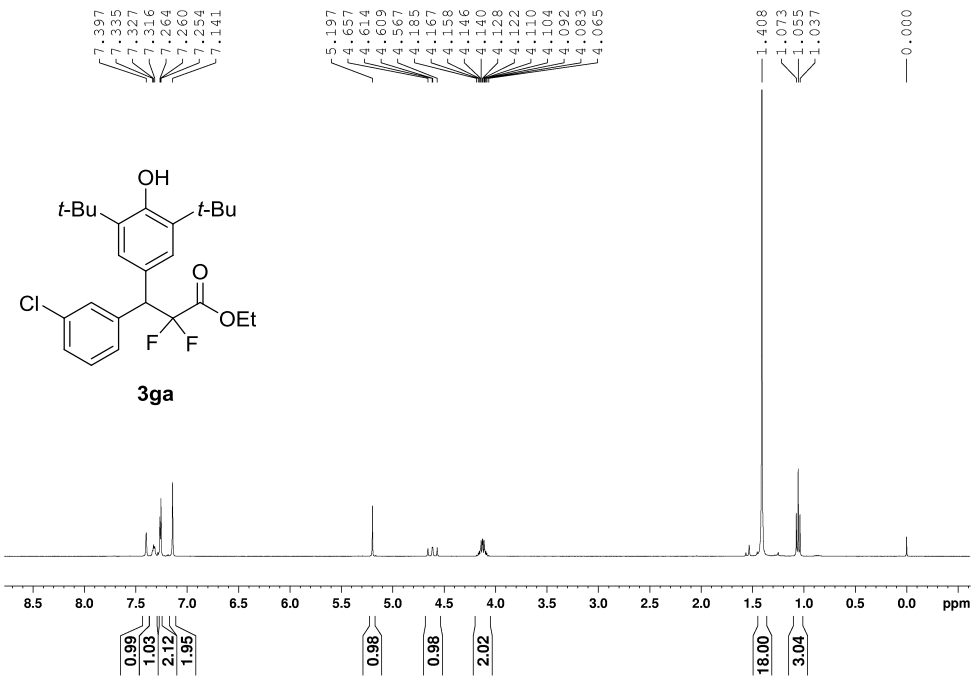
-104.247
-106.675
-107.358
OH
t-Bu
t-Bu
Cl
O
OEt
F
F
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

3fa


7.397
7.335
7.327
7.316
7.264
7.260
7.254
7.141
5.197
4.657
4.614
4.609
4.567
4.185
4.167
4.158
4.146
4.140
4.128
4.122
4.110
4.104
4.092
4.083
4.065
1.408
1.073
1.055
1.037
0.000
OH
t-Bu
t-Bu
O
Cl
OEt
F
F
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
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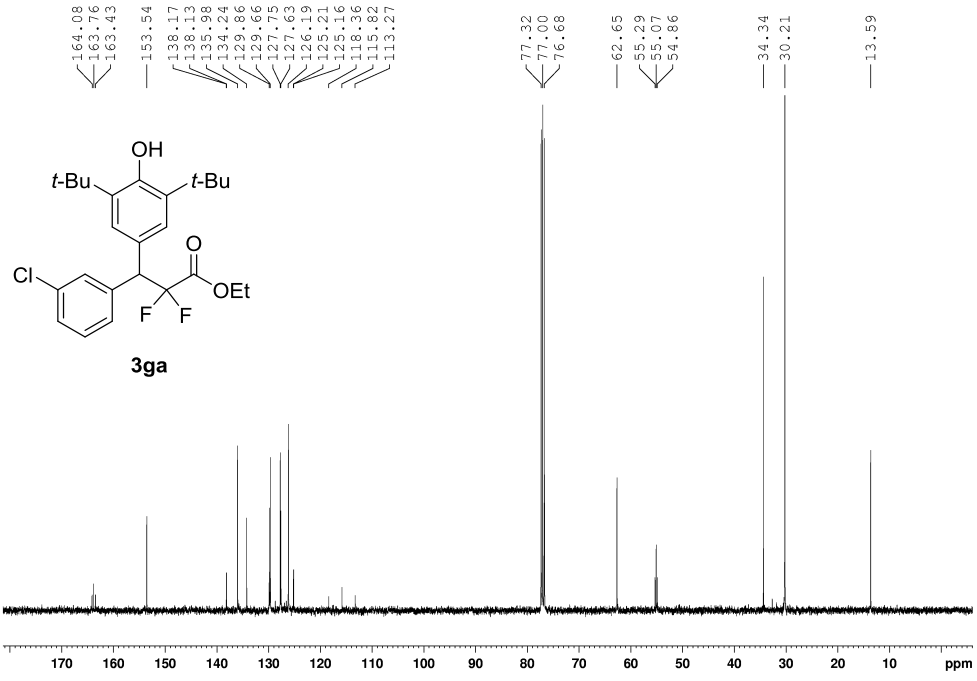
0.99
1.03
2.12
1.95
0.98
0.98
2.02
18.00
3.04

3ga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163.76
163.43
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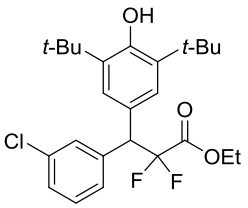
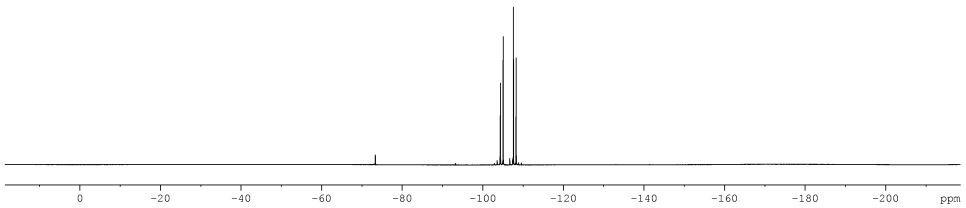
138.17
138.13
135.98
134.24
129.86
129.66
127.75
127.63
126.19
125.21
125.16
118.36
115.82
113.27
77.32
77.00
76.68
62.65
55.29
55.07
54.86
34.34
30.21
13.59
OH
t-Bu
t-Bu
O
Cl
OEt
F
F
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

3ga

-104.371
-105.052
-107.596
-108.277



3ga



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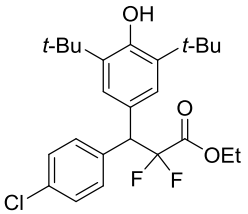
7.307
7.286
7.257
7.128

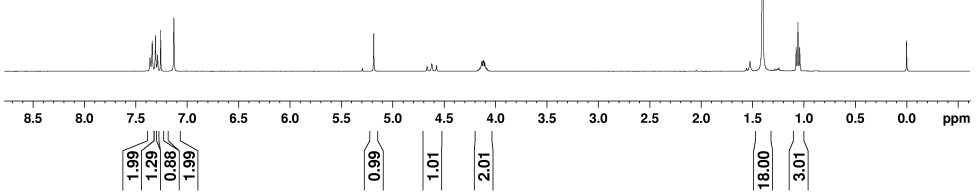
5.184
4.665
4.620
4.574
4.179
4.161
4.152
4.134
4.122
4.116
4.105
4.087
4.078
4.060

1.402
1.075
1.057
1.039

0.000



3ha



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1.29
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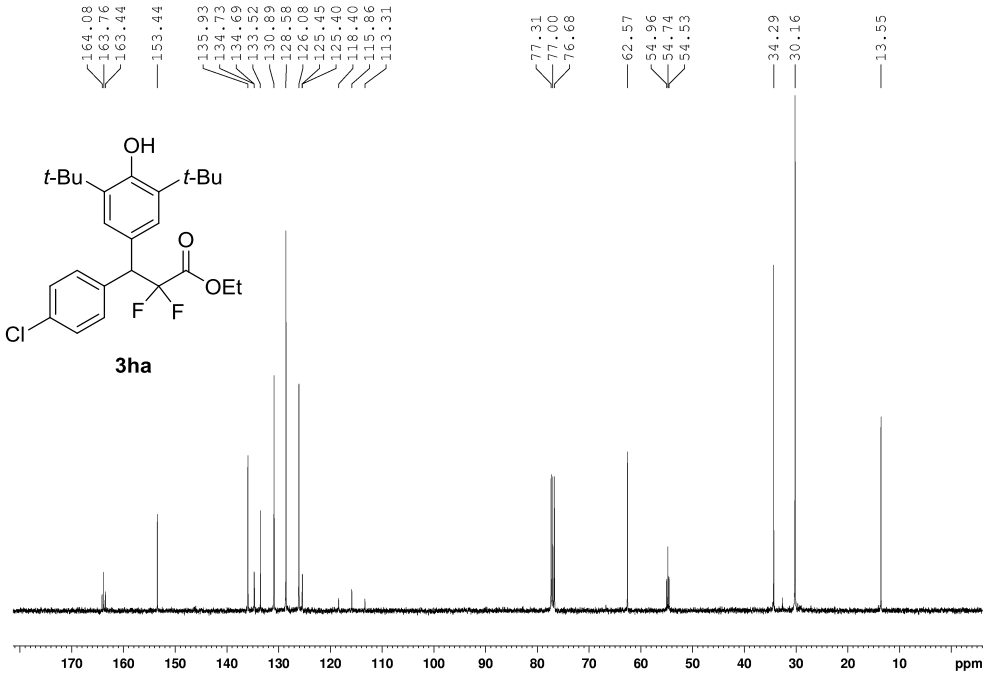
1.99
0.99
1.01
2.01
18.00
3.01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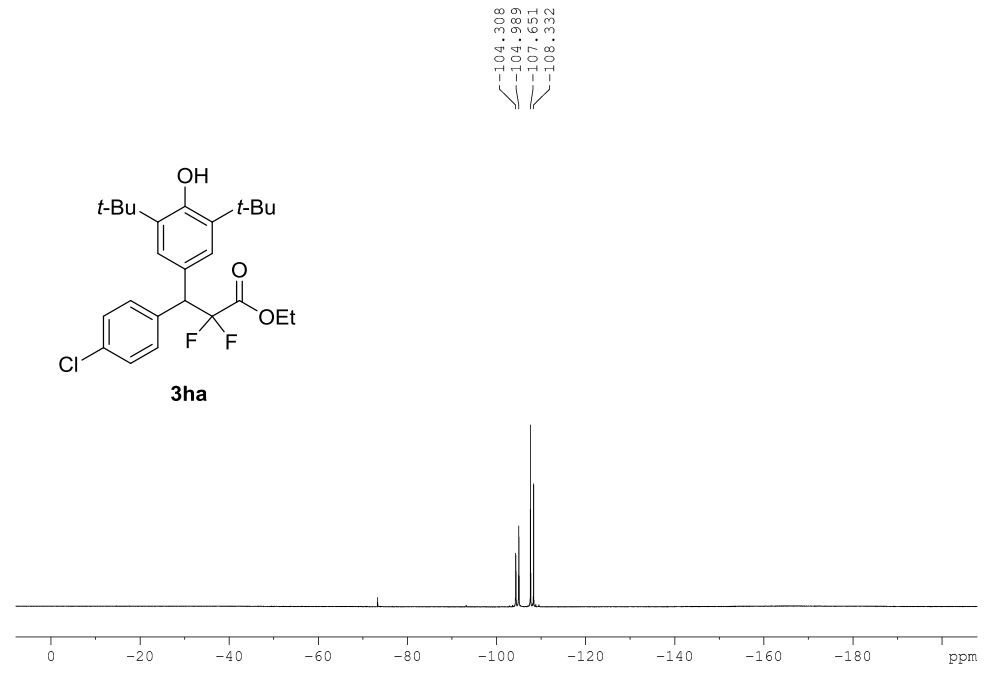
163.76
163.44
153.44
135.93
134.73
134.69
133.52
130.89
128.58
126.08
125.45
125.40
118.40
115.86
113.31
77.31
77.00
76.68
62.57
54.96
54.74
54.53
34.29
30.16
13.55
OH
t-Bu
t-Bu
O
OEt
F
F
Cl
3ha
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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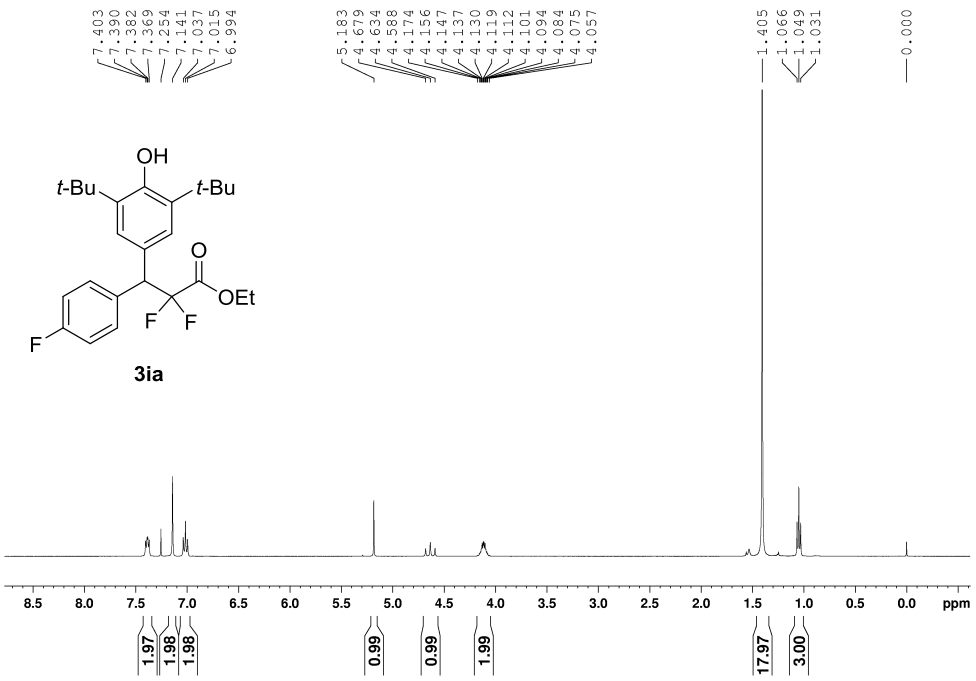
-104.989
-107.651
-108.332
OH
t-Bu
t-Bu
O
OEt
F
F
Cl
3ha
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm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7.254
7.141
7.037
7.015
6.994
5.183
4.679
4.634
4.588
4.174
4.156
4.147
4.137
4.130
4.119
4.112
4.101
4.094
4.084
4.075
4.057
1.405
1.066
1.049
1.031
0.000
OH
t-Bu
t-Bu
O
OEt
F
F
F
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
ppm
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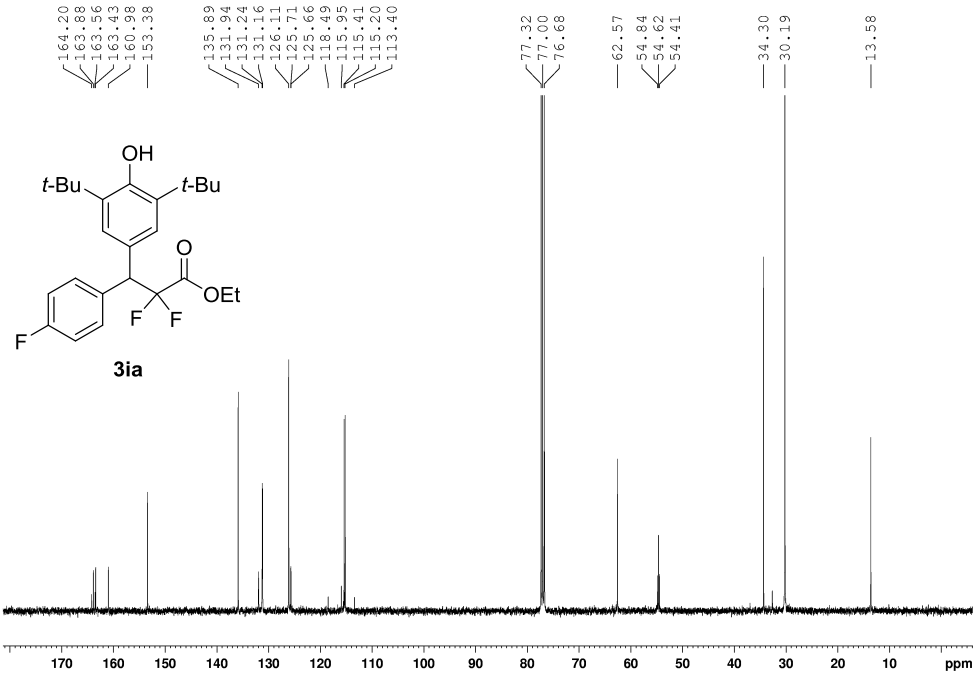
1.98
1.98
0.99
0.99
1.99
17.97
3.00

3ia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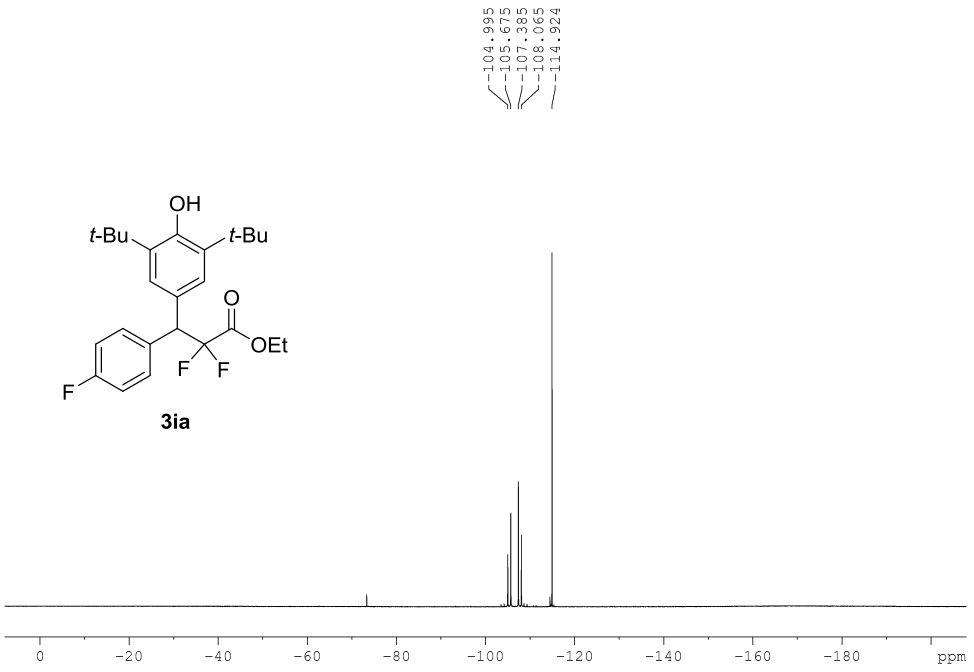
153.38
135.89
131.94
131.24
131.16
126.11
125.71
125.66
118.49
115.95
115.41
115.20
113.40
77.32
77.00
76.68
62.57
54.84
54.62
54.41
34.30
30.19
13.58
OH
t-Bu
t-Bu
O
OEt
F
F
F
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

3ia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-114.924
OH
t-Bu
t-Bu
O
OEt
F
F
F
0
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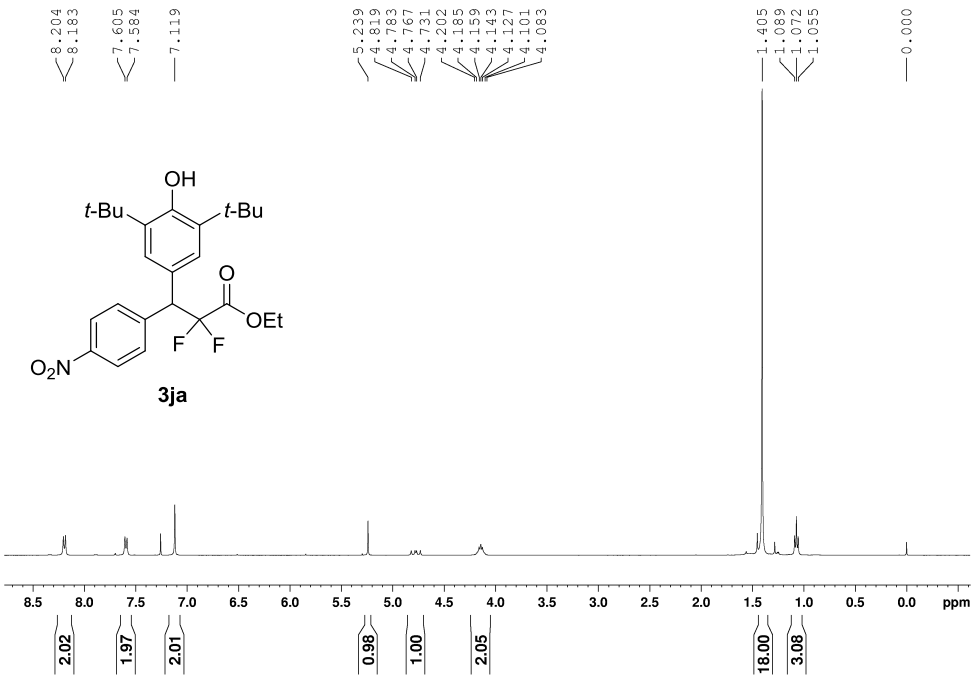
-40
-60
-80
-100
-120
-140
-160
-180
ppm

3ia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7.119
5.239
4.819
4.783
4.767
4.731
4.202
4.185
4.159
4.143
4.127
4.101
4.083
1.405
1.089
1.072
1.055
0.000
OH
t-Bu
t-Bu
O
OEt
F
F
O2N
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
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ppm
2.02
1.97
2.01
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1.00
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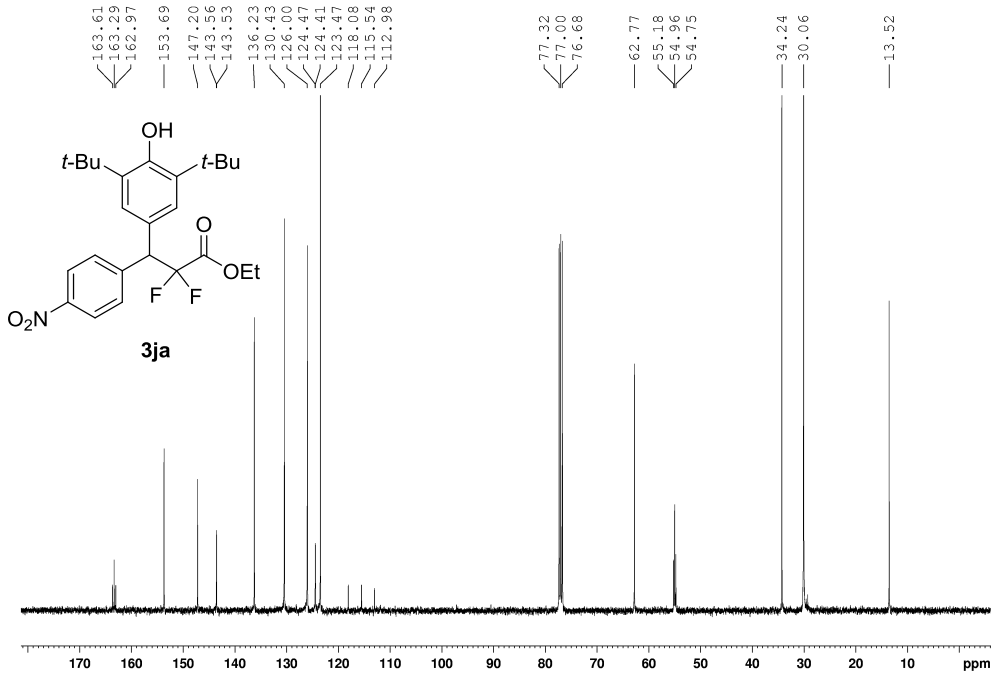
18.00
3.08

3ja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143.56
143.53
136.23
130.43
126.00
124.47
124.41
123.47
118.08
115.54
112.98
77.32
77.00
76.68
62.77
55.18
54.96
54.75
34.24
30.06
13.52
OH
t-Bu
t-Bu
O
OEt
F
F
O2N
3ja
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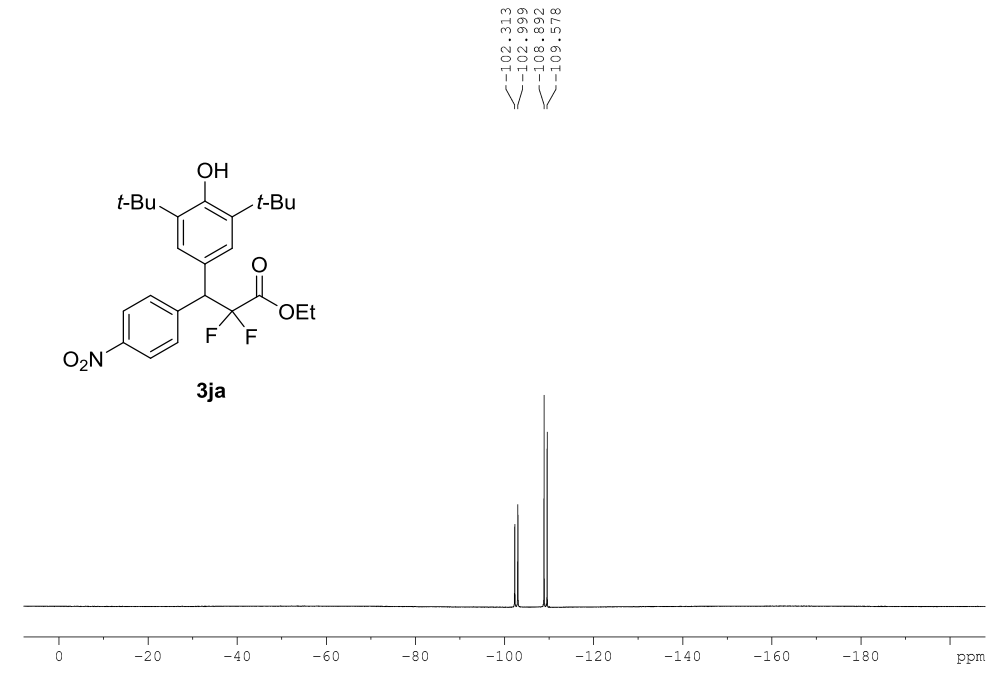
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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t-Bu
O
OEt
F
F
O2N
3ja
0
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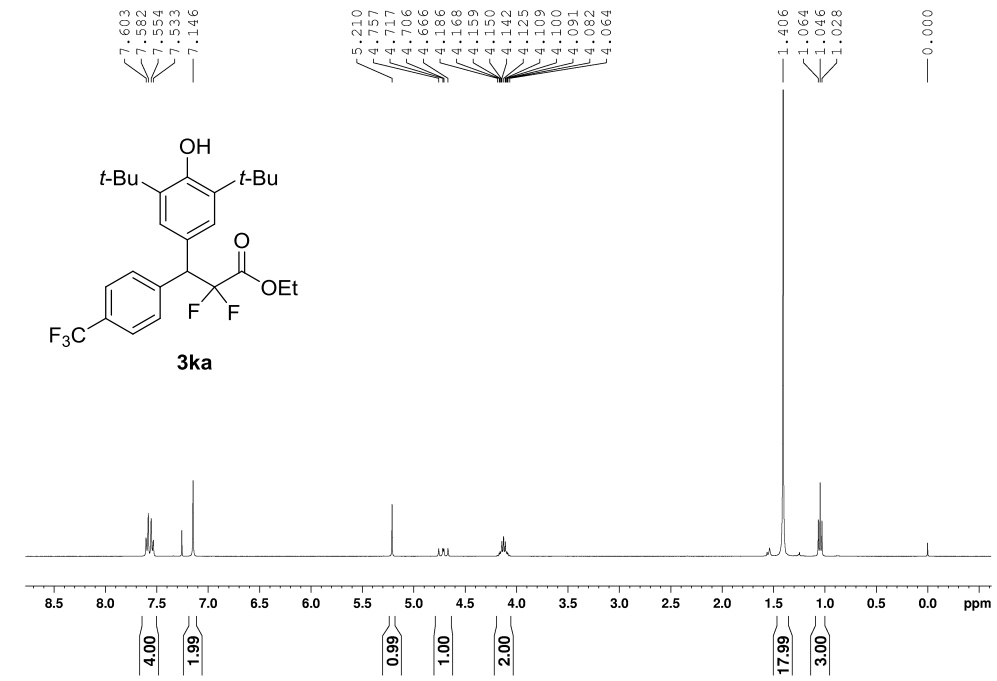
-40
-60
-80
-100
-120
-140
-160
-180
ppm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4.757
4.717
4.706
4.666
4.186
4.168
4.159
4.150
4.142
4.125
4.109
4.100
4.091
4.082
4.064
1.406
1.064
1.046
1.028
0.000
OH
t-Bu
t-Bu
O
OEt
F
F
F3C
3ka
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
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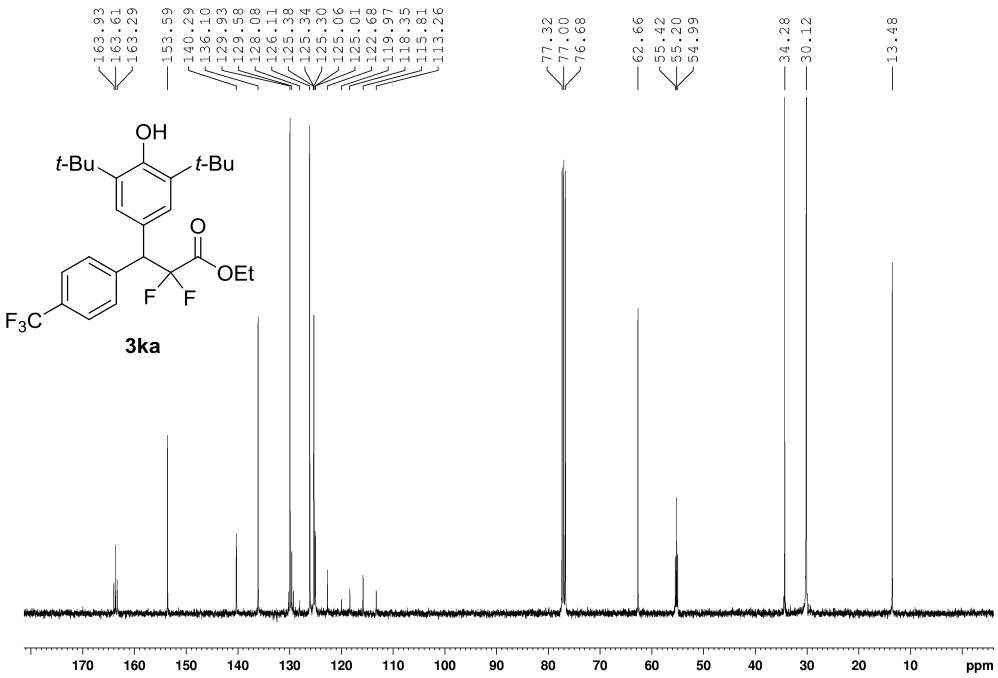
3.00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136.10
129.93
129.58
128.08
126.11
125.38
125.34
125.30
125.06
125.01
122.68
119.97
118.35
115.81
113.26
77.32
77.00
76.68
62.66
55.42
55.20
54.99
34.28
30.12
13.48
OH
t-Bu
t-Bu
O
OEt
F
F
F3C
3ka
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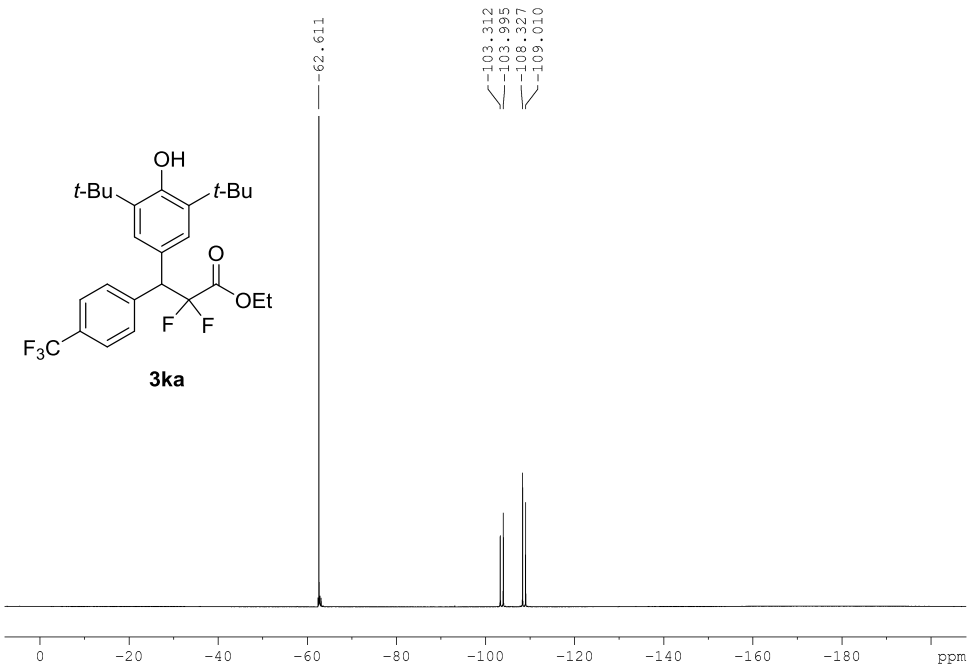
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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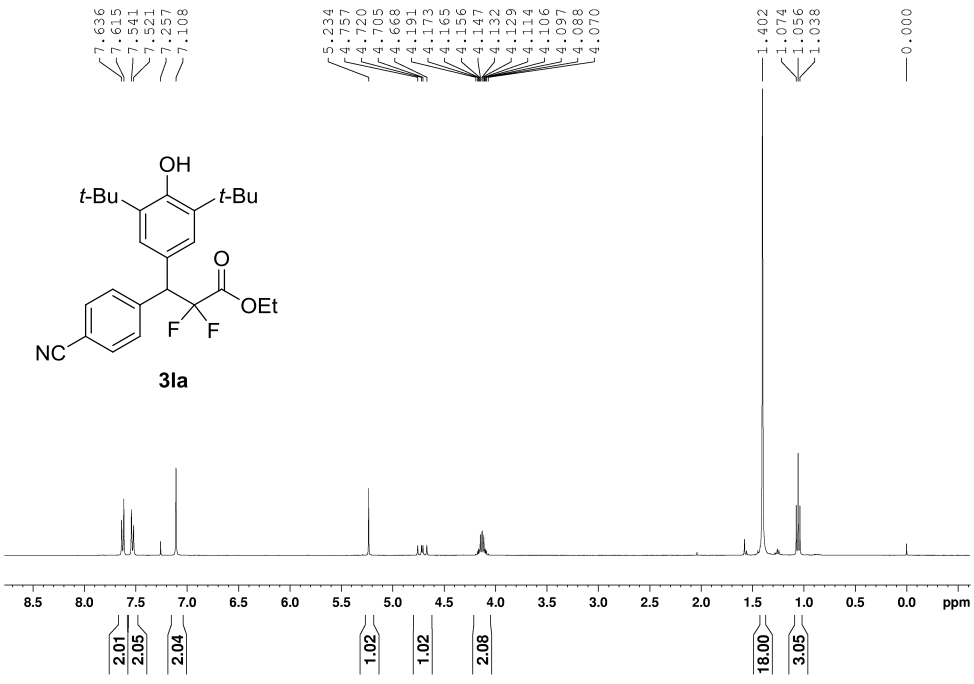
-103.995
-108.327
-109.010
OH
t-Bu
t-Bu
O
OEt
F
F
F3C
3ka
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm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7.521
7.257
7.108
5.234
4.757
4.720
4.705
4.668
4.191
4.173
4.165
4.156
4.147
4.132
4.129
4.114
4.106
4.097
4.088
4.070
1.402
1.074
1.056
1.038
0.000
OH
t-Bu
t-Bu
O
OEt
F
F
NC
3la
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
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0.0
ppm
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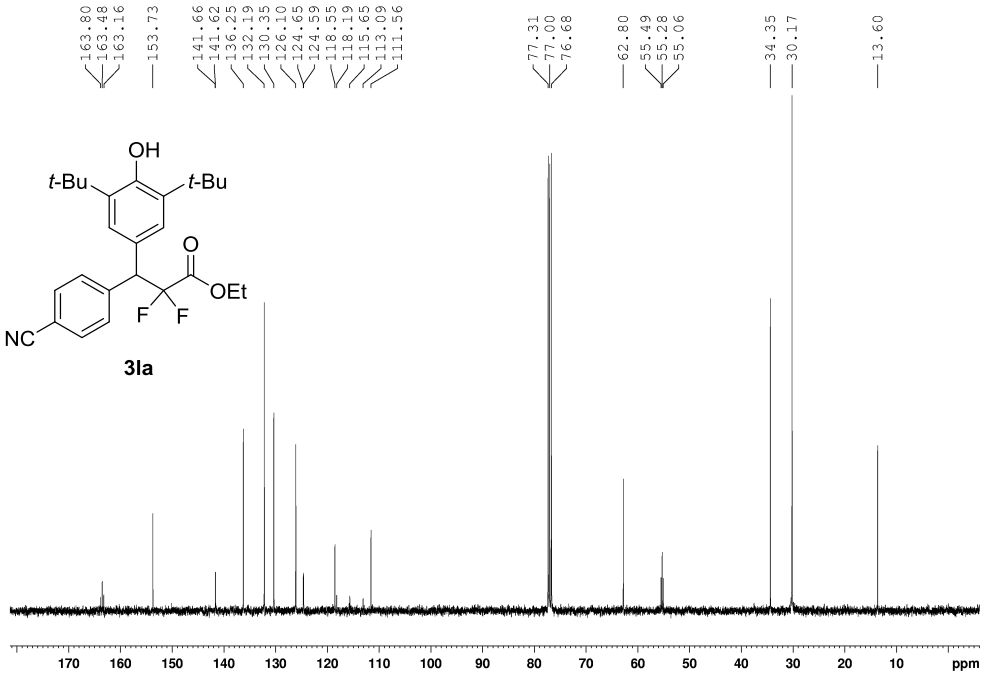
2.05
2.04
1.02
1.02
2.08
18.00
3.05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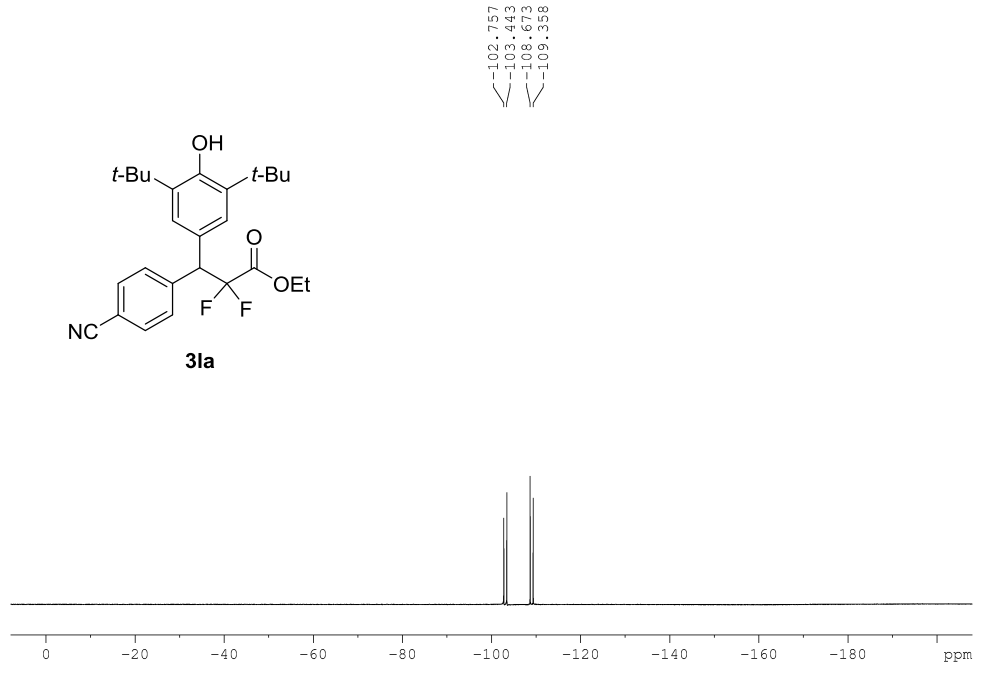
163.48
163.16
153.73
141.66
141.62
136.25
132.19
130.35
126.10
124.65
124.59
118.55
118.19
115.65
113.09
111.56
77.31
77.00
76.68
62.80
55.49
55.28
55.06
34.35
30.17
13.60
OH
t-Bu
t-Bu
O
OEt
F
F
NC
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

3la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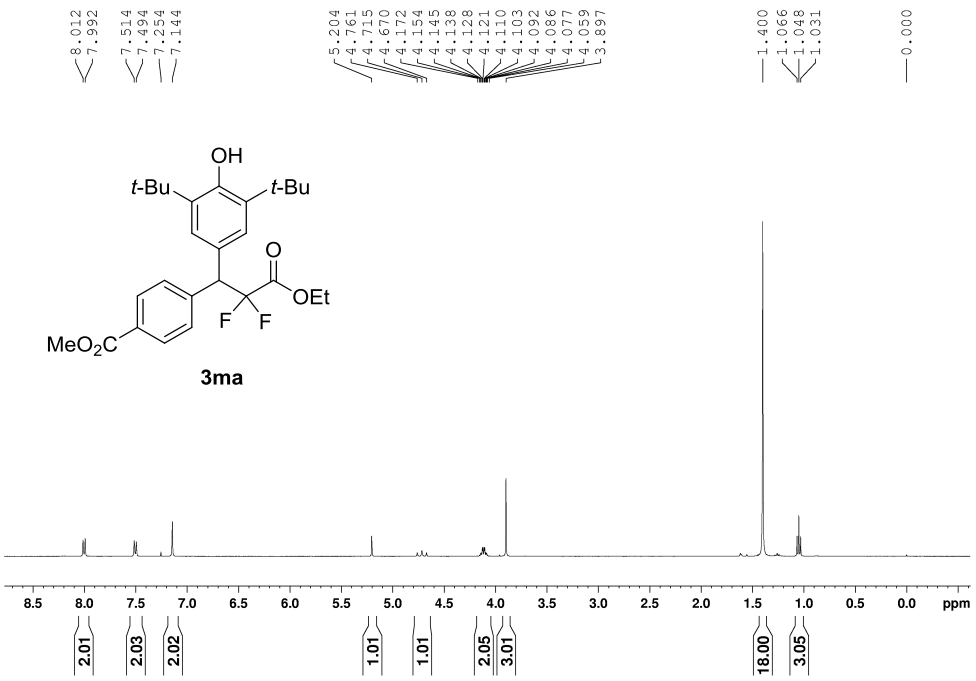
-103.443
-108.673
-109.358
OH
t-Bu
t-Bu
O
OEt
F
F
NC
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

3la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7.992
7.514
7.494
7.254
7.144
5.204
4.761
4.715
4.670
4.172
4.154
4.145
4.138
4.128
4.121
4.110
4.103
4.092
4.086
4.077
4.059
3.897
1.400
1.066
1.048
1.031
0.000
OH
t-Bu
t-Bu
O
OEt
F
F
MeO2C
3ma
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
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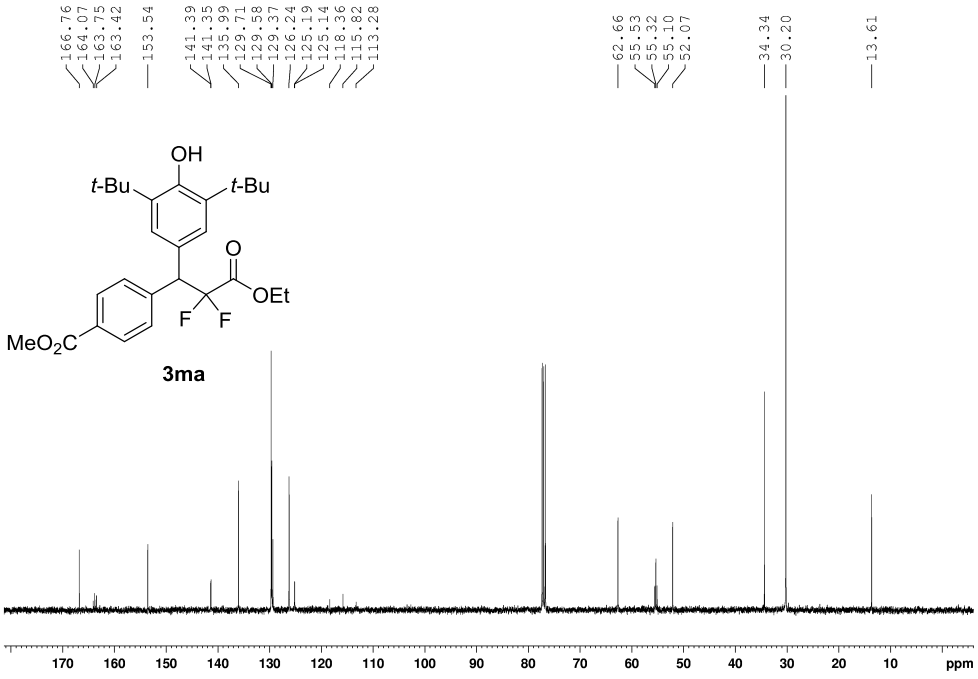
ppm
2.01
2.03
2.02
1.01
1.01
2.05
3.01
18.00
3.05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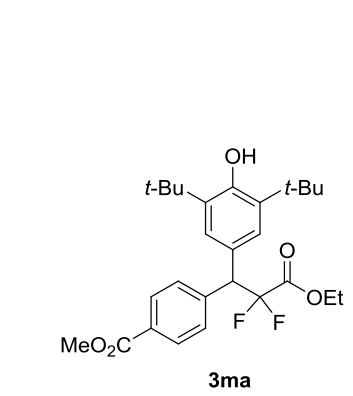
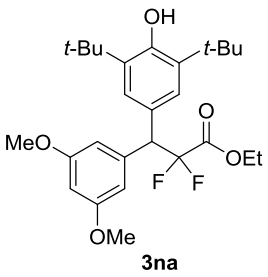
164.07
163.75
163.42
153.54
141.39
141.35
135.99
129.71
129.58
129.37
126.24
125.19
125.14
118.36
115.82
113.28
62.66
55.53
55.32
55.10
52.07
34.34
30.20
13.61
OH
t-Bu
t-Bu
O
OEt
F
F
MeO2C
3ma
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


OH
t-Bu
t-Bu
O
OEt
F
F
MeO2C

3ma

-104.582
-105.265
-107.150
-107.833
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm


OH
t-Bu
t-Bu
O
MeO
OEt
F
F
OMe

3na

7.257
7.191
6.976
6.965
6.833
6.822
6.811
5.166
4.623
4.577
4.531
4.149
4.138
4.122
4.120
4.104
4.086
4.075
3.867
3.854
1.410
1.073
1.056
1.038
0.000
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
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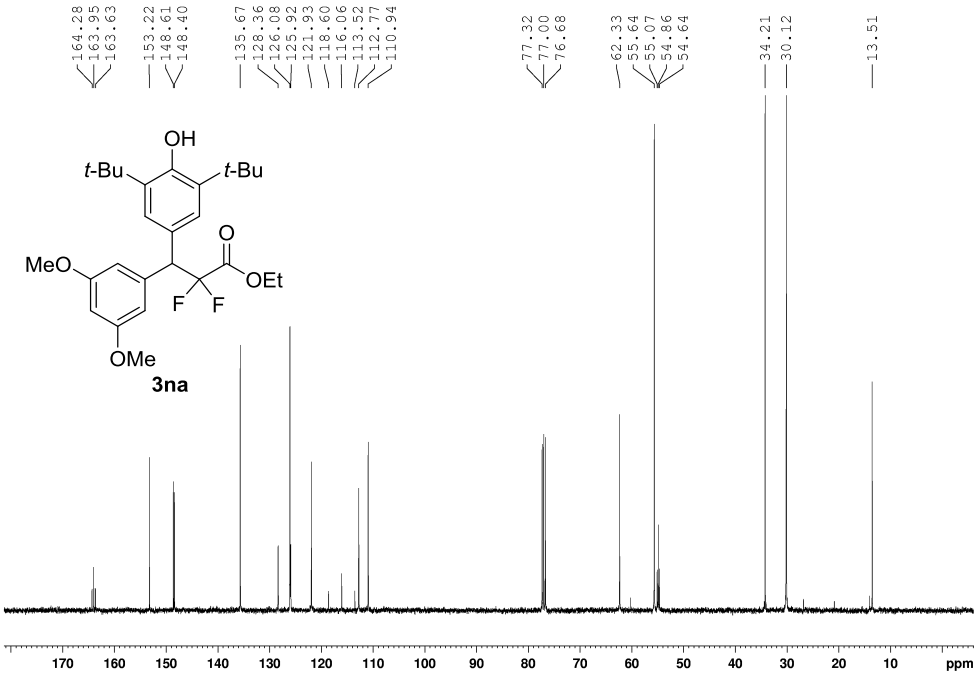
0.0
ppm
1.97
1.99
0.99
0.98
0.99
2.05
2.91
2.97
18.00
3.03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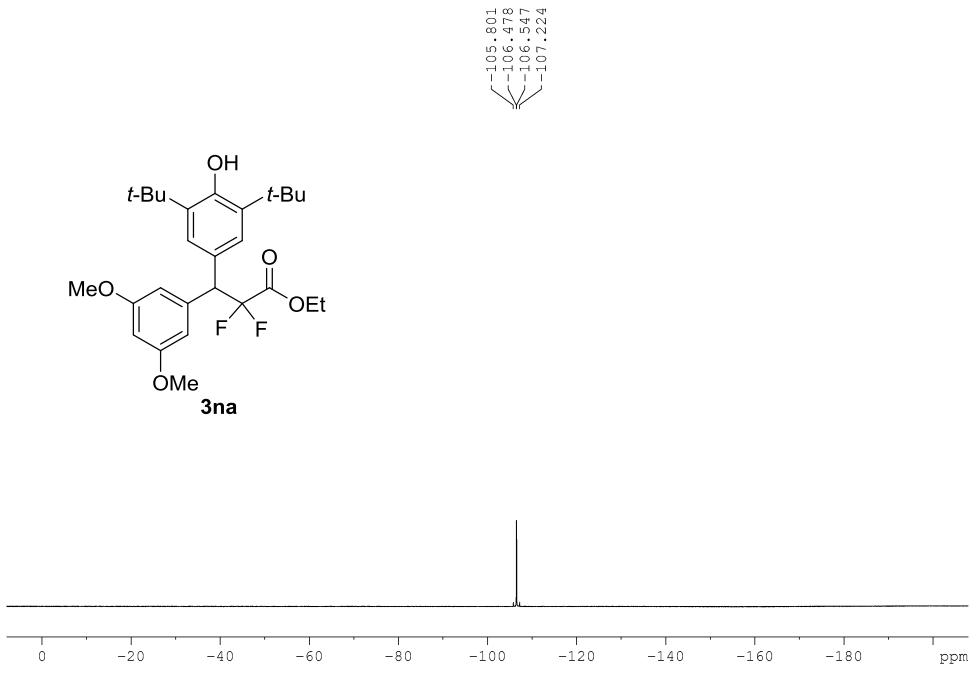
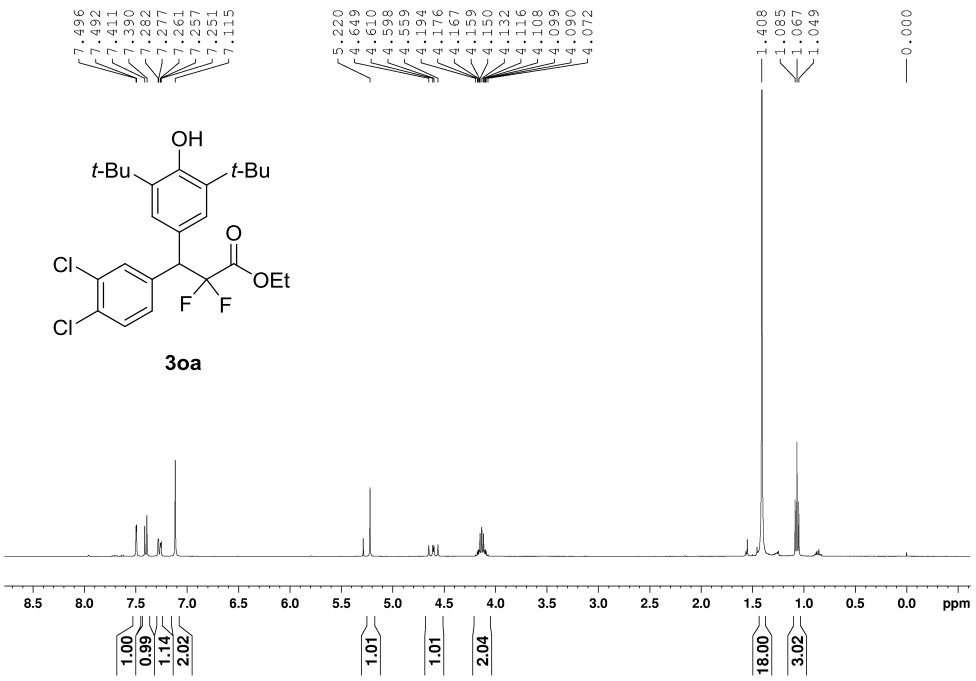
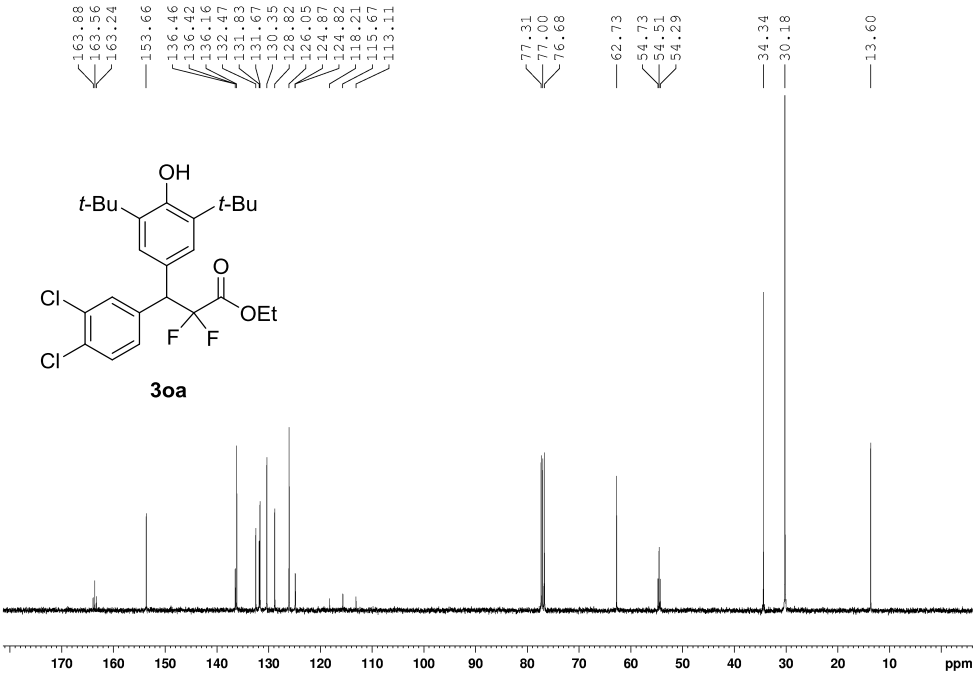
163.95
163.63
153.22
148.61
148.40
135.67
128.36
126.08
125.92
121.93
118.60
116.06
113.52
112.77
110.94
77.32
77.00
76.68
62.33
55.64
55.07
54.86
54.64
34.21
30.12
13.51
OH
t-Bu
t-Bu
O
MeO
OEt
F
F
OMe
3na
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-105.801
-106.478
-106.547
-107.224
OH
t-Bu
t-Bu
O
MeO
OEt
F
F
OMe
3na
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm


7.496
7.492
7.411
7.390
7.282
7.277
7.261
7.257
7.251
7.115
5.220
4.649
4.610
4.598
4.559
4.194
4.176
4.167
4.159
4.150
4.132
4.116
4.108
4.099
4.090
4.072
1.408
1.085
1.067
1.049
0.000
OH
t-Bu
t-Bu
O
Cl
OEt
F
F
Cl
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
ppm
1.00
0.99
1.14
2.02
1.01
1.01
2.04
18.00
3.02

3oa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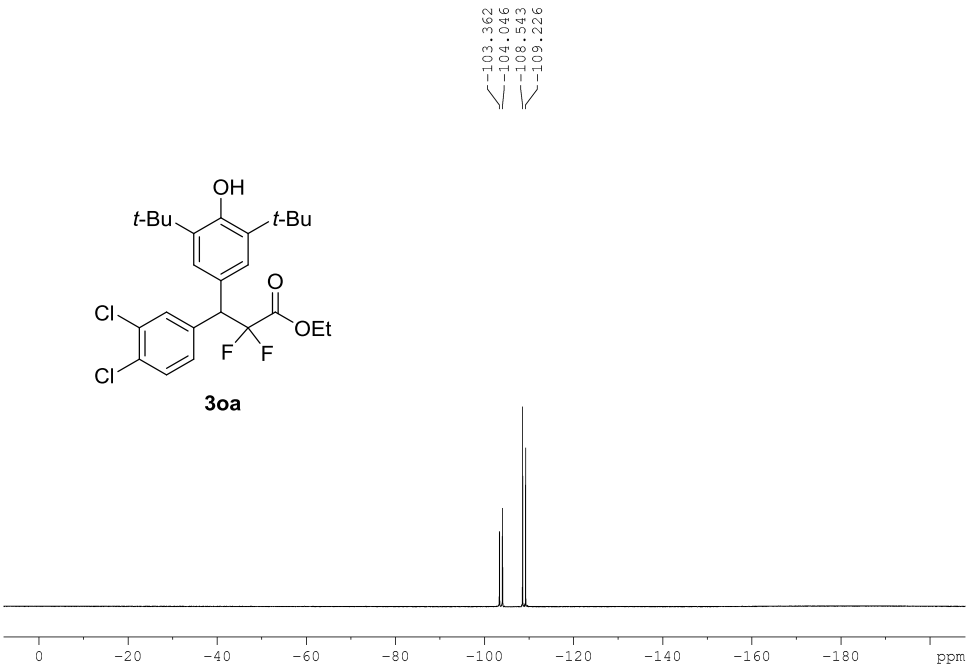
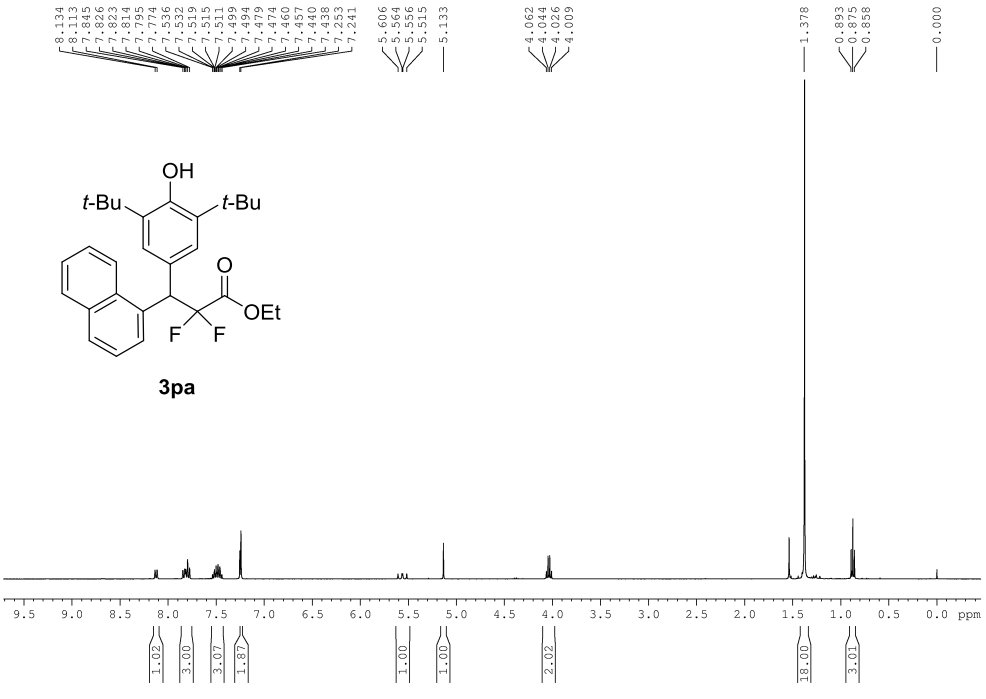
163.56
163.24
153.66
136.46
136.42
136.16
132.47
131.83
131.67
130.35
128.82
126.05
124.87
124.82
118.21
115.67
113.11
77.31
77.00
76.68
62.73
54.73
54.51
54.29
34.34
30.18
13.60
OH
t-Bu
t-Bu
O
Cl
OEt
F
F
Cl
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

3oa


-103.362
-104.046
-108.543
-109.226
OH
t-Bu
t-Bu
O
Cl
OEt
F
F
Cl
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

3oa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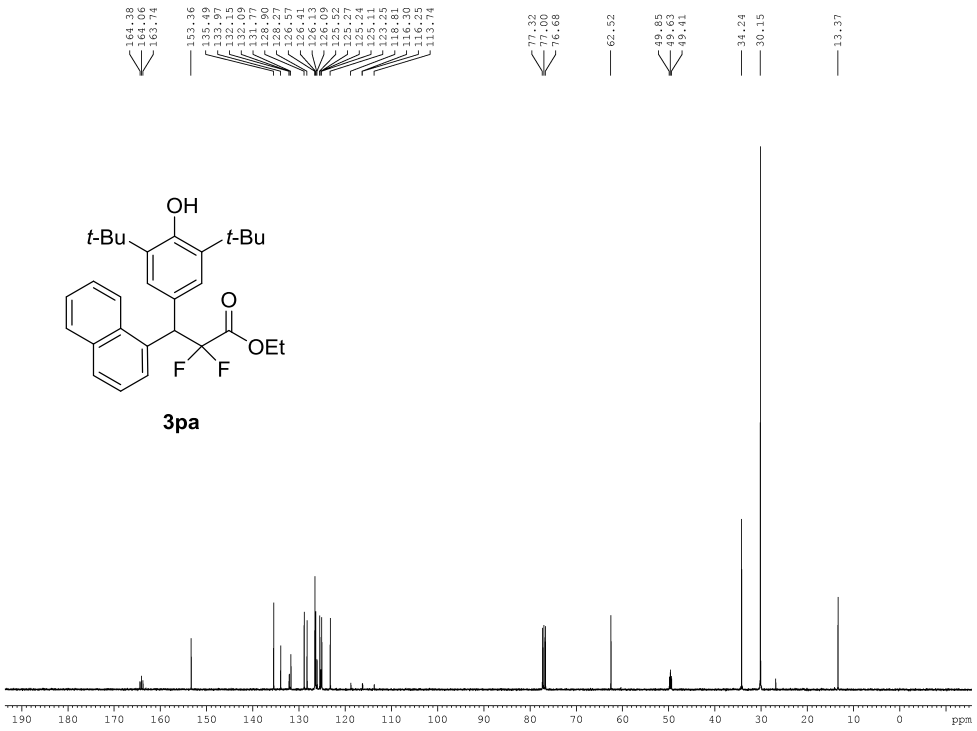
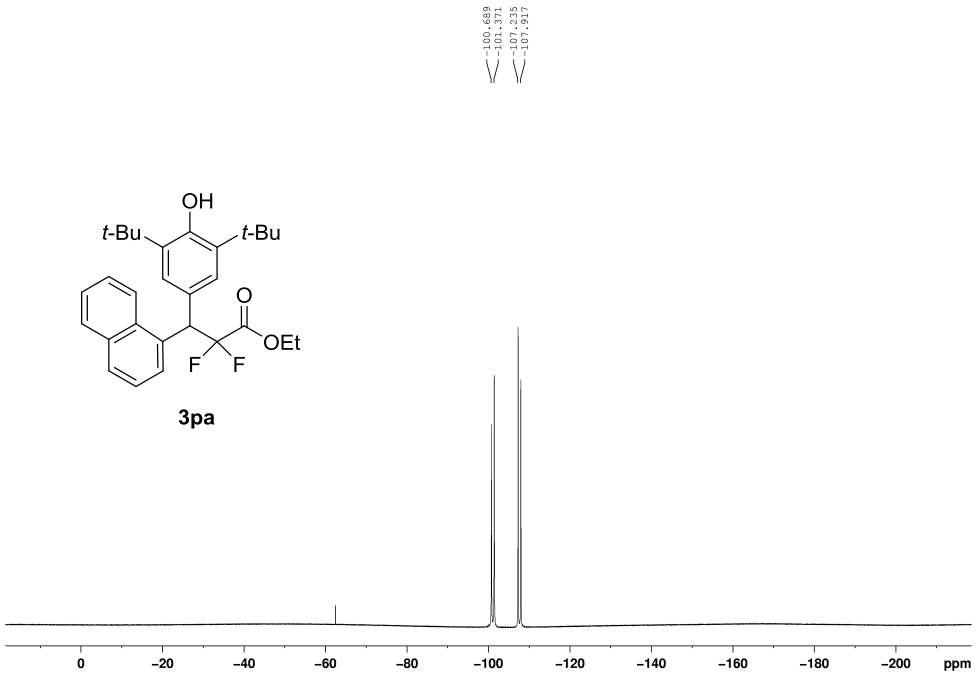
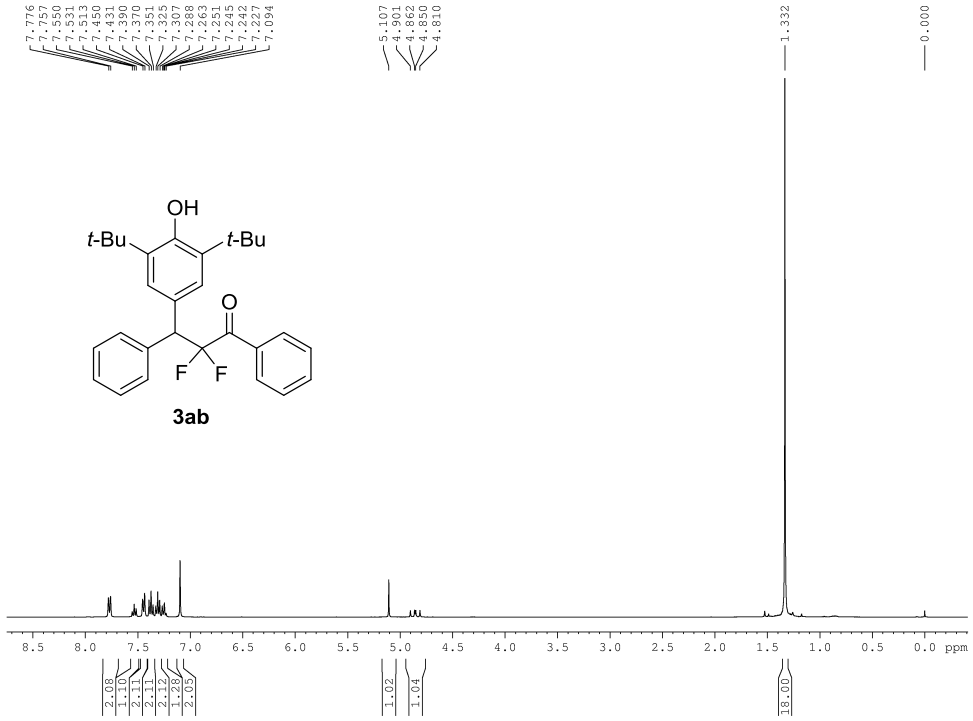
8.113
7.845
7.826
7.823
7.814
7.795
7.774
7.536
7.532
7.519
7.515
7.511
7.499
7.494
7.479
7.474
7.460
7.457
7.440
7.438
7.253
7.241
5.606
5.564
5.556
5.515
5.133
4.062
4.044
4.026
4.009
1.378
0.893
0.875
0.858
0.000
OH
t-Bu
t-Bu
O
OEt
F
F
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.02
3.00
3.07
1.87
1.00
1.00
2.02
18.00
3.01

3pa


164.38
164.06
163.74
153.36
135.49
133.97
132.15
132.09
131.77
128.90
128.27
126.57
126.41
126.13
126.09
125.52
125.27
125.24
125.11
123.25
118.81
116.30
116.25
113.74
77.32
77.00
76.68
62.52
49.85
49.63
49.41
34.24
30.15
13.37
OH
t-Bu
t-Bu
O
OEt
F
F
3pa
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


-100.689
-101.371
-107.235
-107.917
OH
t-Bu
t-Bu
O
OEt
F
F
3pa
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm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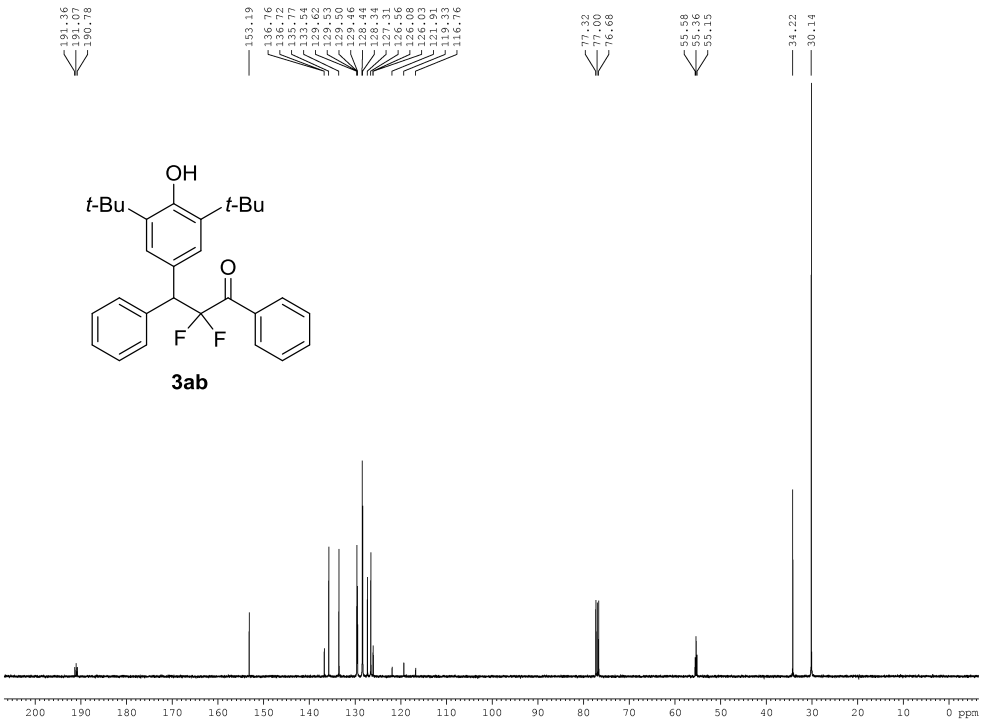
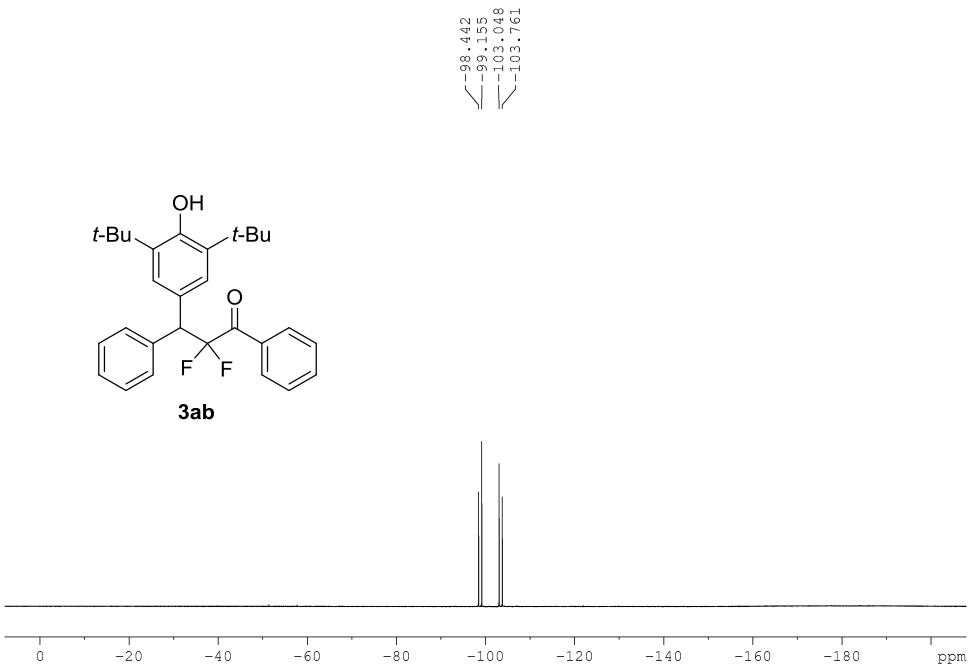
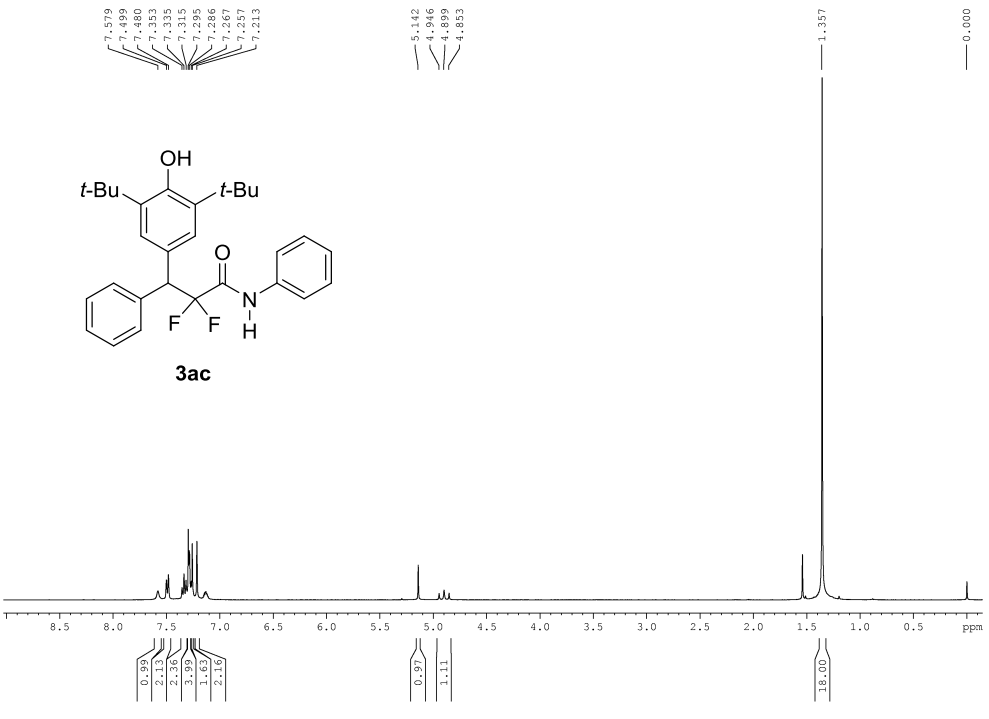
7.757
7.550
7.531
7.513
7.450
7.431
7.390
7.370
7.351
7.325
7.307
7.288
7.263
7.251
7.245
7.242
7.227
7.094
5.107
4.901
4.862
4.850
4.810
1.332
0.000
OH
t-Bu
t-Bu
O
F
F
3ab
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.08
1.10
2.11
2.11
2.12
1.28
2.05
1.02
1.04
18.00


191.36
191.07
190.78
153.19
136.76
136.72
135.77
133.54
129.62
129.53
129.50
129.46
128.44
128.34
127.31
126.56
126.08
126.03
121.91
119.33
116.76
77.32
77.00
76.68
55.58
55.36
55.15
34.22
30.14
OH
t-Bu
t-Bu
O
F
F
3ab
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


-98.442
-99.155
-103.048
-103.761
OH
t-Bu
t-Bu
O
F
F
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

3ab


7.579
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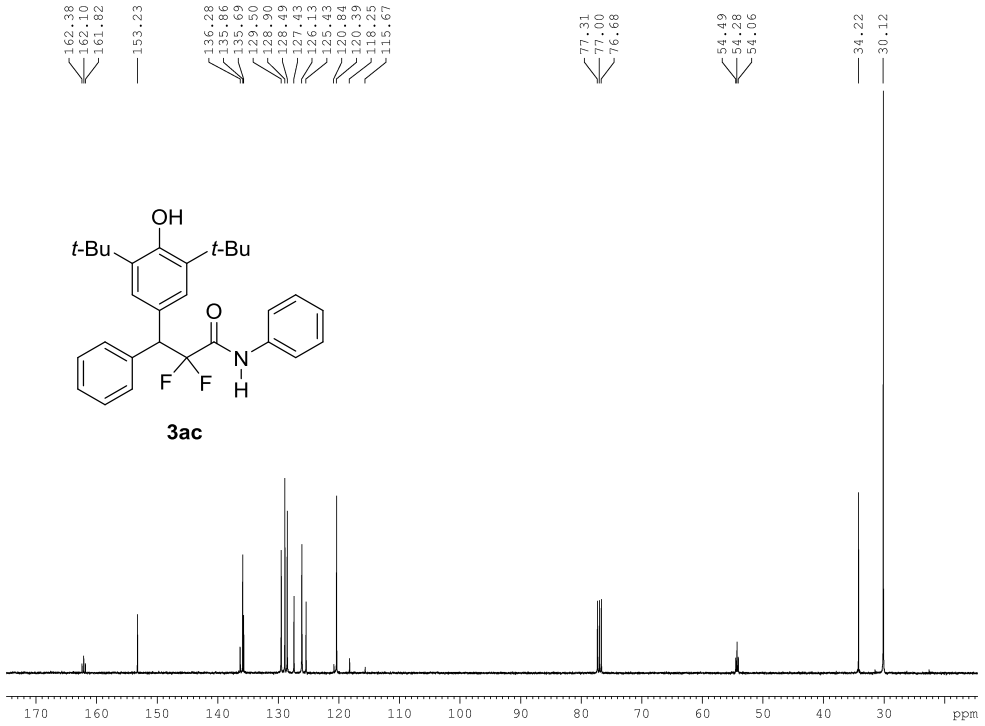
7.480
7.353
7.335
7.315
7.295
7.286
7.267
7.257
7.213
5.142
4.946
4.899
4.853
1.357
0.000
OH
t-Bu
t-Bu
O
N
H
F
F
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.99
2.13
2.36
3.99
1.63
2.16
0.97
1.11
18.00

3ac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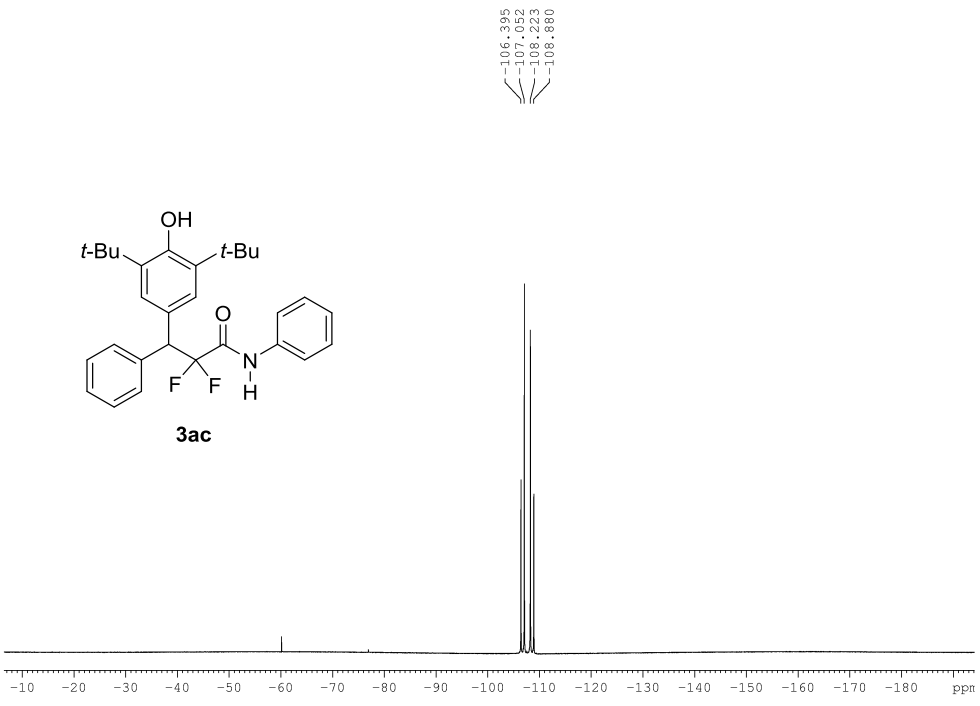
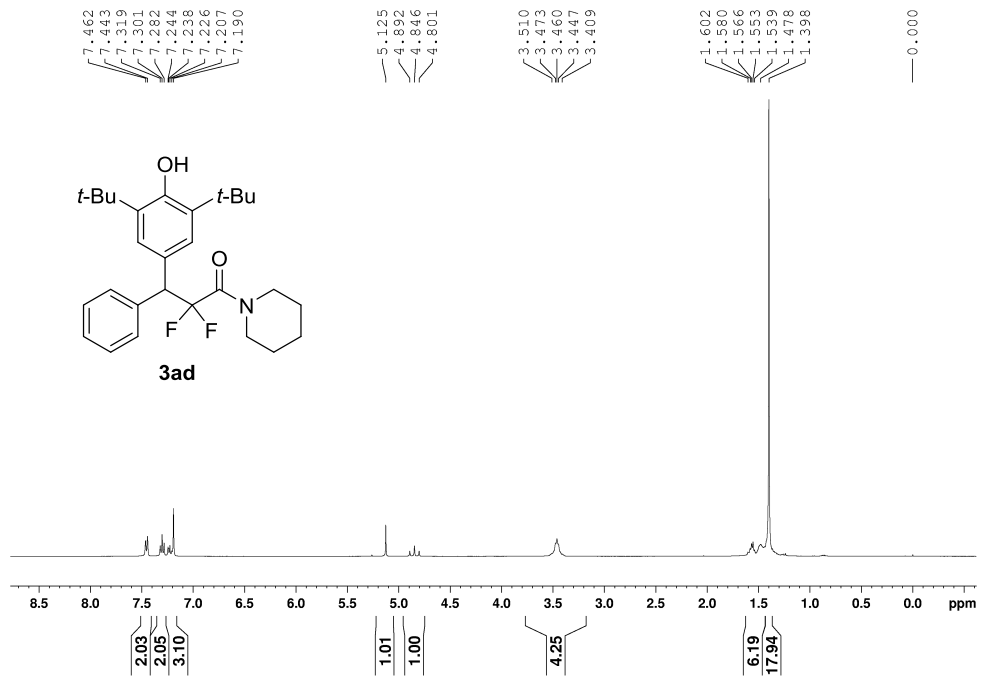
162.10
161.82
153.23
136.28
135.86
135.69
129.50
128.90
128.49
127.43
126.13
125.43
120.84
120.39
118.25
115.67
77.31
77.00
76.68
54.49
54.28
54.06
34.22
30.12
OH
t-Bu
t-Bu
O
N
H
F
F
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm

3ac


-106.395
-107.052
-108.223
-108.880
OH
t-Bu
t-Bu
O
N
H
F
F
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
ppm

3ac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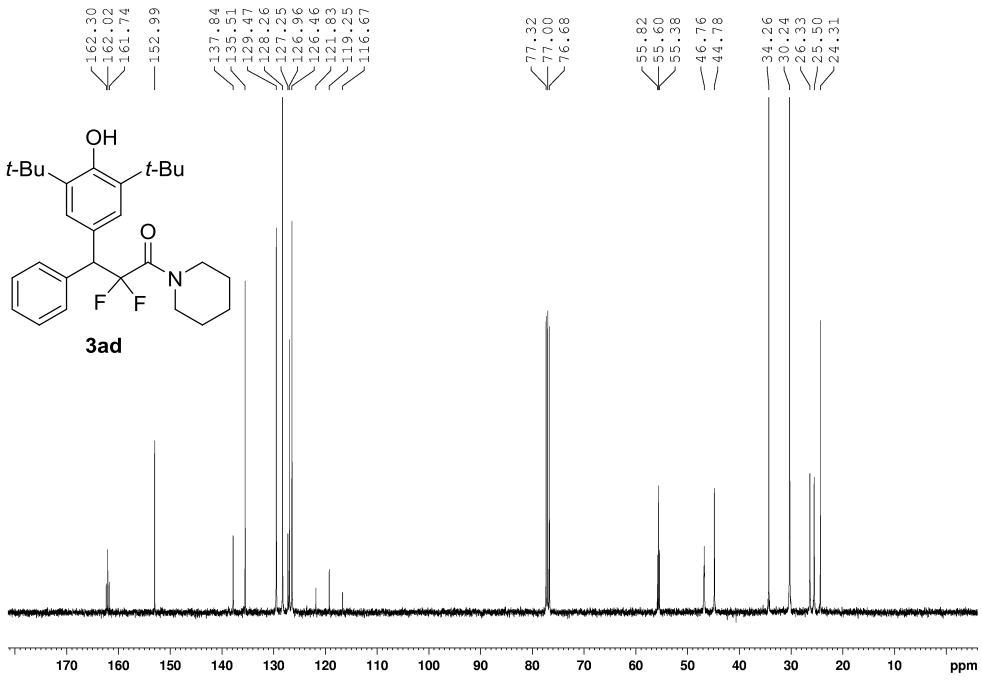
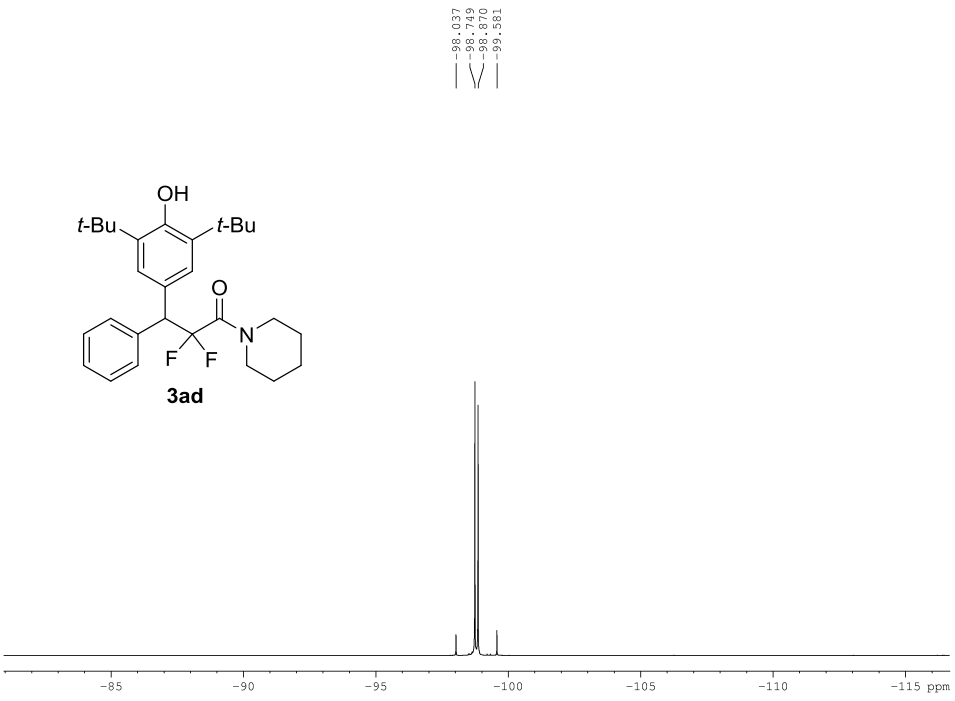
7.319
7.301
7.282
7.244
7.238
7.226
7.207
7.190
5.125
4.892
4.846
4.801
3.510
3.473
3.460
3.447
3.409
1.602
1.580
1.566
1.553
1.539
1.478
1.398
0.000
OH
t-Bu
t-Bu
O
N
F
F
3ad
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.03
2.05
3.10
1.01
1.00
4.25
6.19
17.94


162.30
162.02
161.74
152.99
137.84
135.51
129.47
128.26
127.25
126.96
126.46
121.83
119.25
116.67
77.32
77.00
76.68
55.82
55.60
55.38
46.76
44.78
34.26
30.24
26.33
25.50
24.31
OH
t-Bu
t-Bu
O
N
F
F
3ad
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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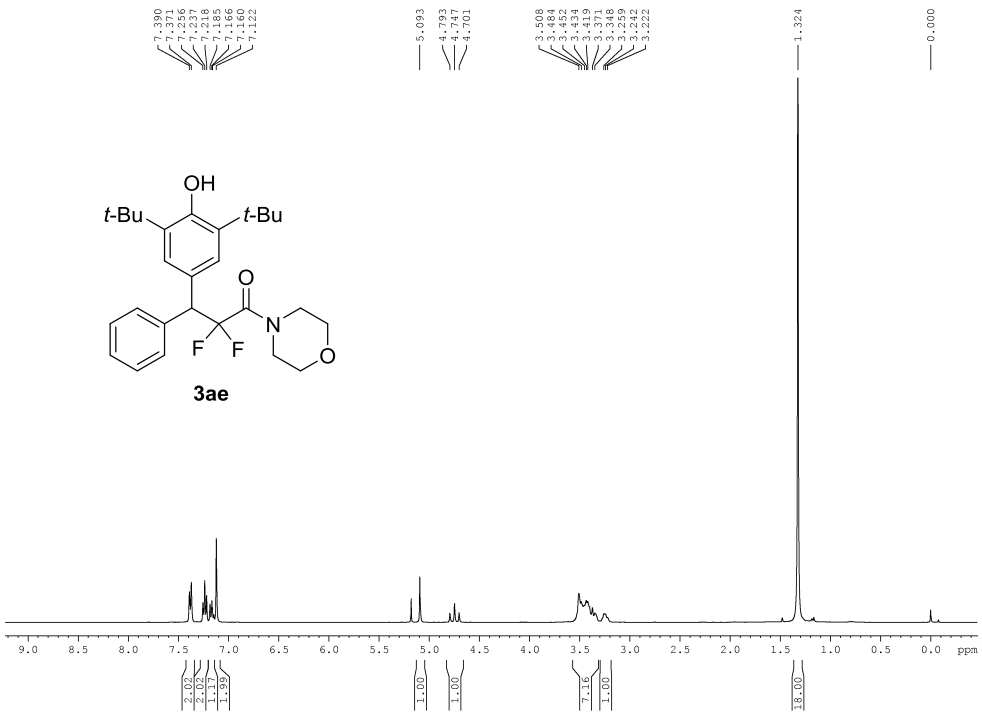
-98.749
-98.870
-99.581
OH
t-Bu
t-Bu
O
N
F
F
-85
-90
-95
-100
-105
-110
-115 ppm

3ad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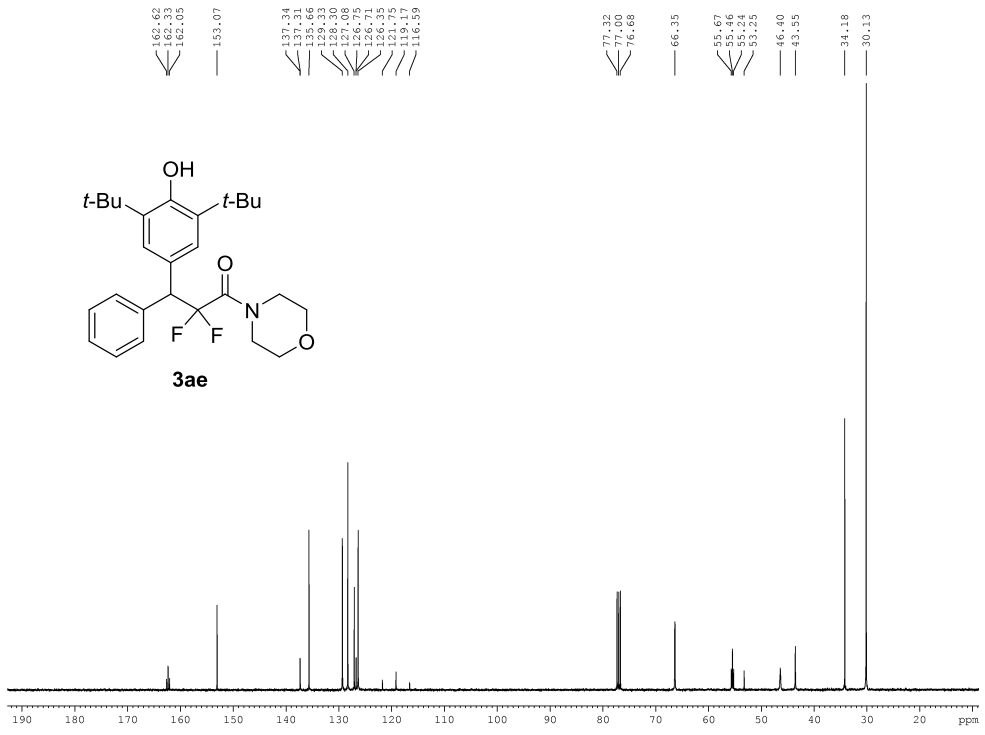
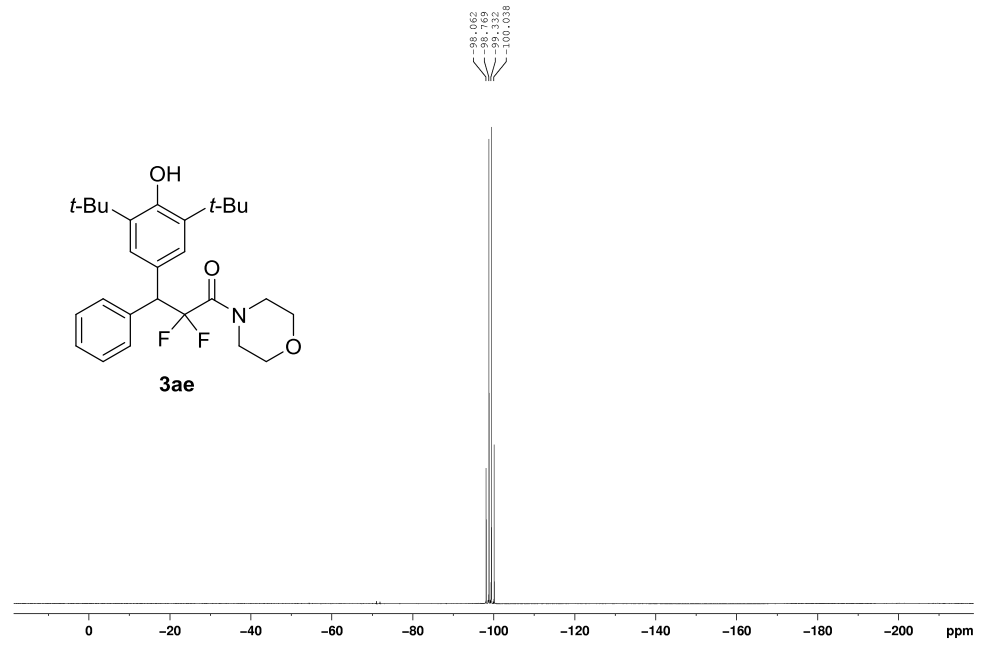
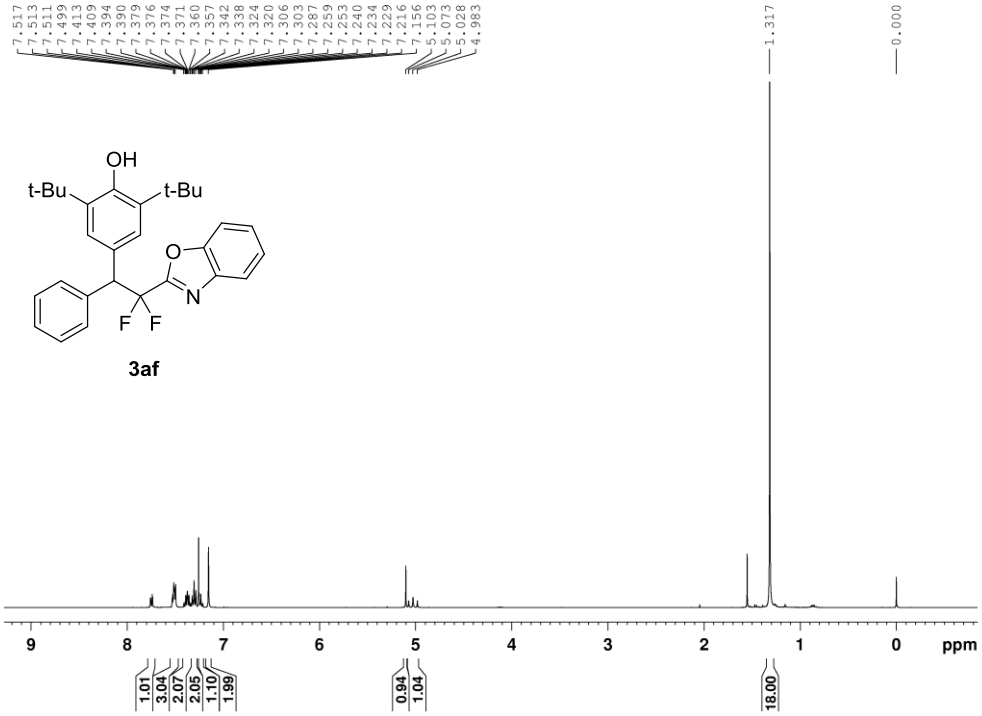
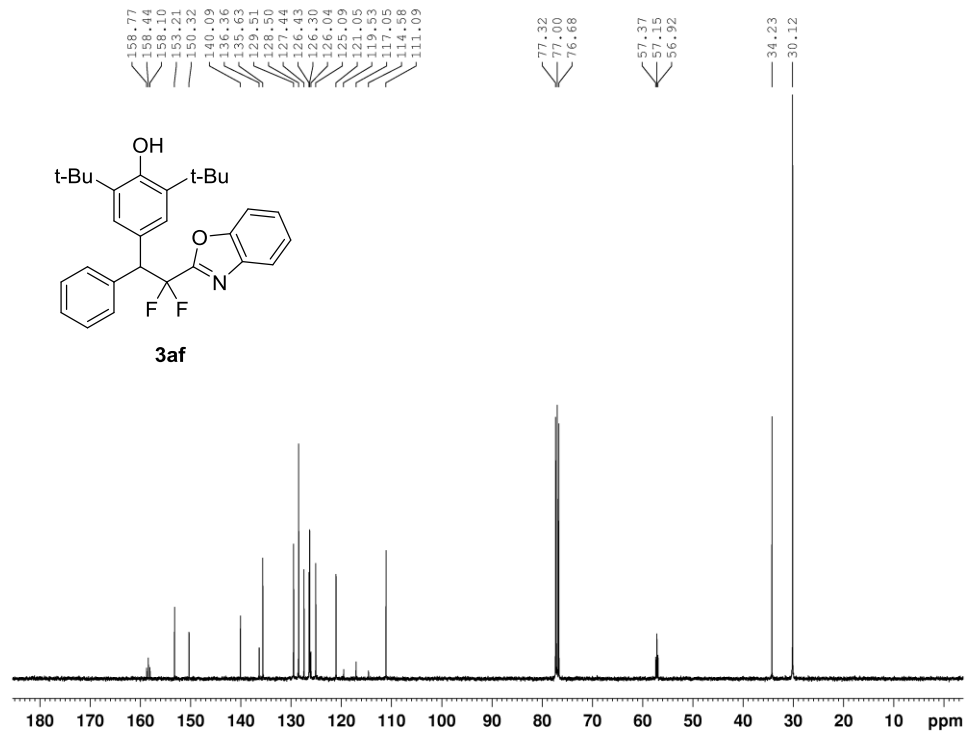
7.256
7.237
7.218
7.185
7.166
7.160
7.122
5.093
4.793
4.747
4.701
3.508
3.484
3.452
3.434
3.419
3.371
3.348
3.259
3.242
3.222
1.324
0.000
OH
t-Bu
t-Bu
O
N
F
F
O
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.02
2.02
2.02
1.17
1.39
1.00
1.00
7.16
1.00
18.00

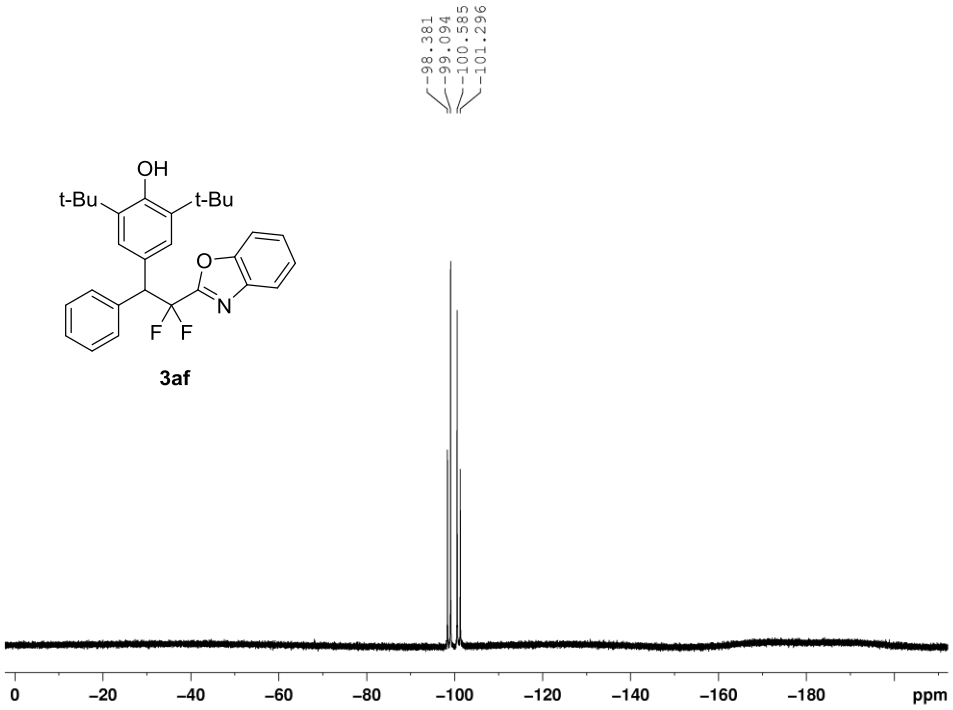
3ae


162.62
162.33
162.05
153.07
137.34
137.31
135.66
129.33
128.30
127.08
127.05
126.71
126.35
121.75
119.17
116.59
77.32
77.00
76.68
66.35
55.67
55.46
55.24
53.25
46.40
43.55
34.18
30.13
OH
t-Bu
t-Bu
O
N
F
F
O
3ae
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

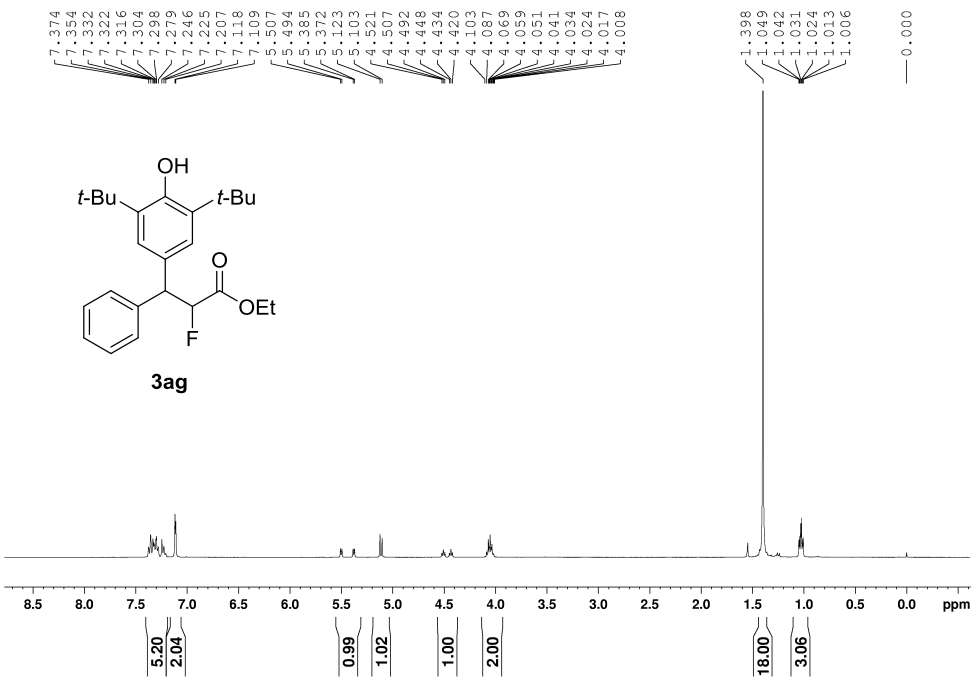

-98.062
-98.758
-99.332
-100.038
OH
t-Bu
t-Bu
O
N
F
F
O
3ae
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm


7.517
7.513
7.511
7.499
7.413
7.409
7.394
7.390
7.379
7.376
7.374
7.371
7.360
7.357
7.342
7.338
7.324
7.320
7.306
7.303
7.287
7.259
7.253
7.240
7.234
7.229
7.216
7.156
5.103
5.073
5.028
4.983
1.317
0.000
OH
t-Bu
t-Bu
O
N
F F
3af
9 8 7 6 5 4 3 2 1 0 ppm
1.01
3.04
2.07
2.05
1.10
1.99
0.94
1.04
18.00

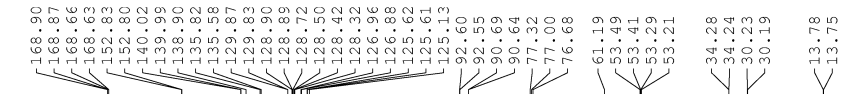

158.77
158.44
158.10
153.21
150.32
140.09
136.36
135.63
129.51
128.50
127.44
126.43
126.30
126.04
125.09
121.05
119.53
117.05
114.58
111.09
77.32
77.00
76.68
57.37
57.15
56.92
34.23
30.12
OH
t-Bu
t-Bu
O
N
F F
3af
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

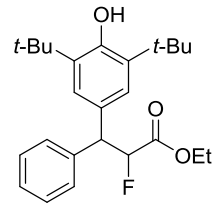

-98.381
-99.094
-100.585
-101.296
OH
t-Bu
t-Bu
O
N
F
F
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
ppm

3af


7.374
7.354
7.332
7.322
7.316
7.304
7.298
7.279
7.246
7.225
7.207
7.118
7.109
5.507
5.494
5.385
5.372
5.123
5.103
4.521
4.507
4.492
4.448
4.434
4.420
4.103
4.087
4.069
4.059
4.051
4.041
4.034
4.024
4.017
4.008
1.398
1.049
1.042
1.031
1.024
1.013
1.006
0.000
OH
t-Bu
t-Bu
O
OEt
F
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
ppm
5.20
2.04
0.99
1.02
1.00
2.00
18.00
3.06

3ag

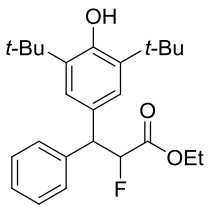

168.90
168.87
168.66
168.63
152.83
152.80
140.02
139.99
138.90
135.82
135.58
129.87
129.83
128.90
128.89
128.72
128.50
128.42
128.32
126.96
126.88
125.62
125.61
125.13
92.60
92.55
90.69
90.64
77.32
77.00
76.68
61.19
53.49
53.41
53.29
53.21
34.28
34.24
30.23
30.19
13.78
13.75


OH
t-Bu
t-Bu
O
OEt
F

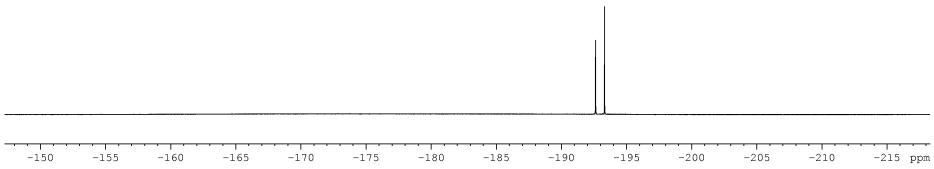
3ag

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


-192.626
-193.318


OH
t-Bu
t-Bu
O
OEt
F

3ag


-150 -155 -160 -165 -170 -175 -180 -185 -190 -195 -200 -205 -210 -215 ppm