

## **Supporting Information**

# **Iridium-Catalyzed Regioselective Synthesis of Trifluoromethylated Isocoumarins through Annulation of Benzoic Acids with Trifluoromethylated Alkynes**

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## General information

Reactions were monitored by TLC analysis which was performed on aluminum plates pre-coated with silica gel (MERCK, 60 F-254), and visualized by UV fluorescence ( $\lambda_{\text{max}} = 254 \text{ nm}$ ) and/or by staining with 1% w/v KMnO<sub>4</sub> in 0.5 M aqueous K<sub>2</sub>CO<sub>3</sub>. Products were purified by flash column chromatography which was performed using silica gel 60® (300-400 mesh).

NMR (Nuclear Magnetic Resonance) spectra were acquired on a BRUKER Avance 400 spectrometer. Chemical shifts for <sup>1</sup>H NMR spectra are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard (CDCl<sub>3</sub>, 7.26 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constants (Hz) and integration. Chemical shifts for <sup>13</sup>C NMR spectra are reported in ppm from the tetramethylsilane with the solvent resonance as internal standard (CDCl<sub>3</sub>, 77.16 ppm) and with complete proton decoupling. No internal standard was used for <sup>19</sup>F NMR spectra.

HRMS (High Resolution Mass Spectra) was measured on a instrument equipped with an APCI or ESI source in the positive-ion mode.

All the trifluoromethylated alkynes **2** were prepared according to Organic Syntheses, Coll. Vol. 9, p. 436 (1998); Vol. 70, p. 246 (1992).

The structures of **3a**, **4a**, **3p** and **4p** were assigned by X-ray crystallographic analysis.

Melting points for solids were measured on a melting point apparatus and are given uncorrected.

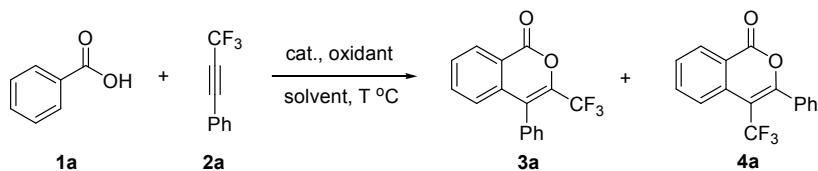
Solvents: Petroleum ether and ethyl acetate for column chromatography were purified prior to use by evaporation on a rotary evaporator. Unless performing reactions sensitive to air and/or moisture, the solvents were bought in p.a. quality and used without further purification. Flasks for absolute solvents were flame-dried three times under oil pump vacuum and back filled with argon.

Transition metal catalysts were purchased and used as received.

## Optimization of parameters for the reaction

Benzoic acid **1a** and trifluoromethylated phenylacetylene **2a** were selected as model substrates to optimize the reaction parameters. The results are summarized in Table S1. The solvent investigation showed that reaction medium played a pivotal role in the transformation (Table S1, entries 1-8). In most cases of tested solvents, the reaction did not occur or only trace amount of product was detected. To our delight, fluoride alcohols were found to be superior to all the others, and TFE gave the best results (Table S1, entry 7). Subsequent temperature evaluation revealed that 50 °C is better than 80 °C (Table S1, entry 9). Then a group of widely used transition metal catalysts were examined (Table S1, entries 10-12). Both Rh and Ru catalysts could generate good yields albeit with poor regioselectivities, while Pd catalyst was completely inert for this transformation and only gave trace amount of product. Finally, a series silver salts as oxidants were investigated, but none of them could deliver better outcomes (Table S1, entries 13-17). Copper salt was also inefficient to promote the coupling to get desired adducts (Table S1, entry 18).

**Table S1.** Comprehensive optimization for the reaction<sup>a</sup>



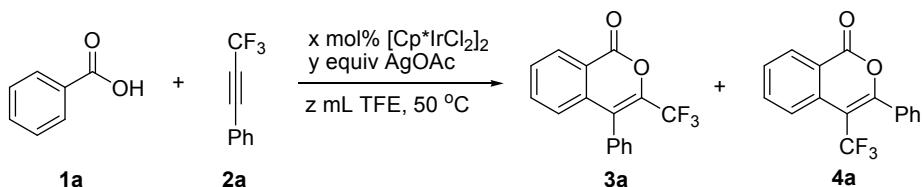
entry	catalyst	oxidant	solvent	T °C	yield of <b>3a</b> %	yield of <b>4a</b> %
1	[Cp*IrCl <sub>2</sub> ] <sub>2</sub>	AgOAc	MeOH	80	10	3
2	[Cp*IrCl <sub>2</sub> ] <sub>2</sub>	AgOAc	EtOH	80	trace	trace
3	[Cp*IrCl <sub>2</sub> ] <sub>2</sub>	AgOAc	t-AmOH	80	NR	NR
4	[Cp*IrCl <sub>2</sub> ] <sub>2</sub>	AgOAc	DCE	80	NR	NR
5	[Cp*IrCl <sub>2</sub> ] <sub>2</sub>	AgOAc	MeCN	80	trace	trace
6	[Cp*IrCl <sub>2</sub> ] <sub>2</sub>	AgOAc	Dioxane	80	trace	trace
7	[Cp*IrCl <sub>2</sub> ] <sub>2</sub>	AgOAc	TFE	80	66	10
8	[Cp*IrCl <sub>2</sub> ] <sub>2</sub>	AgOAc	HFIP	80	56	10
9	[Cp*IrCl <sub>2</sub> ] <sub>2</sub>	AgOAc	TFE	50	81	12
10	[Cp*RhCl <sub>2</sub> ] <sub>2</sub>	AgOAc	TFE	50	45	38
11	[Ru(p-cymene)Cl <sub>2</sub> ] <sub>2</sub>	AgOAc	TFE	50	35	30
12	(PPh <sub>3</sub> ) <sub>2</sub> PdCl <sub>2</sub>	AgOAc	TFE	50	trace	trace
13	[Cp*IrCl <sub>2</sub> ] <sub>2</sub>	Ag <sub>2</sub> CO <sub>3</sub>	TFE	50	46	8
14	[Cp*IrCl <sub>2</sub> ] <sub>2</sub>	AgTFA	TFE	50	17	5
15	[Cp*IrCl <sub>2</sub> ] <sub>2</sub>	AgO	TFE	50	15	5
16	[Cp*IrCl <sub>2</sub> ] <sub>2</sub>	Ag <sub>2</sub> O	TFE	50	trace	trace

17	$[\text{Cp}^*\text{IrCl}_2]_2$	$\text{AgNO}_3$	TFE	50	trace	trace
18	$[\text{Cp}^*\text{IrCl}_2]_2$	$\text{Cu}(\text{OAc})_2$	TFE	50	trace	trace

<sup>a</sup>0.2 mmol of **1a** with 0.3 mmol of **2a**, catalyst (3.5 mol%), oxidant (2 equiv) in 2 mL solvent at 80 or 50 °C for 24 h. Isolated yield.

Encouraged by the preliminary results, the amount of Ir catalyst and Ag oxidant as well as TFE solvent were further investigated based on the practical usage consideration. The results are presented in Table S2. The control experiment showed that both iridium catalyst and silver salt oxidant were necessary for the success, no reaction occurred in the absence of either iridium catalyst or silver salt. (Table S2, entries 1 and 2). It was noteworthy to find that low to 1.5 mol% Ir catalyst was sufficient to provide good yields (Table S2, entry 3). Then reaction concentration was investigated (Table S2, entries 7-9). High concentration was not favourable for the reaction, while satisfactory results in term of yield and selectivity was obtained in a dilute concentration (Table S2, entries 8 and 9). On the other hand, the amount of oxidant silver salt also influenced the process greatly. The yield decreased significantly in presence of one equivalent of Ag salt (Table S2, entry 10). However more oxidant could not improve the outcome further (Table S2, entry 11).

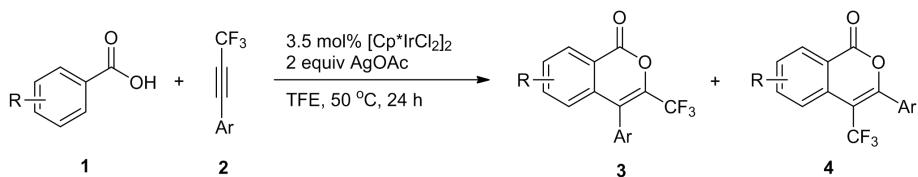
**Table S2.** Catalyst and reagent loading investigation<sup>a</sup>



entry	x	y	z	yield of <b>3a</b> %	yield of <b>4a</b> %
1	0	2	2	NR	NR
2	2.5	0	2	NR	NR
3	1.5	2	2	67	10
4	2.5	2	2	77	12
5	3.5	2	2	81	12
6	4.5	2	2	75	10
7	3.5	2	1	58	7
8	3.5	2	4	85	13
9	3.5	2	8	84	13
10	3.5	1	4	50	8
11	3.5	3	4	75	12

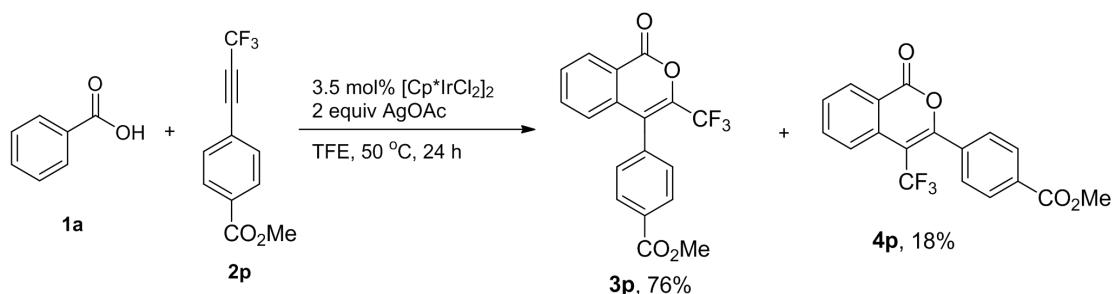
<sup>a</sup>0.2 mmol of **1a** with 0.3 mmol of **2a**,  $[\text{Cp}^*\text{IrCl}_2]_2$  (x mol%),  $\text{AgOAc}$  (y equiv) in z mL solvent at 50 °C for 24 h. Isolated yield.

## General procedure and characterization for the products



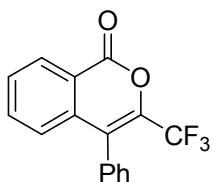
A 10 ml reaction tube was charged with benzoic acid **1** (0.2 mmol, 1.0 equiv), trifluoromethylated internal alkyne **2** (0.3 mmol, 1.5 equiv),  $[\text{Cp}^*\text{IrCl}_2]_2$  (5.6 mg, 0.007 mmol, 3.5 mol%), AgOAc (0.4 mmol, 2 equiv). Then 4 mL TFE was added by syringe. The reaction tube was sealed and the resulting mixture was stirred at  $50^\circ\text{C}$  for 24 hours. The mixture was cooled down to room temperature and the solvent was removed with rotary evaporator. The residue was purified with column chromatography on silica gel, eluting with petroleum ether and ethyl acetate to afford the corresponding product **3** and **4**.

### A 1 mmol scale reaction for **3p** and **4p**.



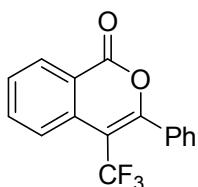
A 50 ml flask was charged with benzoic acid **1a** (1.0 mmol, 1.0 equiv), methyl 4-(3,3,3-trifluoroprop-1-yn-1-yl)benzoate **2p** (1.5 mmol, 1.5 equiv),  $[\text{Cp}^*\text{IrCl}_2]_2$  (28 mg, 0.035 mmol, 3.5 mol%), AgOAc (2.0 mmol, 2 equiv). Then 20 mL TFE was added by syringe. The reaction tube was sealed and the resulting mixture was stirred at  $50^\circ\text{C}$  for 24 hours. The mixture was cooled down to room temperature and the solvent was removed with rotary evaporator. The residue was purified with column chromatography on silica gel, eluting with petroleum ether and ethyl acetate to afford the corresponding product **3p** (264.5 mg, yield 76%) and **4p** (62.6 mg, yield 18%).

## Characterization data of the products



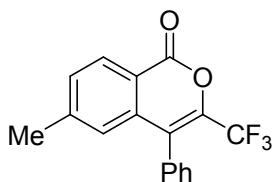
**3a**

3-(trifluoromethyl)-4-phenyl-1*H*-isochromen-1-one (**3a**). White solid, 49.3 mg, yield 85%, mp: 139–140 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.42 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.73 – 7.62 (m, 2H), 7.55 – 7.46 (m, 3H), 7.34 – 7.27 (m, 2H), 7.07 (d, *J* = 8.0 Hz, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 159.4, 138.9 (q, *J*<sub>C-F</sub> = 35.9 Hz), 137.1, 135.2, 130.5, 130.4, 129.9, 129.8 (q, *J*<sub>C-F</sub> = 1.3 Hz), 129.1, 128.7, 126.9, 121.6, 121.0 (q, *J*<sub>C-F</sub> = 2.2 Hz), 119.2 (q, *J*<sub>C-F</sub> = 272.8 Hz); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -63.18; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>16</sub>H<sub>10</sub>F<sub>3</sub>O<sub>2</sub> calcd: 291.0627, found: 291.0630. IR(neat) 3452, 1741, 1602, 1360, 1305, 1196, 1146, 1106, 775, 703, 678 cm<sup>-1</sup>.



**4a**

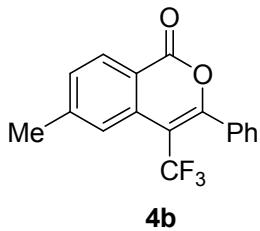
4-(trifluoromethyl)-3-phenyl-1*H*-isochromen-1-one (**4a**). White solid, 7.5 mg, yield 13%, mp: 120–123 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.39 (d, *J* = 8.0 Hz, 1H), 7.86 (d, *J* = 4.0 Hz, 2H), 7.65 (p, *J* = 4.0 Hz, 1H), 7.56 – 7.45 (m, 5H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 160.4, 157.6 (q, *J*<sub>C-F</sub> = 3.5 Hz), 135.4, 133.1, 132.6, 130.7, 130.0, 129.2, 129.1 (q, *J*<sub>C-F</sub> = 1.8 Hz), 128.2, 124.6 (q, *J*<sub>C-F</sub> = 3.6 Hz), 123.5 (q, *J*<sub>C-F</sub> = 271.6 Hz), 120.2, 107.0 (q, *J*<sub>C-F</sub> = 31.6 Hz); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -53.60; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>16</sub>H<sub>10</sub>F<sub>3</sub>O<sub>2</sub> calcd: 291.0627, found: 291.0631. IR(neat) 3444, 1728, 1641, 1487, 1360, 1118, 1157, 1083, 979, 777, 763, 698 cm<sup>-1</sup>.



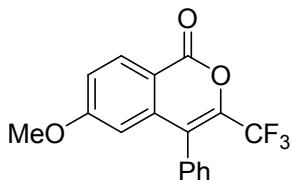
**3b**

3-(trifluoromethyl)-6-methyl-4-phenyl-1*H*-isochromen-1-one (**3b**). White solid, 49.9 mg, yield 82%, mp: 117–119 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.29 (d, *J* = 8.4 Hz,

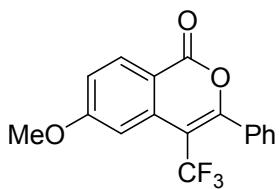
1H), 7.57 – 7.48 (m, 3H), 7.46 (d,  $J$  = 8.0 Hz, 1H), 7.32 – 7.27 (m, 2H), 6.81 (s, 1H), 2.38 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.5, 146.7, 139.0 (q,  $J_{\text{C}-\text{F}} = 35.7$  Hz), 137.1, 131.6, 130.6, 129.9, 129.8 (q,  $J_{\text{C}-\text{F}} = 1.3$  Hz), 129.0, 128.7, 126.8, 120.9 (q,  $J_{\text{C}-\text{F}} = 2.2$  Hz), 119.3 (q,  $J_{\text{C}-\text{F}} = 272.9$  Hz), 119.1, 22.1;  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -63.11; HRMS (pos. ESI): m/z [M + H] $^+$  for  $\text{C}_{17}\text{H}_{12}\text{F}_3\text{O}_2$  calcd: 305.0784, found: 305.0788. IR(neat) 3480, 1751, 1610, 1360, 1296, 1201, 1134, 1029, 777, 700, 611  $\text{cm}^{-1}$ .



**4-(trifluoromethyl)-6-methyl-3-phenyl-1*H*-isochromen-1-one (4b).** White solid, 6.1 mg, yield 10%, mp: 124–125 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.27 (d,  $J$  = 8.0 Hz, 1H), 7.62 (s, 1H), 7.55 – 7.45 (m, 6H), 2.56 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  160.4, 157.6 (q,  $J_{\text{C}-\text{F}} = 3.7$  Hz), 146.6, 133.2, 132.8, 130.6, 130.5, 130.0, 129.1 (q,  $J_{\text{C}-\text{F}} = 1.9$  Hz), 128.2, 124.6 (q,  $J_{\text{C}-\text{F}} = 3.6$  Hz), 123.6 (q,  $J_{\text{C}-\text{F}} = 271.5$  Hz), 117.7, 106.9 (q,  $J_{\text{C}-\text{F}} = 31.3$  Hz), 22.5;  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -53.48; HRMS (pos. ESI): m/z [M + H] $^+$  for  $\text{C}_{17}\text{H}_{12}\text{F}_3\text{O}_2$  calcd: 305.0784, found: 305.0788. IR(neat) 3460, 2927, 1743, 1641, 1367, 1319, 1170, 1118, 1043, 781, 709, 617  $\text{cm}^{-1}$ .

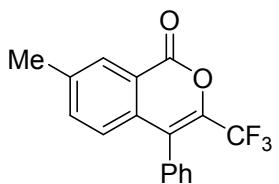


**3-(trifluoromethyl)-6-methoxy-4-phenyl-1*H*-isochromen-1-one (3c).** White solid, 32.6 mg, yield 51%, mp: 143–144 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.34 (d,  $J$  = 8.8 Hz, 1H), 7.51 – 7.49 (m, 3H), 7.30 – 7.28 (m, 2H), 7.15 (dd,  $J$  = 8.8, 2.4 Hz, 1H), 6.41 (d,  $J$  = 2.4 Hz, 1H), 3.74 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  165.0, 159.2, 139.5, 139.4 (q,  $J_{\text{C}-\text{F}} = 35.7$  Hz), 132.3, 130.6, 129.8 (q,  $J_{\text{C}-\text{F}} = 1.4$  Hz), 129.1, 128.7, 120.7 (q,  $J_{\text{C}-\text{F}} = 2.3$  Hz), 119.2 (q,  $J_{\text{C}-\text{F}} = 272.9$  Hz), 117.4, 114.5, 110.4, 55.6;  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -63.22; HRMS (pos. ESI): m/z [M + H] $^+$  for  $\text{C}_{17}\text{H}_{12}\text{F}_3\text{O}_3$  calcd: 321.0733, found: 321.0735. IR(neat) 3440, 2923, 1741, 1641, 1365, 1169, 1118, 1083, 781, 709, 617  $\text{cm}^{-1}$ .



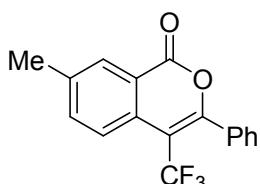
**4c**

**4-(trifluoromethyl)-6-methoxy-3-phenyl-1*H*-isochromen-1-one (**4c**).** White solid, 7.7 mg, yield 12%, mp: 120–121 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.31 (d, *J* = 9.2 Hz, 1H), 7.55 – 7.45 (m, 5H), 7.24 – 7.21 (m, 1H), 7.17 (dd, *J* = 8.8, 2.0 Hz, 1H), 3.97 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 165.0, 160.1, 158.3 (q, *J*<sub>C-F</sub> = 3.4 Hz), 135.3, 132.8, 132.3, 130.7, 129.0 (q, *J*<sub>C-F</sub> = 1.8 Hz), 128.2, 123.6 (q, *J*<sub>C-F</sub> = 271.5 Hz), 116.8, 113.1, 107.9 (q, *J*<sub>C-F</sub> = 3.7 Hz), 106.7 (q, *J*<sub>C-F</sub> = 31.4 Hz), 55.8; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -53.73; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>17</sub>H<sub>12</sub>F<sub>3</sub>O<sub>3</sub> calcd: 321.0733, found: 321.0735. IR(neat) 3448, 2925, 1740, 1610, 1492, 1360, 1276, 1110, 1081, 1020, 827, 773, 711 cm<sup>-1</sup>.



**3d**

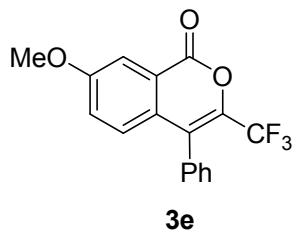
**3-(trifluoromethyl)-7-methyl-4-phenyl-1*H*-isochromen-1-one (**3d**).** White solid, 45.6 mg, yield 75%, mp: 154–155 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.22 (s, 1H), 7.51 – 7.49 (m, 4H), 7.30 – 7.27 (m, 2H), 6.95 (d, *J* = 8.0 Hz, 1H), 2.50 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 159.6, 141.1, 138.1 (q, *J*<sub>C-F</sub> = 35.9 Hz), 136.4, 134.6, 130.7, 129.8, 129.7, 128.9, 128.7, 126.8, 121.5, 121.0 (q, *J*<sub>C-F</sub> = 2.3 Hz), 119.3 (q, *J*<sub>C-F</sub> = 272.6 Hz), 21.4; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -63.05; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>17</sub>H<sub>12</sub>F<sub>3</sub>O<sub>2</sub> calcd: 305.0784, found: 305.0789. IR(neat) 3451, 3066, 1739, 1360, 1305, 1261, 1191, 1137, 1116, 842, 715, 703 cm<sup>-1</sup>.



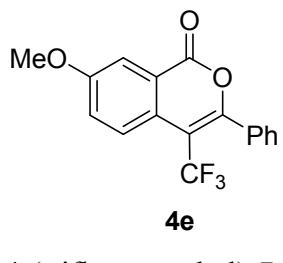
**4d**

**4-(trifluoromethyl)-7-methyl-3-phenyl-1*H*-isochromen-1-one (**4d**).** White solid, 6.7 mg, yield 11%, mp: 135–136 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.20 (q, *J* = 0.4 Hz, 1H), 7.75 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.66 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.55 – 7.46 (m, 5H),

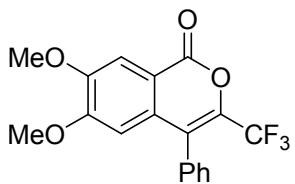
2.52 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  160.6, 156.6 (q,  $J_{\text{C-F}} = 3.7$  Hz), 139.8, 136.5, 132.7, 130.6, 130.5, 129.7, 129.2 (q,  $J_{\text{C-F}} = 1.9$  Hz), 128.2, 124.5 (q,  $J_{\text{C-F}} = 3.6$  Hz), 123.6 (q,  $J_{\text{C-F}} = 271.5$  Hz), 120.1, 107.0 (q,  $J_{\text{C-F}} = 31.7$  Hz), 21.2;  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -53.66. HRMS (pos. ESI): m/z [M + H] $^+$  for  $\text{C}_{17}\text{H}_{12}\text{F}_3\text{O}_2$  calcd: 305.0784, found: 305.0788. IR(neat) 3448, 2921, 1737, 1643, 1502, 1362, 1162, 1106, 1081, 979, 784, 700  $\text{cm}^{-1}$ .



**3-(trifluoromethyl)-7-methoxy-4-phenyl-1*H*-isochromen-1-one (3e).** White solid, 24.3 mg, yield 38%, mp: 97-98 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.81 (d,  $J = 2.8$  Hz, 1H), 7.51 – 7.49 (m, 3H), 7.30 – 7.27 (m, 2H), 7.24 (dd,  $J = 9.2, 2.8$  Hz, 1H), 6.98 (d,  $J = 8.8$  Hz, 1H), 3.94 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  161.1, 159.7, 130.8, 130.4, 129.7 (q,  $J_{\text{C-F}} = 1.3$  Hz), 129.0, 128.7, 128.5, 124.3, 123.1, 121.0 (q,  $J_{\text{C-F}} = 2.3$  Hz), 119.4 (q,  $J_{\text{C-F}} = 272.2$  Hz), 110.7, 56.0 (one carbon missing);  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -62.80; HRMS (pos. ESI): m/z [M + H] $^+$  for  $\text{C}_{17}\text{H}_{12}\text{F}_3\text{O}_3$  calcd: 321.0733, found: 321.0738. IR(neat) 3450, 2930, 1745, 1630, 1480, 1250, 1210, 1130, 877, 787, 655  $\text{cm}^{-1}$ .

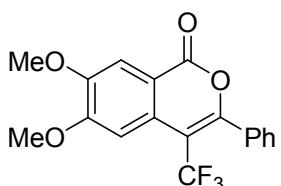


**4-(trifluoromethyl)-7-methoxy-3-phenyl-1*H*-isochromen-1-one (4e).** White solid, 5.1 mg, yield 8%, mp: 128-129 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.79 – 7.76 (m, 2H), 7.55 – 7.47 (m, 5H), 7.42 (dd,  $J = 9.2, 2.8$  Hz, 1H), 3.96 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  160.6, 160.1, 155.3 (q,  $J_{\text{C-F}} = 3.4$  Hz), 132.7, 130.5, 129.2 (q,  $J_{\text{C-F}} = 1.8$  Hz), 128.1, 126.4, 126.3 (q,  $J_{\text{C-F}} = 3.7$  Hz), 124.7, 123.6 (q,  $J_{\text{C-F}} = 271.4$  Hz), 121.7, 110.6, 106.9 (q,  $J_{\text{C-F}} = 31.4$  Hz), 55.9;  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -53.62; HRMS (pos. ESI): m/z [M + H] $^+$  for  $\text{C}_{17}\text{H}_{12}\text{F}_3\text{O}_3$  calcd: 321.0733, found: 321.0738. IR(neat) 3442, 2927, 1747, 1644, 1502, 1332, 1265, 1164, 1116, 1022, 835, 700  $\text{cm}^{-1}$ .



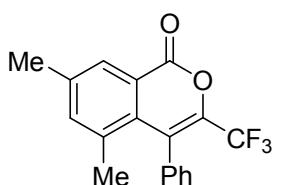
**3f**

3-(trifluoromethyl)-6,7-dimethoxy-4-phenyl-1*H*-isochromen-1-one (**3f**). White solid, 42.0 mg, yield 60%, mp: 126–127 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.76 (s, 1H), 7.52 – 7.50 (m, 3H), 7.32 – 7.29 (m, 2H), 6.38 (s, 1H), 4.02 (s, 3H), 3.70 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 159.4, 155.2, 151.2, 137.9 (q, J<sub>C-F</sub> = 35.8 Hz), 132.5, 130.9, 129.7 (q, J<sub>C-F</sub> = 1.3 Hz), 129.1, 128.7, 120.7 (q, J<sub>C-F</sub> = 2.4 Hz), 119.3 (q, J<sub>C-F</sub> = 272.6 Hz), 115.1, 109.8, 107.4, 56.5, 56.0; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -62.86; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>18</sub>H<sub>14</sub>F<sub>3</sub>O<sub>4</sub> calcd: 351.0839, found: 351.0840. IR(neat) 3448, 2948, 1733, 1606, 1515, 1392, 1351, 1274, 1213, 1126, 1049, 871, 767, 713 cm<sup>-1</sup>.



**4f**

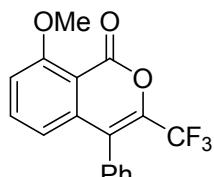
4-(trifluoromethyl)-6,7-dimethoxy-3-phenyl-1*H*-isochromen-1-one (**4f**). White solid, 4.9 mg, yield 7%, mp: 134–135 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.74 (s, 1H), 7.55 – 7.47 (m, 4H), 7.19 (d, J = 1.2 Hz, 1H), 4.04 (s, 3H), 4.03 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 159.4, 155.5 (q, J<sub>C-F</sub> = 3.4 Hz), 154.2, 149.3, 131.8, 129.5, 128.2, 127.5, 127.1, 126.5, 122.7 (q, J<sub>C-F</sub> = 272.6 Hz), 112.7, 108.7, 104.6 (q, J<sub>C-F</sub> = 33.9 Hz), 55.4, 55.3; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -53.73; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -53.58; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>18</sub>H<sub>14</sub>F<sub>3</sub>O<sub>4</sub> calcd: 351.0839, found: 351.0840. IR(neat) 3463, 2915, 1745, 1610, 1519, 1467, 1346, 1284, 1110, 1054, 881, 775, 713 cm<sup>-1</sup>.



**3g**

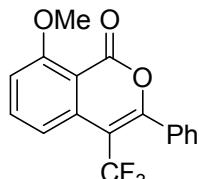
3-(trifluoromethyl)-5,7-dimethyl-4-phenyl-1*H*-isochromen-1-one (**3g**). White solid, 50.2 mg, yield 79%, mp: 121–122 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.17 (s, 1H),

7.47 – 7.41 (m, 3H), 7.32 – 7.31 (m, 3H), 2.44 (s, 3H), 1.66 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 160.2, 141.1, 140.7, 138.4 (q, *J*<sub>C-F</sub> = 34.6 Hz), 137.5, 133.3, 131.2, 130.5 (q, *J*<sub>C-F</sub> = 1.5 Hz), 129.0, 128.8, 128.3, 122.6, 121.4 (q, *J*<sub>C-F</sub> = 2.2 Hz), 119.6 (q, *J*<sub>C-F</sub> = 273.0 Hz), 22.5, 21.0; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -61.27; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>18</sub>H<sub>14</sub>F<sub>3</sub>O<sub>2</sub> calcd: 319.0940, found: 319.0944. IR(neat) 3435, 2933, 1730, 1608, 1346, 1298, 1184, 1124, 881, 776, 715 cm<sup>-1</sup>.



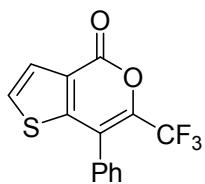
**3h**

3-(trifluoromethyl)-8-methoxy-4-phenyl-1*H*-isochromen-1-one (**3h**). White solid, 15.4 mg, yield 24%, mp: 147-149 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.59 (t, *J* = 8.2 Hz, 1H), 7.49 (s, 3H), 7.26 (s, 2H), 7.10 (d, *J* = 8.4 Hz, 1H), 6.56 (d, *J* = 8.0 Hz, 1H), 4.05 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 161.9, 155.9, 140.0, 136.0, 131.1, 129.9 (q, *J*<sub>C-F</sub> = 1.0 Hz), 128.9, 128.6, 120.2 (q, *J*<sub>C-F</sub> = 1.8 Hz), 119.1 (q, *J*<sub>C-F</sub> = 272.6 Hz), 118.8, 112.2, 110.2, 56.6 (one carbon missing); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -63.38; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>17</sub>H<sub>12</sub>F<sub>3</sub>O<sub>3</sub> calcd: 321.0733, found: 321.0738. IR(neat) 3437, 2915, 1741, 1397, 1270, 1137, 1000, 811, 684 cm<sup>-1</sup>.



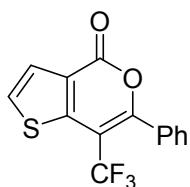
**4h**

4-(trifluoromethyl)-8-methoxy-3-phenyl-1*H*-isochromen-1-one (**3h**). White solid, 6.4 mg, yield 10%, mp: 130-131 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.74 (t, *J* = 8.4 Hz, 1H), 7.55 (d, *J* = 1.9 Hz, 2H), 7.51 – 7.44 (m, 3H), 7.37 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.09 (d, *J* = 8.4 Hz, 1H), 4.03 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 161.7, 158.2 (q, *J*<sub>C-F</sub> = 3.5 Hz), 156.7, 136.2, 135.9, 132.7, 130.7, 129.1 (q, *J*<sub>C-F</sub> = 1.8 Hz), 128.1, 123.6 (q, *J*<sub>C-F</sub> = 271.4 Hz), 116.1 (q, *J*<sub>C-F</sub> = 3.8 Hz), 111.1, 109.0, 106.3 (q, *J*<sub>C-F</sub> = 31.4 Hz), 56.5; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -53.57; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>17</sub>H<sub>12</sub>F<sub>3</sub>O<sub>3</sub> calcd: 321.0733, found: 321.0738. IR(neat) 3430, 2920, 2850, 1738, 1633, 1463, 1398, 1267, 1200, 1108 cm<sup>-1</sup>.



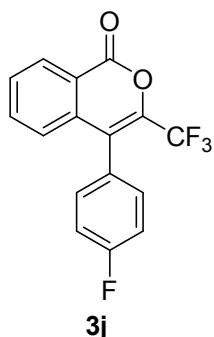
**3i**

6-(trifluoromethyl)-7-phenyl-4*H*-thieno[3,2-*c*]pyran-4-one (**3i**). White solid, 20.7 mg, yield 35%, mp: 110–111 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.72 (d, *J* = 5.2 Hz, 1H), 7.55 – 7.51 (m, 4H), 7.42 – 7.39 (m, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 155.4, 152.5, 131.1, 129.9, 129.8, 129.0, 128.8 (q, *J*<sub>C-F</sub> = 1.3 Hz), 126.6, 125.7, 119.2 (q, *J*<sub>C-F</sub> = 272.8 Hz), 119.0 (q, *J*<sub>C-F</sub> = 2.3 Hz) (one carbon missing); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -62.64; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>14</sub>H<sub>8</sub>F<sub>3</sub>O<sub>2</sub>S calcd: 297.0192, found: 297.0195. IR(neat) 3446, 3114, 2923, 1739, 1509, 1407, 1303, 1196, 1143, 906, 723, 701 cm<sup>-1</sup>.



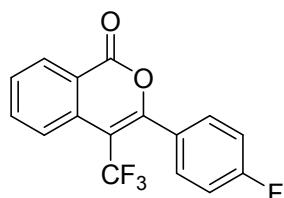
**4i**

7-(trifluoromethyl)-6-phenyl-4*H*-thieno[3,2-*c*]pyran-4-one (**4i**). White solid, 2.9 mg, yield 5%, mp: 102–103 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.68 (d, *J* = 5.6 Hz, 1H), 7.58 (d, *J* = 7.2 Hz, 2H), 7.53 – 7.47 (m, 4H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 158.3 (q, *J*<sub>C-F</sub> = 3.4 Hz), 156.5, 145.5, 131.4, 131.0, 129.0 (q, *J*<sub>C-F</sub> = 1.7 Hz), 128.3, 127.9 (q, *J*<sub>C-F</sub> = 2.0 Hz), 125.6, 124.2, 123.2 (q, *J*<sub>C-F</sub> = 271.0 Hz), 106.8 (q, *J*<sub>C-F</sub> = 34.7 Hz); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -55.06; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>14</sub>H<sub>8</sub>F<sub>3</sub>O<sub>2</sub>S calcd: 297.0192, found: 297.0195. IR(neat) 3442, 2927, 1737, 1617, 1350, 1174, 1126, 1080, 985, 717, 701 cm<sup>-1</sup>.



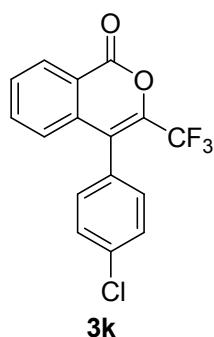
**3j**

**3-(trifluoromethyl)-4-(4-fluorophenyl)-1*H*-isochromen-1-one (**3j**).** White solid, 47.4 mg, yield 77%, mp: 130-131 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.32 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.65 (td, *J* = 7.6, 1.2 Hz, 1H), 7.58 (td, *J* = 7.2, 0.8 Hz, 1H), 7.23 – 7.19 (m, 2H), 7.15 – 7.10 (m, 2H), 6.98 (d, *J* = 7.6 Hz, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 163.1 (d, *J*<sub>C-F</sub> = 247.6 Hz), 159.2, 139.2 (q, *J*<sub>C-F</sub> = 36.0 Hz), 136.9, 135.3, 131.7 (dd, *J*<sub>C-F</sub> = 8.2, 1.2 Hz), 130.5, 130.0, 126.6, 126.3 (q, *J*<sub>C-F</sub> = 3.5 Hz), 121.6, 120.0 (q, *J*<sub>C-F</sub> = 2.2 Hz), 119.2 (q, *J*<sub>C-F</sub> = 272.9 Hz), 116.0 (d, *J*<sub>C-F</sub> = 21.7 Hz); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -63.13, -111.94; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>16</sub>H<sub>9</sub>F<sub>4</sub>O<sub>2</sub> calcd: 309.0533, found: 309.0536. IR(neat) 3450, 3072, 1743, 1606, 1513, 1353, 1307, 1190, 1149, 833, 781, 709 cm<sup>-1</sup>.



**4j**

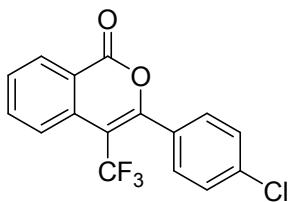
**4-(trifluoromethyl)-3-(4-fluorophenyl)-1*H*-isochromen-1-one (**4j**).** White solid, 6.7 mg, yield 11%, mp: 140-142 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.39 (d, *J* = 8.0 Hz, 1H), 7.86 – 7.85 (m, 2H), 7.68 – 7.64 (m, 1H), 7.57 (dd, *J* = 8.4, 5.2 Hz, 2H), 7.17 (t, *J* = 8.6 Hz, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 164.1 (d, *J*<sub>C-F</sub> = 250.3 Hz), 160.2, 156.4 (q, *J*<sub>C-F</sub> = 3.6 Hz), 135.4, 133.0, 131.3 (dd, *J*<sub>C-F</sub> = 8.8, 1.8 Hz), 130.0, 129.3, 128.7 (d, *J*<sub>C-F</sub> = 3.4 Hz), 124.6 (q, *J*<sub>C-F</sub> = 3.6 Hz), 123.5 (q, *J*<sub>C-F</sub> = 271.6 Hz), 120.2, 115.5 (d, *J*<sub>C-F</sub> = 22.0 Hz), 106.2 (q, *J*<sub>C-F</sub> = 31.6 Hz); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -53.61, -108.55; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>16</sub>H<sub>9</sub>F<sub>4</sub>O<sub>2</sub> calcd: 309.0533, found: 309.0537. IR(neat) 3432, 2915, 1735, 1639, 1511, 1359, 1162, 1122, 1079, 979, 850, 777 cm<sup>-1</sup>.



**3k**

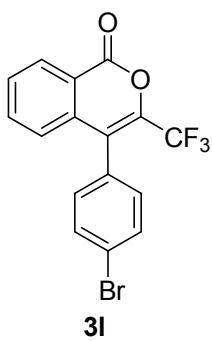
**4-(4-chlorophenyl)-3-(trifluoromethyl)-1*H*-isochromen-1-one (**3k**).** White solid, 40.8 mg, yield 63%, mp: 125-127 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.41 (dd, *J* = 7.8, 1.0

Hz, 1H), 7.75 – 7.65 (m, 2H), 7.50 (d,  $J$  = 8.4 Hz, 2H), 7.25 (d,  $J$  = 8.4 Hz, 2H), 7.06 (d,  $J$  = 8.0 Hz, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.2, 139.2 (q,  $J_{\text{C-F}} = 36.0$  Hz), 136.7, 135.4, 135.3, 131.2 (q,  $J_{\text{C-F}} = 1.4$  Hz), 130.6, 130.1, 129.1, 129.0, 126.6, 121.6, 119.8 (q,  $J_{\text{C-F}} = 2.1$  Hz), 119.1 (q,  $J_{\text{C-F}} = 273.0$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -63.11; HRMS (pos. ESI): m/z [M + H] $^+$  for  $\text{C}_{16}\text{H}_9\text{F}_3\text{O}_2\text{Cl}$  calcd: 325.0238, found: 325.0248. IR(neat) 3460, 1735, 1597, 1492, 1355, 1303, 1199, 1110, 966, 827, 781  $\text{cm}^{-1}$ .



**4k**

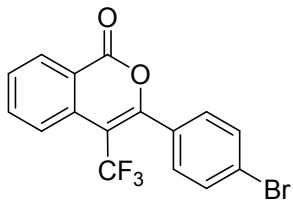
3-(4-chlorophenyl)-4-(trifluoromethyl)-1*H*-isochromen-1-one (**4k**). White solid, 10.4 mg, yield 16%, mp: 112-114 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.39 (d,  $J$  = 8.0 Hz, 1H), 7.89 – 7.85 (m, 2H), 7.68 – 7.65 (m, 1H), 7.47 (dt,  $J$  = 6.6, 5.2 Hz, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  160.1, 156.2 (q,  $J_{\text{C-F}} = 3.4$  Hz), 137.1, 135.4, 132.9, 131.0, 130.5 (q,  $J_{\text{C-F}} = 1.9$  Hz), 130.1, 129.4, 128.6, 124.6 (q,  $J_{\text{C-F}} = 3.6$  Hz), 123.4 (q,  $J_{\text{C-F}} = 271.6$  Hz), 120.2, 107.3 (q,  $J_{\text{C-F}} = 31.7$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -53.59; HRMS (pos. ESI): m/z [M + H] $^+$  for  $\text{C}_{16}\text{H}_9\text{F}_3\text{O}_2\text{Cl}$  calcd: 325.0238, found: 325.0247. IR(neat) 3440, 2915, 1754, 1633, 1486, 1355, 1160, 1122, 977, 780, 701  $\text{cm}^{-1}$ .



**3l**

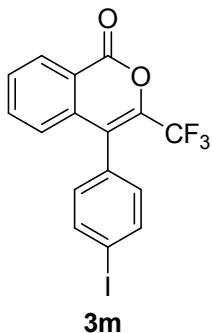
4-(4-bromophenyl)-3-(trifluoromethyl)-1*H*-isochromen-1-one (**3l**). White solid, 55.9 mg, yield 76%, mp: 127-128 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.41 (dd,  $J$  = 8.0, 1.2 Hz, 1H), 7.74 – 7.67 (m, 2H), 7.66 (d,  $J$  = 8.4 Hz, 2H), 7.19 (d,  $J$  = 8.4 Hz, 2H), 7.06 (d,  $J$  = 8.0 Hz, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.2, 139.1 (q,  $J_{\text{C-F}} = 36.0$  Hz), 136.6, 135.3, 132.1, 131.5 (q,  $J_{\text{C-F}} = 1.3$  Hz), 130.6, 130.1, 129.5, 126.6, 123.6, 121.6, 119.8 (q,  $J_{\text{C-F}} = 2.3$  Hz), 119.1 (q,  $J_{\text{C-F}} = 272.9$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -63.09; HRMS (pos. ESI): m/z [M + H] $^+$  for  $\text{C}_{16}\text{H}_9\text{F}_3\text{BrO}_2$  calcd: 368.9733, found:

368.9745. IR(neat) 3450, 1741, 1590, 1358, 1303, 1197, 1110, 964, 821, 775, 707 cm<sup>-1</sup>.



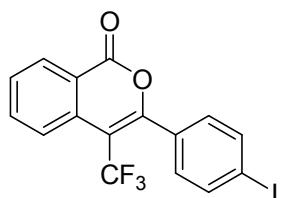
**4l**

**3-(4-bromophenyl)-4-(trifluoromethyl)-1*H*-isochromen-1-one (4l).** White solid, 11.0 mg, yield 15%, mp: 106-107 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.39 (d, *J* = 8.0 Hz, 1H), 7.89 – 7.83 (m, 2H), 7.68 – 7.66 (m, 1H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.43 (d, *J* = 8.4 Hz, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 160.1, 156.3 (q, *J*<sub>C-F</sub> = 3.5 Hz), 135.4, 132.6, 131.6, 131.4, 130.7 (q, *J*<sub>C-F</sub> = 1.9 Hz), 130.1, 129.4, 125.5, 124.6 (q, *J*<sub>C-F</sub> = 3.6 Hz), 123.4 (q, *J*<sub>C-F</sub> = 271.7 Hz), 120.2, 107.3 (q, *J*<sub>C-F</sub> = 31.6 Hz); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -53.58; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>16</sub>H<sub>9</sub>F<sub>3</sub>BrO<sub>2</sub> calcd: 368.9733, found: 368.9743. IR(neat) 3440, 2923, 1754, 1635, 1484, 1355, 1160, 1122, 1083, 1010, 779, 701 cm<sup>-1</sup>.



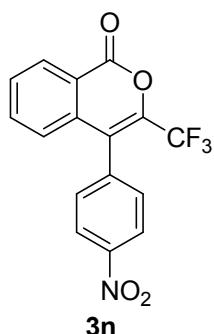
**3m**

**3-(trifluoromethyl)-4-(4-iodophenyl)-1*H*-isochromen-1-one (3m).** White solid, 59.1 mg, yield 71%, mp: 148-149 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.41 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 2H), 7.76 – 7.65 (m, 2H), 7.06 (d, *J* = 8.4 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 159.1, 139.0 (q, *J*<sub>C-F</sub> = 36.0 Hz), 138.0, 136.6, 135.3, 131.6 (q, *J*<sub>C-F</sub> = 1.3 Hz), 130.6, 130.1, 130.0, 126.6, 121.6, 119.9 (q, *J*<sub>C-F</sub> = 2.1 Hz), 119.1 (q, *J*<sub>C-F</sub> = 273.0 Hz), 95.2; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -63.07; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>16</sub>H<sub>9</sub>F<sub>3</sub>O<sub>2</sub>I calcd: 416.9594, found: 416.9596. IR(neat) 3455, 2927, 1740, 1487, 1357, 1303, 1195, 1108, 964, 819, 777, 707 cm<sup>-1</sup>.



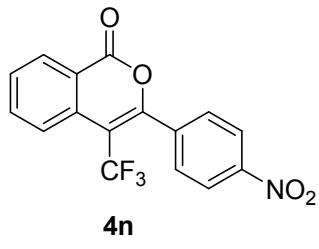
**4m**

**4-(trifluoromethyl)-3-(4-iodophenyl)-1*H*-isochromen-1-one (**4m**).** White solid, 16.6 mg, yield 20%, mp: 125-126 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.39 (d,  $J = 7.6$  Hz, 1H), 7.89 – 7.82 (m, 4H), 7.68 – 7.64 (m, 1H), 7.29 (d,  $J = 8.4$  Hz, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  160.1, 156.4 (q,  $J_{\text{C}-\text{F}} = 3.6$  Hz), 137.5, 135.4, 132.8, 130.7 (q,  $J_{\text{C}-\text{F}} = 1.5$  Hz), 130.1, 129.4, 128.2, 124.6 (q,  $J_{\text{C}-\text{F}} = 3.7$  Hz), 123.4 (q,  $J_{\text{C}-\text{F}} = 271.7$  Hz), 120.2, 107.2 (q,  $J_{\text{C}-\text{F}} = 31.7$  Hz), 97.5;  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -53.56; HRMS (pos. ESI): m/z [M + H] $^+$  for  $\text{C}_{16}\text{H}_9\text{F}_3\text{O}_2\text{I}$  calcd: 416.9594, found: 416.9597. IR(neat) 3445, 1751, 1633, 1481, 1357, 1178, 1112, 977, 836, 775  $\text{cm}^{-1}$ .

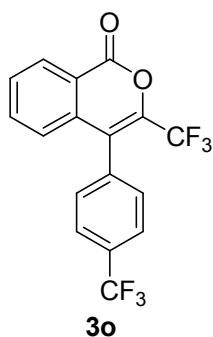


**3n**

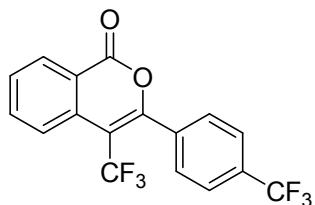
**3-(trifluoromethyl)-4-(4-nitrophenyl)-1*H*-isochromen-1-one (**3n**).** White solid, 44.2 mg, yield 66%, mp: 133-134 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.45 (dd,  $J = 7.2, 1.2$  Hz, 1H), 8.40 (d,  $J = 8.4$  Hz, 2H), 7.77 – 7.70 (m, 2H), 7.55 (d,  $J = 8.4$  Hz, 2H), 6.96 (d,  $J = 7.6$  Hz, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.8, 148.5, 139.3 (q,  $J_{\text{C}-\text{F}} = 36.4$  Hz), 137.5, 135.8, 135.6, 131.1 (q,  $J_{\text{C}-\text{F}} = 1.4$  Hz), 131.0, 130.4, 126.2, 124.0, 121.5, 119.0 (q,  $J_{\text{C}-\text{F}} = 2.2$  Hz), 118.9 (q,  $J_{\text{C}-\text{F}} = 273.1$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -63.16; HRMS (pos. ESI): m/z [M + H] $^+$  for  $\text{C}_{16}\text{H}_9\text{F}_3\text{NO}_4$  calcd: 336.0478, found: 336.0485. IR(neat) 3450, 2929, 3104, 1754, 1600, 1525, 1351, 1307, 1201, 1137, 1112, 848, 782, 709  $\text{cm}^{-1}$ .



**4-(trifluoromethyl)-3-(4-nitrophenyl)-1*H*-isochromen-1-one (4n).** White solid, 16.1 mg, yield 24%, mp: 131–132 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.42 (d, *J* = 8.0 Hz, 1H), 8.35 (d, *J* = 8.8 Hz, 2H), 7.93 – 7.86 (m, 2H), 7.75 (d, *J* = 8.8 Hz, 2H), 7.71 – 7.69 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 159.6, 154.7 (q, *J*<sub>C-F</sub> = 3.4 Hz), 149.1, 138.5, 135.7, 132.3, 130.3 (q, *J*<sub>C-F</sub> = 1.9 Hz), 130.2, 130.0, 124.8 (q, *J*<sub>C-F</sub> = 3.5 Hz), 123.5, 123.1 (q, *J*<sub>C-F</sub> = 271.9 Hz), 120.3, 108.3 (q, *J*<sub>C-F</sub> = 31.9 Hz); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -53.59; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>16</sub>H<sub>9</sub>F<sub>3</sub>NO<sub>4</sub> calcd: 336.0478, found: 336.0485. IR(neat) 3440, 2915, 1766, 1600, 1523, 1349, 1162, 1122, 1083, 981, 844, 777, 700 cm<sup>-1</sup>.

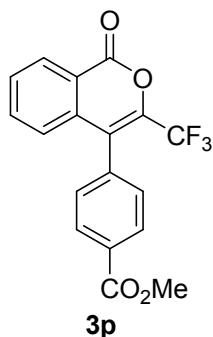


**3-(trifluoromethyl)-4-(4-(trifluoromethyl)phenyl)-1*H*-isochromen-1-one (3o).** White solid, 52.3 mg, yield 73%, mp: 136–137 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.43 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 2H), 7.76 – 7.68 (m, 2H), 7.47 (d, *J* = 8.0 Hz, 2H), 6.99 (d, *J* = 7.6 Hz, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 159.0, 139.2 (q, *J*<sub>C-F</sub> = 36.3 Hz), 136.3, 135.4, 134.5, 131.5 (q, *J*<sub>C-F</sub> = 32.7 Hz), 130.7, 130.4 (q, *J*<sub>C-F</sub> = 1.4 Hz), 130.2, 126.5, 125.8 (q, *J*<sub>C-F</sub> = 3.7 Hz), 123.8 (q, *J*<sub>C-F</sub> = 270.7 Hz), 121.6, 119.6 (q, *J*<sub>C-F</sub> = 2.0 Hz), 119.0 (q, *J*<sub>C-F</sub> = 272.9 Hz); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -62.83, -63.21; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>17</sub>H<sub>9</sub>F<sub>6</sub>O<sub>2</sub> calcd: 359.0501, found: 359.0501. IR(neat) 3450, 1733, 1620, 1357, 1328, 1203, 1110, 1068, 835, 781, 711, 622 cm<sup>-1</sup>.



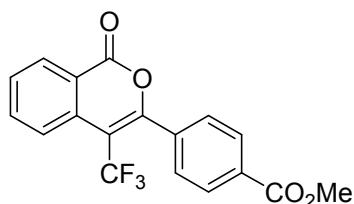
**4o**

**4-(trifluoromethyl)-3-(4-(trifluoromethyl)phenyl)-1*H*-isochromen-1-one (4o).** White solid, 13.6 mg, yield 19%, mp: 89–90 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.41 (d, *J* = 8.0 Hz, 1H), 7.89 – 7.87 (m, 2H), 7.75 (d, *J* = 8.4 Hz, 2H), 7.71 – 7.67 (m, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 159.9, 155.7 (q, *J*<sub>C-F</sub> = 3.5 Hz), 136.0, 135.5, 132.6 (q, *J*<sub>C-F</sub> = 32.7 Hz), 132.5, 130.2, 129.7, 129.6 (q, *J*<sub>C-F</sub> = 1.9 Hz), 125.3 (q, *J*<sub>C-F</sub> = 3.7 Hz), 124.7 (q, *J*<sub>C-F</sub> = 3.5 Hz), 123.6 (q, *J*<sub>C-F</sub> = 270.9 Hz), 123.3 (q, *J*<sub>C-F</sub> = 271.8 Hz), 120.3, 107.8 (q, *J*<sub>C-F</sub> = 31.8 Hz); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -53.63, -62.98; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>17</sub>H<sub>9</sub>F<sub>6</sub>O<sub>2</sub> calcd: 359.0501, found: 359.0501. IR(neat) 3463, 1760, 1616, 1324, 1182, 1120, 1062, 852, 775, 711 cm<sup>-1</sup>.



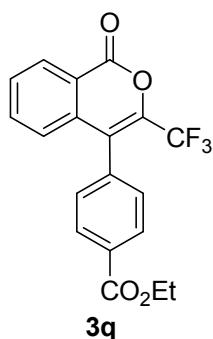
**3p**

**methyl 4-(3-(trifluoromethyl)-1-oxo-1*H*-isochromen-4-yl)benzoate (3p).** White solid, 51.5 mg, yield 74%, mp: 157–158 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.43 (d, *J* = 7.2 Hz, 1H), 8.19 (d, *J* = 8.0 Hz, 2H), 7.74 – 7.67 (m, 2H), 7.41 (d, *J* = 8.4 Hz, 2H), 7.00 (d, *J* = 7.6 Hz, 1H), 3.98 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 166.4, 159.2, 138.9 (q, *J*<sub>C-F</sub> = 36.2 Hz), 136.4, 135.4, 135.3, 131.0, 130.7, 130.1, 130.0 (q, *J*<sub>C-F</sub> = 1.3 Hz), 129.9, 126.6, 121.5, 120.1 (q, *J*<sub>C-F</sub> = 2.2 Hz), 119.2 (q, *J*<sub>C-F</sub> = 272.9 Hz) 52.4; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -63.21; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>18</sub>H<sub>12</sub>F<sub>3</sub>O<sub>4</sub> calcd: 349.0682, found: 349.0684. IR(neat) 3442, 1745, 1727, 1603, 1461, 1357, 1290, 1191, 1147, 1116, 1058, 1024, 966, 782, 711 cm<sup>-1</sup>.



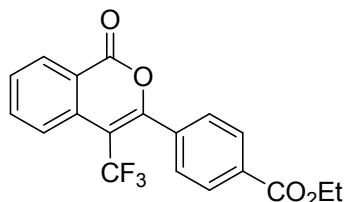
**4p**

methyl 4-(4-(trifluoromethyl)-1-oxo-1*H*-isochromen-3-yl)benzoate (**4p**). White solid, 10.4 mg, yield 15%, mp: 122–123 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.41 (d, *J* = 8.0 Hz, 1H), 8.15 (d, *J* = 8.4 Hz, 2H), 7.88 – 7.87 (m, 2H), 7.70 – 7.60 (m, 1H), 7.64 (d, *J* = 8.4 Hz, 2H), 3.97 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 166.2, 160.0, 156.3 (q, *J*<sub>C-F</sub> = 3.6 Hz), 136.7, 135.5, 132.7, 132.1, 130.1, 129.5, 129.4, 129.2 (q, *J*<sub>C-F</sub> = 1.8 Hz), 124.6 (q, *J*<sub>C-F</sub> = 3.7 Hz), 123.3 (q, *J*<sub>C-F</sub> = 271.8 Hz), 119.2, 107.6 (q, *J*<sub>C-F</sub> = 31.7 Hz), 52.4; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -53.63; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>18</sub>H<sub>12</sub>F<sub>3</sub>O<sub>4</sub> calcd: 349.0682, found: 349.0685. IR(neat) 3459, 1754, 1727, 1648, 1606, 1490, 1436, 1361, 1278, 1162, 1120, 1020, 981, 862, 777, 709 cm<sup>-1</sup>.



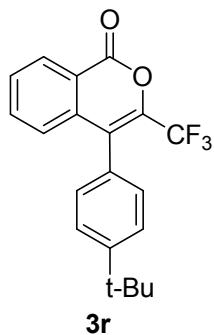
**3q**

ethyl 4-(3-(trifluoromethyl)-1-oxo-1*H*-isochromen-4-yl)benzoate (**3q**). White solid, 46.3 mg, yield 64%, mp: 148–149 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.43 (d, *J* = 7.2 Hz, 1H), 8.20 (d, *J* = 8.4 Hz, 2H), 7.73–7.66 (m, 2H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.00 (d, *J* = 7.6 Hz, 1H), 4.44 (q, *J* = 7.2 Hz, 2H), 1.44 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 165.9, 159.1, 139.0 (q, *J*<sub>C-F</sub> = 36.3 Hz), 136.5, 135.3, 135.2, 131.4, 130.6, 130.1, 130.0 (q, *J*<sub>C-F</sub> = 1.1 Hz), 129.9, 126.5, 121.6, 120.1 (q, *J*<sub>C-F</sub> = 2.2 Hz), 119.1 (q, *J*<sub>C-F</sub> = 272.9 Hz), 61.3, 14.3; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -63.23; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>19</sub>H<sub>14</sub>F<sub>3</sub>O<sub>4</sub> calcd: 363.0839, found: 363.0840. IR(neat) 3448, 2985, 2919, 1751, 1716, 1629, 1610, 1486, 1409, 1357, 1276, 1176, 1164, 1103, 1081, 1020, 979, 771, 703 cm<sup>-1</sup>.



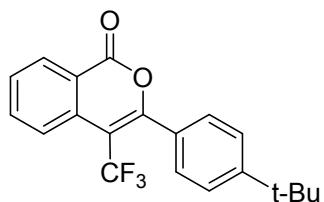
**4q**

ethyl 4-(4-(trifluoromethyl)-1-oxo-1*H*-isochromen-3-yl)benzoate (**4q**). White solid, 13.0 mg, yield 18%, mp: 108–110 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.40 (d, *J* = 7.6 Hz, 1H), 8.15 (d, *J* = 8.4 Hz, 2H), 7.88 – 7.86 (m, 2H), 7.69 – 7.65 (m, 1H), 7.63 (d, *J* = 8.4 Hz, 2H), 4.42 (q, *J* = 7.2 Hz, 2H), 1.43 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 165.7, 160.0, 156.3 (q, *J*<sub>C-F</sub> = 3.5 Hz), 136.5, 135.5, 132.7, 132.5, 130.1, 129.6, 129.4, 129.2 (q, *J*<sub>C-F</sub> = 1.8 Hz), 124.6 (q, *J*<sub>C-F</sub> = 3.5 Hz), 123.3 (q, *J*<sub>C-F</sub> = 271.8 Hz), 120.2, 107.6 (q, *J*<sub>C-F</sub> = 31.8 Hz), 61.4, 14.3; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -53.62; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>19</sub>H<sub>14</sub>F<sub>3</sub>O<sub>4</sub> calcd: 363.0839, found: 363.0841. IR(neat) 3463, 2977, 2913, 1752, 1716, 1629, 1605, 1486, 1409, 1359, 1272, 1176, 1166, 1105, 1079, 1018, 977, 771, 703 cm<sup>-1</sup>.



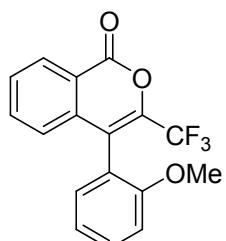
**3r**

4-(4-*tert*-butylphenyl)-3-(trifluoromethyl)-1*H*-isochromen-1-one (**3r**). White solid, 57.4 mg, yield 83%, mp: 126–127 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.40 (d, *J* = 7.2 Hz, 1H), 7.67 (dt, *J* = 24.4, 6.8 Hz, 2H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.21 (d, *J* = 8.4 Hz, 2H), 7.11 (d, *J* = 7.6 Hz, 1H), 1.39 (s, 9H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 159.5, 152.1, 138.8 (q, *J*<sub>C-F</sub> = 35.7 Hz), 137.3, 135.1, 130.3, 129.8, 129.5 (q, *J*<sub>C-F</sub> = 1.1 Hz), 127.3, 127.0, 125.6, 121.6, 121.1 (q, *J*<sub>C-F</sub> = 2.2 Hz), 119.3 (q, *J*<sub>C-F</sub> = 272.8 Hz), 34.8, 31.3; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -63.12; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>20</sub>H<sub>18</sub>F<sub>3</sub>O<sub>2</sub> calcd: 347.1253, found: 347.1265. IR(neat) 3457, 2965, 1749, 1600, 1457, 1355, 1305, 1189, 1139, 1116, 966, 826, 777, 707 cm<sup>-1</sup>.



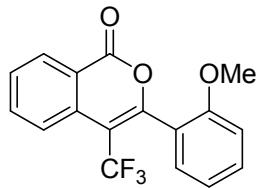
**4r**

3-(4-*tert*-butylphenyl)-4-(trifluoromethyl)-1*H*-isochromen-1-one (**4r**). White solid, 11.1 mg, yield 16%, mp: 106–107 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.38 (d, *J* = 8.0 Hz, 1H), 7.84 (d, *J* = 2.8 Hz, 2H), 7.67–7.62 (m, 1H), 7.49 (s, 4H), 1.36 (s, 9H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 160.5, 157.8 (*q*, *J*<sub>C-F</sub> = 3.5 Hz), 154.2, 135.2, 133.3, 130.0, 129.7, 129.0, 128.9 (*q*, *J*<sub>C-F</sub> = 1.8 Hz), 125.2, 124.5 (*q*, *J*<sub>C-F</sub> = 3.6 Hz), 123.6 (*q*, *J*<sub>C-F</sub> = 271.6 Hz), 120.2, 106.6 (*q*, *J*<sub>C-F</sub> = 31.6 Hz), 35.0, 31.2; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -53.57; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>20</sub>H<sub>18</sub>F<sub>3</sub>O<sub>2</sub> calcd: 347.1253, found: 347.1264. IR(neat) 3463, 2967, 1741, 1644, 1360, 1263, 1108, 1079, 1022, 800, 711 cm<sup>-1</sup>.



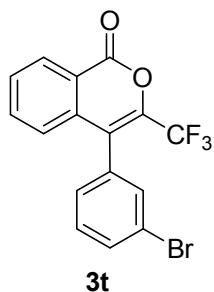
**3s**

3-(trifluoromethyl)-4-(2-methoxyphenyl)-1*H*-isochromen-1-one (**3s**). White solid, 47.4 mg, yield 74%, mp: 123–124 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.39 (d, *J* = 8.0 Hz, 1H), 7.65 (dt, *J* = 21.2, 7.4 Hz, 2H), 7.49 (t, *J* = 7.8 Hz, 1H), 7.18 (d, *J* = 7.2 Hz, 1H), 7.08 (t, *J* = 7.4 Hz, 1H), 7.05 (d, *J* = 8.4 Hz, 2H), 3.73 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 158.7, 156.4, 138.1 (*q*, *J*<sub>C-F</sub> = 35.8 Hz), 135.8, 134.0, 130.2 (*q*, *J*<sub>C-F</sub> = 1.4 Hz), 129.8, 129.1, 128.8, 125.3, 120.7, 119.9, 118.3, 18.2 (*q*, *J*<sub>C-F</sub> = 272.5 Hz), 116.7 (*q*, *J*<sub>C-F</sub> = 2.1 Hz), 110.0, 54.5; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -64.97; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>17</sub>H<sub>12</sub>F<sub>3</sub>O<sub>3</sub> calcd: 321.0733, found: 321.0740. IR(neat) 3471, 3018, 2844, 1751, 1602, 1494, 1457, 1355, 1305, 1261, 1197, 1114, 1018, 964, 761, 705 cm<sup>-1</sup>.



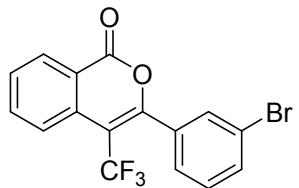
**4s**

4-(trifluoromethyl)-3-(2-methoxyphenyl)-1*H*-isochromen-1-one (**4s**). White solid, 1.9 mg, yield 3%, mp: 104–106 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.40 (d, *J* = 8.0 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 2H), 7.66–7.63 (m, 1H), 7.46 (t, *J* = 8.0 Hz, 1H), 7.37 (d, *J* = 7.6 Hz, 1H), 7.04 (t, *J* = 7.6 Hz, 1H), 6.97 (d, *J* = 8.0 Hz, 1H), 3.82 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 160.9, 157.1, 154.1 (q, *J*<sub>C-F</sub> = 3.6 Hz), 135.2, 133.1, 132.0, 131.6, 130.2 (q, *J*<sub>C-F</sub> = 1.2 Hz), 130.0, 129.1, 124.4 (q, *J*<sub>C-F</sub> = 3.4 Hz), 123.4 (q, *J*<sub>C-F</sub> = 271.8 Hz), 122.1, 120.3, 110.9, 108.6 (q, *J*<sub>C-F</sub> = 31.3 Hz), 55.6; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -56.86; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>17</sub>H<sub>12</sub>F<sub>3</sub>O<sub>3</sub> calcd: 321.0733, found: 321.0741. IR(neat) 3448, 2923, 1749, 1637, 1490, 1398, 1359, 1253, 1162, 1108, 1074, 1018, 977, 755 cm<sup>-1</sup>.



**3t**

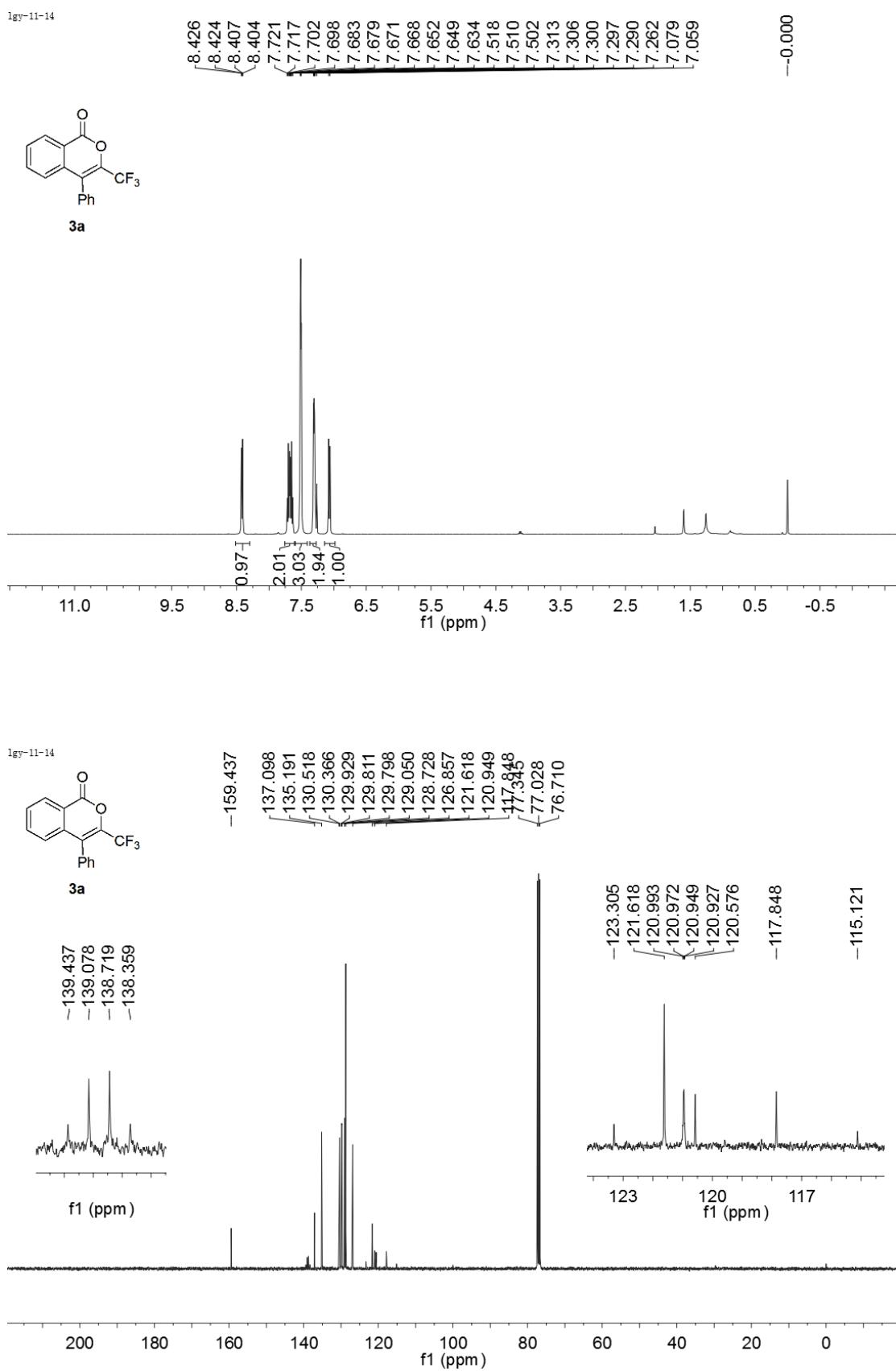
4-(3-bromophenyl)-3-(trifluoromethyl)-1*H*-isochromen-1-one (**3t**). White solid, 36.8 mg, yield 50%, mp: 116–117 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.42 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.74 (td, *J* = 7.6, 1.2 Hz, 2H), 7.70 – 7.65 (m, 2H), 7.48 (s, 1H), 7.40 (t, *J* = 8.0 Hz, 1H), 7.25 (d, *J* = 7.2 Hz, 1H), 7.05 (d, *J* = 8.0 Hz, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 159.1, 139.2 (q, *J*<sub>C-F</sub> = 36.2 Hz), 136.5, 135.4, 132.7 (q, *J*<sub>C-F</sub> = 1.3 Hz), 132.6, 132.3, 130.6, 130.3, 130.1, 128.6 (q, *J*<sub>C-F</sub> = 1.4 Hz), 126.6, 122.8, 121.5, 119.5 (q, *J*<sub>C-F</sub> = 2.2 Hz), 119.1 (q, *J*<sub>C-F</sub> = 273.0 Hz); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -63.19; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>16</sub>H<sub>9</sub>F<sub>3</sub>BrO<sub>2</sub> calcd: 368.9733, found: 368.9743. IR(neat) 3446, 1745, 1353, 1307, 1191, 1147, 1114, 979, 781, 703 cm<sup>-1</sup>.



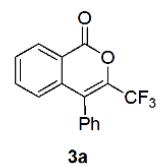
**4t**

3-(3-bromophenyl)-4-(trifluoromethyl)-1*H*-isochromen-1-one (**4t**). White solid, 11.0 mg, yield 15%, mp: 118–119 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.40 (d, *J* = 8.0 Hz, 1H), 7.88 – 7.86 (m, 2H), 7.69 – 7.65 (m, 1H), 7.56 (s, 1H), 7.52 – 7.49 (m, 1H), 7.43 – 7.41 (m, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 160.0, 155.7 (q, *J*<sub>C-F</sub> = 3.5 Hz), 135.5, 134.4, 133.8, 132.7, 131.9 (q, *J*<sub>C-F</sub> = 1.7 Hz), 130.1, 129.7, 129.6, 127.8 (q, *J*<sub>C-F</sub> = 2.0 Hz), 124.7 (q, *J*<sub>C-F</sub> = 3.6 Hz), 123.3 (q, *J*<sub>C-F</sub> = 271.7 Hz), 122.2, 120.2, 107.5 (q, *J*<sub>C-F</sub> = 31.8 Hz); <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -53.68; HRMS (pos. ESI): m/z [M + H]<sup>+</sup> for C<sub>16</sub>H<sub>9</sub>F<sub>3</sub>BrO<sub>2</sub> calcd: 368.9733, found: 368.9743. IR(neat) 3463, 2921, 1758, 1629, 1355, 1155, 1126, 983, 769, 692 cm<sup>-1</sup>.

## Copies of NMR spectra of the products

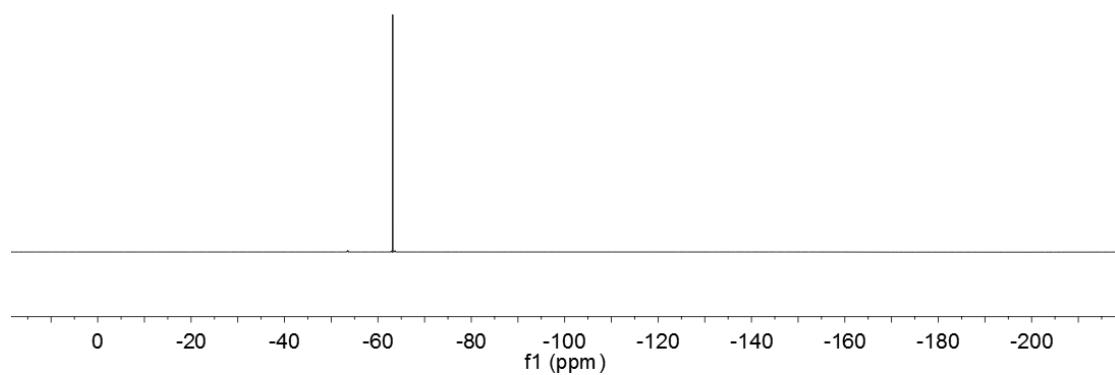


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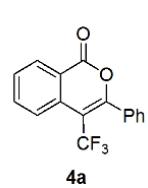


3a

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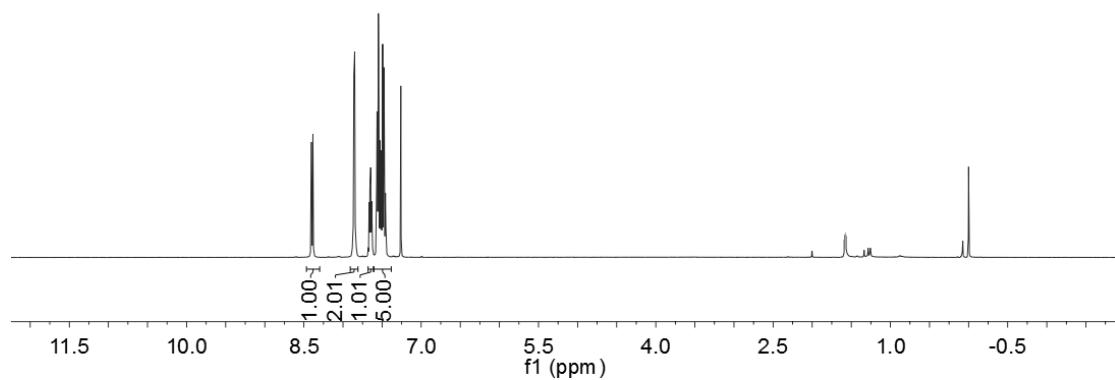


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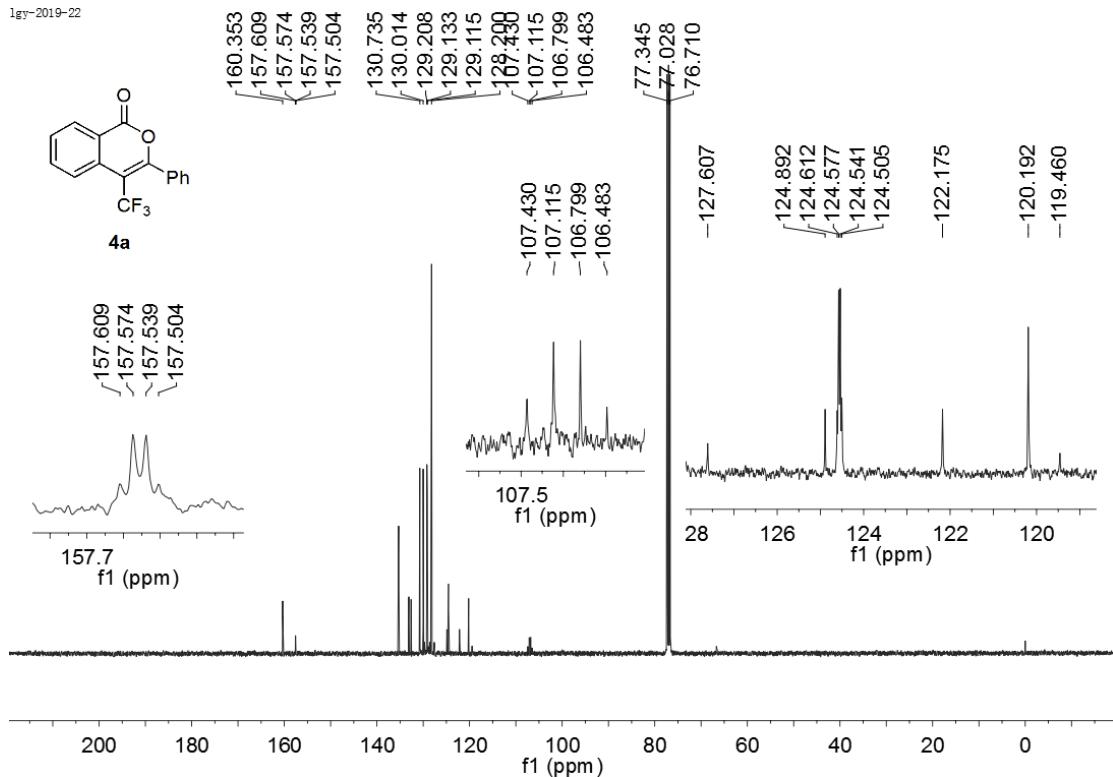


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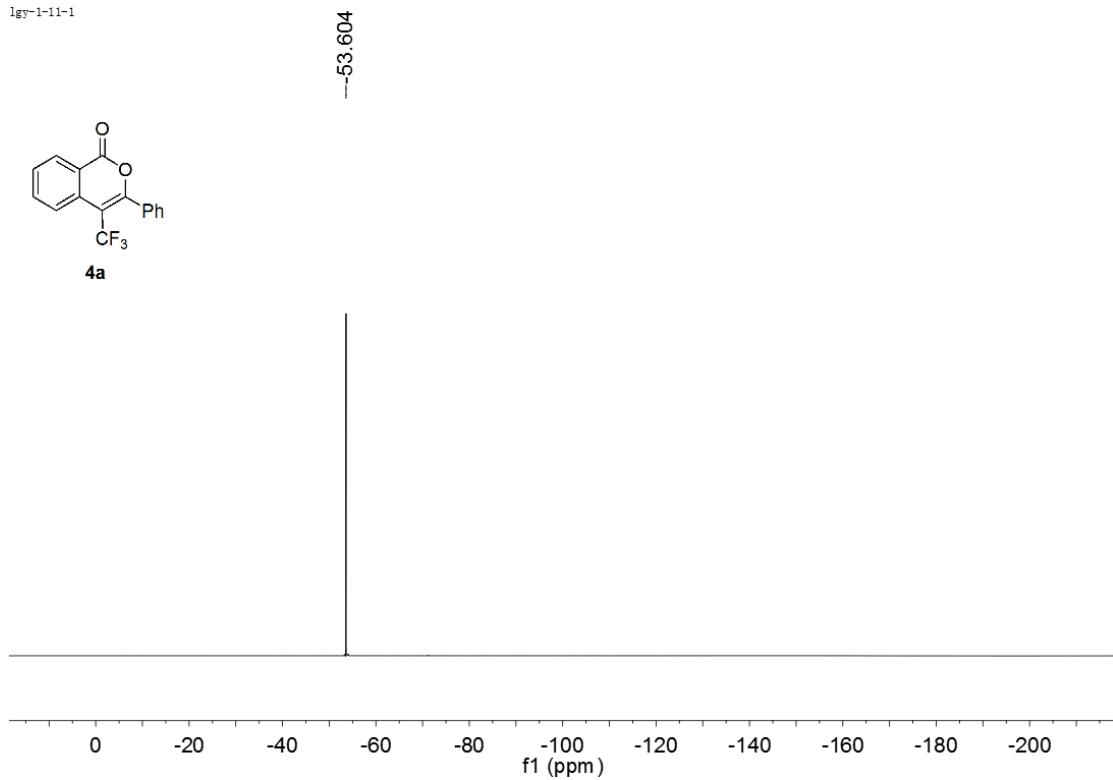
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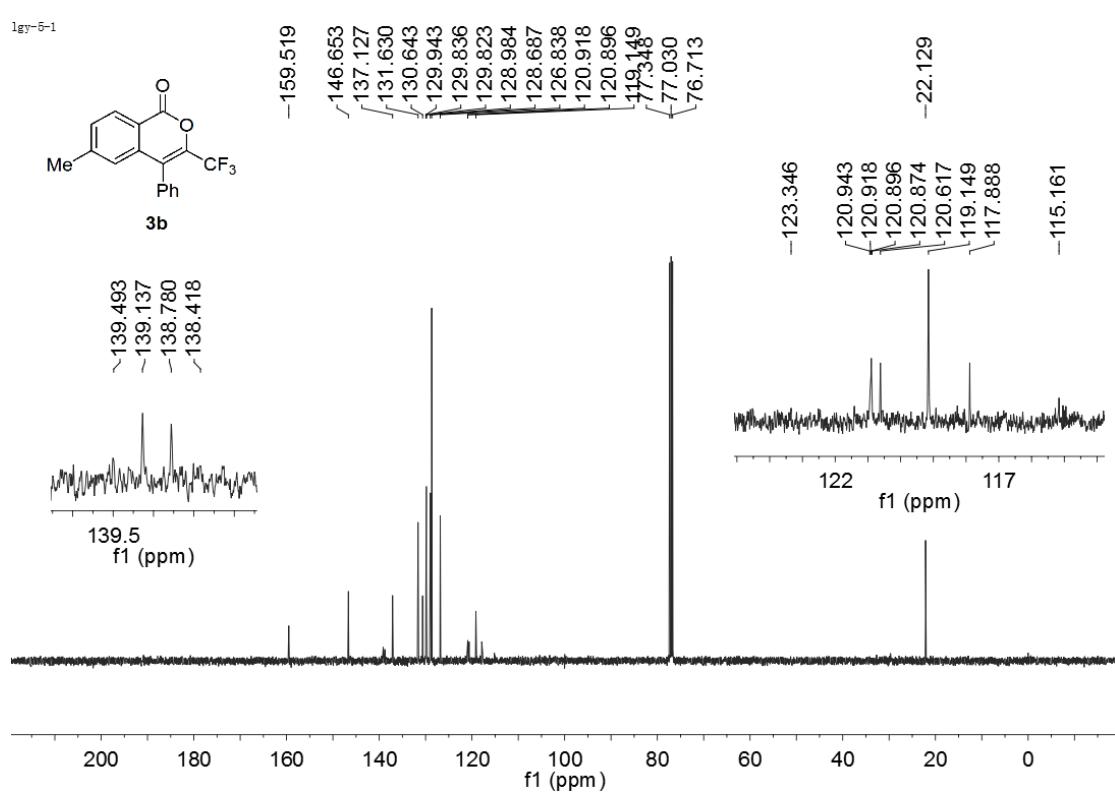
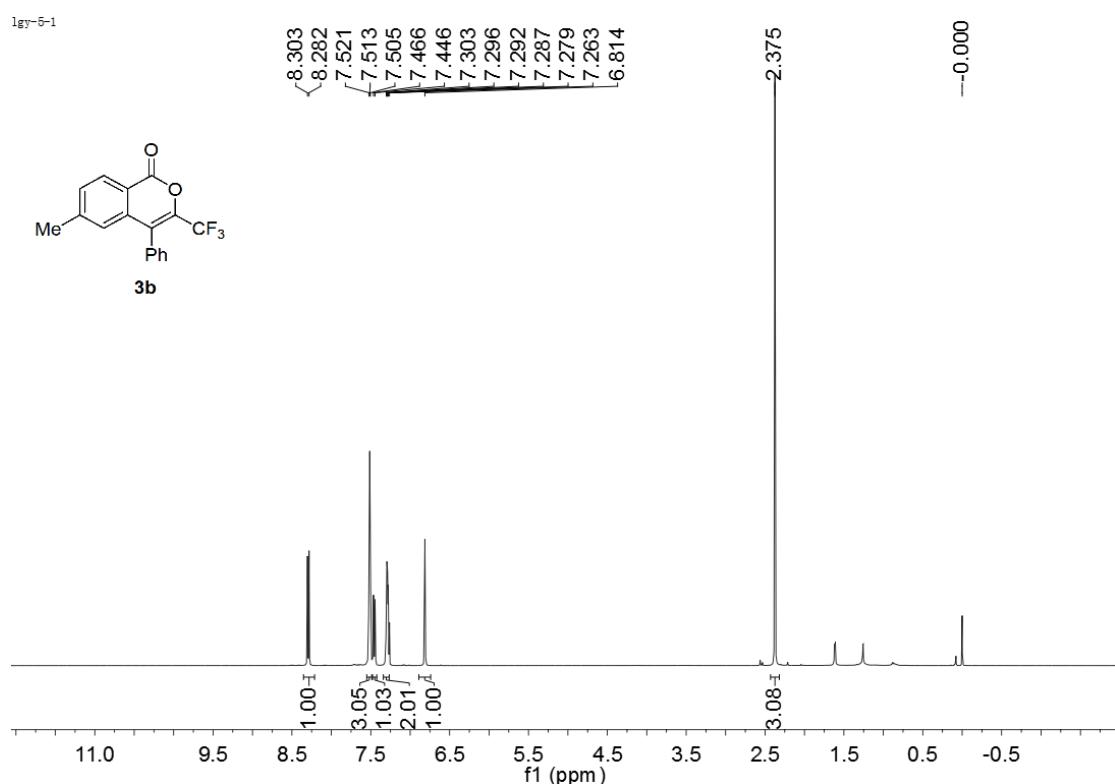


lgy-2019-22



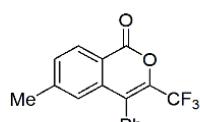
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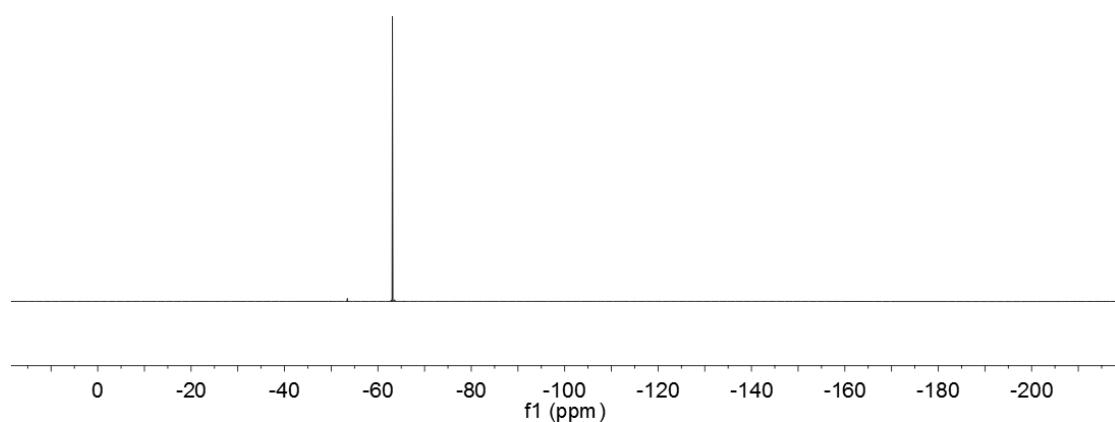


lgy-5-1

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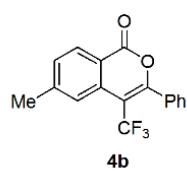


**3b**

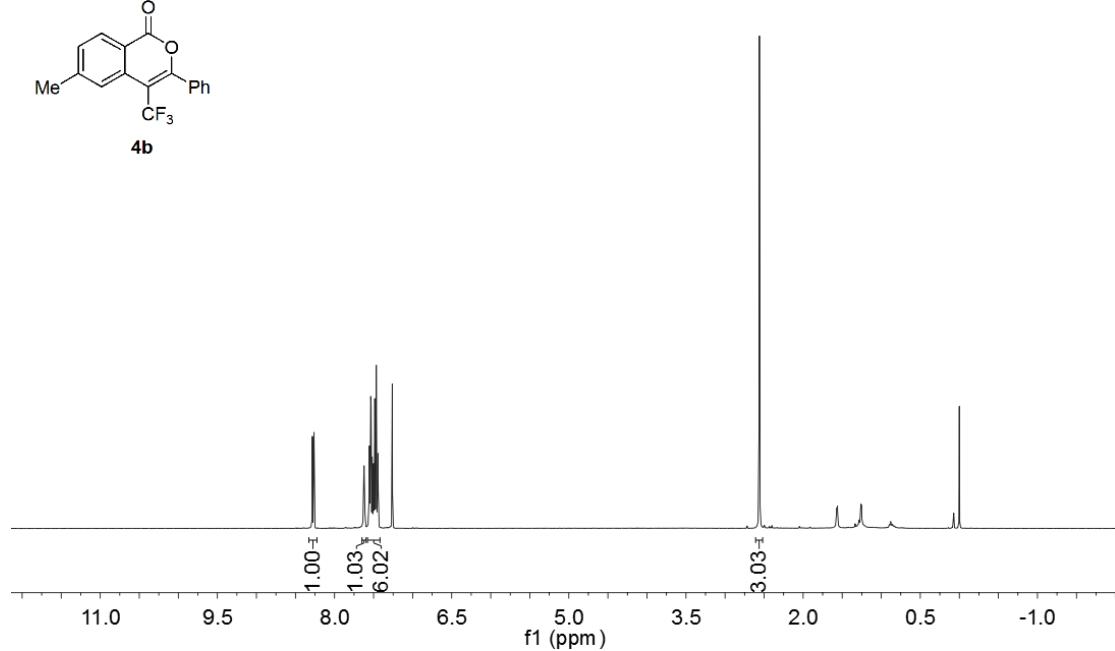


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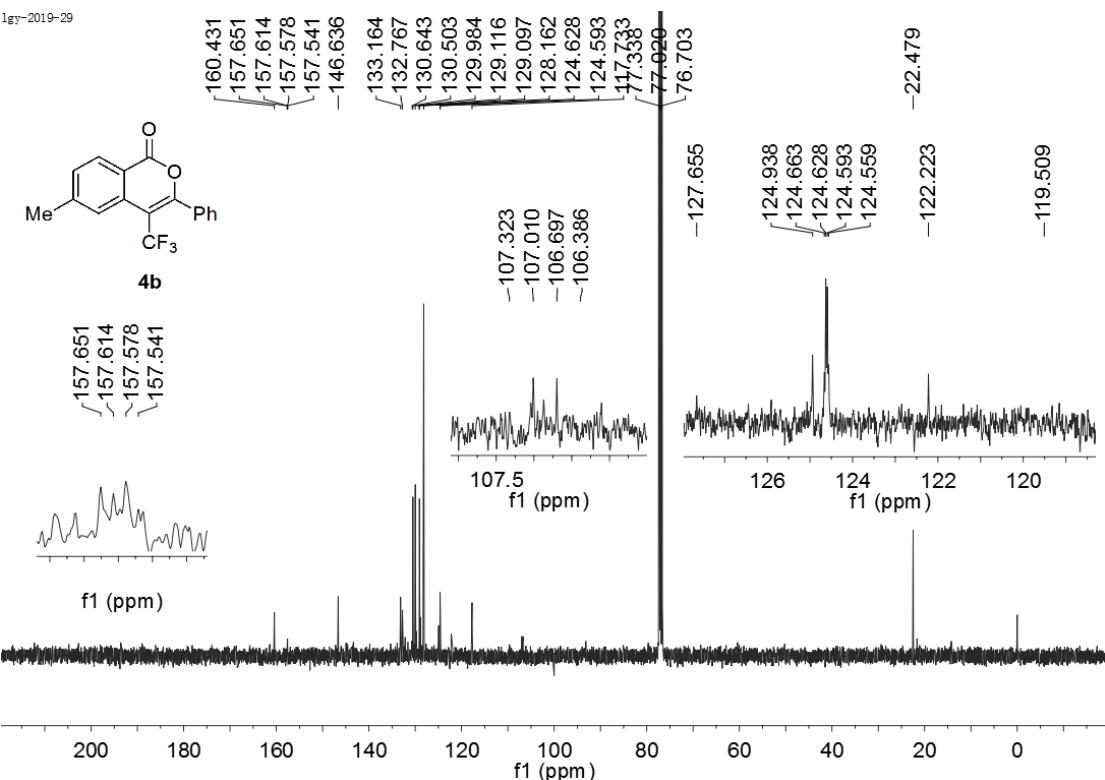
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7.536  
7.532  
7.519  
7.505  
7.501  
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7.484  
7.470  
7.466  
7.449  
7.445  
7.260  
-2.560  
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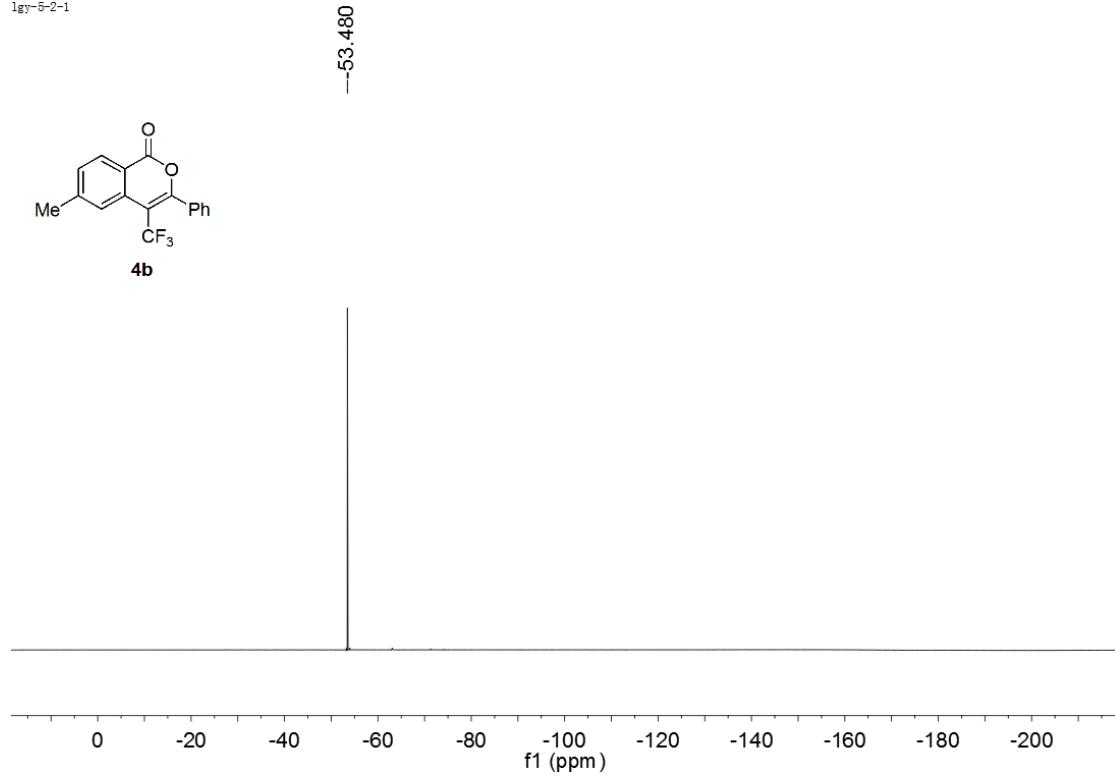
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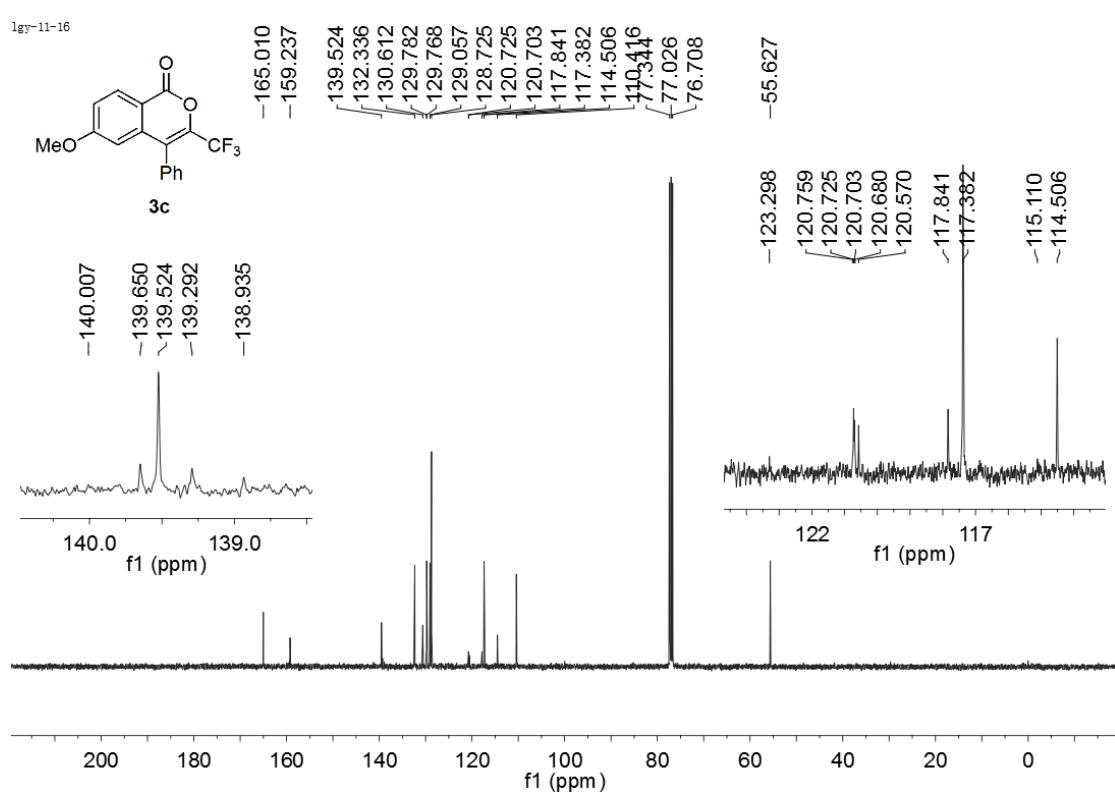
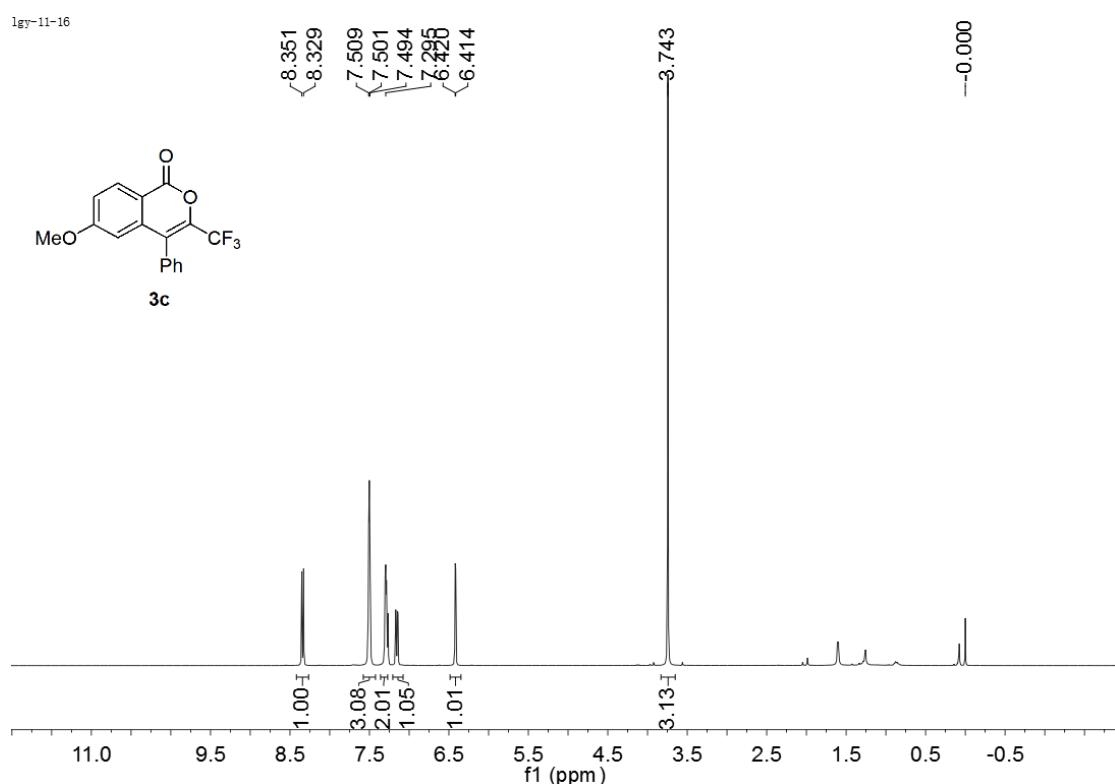


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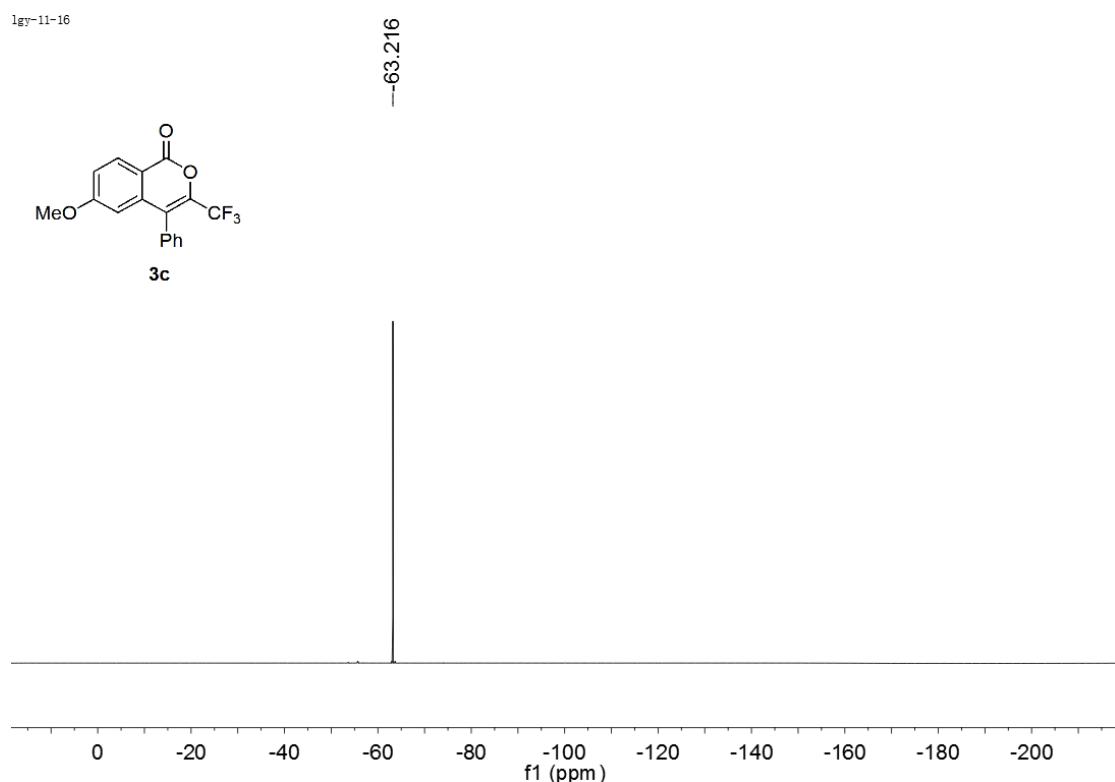
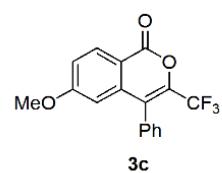


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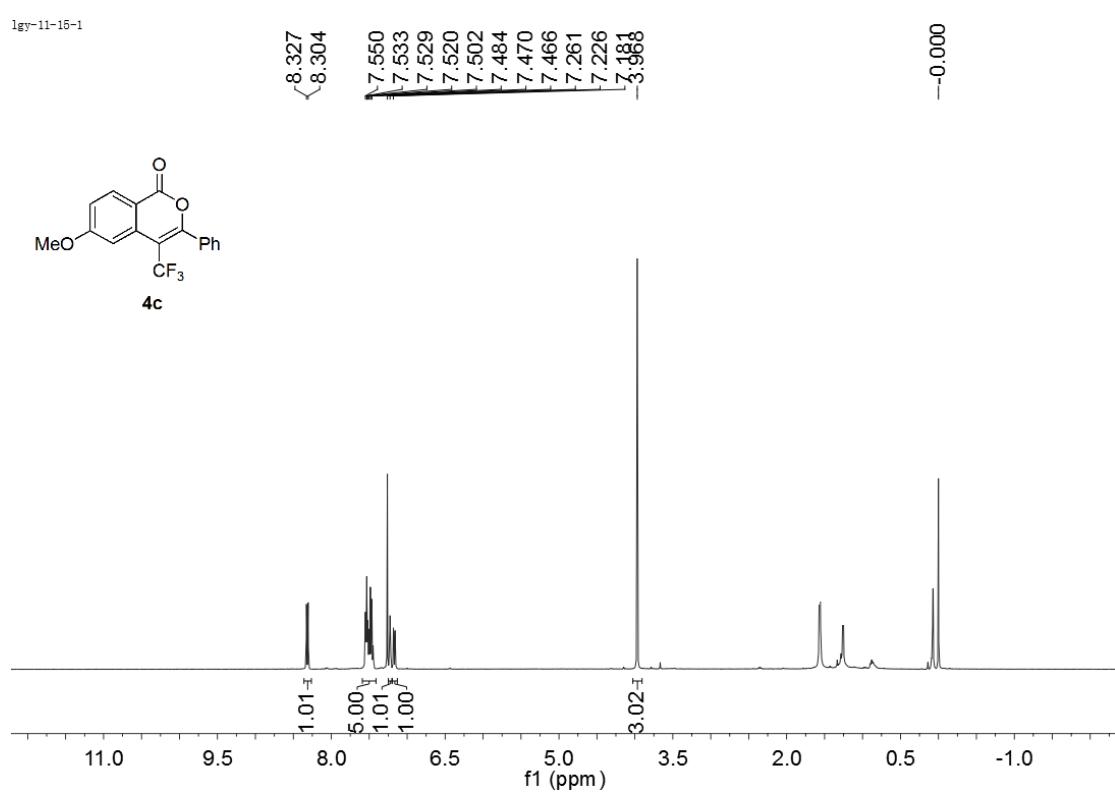
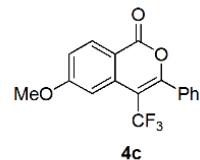




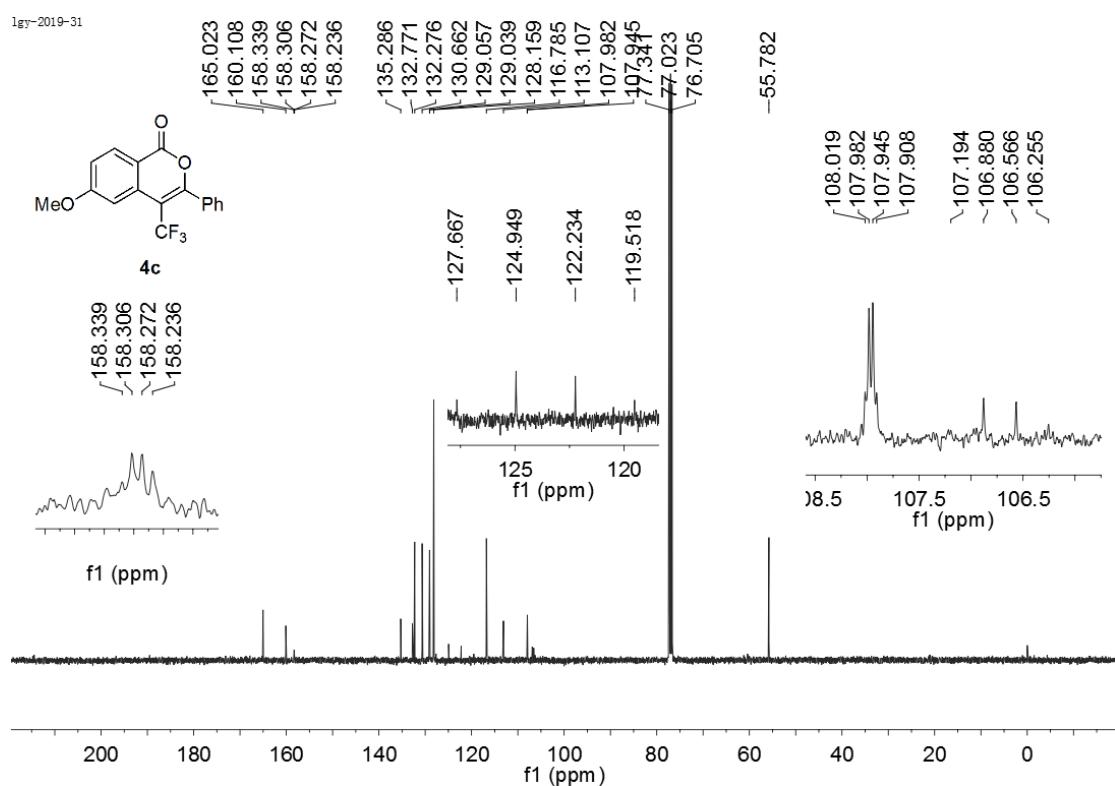
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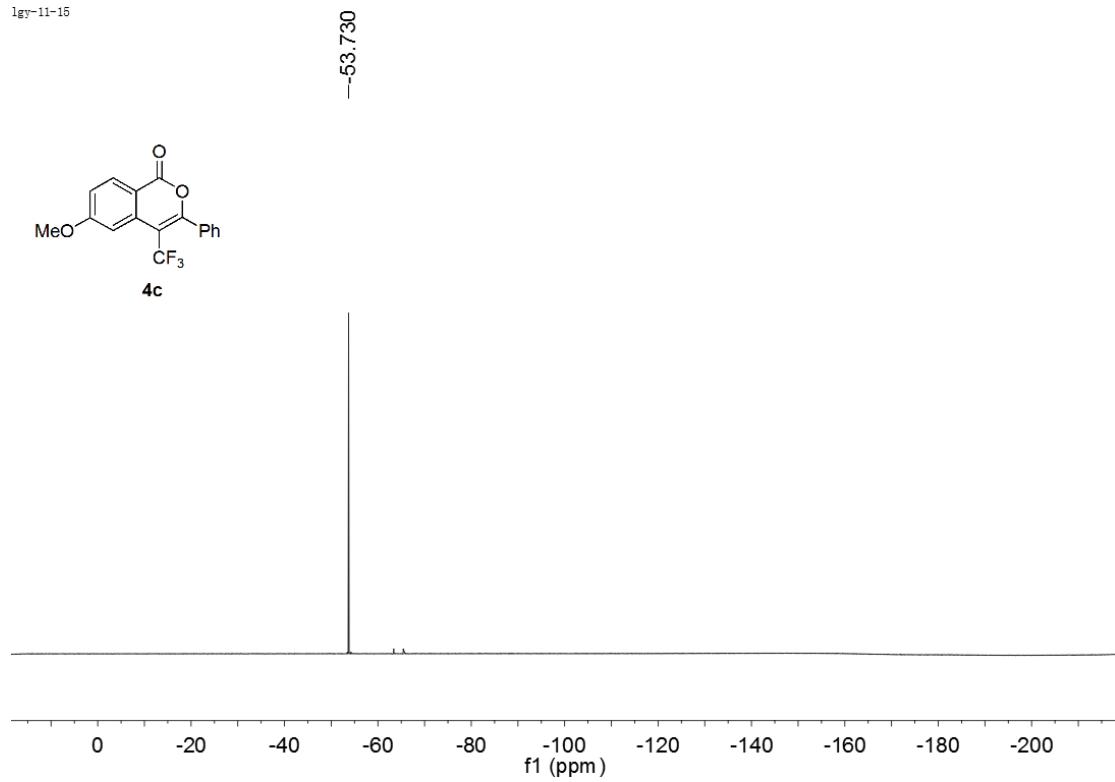
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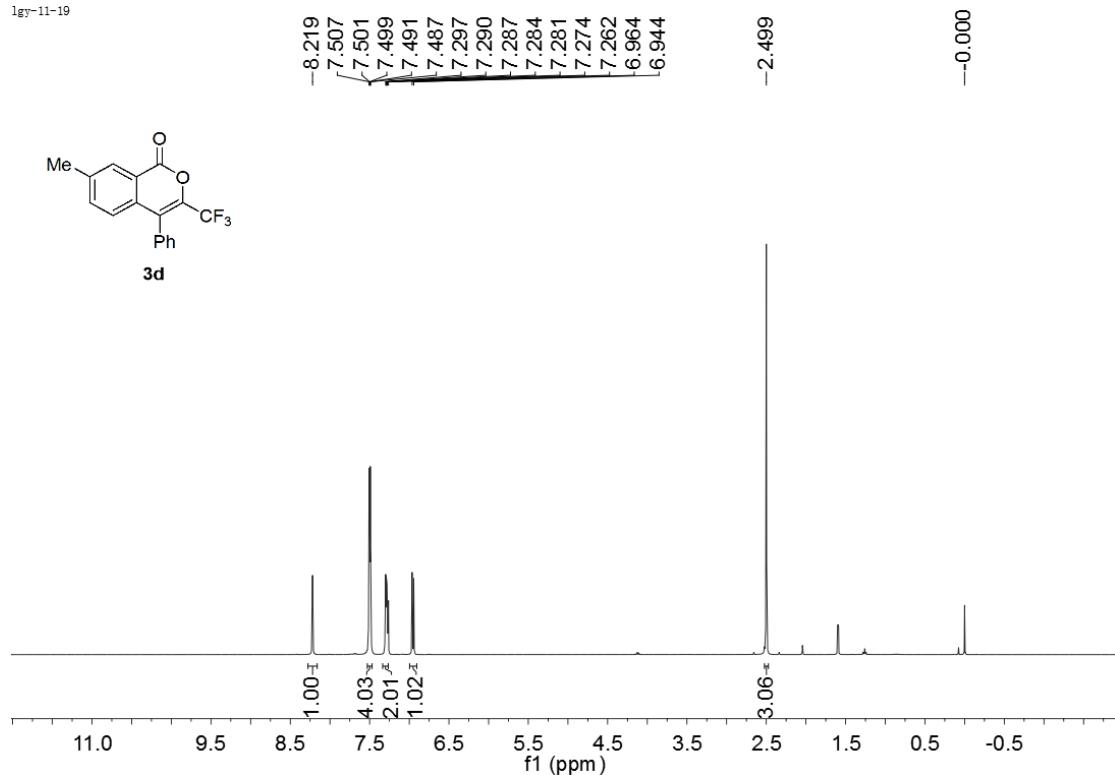
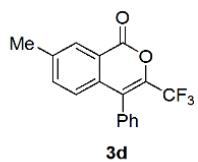
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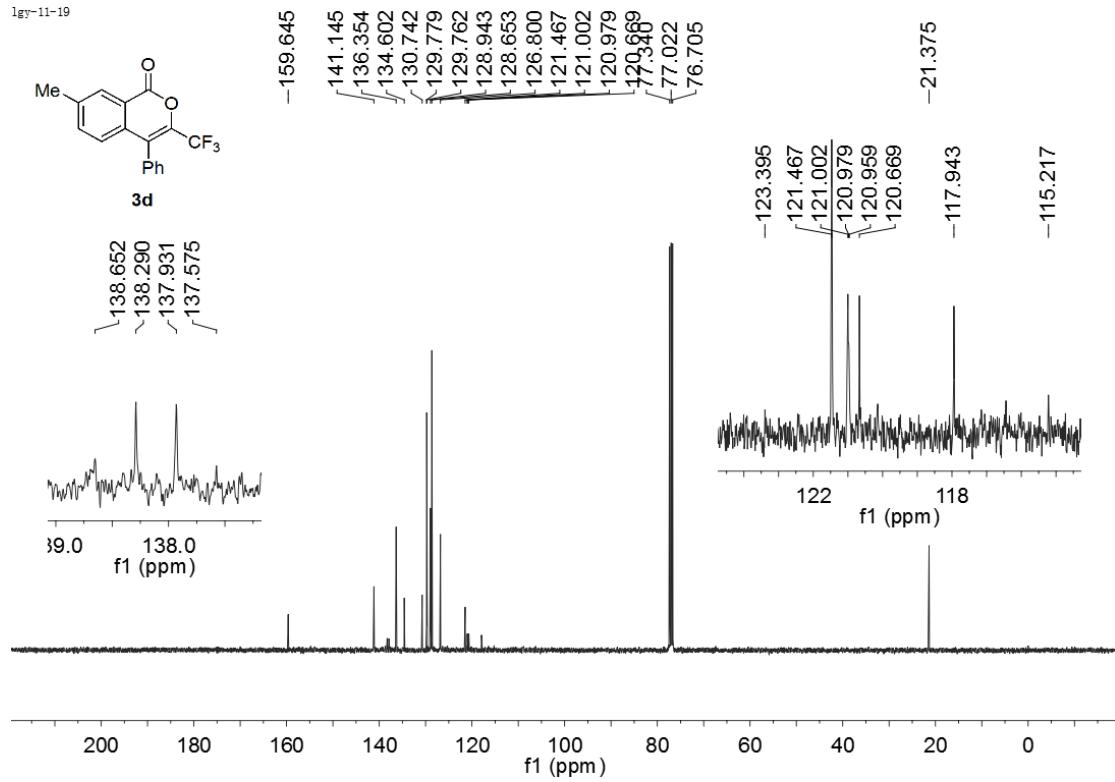
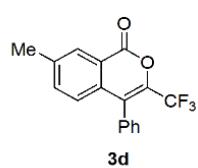
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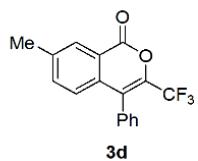


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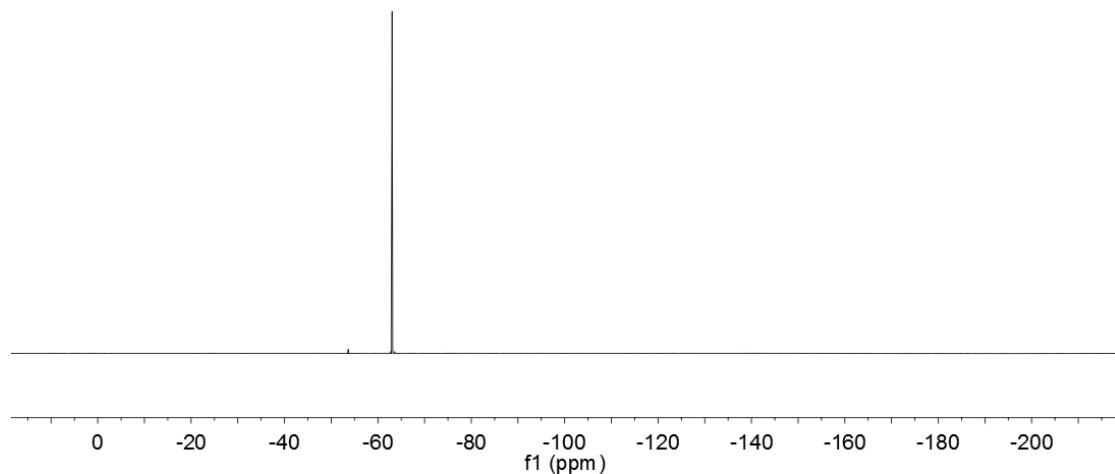


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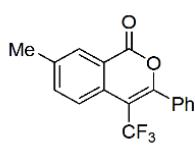


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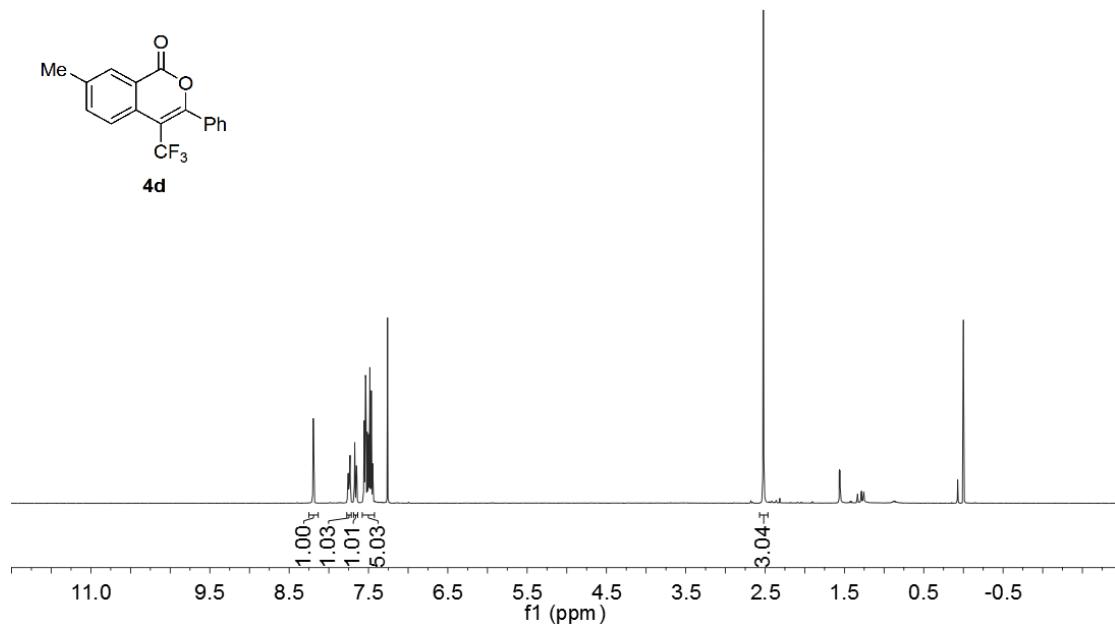


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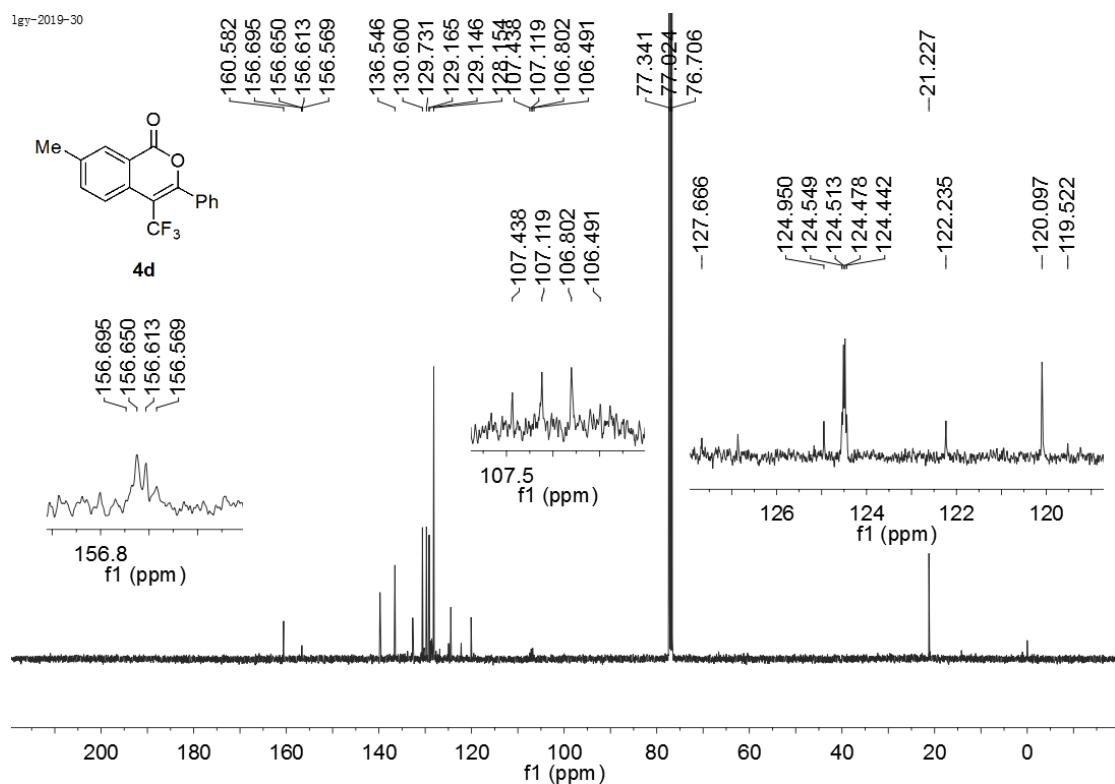
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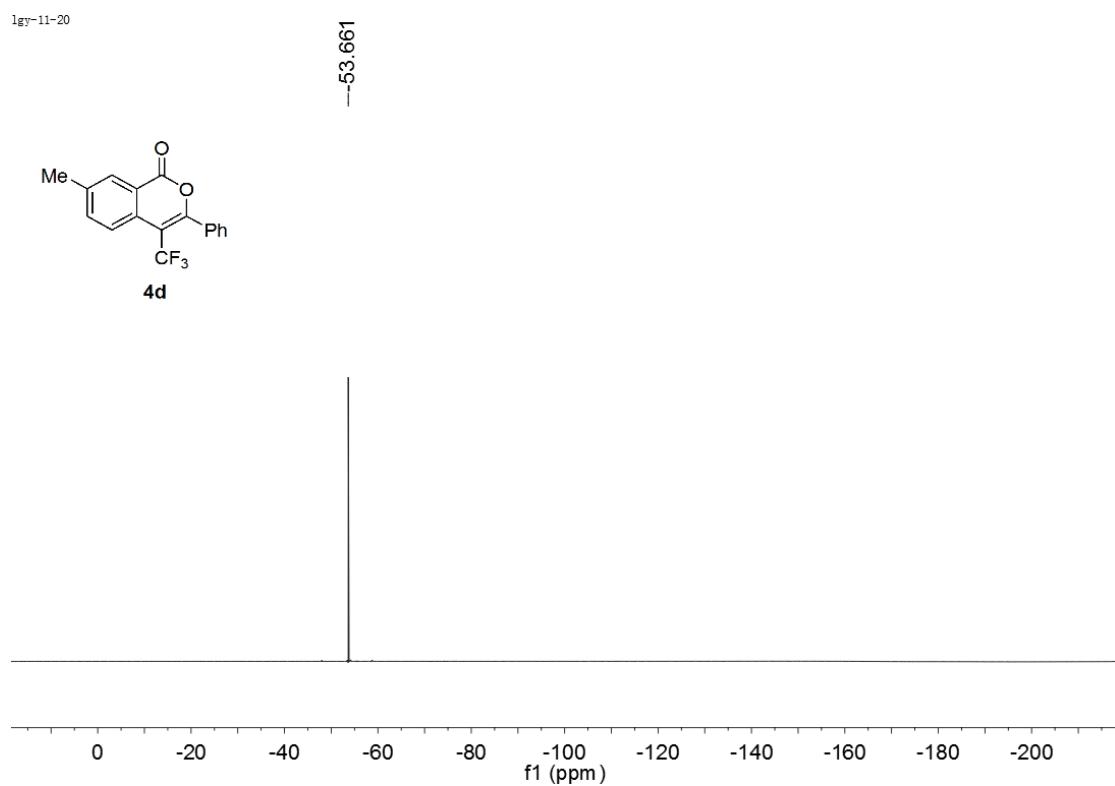
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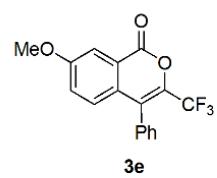
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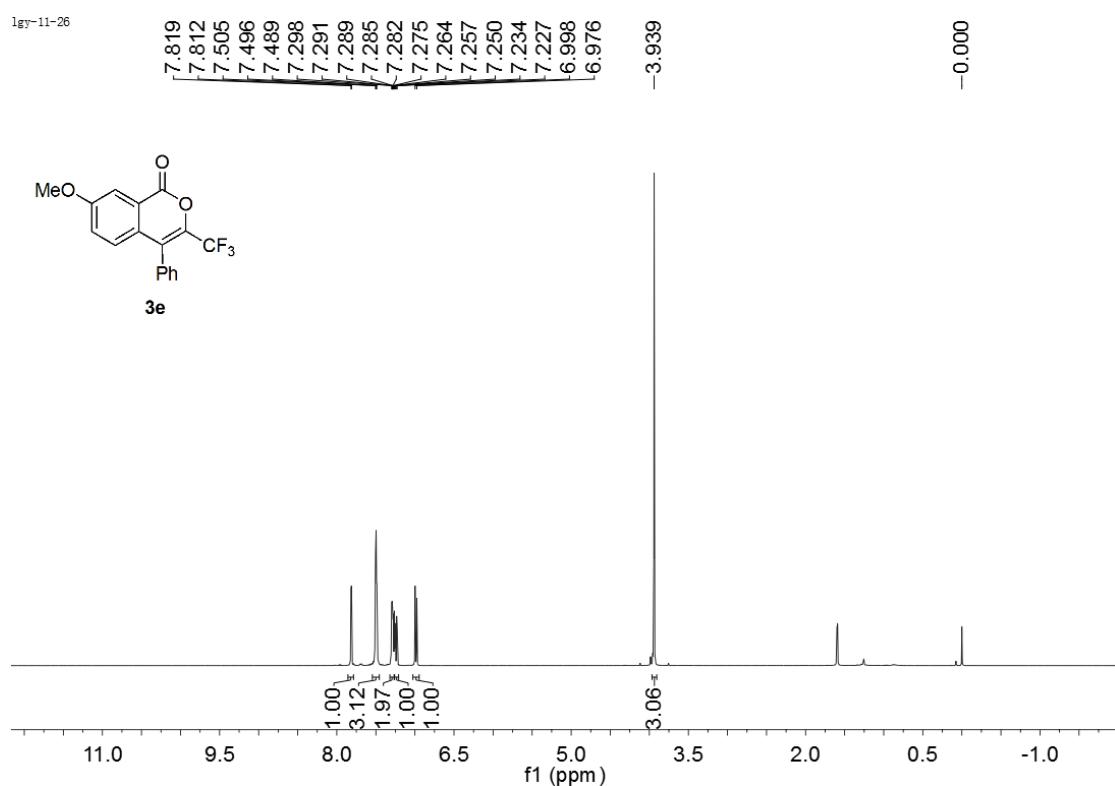
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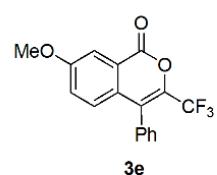
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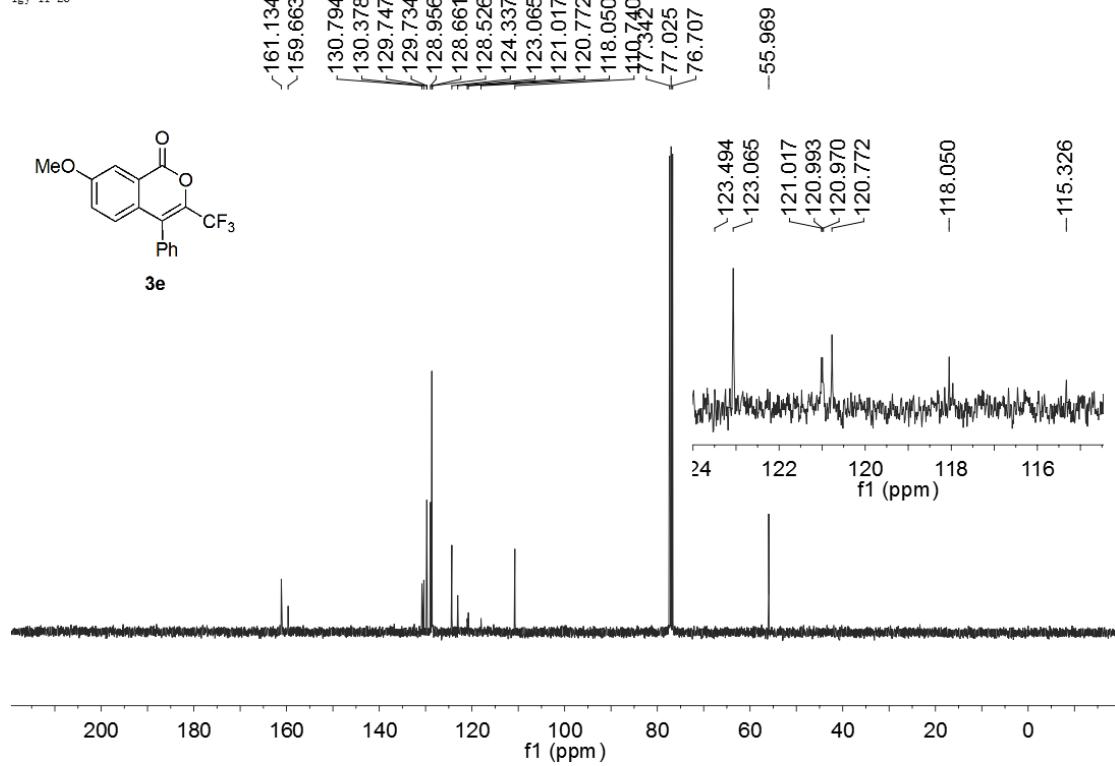
**3e**



lgy-11-26

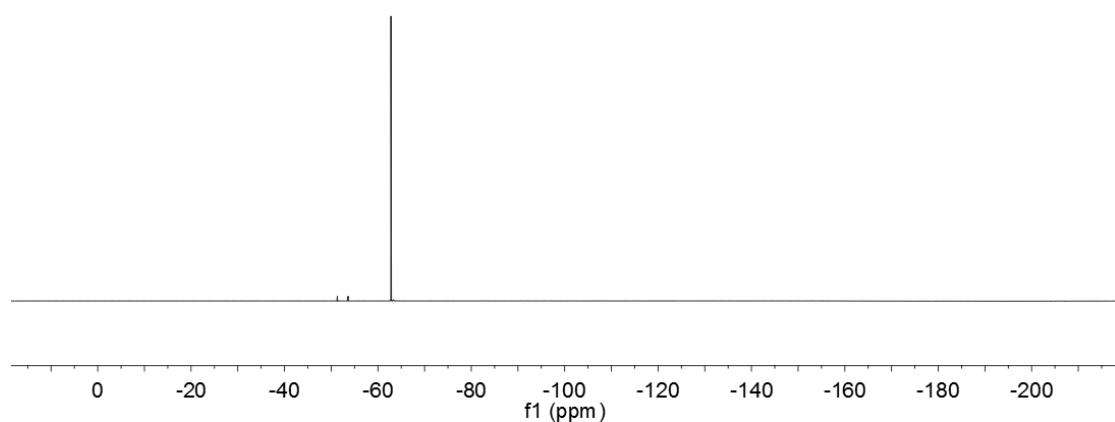
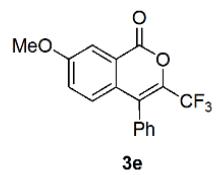


**3e**



lgy-11-26

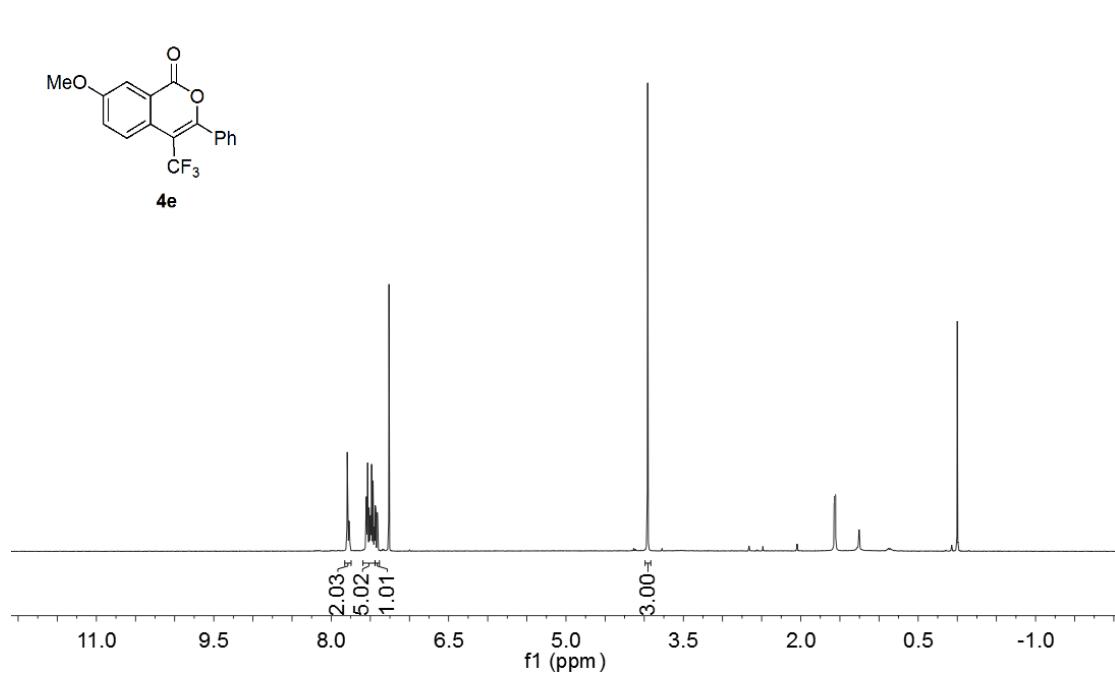
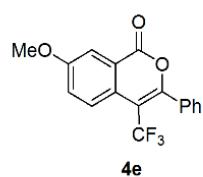
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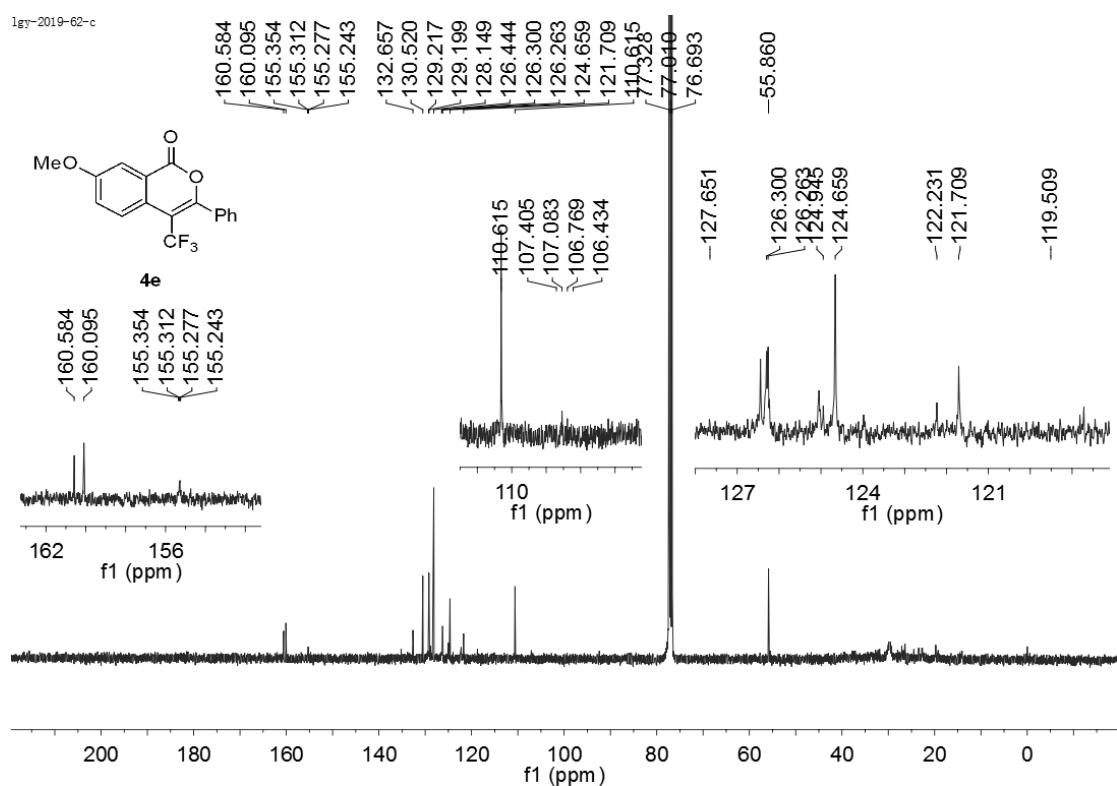
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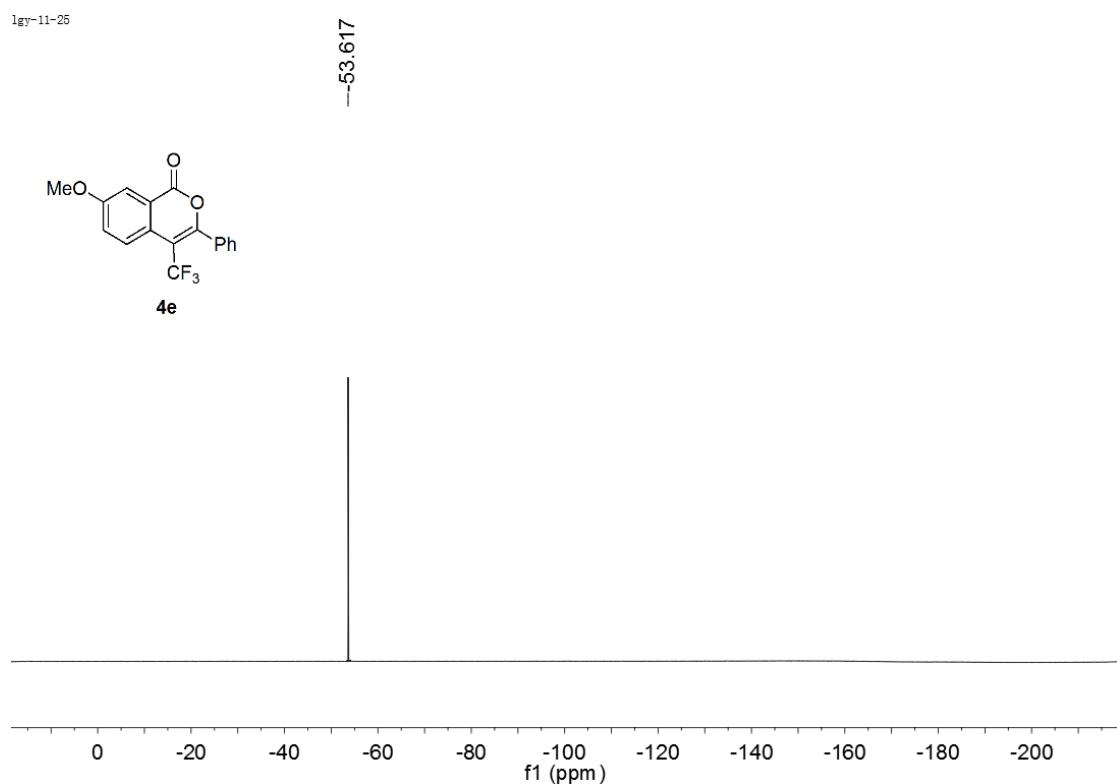
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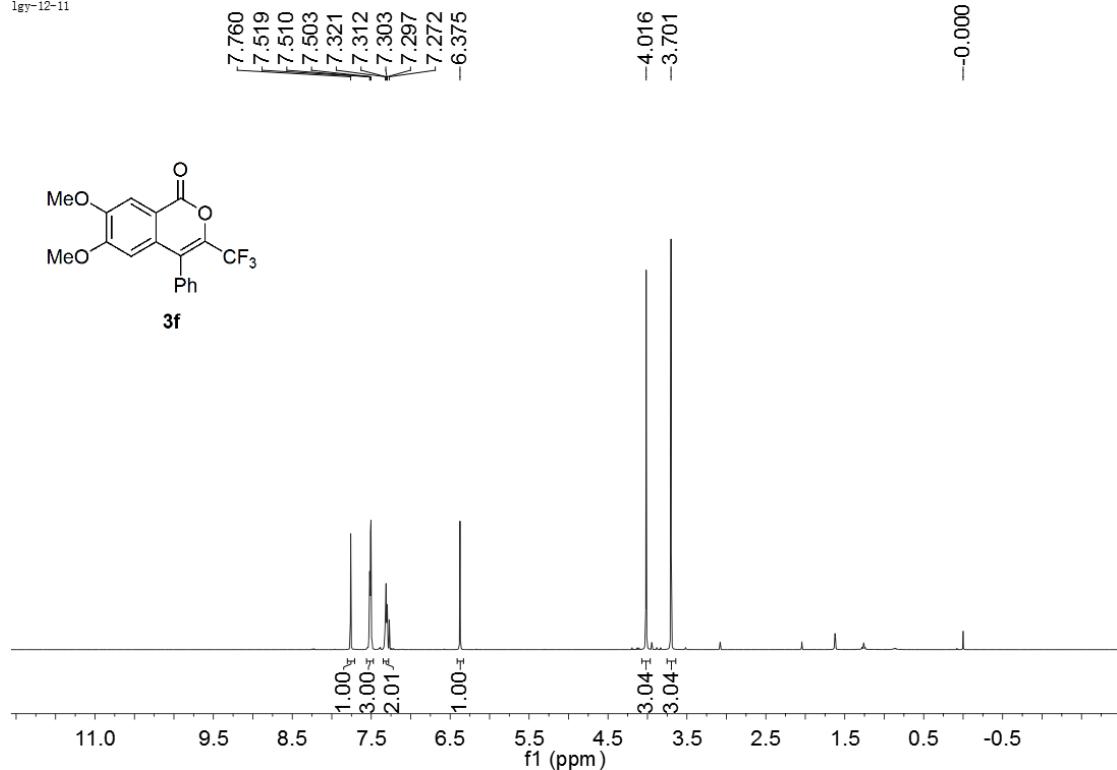
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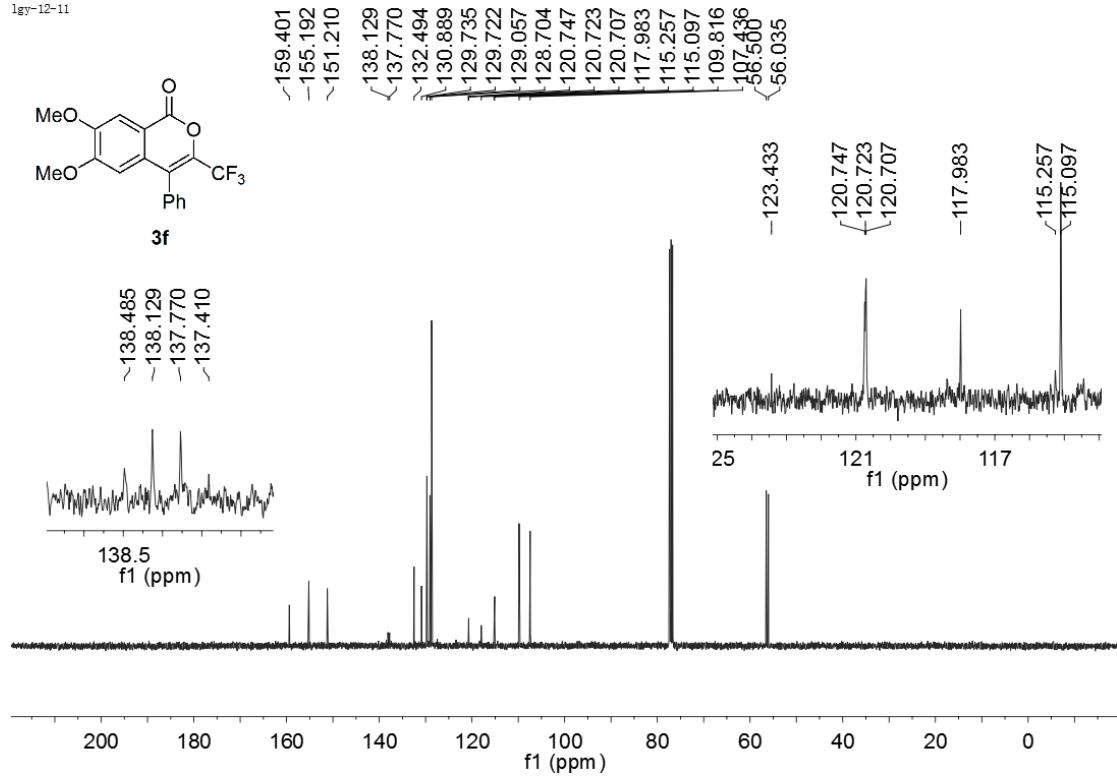
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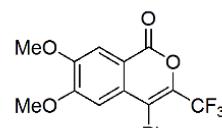
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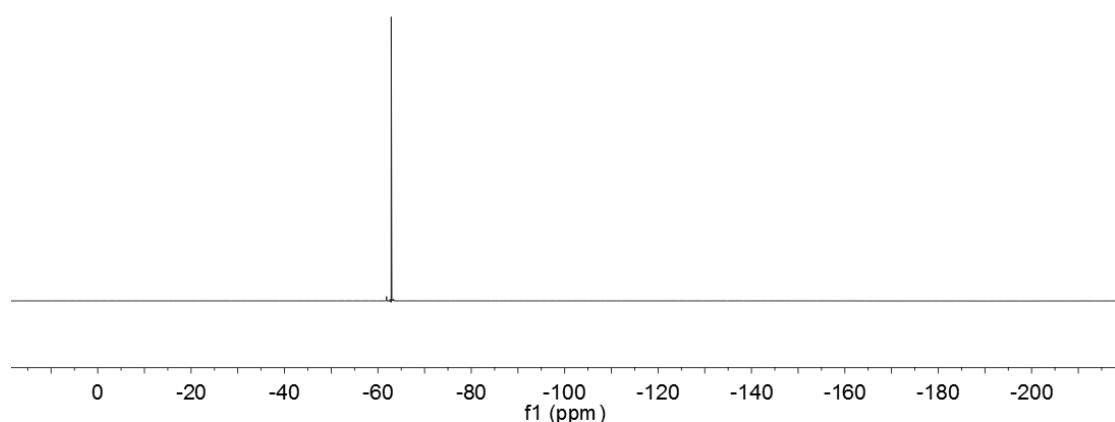
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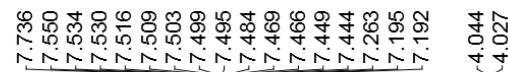
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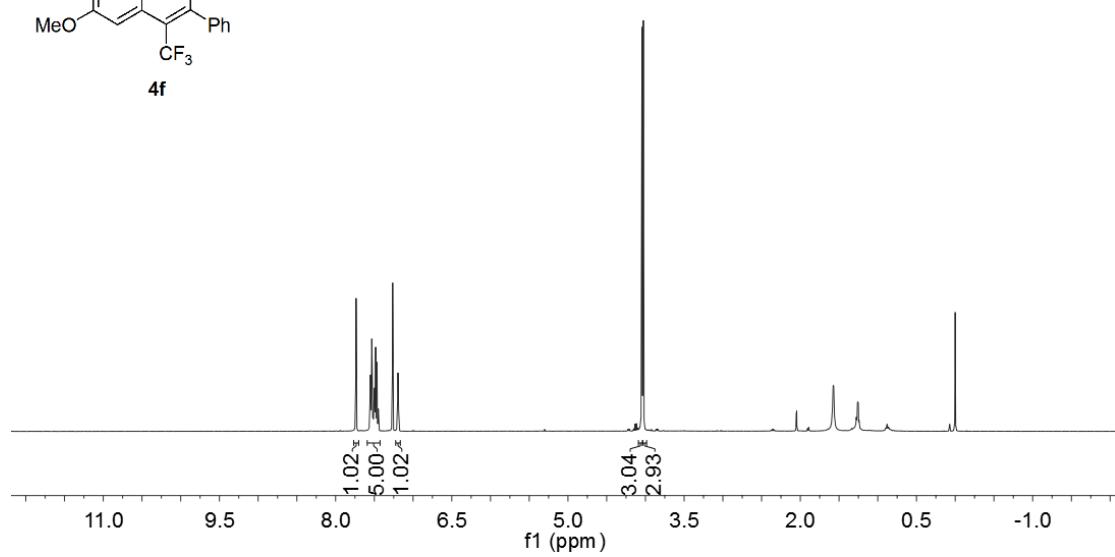
**3f**



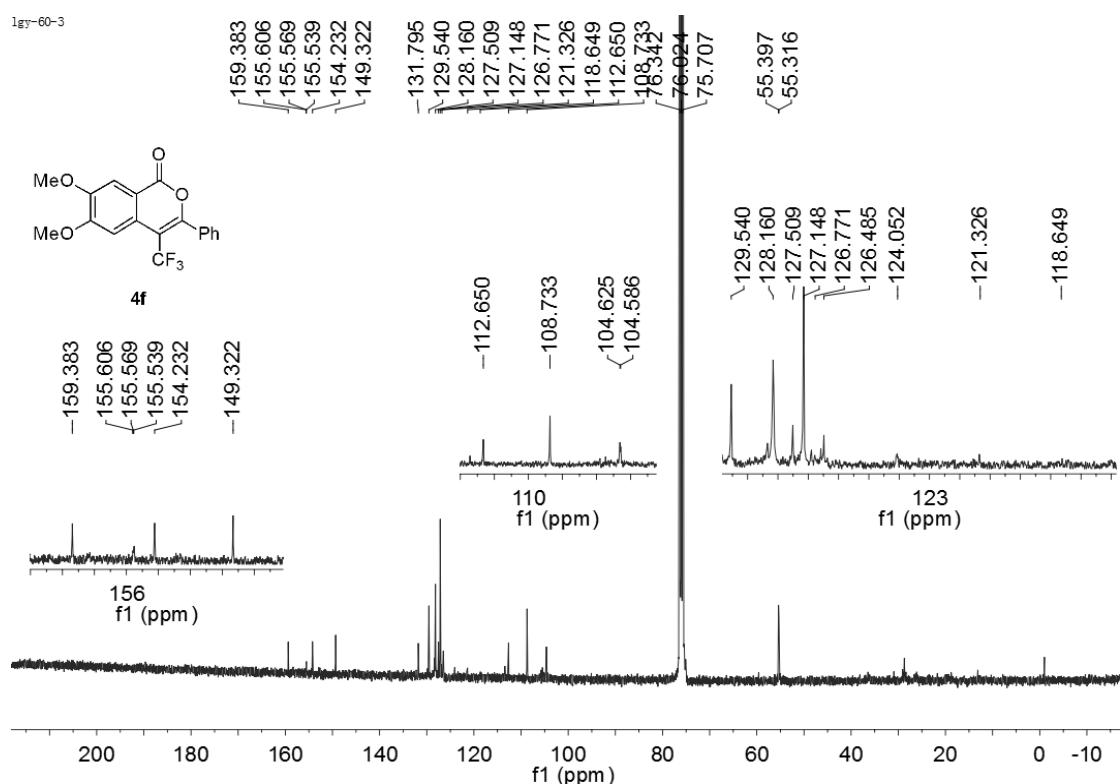
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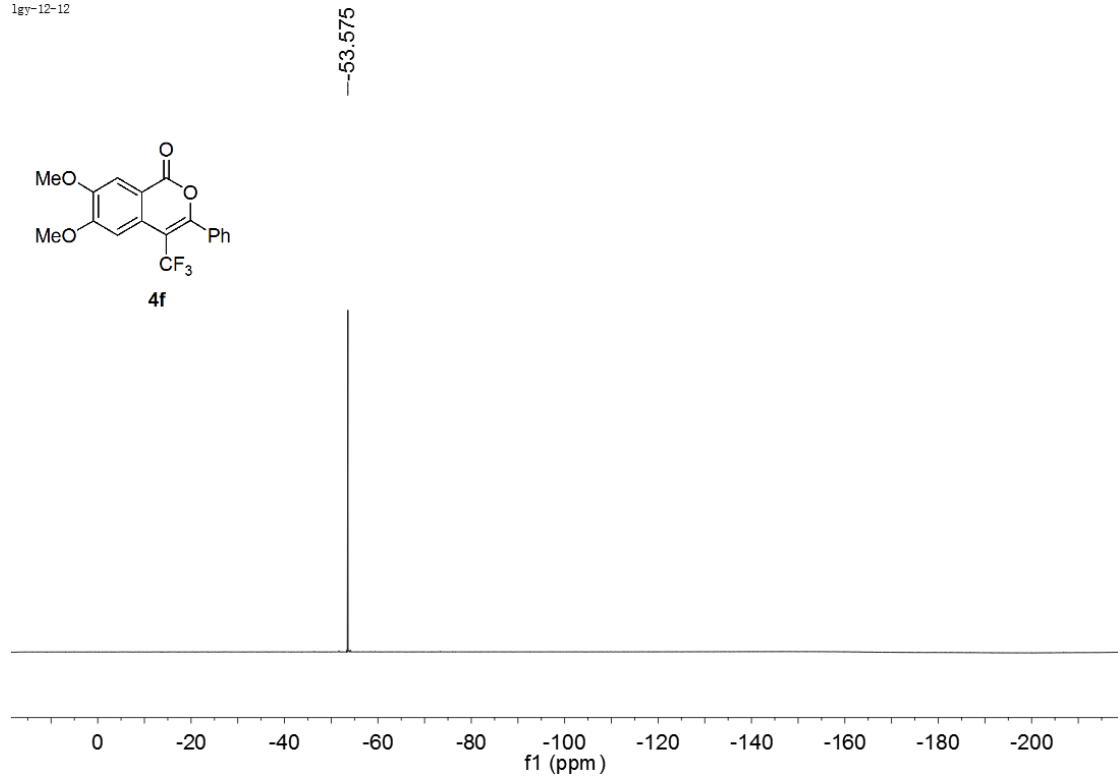
**4f**



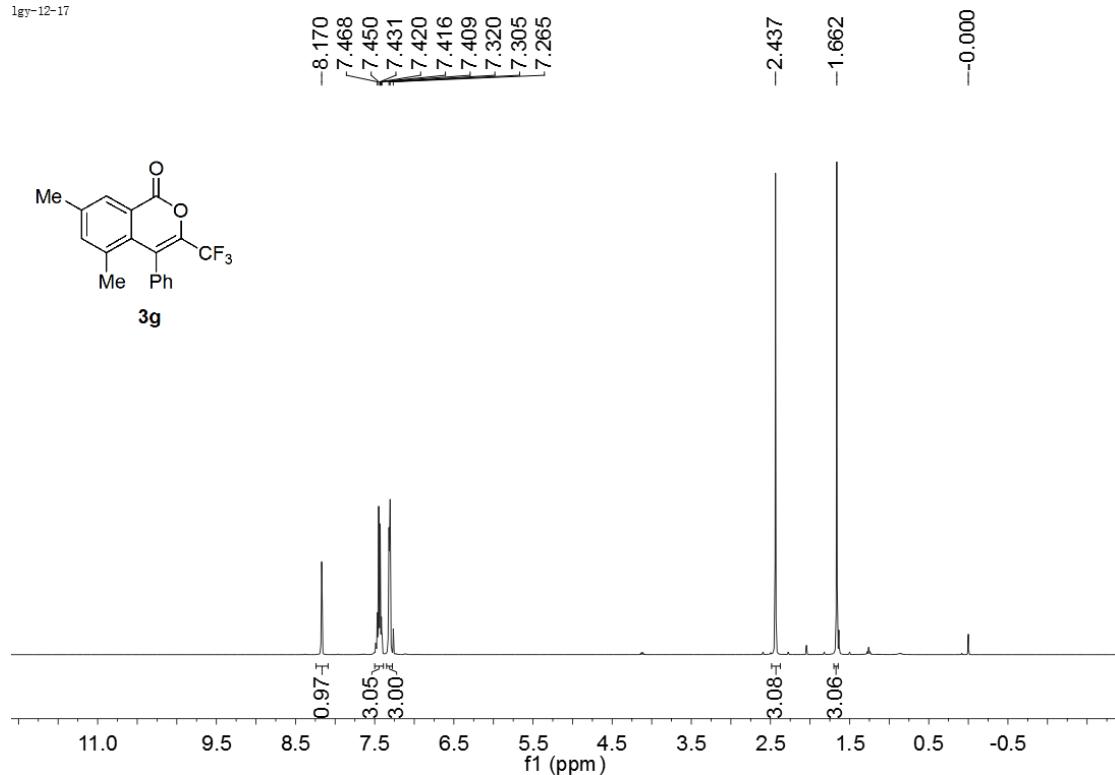
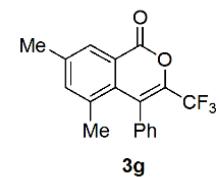
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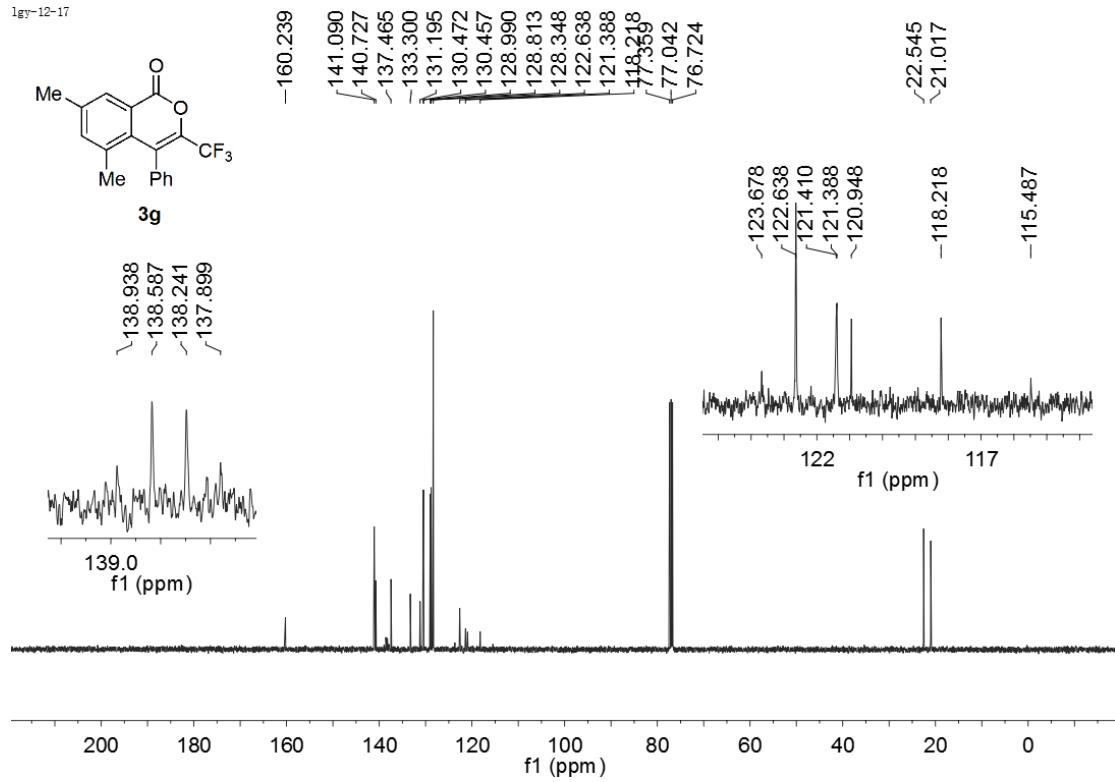
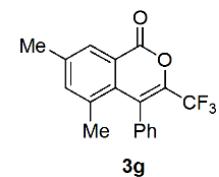
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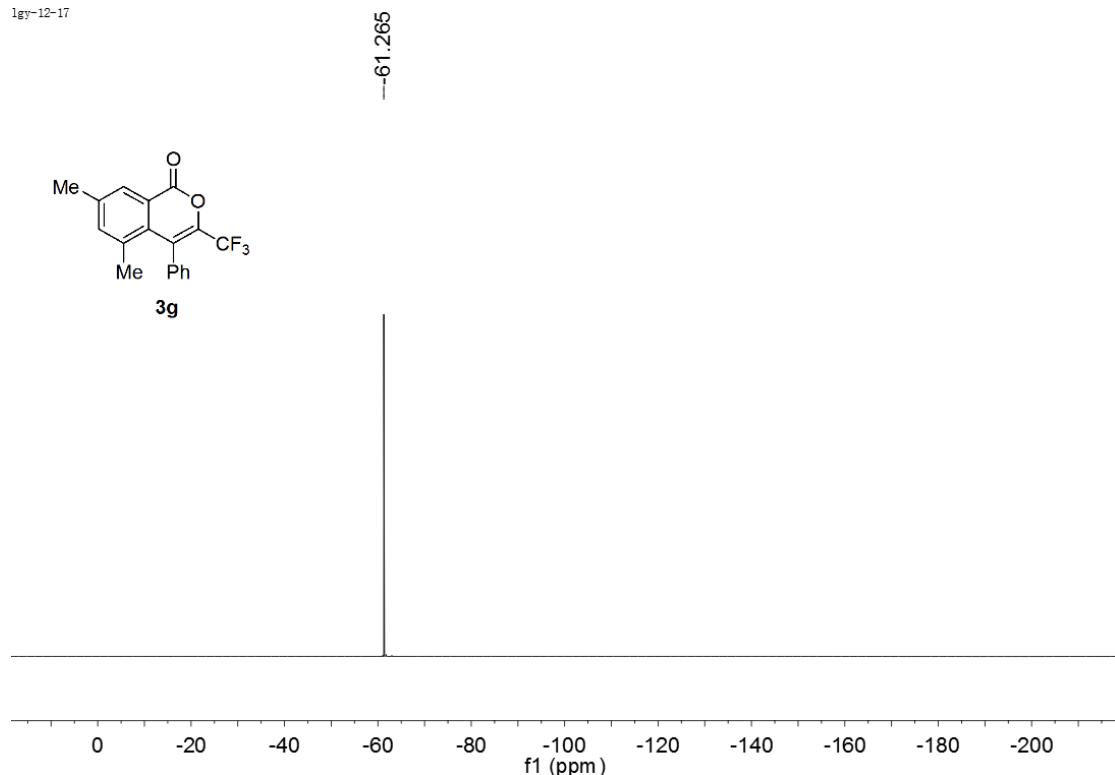
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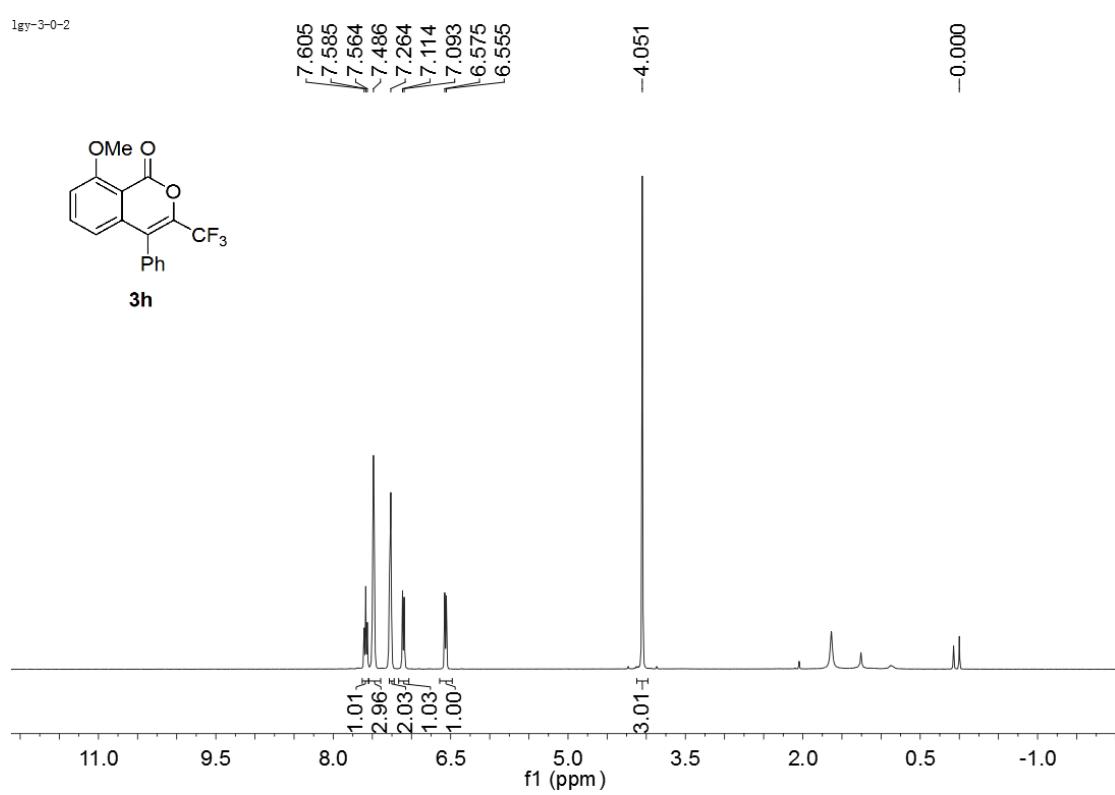
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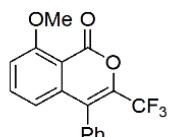
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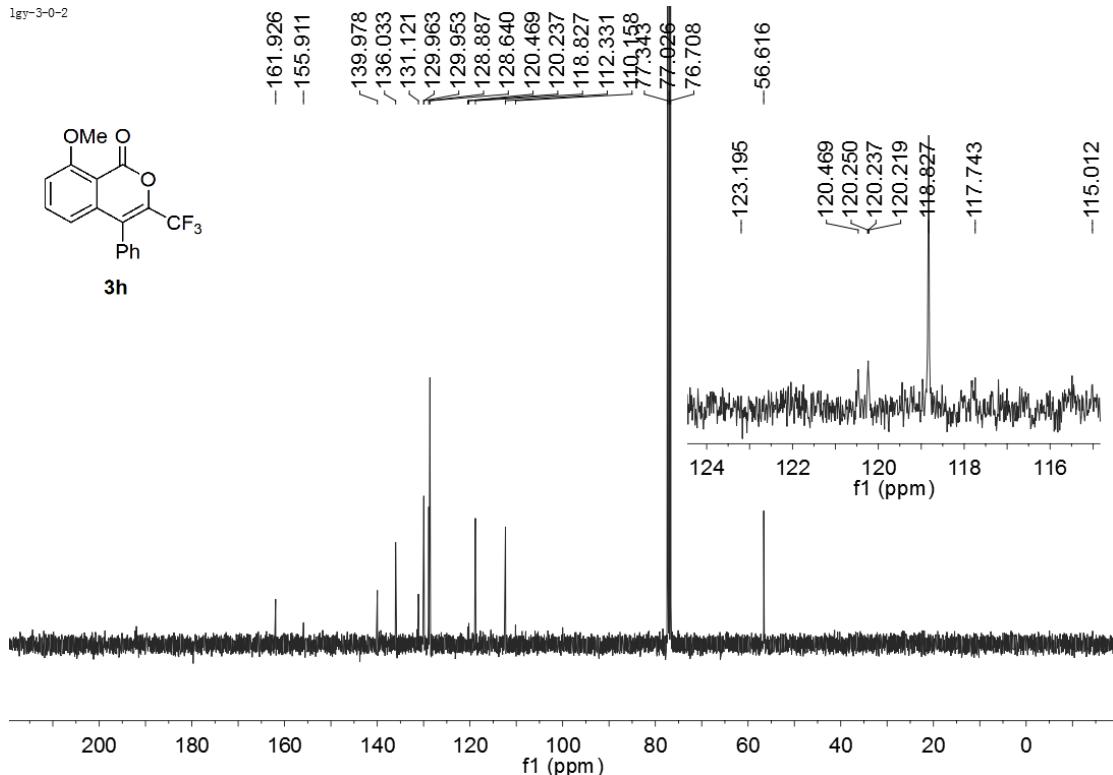
lgy-3-0-2



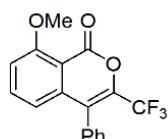
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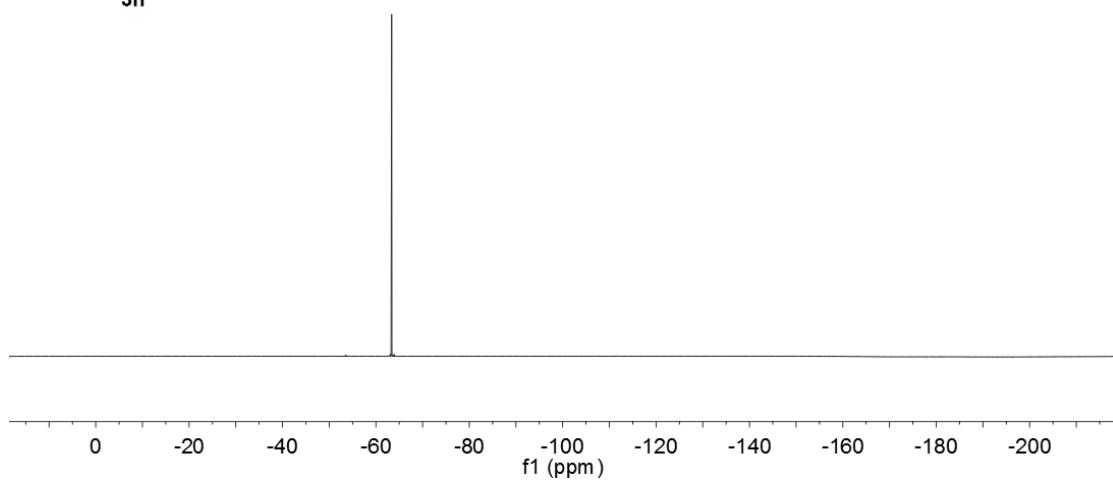
3h



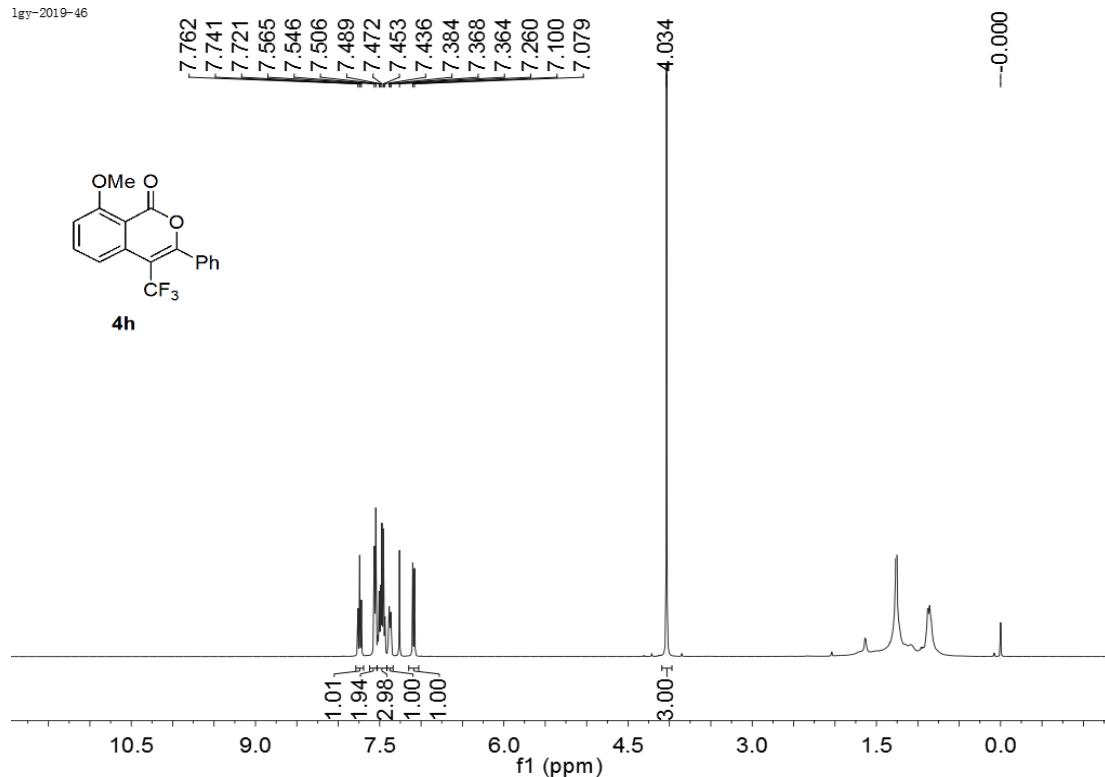
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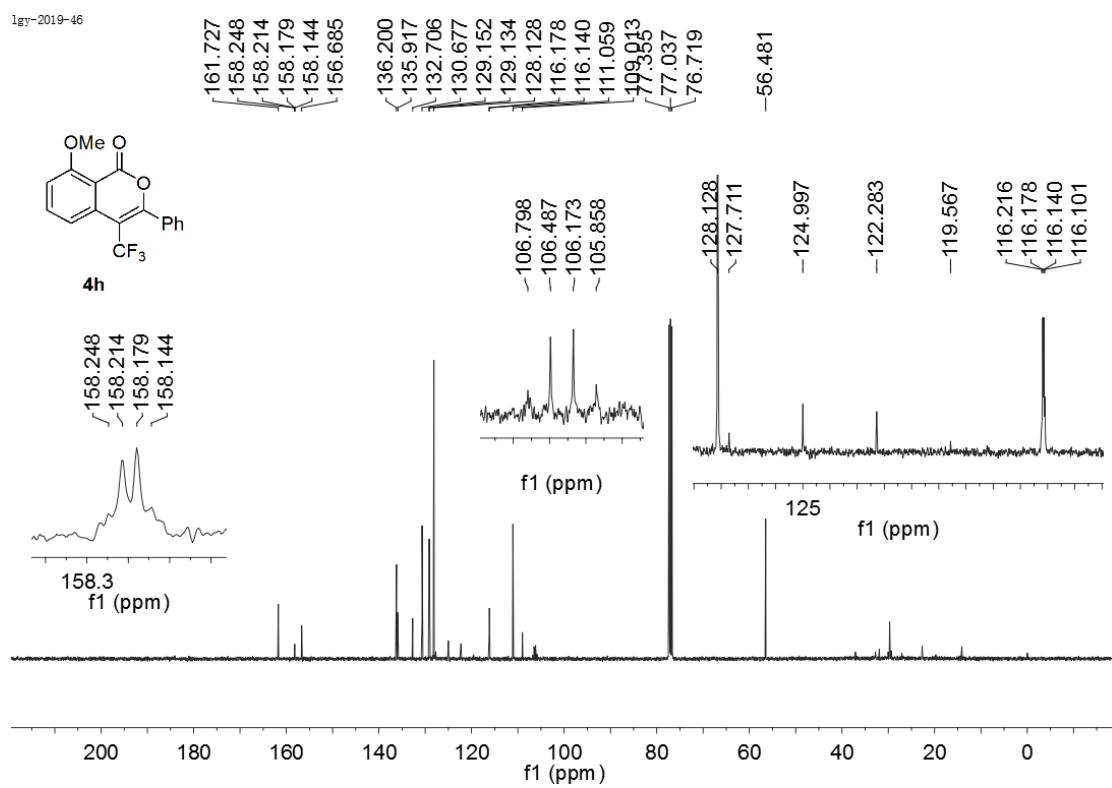
3h



lgy-2019-46

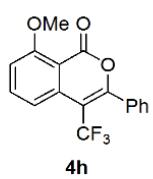


lgy-2019-46

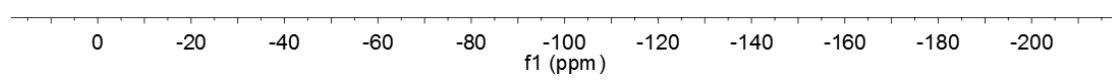


lgy-3-0-1

-53.566



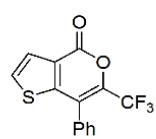
**4h**



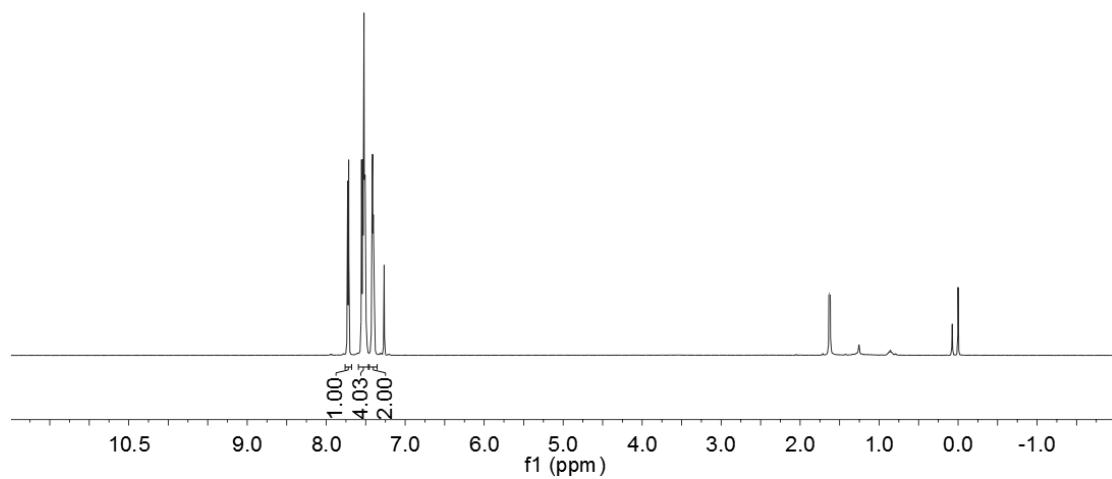
lgy-12-6

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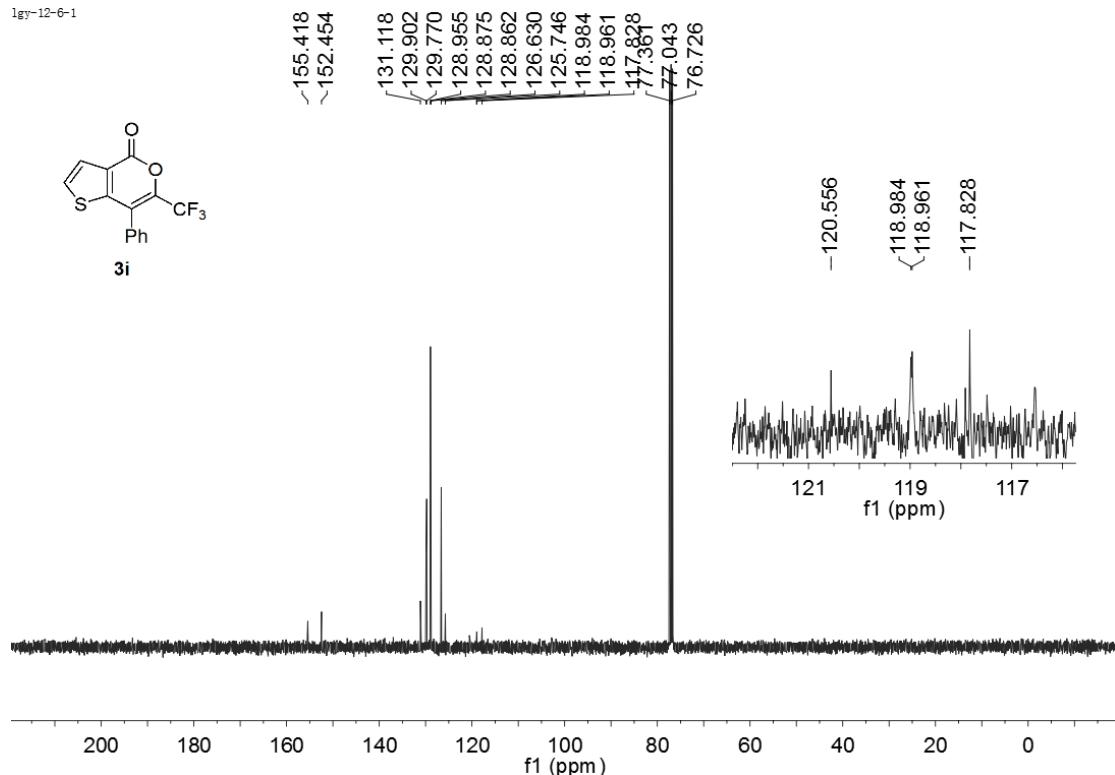
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7.522  
7.514  
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7.418  
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7.405  
7.394  
7.266



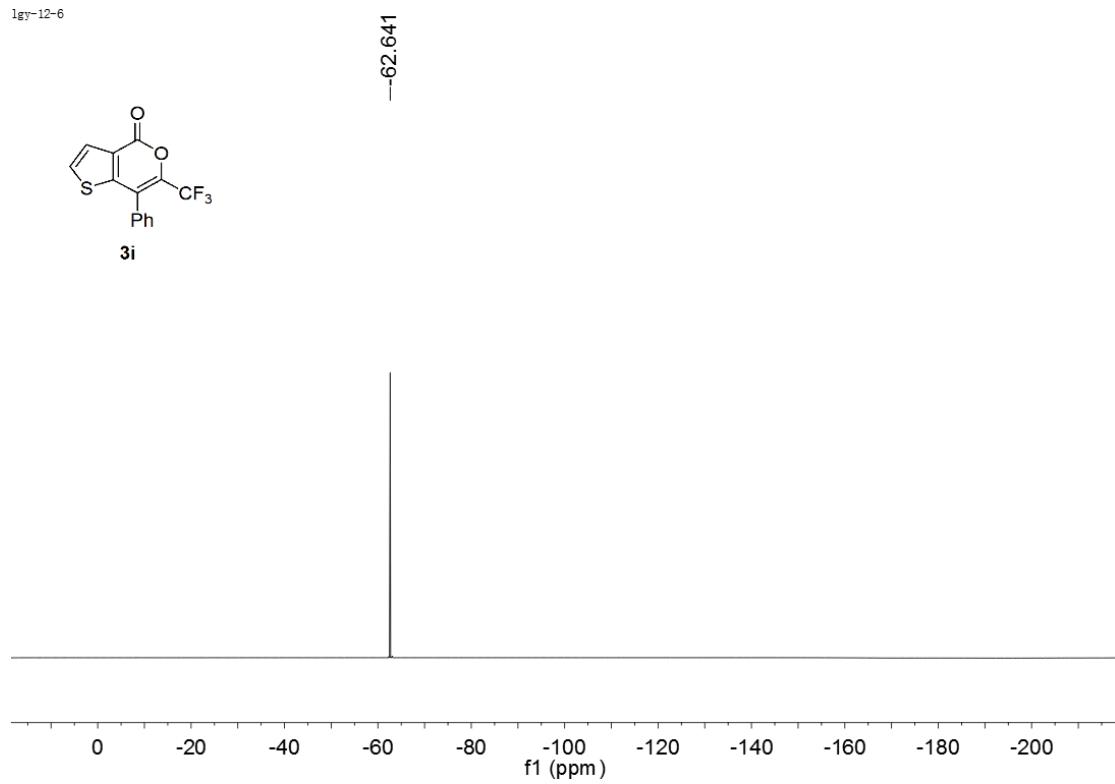
**3i**



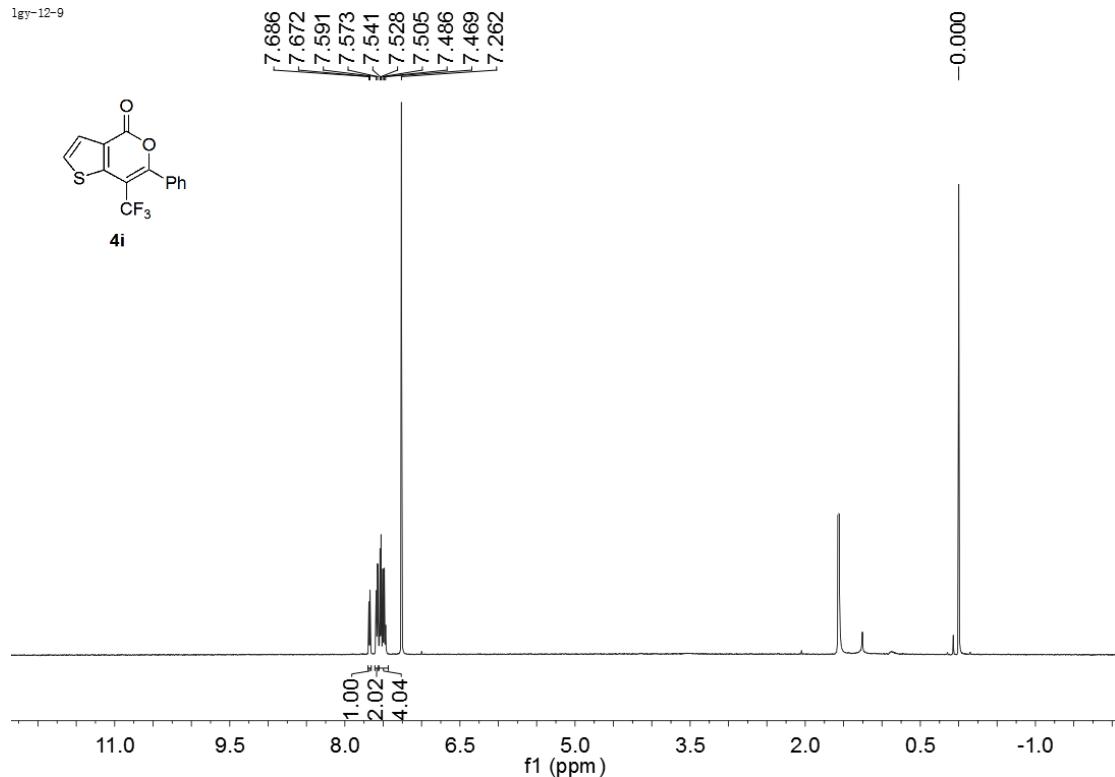
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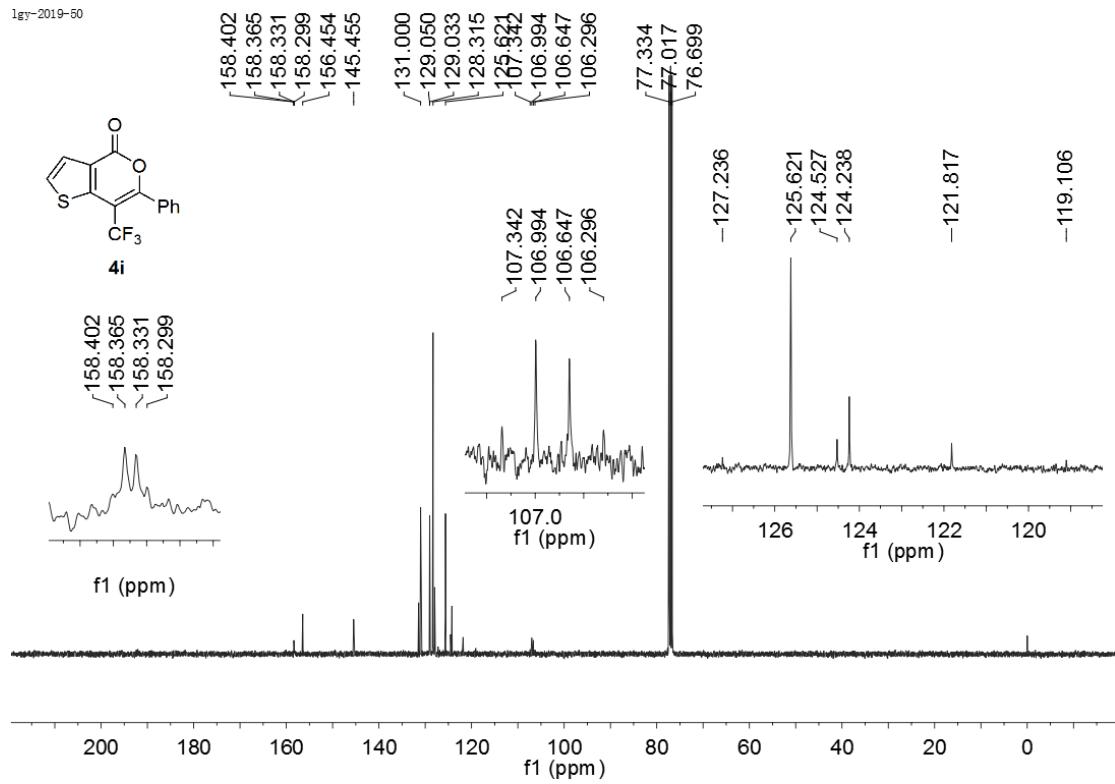
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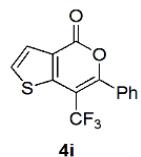
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lgy-2019-50

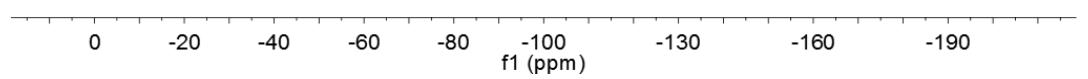


lgy-12-9

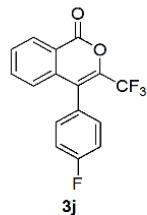


**4i**

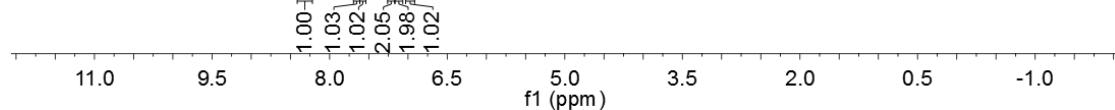
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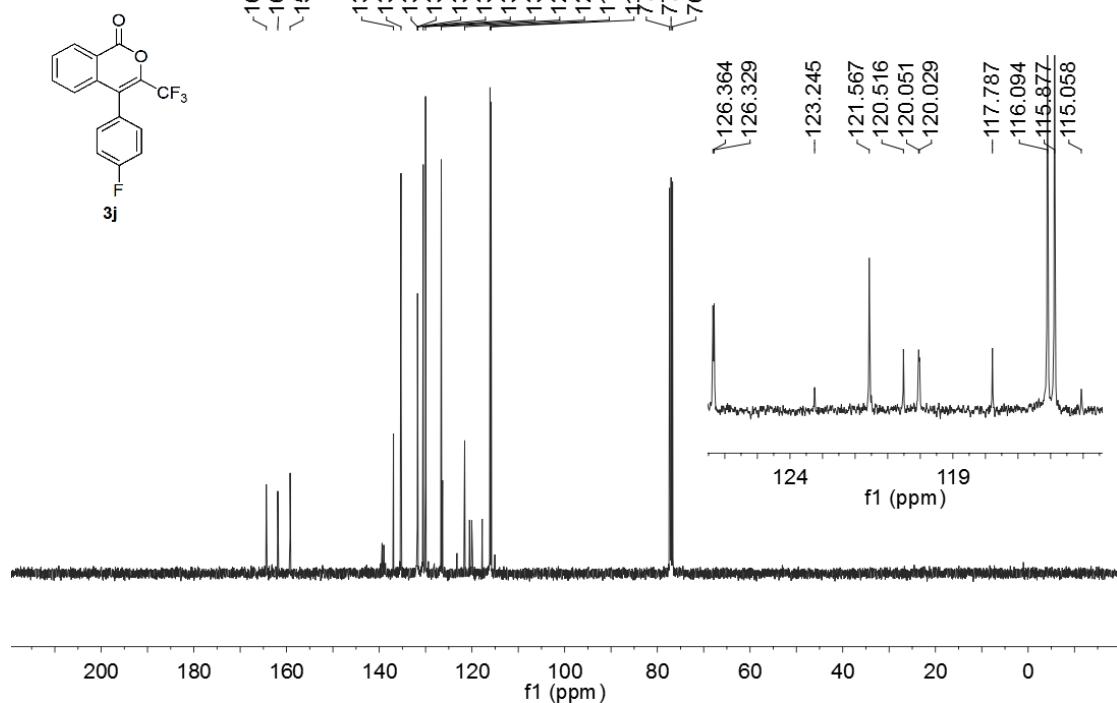
lgy-3-0-8



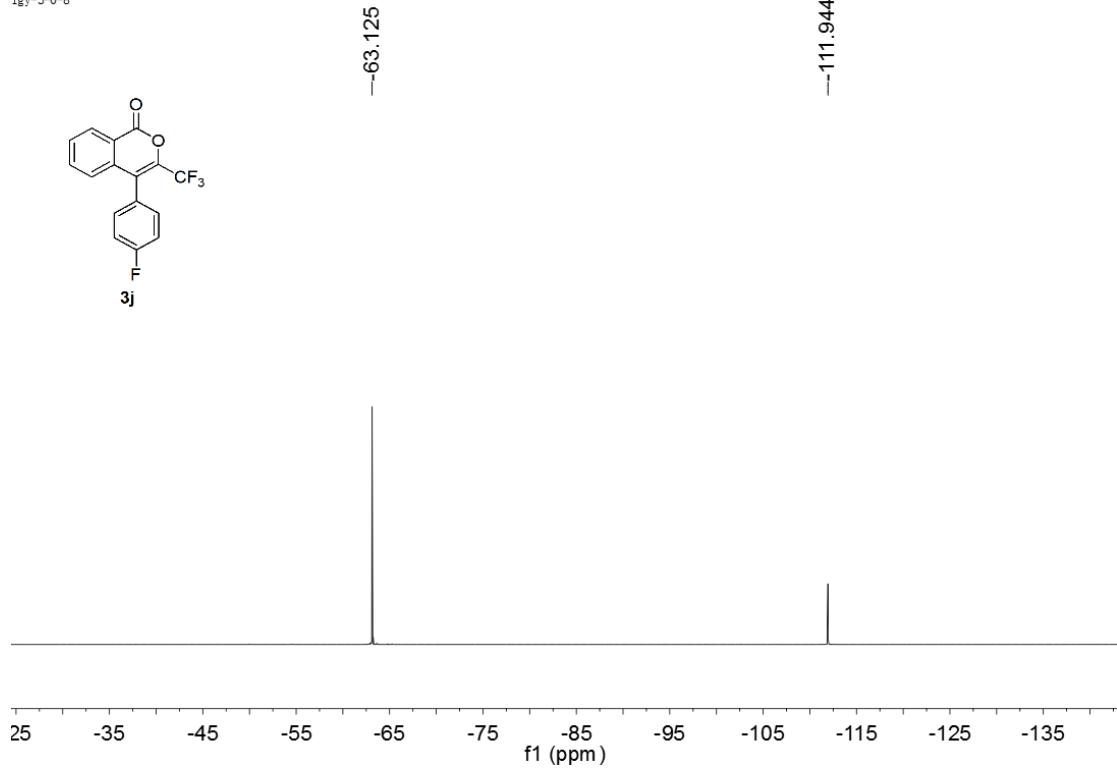
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8.309  
8.306  
7.666  
7.663  
7.647  
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7.562  
7.228  
7.223  
7.214  
7.206  
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7.125  
7.109  
7.104  
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6.971  
-0.000

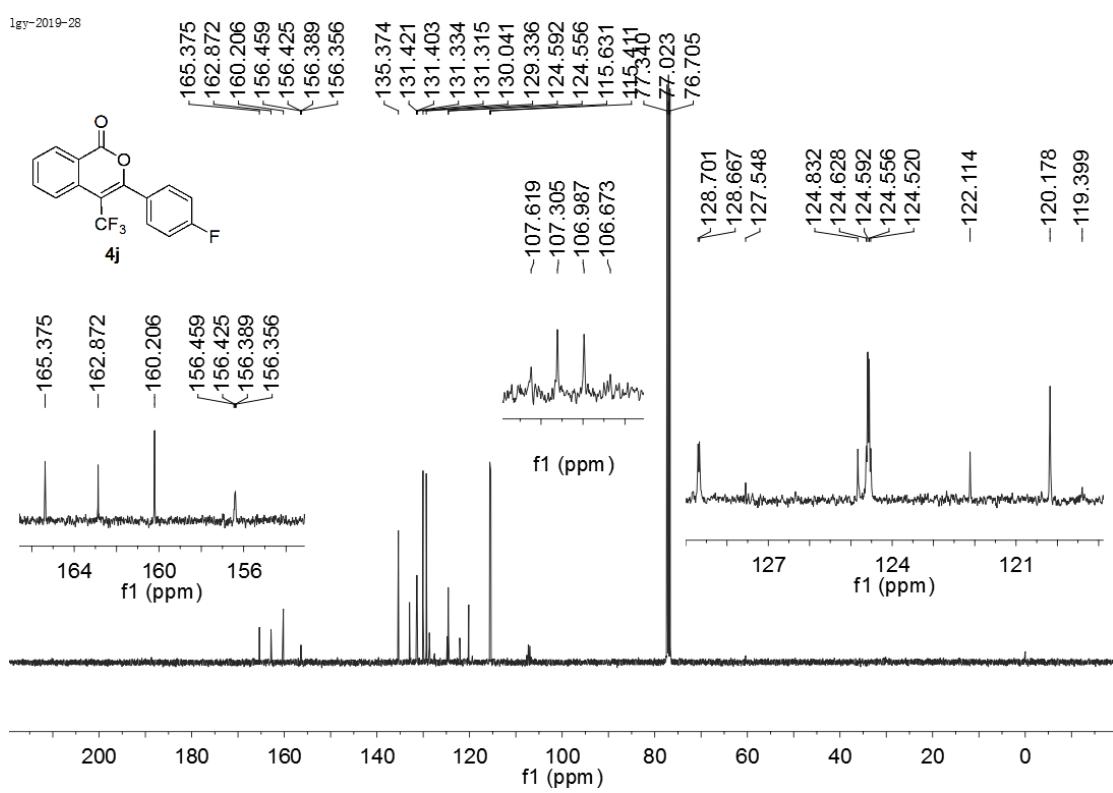
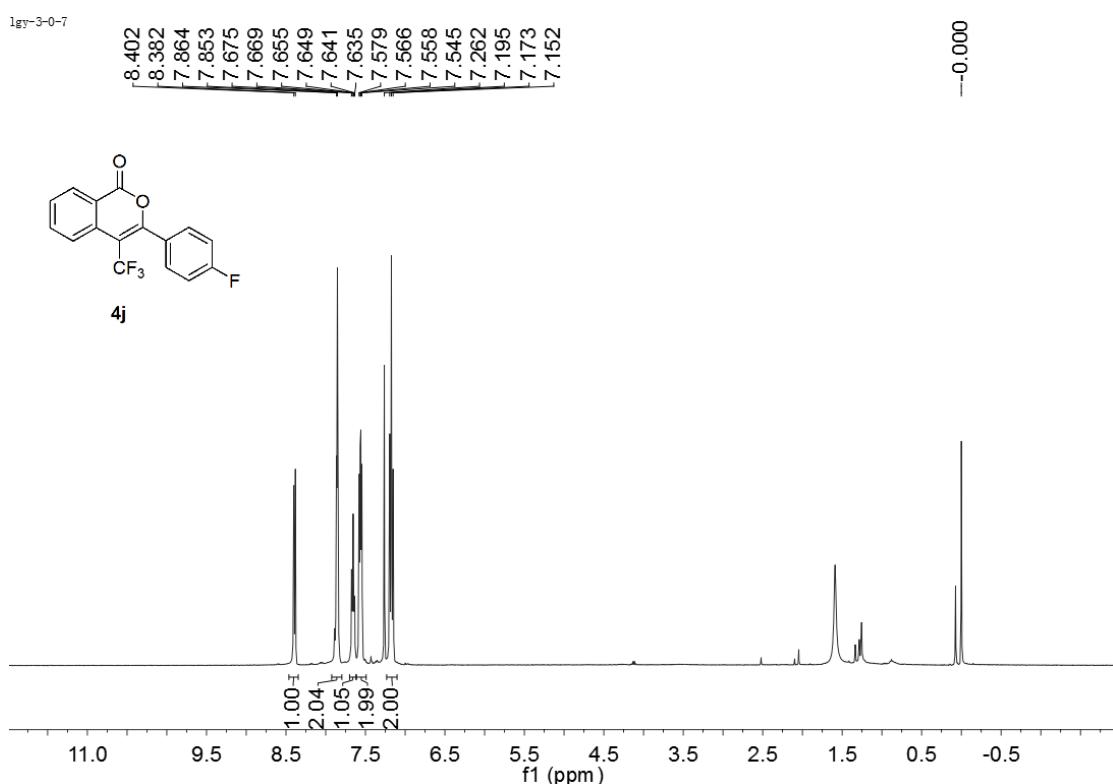


lgy-3-0-8

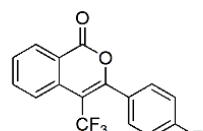


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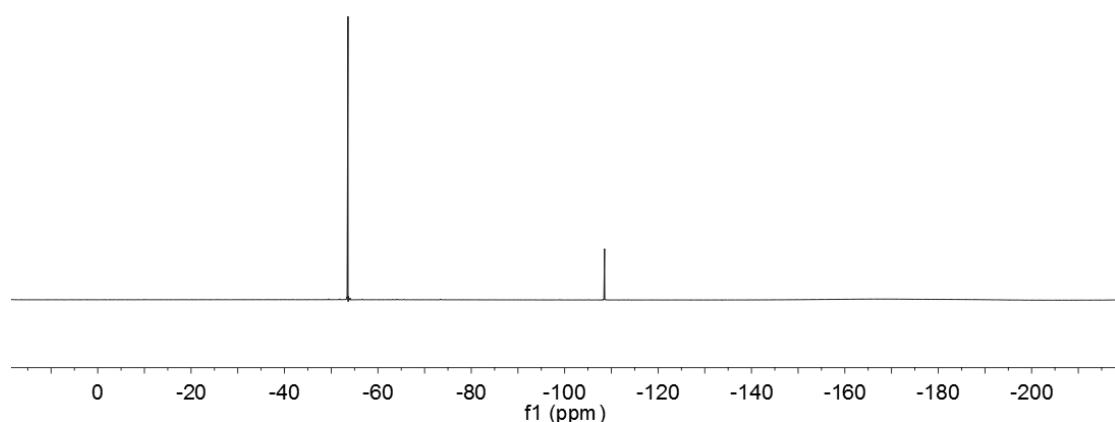




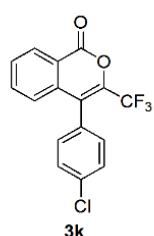
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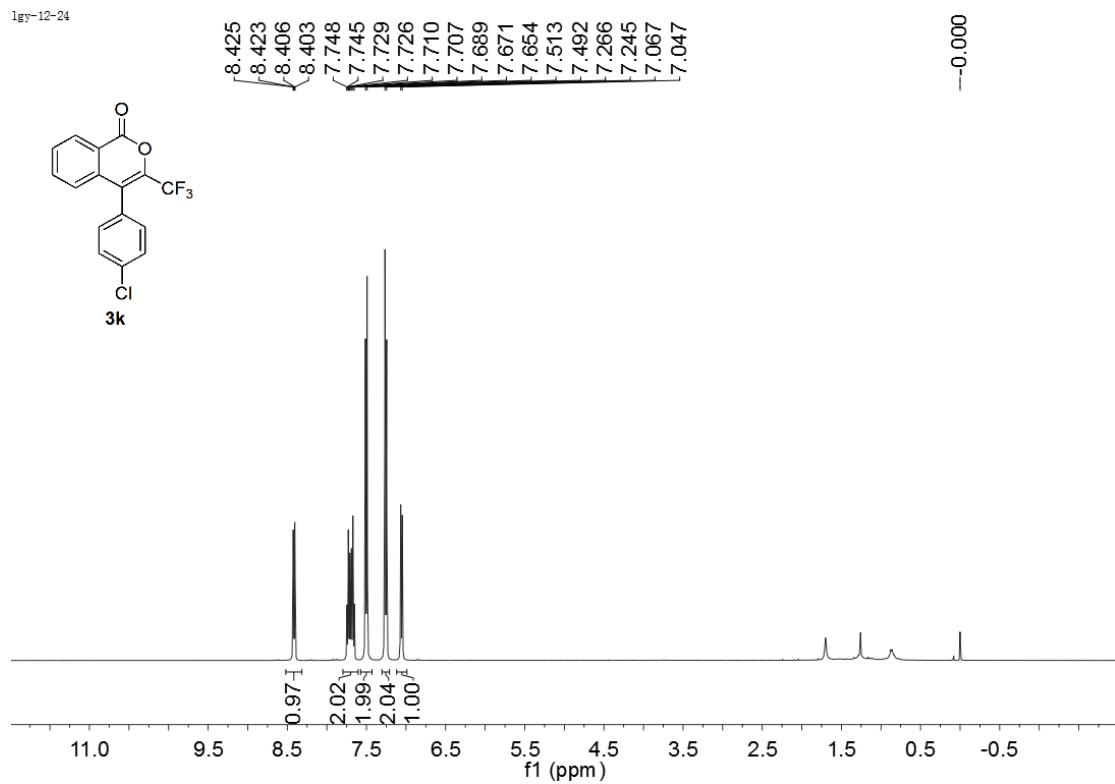
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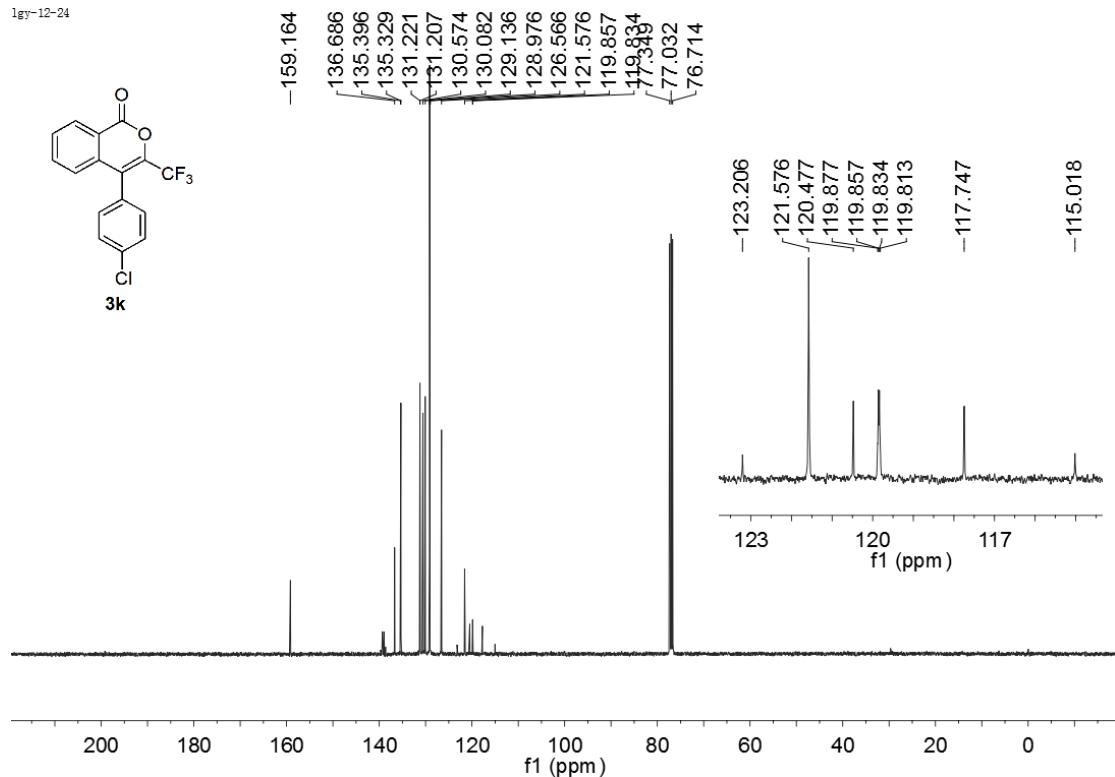
lgy-12-24



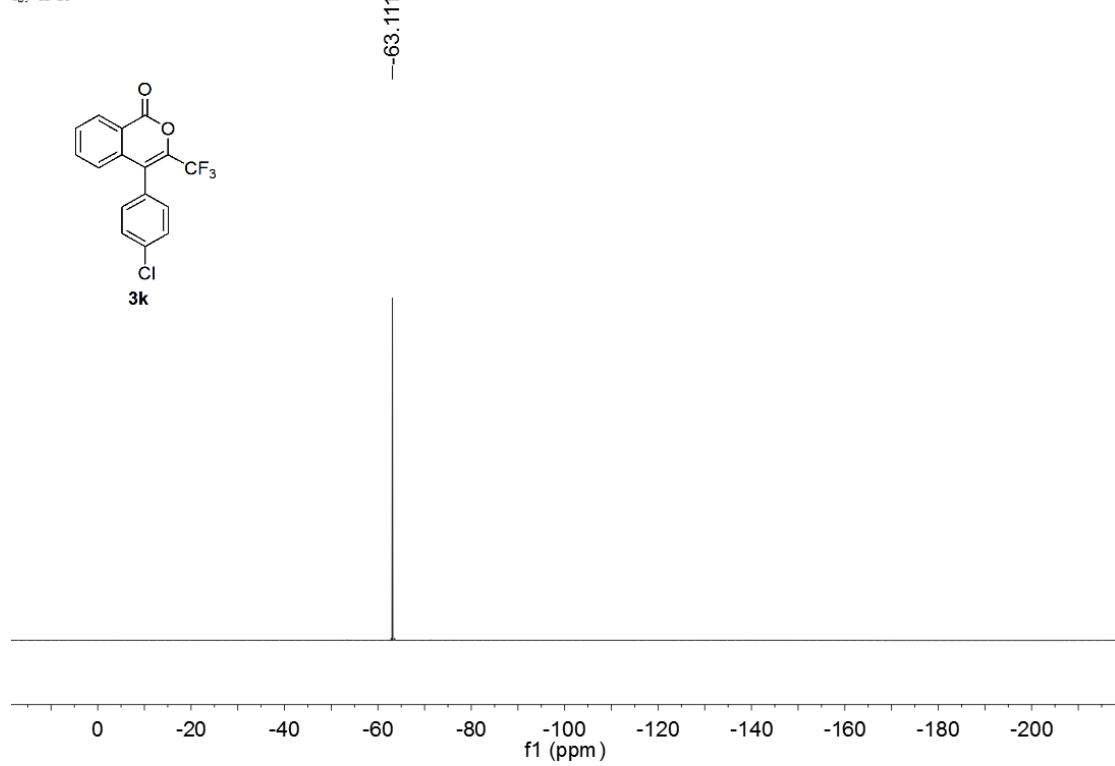
**3k**

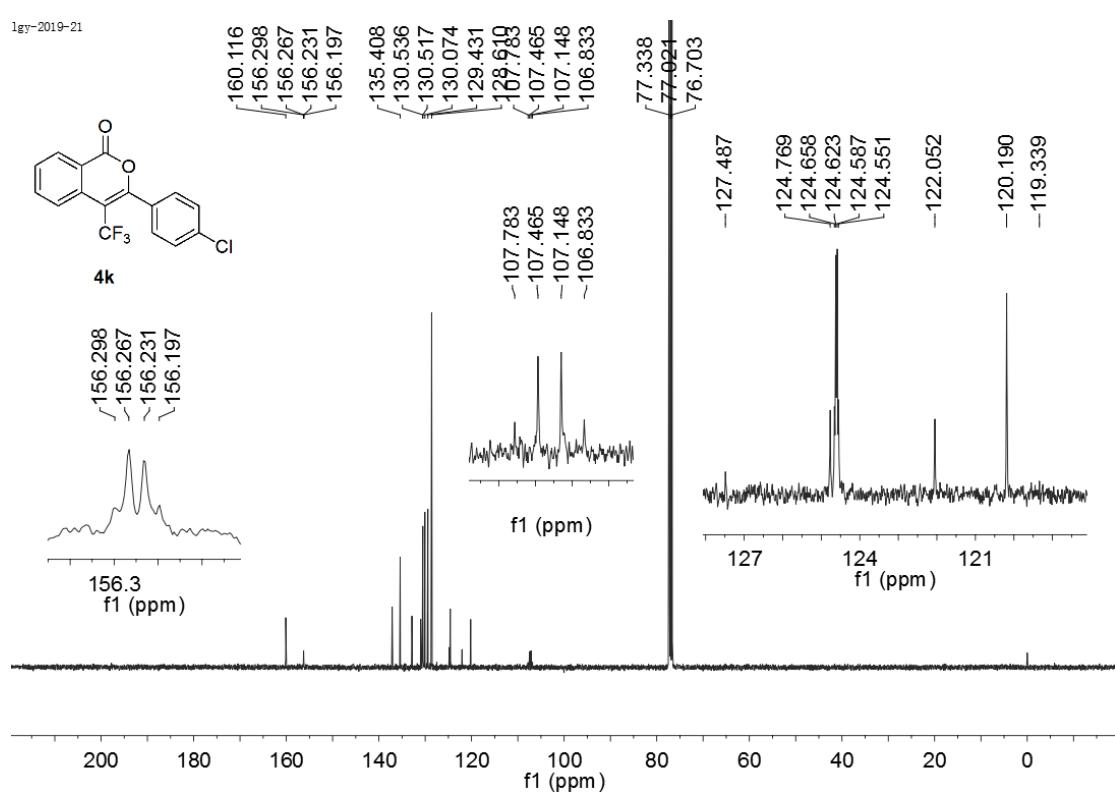
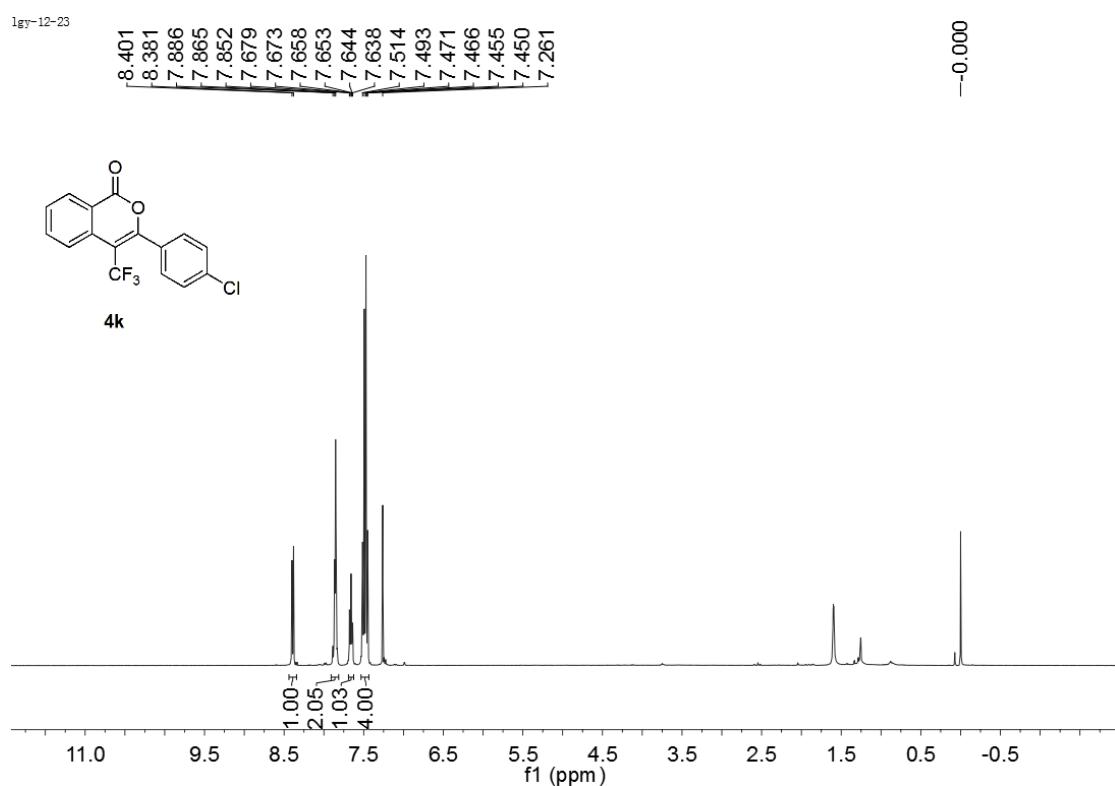


lgy-12-24



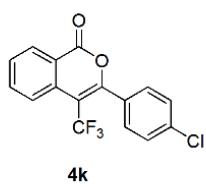
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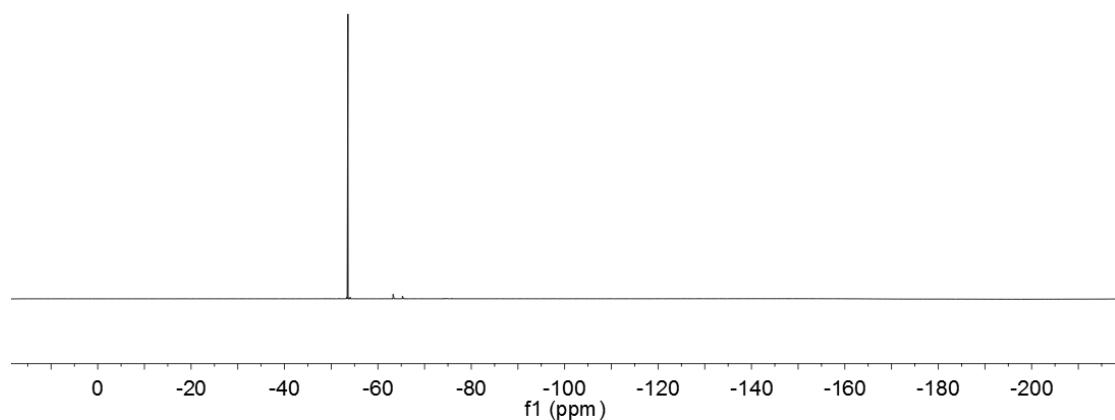


lgy-12-23

-53.587

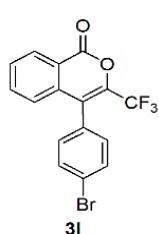


**4k**

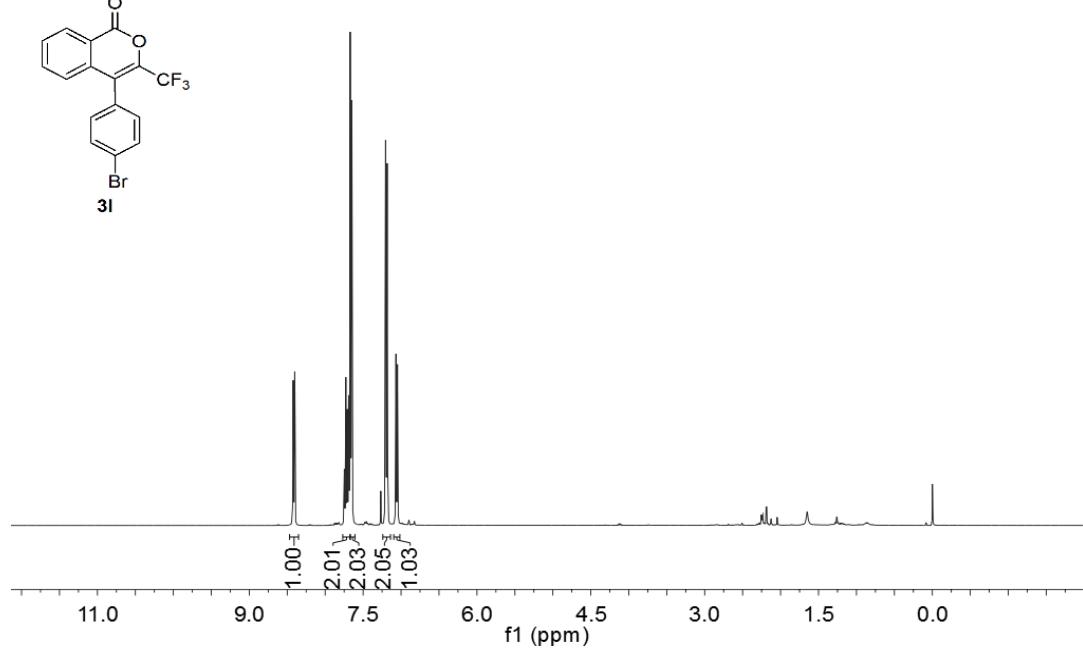


lgy-12-28

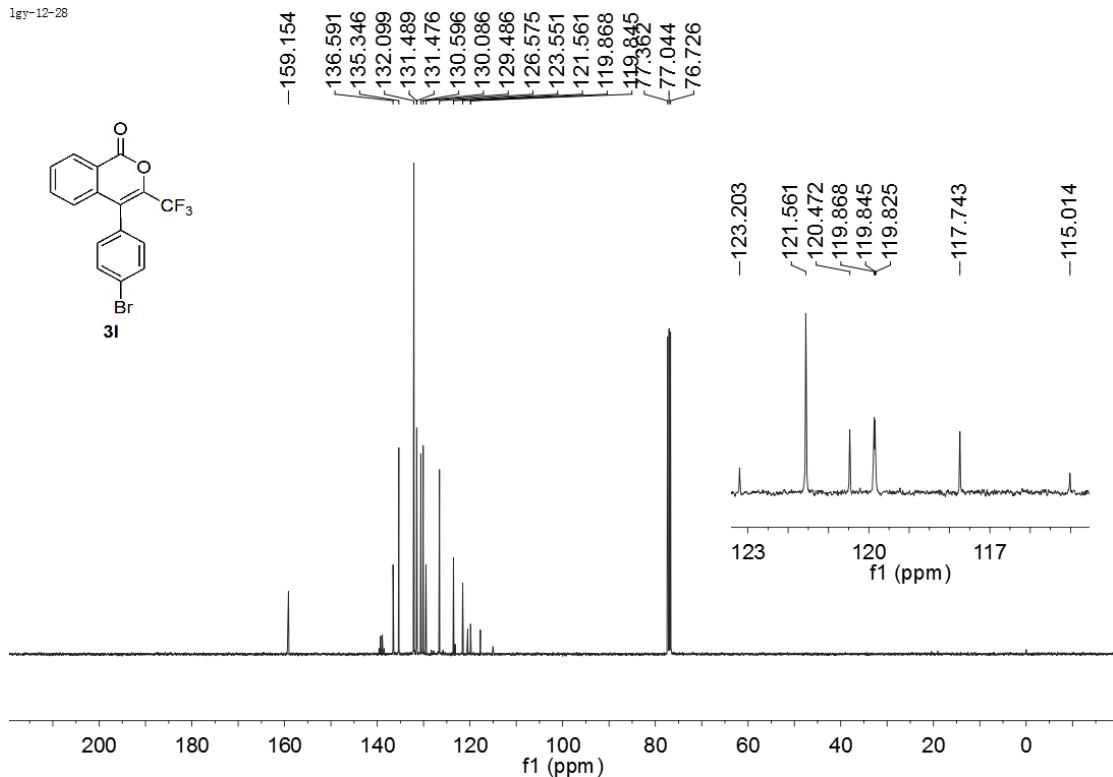
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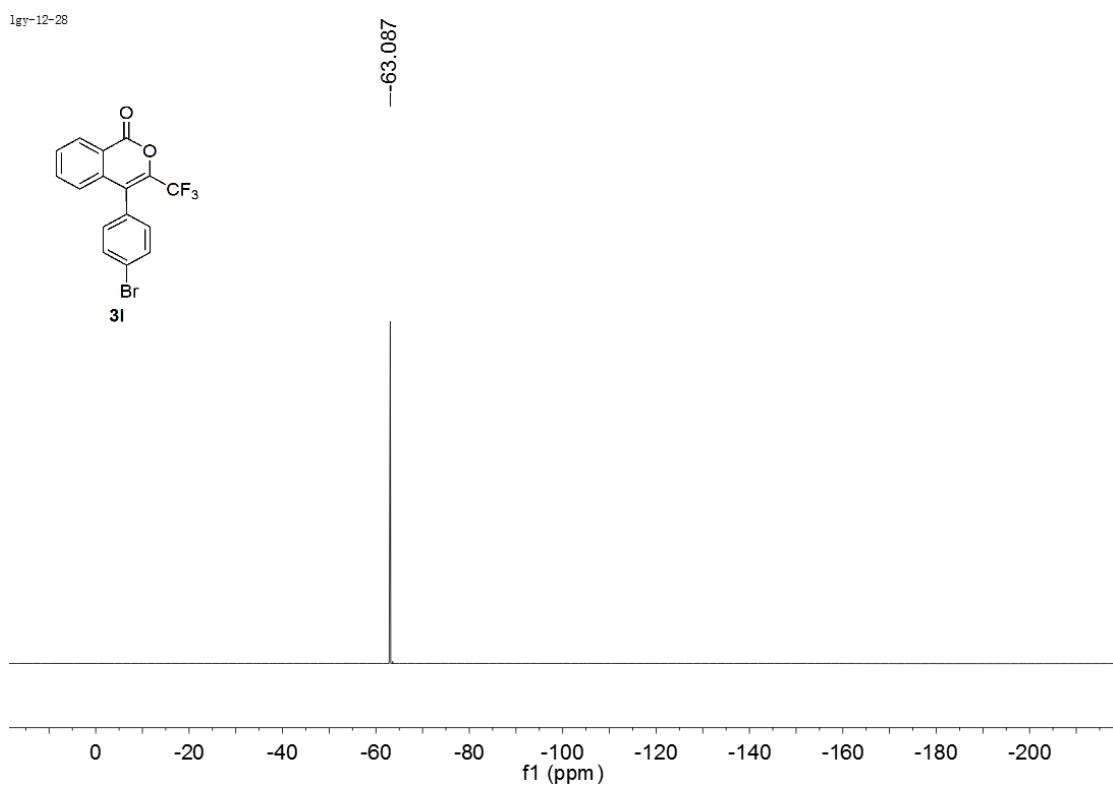
**3l**

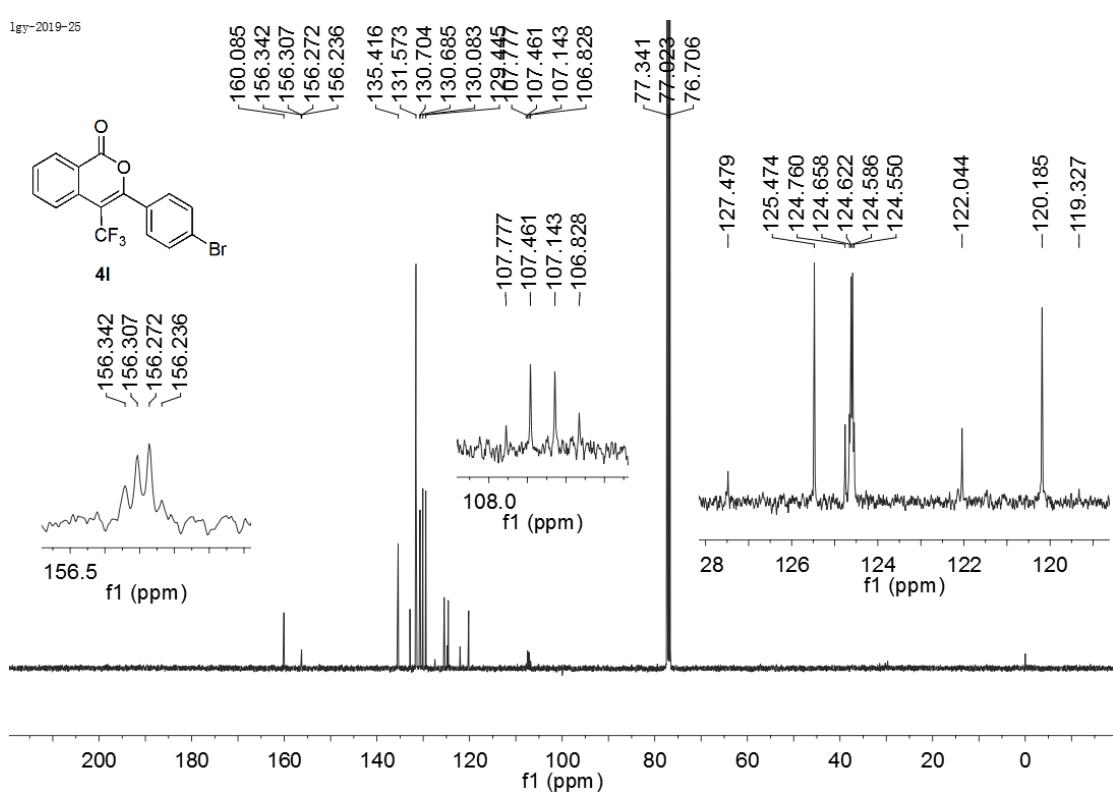
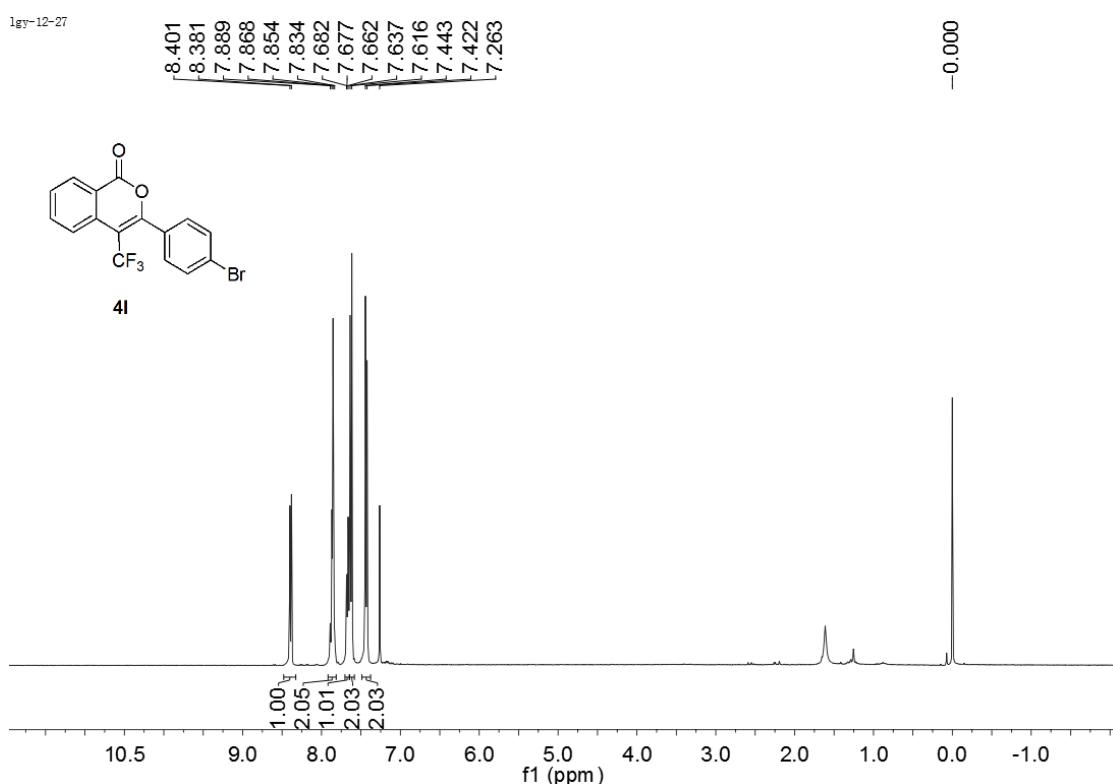


lgy-12-28

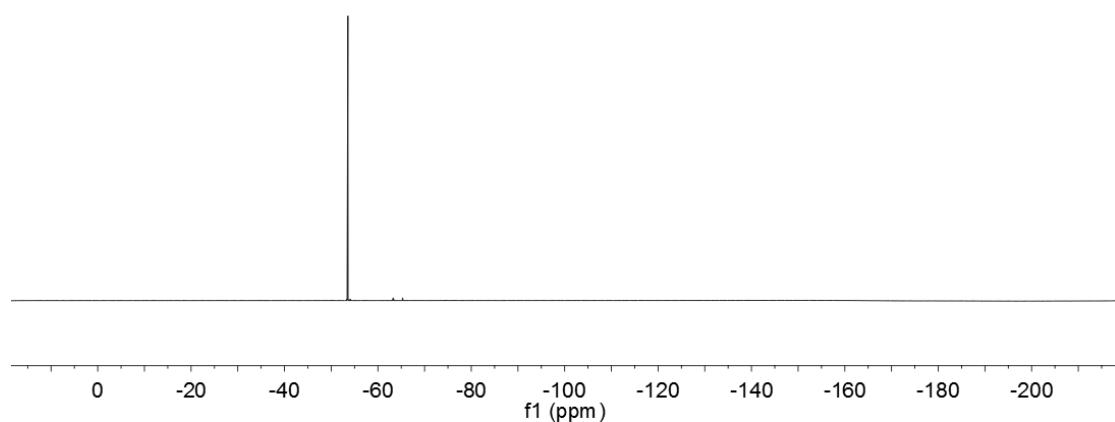
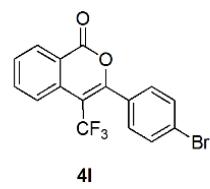


lgy-12-28

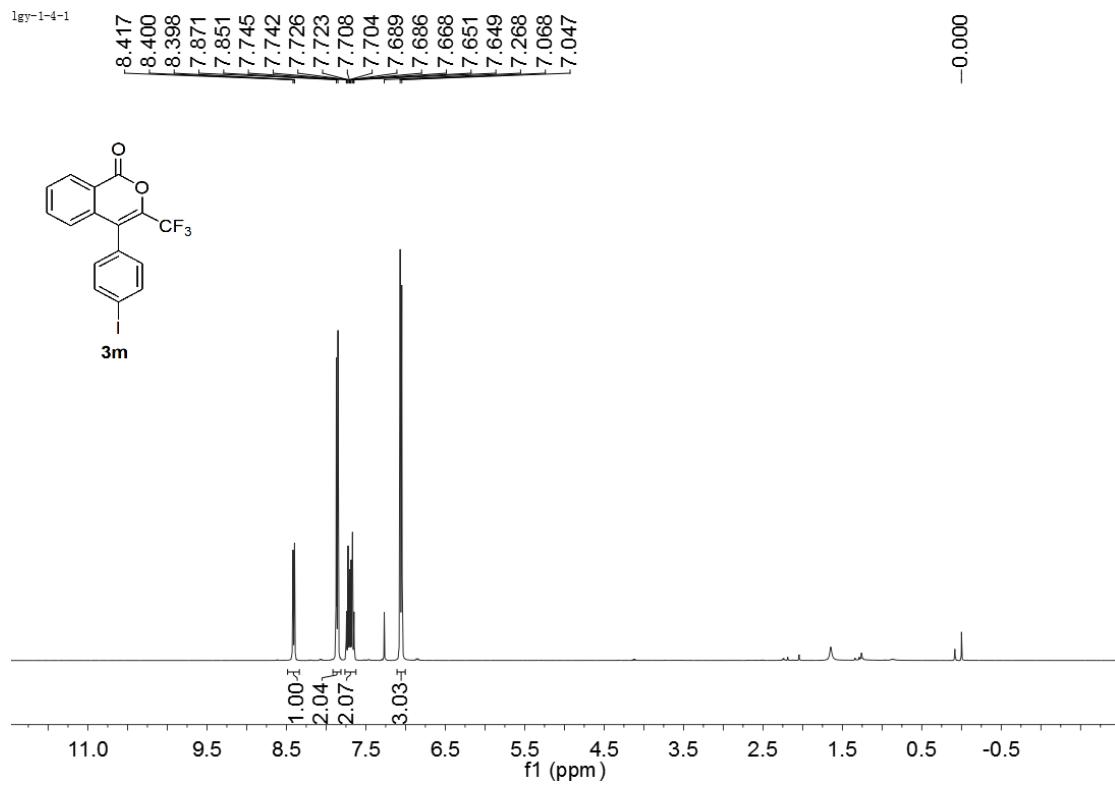
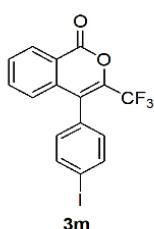




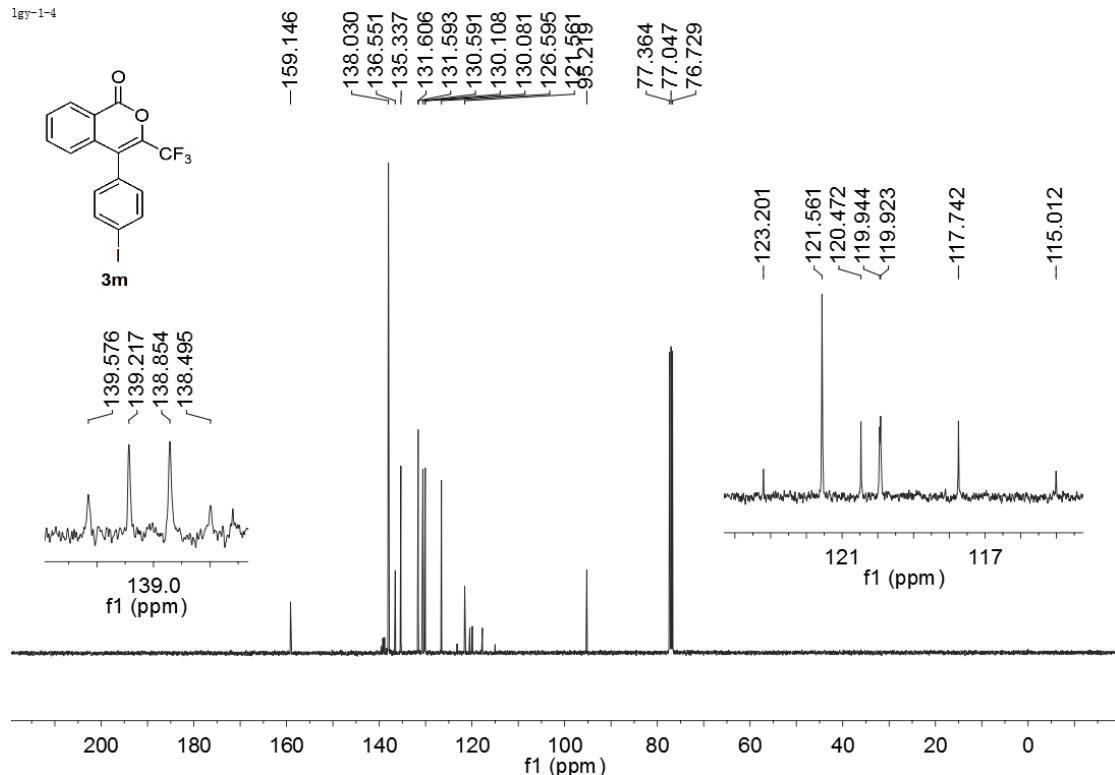
lgy-12-27



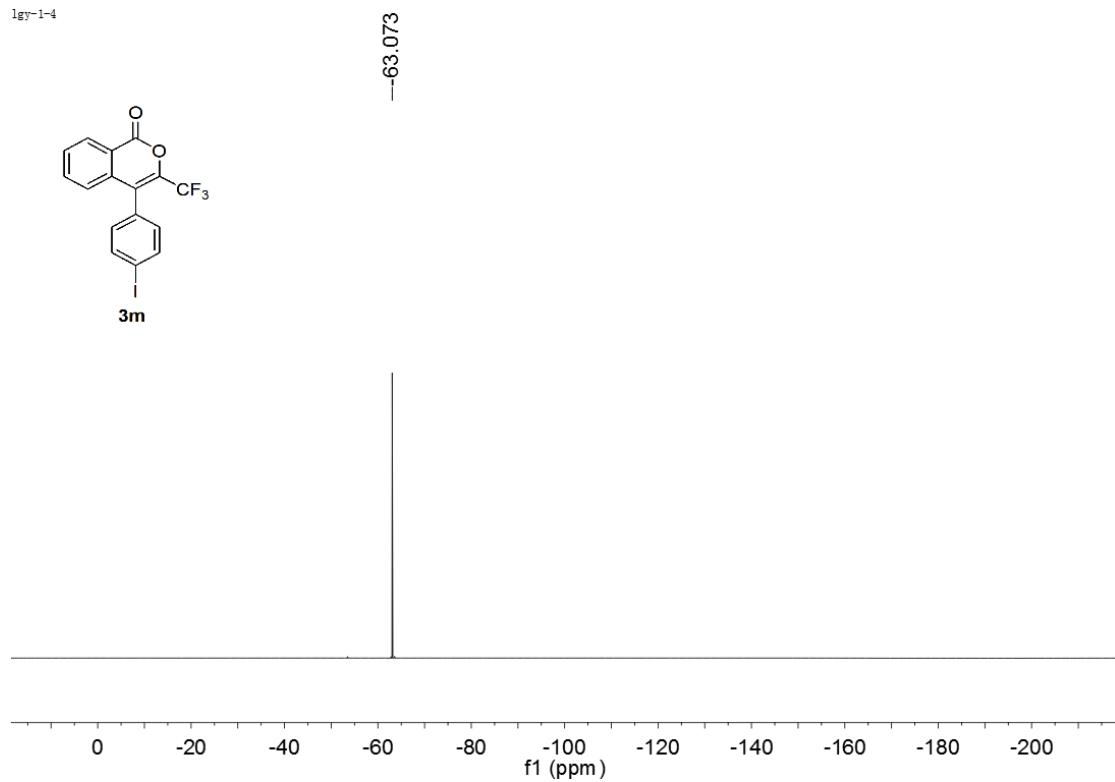
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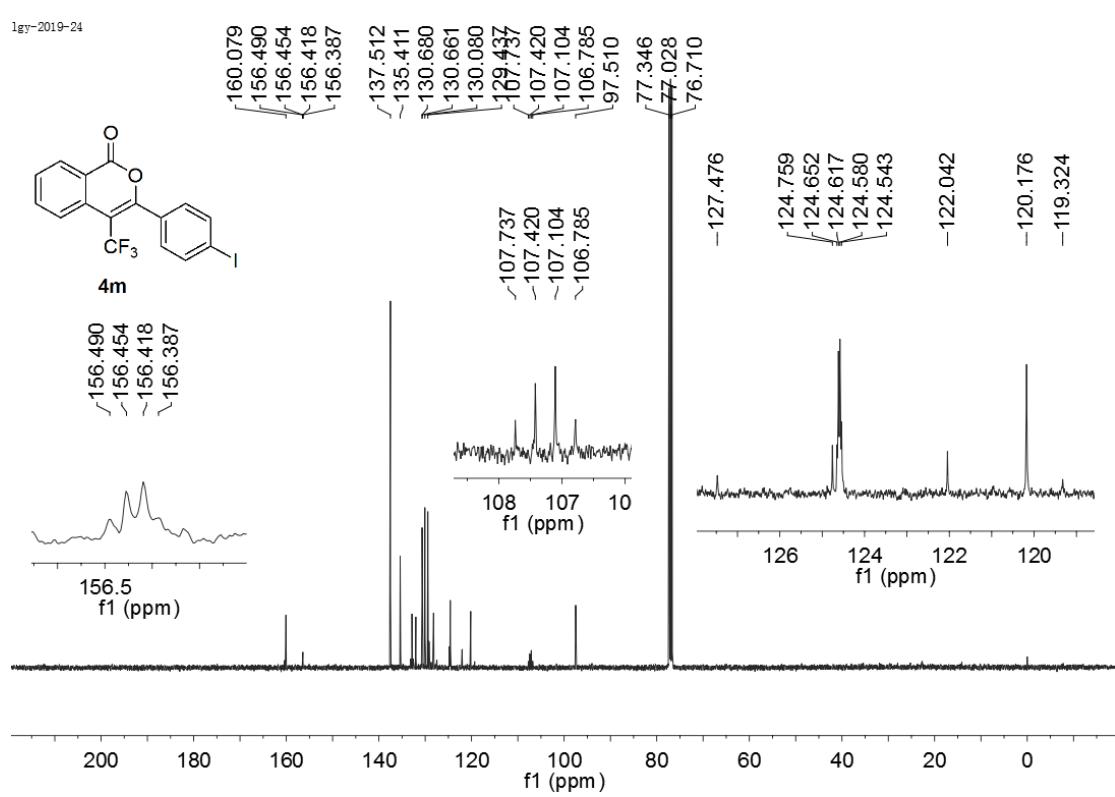
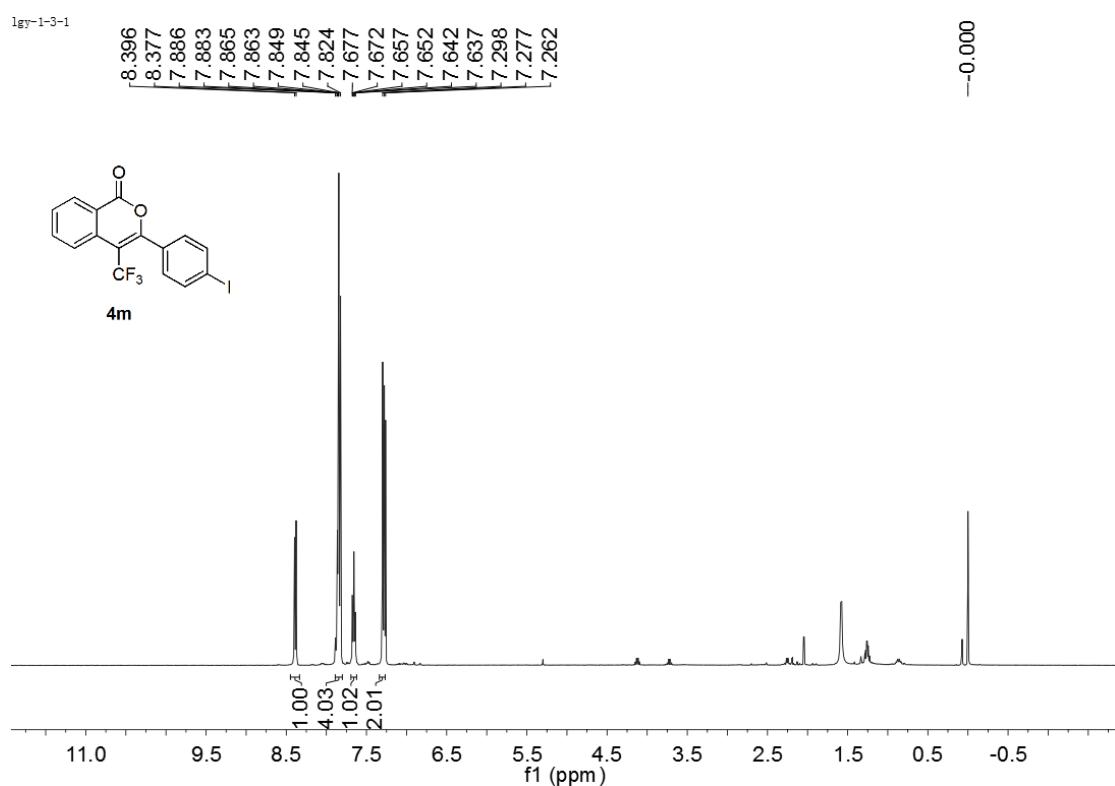


lgy-1-4



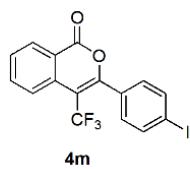
lgy-1-4



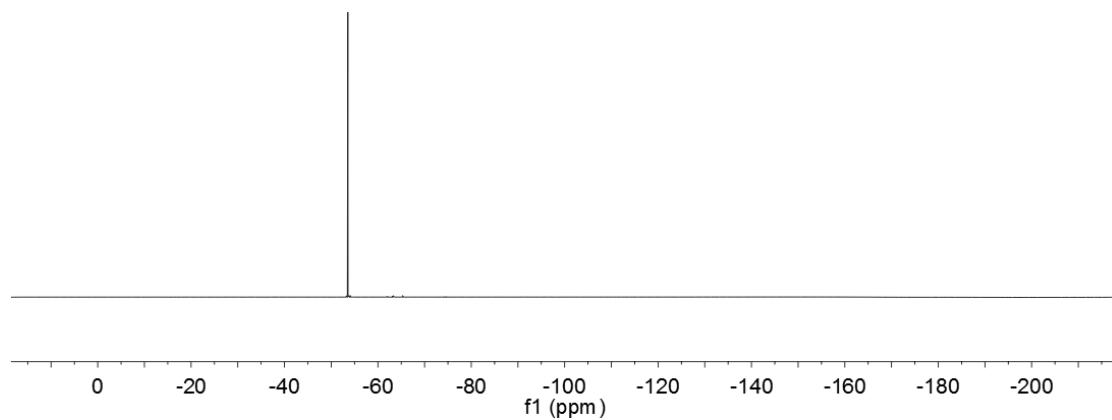


lgy-1-3

-53.563

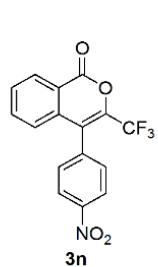


**4m**

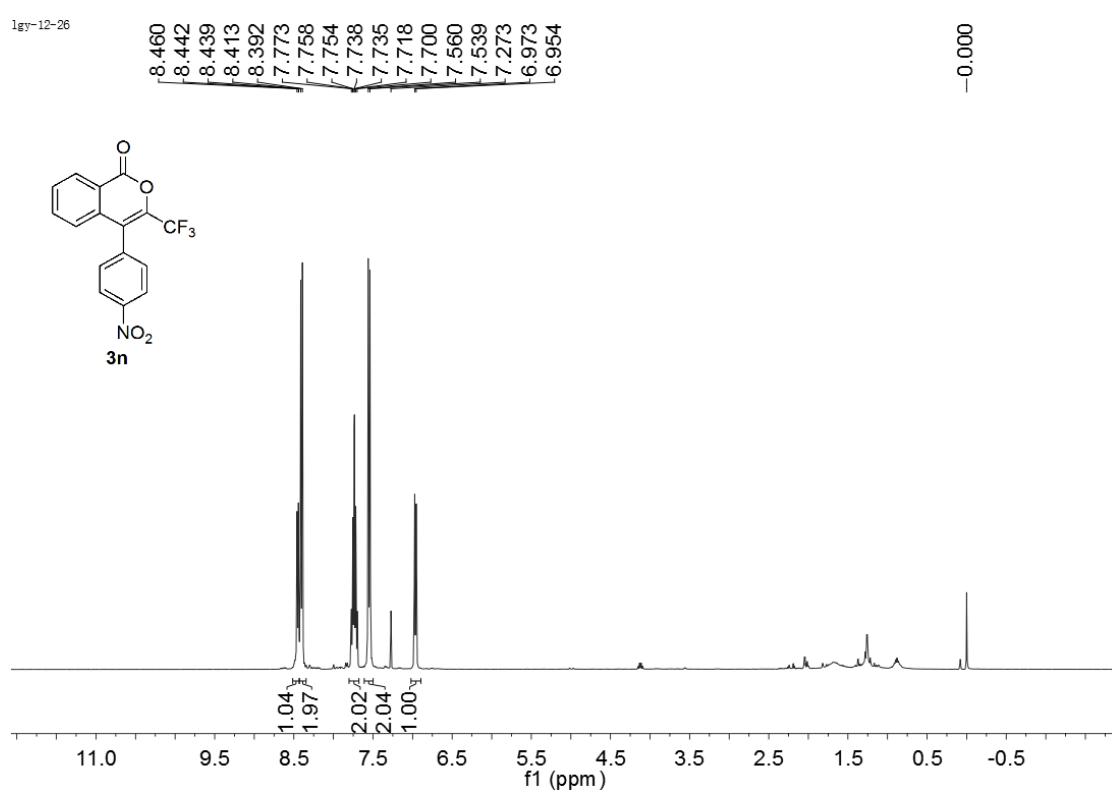


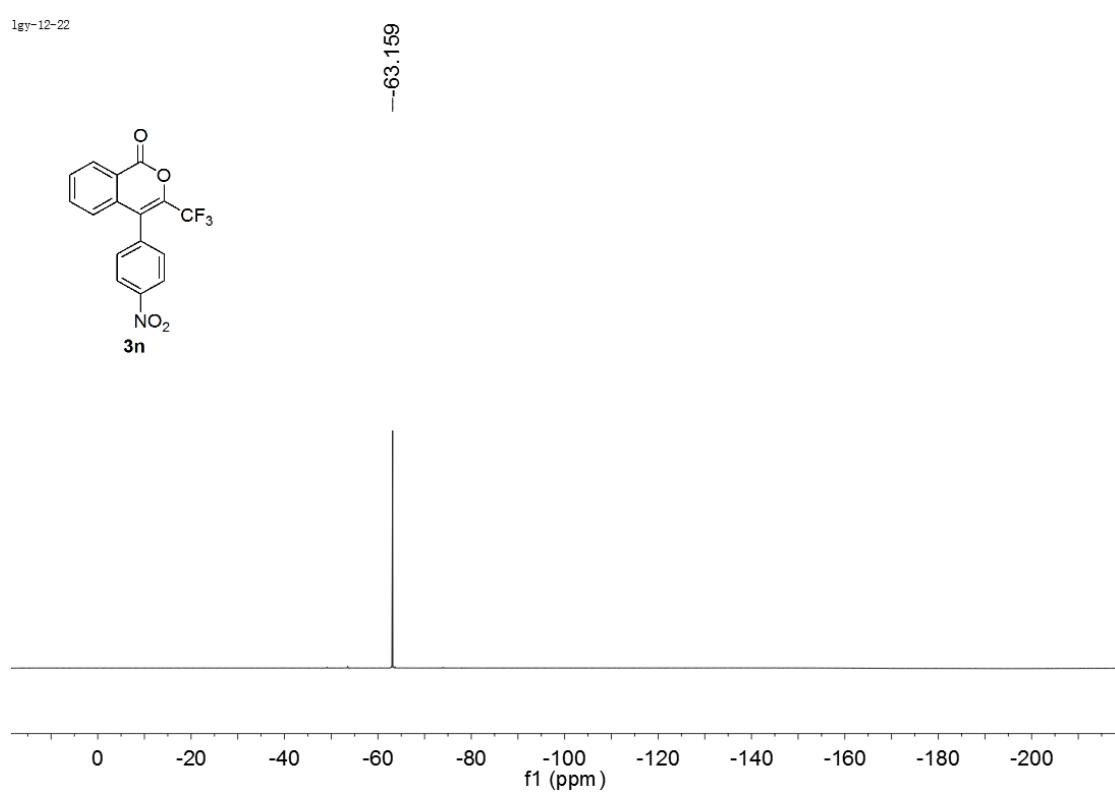
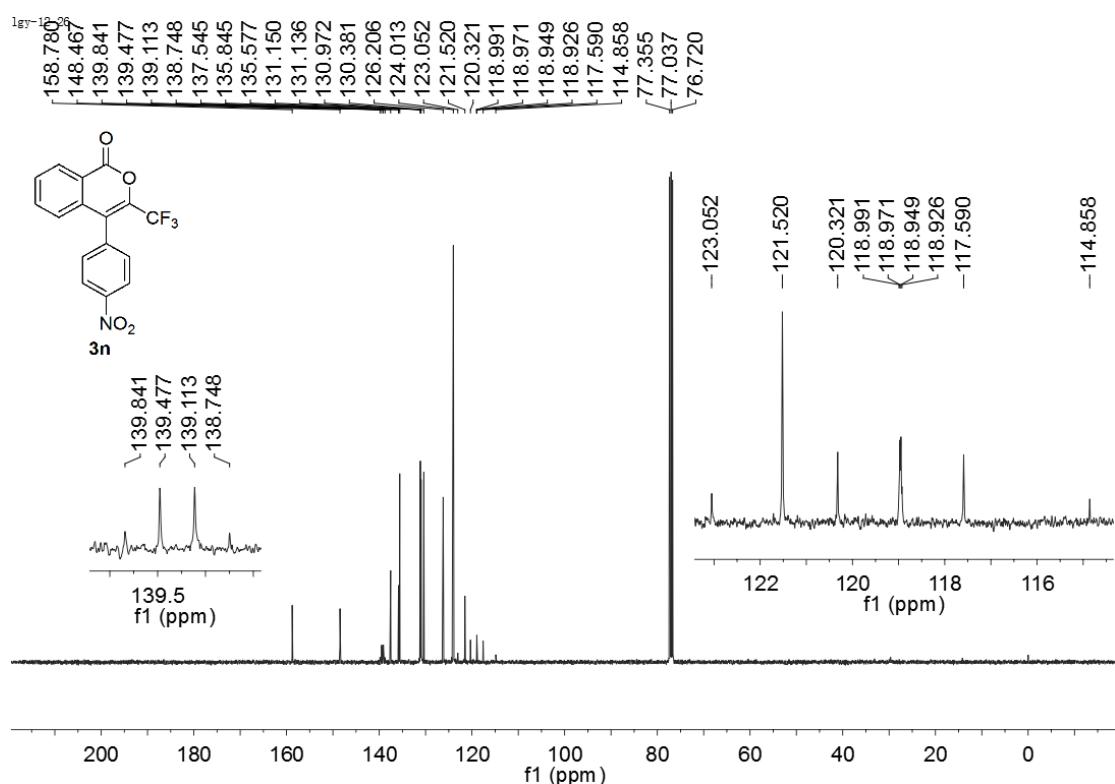
lgy-12-26

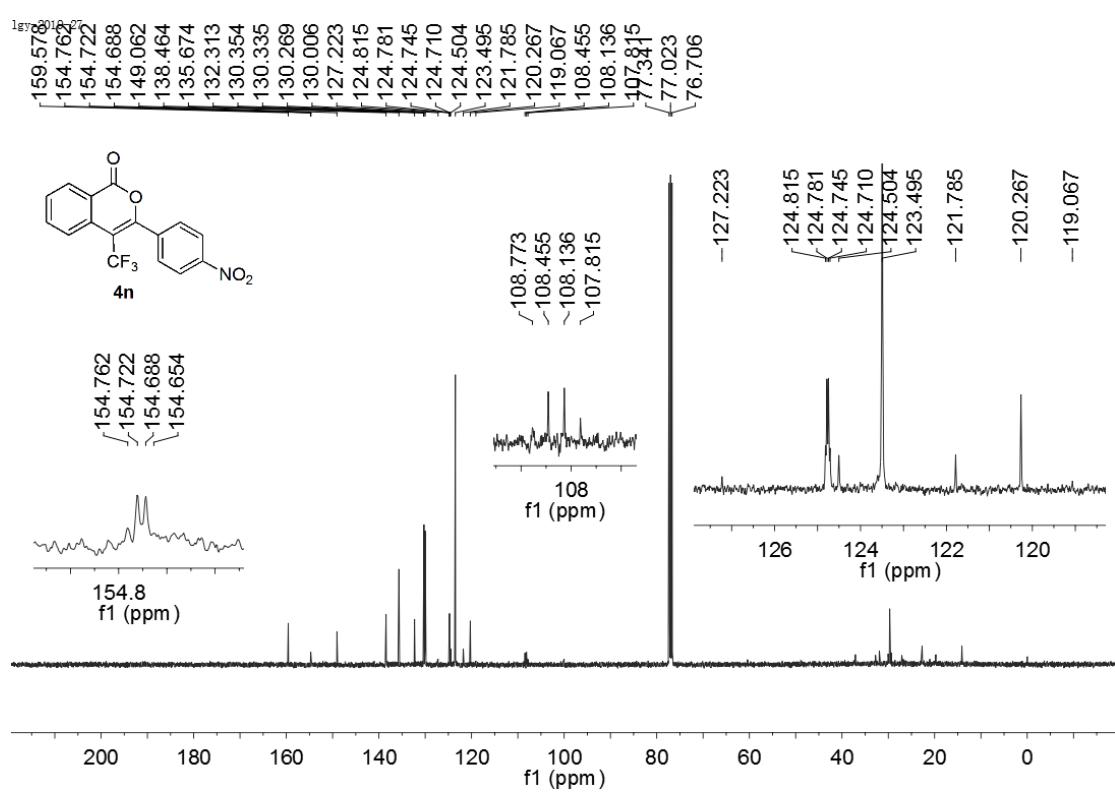
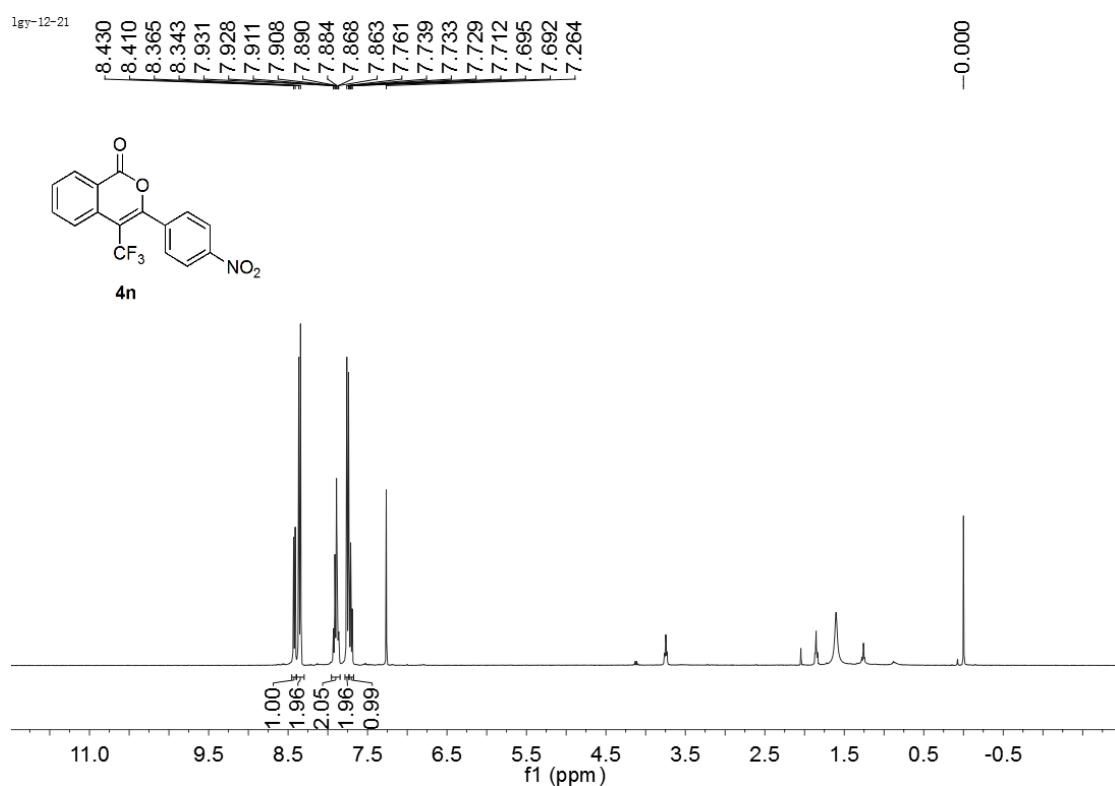
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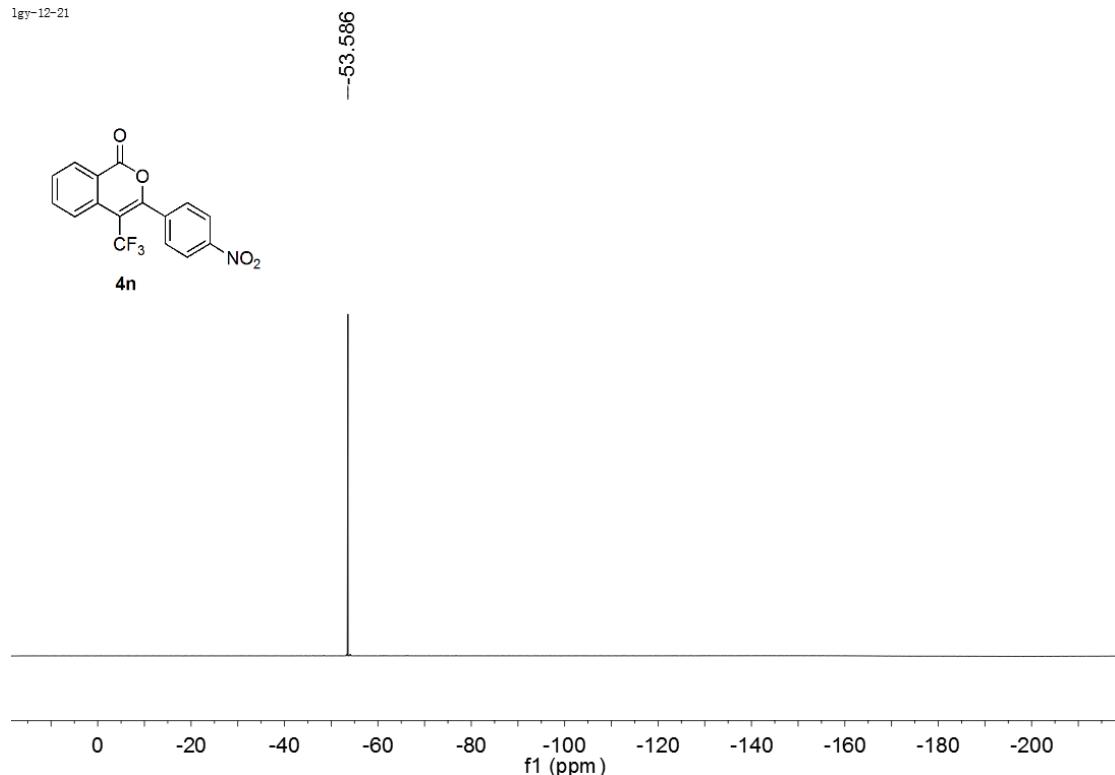
**3n**



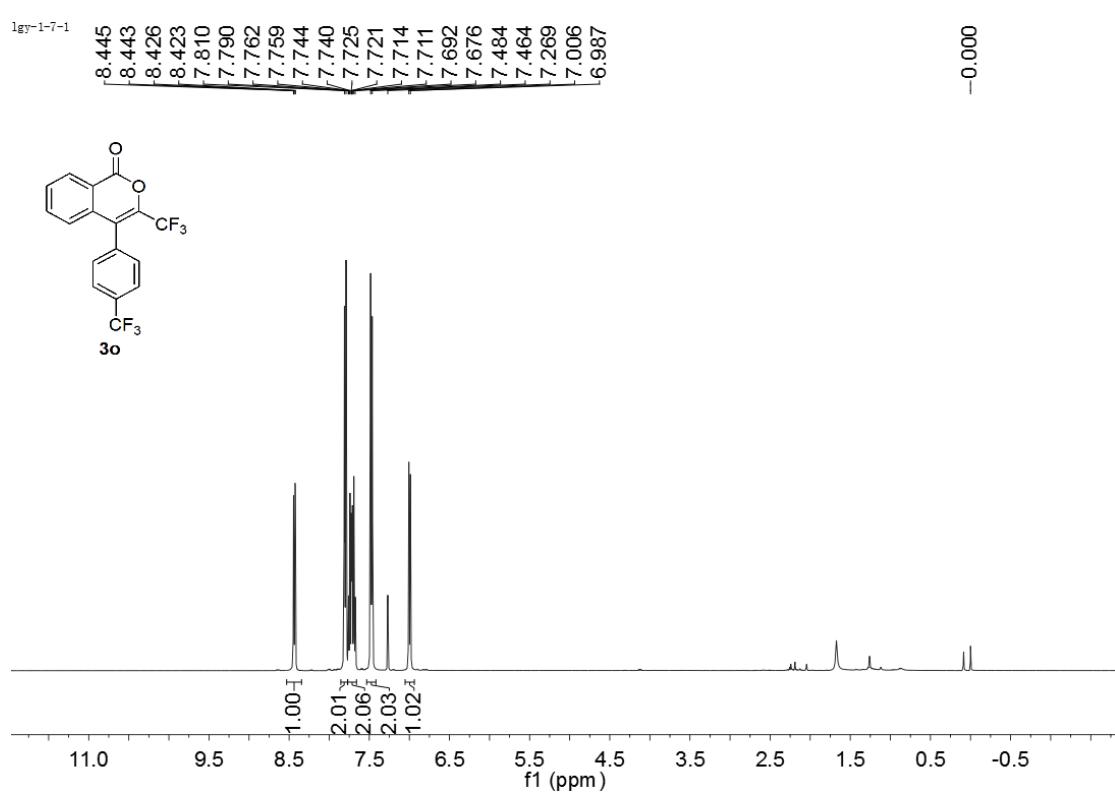




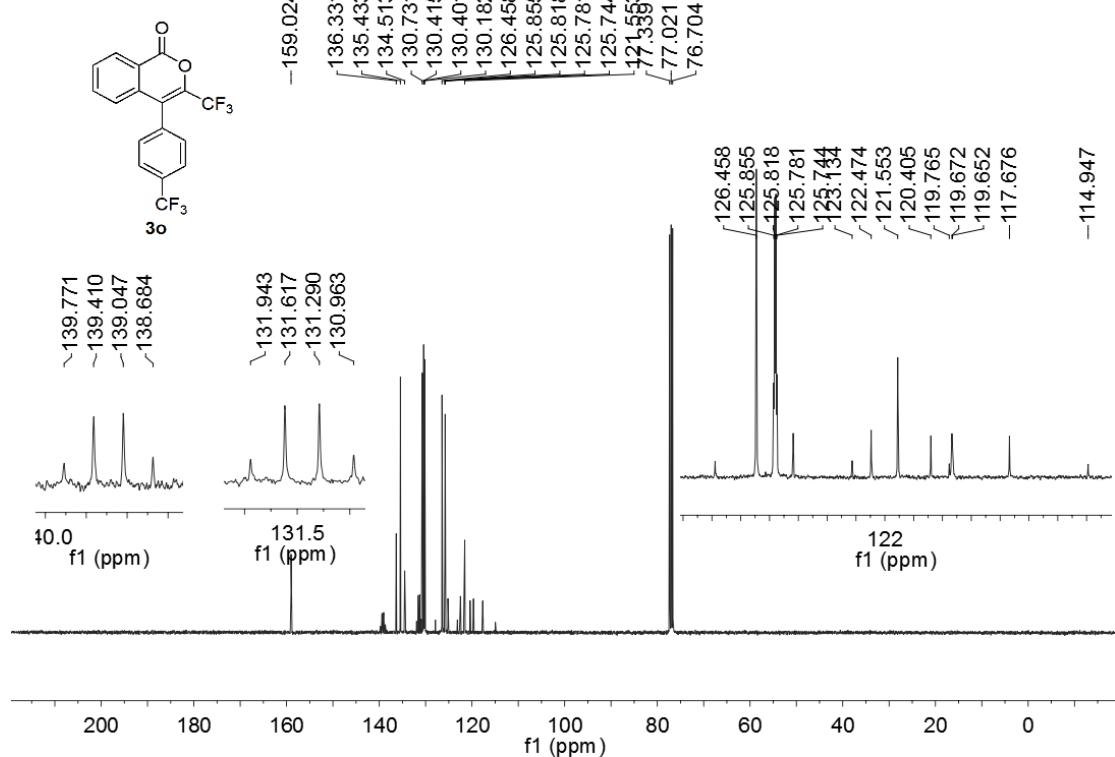
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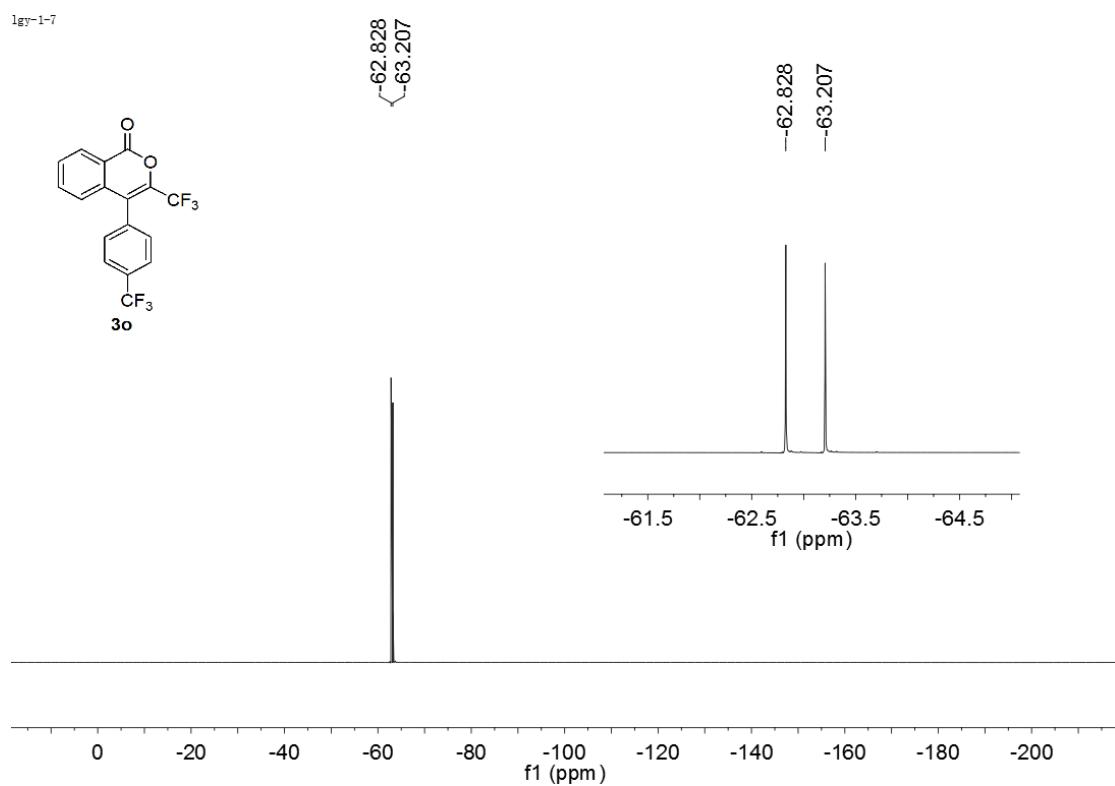
lgy-1-7-1



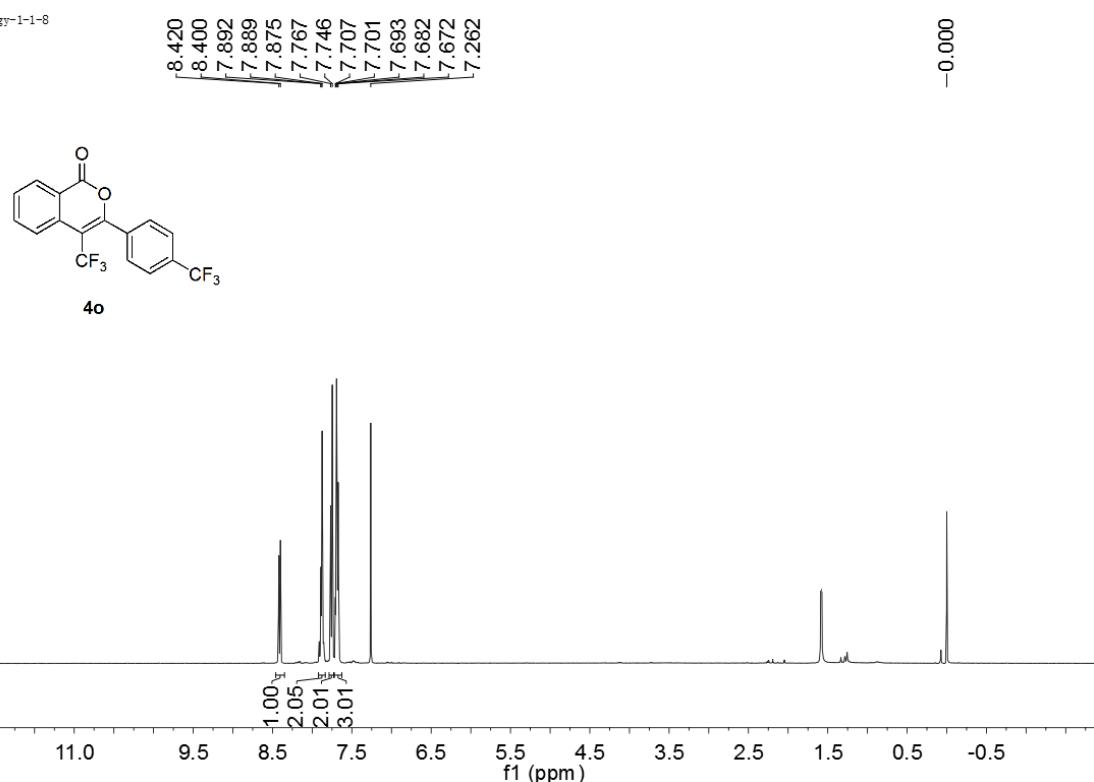
1gyc-1-7



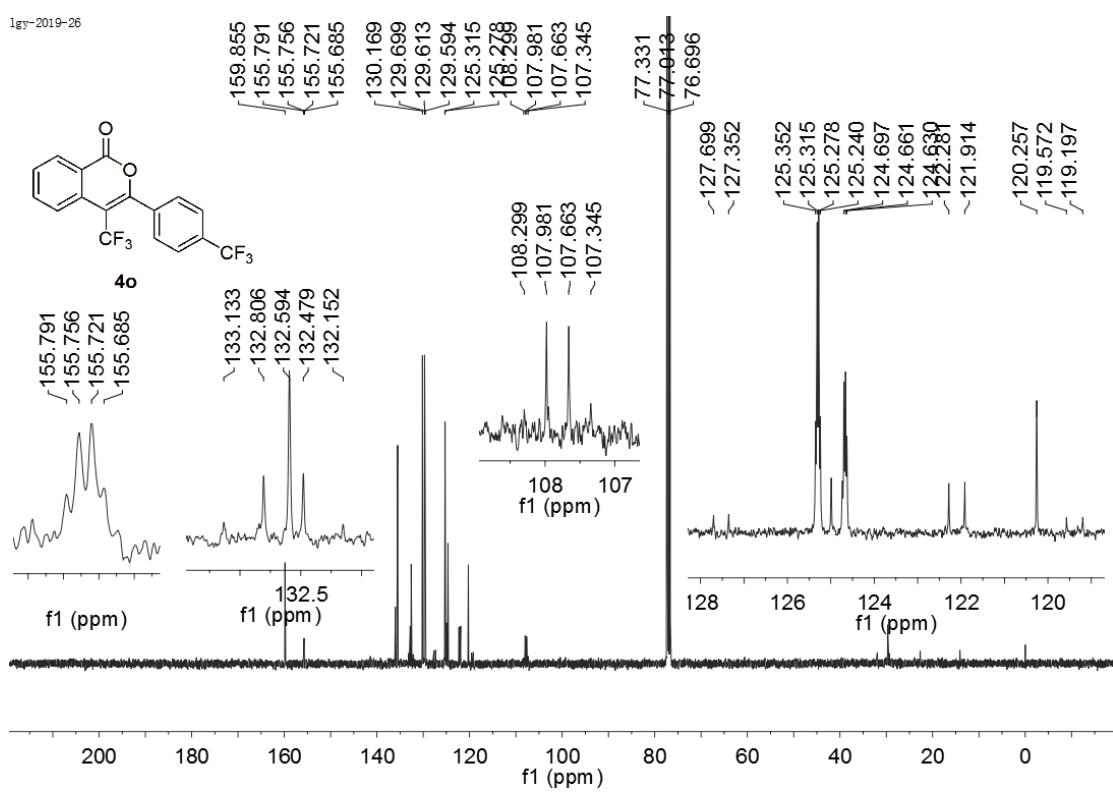
1gyc-1-7



lgy-1-1-8

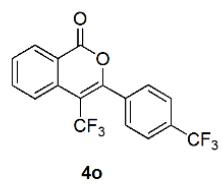


lgy-2019-26

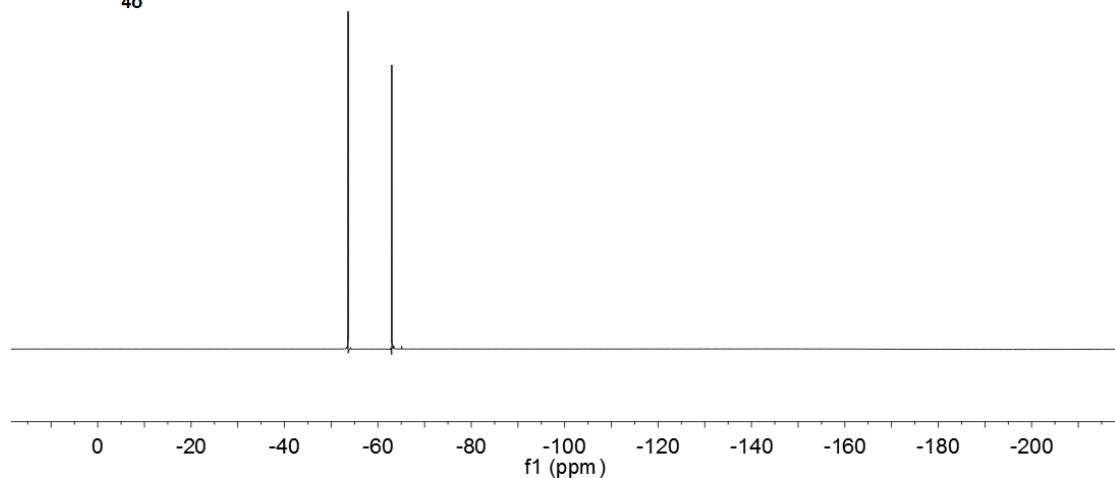


lgy-1-1-8

-53.626  
-62.978

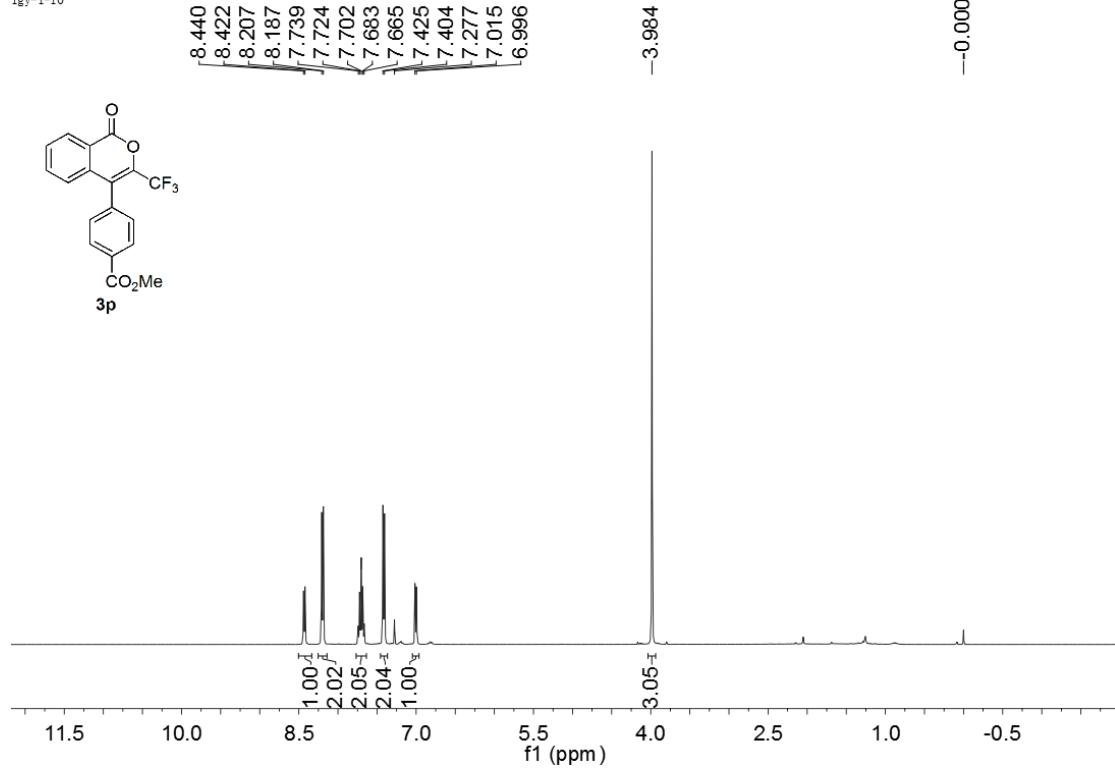
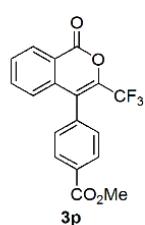


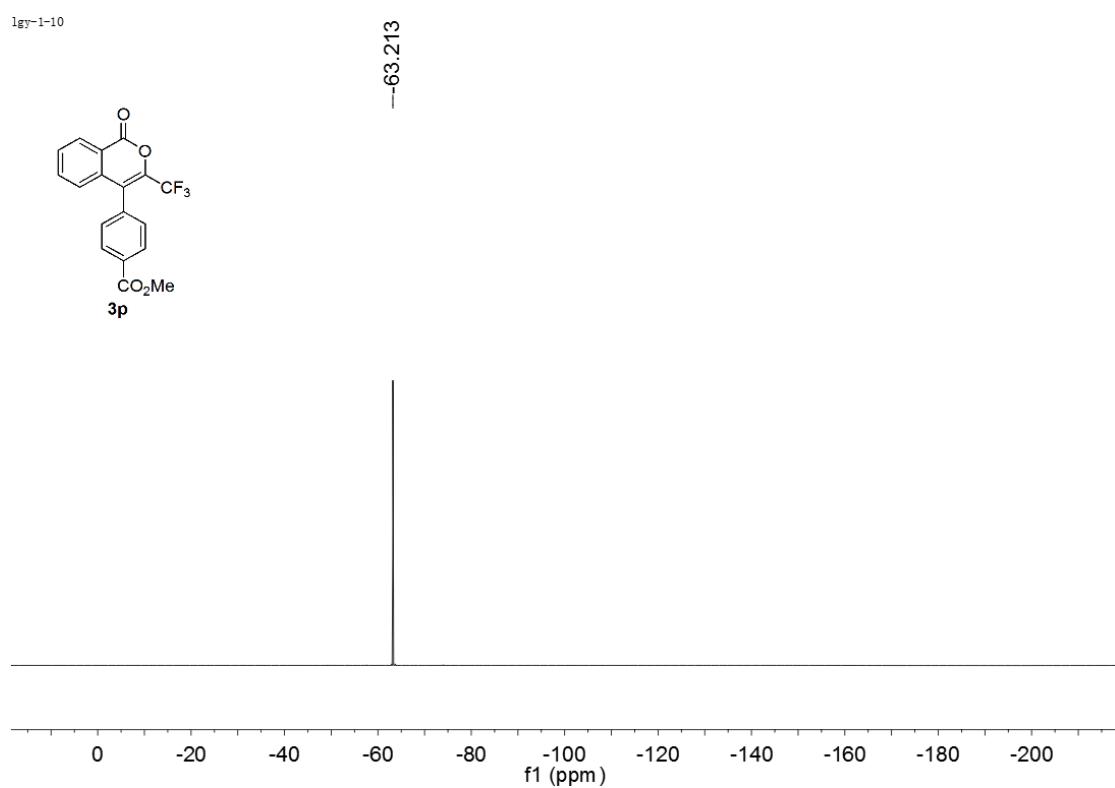
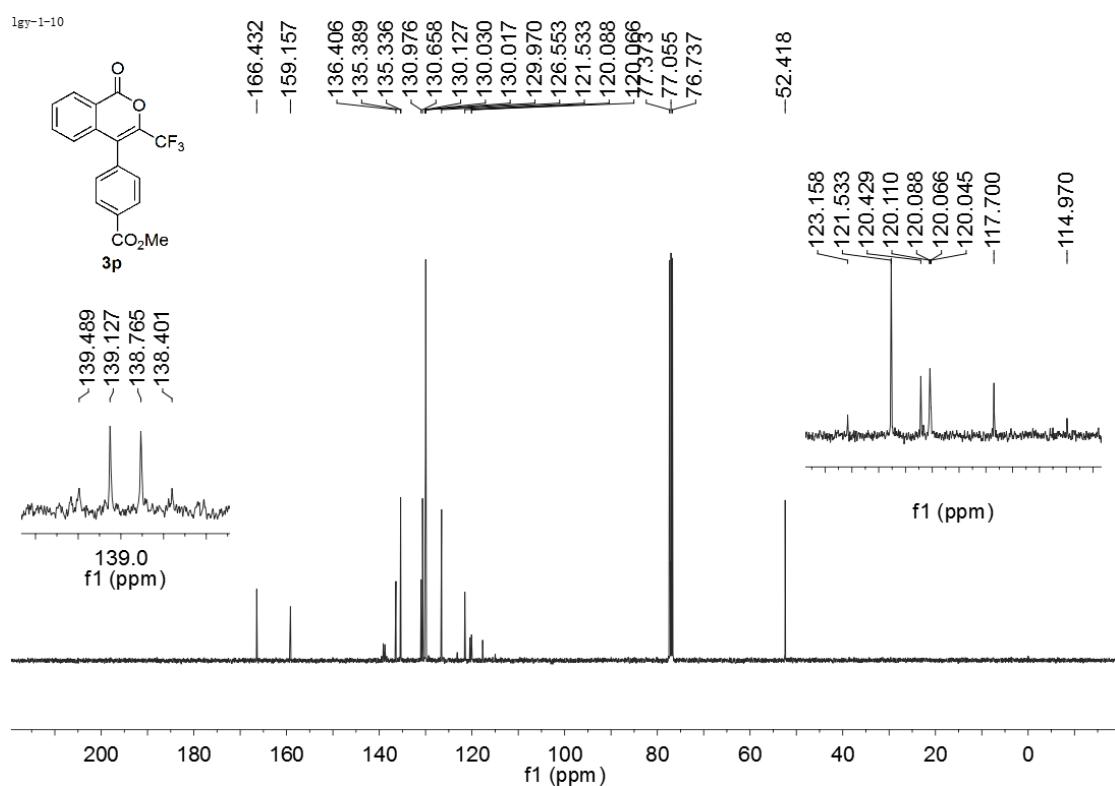
4o

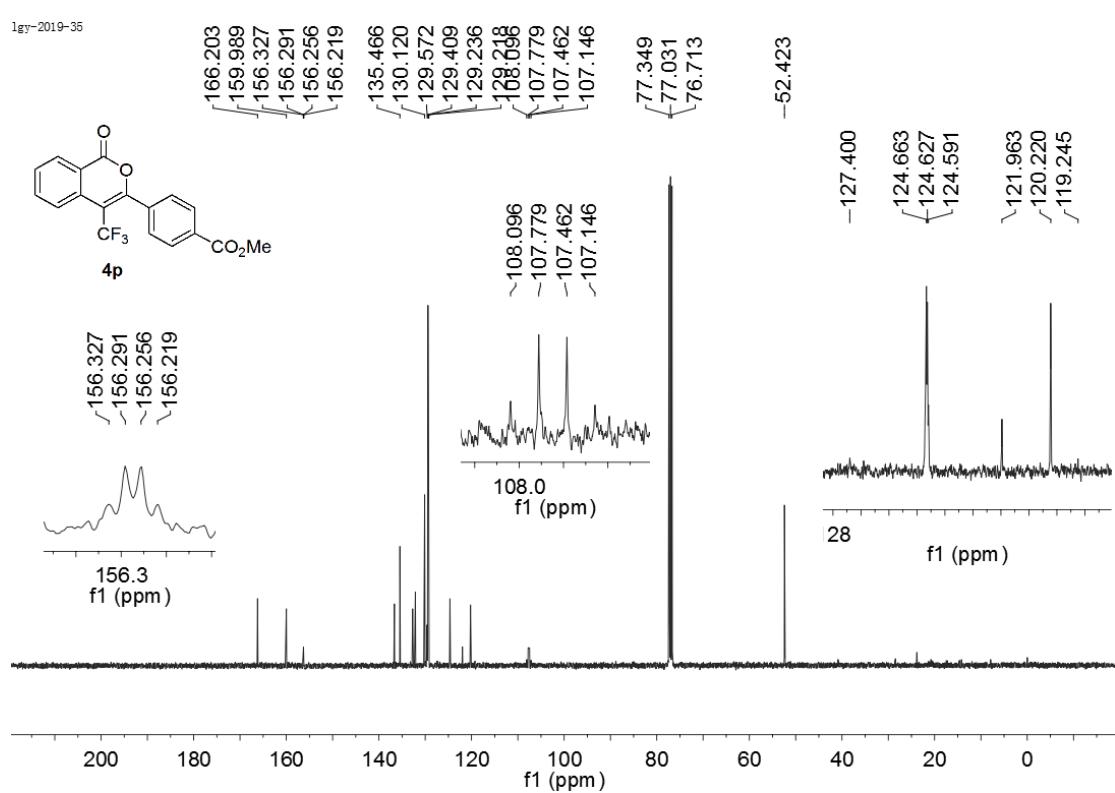
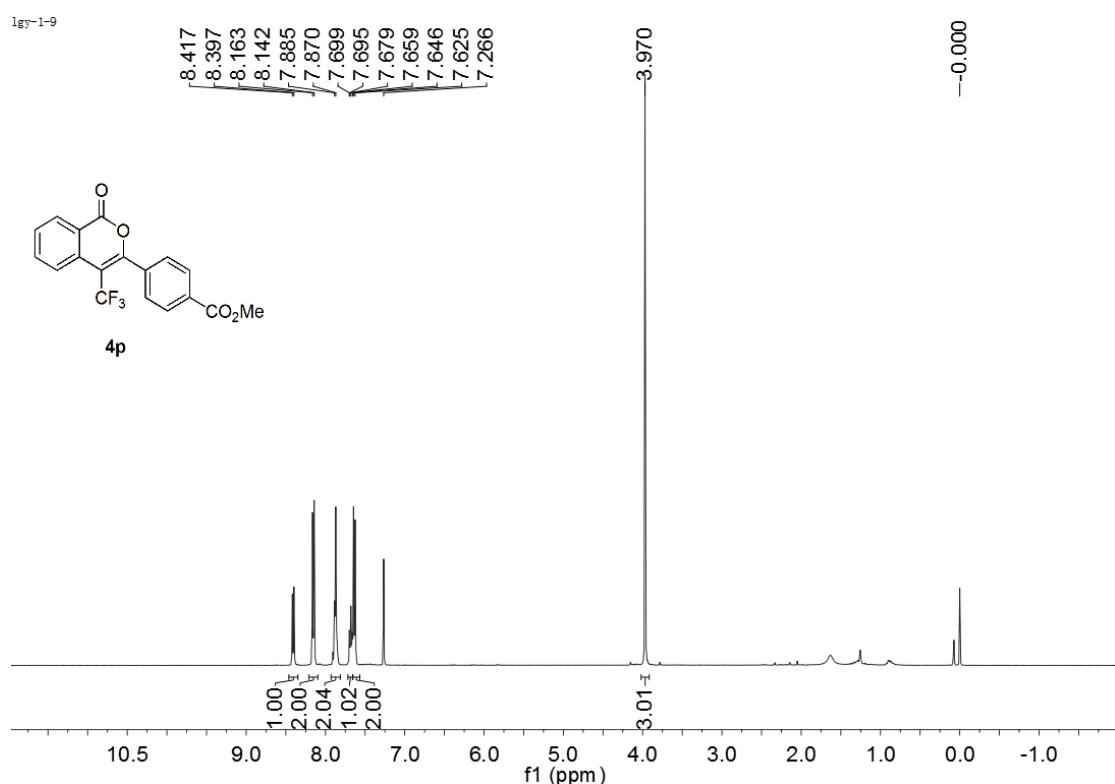


lgy-1-10

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8.207  
8.187  
7.739  
7.724  
7.724  
7.702  
7.683  
7.665  
7.425  
7.404  
7.277  
7.015  
6.996  
-3.984  
-0.000

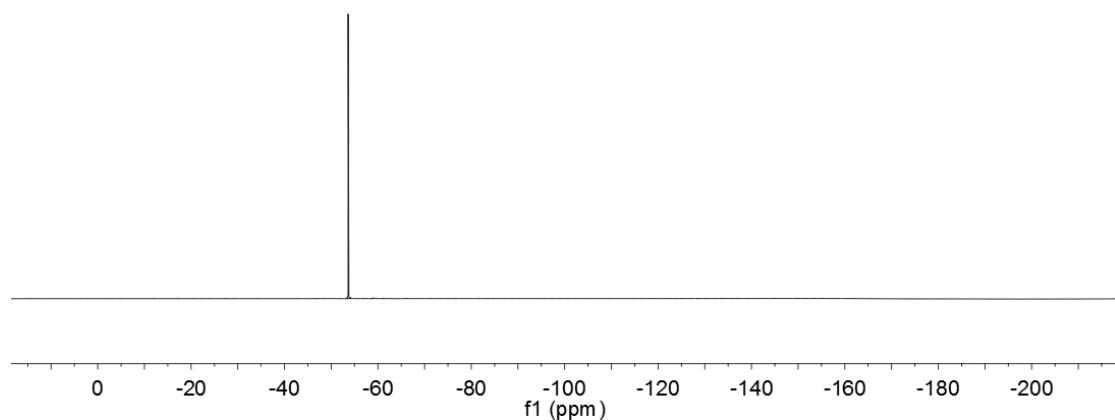
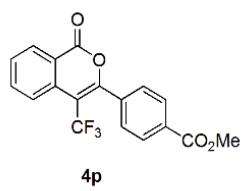






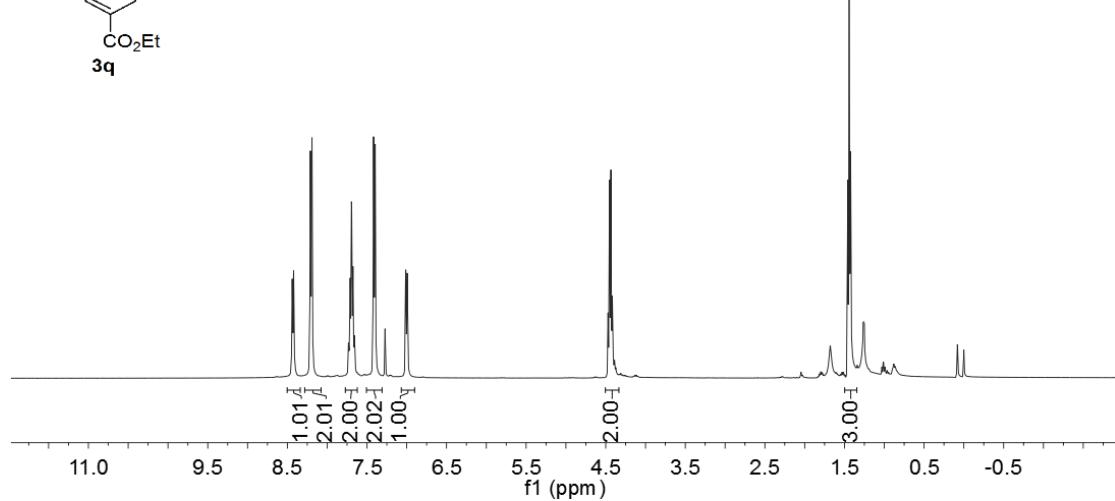
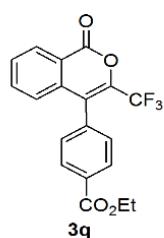
lgy-1-9

-53.629

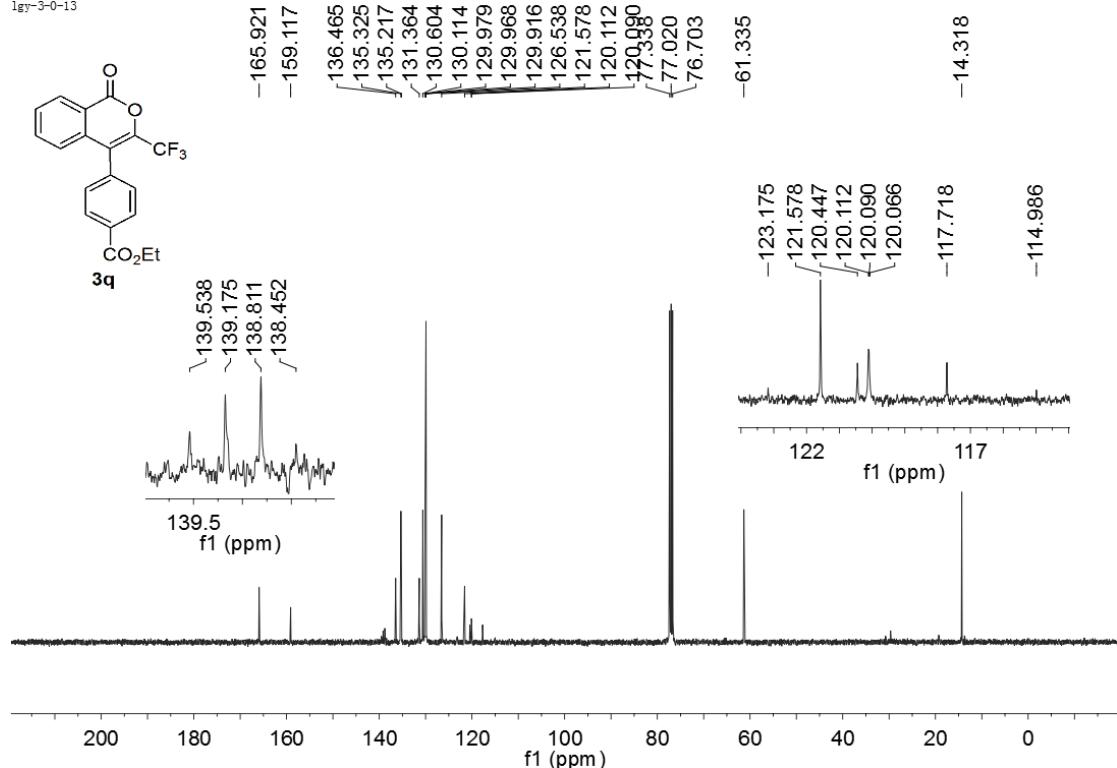


lgy-3-0-13

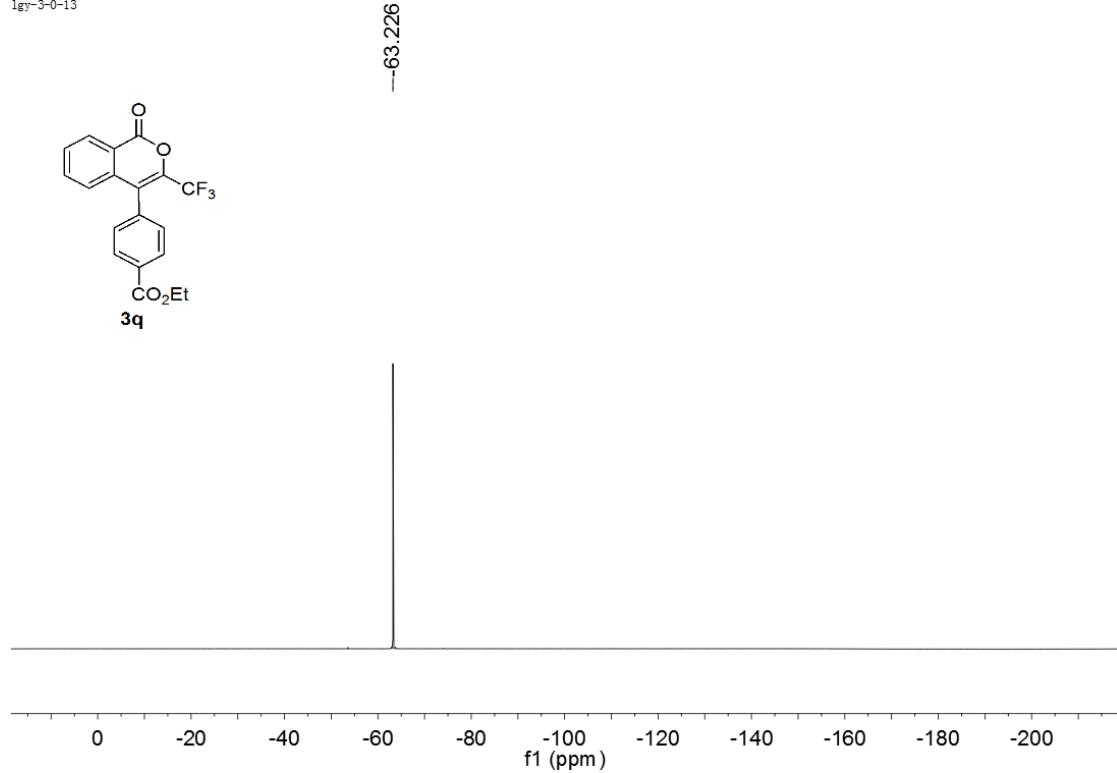
1.459  
1.442  
1.424  
-0.000



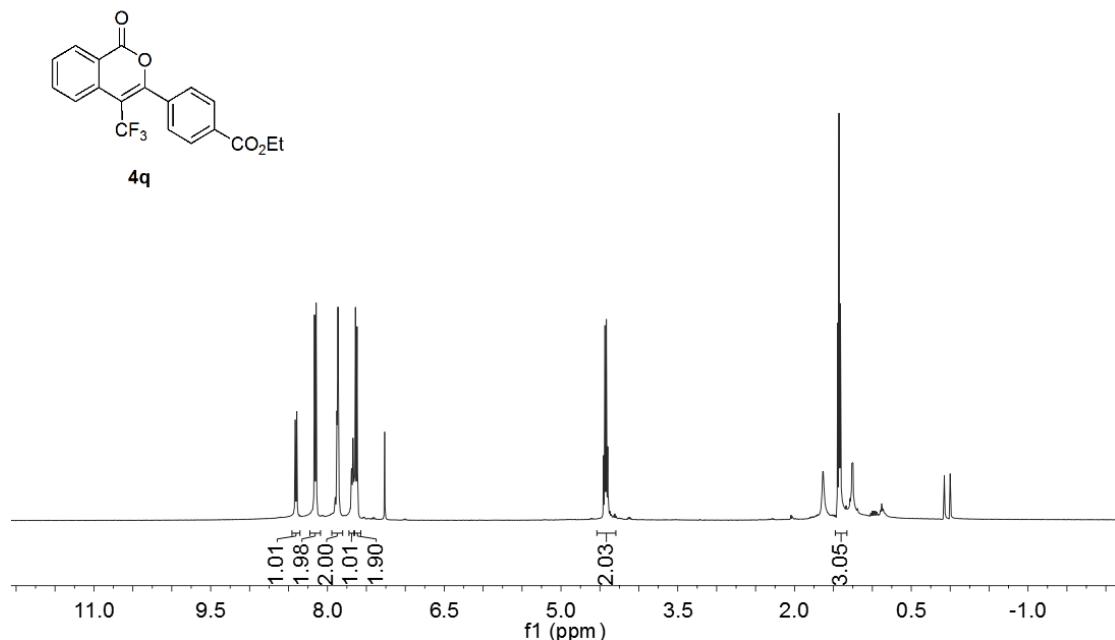
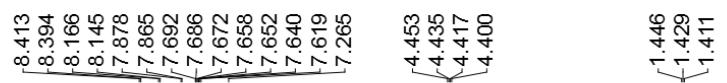
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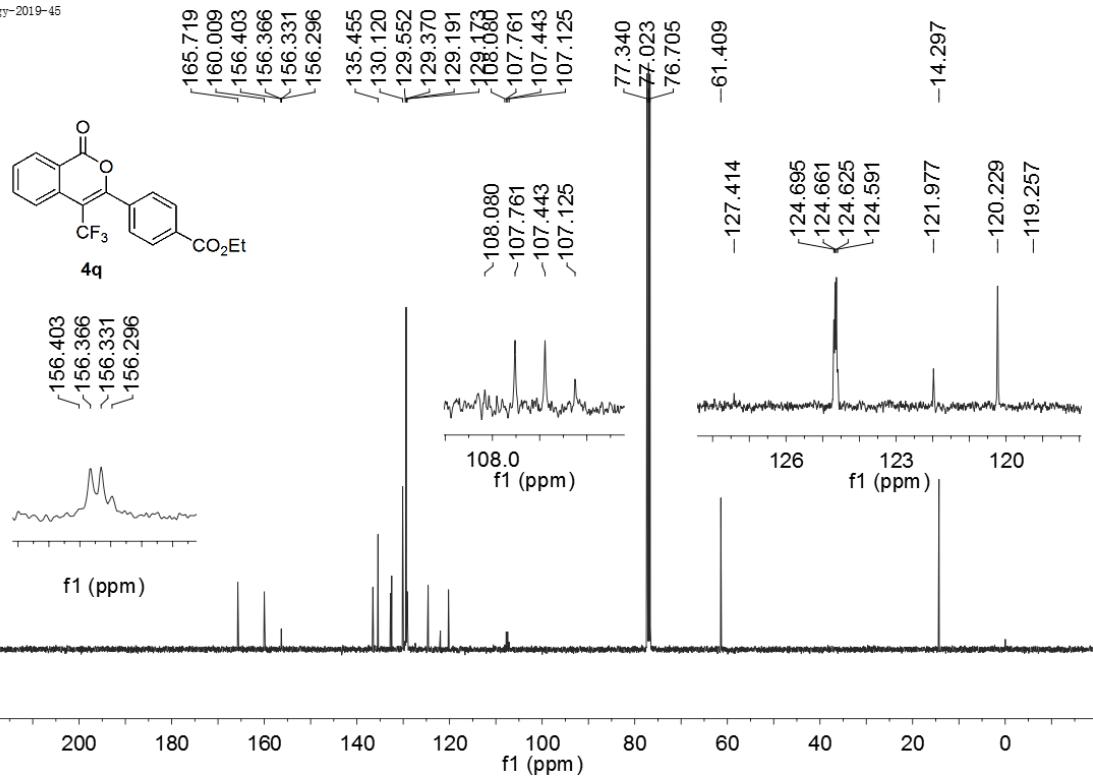
lgy-3-0-13



lgy-3-0-12

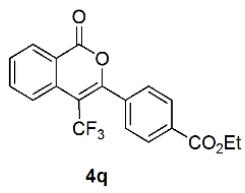


lgy-2019-45

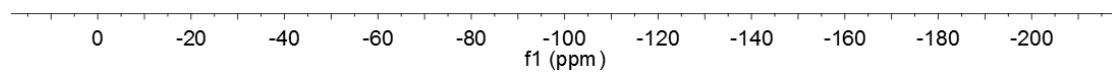


lgy-3-0-12

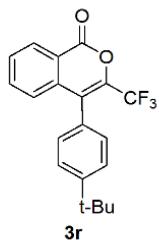
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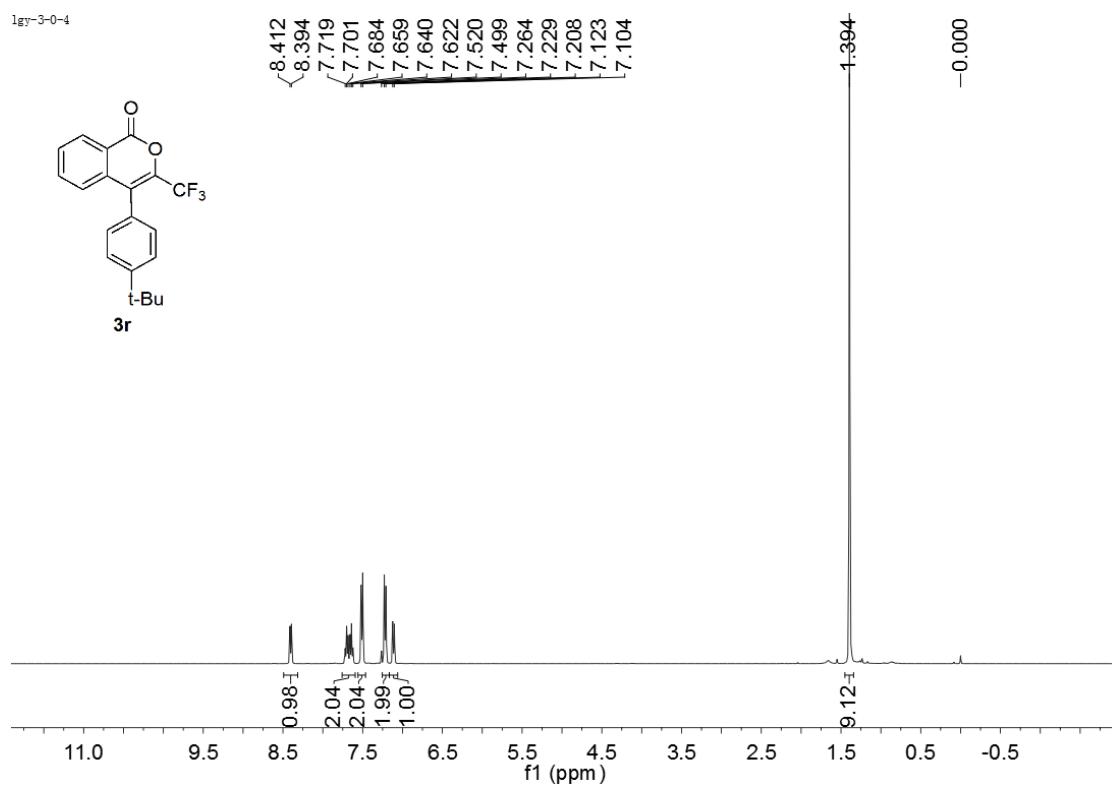
**4q**



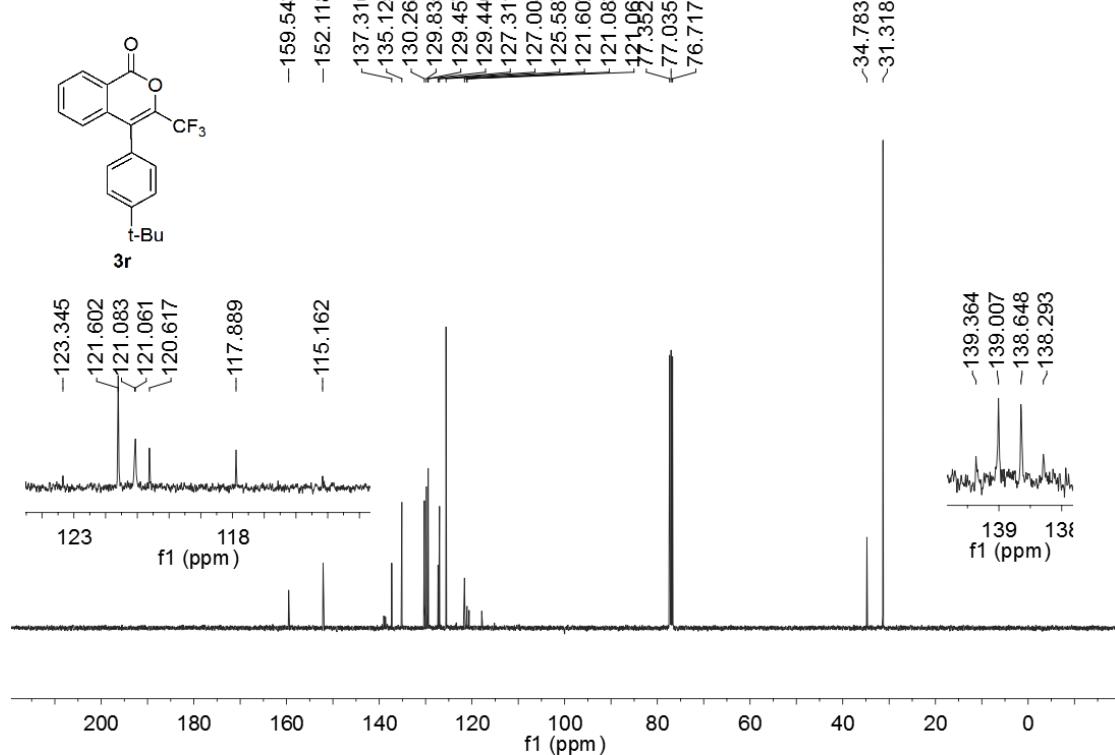
lgy-3-0-4



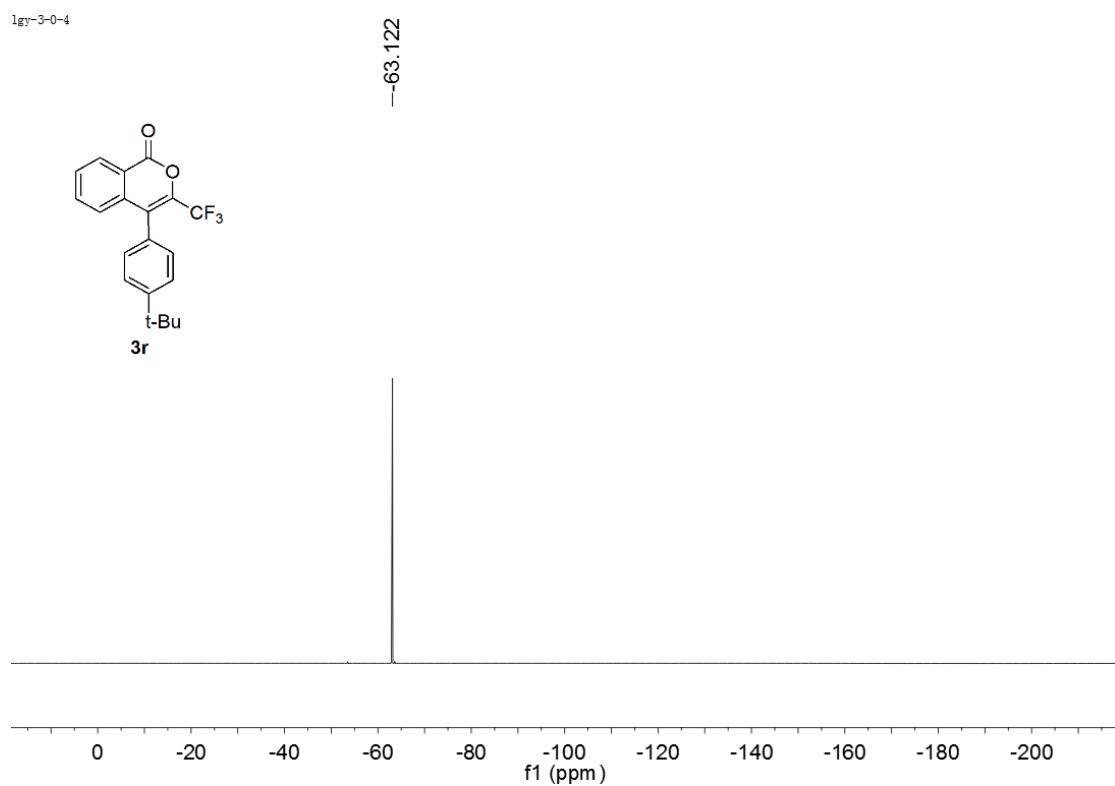
**3r**



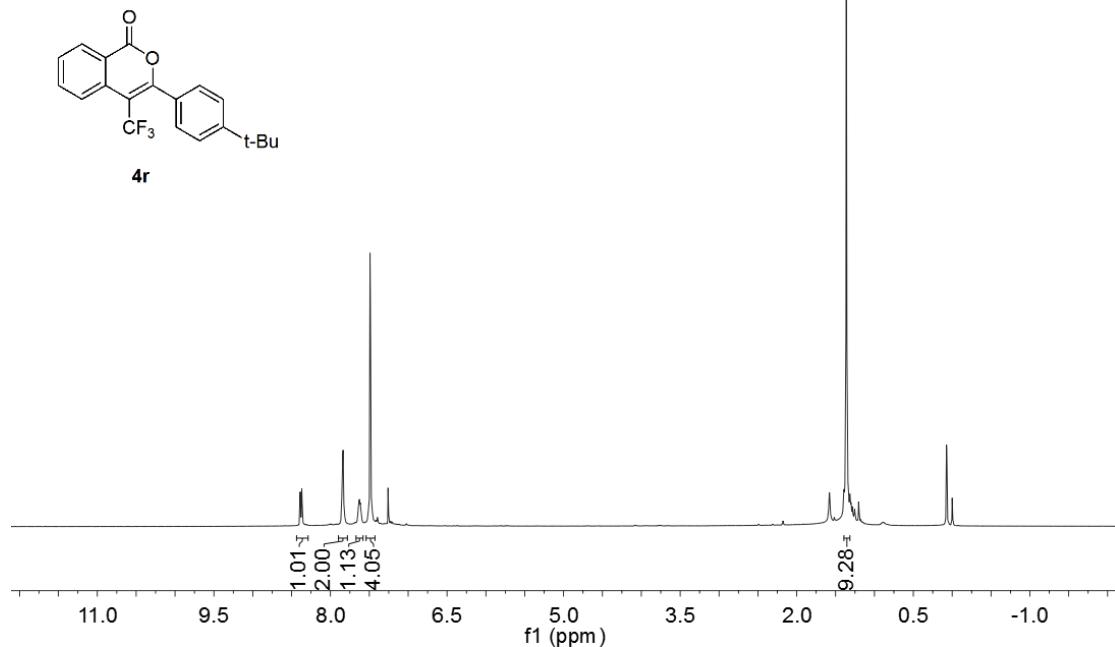
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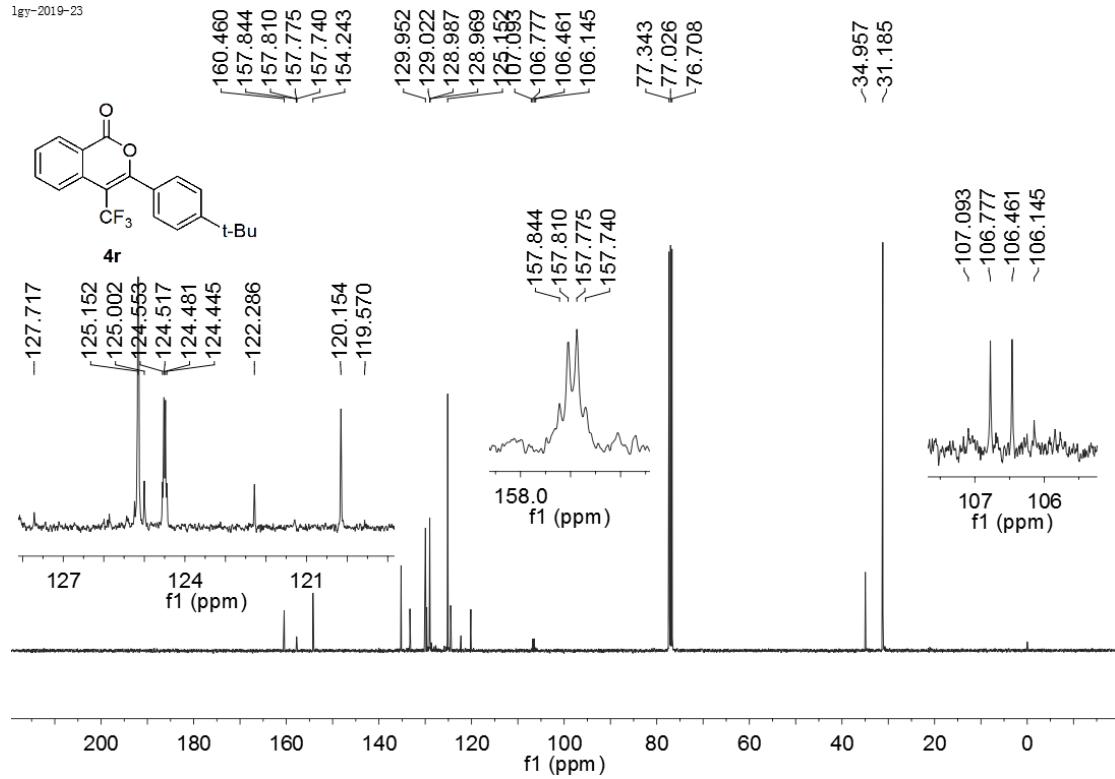
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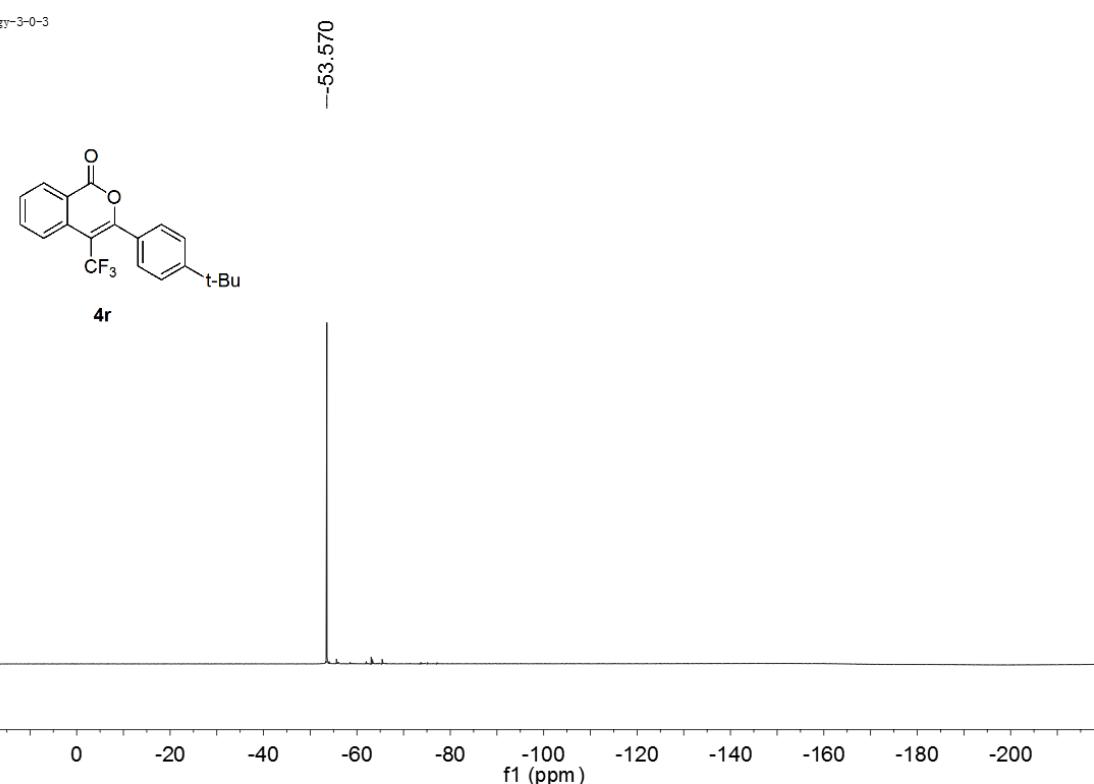
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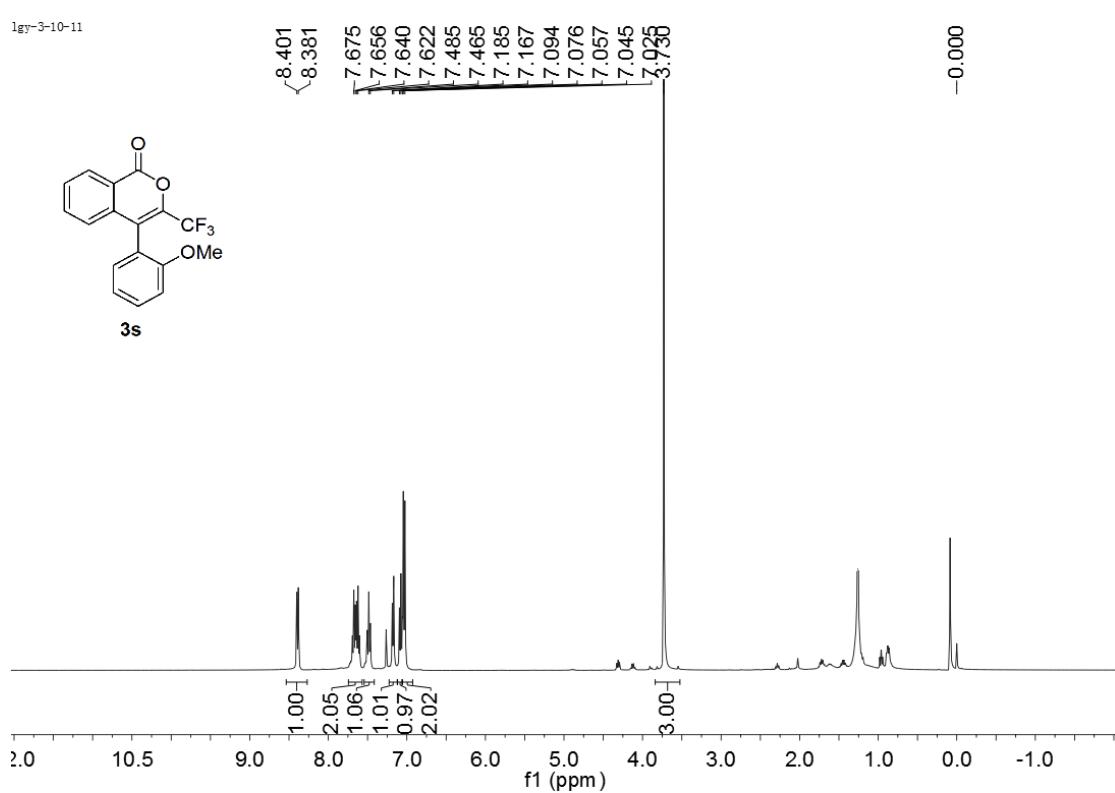
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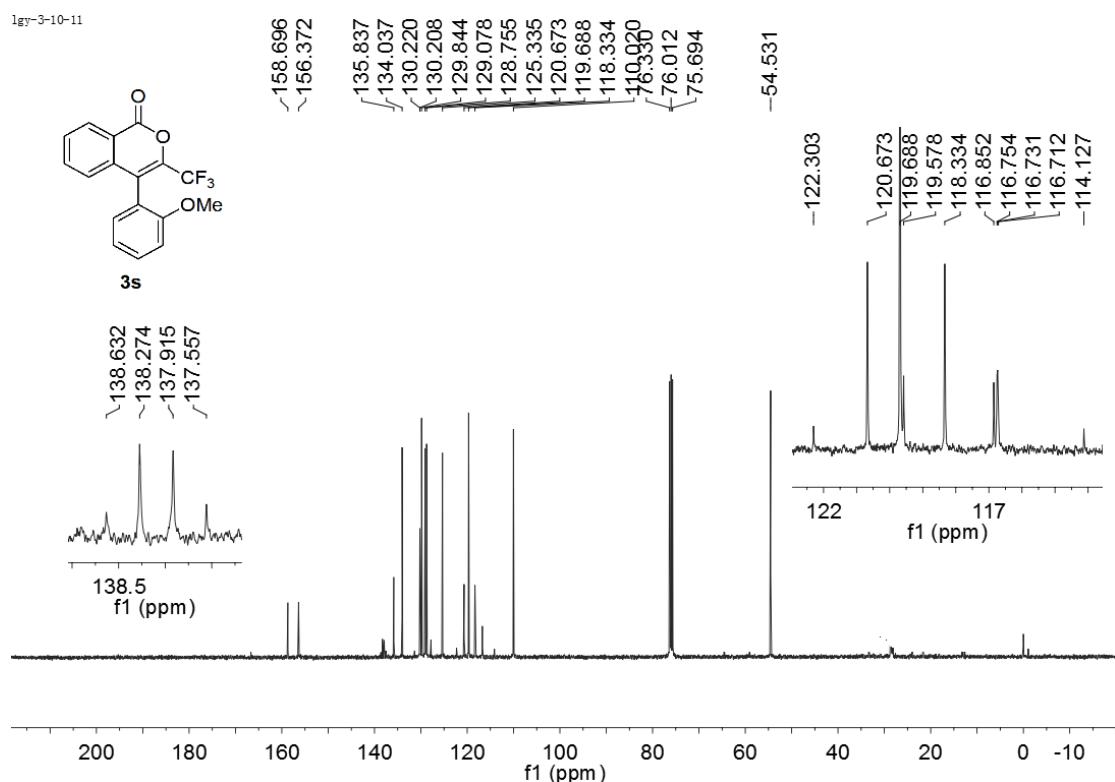
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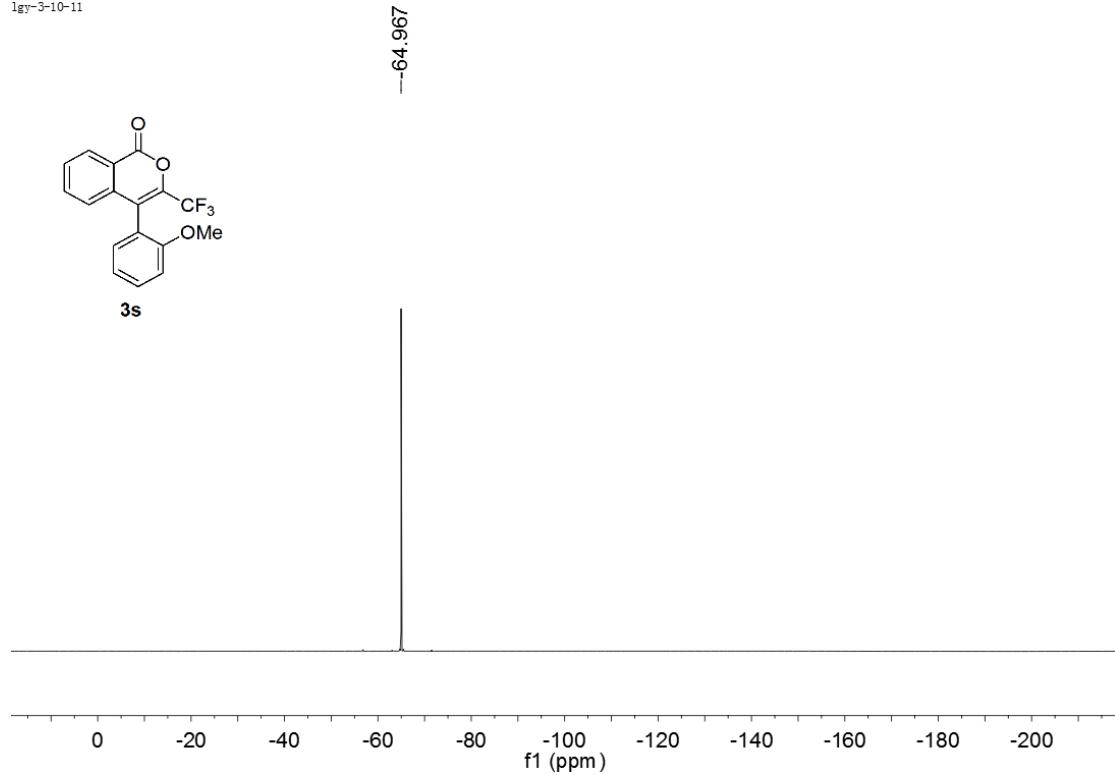
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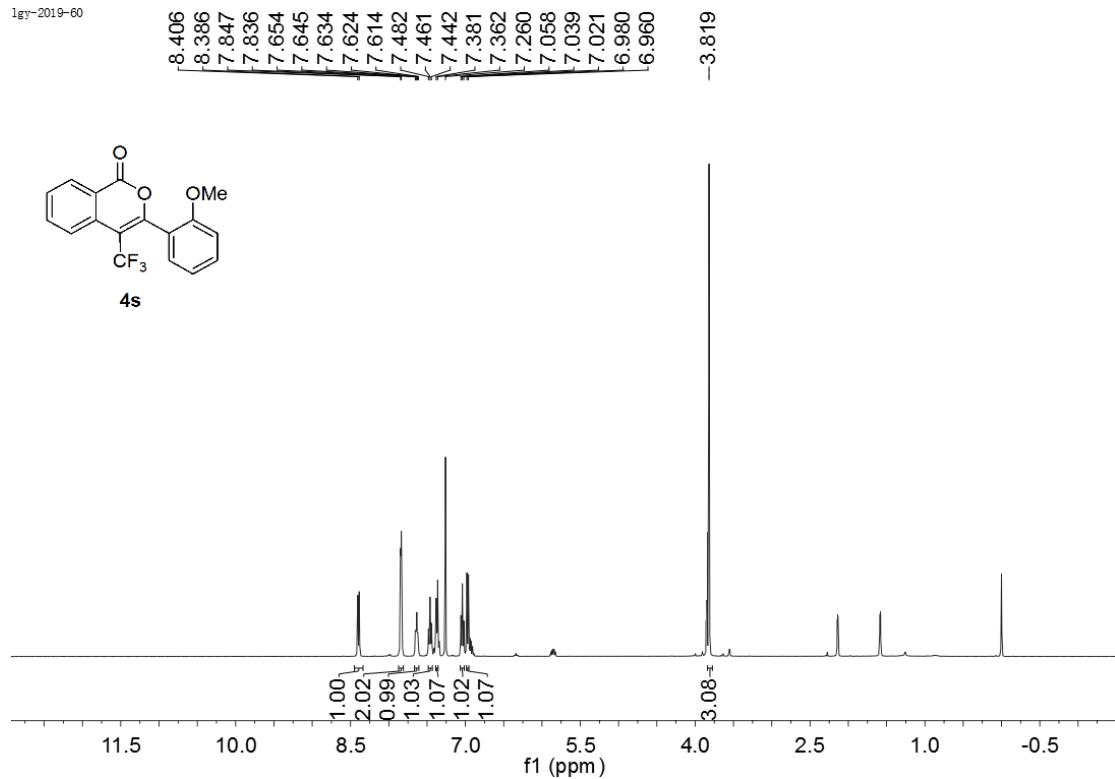
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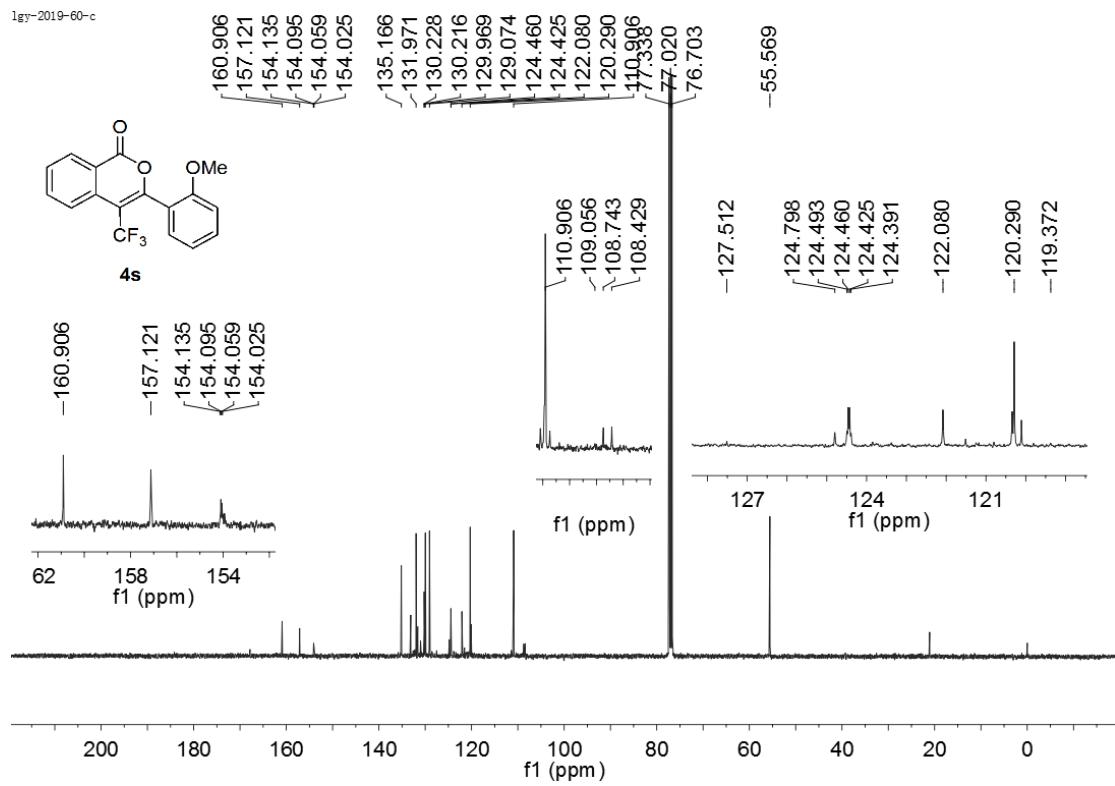
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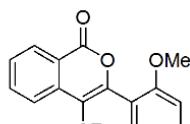
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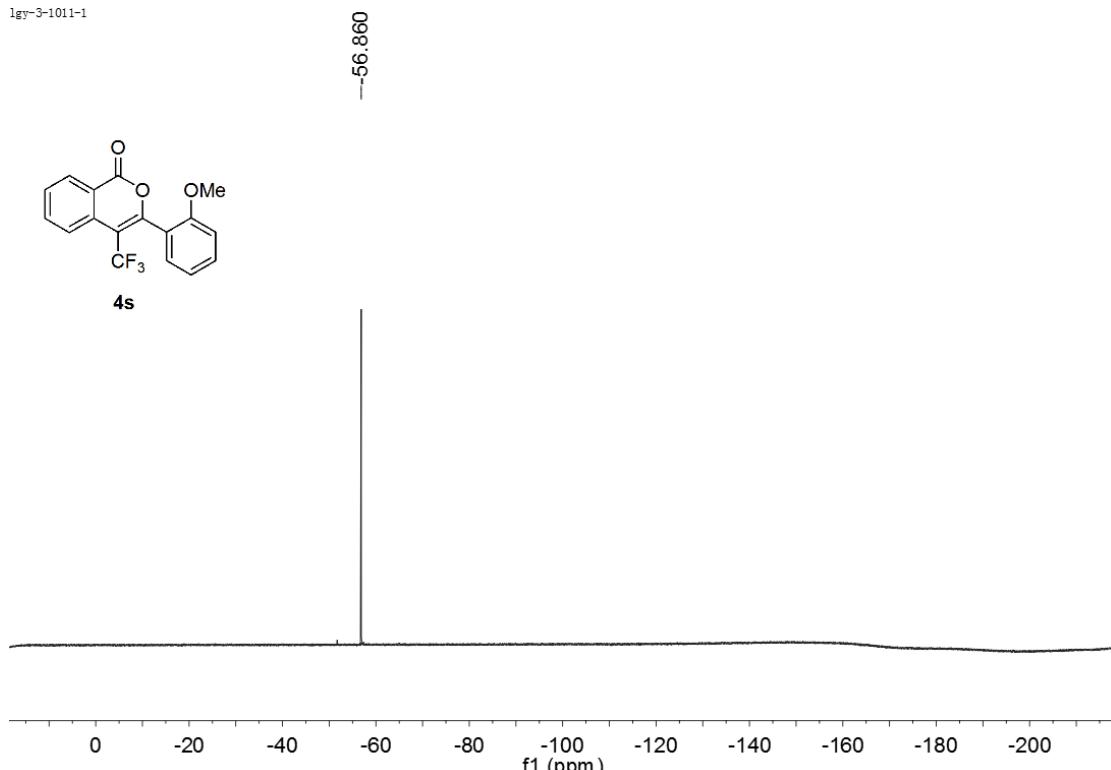
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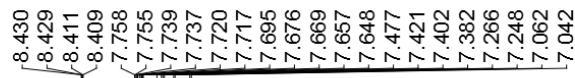
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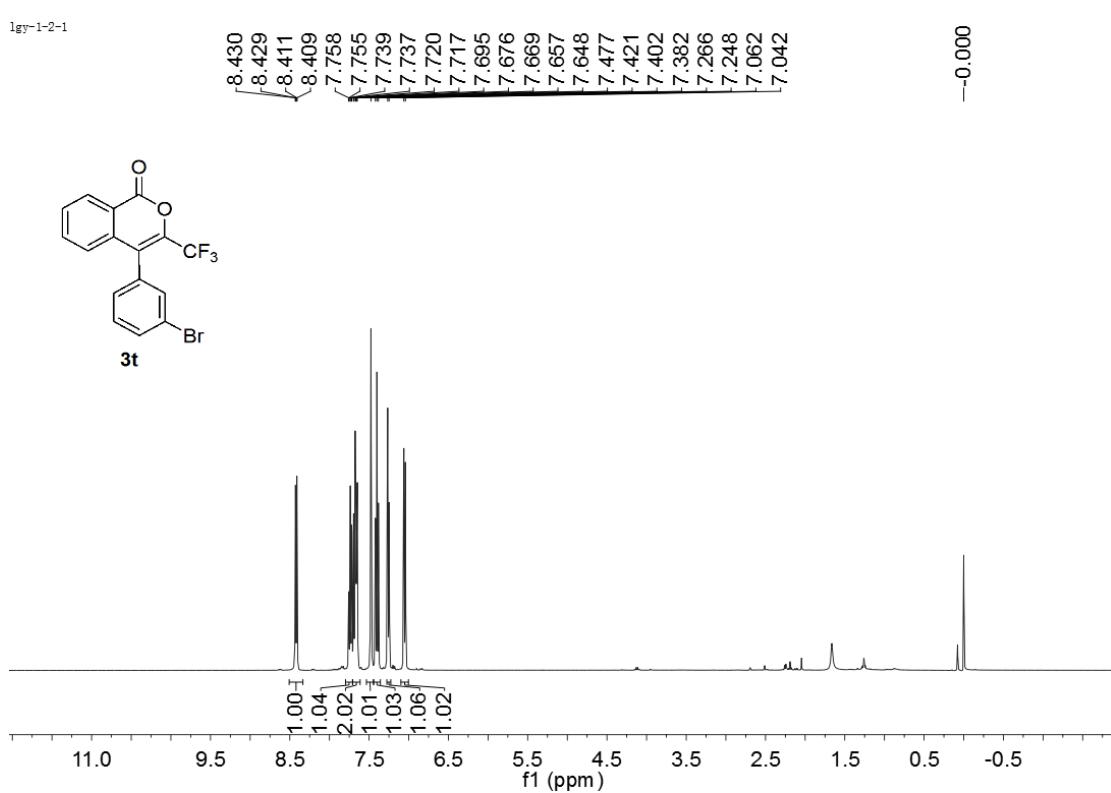
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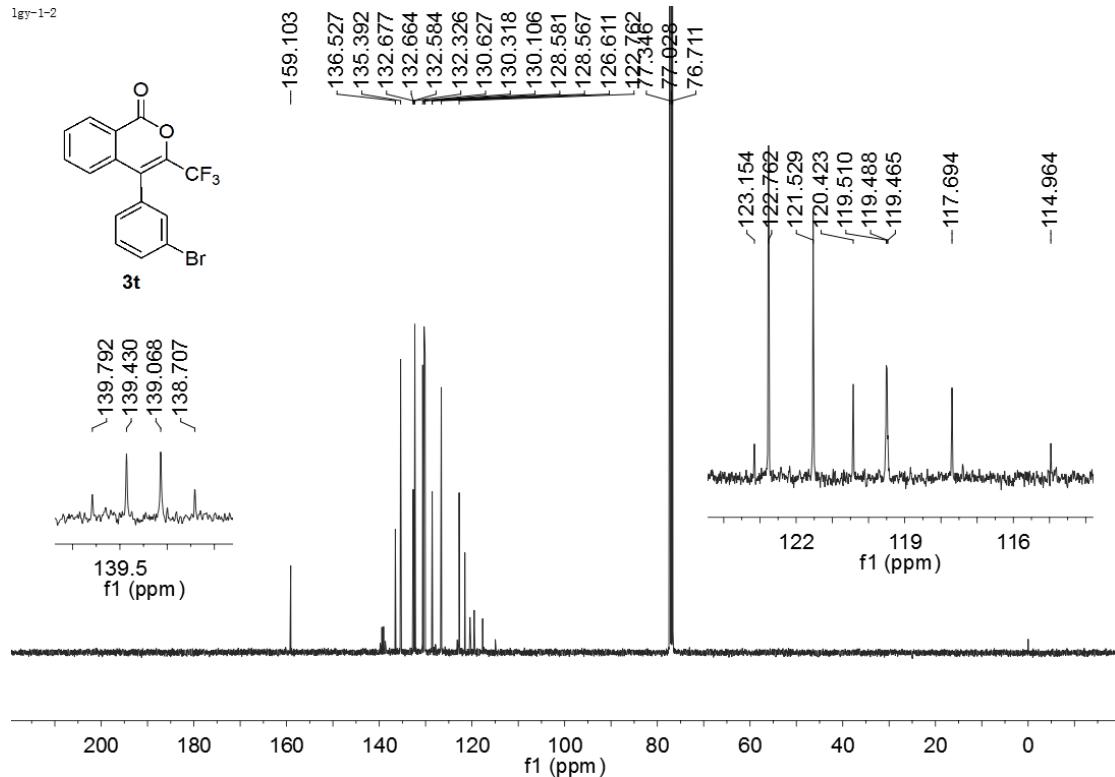
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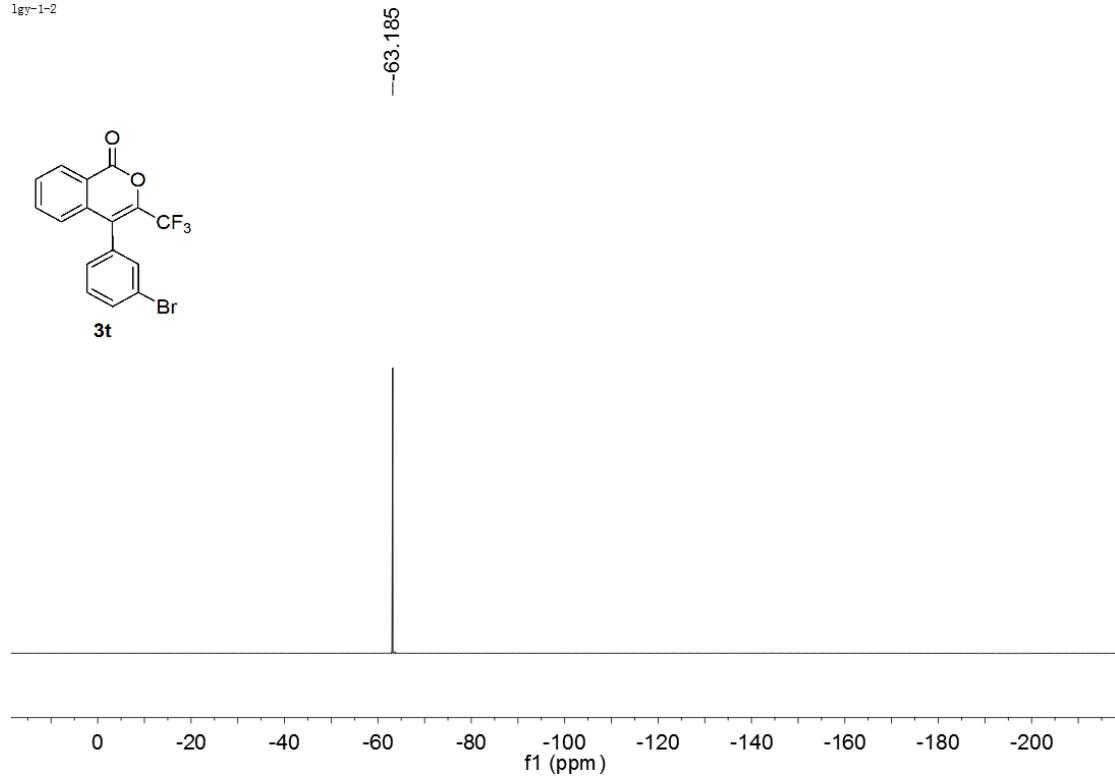
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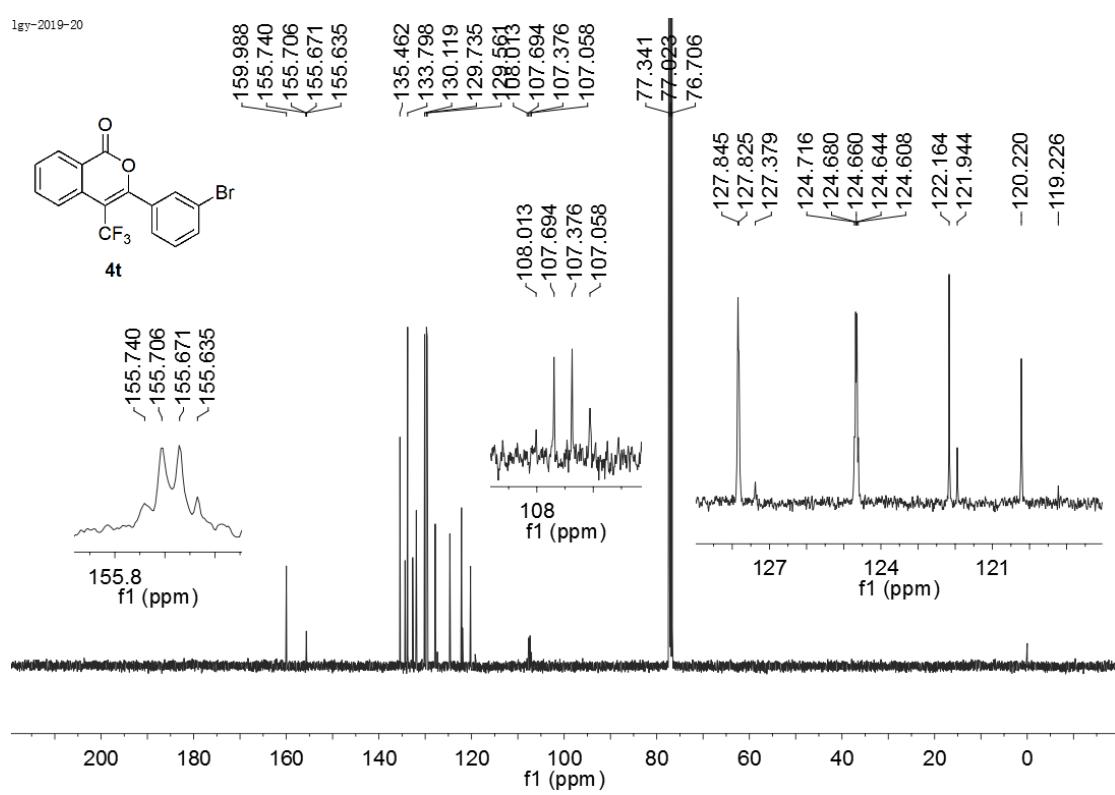
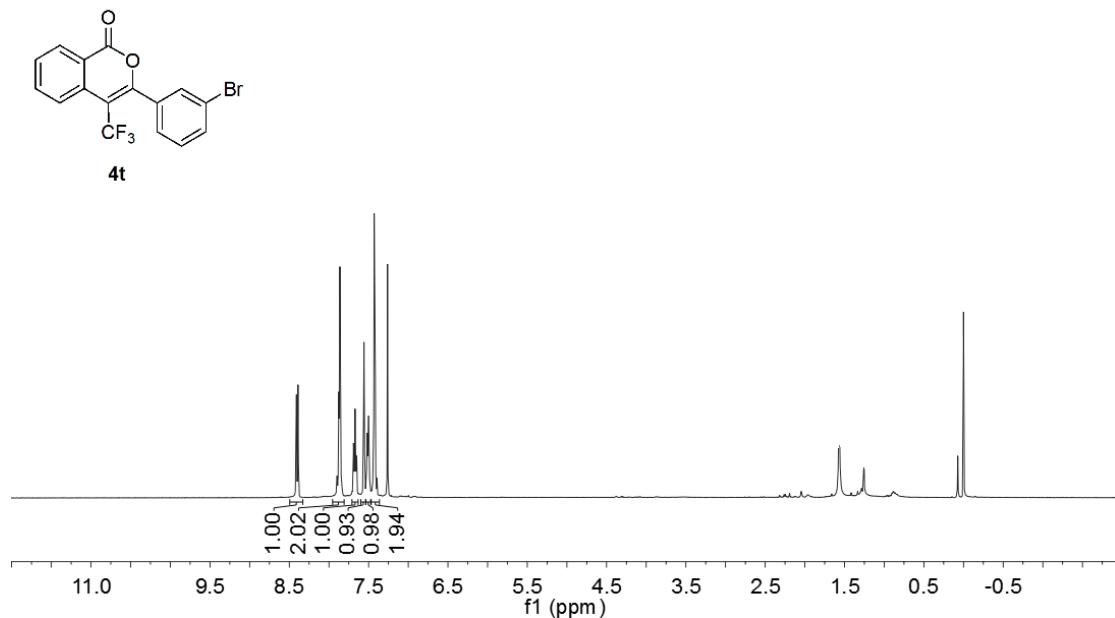
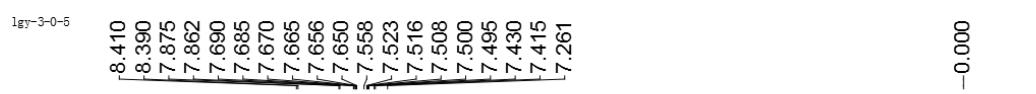


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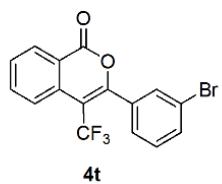


lgy-1-2





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**4t**