

# Supporting Information

## Two-step synthesis of vicinal trifluoromethyl primary amines from $\alpha$ -trifluoromethyl styrenes and phthalimide

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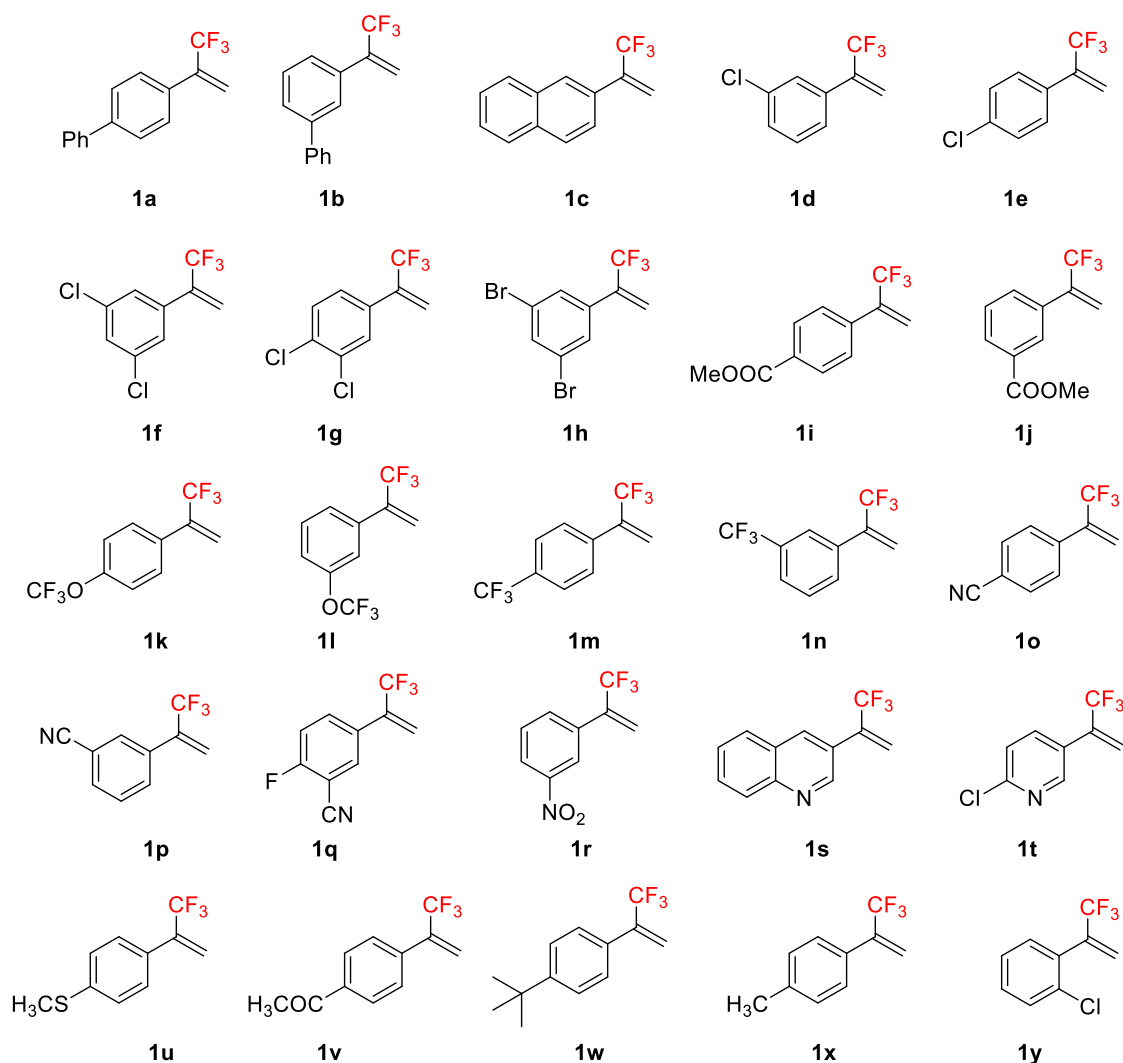
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## 1. General information

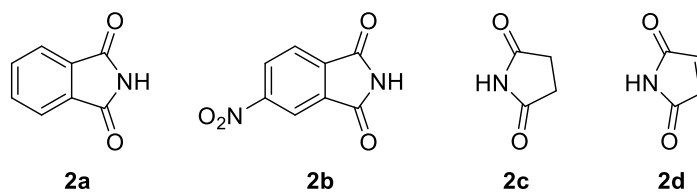
All reagents were of analytical grade, and obtained from commercial suppliers and used without further purification. Melting points were measured in an open capillary using EZ-Melt automated melting point apparatus and were uncorrected.  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra were recorded on a 400 spectrometer (400 MHz for  $^1\text{H}$  and 100 MHz for  $^{13}\text{C}$ , respectively) using TMS as an internal standard. The  $^{19}\text{F}$  NMR spectra were obtained on a 400 spectrometer (376 MHz) with  $\text{CF}_3\text{COOH}$  as an internal standard.  $\text{CDCl}_3$  or  $\text{DMSO}-d_6$  were used as the NMR solvents. High resolution mass spectra (HRMS) were acquired in the ESI mode using a TOF mass analyzer. The GC and GC-MS were recorded on HP 5973 MSD with 6890 GC. Silica gel (300–400 mesh size) was used for column chromatography. TLC analysis of reaction mixtures was performed using silica gel plates.

## 2. $\alpha$ -(Trifluoromethyl)styrenes (**1a–y**) and imides (**2a–d**) used in this reaction



The  $\alpha$ -(trifluoromethyl)styrenes (**1a–y**) were prepared according to the reported procedure.<sup>1–5</sup>

The imides **2a–d** were obtained from commercial suppliers.



### 3. General procedure for the synthesis of compounds **3a–v**

To a glass tube charged with a stirring bar were added DBU or DABCO or TMG or CsF (2.0 mmol, 2.0 equiv), **2a** (220.5 mg, 1.5 mmol, 1.5 equiv),  $\alpha$ -(trifluoromethyl)styrenes **1a–v** (1.0 mmol, 1.0 equiv), and DMF (4 mL). The reaction vial was sealed with a rubber septum and then the reaction mixture was stirred at 80 °C for 16 h (monitored by TLC or GC/MS). After completion of the reaction, the reaction mixture was quenched with saturated aqueous solution of NH<sub>4</sub>Cl (20 mL) and extracted with ethyl acetate (3 × 10 mL). The organic layer was separated and dried over Na<sub>2</sub>SO<sub>4</sub>, filtered and concentrated in vacuo. The resultant residue was purified by column chromatography on silica gel using *n*-hexane/ ethyl acetate (5/1) as eluent to afford the pure compounds **3a–v**.

### 4. General procedure for the synthesis of the target compounds **4a–u**

To a flask charged with a stirring bar were added **3a–u** (1.0 mmol, 2.0 equiv), NH<sub>2</sub>NH<sub>2</sub>·H<sub>2</sub>O (500.6 mg, 10.0 mmol, 10.0 equiv) and CH<sub>3</sub>OH (10 mL). The reaction mixture was refluxed at 70 °C for 5 h (monitored by TLC and GC/MS). After completion of the reaction, the reaction mixture was quenched with saturated aqueous solution of NH<sub>4</sub>Cl (20 mL) and extracted with ethyl acetate (3 × 10 mL). The organic layer was separated and dried over Na<sub>2</sub>SO<sub>4</sub>, filtered and concentrated in vacuo. The resultant residue was purified by column chromatography on silica gel using *n*-hexane/ ethyl acetate (2/1) as eluent to afford the pure target compounds **4a–u**.

### 5. General procedure for the synthesis of compounds **5a–c**

To a glass tube charged with a stirring bar were added DBU or CsF (2.0 mmol, 2.0 equiv), **2a** (221 mg, 1.5 mmol, 1.5 equiv),  $\alpha$ -(trifluoromethyl)styrenes **1w–y** (1.0 mmol, 1.0 equiv), and DMF (4 mL). The reaction vial was sealed with a rubber septum and then the reaction mixture was stirred at 80 °C for 16 h (monitored by TLC and GC/MS). After completion of the reaction, the reaction mixture was quenched with saturated aqueous solution of NH<sub>4</sub>Cl (20 mL) and extracted with ethyl acetate (3 × 10 mL). The organic layer was separated and dried over Na<sub>2</sub>SO<sub>4</sub>, filtered and concentrated in vacuo. The resultant residue was purified by column chromatography on silica gel using *n*-hexane/ ethyl acetate (5/1) as eluent to afford the pure compounds **5a–c**.

### 6. General procedure for the synthesis of compounds **7a–c**

To a glass tube charged with a stirring bar were added DBU (305 mg, 2.0 mmol, 2.0 equiv), **2b–d** (1.5 mmol, 1.5 equiv),  $\alpha$ -(trifluoromethyl)styrene **1a** (248 mg, 1.0 mmol, 1.0 equiv), and DMF (4 mL). The reaction vial was

sealed with a rubber septum and then the reaction mixture was stirred at 80 °C for 16 h (monitored by TLC and GC/MS). After completion of the reaction, the reaction mixture was quenched with saturated aqueous solution of NH<sub>4</sub>Cl (20 mL) and extracted with ethyl acetate (3 × 10 mL). The organic layer was separated and dried over Na<sub>2</sub>SO<sub>4</sub>, filtered and concentrated in vacuo. The resultant residue was purified by column chromatography on silica gel using *n*-hexane/ ethyl acetate (5/1) as eluent to afford the pure compounds **7a–c**.

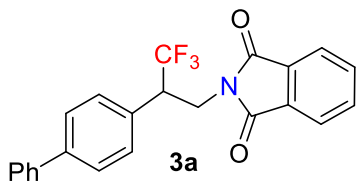
**7. Table S1 Screening various bases for hydroamination reaction (yields of hydroamination products **3a–v**, based on GC-MS)**

Reaction scheme: **1a–v** + **2a** (PhthNH)  $\xrightarrow[\text{DMF, 80 °C, 16 h}]{\text{Base (2.0 equiv.)}}$  **3a–v**

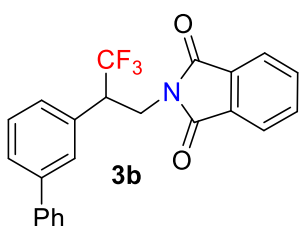
Substrate	Base			
	DBU	DABCO	CsF	TMG
<b>1a</b>	81%	0	2%	33%
<b>1b</b>	56%	0	17%	11%
<b>1c</b>	72%	0	1%	20%
<b>1d</b>	80%	0	2%	50%
<b>1e</b>	69%	1%	3%	60%
<b>1f</b>	78%	88%	2%	73%
<b>1g</b>	0	67%	1%	2%
<b>1h</b>	2%	1%	83%	43%
<b>1i</b>	72%	61%	4%	3%
<b>1j</b>	68%	1%	16%	39%
<b>1k</b>	63%	2%	12%	37%
<b>1l</b>	1%	9%	60%	10%
<b>1m</b>	61%	90%	7%	5%
<b>1n</b>	0	4%	61%	6%
<b>1o</b>	82%	72%	3%	0
<b>1p</b>	70%	65%	21%	3%
<b>1q</b>	41%	22%	53%	58%
<b>1r</b>	0	82%	3%	6%
<b>1s</b>	69%	0	24%	36%
<b>1t</b>	72%	4%	3%	41%
<b>1u</b>	64%	0	0	6%
<b>1v</b>	63%	0	4%	5%



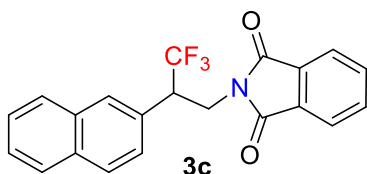
## 8. Analytical data of the intermediates and target compounds



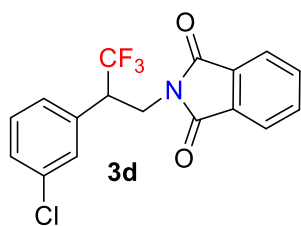
**2-(2-([1,1'-Biphenyl]-4-yl)-3,3,3-trifluoropropyl)isoindoline-1,3-dione (3a).** White solid, m.p. 126.7–128.5 °C, yield 76% (300.2 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80–7.75 (m, 2H), 7.69–7.64 (m, 2H), 7.55–7.51 (m, 4H), 7.43–7.39 (m, 4H), 7.35–7.30 (m, 1H), 4.35–4.16 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  166.7, 140.5, 139.1, 133.1, 130.6, 129.4, 128.6, 127.8, 126.5, 126.4, 126.0, 124.9 (d,  $^1J_{\text{CF}} = 279.0$  Hz), 122.4, 46.3 (q,  $^2J_{\text{CF}} = 26.2$  Hz), 36.1 (d,  $^3J_{\text{CF}} = 2.7$  Hz); HRMS (ESI): calcd for  $\text{C}_{23}\text{H}_{16}\text{F}_3\text{O}_2\text{N}+\text{Na}$   $[\text{M}+\text{Na}]^+$ : 418.1031, found: 418.1034.



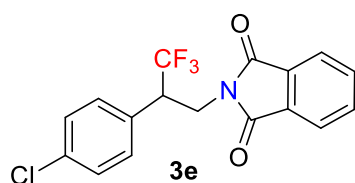
**2-(2-([1,1'-Biphenyl]-3-yl)-3,3,3-trifluoropropyl)isoindoline-1,3-dione (3b).** Yellow oil, yield 42% (165.9 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.83–7.80 (m, 2H), 7.71–7.69 (m, 2H), 7.60–7.54 (m, 4H), 7.49–7.36 (m, 5H), 4.42–4.36 (m, 1H), 4.32–4.19 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  166.7, 140.7, 139.4, 133.1, 131.0, 130.5, 128.1, 127.8, 127.0 (d,  $^3J_{\text{CF}} = 2.7$  Hz), 126.6, 126.5, 126.1, 124.8 (d,  $^1J_{\text{CF}} = 278.7$  Hz), 122.4, 46.7 (q,  $^2J_{\text{CF}} = 26.4$  Hz), 36.0 (d,  $^3J_{\text{CF}} = 2.5$  Hz); HRMS (ESI): calcd for  $\text{C}_{23}\text{H}_{16}\text{F}_3\text{O}_2\text{N}+\text{Na}$   $[\text{M}+\text{Na}]^+$ : 418.1031, found: 418.1036.



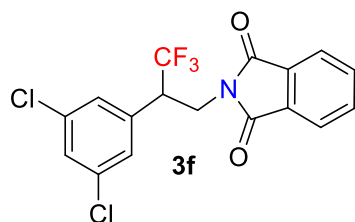
**2-(3,3,3-Trifluoro-2-(naphthalen-2-yl)propyl)isoindoline-1,3-dione (3c).** White solid, m.p. 138.9–140.3 °C, yield 53% (195.6 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.82–7.78 (m, 4H), 7.74–7.71 (m, 2H), 7.64–7.61 (m, 2H), 7.50–7.43 (m, 3H), 4.44–4.27 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  166.7, 133.1, 132.2, 132.0, 130.5, 128.2, 127.9, 127.6, 127.0, 126.6, 125.5, 125.4, 125.0, 124.9 (d,  $^1J_{\text{CF}} = 279.0$  Hz), 122.4, 46.8 (q,  $^2J_{\text{CF}} = 26.3$  Hz), 36.0 (d,  $^3J_{\text{CF}} = 2.8$  Hz); HRMS (ESI): calcd for  $\text{C}_{21}\text{H}_{14}\text{F}_3\text{O}_2\text{N}+\text{Na}$   $[\text{M}+\text{Na}]^+$ : 392.0874, found: 392.0877.



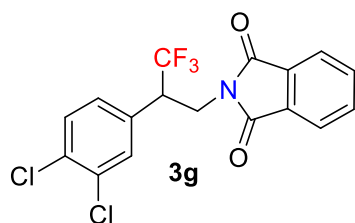
**2-(2-(3-Chlorophenyl)-3,3,3-trifluoropropyl)isoindoline-1,3-dione (3d).** White solid, m.p. 121.5–122.7 °C, yield 59% (208.3 mg);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.81–7.78 (m, 2H), 7.72–7.68 (m, 2H), 7.34 (s, 1H), 7.29–7.26 (m, 3H), 4.27–4.07 (m, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  166.6, 133.6, 133.2, 132.5, 130.5, 129.0, 128.5, 128.1, 126.2, 124.5 (q,  $^1J_{\text{CF}} = 278.9$  Hz), 122.5, 46.5 (q,  $^2J_{\text{CF}} = 26.6$  Hz), 35.9 (d,  $^3J_{\text{CF}} = 2.7$  Hz); HRMS (ESI): calcd for  $\text{C}_{17}\text{H}_{11}\text{F}_3\text{O}_2\text{NCl} + \text{Na}$   $[\text{M} + \text{Na}]^+$ : 376.0328, found: 376.0331.



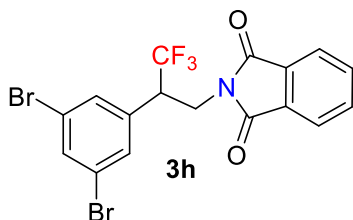
**2-(2-(4-Chlorophenyl)-3,3,3-trifluoropropyl)isoindoline-1,3-dione (3e).** White solid, m.p. 70.9–80.4 °C, yield 46% (162.4 mg);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80–7.78 (m, 2H), 7.71–7.68 (m, 2H), 7.29–7.25 (m, 4H), 4.30–4.13 (m, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  166.6, 133.9, 133.2, 130.5, 129.6, 128.9, 128.0, 124.6 (d,  $^1J_{\text{CF}} = 278.6$  Hz), 122.5, 46.2 (q,  $^2J_{\text{CF}} = 25.0$  Hz), 35.9 (d,  $^3J_{\text{CF}} = 2.8$  Hz); HRMS (ESI): calcd for  $\text{C}_{17}\text{H}_{11}\text{F}_3\text{O}_2\text{NCl} + \text{Na}$   $[\text{M} + \text{Na}]^+$ : 376.0328, found: 376.0326.



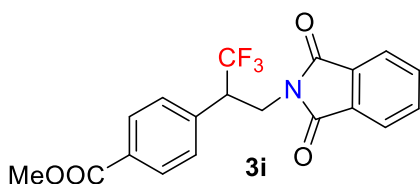
**2-(2-(3,5-Dichlorophenyl)-3,3,3-trifluoropropyl)isoindoline-1,3-dione (3f).** White solid, m.p. 109.8–111.6 °C, yield 72% (278.6 mg);  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.84–7.81 (m, 2H), 7.73–7.71 (m, 2H), 7.32–7.26 (m, 3H), 4.21–4.04 (m, 3H);  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.7, 135.5, 134.9, 134.5, 131.6, 129.4, 128.0, 125.4 (d,  $^1J_{\text{CF}} = 279.1$  Hz), 123.8, 47.5 (q,  $^2J_{\text{CF}} = 26.9$  Hz), 36.9 (d,  $^3J_{\text{CF}} = 2.6$  Hz); HRMS (ESI): calcd for  $\text{C}_{17}\text{H}_{10}\text{F}_3\text{O}_2\text{NCl}_2 + \text{Na}$   $[\text{M} + \text{Na}]^+$ : 409.9938, found: 409.9934.



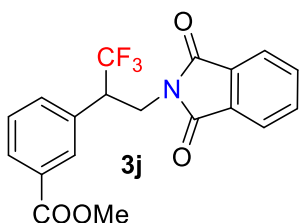
**2-(2-(3,4-Dichlorophenyl)-3,3,3-trifluoropropyl)isoindoline-1,3-dione (3g).** White solid, m.p. 112.4–113.2 °C, yield 64% (247.7 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.82–7.78 (m, 2H), 7.73–7.68 (m, 2H), 7.48–7.37 (m, 2H), 7.25–7.22 (m, 1H), 4.29–4.06 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.7, 134.4, 134.3, 133.5, 133.1, 131.5, 130.9, 128.5, 125.4 (d,  $^1J_{\text{CF}} = 278.9$  Hz), 123.7, 123.6, 47.2 (q,  $^2J_{\text{CF}} = 26.8$  Hz), 36.8 (d,  $^3J_{\text{CF}} = 3.3$  Hz); HRMS (ESI): calcd for  $\text{C}_{17}\text{H}_{10}\text{F}_3\text{O}_2\text{NCl}_2 + \text{Na}$   $[\text{M} + \text{Na}]^+$ : 409.9938, found: 409.9936.



**2-(2-(3,5-Dibromophenyl)-3,3,3-trifluoropropyl)isoindoline-1,3-dione (3h).** White solid, m.p. 104.1–105.2 °C, yield 70% (333.2 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.84–7.81 (m, 2H), 7.75–7.70 (m, 2H), 7.62 (t,  $J = 1.6$  Hz, 1H), 7.46 (s, 2H), 4.21–4.00 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.7, 135.4, 134.9, 134.5, 131.6, 131.2, 125.3 (d,  $^1J_{\text{CF}} = 279.0$  Hz), 123.8, 123.3, 47.3 (q,  $^2J_{\text{CF}} = 26.8$  Hz), 36.9 (d,  $^3J_{\text{CF}} = 3.1$  Hz); HRMS (ESI): calcd for  $\text{C}_{17}\text{H}_{10}\text{F}_3\text{O}_2\text{NBBr}_2 + \text{Na}$   $[\text{M} + \text{Na}]^+$ : 497.8928, found: 497.8935.

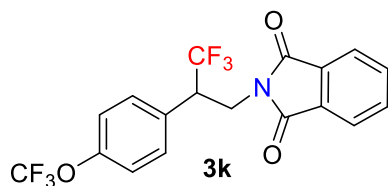


**Methyl 4-(3-(1,3-dioxisoindolin-2-yl)-1,1,1-trifluoropropan-2-yl)benzoate (3i).** White solid, m.p. 144.9–146.8 °C, yield 55% (207.4 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.98 (d,  $J = 8.0$  Hz, 2H), 7.78–7.75 (m, 2H), 7.71–7.67 (m, 2H), 7.44 (d,  $J = 8.0$  Hz, 2H), 4.34–4.18 (m, 3H), 3.88 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.7, 166.6, 136.6, 134.4, 131.6, 130.8, 130.1, 129.5, 125.7 (d,  $^1J_{\text{CF}} = 278.9$  Hz), 123.6, 52.3, 47.9 (q,  $^2J_{\text{CF}} = 26.6$  Hz), 37.1 (d,  $^3J_{\text{CF}} = 2.6$  Hz); HRMS (ESI): calcd for  $\text{C}_{19}\text{H}_{14}\text{F}_3\text{O}_4\text{N} + \text{Na}$   $[\text{M} + \text{Na}]^+$ : 400.0773, found: 400.0776.

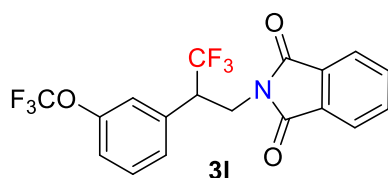


**Methyl 3-(3-(1,3-dioxisoindolin-2-yl)-1,1,1-trifluoropropan-2-yl)benzoate (3j).** White solid, m.p. 134.3–135.1 °C, yield 43% (162.1 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.02–7.98 (m, 2H), 7.80–7.76 (m, 2H), 7.71–7.68 (m, 2H), 7.60 (d,  $J = 7.6$  Hz, 1H), 7.43 (t,  $J = 7.6$  Hz, 1H), 4.28–4.13 (m, 3H), 3.90 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  168.1, 166.4, 134.3, 133.5, 132.1, 131.6, 130.8, 130.7, 130.2, 129.0, 125.7 (d,  $^1J_{\text{CF}} = 278.9$

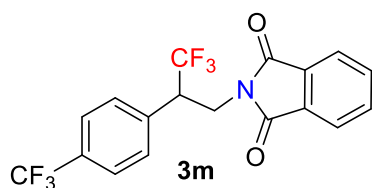
Hz), 123.6, 52.3, 47.7 (q,  $^2J_{\text{CF}} = 26.6$  Hz), 37.0 (d,  $^3J_{\text{CF}} = 3.0$  Hz); HRMS (ESI): calcd for  $\text{C}_{19}\text{H}_{14}\text{F}_3\text{O}_4\text{N}+\text{Na}$   $[\text{M}+\text{Na}]^+$ : 400.0773, found: 400.0777.



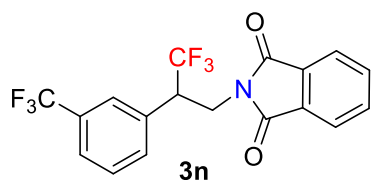
**2-(3,3,3-Trifluoro-2-(4-(trifluoromethoxy)phenyl)propyl)isoindoline-1,3-dione (3k).** White solid, m.p. 79.9–81.8 °C, yield 57% (229.7 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.81–7.77 (m, 2H), 7.72–7.67 (m, 2H), 7.40 (d,  $J = 8.8$  Hz, 2H), 7.16 (d,  $J = 8.0$  Hz, 2H), 4.31–4.11 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.7, 149.6, 134.4, 131.6, 130.9, 130.2, 125.7 (d,  $^1J_{\text{CF}} = 278.9$  Hz), 123.6, 121.2, 120.4 (d,  $^1J_{\text{CF}} = 256.2$  Hz), 47.3 (q,  $^2J_{\text{CF}} = 26.6$  Hz), 37.0 (d,  $^3J_{\text{CF}} = 3.2$  Hz); HRMS (ESI): calcd for  $\text{C}_{18}\text{H}_{11}\text{F}_6\text{O}_3\text{N}+\text{H}$   $[\text{M}+\text{H}]^+$ : 404.0721, found: 404.0720.



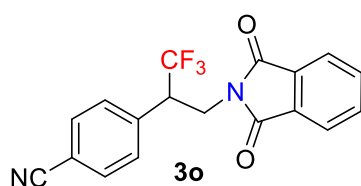
**2-(3,3,3-Trifluoro-2-(3-(trifluoromethoxy)phenyl)propyl)isoindoline-1,3-dione (3l).** White solid, m.p. 80.0–81.9 °C, yield 44% (177.3 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.79–7.77 (m, 2H), 7.71–7.66 (m, 2H), 7.37–7.30 (m, 2H), 7.22–7.15 (m, 2H), 4.30–4.10 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.6, 149.3, 134.3, 133.8, 131.5, 130.3, 127.6, 125.5 (d,  $^1J_{\text{CF}} = 278.7$  Hz), 123.5, 122.1, 121.4, 120.3 (d,  $^1J_{\text{CF}} = 256.1$  Hz), 47.5 (q,  $^2J_{\text{CF}} = 26.8$  Hz), 37.0 (d,  $^3J_{\text{CF}} = 3.3$  Hz); HRMS (ESI): calcd for  $\text{C}_{18}\text{H}_{11}\text{F}_6\text{O}_3\text{N}+\text{Na}$   $[\text{M}+\text{Na}]^+$ : 426.0541, found: 426.0542.



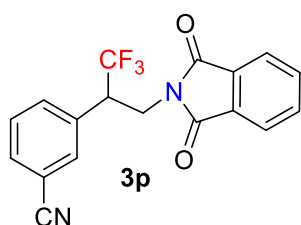
**2-(3,3,3-Trifluoro-2-(4-(trifluoromethyl)phenyl)propyl)isoindoline-1,3-dione (3m).** White solid, m.p. 81.0–81.7 °C, yield 85% (329.0 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80–7.77 (m, 2H), 7.72–7.69 (m, 2H), 7.59 (d,  $J = 8.0$  Hz, 2H), 7.50 (d,  $J = 8.0$  Hz, 2H), 4.35–4.20 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.6, 135.6, 134.3, 131.5, 131.2 (q,  $^2J_{\text{CF}} = 32.5$  Hz), 129.8, 125.8 (q,  $^3J_{\text{CF}} = 3.8$  Hz), 125.5 (d,  $^1J_{\text{CF}} = 278.9$  Hz), 123.8 (q,  $^1J_{\text{CF}} = 270.5$  Hz), 123.6, 47.7 (q,  $^2J_{\text{CF}} = 26.6$  Hz), 36.9 (d,  $^3J_{\text{CF}} = 2.6$  Hz); HRMS (ESI): calcd for  $\text{C}_{18}\text{H}_{11}\text{F}_6\text{O}_2\text{N}+\text{Na}$   $[\text{M}+\text{Na}]^+$ : 410.0592, found: 410.0594.



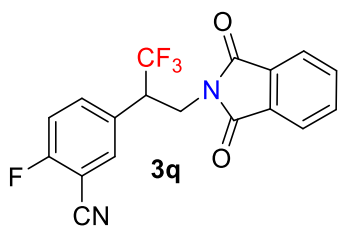
**2-(3,3,3-Trifluoro-2-(3-(trifluoromethyl)phenyl)propyl)isoindoline-1,3-dione (3n).** White solid, m.p. 96.1–96.5 °C, yield 42% (162.5 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80–7.75 (m, 2H), 7.72–7.66 (m, 2H), 7.60–7.57 (m, 3H), 7.47 (t,  $J = 7.4$  Hz, 1H), 4.32–4.17 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.7, 134.4, 132.7, 132.5, 131.5, 131.3 (q,  $^2J_{\text{CF}} = 32.4$  Hz), 129.4, 126.3 (d,  $^3J_{\text{CF}} = 3.3$  Hz), 125.9 (q,  $^3J_{\text{CF}} = 3.8$  Hz), 125.6 (d,  $^1J_{\text{CF}} = 278.8$  Hz), 123.7 (d,  $^1J_{\text{CF}} = 270.8$  Hz), 123.6, 47.7 (q,  $^2J_{\text{CF}} = 26.7$  Hz), 36.9 (d,  $^3J_{\text{CF}} = 2.6$  Hz); HRMS (ESI): calcd for  $\text{C}_{18}\text{H}_{11}\text{F}_6\text{O}_2\text{N} + \text{Na}$   $[\text{M} + \text{Na}]^+$ : 410.0592, found: 410.0591.



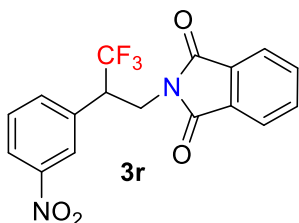
**4-(3-(1,3-Dioxisoindolin-2-yl)-1,1,1-trifluoropropan-2-yl)benzotrile (3o).** White solid, m.p. 121.3–122.1 °C, yield 76% (261.4 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.81–7.77 (m, 2H), 7.73–7.69 (m, 2H), 7.62 (d,  $J = 8.4$  Hz, 2H), 7.49 (d,  $J = 8.4$  Hz, 2H), 4.33–4.17 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.6, 136.8, 134.5, 132.6, 131.4, 130.2, 125.3 (d,  $^1J_{\text{CF}} = 279.0$  Hz), 123.6, 118.1, 113.1, 48.0 (q,  $^2J_{\text{CF}} = 26.8$  Hz), 36.7 (d,  $^3J_{\text{CF}} = 2.8$  Hz); HRMS (ESI): calcd for  $\text{C}_{18}\text{H}_{11}\text{F}_3\text{O}_2\text{N}_2 + \text{Na}$   $[\text{M} + \text{Na}]^+$ : 367.0670, found: 367.0670.



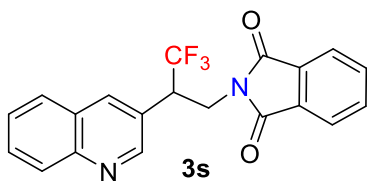
**3-(3-(1,3-Dioxisoindolin-2-yl)-1,1,1-trifluoropropan-2-yl)benzotrile (3p).** White solid, m.p. 148.9–150.7 °C, yield 55% (189.2 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.81–7.78 (m, 2H), 7.74–7.71 (m, 2H), 7.67–7.61 (m, 3H), 7.48 (t,  $J = 7.6$  Hz, 1H), 4.33–4.13 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.6, 134.5, 133.6, 133.3, 133.1, 132.7, 131.5, 129.8, 125.4 (d,  $^1J_{\text{CF}} = 278.8$  Hz), 123.7, 118.1, 113.2, 47.7 (q,  $^2J_{\text{CF}} = 26.8$  Hz), 36.8 (d,  $^3J_{\text{CF}} = 3.4$  Hz); HRMS (ESI): calcd for  $\text{C}_{18}\text{H}_{11}\text{F}_3\text{O}_2\text{N}_2 + \text{Na}$   $[\text{M} + \text{Na}]^+$ : 367.0670, found: 367.0673.



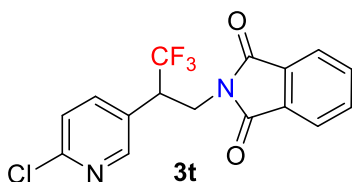
**5-(3-(1,3-Dioxoisindolin-2-yl)-1,1,1-trifluoropropan-2-yl)-2-fluorobenzonitrile (3q).** White solid, m.p. 143.4–143.6 °C, yield 40% (144.8 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.84–7.81 (m, 2H), 7.77–7.74 (m, 2H), 7.70–7.63 (m, 2H), 7.23 (t,  $J = 8.6$  Hz, 1H), 4.35–4.14 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.7, 163.3 (d,  $^1J_{\text{CF}} = 260.1$  Hz), 135.9 (d,  $^3J_{\text{CF}} = 8.7$  Hz), 134.7, 134.6, 131.4, 128.9, 128.0 (d,  $^1J_{\text{CF}} = 278.9$  Hz), 123.8, 117.3 (d,  $^2J_{\text{CF}} = 19.8$  Hz), 113.3, 102.3 (q,  $^2J_{\text{CF}} = 15.7$  Hz), 47.2 (q,  $^2J_{\text{CF}} = 27.0$  Hz), 36.7 (d,  $^3J_{\text{CF}} = 3.2$  Hz); HRMS (ESI): calcd for  $\text{C}_{18}\text{H}_{10}\text{F}_4\text{O}_2\text{N}_2 + \text{Na}$   $[\text{M} + \text{Na}]^+$ : 385.0576, found: 385.0579.



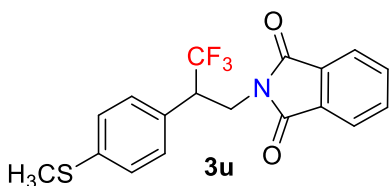
**2-(3,3,3-Trifluoro-2-(3-nitrophenyl)propyl)isoindoline-1,3-dione (3r).** White solid, m.p. 122.8–123.6 °C, yield 67% (243.9 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.26–8.17 (m, 2H), 7.79–7.68 (m, 5H), 7.54 (t,  $J = 8.0$  Hz, 1H), 4.36–4.21 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.6, 148.3, 135.2, 134.5, 133.6, 131.4, 130.0, 125.3 (d,  $^1J_{\text{CF}} = 279.0$  Hz), 124.6, 124.1, 123.7, 47.7 (q,  $^2J_{\text{CF}} = 26.9$  Hz), 36.8 (d,  $^3J_{\text{CF}} = 3.2$  Hz); HRMS (ESI): calcd for  $\text{C}_{17}\text{H}_{11}\text{F}_3\text{O}_4\text{N}_2 + \text{Na}$   $[\text{M} + \text{Na}]^+$ : 387.0569, found: 387.0574.



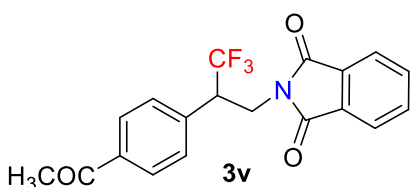
**2-(3,3,3-Trifluoro-2-(quinolin-3-yl)propyl)isoindoline-1,3-dione (3s).** White solid, m.p. 135.1–135.3 °C, yield 51% (188.7 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.82 (d,  $J = 1.6$  Hz, 1H), 8.29 (s, 1H), 8.08 (d,  $J = 8.4$  Hz, 1H), 7.86 (d,  $J = 8.0$  Hz, 1H), 7.76–7.71 (m, 3H), 7.68–7.65 (m, 2H), 7.58 (t,  $J = 7.6$  Hz, 1H), 4.47–4.30 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.8, 151.1, 148.2, 136.6, 134.4, 131.5, 130.4, 129.3, 128.2, 127.5, 127.4, 125.7 (d,  $^1J_{\text{CF}} = 279.0$  Hz), 124.7, 123.7, 45.9 (q,  $^2J_{\text{CF}} = 26.9$  Hz), 36.8 (d,  $^3J_{\text{CF}} = 2.6$  Hz); HRMS (ESI): calcd for  $\text{C}_{20}\text{H}_{13}\text{F}_3\text{O}_2\text{N}_2 + \text{H}$   $[\text{M} + \text{H}]^+$ : 371.1007, found: 371.0999.



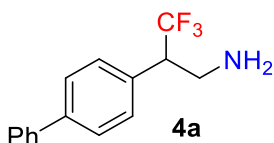
**2-(2-(6-Chloropyridin-3-yl)-3,3,3-trifluoropropyl)isoindoline-1,3-dione (3t).** White solid, m.p. 126.8–127.7 °C, yield 59% (208.9 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.25 (d,  $J = 2.0$  Hz, 1H), 7.79–7.77 (m, 3H), 7.72–7.69 (m, 2H), 7.33 (d,  $J = 8.4$  Hz, 1H), 4.33–4.10 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.6, 152.4, 150.8, 138.8, 134.5, 131.4, 126.4, 125.2 (d,  $^1J_{\text{CF}} = 279.0$  Hz), 124.6, 123.7, 45.2 (q,  $^2J_{\text{CF}} = 27.2$  Hz), 36.5 (d,  $^3J_{\text{CF}} = 2.8$  Hz); HRMS (ESI): calcd for  $\text{C}_{16}\text{H}_{10}\text{F}_3\text{O}_2\text{N}_2\text{Cl}+\text{H}$   $[\text{M}+\text{H}]^+$ : 355.0461, found: 355.0466.



**2-(3,3,3-Trifluoro-2-(4-(methylthio)phenyl)propyl)isoindoline-1,3-dione (3u).** White solid, m.p. 115.8–116.4 °C, yield 46% (167.9 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.82–7.79 (m, 2H), 7.72–7.69 (m, 2H), 7.28 (d,  $J = 7.2$  Hz, 2H), 7.19 (d,  $J = 7.6$  Hz, 2H), 4.33–4.10 (m, 3H), 2.45 (d,  $J = 1.6$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.7, 139.7, 134.2, 131.6, 129.7, 127.9, 126.3, 125.9 (d,  $^1J_{\text{CF}} = 278.8$  Hz), 123.5, 47.3 (q,  $^2J_{\text{CF}} = 26.4$  Hz), 37.0 (d,  $^3J_{\text{CF}} = 3.3$  Hz), 15.3; HRMS (ESI): calcd for  $\text{C}_{18}\text{H}_{14}\text{F}_3\text{O}_2\text{NS}+\text{Na}$   $[\text{M}+\text{Na}]^+$ : 388.0595, found: 388.0596.

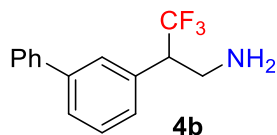


**2-(2-(4-acetylphenyl)-3,3,3-trifluoropropyl)isoindoline-1,3-dione (3v).** White solid, m.p. 88.3–88.6 °C, yield 51% (184.1 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.89 (d,  $J = 8.4$  Hz, 2H), 7.78–7.75 (m, 2H), 7.70–7.67 (m, 2H), 7.45 (d,  $J = 8.4$  Hz, 2H), 4.35–4.17 (m, 3H), 2.55 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  197.5, 167.6, 137.5, 136.6, 134.3, 131.5, 129.6, 128.7, 125.6 (d,  $^1J_{\text{CF}} = 278.8$  Hz), 123.6, 47.7 (q,  $^2J_{\text{CF}} = 26.6$  Hz), 36.9 (d,  $^3J_{\text{CF}} = 2.7$  Hz), 26.6; HRMS (ESI): calcd for  $\text{C}_{19}\text{H}_{14}\text{F}_3\text{O}_3\text{N}+\text{Na}$   $[\text{M}+\text{Na}]^+$ : 384.0823, found: 384.0827.

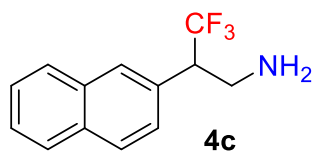


**2-([1,1'-Biphenyl]-4-yl)-3,3,3-trifluoropropan-1-amine (4a).** Yellow oil, yield 76% (201.4 mg);  $^1\text{H}$  NMR (400

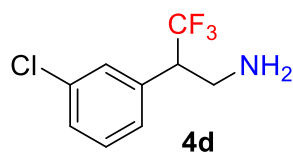
MHz, DMSO-*d*<sub>6</sub>) δ 7.72–7.69 (m, 4H), 7.52–7.47 (m, 4H), 7.40 (t, *J* = 7.2 Hz, 1H), 3.75–3.64 (m, 1H), 3.25–3.21 (m, 1H), 3.12–3.07 (m, 1H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) δ 140.4, 140.1, 133.5, 130.4, 129.5, 128.1, 127.4, 127.3 (d, <sup>1</sup>*J*<sub>CF</sub> = 278.9 Hz), 127.2, 52.2 (q, <sup>2</sup>*J*<sub>CF</sub> = 23.7 Hz), 41.4 (d, <sup>3</sup>*J*<sub>CF</sub> = 2.1 Hz); <sup>19</sup>F NMR (376 MHz, DMSO-*d*<sub>6</sub>) δ –62.0 (s, 3F); HRMS (ESI): calcd for C<sub>15</sub>H<sub>14</sub>F<sub>3</sub>N+H [M+H]<sup>+</sup>: 266.1157, found: 266.1154.



**2-([1,1'-Biphenyl]-3-yl)-3,3,3-trifluoropropan-1-amine (4b).** Yellow oil, yield 85% (225.3 mg); <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 7.70–7.47 (m, 7H), 7.39 (t, *J* = 6.6 Hz, 2H), 3.79–3.68 (m, 1H), 3.28–3.23 (m, 1H), 3.18–3.12 (m, 1H), 2.38 (s, 2H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) δ 141.1, 140.3, 135.0 (d, <sup>3</sup>*J*<sub>CF</sub> = 1.3 Hz), 129.8, 129.5, 128.7, 128.4, 128.1, 127.3, 127.0, 127.4 (q, <sup>1</sup>*J*<sub>CF</sub> = 279.1 Hz), 52.5 (q, <sup>2</sup>*J*<sub>CF</sub> = 23.8 Hz), 41.3 (d, <sup>3</sup>*J*<sub>CF</sub> = 1.9 Hz); <sup>19</sup>F NMR (376 MHz, DMSO-*d*<sub>6</sub>) δ –62.0 (s, 3F); HRMS (ESI): calcd for C<sub>15</sub>H<sub>14</sub>F<sub>3</sub>N+H [M+H]<sup>+</sup>: 266.1157, found: 266.1157.

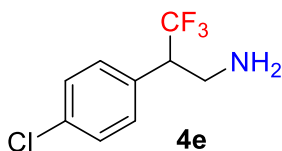


**3,3,3-Trifluoro-2-(naphthalen-2-yl)propan-1-amine (4c).** Yellow oil, yield 96% (229.4 mg); <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 7.97–7.93 (m, 4H), 7.57–7.51 (m, 3H), 3.85–3.74 (m, 1H), 3.28 (dd, *J*<sub>1</sub> = 4.8 Hz, *J*<sub>2</sub> = 12.8 Hz, 1H), 3.18 (dd, *J*<sub>1</sub> = 9.2 Hz, *J*<sub>2</sub> = 12 Hz, 1H), 1.55 (s, 2H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) δ 133.4, 133.1, 131.9 (d, <sup>3</sup>*J*<sub>CF</sub> = 1.5 Hz), 131.6, 129.3, 128.7, 128.3, 128.0, 127.4 (q, <sup>1</sup>*J*<sub>CF</sub> = 279.1 Hz), 127.2, 126.9 (d, <sup>3</sup>*J*<sub>CF</sub> = 4.4 Hz), 52.8 (q, <sup>2</sup>*J*<sub>CF</sub> = 23.8 Hz), 41.4 (d, <sup>3</sup>*J*<sub>CF</sub> = 2.0 Hz); <sup>19</sup>F NMR (376 MHz, DMSO-*d*<sub>6</sub>) δ –66.7 (s, 3F); HRMS (ESI): calcd for C<sub>13</sub>H<sub>12</sub>F<sub>3</sub>N+H [M+H]<sup>+</sup>: 240.1000, found: 240.1000.

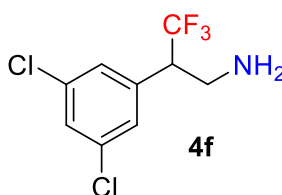


**2-(3-Chlorophenyl)-3,3,3-trifluoropropan-1-amine (4d).** Yellow oil, yield 76% (169.5 mg); <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 7.46–7.33 (m, 4H), 3.75–3.64 (m, 1H), 3.20–3.16 (m, 1H), 3.08–3.02 (m, 1H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) δ 136.8 (d, <sup>3</sup>*J*<sub>CF</sub> = 1.6 Hz), 133.7, 131.0, 129.8, 128.7, 128.5, 124.2 (d, <sup>1</sup>*J*<sub>CF</sub> = 279.0 Hz), 52.0 (q, <sup>2</sup>*J*<sub>CF</sub> = 23.9 Hz), 41.4 (d, <sup>3</sup>*J*<sub>CF</sub> = 2.3 Hz); <sup>19</sup>F NMR (376 MHz, DMSO-*d*<sub>6</sub>) δ –66.9 (s, 3F); HRMS (ESI): calcd for C<sub>9</sub>H<sub>9</sub>F<sub>3</sub>NCl+H [M+H]<sup>+</sup>: 224.0454, found: 224.0459.

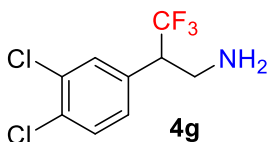




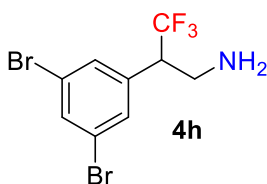
**2-(4-Chlorophenyl)-3,3,3-trifluoropropan-1-amine (4e).** Yellow oil, yield 74% (165.0 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  7.49–7.46 (m, 2H), 7.42–7.40 (m, 2H), 3.70–3.64 (m, 1H), 3.21–3.16 (m, 1H), 3.06–3.00 (m, 1H), 1.71 (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ )  $\delta$  133.4, 131.6, 129.1, 127.1 (q,  $^1J_{\text{CF}} = 278.9$  Hz), 51.9 (q,  $^2J_{\text{CF}} = 23.9$  Hz), 41.2 (d,  $^3J_{\text{CF}} = 2.3$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  –67.1 (s, 3F); HRMS (ESI): calcd for  $\text{C}_9\text{H}_9\text{F}_3\text{NCl} + \text{H}$   $[\text{M} + \text{H}]^+$ : 224.0454, found: 224.0455.



**2-(3,5-Dichlorophenyl)-3,3,3-trifluoropropan-1-amine (4f).** Yellow oil, yield 87% (223.6 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  7.62 (t,  $J = 1.8$  Hz, 1H), 7.47 (d,  $J = 1.2$  Hz, 2H), 3.82–3.71 (m, 1H), 3.20–3.15 (m, 1H), 3.11–3.05 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ )  $\delta$  138.6, 134.7, 128.8, 128.4, 126.7 (d,  $^1J_{\text{CF}} = 279.0$  Hz), 51.6 (q,  $^2J_{\text{CF}} = 24.2$  Hz), 40.9 (d,  $^3J_{\text{CF}} = 1.9$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  –66.9 (s, 3F); HRMS (ESI): calcd for  $\text{C}_9\text{H}_8\text{F}_3\text{NCl}_2 + \text{H}$   $[\text{M} + \text{H}]^+$ : 258.0064, found: 258.0070.

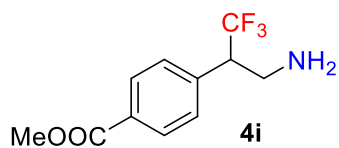


**2-(3,4-Dichlorophenyl)-3,3,3-trifluoropropan-1-amine (4g).** Yellow oil, yield 75% (192.8 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  7.69–7.67 (m, 2H), 7.41 (dd,  $J_1 = 2.0$  Hz,  $J_2 = 8.4$  Hz, 1H), 3.83–3.72 (m, 1H), 3.22–3.18 (m, 1H), 3.11–3.06 (m, 1H), 2.45 (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ )  $\delta$  135.3 (d,  $^3J_{\text{CF}} = 1.6$  Hz), 132.0, 131.7, 131.5, 131.2, 130.1, 126.8 (q,  $^1J_{\text{CF}} = 278.9$  Hz), 51.2 (q,  $^2J_{\text{CF}} = 24.3$  Hz), 40.8 (d,  $^3J_{\text{CF}} = 2.2$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  –67.0 (s, 3F); HRMS (ESI): calcd for  $\text{C}_9\text{H}_8\text{F}_3\text{NCl}_2 + \text{H}$   $[\text{M} + \text{H}]^+$ : 258.0064, found: 258.0062.

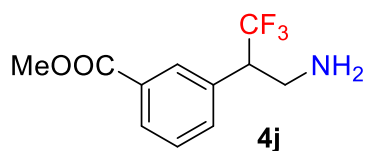


**2-(3,5-Dibromophenyl)-3,3,3-trifluoropropan-1-amine (4h).** Yellow oil, yield 60% (207.0 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  7.86 (t,  $J = 1.8$  Hz, 1H), 7.64 (s, 2H), 3.80–3.69 (m, 1H), 3.19–3.14 (m, 1H), 3.09–3.04 (m, 1H), 1.54 (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ )  $\delta$  139.1, 133.7, 131.9, 126.8 (q,  $^1J_{\text{CF}} = 279.0$  Hz), 122.6, 51.6

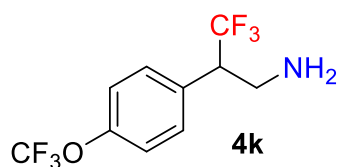
(q,  $^2J_{CF} = 24.2$  Hz), 40.9 (d,  $^3J_{CF} = 1.9$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  -66.8 (s, 3F); HRMS (ESI): calcd for  $\text{C}_9\text{H}_8\text{F}_3\text{NBr}_2+\text{H}$   $[\text{M}+\text{H}]^+$ : 345.9054, found: 345.9061.



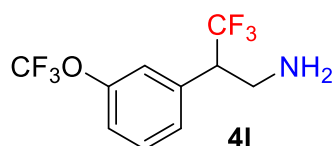
**Methyl 4-(3-amino-1,1,1-trifluoropropan-2-yl)benzoate (4i).** Yellow oil, yield 68% (168.0mg);  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  7.99 (d,  $J = 8.0$  Hz, 2H), 7.53 (d,  $J = 8.0$  Hz, 2H), 3.87 (s, 3H), 3.79–3.73 (m, 1H), 3.23–3.18 (m, 1H), 3.09–3.03 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ )  $\delta$  166.5, 139.8 (d,  $^3J_{CF} = 1.6$  Hz), 130.3, 129.9, 127.0 (d,  $^1J_{CF} = 279.1$  Hz), 52.7, 52.3 (q,  $^2J_{CF} = 25.2$  Hz), 41.3 (d,  $^3J_{CF} = 2.1$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  -66.6 (s, 3F); HRMS (ESI): calcd for  $\text{C}_{11}\text{H}_{12}\text{F}_3\text{NO}_2+\text{H}$   $[\text{M}+\text{H}]^+$ : 248.0898, found: 248.0897.



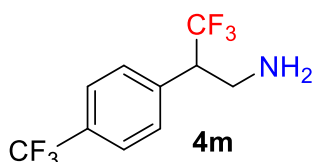
**Methyl 3-(3-amino-1,1,1-trifluoropropan-2-yl)benzoate (4j).** Yellow oil, yield 68% (168.0 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  7.99–7.97 (m, 2H), 7.69 (d,  $J = 8.0$  Hz, 1H), 7.58 (d,  $J = 7.8$  Hz, 1H), 3.89 (s, 3H), 3.83–3.77 (m, 1H), 3.26–3.22 (m, 1H), 3.11–3.06 (m, 1H), 2.11 (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ )  $\delta$  166.46, 135.1 (d,  $^3J_{CF} = 1.5$  Hz), 134.5, 130.5, 130.5, 129.6, 129.3, 127.1 (d,  $^1J_{CF} = 278.8$  Hz), 52.6, 52.2 (q,  $^2J_{CF} = 23.9$  Hz), 41.3 (d,  $^3J_{CF} = 2.9$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  -67.0 (s, 3F); HRMS (ESI): calcd for  $\text{C}_{11}\text{H}_{12}\text{F}_3\text{NO}_2+\text{H}$   $[\text{M}+\text{H}]^+$ : 248.0898, found: 248.0905.



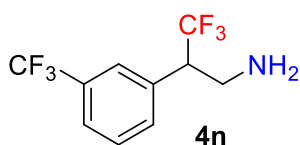
**3,3,3-Trifluoro-2-(4-(trifluoromethoxy)phenyl)propan-1-amine (4k).** Yellow oil, yield 51% (139.2 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  7.52 (d,  $J = 8.4$  Hz, 2H), 7.40 (d,  $J = 8.0$  Hz, 2H), 3.79–3.68 (m, 1H), 3.22–3.18 (m, 1H), 3.08–3.03 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ )  $\delta$  148.6, 133.7 (d,  $^3J_{CF} = 2.0$  Hz), 131.8, 127.1 (d,  $^1J_{CF} = 279.2$  Hz), 121.6, 120.6 (d,  $^1J_{CF} = 254.7$  Hz), 51.5 (q,  $^2J_{CF} = 24.3$  Hz), 41.1 (d,  $^3J_{CF} = 2.0$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  -52.1 (s, 3F), -62.3 (s, 3F); HRMS (ESI): calcd for  $\text{C}_{10}\text{H}_9\text{F}_6\text{NO}+\text{H}$   $[\text{M}+\text{H}]^+$ : 274.0667, found: 274.0665.



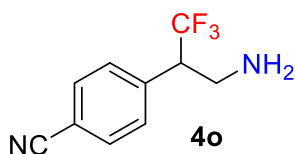
**3,3,3-Trifluoro-2-(3-(trifluoromethoxy)phenyl)propan-1-amine (4l).** Yellow oil, yield 90% (245.7 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  7.56 (t,  $J = 8.0$  Hz, 1H), 7.45–7.36 (m, 3H), 3.83–3.72 (m, 1H), 3.23–3.19 (m, 1H), 3.10–3.05 (m, 1H), 1.79 (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ )  $\delta$  148.4, 137.1, 131.0, 128.8, 127.0 (q,  $^1J_{\text{CF}} = 278.8$  Hz), 122.5, 121.0, 120.5 (d,  $^1J_{\text{CF}} = 254.8$  Hz), 52.0 (q,  $^2J_{\text{CF}} = 24.0$  Hz), 41.1 (d,  $^3J_{\text{CF}} = 3.1$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  -57.0 (d,  $J = 5.3$  Hz, 3F), -67.1 (s, 3F); HRMS (ESI): calcd for  $\text{C}_{10}\text{H}_9\text{F}_6\text{NO}+\text{H}$   $[\text{M}+\text{H}]^+$ : 274.0667, found: 274.0673.



**3,3,3-Trifluoro-2-(4-(trifluoromethyl)phenyl)propan-1-amine (4m).** Yellow oil, yield 69% (177.3 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  7.78 (d,  $J = 8.0$  Hz, 2H), 7.63 (d,  $J = 8.0$  Hz, 2H), 3.87–3.76 (m, 1H), 3.26–3.22 (m, 1H), 3.13–3.07 (m, 1H), 2.46 (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ )  $\delta$  139.2, 130.7, 129.2 (q,  $^2J_{\text{CF}} = 31.7$  Hz), 127.0 (d,  $^1J_{\text{CF}} = 278.9$  Hz), 125.9 (q,  $^3J_{\text{CF}} = 3.8$  Hz), 124.6 (d,  $^1J_{\text{CF}} = 270.4$  Hz), 52.2 (q,  $^2J_{\text{CF}} = 24.0$  Hz), 41.2 (d,  $^3J_{\text{CF}} = 2.0$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  -61.3 (s, 3F), -66.9 (s, 3F); HRMS (ESI): calcd for  $\text{C}_{10}\text{H}_9\text{F}_6\text{N}+\text{H}$   $[\text{M}+\text{H}]^+$ : 258.0717, found: 258.0718.

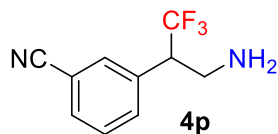


**3,3,3-Trifluoro-2-(3-(trifluoromethyl)phenyl)propan-1-amine (4n).** Yellow oil, yield 76% (195.3 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  7.76–7.64 (m, 4H), 3.95–3.84 (m, 1H), 3.27–3.23 (m, 1H), 3.18–3.13 (m, 1H), 2.97 (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ )  $\delta$  135.5 (d,  $^3J_{\text{CF}} = 1.8$  Hz), 133.8, 130.3, 129.8 (q,  $^2J_{\text{CF}} = 31.4$  Hz), 129.7 (d,  $^1J_{\text{CF}} = 279.0$  Hz), 126.7 (d,  $^3J_{\text{CF}} = 3.6$  Hz), 125.6 (q,  $^3J_{\text{CF}} = 3.5$  Hz), 124.6 (d,  $^1J_{\text{CF}} = 270.5$  Hz), 51.4 (q,  $^2J_{\text{CF}} = 24.2$  Hz), 40.6 (d,  $^3J_{\text{CF}} = 5.8$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  -61.1 (s, 3F), -67.0 (s, 3F); HRMS (ESI): calcd for  $\text{C}_{10}\text{H}_9\text{F}_6\text{N}+\text{H}$   $[\text{M}+\text{H}]^+$ : 258.0717, found: 258.0726.

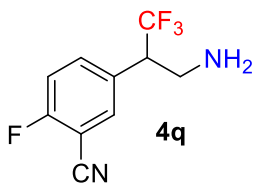


**4-(3-Amino-1,1,1-trifluoropropan-2-yl)benzonitrile (4o).** Yellow oil, yield 73% (156.2 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  7.88 (d,  $J = 8.4$  Hz, 2H), 7.59 (d,  $J = 8.0$  Hz, 2H), 3.86–3.75 (m, 1H), 3.22–3.17 (m, 1H), 3.09–3.03 (m, 1H), 1.56 (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ )  $\delta$  140.1, 133.0, 131.0, 126.9 (d,  $^1J_{\text{CF}} = 279.1$

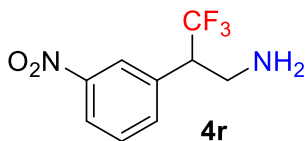
Hz), 119.1, 111.5, 52.3 (q,  $^2J_{\text{CF}} = 24.0$  Hz), 41.1 (d,  $^3J_{\text{CF}} = 2.1$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  -66.3 (s, 3F); HRMS (ESI): calcd for  $\text{C}_{10}\text{H}_9\text{F}_3\text{N}_2+\text{H}$   $[\text{M}+\text{H}]^+$ : 215.0796, found: 215.0795.



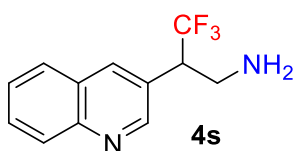
**3-(3-Amino-1,1,1-trifluoropropan-2-yl)benzonitrile (4p).** Yellow oil, yield 65% (139.1 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  7.89–7.85 (m, 2H), 7.75 (d,  $J = 7.6$  Hz, 1H), 7.63 (t,  $J = 7.8$  Hz, 1H), 3.84–3.73 (m, 1H), 3.23–3.19 (m, 1H), 3.14–3.08 (m, 1H), 2.28 (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ )  $\delta$  136.1 (d,  $^3J_{\text{CF}} = 1.7$  Hz), 134.8, 133.6, 132.4, 130.3, 126.9 (q,  $^1J_{\text{CF}} = 278.9$  Hz), 119.1, 112.2, 51.9 (q,  $^2J_{\text{CF}} = 24.1$  Hz), 40.8 (d,  $^3J_{\text{CF}} = 2.0$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  -62.2 (s, 3F); HRMS (ESI): calcd for  $\text{C}_{10}\text{H}_9\text{F}_3\text{N}_2+\text{H}$   $[\text{M}+\text{H}]^+$ : 215.0796, found: 215.0797.



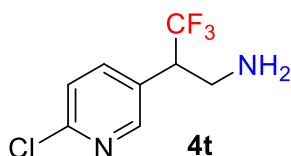
**5-(3-Amino-1,1,1-trifluoropropan-2-yl)-2-fluorobenzonitrile (4q).** Yellow oil, yield 74% (171.7 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  8.00 (dd,  $J_1 = 2.0$  Hz,  $J_2 = 6.4$  Hz, 1H), 7.85–7.81 (m, 1H), 7.58 (t,  $J = 9.0$  Hz, 1H), 3.86–3.75 (m, 1H), 3.22–3.17 (m, 1H), 3.13–3.08 (m, 1H), 2.30 (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ )  $\delta$  162.7 (d,  $^1J_{\text{CF}} = 254.6$  Hz), 137.7 (d,  $^3J_{\text{CF}} = 8.8$  Hz), 135.2, 132.1, 126.8 (q,  $^1J_{\text{CF}} = 278.7$  Hz), 117.3 (d,  $^2J_{\text{CF}} = 19.5$  Hz), 114.3, 101.0 (d,  $^2J_{\text{CF}} = 15.3$  Hz), 51.1 (q,  $^2J_{\text{CF}} = 24.3$  Hz), 40.7 (d,  $^3J_{\text{CF}} = 2.9$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  -67.3 (s, 3F), -109.6 (s, 1F); HRMS (ESI): calcd for  $\text{C}_{10}\text{H}_8\text{F}_4\text{N}_2+\text{H}$   $[\text{M}+\text{H}]^+$ : 233.0702, found: 233.0707.



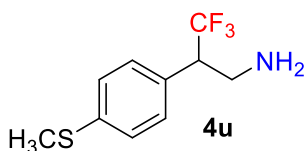
**3,3,3-Trifluoro-2-(3-nitrophenyl)propan-1-amine (4r).** Yellow oil, yield 59% (138.1 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  8.26–8.24 (m, 2H), 7.88 (d,  $J = 7.6$  Hz, 1H), 7.73 (t,  $J = 7.8$  Hz, 1H), 4.00–3.89 (m, 1H), 3.27–3.22 (m, 1H), 3.15–3.10 (m, 1H), 2.15 (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ )  $\delta$  148.4, 136.6 (d,  $^3J_{\text{CF}} = 1.8$  Hz), 136.4, 130.6, 126.9 (q,  $^1J_{\text{CF}} = 278.9$  Hz), 124.7, 123.6, 51.7 (q,  $^2J_{\text{CF}} = 24.2$  Hz), 41.1 (d,  $^3J_{\text{CF}} = 2.2$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  -66.9 (s, 3F); HRMS (ESI): calcd for  $\text{C}_9\text{H}_9\text{F}_3\text{N}_2\text{O}_2+\text{H}$   $[\text{M}+\text{H}]^+$ : 235.0694, found: 235.0699.



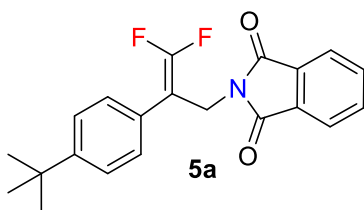
**3,3,3-Trifluoro-2-(quinolin-3-yl)propan-1-amine (4s).** Yellow oil, yield 73% (175.2 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  8.89 (d,  $J = 2.0$  Hz, 1H), 8.42 (d,  $J = 1.2$  Hz, 1H), 8.06–8.03 (m, 2H), 7.82–7.78 (m, 1H), 7.67–7.63 (m, 1H), 4.02–3.91 (m, 1H), 4.35–3.30 (m, 1H), 3.28–3.22 (m, 1H), 2.21 (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ )  $\delta$  152.2, 147.8, 136.7, 130.4, 129.2, 128.7, 127.9, 127.5, 127.1 (q,  $^1J_{\text{CF}} = 278.9$  Hz), 50.0 (q,  $^2J_{\text{CF}} = 24.3$  Hz), 40.8 (d,  $^3J_{\text{CF}} = 2.1$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  -66.9 (s, 3F); HRMS (ESI): calcd for  $\text{C}_{12}\text{H}_{11}\text{F}_3\text{N}_2\text{O}_2+\text{H}$   $[\text{M}+\text{H}]^+$ : 241.0953, found: 241.0951.



**2-(6-chloropyridin-3-yl)-3,3,3-trifluoropropan-1-amine (4t).** Yellow oil, yield 89% (199.4 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  8.42 (d,  $J = 2.0$  Hz, 1H), 7.90–7.88 (m, 1H), 7.57 (d,  $J = 8.0$  Hz, 1H), 3.83–3.72 (m, 1H), 3.21–3.17 (m, 1H), 3.08–3.03 (m, 1H), 1.65 (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ )  $\delta$  151.4, 150.6, 140.6, 129.9, 126.8 (q,  $^1J_{\text{CF}} = 278.9$  Hz), 124.8, 49.3 (q,  $^2J_{\text{CF}} = 24.4$  Hz), 40.7 (d,  $^3J_{\text{CF}} = 2.3$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  -67.1 (s, 3F); HRMS (ESI): calcd for  $\text{C}_8\text{H}_8\text{F}_3\text{N}_2\text{Cl}+\text{H}$   $[\text{M}+\text{H}]^+$ : 225.0406, found: 225.0405.

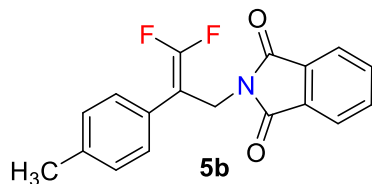


**3,3,3-Trifluoro-2-(4-(methylthio)phenyl)propan-1-amine (4u).** Yellow oil, yield 75% (176.3 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  7.31–7.27 (m, 4H), 3.65–3.54 (m, 1H), 3.19–3.14 (m, 1H), 3.05–3.00 (m, 1H), 2.47 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ )  $\delta$  138.2, 130.0, 129.8, 126.7 (q,  $^1J_{\text{CF}} = 279.0$  Hz), 126.0, 51.3 (q,  $^2J_{\text{CF}} = 23.9$  Hz), 40.6 (d,  $^3J_{\text{CF}} = 2.8$  Hz), 14.5;  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  -67.2 (s, 3F); HRMS (ESI): calcd for  $\text{C}_{10}\text{H}_{12}\text{F}_3\text{NS}+\text{H}$   $[\text{M}+\text{H}]^+$ : 236.0721, found: 236.0728.

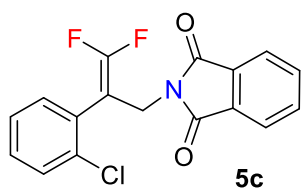


**2-(2-(4-(tert-Butyl)phenyl)-3,3-difluoroallyl)isoindoline-1,3-dione (5a).** Yellow oil, yield 21% (74.6 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.78–7.75 (m, 2H), 7.66–7.64 (m, 2H), 7.32 (s, 4H), 4.70 (t,  $J = 2.0$  Hz, 2H), 1.26 (s,

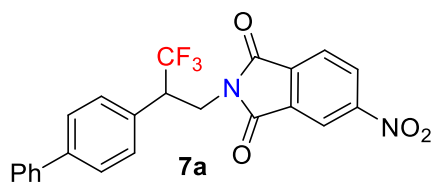
9H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.8, 154.8 (t,  $^1J_{\text{CF}} = 290.5$  Hz), 150.9, 134.0, 131.9, 128.2 (t,  $^4J_{\text{CF}} = 3.2$  Hz), 127.6 (t,  $^3J_{\text{CF}} = 3.2$  Hz), 125.5, 123.4, 88.9 (t,  $^2J_{\text{CF}} = 17.0$  Hz), 35.4 (q,  $^3J_{\text{CF}} = 2.1$  Hz), 34.6, 31.2;  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -86.9 (d,  $J = 32.7$  Hz, 1F), -87.1 (d,  $J = 32.7$  Hz, 1F); HRMS (ESI): calcd for  $\text{C}_{21}\text{H}_{19}\text{F}_2\text{O}_2\text{N}+\text{Na}$   $[\text{M}+\text{Na}]^+$ : 378.1282, found: 378.1284.



**2-(3,3-Difluoro-2-(p-tolyl)allyl)isoindoline-1,3-dione (5b).** White solid, m.p. 119.4–119.6 °C, yield 30% (93.9 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77–7.73 (m, 2H), 7.66–7.63 (m, 2H), 7.25–7.22 (m, 2H), 7.09 (d,  $J = 8.0$  Hz, 2H), 4.67 (t,  $J = 2.0$  Hz, 2H), 2.26 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.8, 154.6, (t,  $^1J_{\text{CF}} = 290.1$  Hz), 137.8, 134.0, 131.8, 129.2, 128.5 (t,  $^4J_{\text{CF}} = 2.8$  Hz), 127.5 (t,  $^3J_{\text{CF}} = 3.1$  Hz), 123.4, 89.0 (t,  $^2J_{\text{CF}} = 17.5$  Hz), 35.5 (q,  $^3J_{\text{CF}} = 2.1$  Hz), 21.2;  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -87.5 (d,  $J = 32.7$  Hz, 1F), -87.8 (d,  $J = 33.8$  Hz, 1F); HRMS (ESI): calcd for  $\text{C}_{18}\text{H}_{13}\text{F}_2\text{O}_2\text{N}+\text{Na}$   $[\text{M}+\text{Na}]^+$ : 336.0812, found: 336.0818.

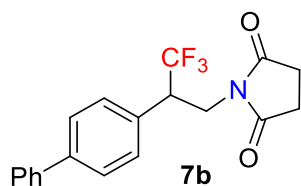


**2-(2-(2-Chlorophenyl)-3,3-difluoroallyl)isoindoline-1,3-dione (5c).** Yellow oil, yield 34% (113.2 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.79–7.74 (m, 2H), 7.71–7.65 (m, 2H), 7.37–7.32 (m, 1H), 7.27–7.13 (m, 3H), 4.66 (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.6, 154.6 (dd,  $^1J_{\text{CF}} = 288.1, 292.7$  Hz), 134.7 (d,  $^4J_{\text{CF}} = 2.6$  Hz), 134.1, 131.8, 131.7 (d,  $^4J_{\text{CF}} = 4.1$  Hz), 130.1, 129.9 (d,  $^3J_{\text{CF}} = 5.0$  Hz), 129.7, 127.0, 123.4, 87.2 (t,  $^2J_{\text{CF}} = 20.7$  Hz), 35.6 (d,  $^3J_{\text{CF}} = 4.2$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -84.3 (d,  $J = 28.6$  Hz, 1F), -88.2 (d,  $J = 28.6$  Hz, 1F); HRMS (ESI): calcd for  $\text{C}_{17}\text{H}_{10}\text{F}_2\text{O}_2\text{NCl}+\text{Na}$   $[\text{M}+\text{Na}]^+$ : 356.0266, found: 356.0272.



**2-(2-([1,1'-Biphenyl]-4-yl)-3,3,3-trifluoropropyl)-5-nitroisoindoline-1,3-dione (7a).** Yellow solid, m.p. 60.9–61.7 °C, yield 40% (176.0 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.61–8.55 (m, 2H), 8.00–7.96 (m, 1H), 7.54 (t,  $J = 8.4$  Hz, 4H), 7.42–7.39 (m, 4H), 7.34 (t,  $J = 7.2$  Hz, 1H), 4.40–4.11 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  165.6, 165.4, 151.9, 141.9, 140.0, 135.9, 133.0, 130.0, 129.6, 129.5, 128.9, 127.8, 127.6, 127.0, 125.8 (d,  $^1J_{\text{CF}} =$

278.9 Hz), 124.8, 119.0, 47.3 (q,  $^2J_{\text{CF}} = 26.6$  Hz), 37.7 (d,  $^3J_{\text{CF}} = 2.0$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -68.5 (s, 3F); HRMS (ESI): calcd for  $\text{C}_{23}\text{H}_{15}\text{F}_3\text{O}_4\text{N}_2+\text{H}$   $[\text{M}+\text{H}]^+$ : 441.1062, found: 441.1056.



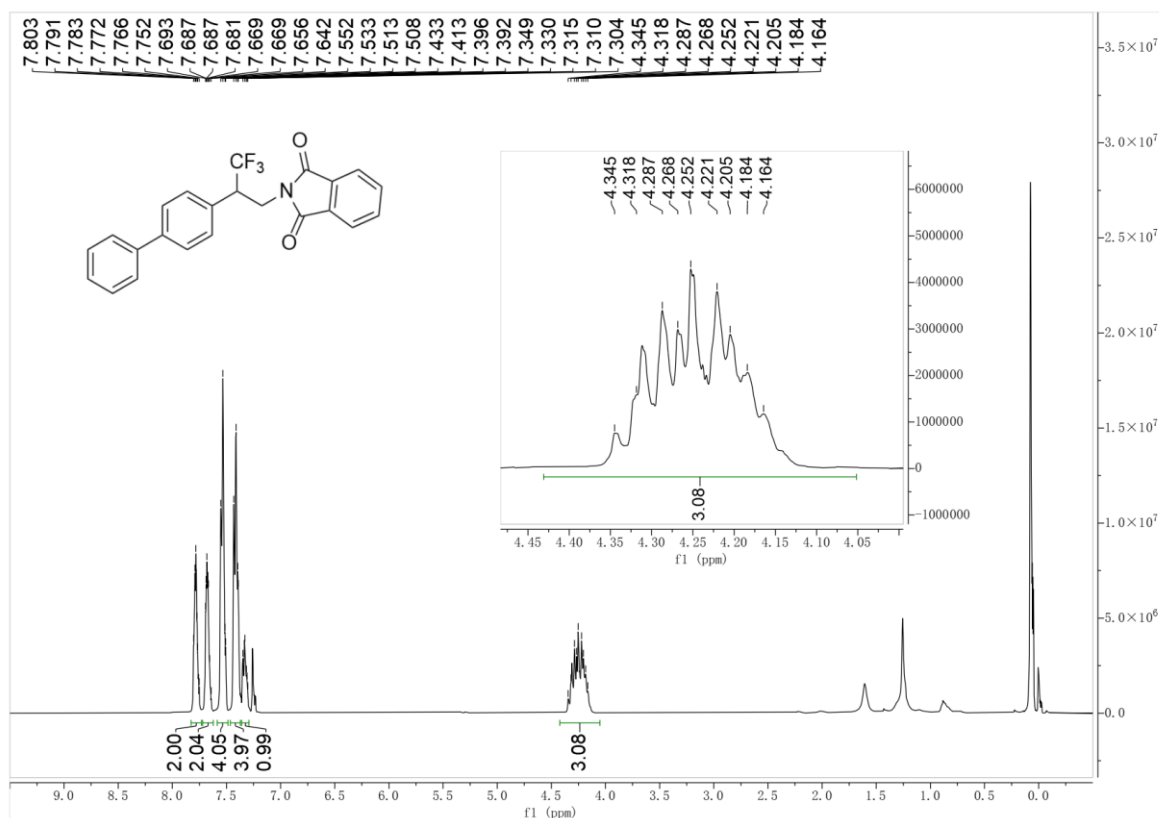
**1-(2-([1,1'-Biphenyl]-4-yl)-3,3,3-trifluoropropyl)pyrrolidine-2,5-dione (7b).** White solid, m.p. 147.9–148.5 °C, yield 76% (263.7 mg);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.57 (d,  $J = 8.4$  Hz, 4H), 7.45–7.33 (m, 5H), 4.17–3.99 (m, 3H), 2.63–2.48 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  176.6, 141.8, 140.2, 130.4, 129.7, 129.0, 127.8, 127.5, 127.1, 126.0 (d,  $^1J_{\text{CF}} = 278.2$  Hz), 46.4 (q,  $^2J_{\text{CF}} = 26.7$  Hz), 37.7 (d,  $^3J_{\text{CF}} = 3.1$  Hz), 28.0;  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -68.5 (s, 3F); HRMS (ESI): calcd for  $\text{C}_{19}\text{H}_{16}\text{F}_3\text{O}_2\text{N}+\text{Na}$   $[\text{M}+\text{Na}]^+$ : 370.1031, found: 370.1032.

## 9. References

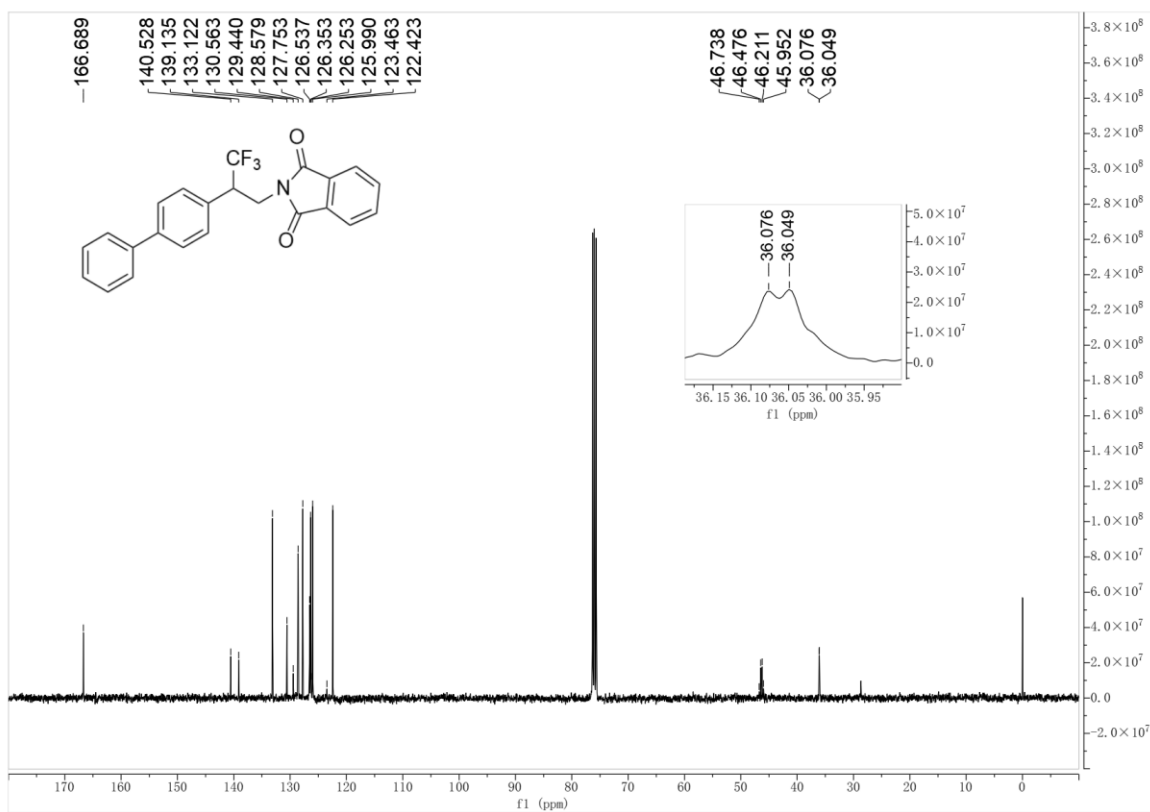
- (1) Y. Q. Guo, Y. P. Cao, H. J. Song, Y. X. Liu and Q. M. Wang, Photoredox relay-catalyzed *gem*-difluoroallylation of alkyl iodides, *Chem. Commun.*, 2021, **57**, 9768.
- (2) F. L. Chen, X. F. Xu, Y. L. He, G. P. Huang and S. L. Zhu, NiH-Catalyzed migratory defluorinative olefin cross-coupling: trifluoromethyl-substituted alkenes as acceptor olefins to form *gem*-difluoroalkenes, *Angew. Chem., Int. Ed.*, 2020, **59**, 5398.
- (3) Y. F. Chen, N. N. Ni, D. P. Cheng and X. L. Xu, The coupling of alkylboronic acids with  $\alpha$ -(trifluoromethyl)styrenes by Lewis base/photoredox dual catalysis, *Tetrahedron Lett.*, 2020, **61**, 152425.
- (4) Y. Li, B. Zhao, K. Dai, D. H. Tu, B. Wang, Y. Y. Wang, Z. T. Liu, Z. W. Liu and J. Lu, Palladium-catalyzed Suzuki-Miyaura reaction of fluorinated vinyl chloride: a new approach for synthesis  $\alpha$  and  $\alpha,\beta$ -difluoromethylstyrenes, *Tetrahedron*, 2016, **72**, 5684.
- (5) W. J. Yue, C. S. Day and R. Martin, Site-selective defluorinative  $\text{sp}^3$  C–H alkylation of secondary amides, *J. Am. Chem. Soc.*, 2021, **143**, 6395.

## 10. $^1\text{H}$ , $^{13}\text{C}$ , $^{19}\text{F}$ NMR and HRMS spectra of the intermediates and target compounds

### $^1\text{H}$ NMR spectrum of 3a (400 MHz, $\text{CDCl}_3$ )



### $^{13}\text{C}$ NMR spectrum of 3a (100 MHz, $\text{CDCl}_3$ )





## HRMS (ESI) spectrum of 3a

Monoisotopic Mass, Even Electron Ions

2752 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

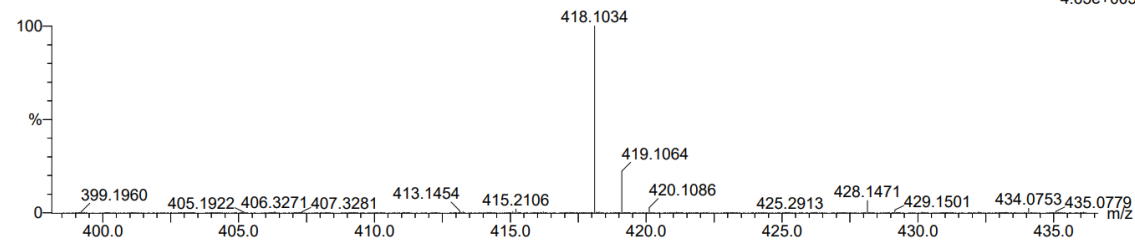
Elements Used:

C: 23-23 H: 16-16 N: 0-100 O: 0-100 F: 3-6 Na: 0-2

32

240511-2-9 13 (0.105)

1: TOF MS ES+  
4.65e+005

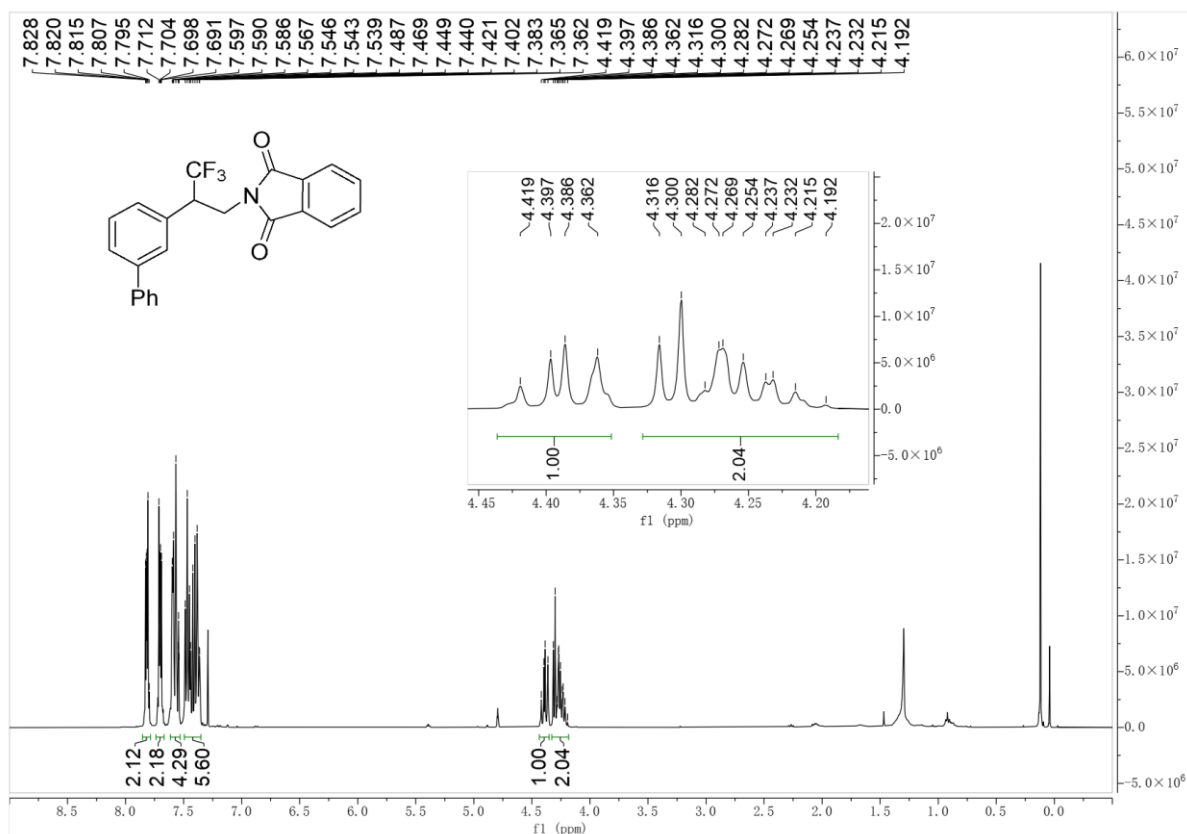


Minimum:

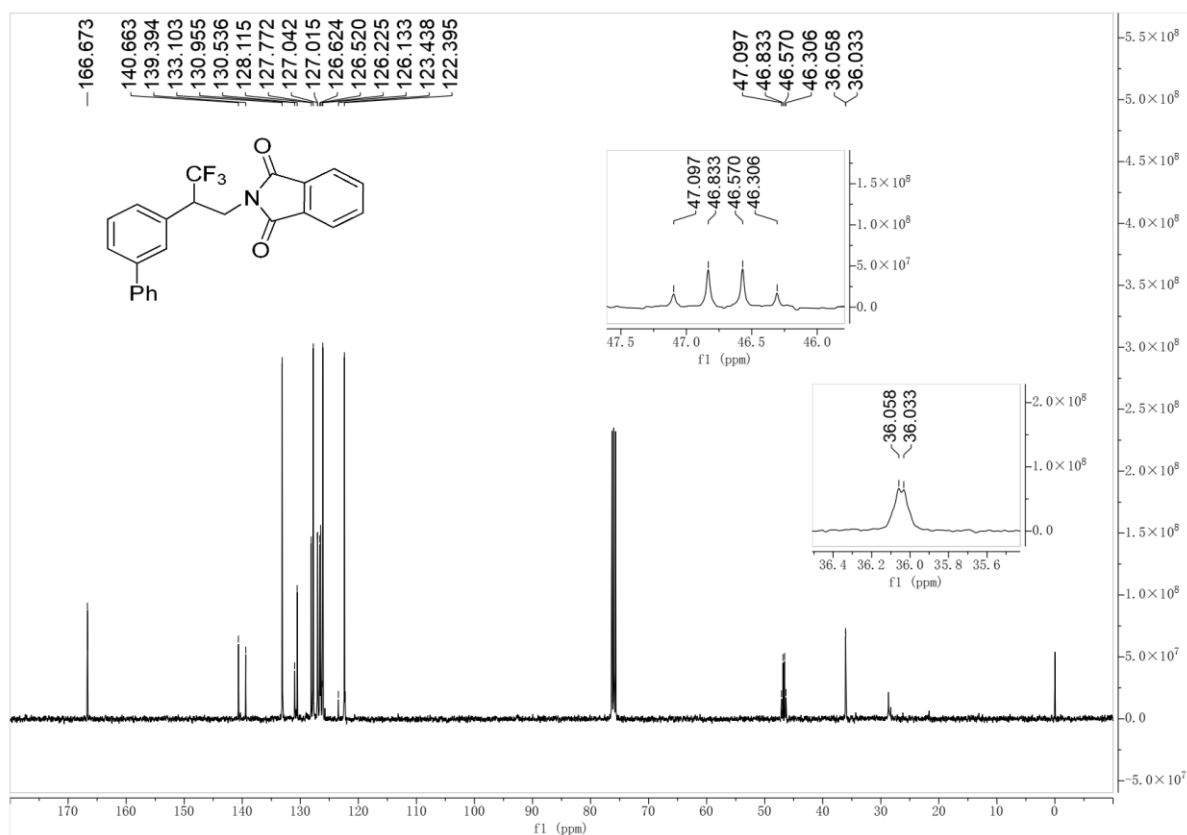
Maximum: 5.0 10.0 -1.5 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
418.1034	418.1031	0.3	0.7	14.5	537.3	n/a	n/a	C23 H16 N O2 F3 Na

## <sup>1</sup>H NMR spectrum of 3b (400 MHz, CDCl<sub>3</sub>)



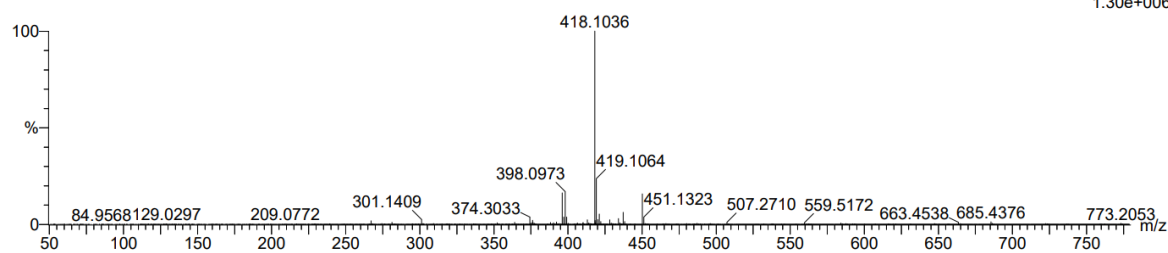
**<sup>13</sup>C NMR spectrum of 3b (100 MHz, CDCl<sub>3</sub>)**



**HRMS (ESI) spectrum of 3b**

Monoisotopic Mass, Even Electron Ions  
 2752 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)  
 Elements Used:  
 C: 23-23 H: 16-16 N: 0-100 O: 0-100 F: 3-6 Na: 0-2  
 32  
 240511-2-21 13 (0.105)

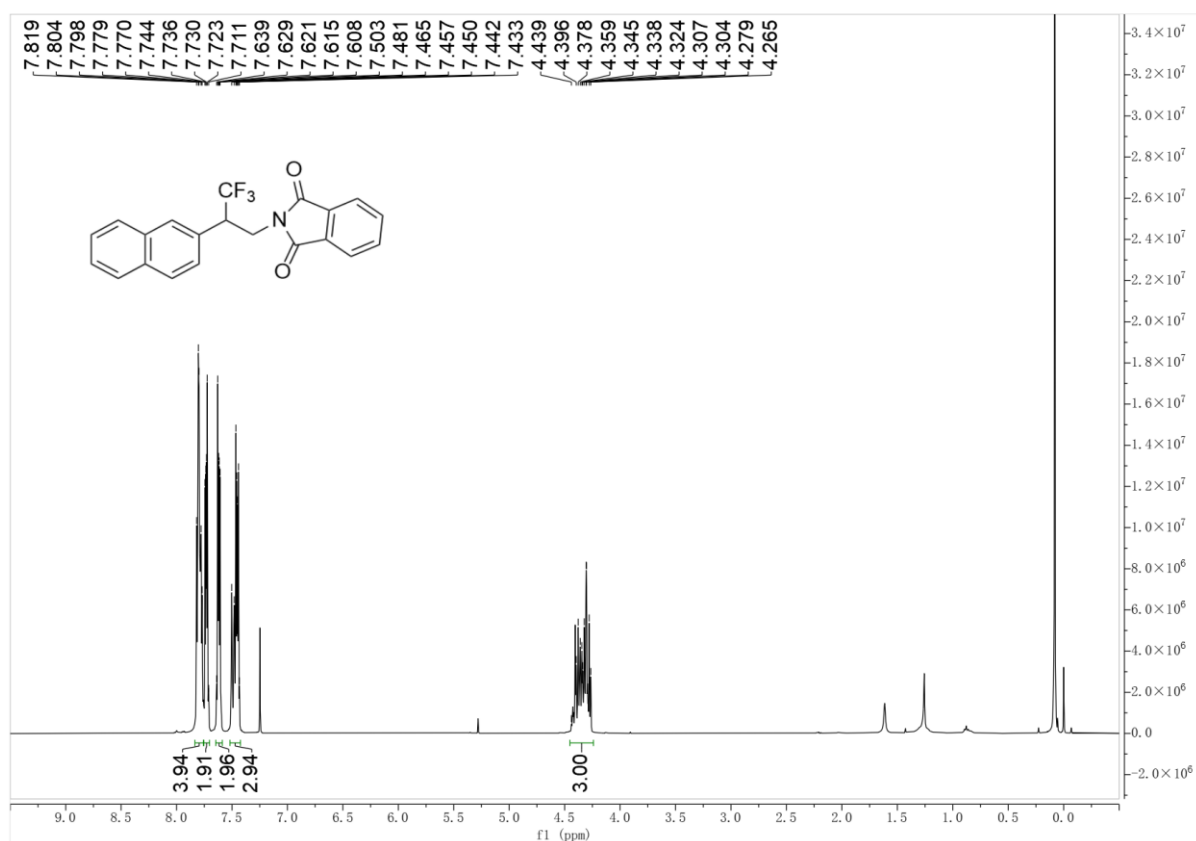
1: TOF MS ES+  
 1.30e+006



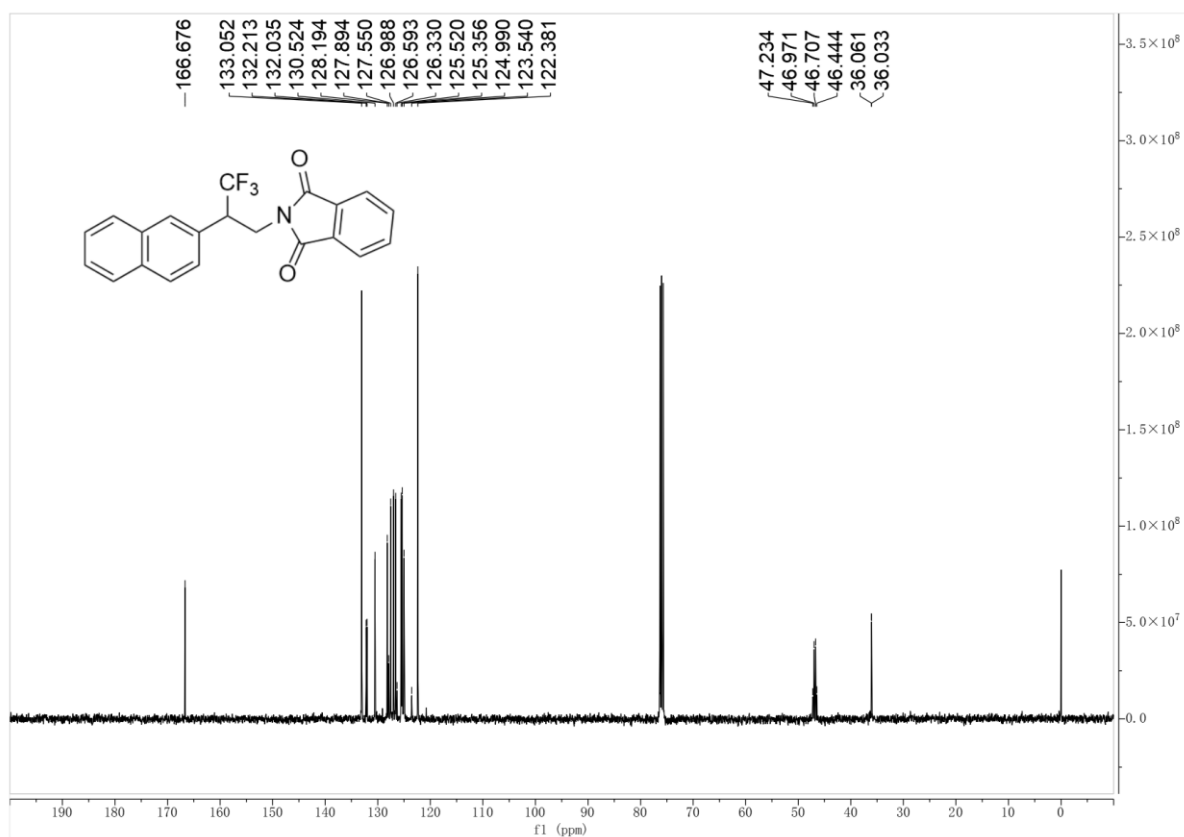
Minimum: -1.5  
 Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
418.1036	418.1031	0.5	1.2	14.5	721.8	n/a	n/a	C23 H16 N 02 F3 Na

**<sup>1</sup>H NMR spectrum of 3c (400 MHz, CDCl<sub>3</sub>)**



**<sup>13</sup>C NMR spectrum of 3c (100 MHz, CDCl<sub>3</sub>)**



## HRMS (ESI) spectrum of 3c

Monoisotopic Mass, Even Electron Ions

2323 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

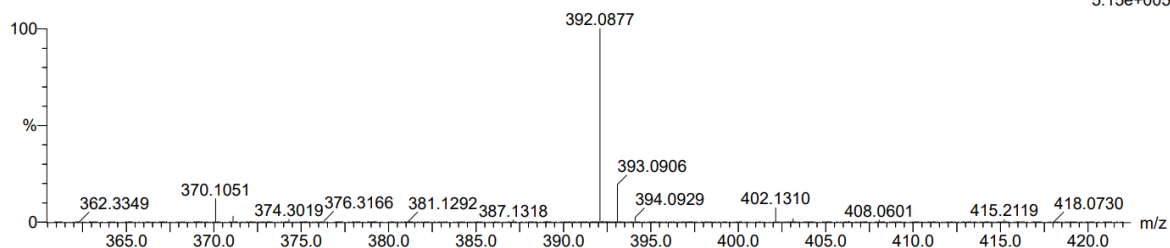
Elements Used:

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32

240511-2-7 14 (0.110)

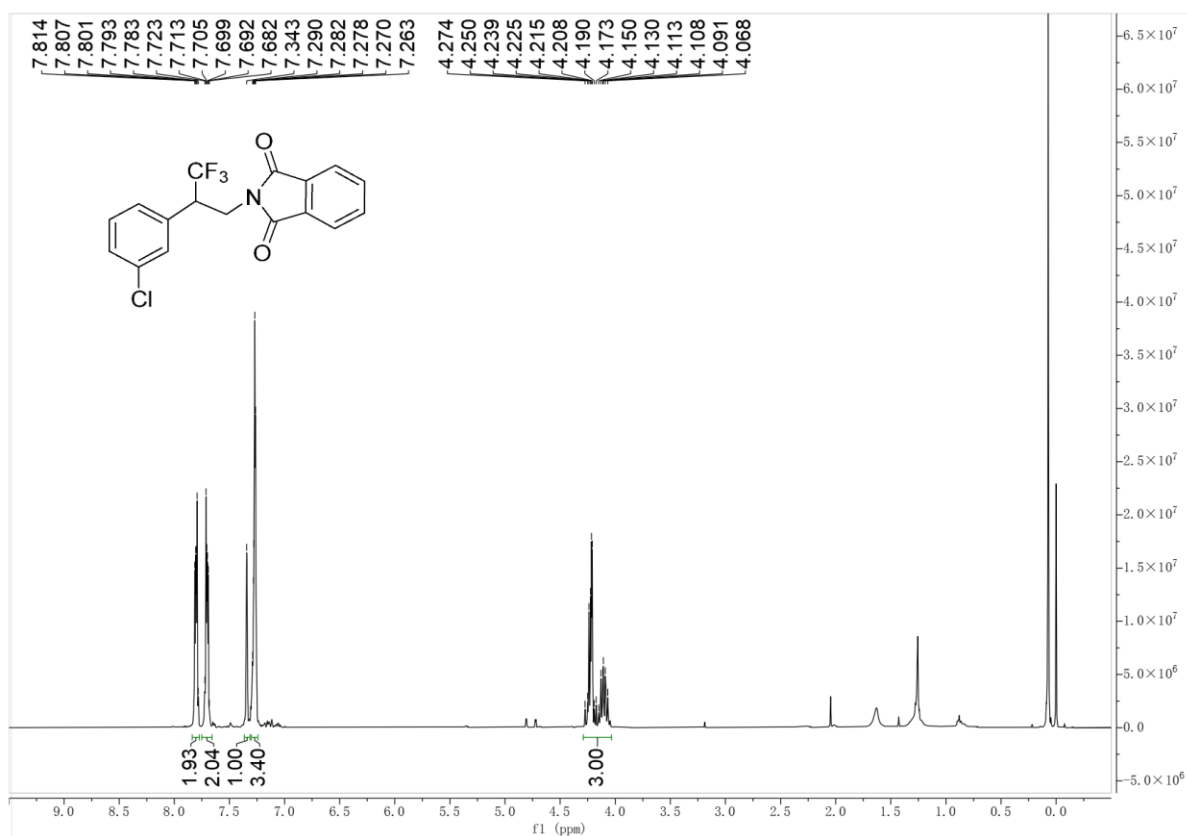
1: TOF MS ES+  
5.15e+005



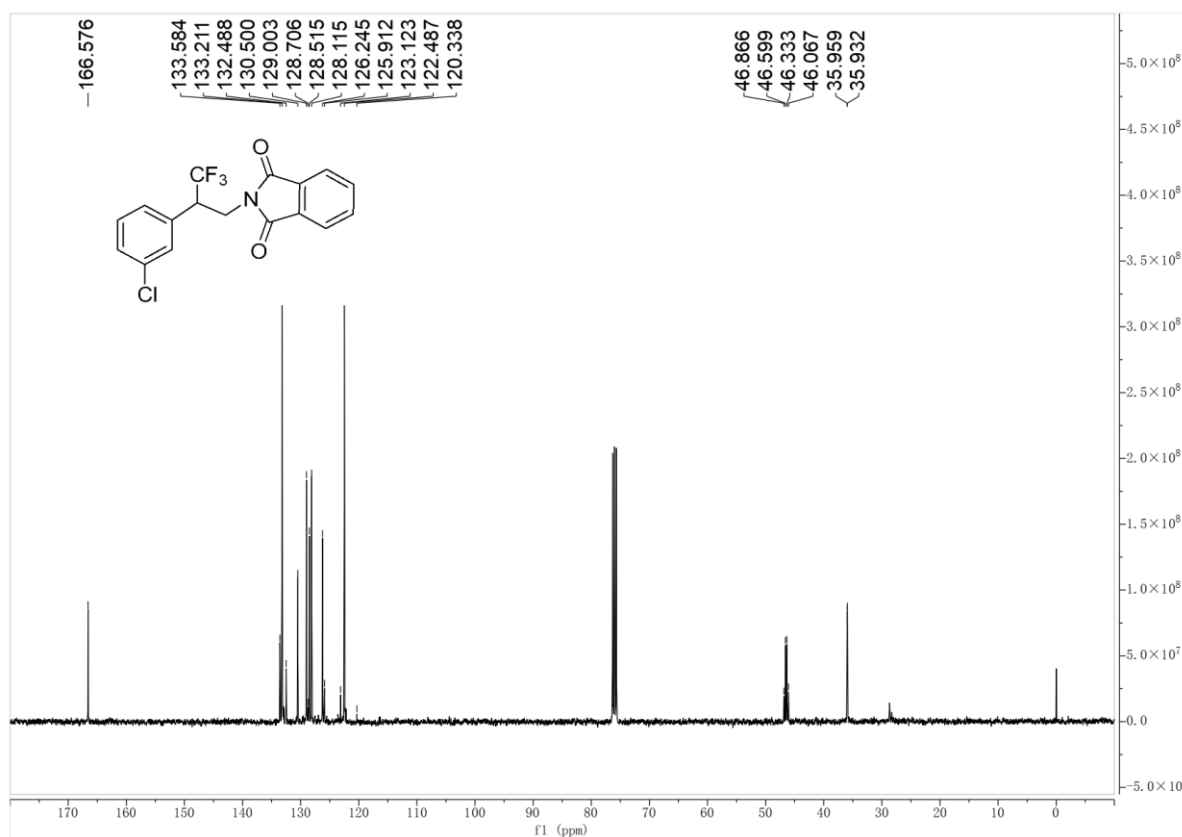
Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
392.0877	392.0874	0.3	0.8	13.5	596.0	n/a	n/a	C21 H14 N O2 F3 Na

## <sup>1</sup>H NMR spectrum of 3d (400 MHz, CDCl<sub>3</sub>)



**<sup>13</sup>C NMR spectrum of 3d (100 MHz, CDCl<sub>3</sub>)**



**HRMS (ESI) spectrum of 3d**

Monoisotopic Mass, Even Electron Ions

2798 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

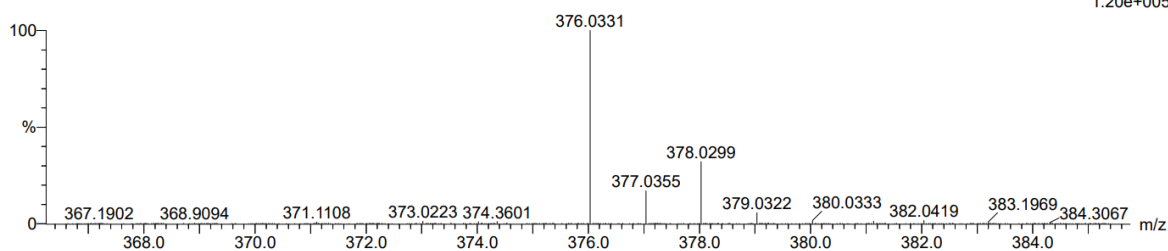
Elements Used:

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32

240511-2-18 11 (0.094)

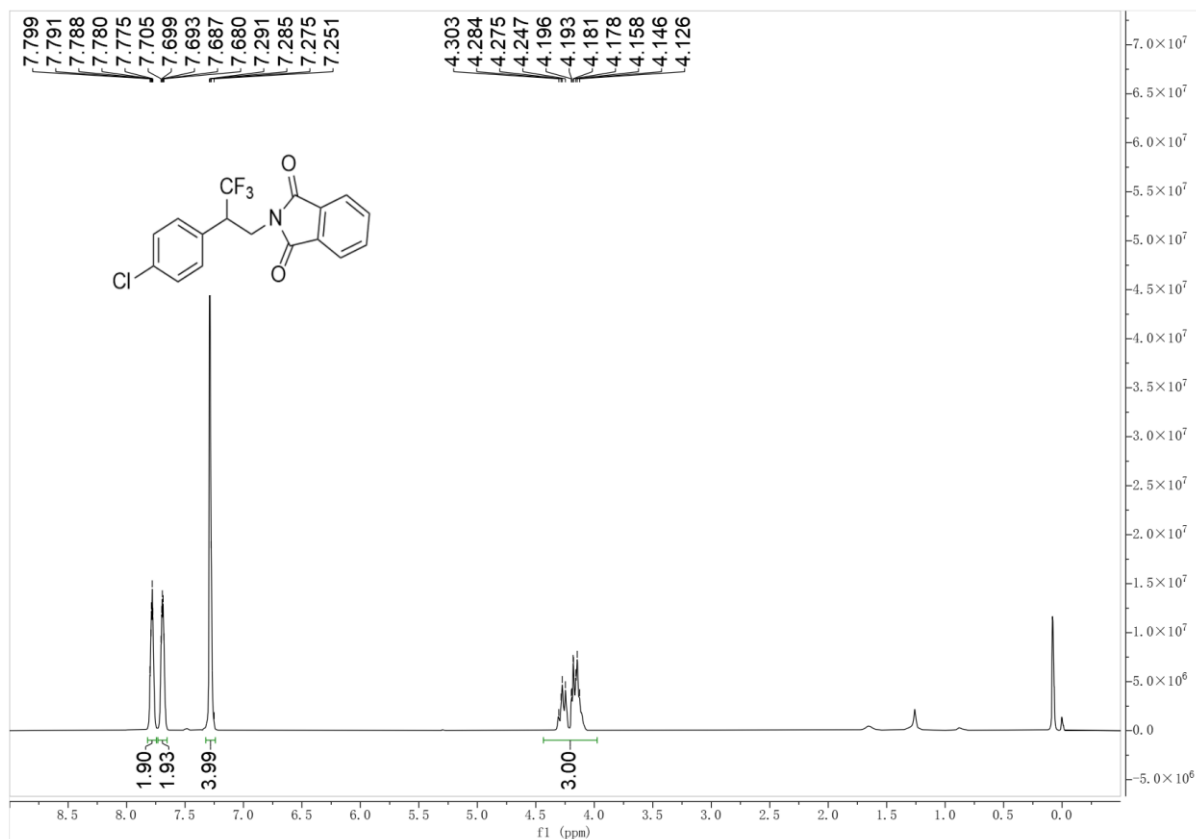
1: TOF MS ES+  
1.20e+005



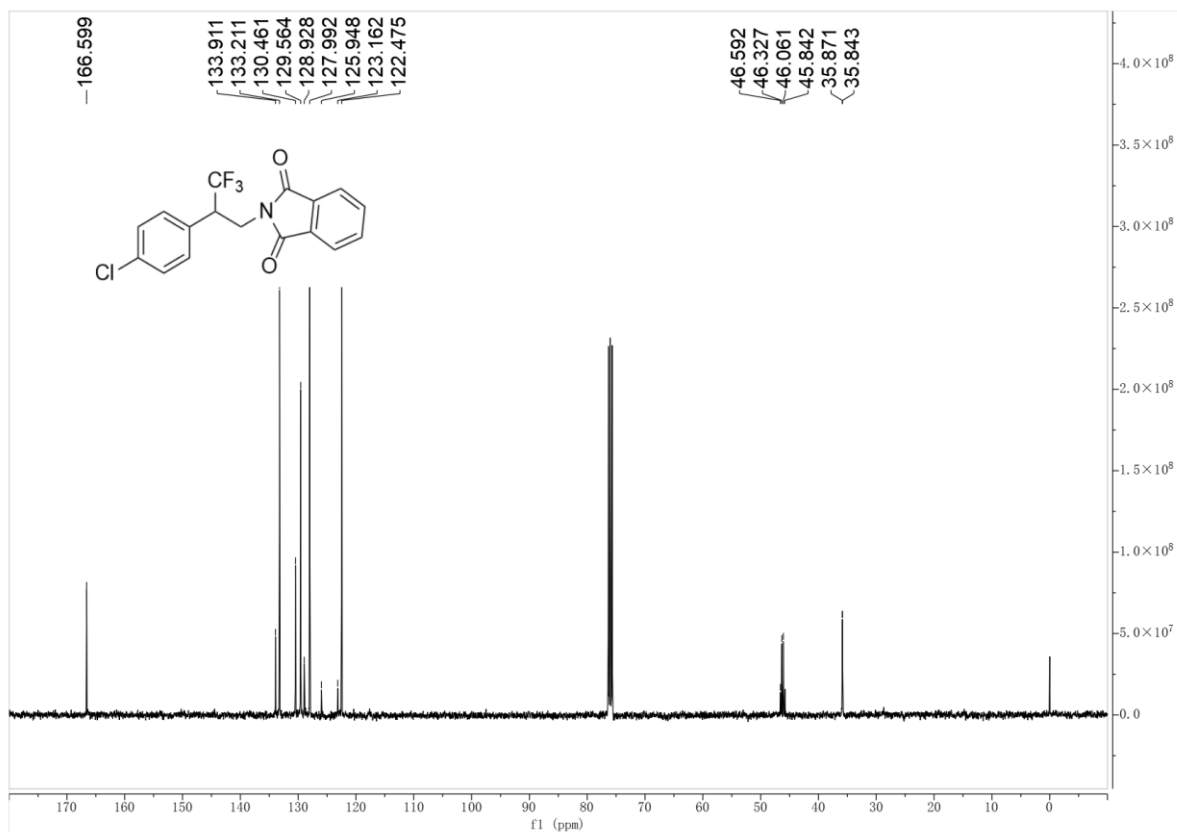
Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
376.0331	376.0328	0.3	0.8	10.5	529.8	n/a	n/a	C17 H11 N O2 F3 Na Cl

**<sup>1</sup>H NMR spectrum of 3e (400 MHz, CDCl<sub>3</sub>)**



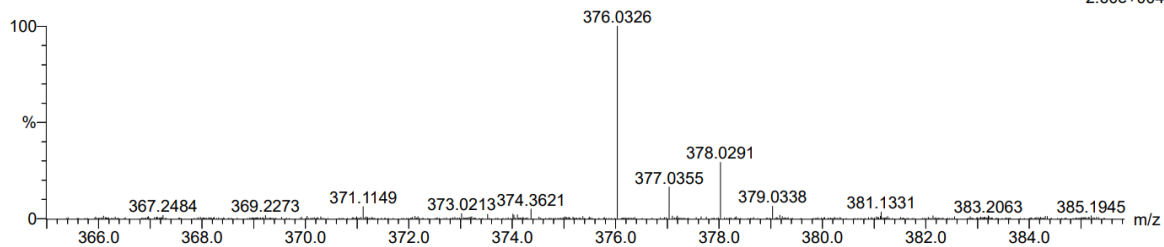
**<sup>13</sup>C NMR spectrum of 3e (100 MHz, CDCl<sub>3</sub>)**



## HRMS (ESI) spectrum of 3e

Monoisotopic Mass, Even Electron Ions  
2798 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)  
Elements Used:  
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32  
240511-2-22 11 (0.094)

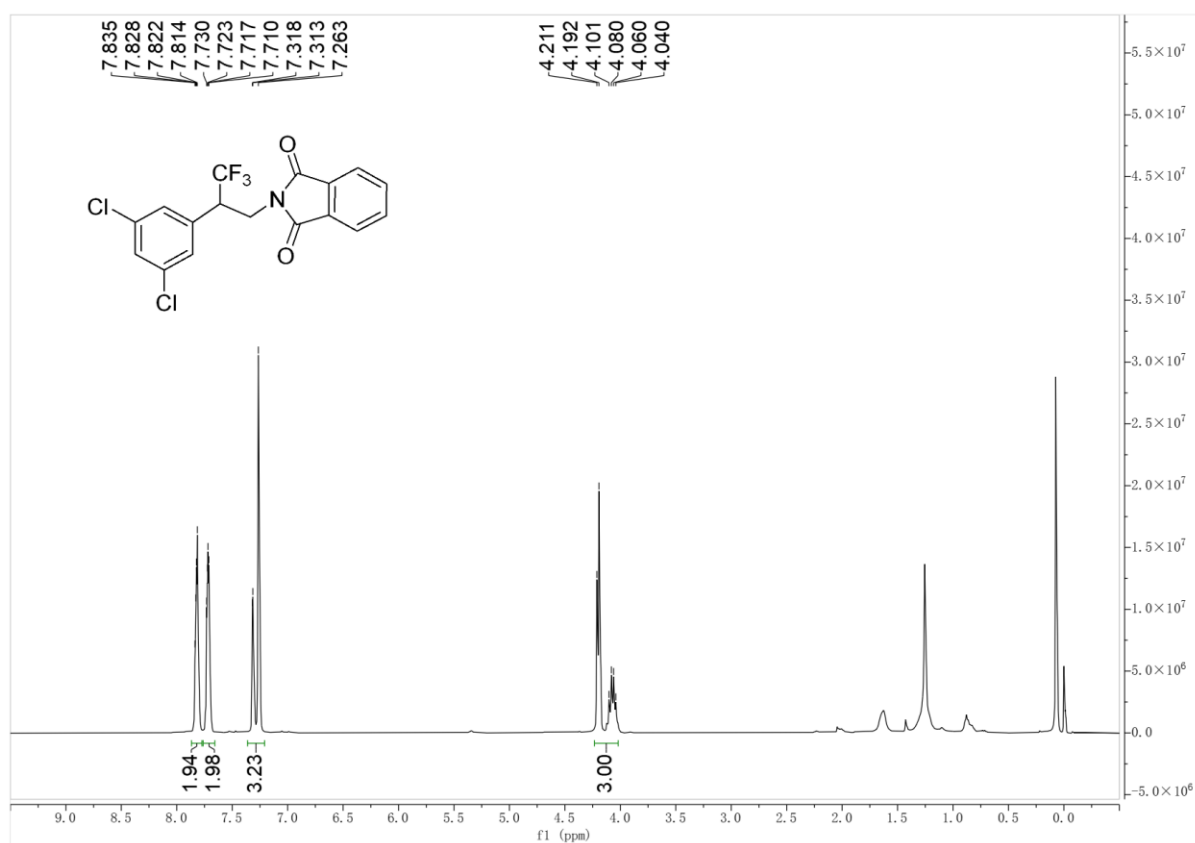
1: TOF MS ES+  
2.60e+004



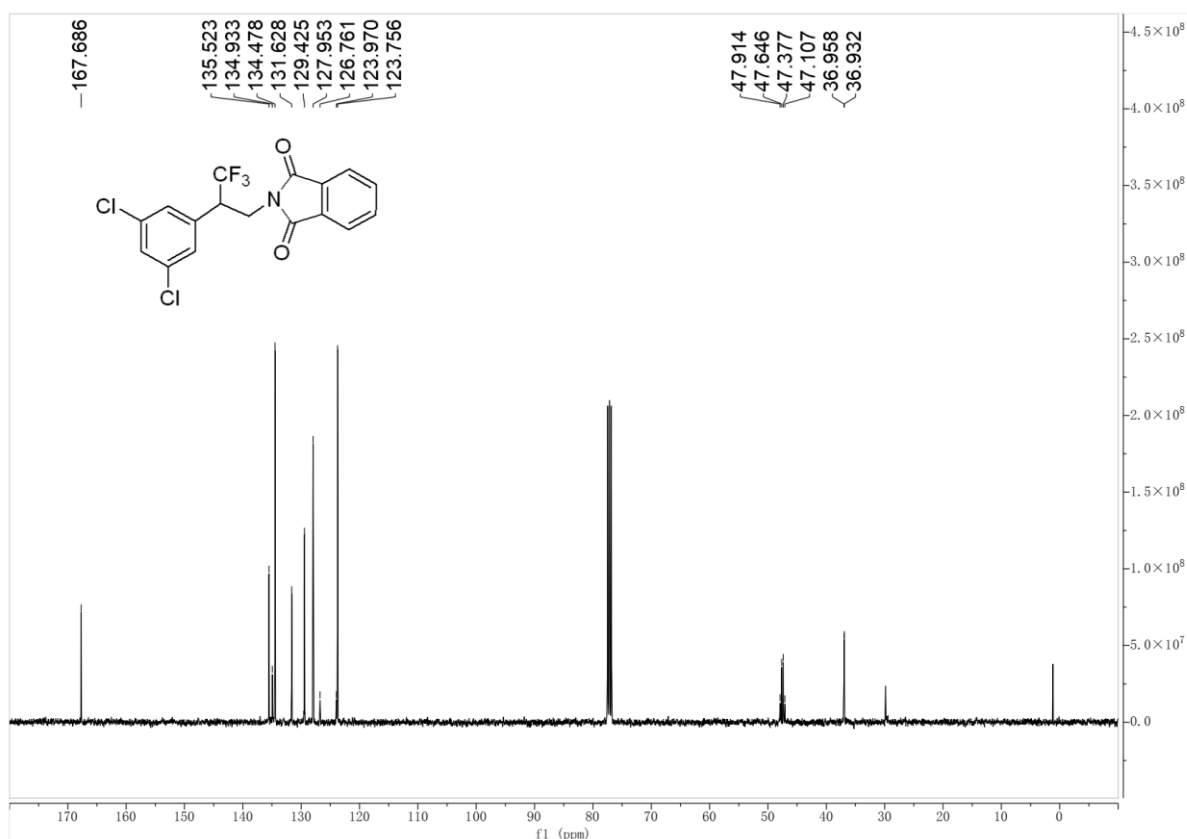
Minimum: -1.5  
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
376.0326	376.0328	-0.2	-0.5	10.5	409.8	n/a	n/a	C17 H11 N O2 F3 Na Cl

## <sup>1</sup>H NMR spectrum of 3f (400 MHz, CDCl<sub>3</sub>)



**<sup>13</sup>C NMR spectrum of 3f (100 MHz, CDCl<sub>3</sub>)**



**HRMS (ESI) spectrum of 3f**

Monoisotopic Mass, Even Electron Ions

3701 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

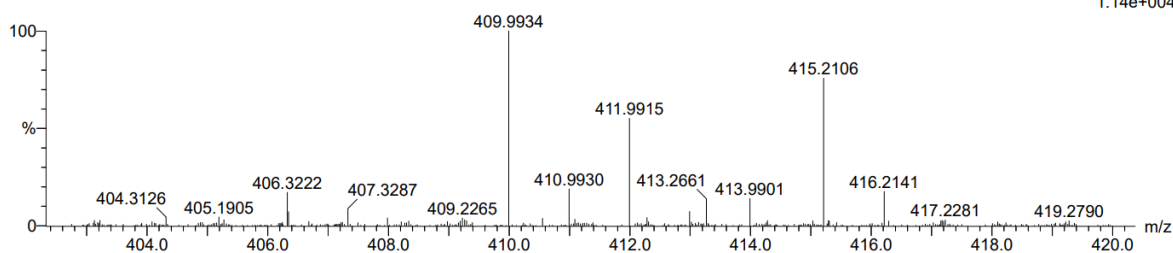
Elements Used:

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32

240511-2-17 14 (0.110)

1: TOF MS ES+  
1.14e+004

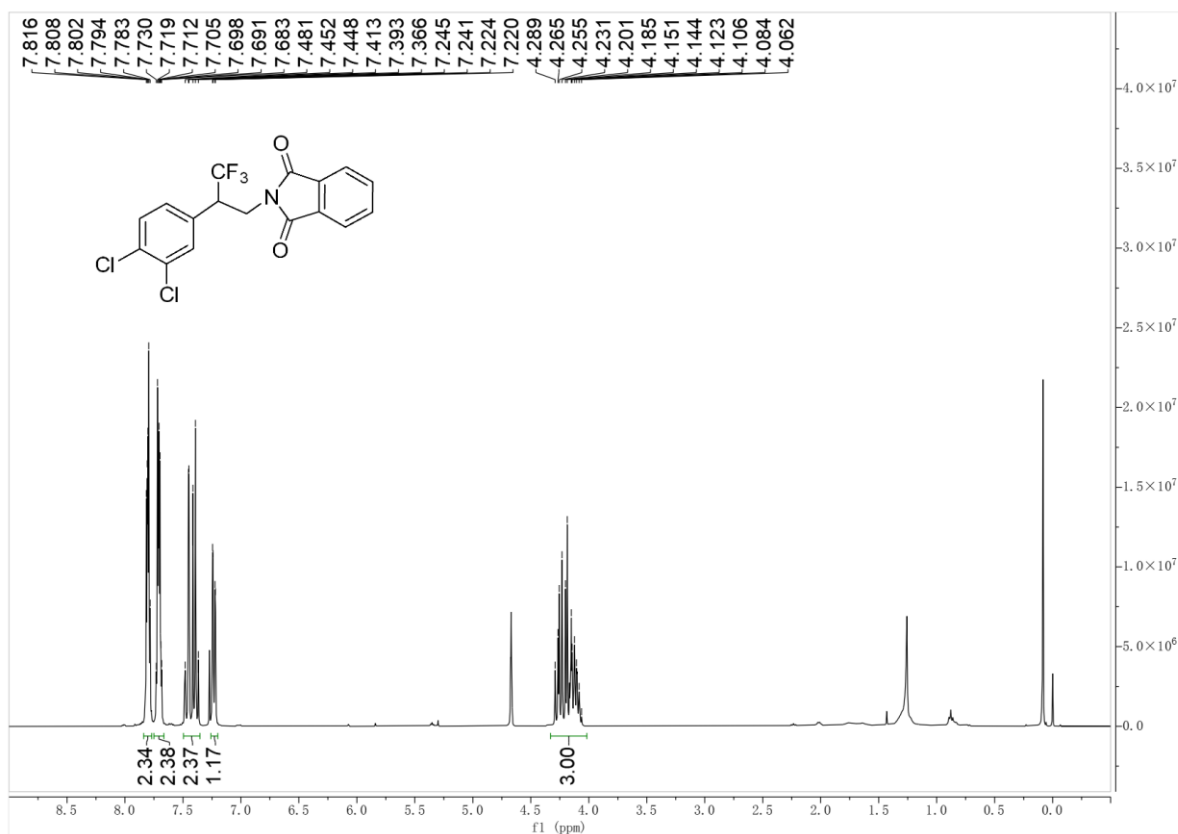


Minimum: -1.5  
Maximum: 5.0 10.0 50.0

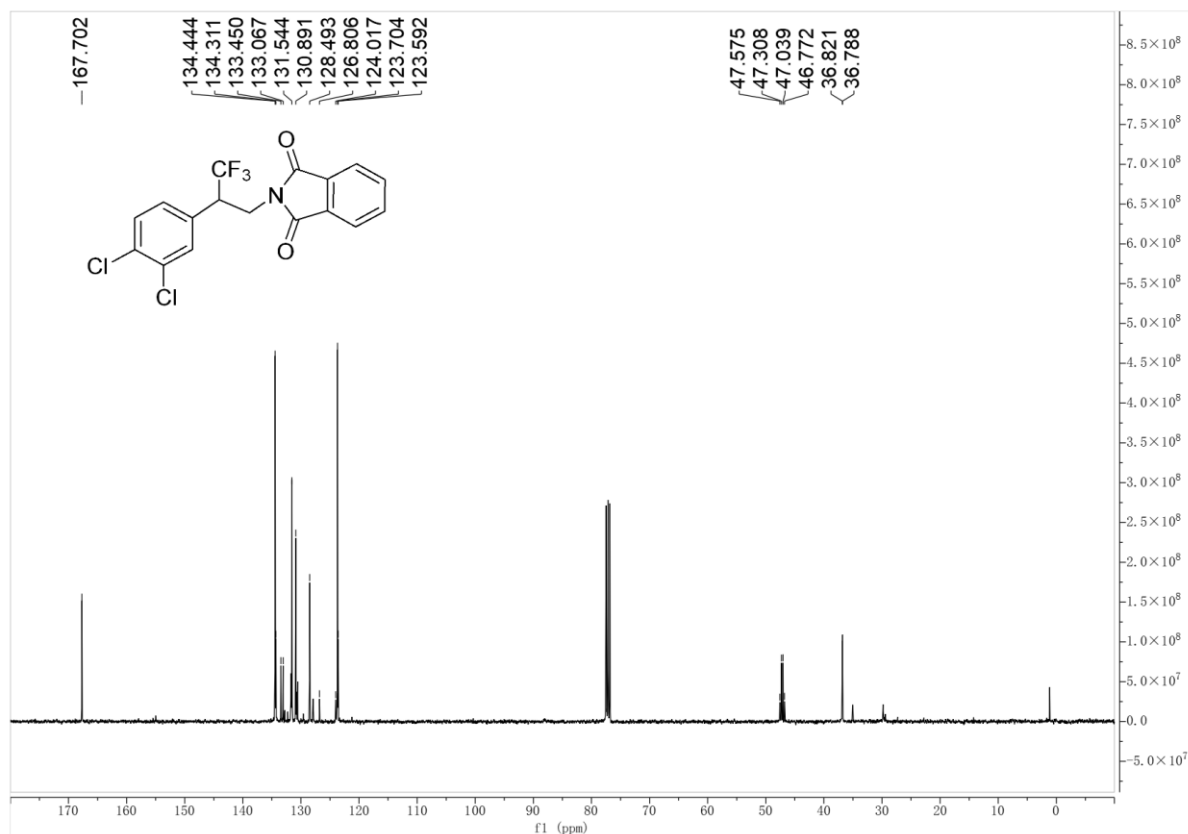
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
409.9934	409.9938	-0.4	-1.0	10.5	383.6	n/a	n/a	C17 H10 N O2 F3 Na Cl2



**<sup>1</sup>H NMR spectrum of 3g (400 MHz, CDCl<sub>3</sub>)**



**<sup>13</sup>C NMR spectrum of 3g (100 MHz, CDCl<sub>3</sub>)**



## HRMS (ESI) spectrum of 3g

Monoisotopic Mass, Even Electron Ions

3555 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

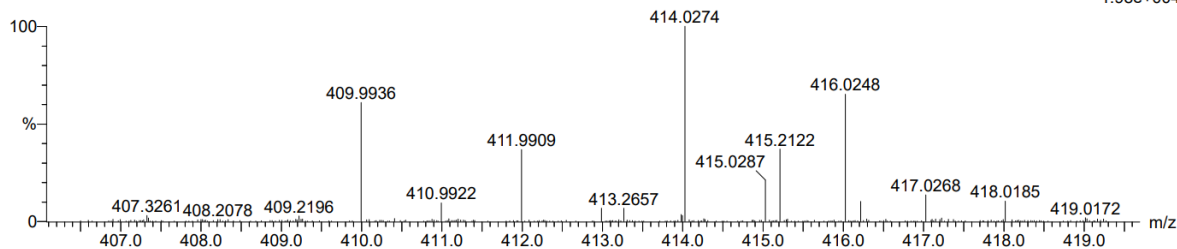
Elements Used:

C: 17-17 H: 10-10 N: 0-100 O: 0-100 F: 3-6 Na: 0-2 Cl: 1-2

32

240511-2-19 13 (0.105)

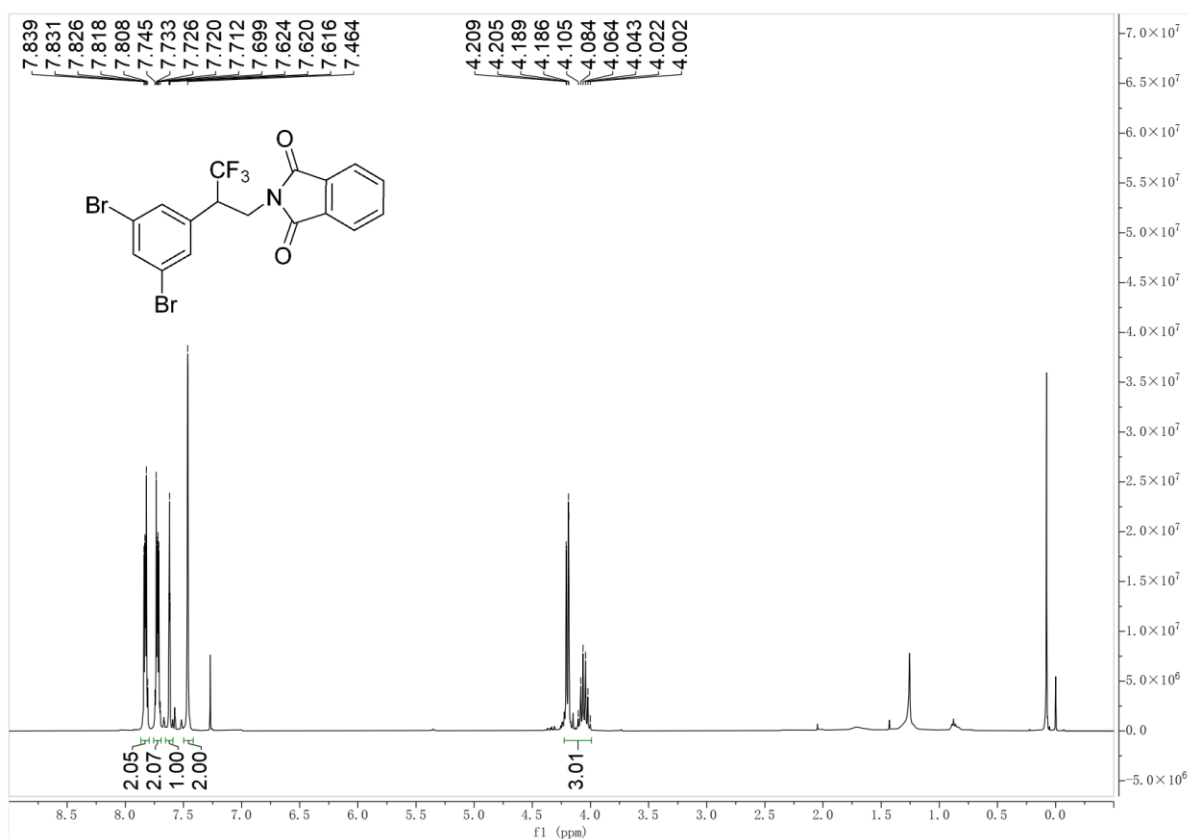
1: TOF MS ES+  
1.98e+004



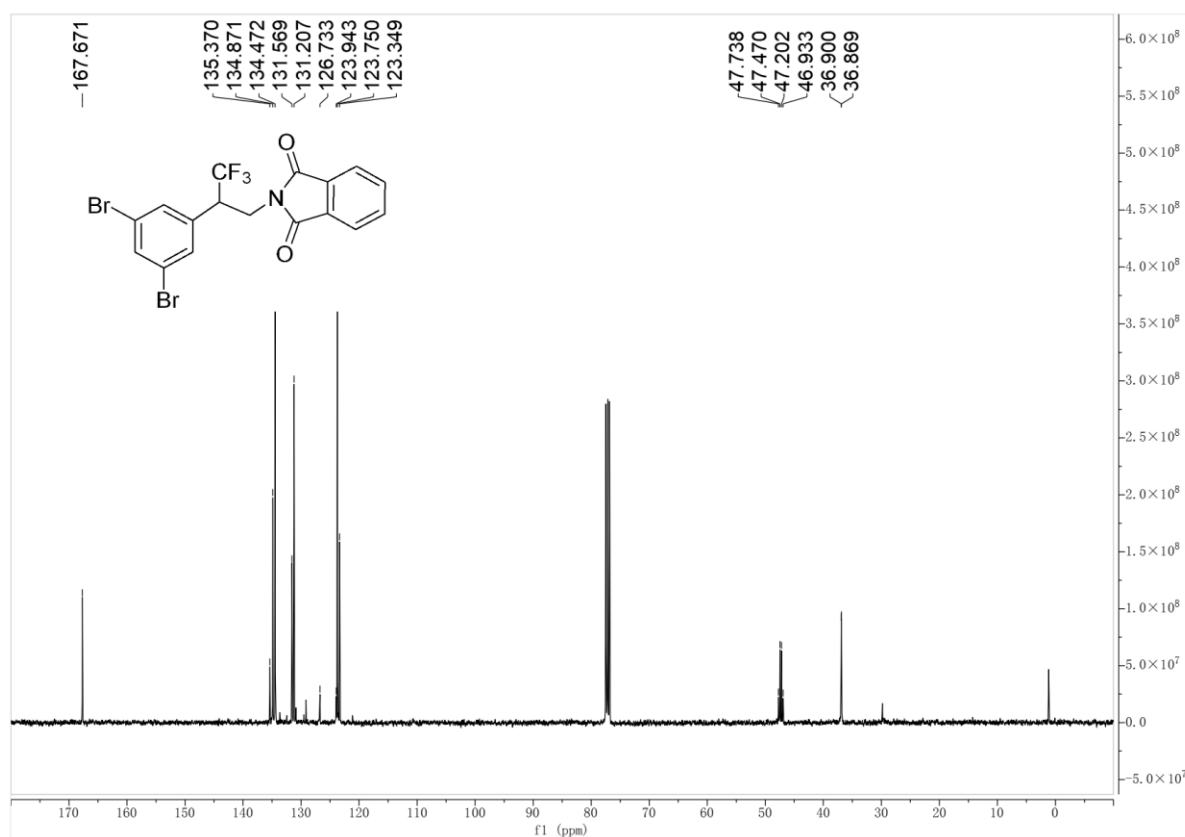
Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
409.9936	409.9938	-0.2	-0.5	10.5	467.8	n/a	n/a	C17 H10 N O2 F3 Na Cl2

## <sup>1</sup>H NMR spectrum of 3h (400 MHz, CDCl<sub>3</sub>)



**<sup>13</sup>C NMR spectrum of 3h (100 MHz, CDCl<sub>3</sub>)**

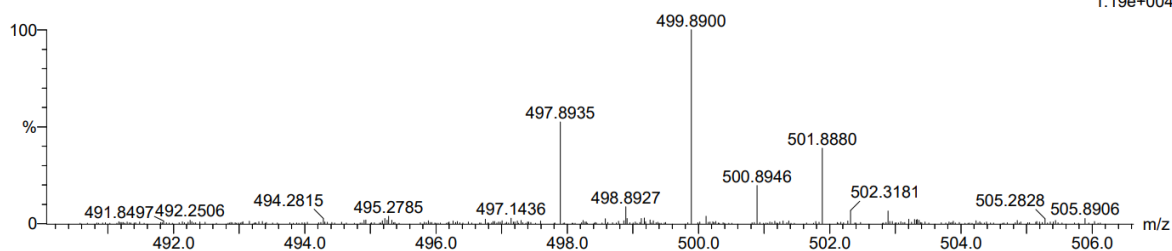


**HRMS (ESI) spectrum of 3h**

Monoisotopic Mass, Even Electron Ions  
 4133 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)  
 Elements Used:  
 C: 17-17 H: 10-10 N: 0-100 O: 0-100 F: 3-6 Na: 0-2 Br: 1-2

32  
 240511-2-12 15 (0.115)

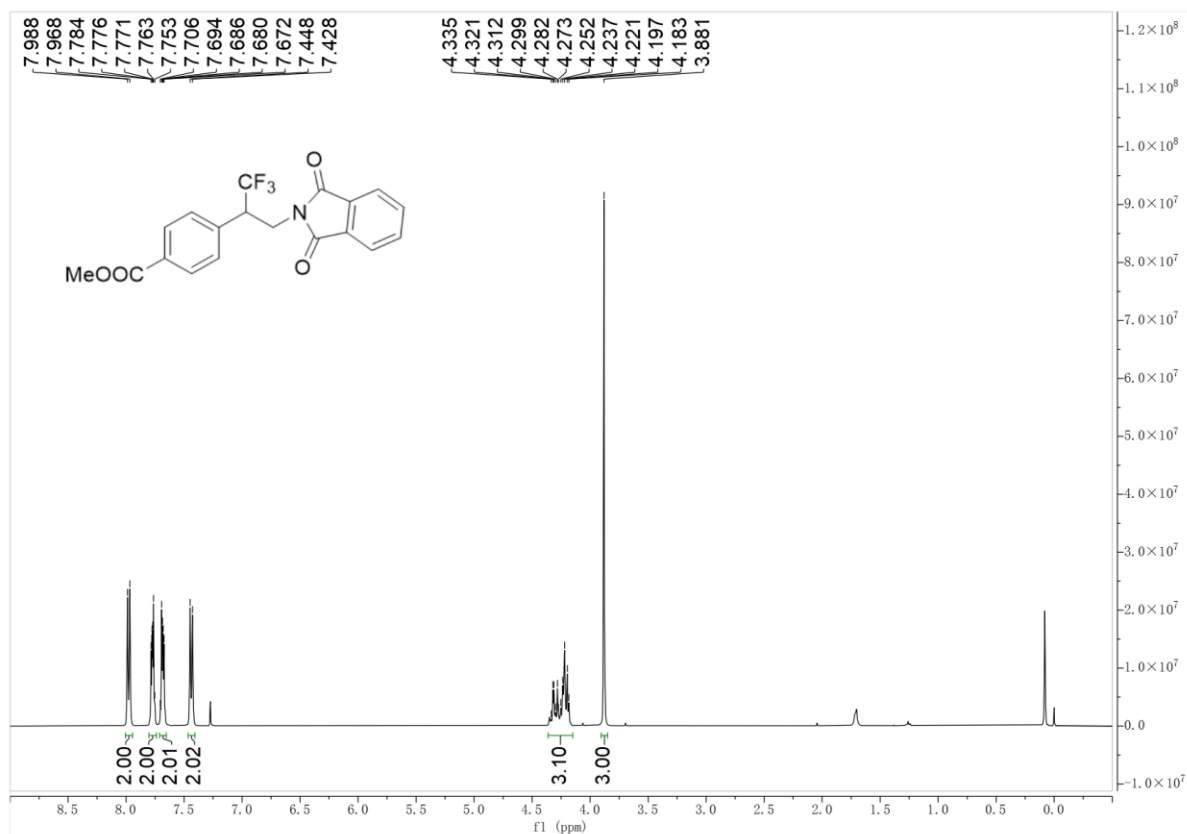
1: TOF MS ES+  
 1.19e+004



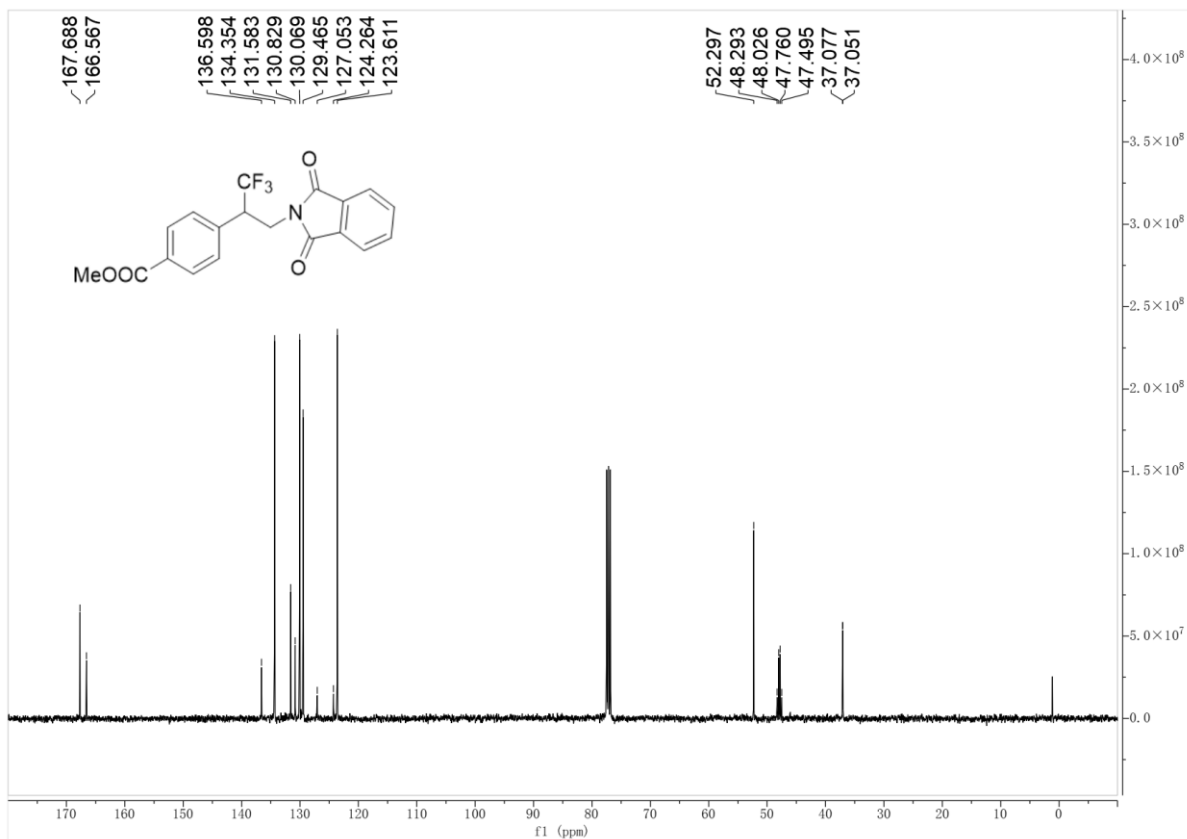
Minimum: -1.5  
 Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
497.8935	497.8928	0.7	1.4	10.5	425.8	n/a	n/a	C17 H10 N 02 F3 Na Br2

**<sup>1</sup>H NMR spectrum of 3i (400 MHz, CDCl<sub>3</sub>)**



**<sup>13</sup>C NMR spectrum of 3i (100 MHz, CDCl<sub>3</sub>)**



## HRMS (ESI) spectrum of 3i

Monoisotopic Mass, Even Electron Ions

2343 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

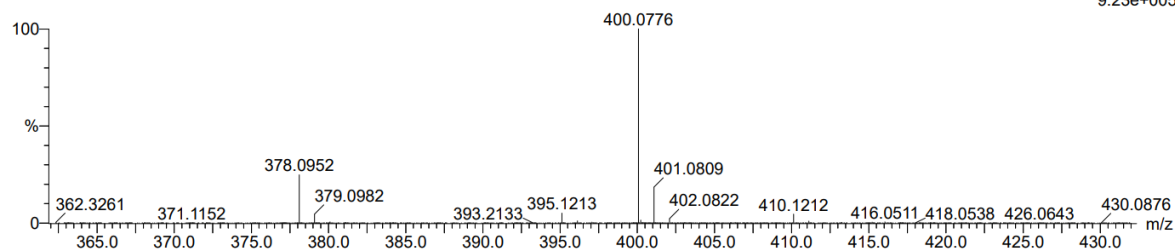
Elements Used:

C: 19-191 H: 14-14 N: 0-100 O: 0-100 F: 3-6 Na: 0-2

32

240511-2-10 14 (0.110)

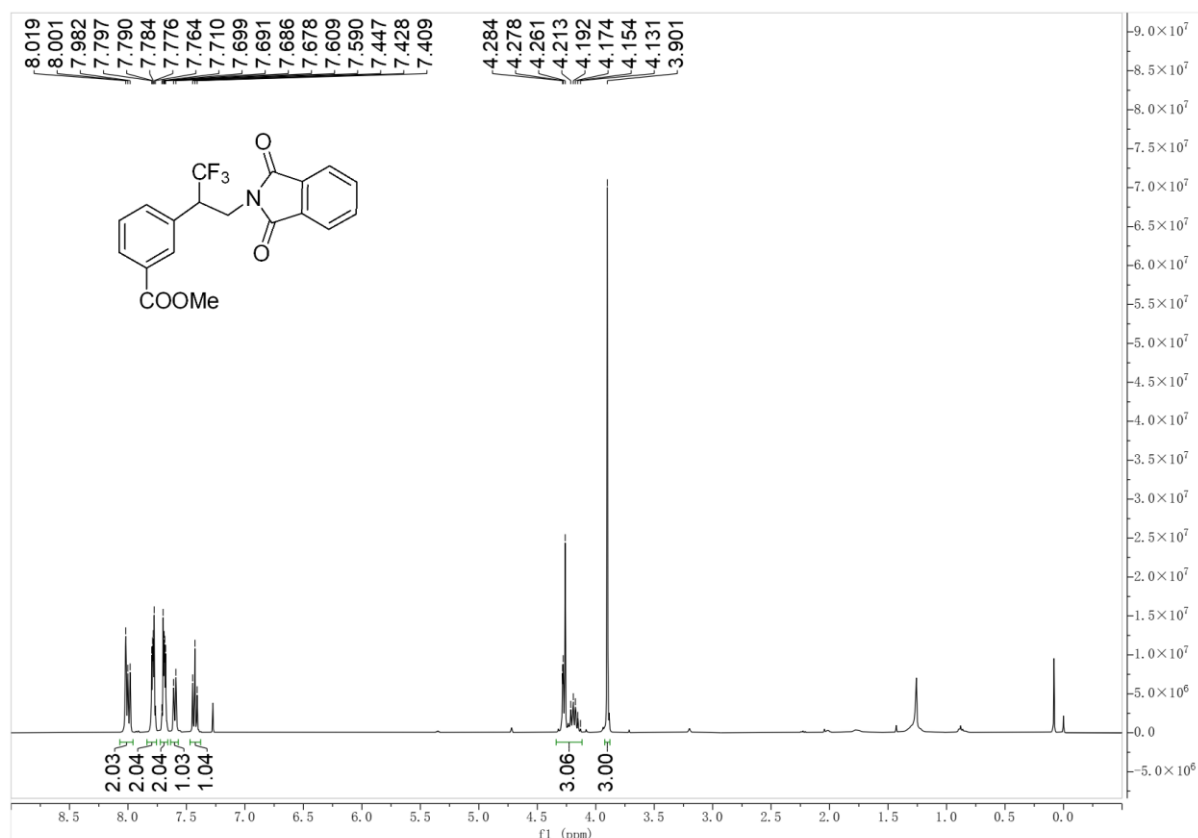
1: TOF MS ES+  
9.23e+005



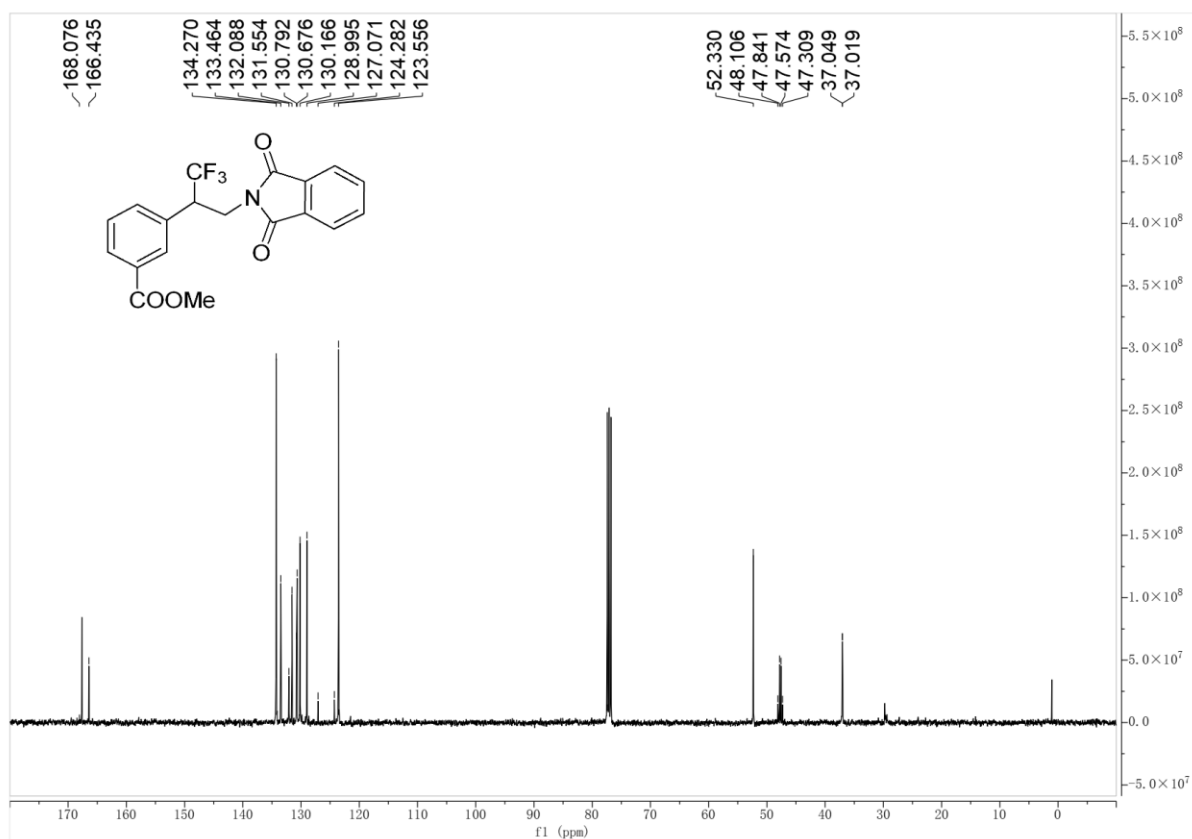
Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
400.0776	400.0773	0.3	0.7	11.5	660.5	n/a	n/a	C19 H14 N O4 F3 Na

## <sup>1</sup>H NMR spectrum of 3j (400 MHz, CDCl<sub>3</sub>)



**<sup>13</sup>C NMR spectrum of 3j (100 MHz, CDCl<sub>3</sub>)**



**HRMS (ESI) spectrum of 3j**

Monoisotopic Mass, Even Electron Ions

2361 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

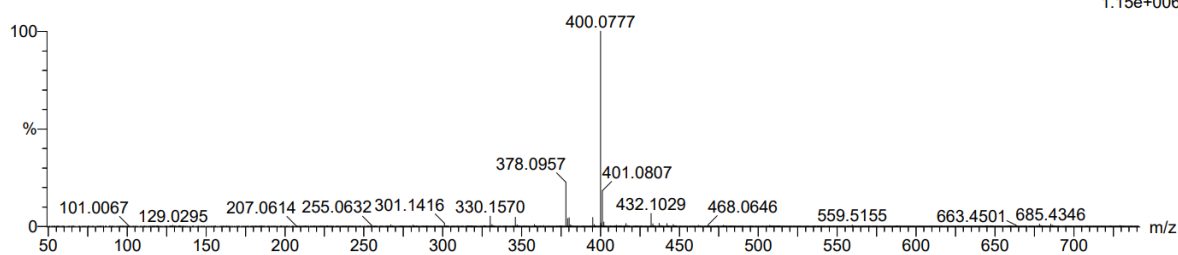
Elements Used:

C: 19-19 H: 14-14 N: 0-100 O: 0-100 F: 3-6 Na: 0-2

32

240511-2-6 16 (0.121)

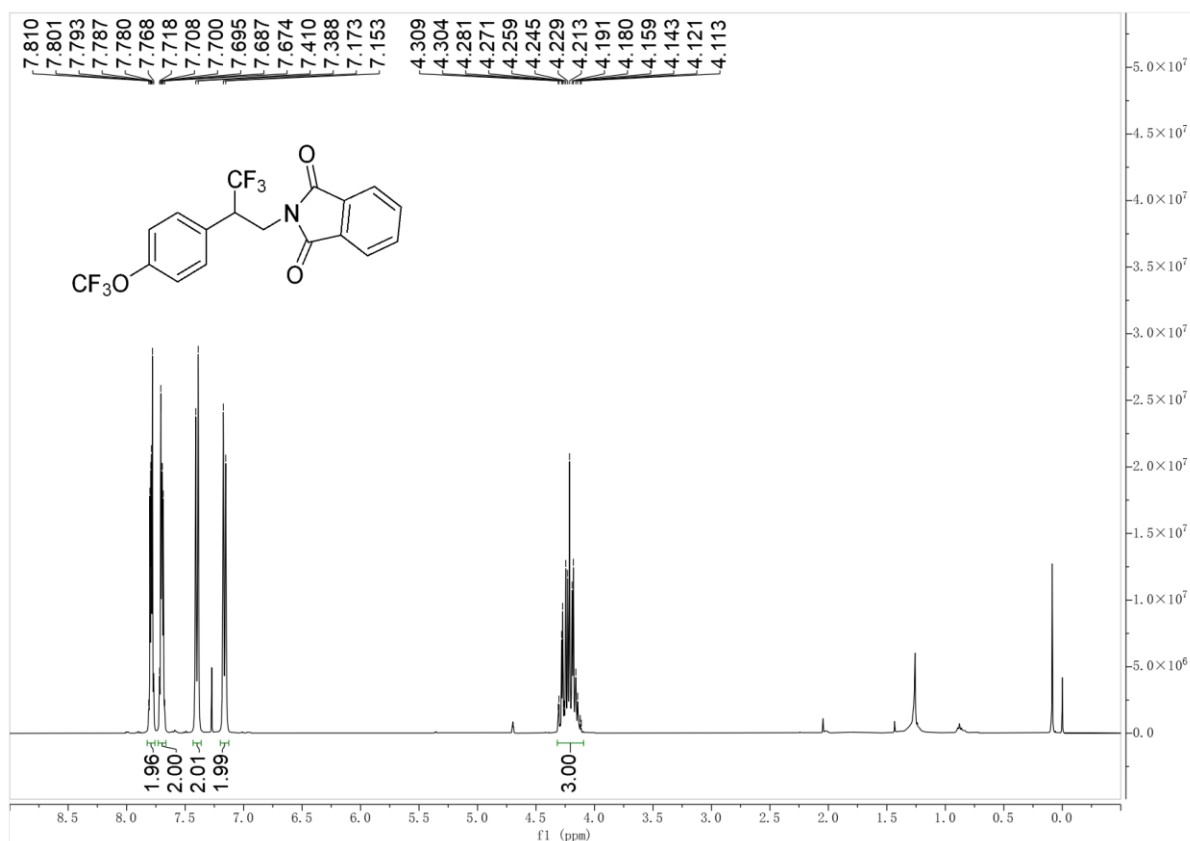
1: TOF MS ES+  
1.15e+006



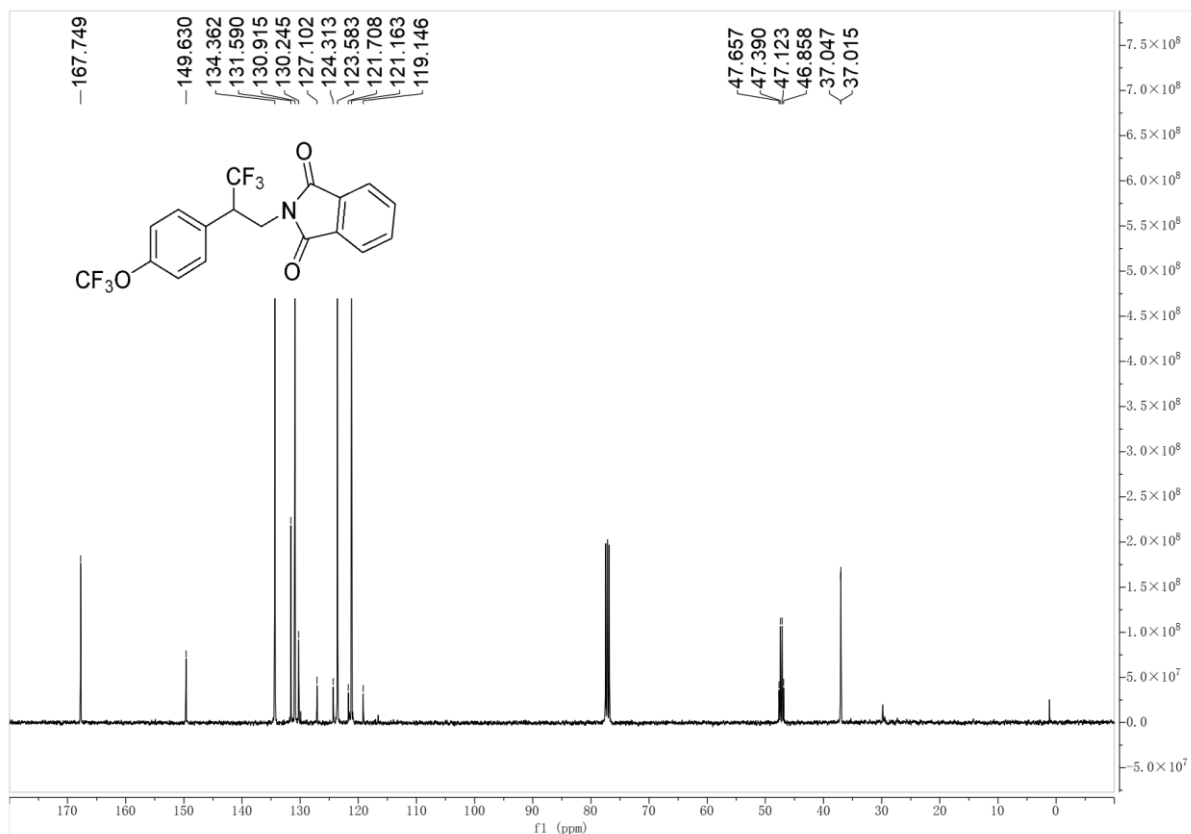
Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
400.0777	400.0773	0.4	1.0	11.5	738.9	n/a	n/a	C <sub>19</sub> H <sub>14</sub> N <sub>04</sub> F <sub>3</sub> Na

**<sup>1</sup>H NMR spectrum of 3k (400 MHz, CDCl<sub>3</sub>)**



**<sup>13</sup>C NMR spectrum of 3k (100 MHz, CDCl<sub>3</sub>)**



## HRMS (ESI) spectrum of 3k

Monoisotopic Mass, Even Electron Ions

2383 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

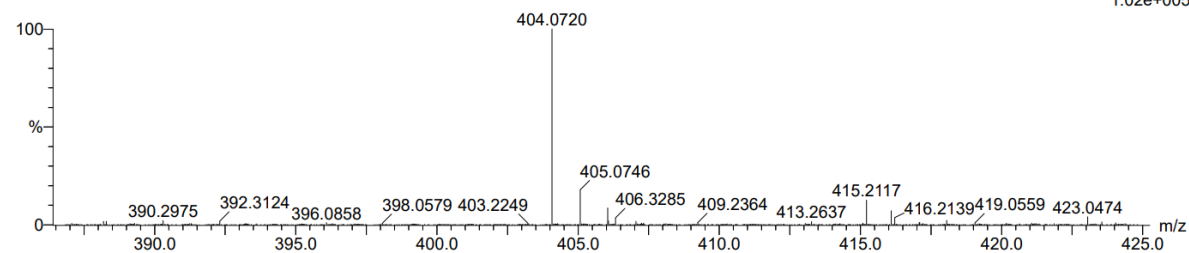
Elements Used:

C: 18-18 H: 12-12 N: 0-100 O: 0-100 F: 3-6 Na: 0-2

32

240511-2-16 12 (0.100)

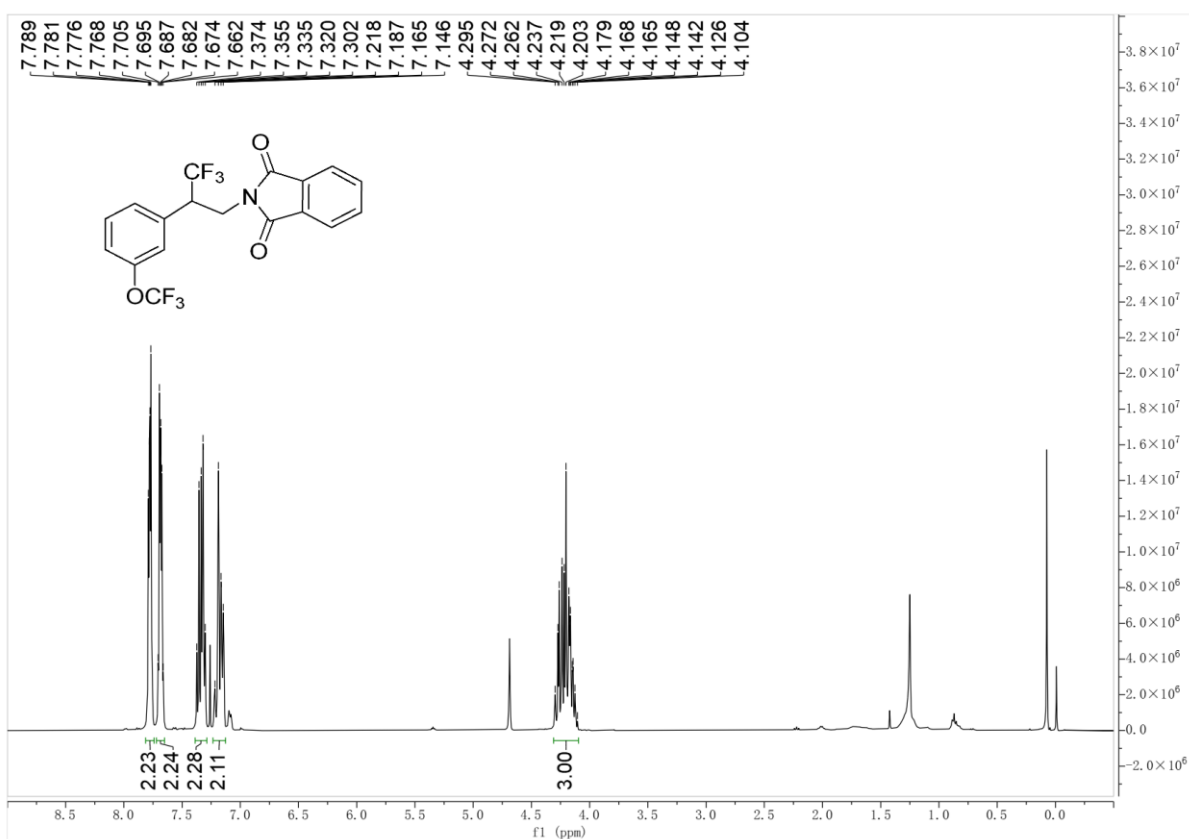
1: TOF MS ES+  
1.02e+005



Minimum: -1.5  
Maximum: 50.0

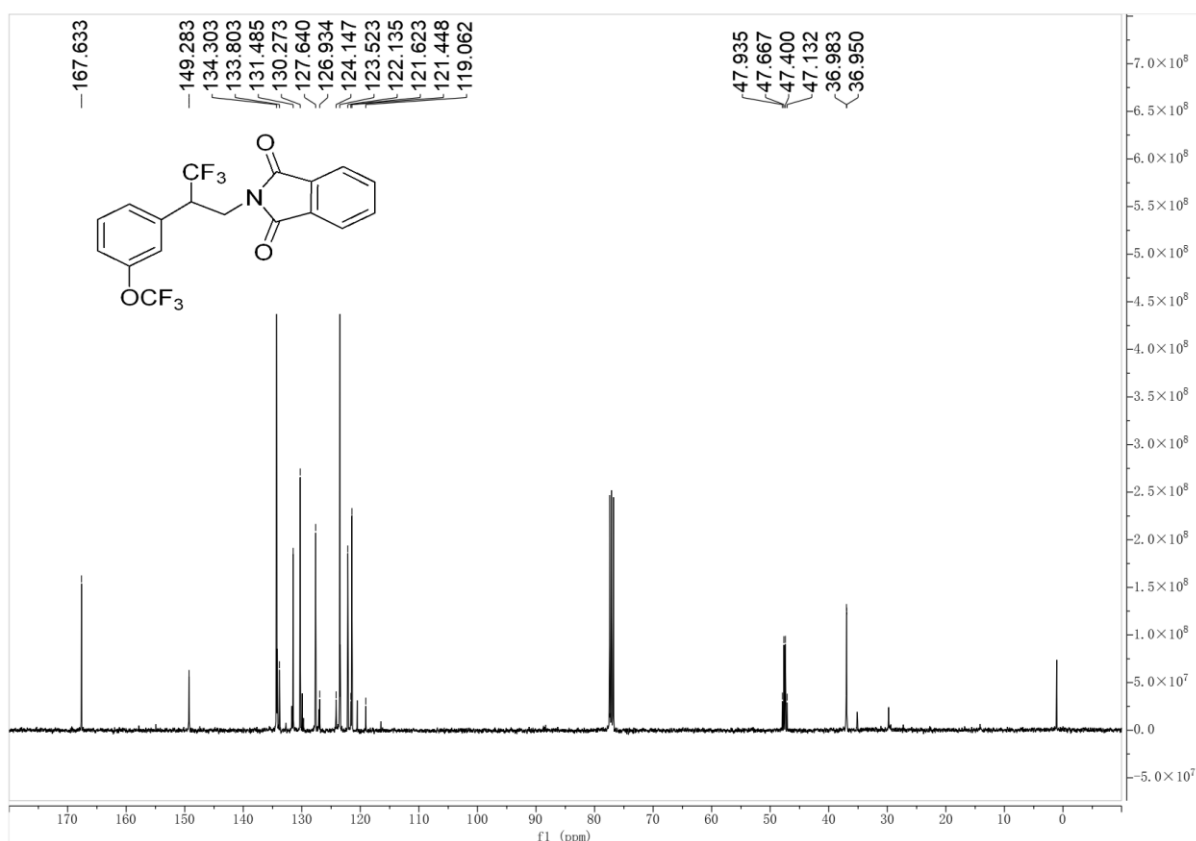
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
404.0720	404.0721	-0.1	-0.2	10.5	626.4	n/a	n/a	C18 H12 N O3 F6

## <sup>1</sup>H NMR spectrum of 3l (400 MHz, CDCl<sub>3</sub>)





**<sup>13</sup>C NMR spectrum of 3l (100 MHz, CDCl<sub>3</sub>)**



**HRMS (ESI) spectrum of 3l**

Monoisotopic Mass, Even Electron Ions

2696 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

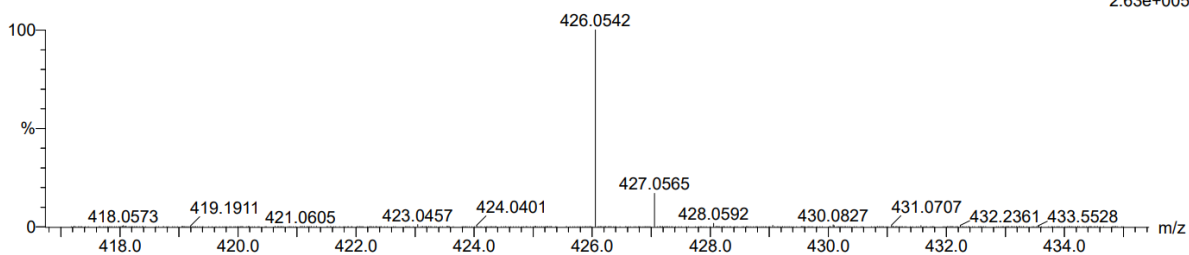
Elements Used:

C: 18-18 H: 11-11 N: 0-100 O: 0-100 F: 3-6 Na: 0-2

32

240511-2-3 12 (0.100)

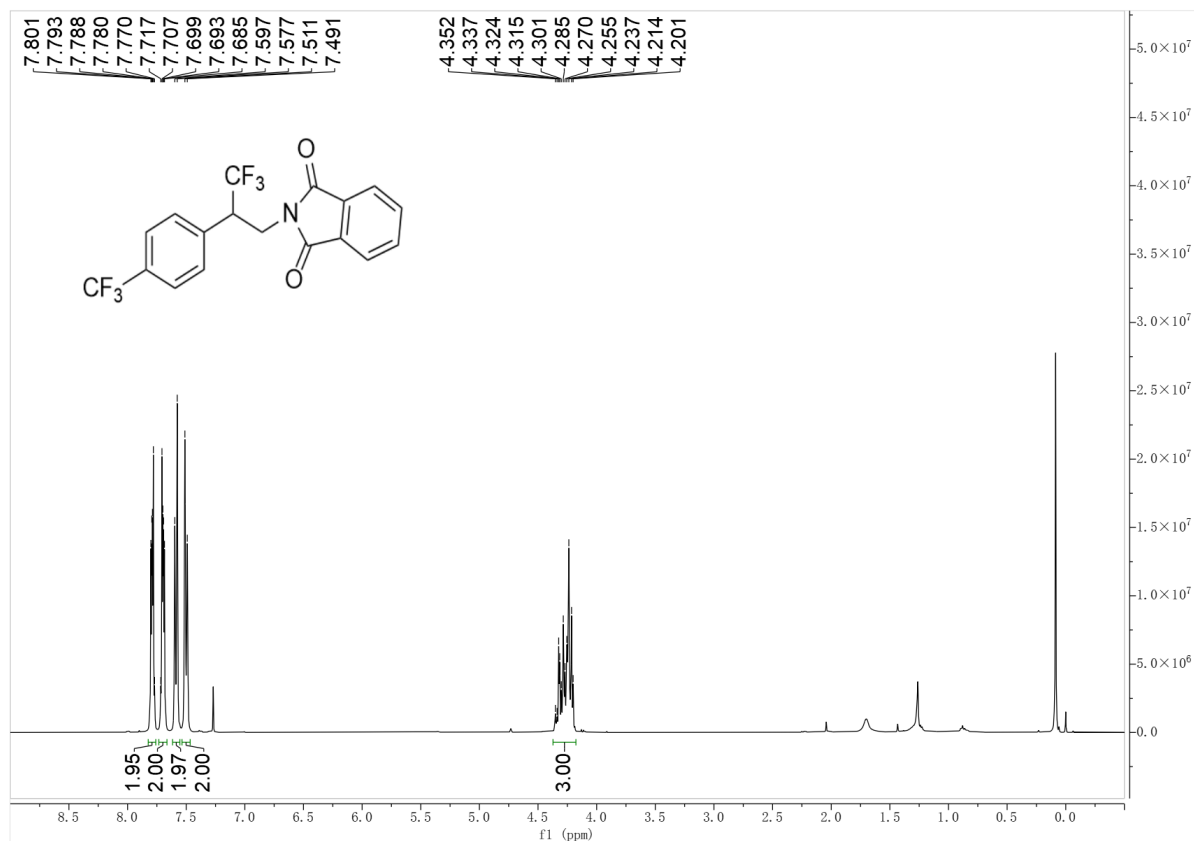
1: TOF MS ES+  
2.63e+005



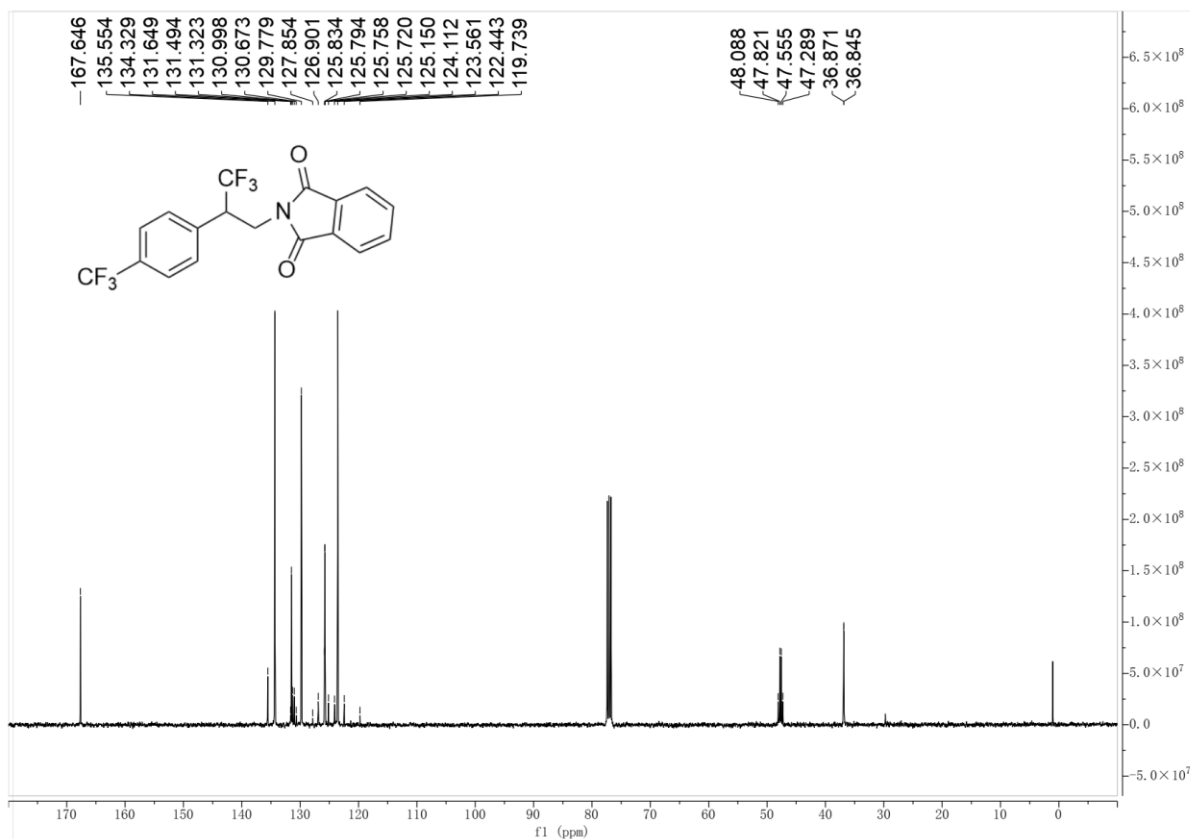
Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
426.0542	426.0541	0.1	0.2	10.5	578.6	n/a	n/a	C <sub>18</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub> F <sub>6</sub> Na

**<sup>1</sup>H NMR spectrum of 3m (400 MHz, CDCl<sub>3</sub>)**



**<sup>13</sup>C NMR spectrum of 3m (100 MHz, CDCl<sub>3</sub>)**



## HRMS (ESI) spectrum of 3m

Monoisotopic Mass, Even Electron Ions

522 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

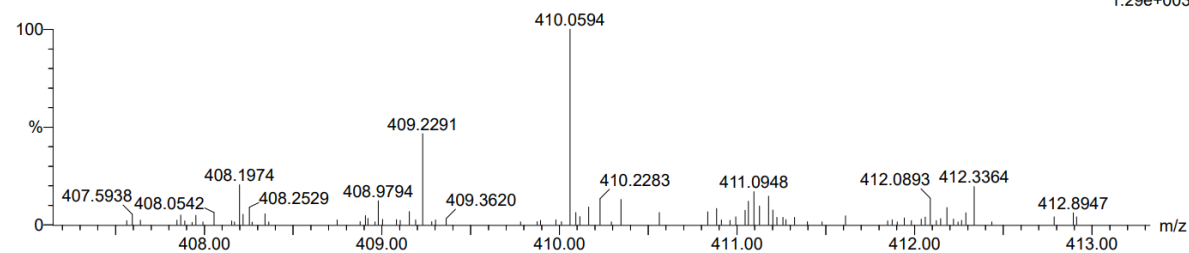
Elements Used:

C: 18-18 H: 11-11 N: 0-100 O: 0-100 F: 6-6 Na: 0-2

37

240511-2-1 9 (0.084)

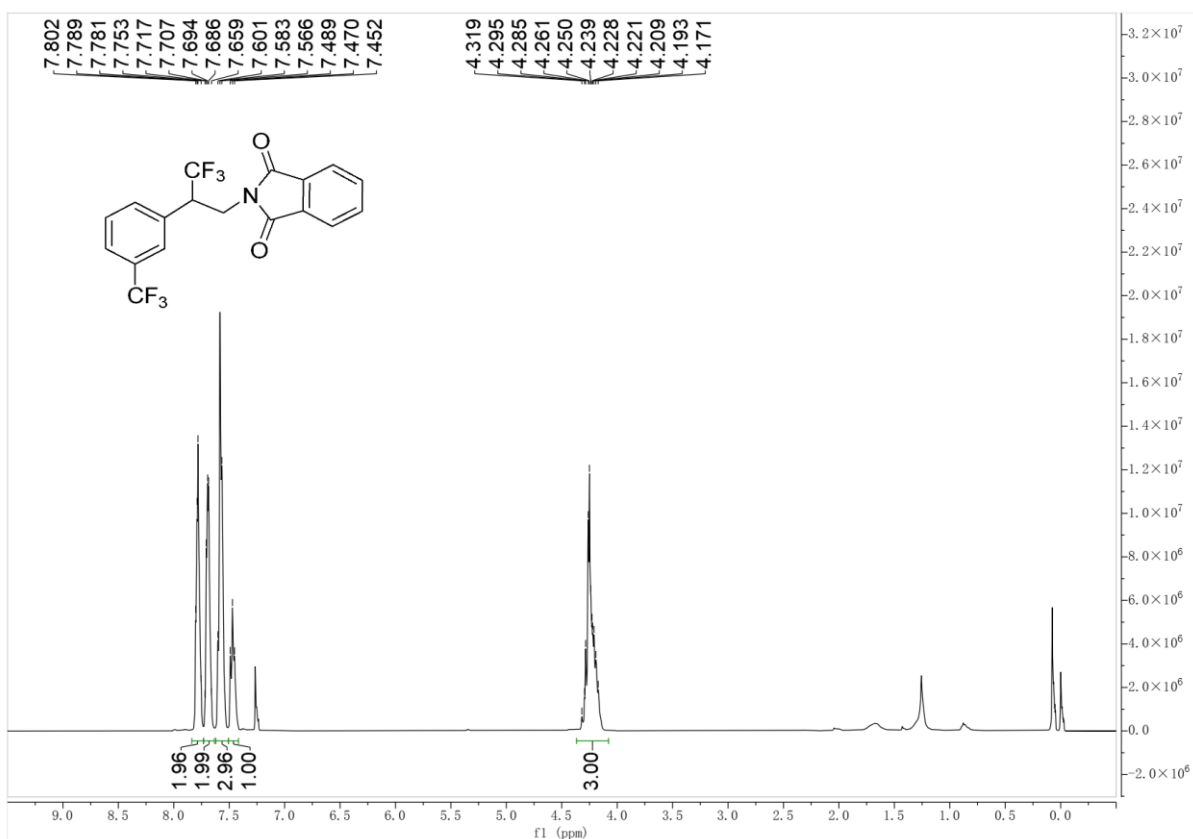
1: TOF MS ES+  
1.29e+003



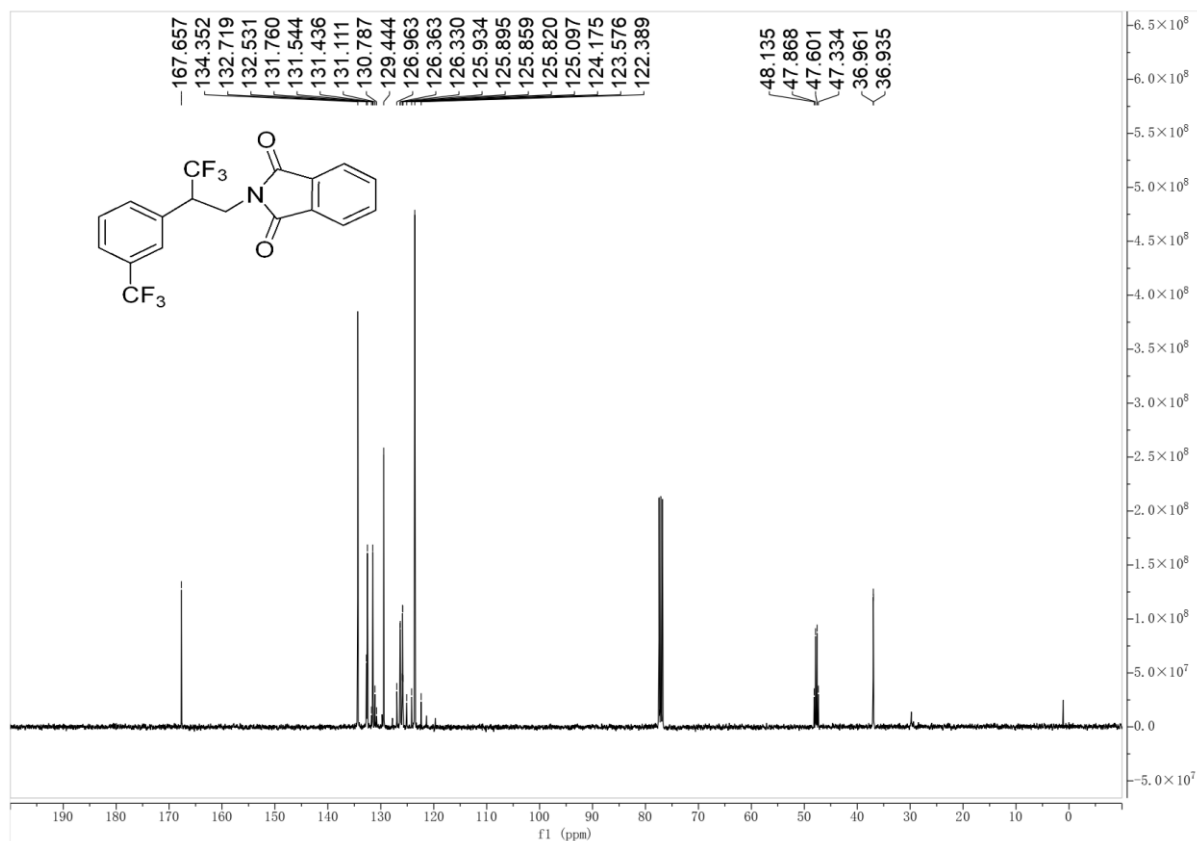
Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
410.0594	410.0592	0.2	0.5	10.5	335.5	n/a	n/a	C18 H11 N O2 F6 Na

## <sup>1</sup>H NMR spectrum of 3n (400 MHz, CDCl<sub>3</sub>)



**<sup>13</sup>C NMR spectrum of 3n (100 MHz, CDCl<sub>3</sub>)**



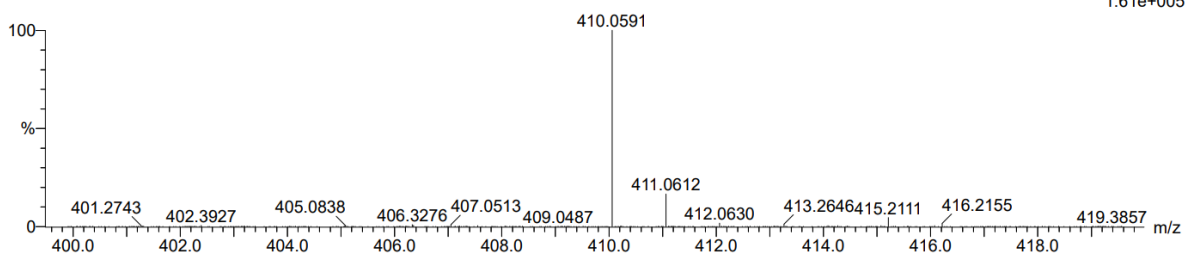
**HRMS (ESI) spectrum of 3n**

Monoisotopic Mass, Even Electron Ions  
 2470 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)  
 Elements Used:

C: 18-18 H: 11-11 N: 0-100 O: 0-100 F: 3-6 Na: 0-2

32  
 240511-2-8 11 (0.094)

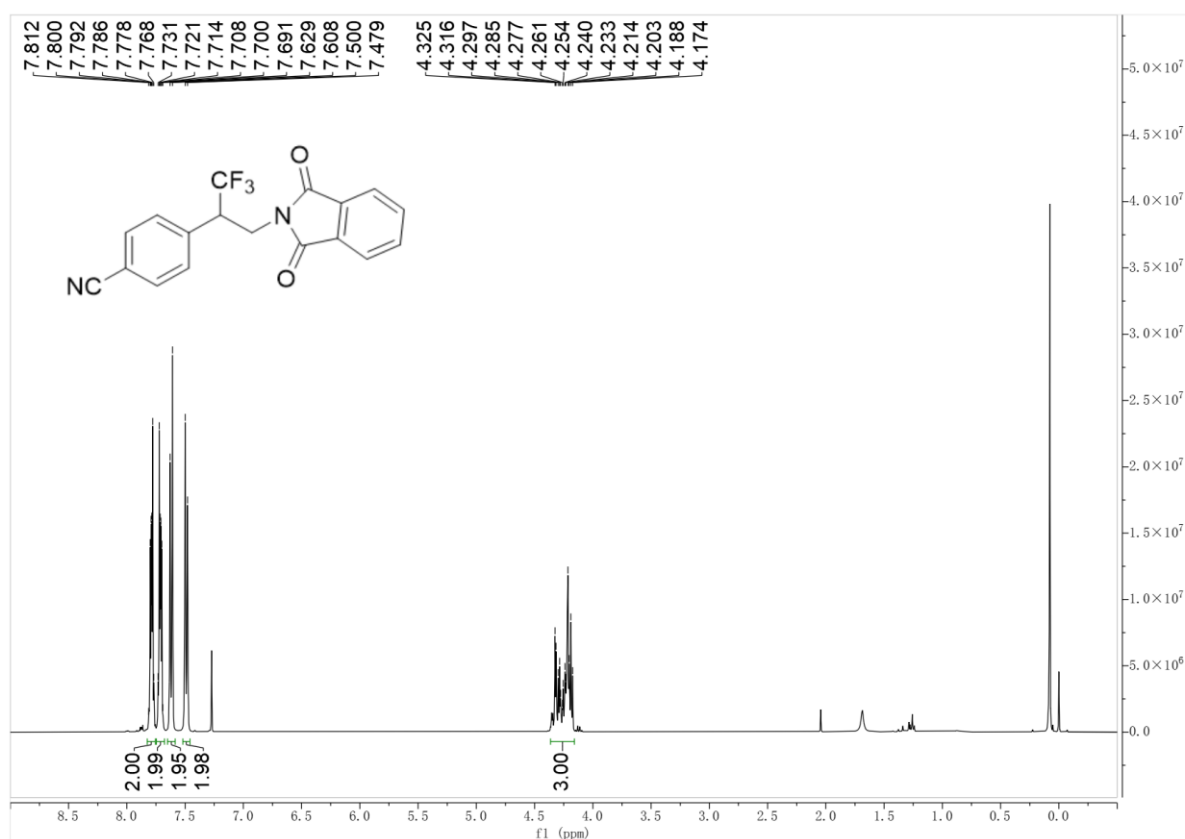
1: TOF MS ES+  
 1.61e+005



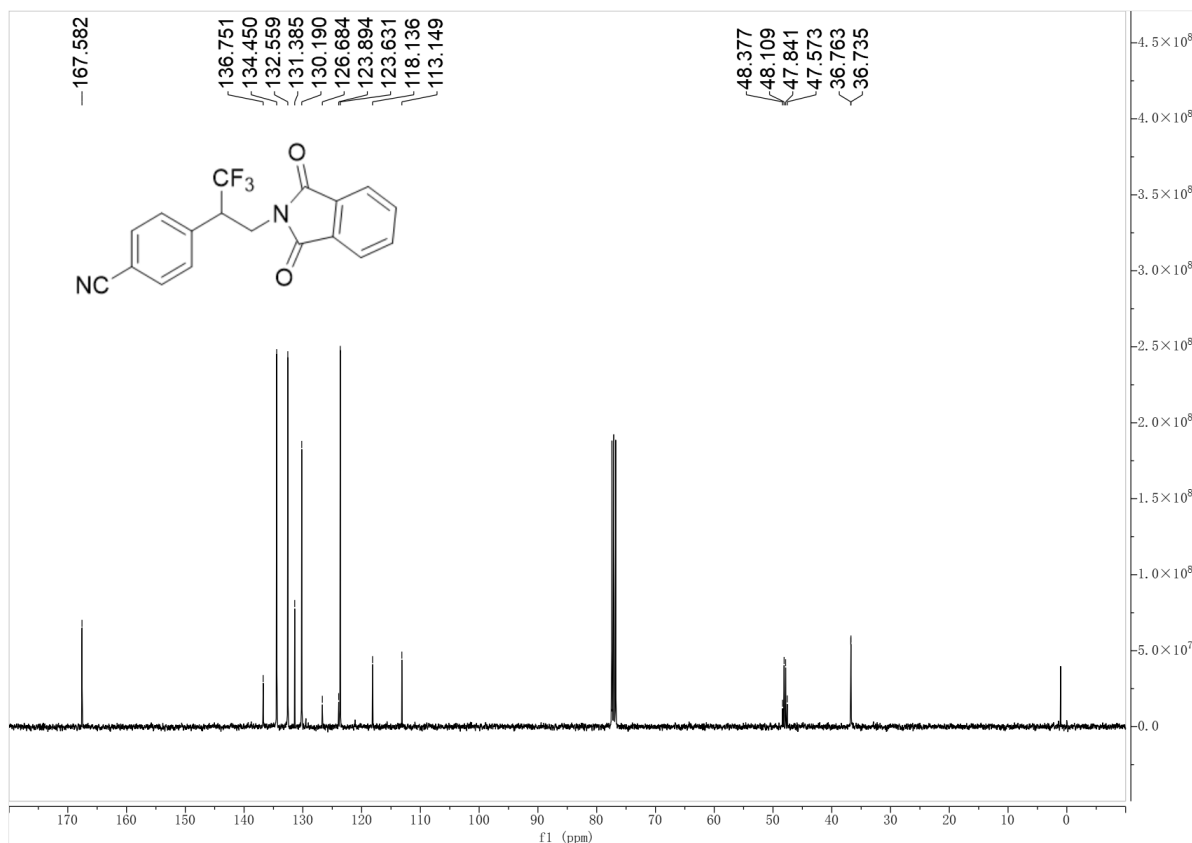
Minimum: -1.5  
 Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
410.0591	410.0592	-0.1	-0.2	10.5	497.9	n/a	n/a	C18 H11 N O2 F6 Na

**<sup>1</sup>H NMR spectrum of 3o (400 MHz, CDCl<sub>3</sub>)**



**<sup>13</sup>C NMR spectrum of 3o (100 MHz, CDCl<sub>3</sub>)**



## HRMS (ESI) spectrum of 3o

Monoisotopic Mass, Even Electron Ions

1916 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

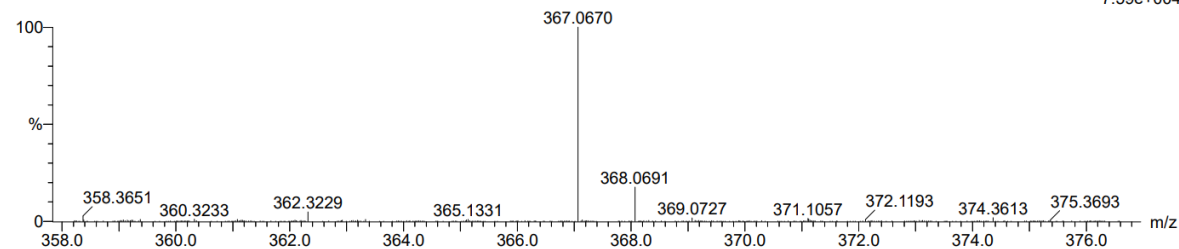
Elements Used:

C: 18-18 H: 11-11 N: 0-100 O: 0-100 F: 3-6 Na: 0-2

32

240511-2-13 10 (0.089)

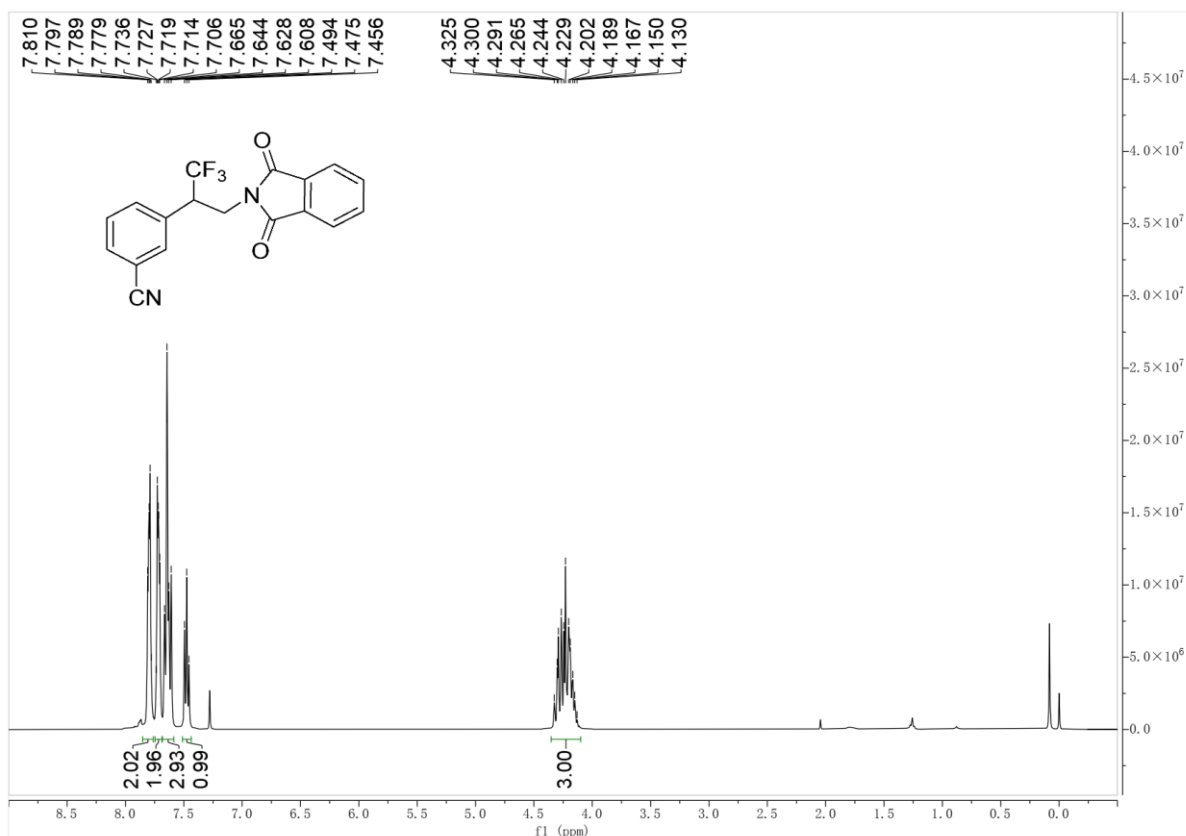
1: TOF MS ES+  
7.59e+004



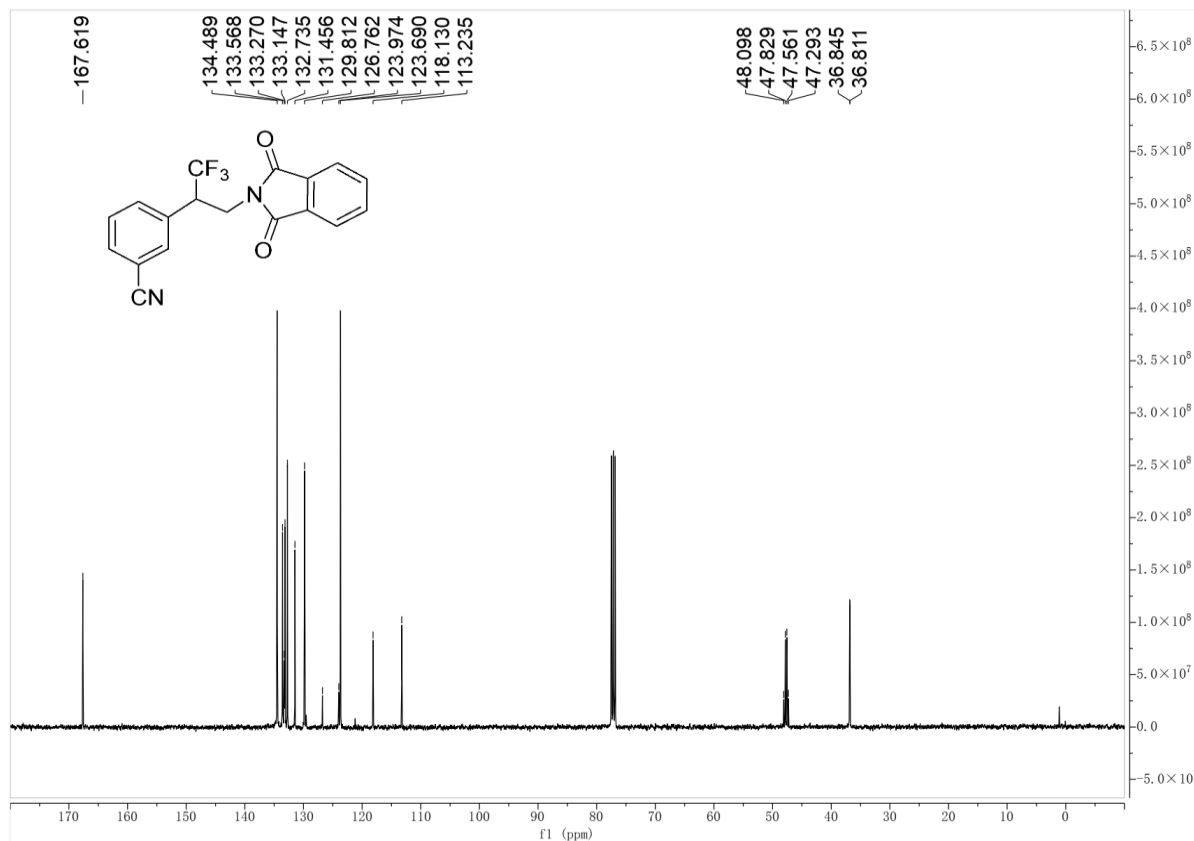
Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
367.0670	367.0670	0.0	0.0	12.5	446.2	n/a	n/a	C18 H11 N2 O2 F3 Na

## <sup>1</sup>H NMR spectrum of 3p (400 MHz, CDCl<sub>3</sub>)



**<sup>13</sup>C NMR spectrum of 3p (100 MHz, CDCl<sub>3</sub>)**



**HRMS (ESI) spectrum of 3p**

Monoisotopic Mass, Even Electron Ions  
 1916 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

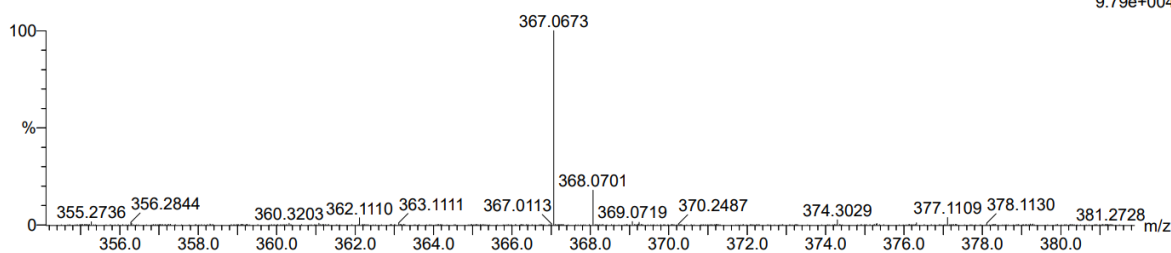
Elements Used:

C: 18-18 H: 11-11 N: 0-100 O: 0-100 F: 3-6 Na: 0-2

32

240511-2-14 20 (0.142)

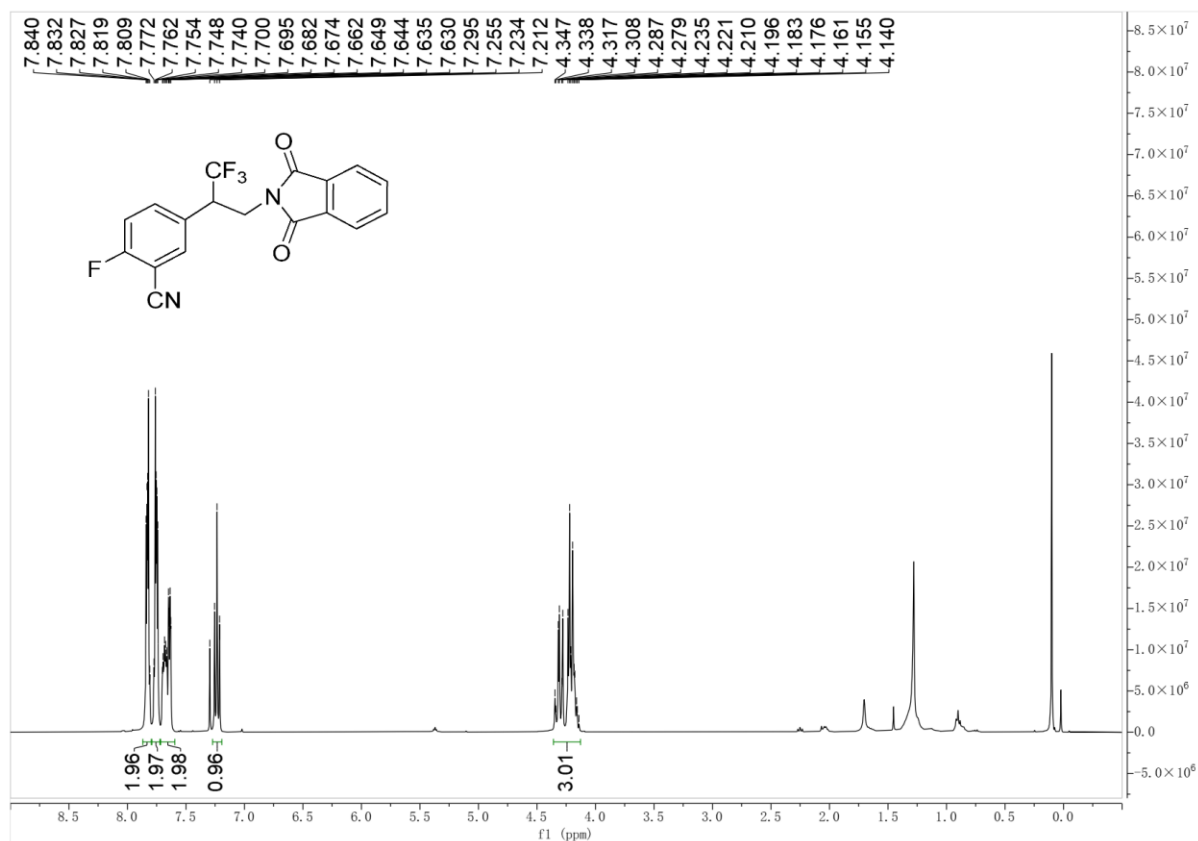
1: TOF MS ES+  
 9.79e+004



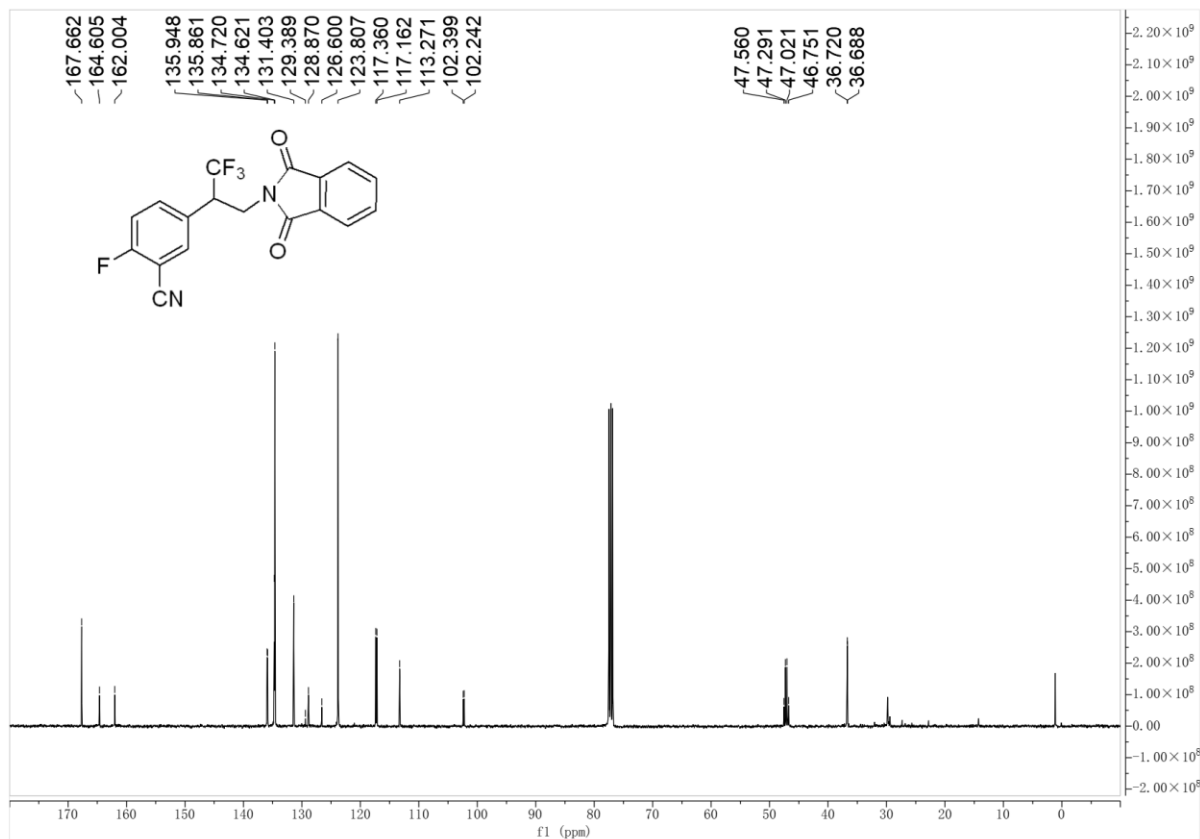
Minimum: -1.5  
 Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
367.0673	367.0670	0.3	0.8	12.5	369.7	n/a	n/a	C18 H11 N2 O2 F3 Na

**<sup>1</sup>H NMR spectrum of 3q (400 MHz, CDCl<sub>3</sub>)**



**<sup>13</sup>C NMR spectrum of 3q (100 MHz, CDCl<sub>3</sub>)**





## HRMS (ESI) spectrum of 3q

Monoisotopic Mass, Even Electron Ions

2140 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

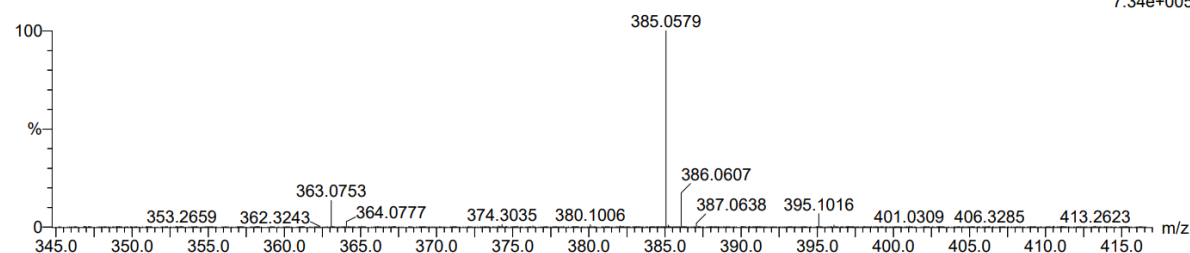
Elements Used:

C: 18-18 H: 10-10 N: 0-100 O: 0-100 F: 3-6 Na: 0-2

32

240511-2-20 16 (0.121)

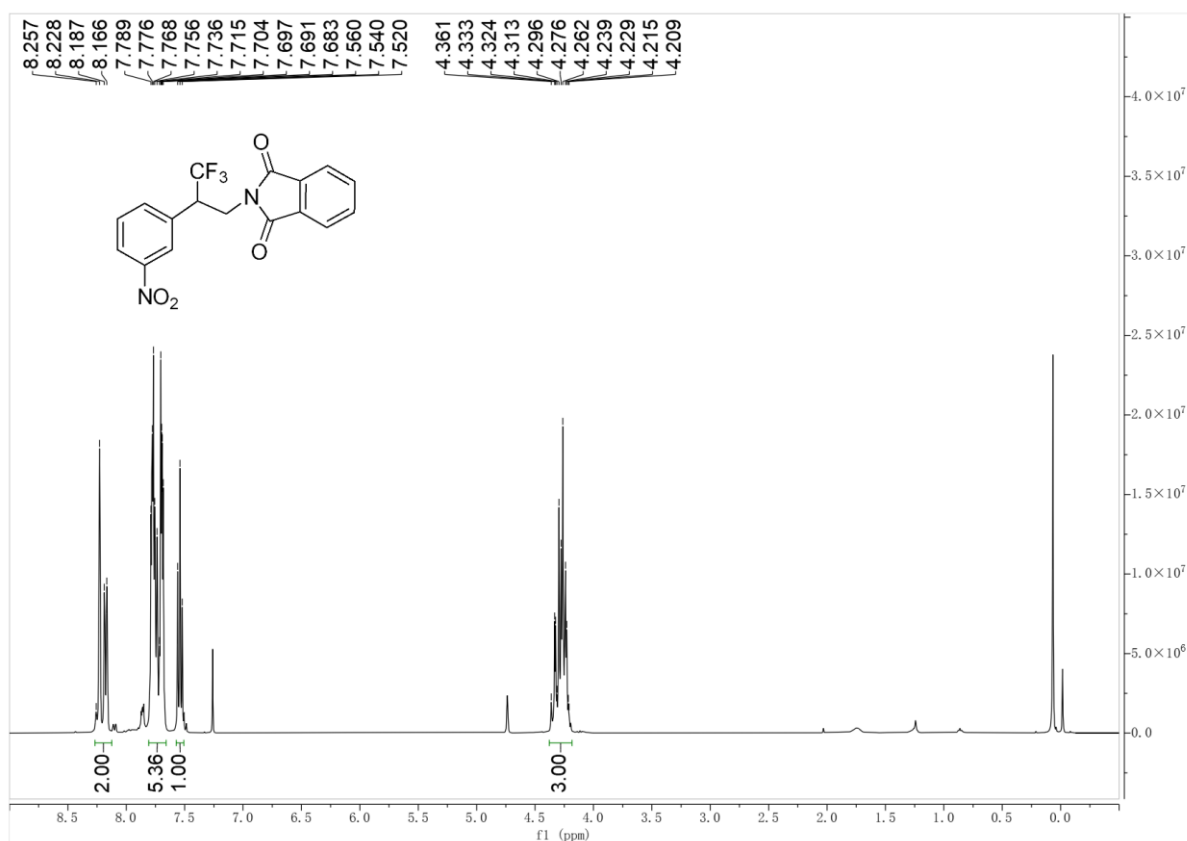
1: TOF MS ES+  
7.34e+005



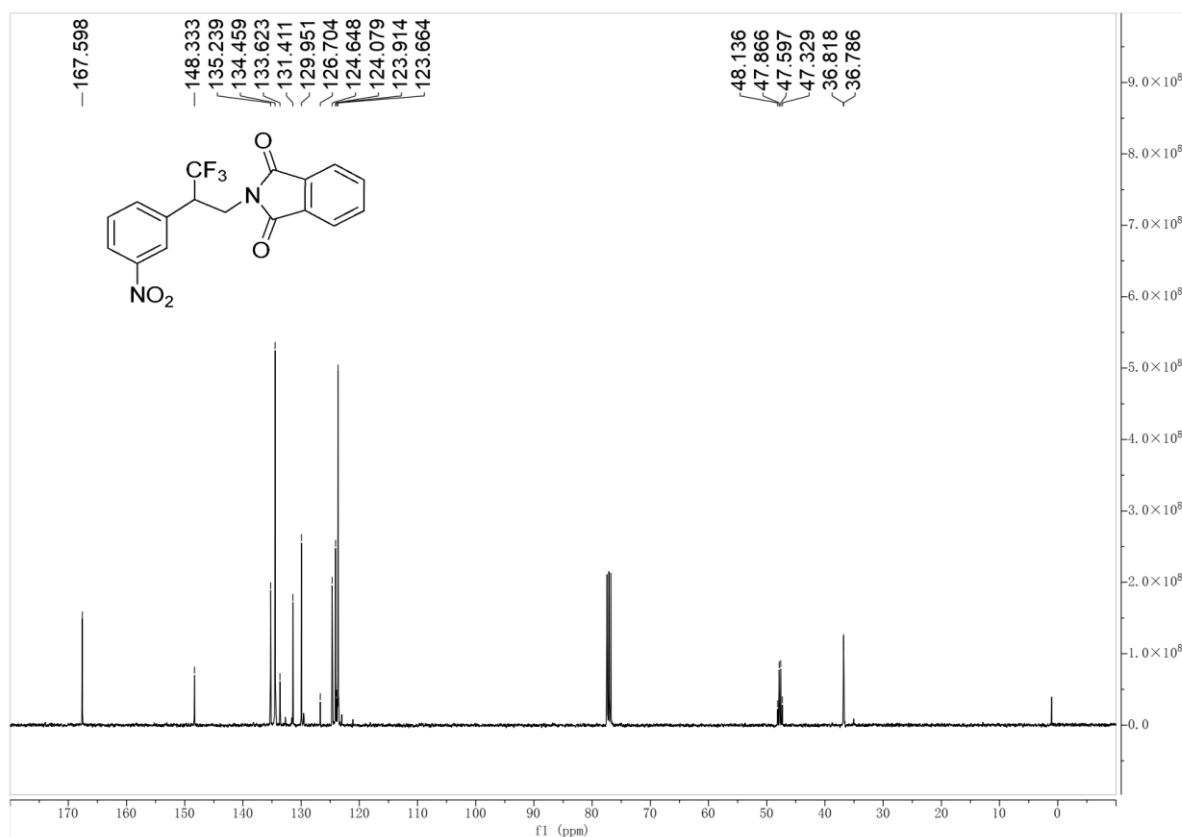
Minimum: -1.5  
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
385.0579	385.0576	0.3	0.8	12.5	627.3	n/a	n/a	C18 H10 N2 O2 F4 Na

## <sup>1</sup>H NMR spectrum of 3r (400 MHz, CDCl<sub>3</sub>)



**<sup>13</sup>C NMR spectrum of 3r (100 MHz, CDCl<sub>3</sub>)**



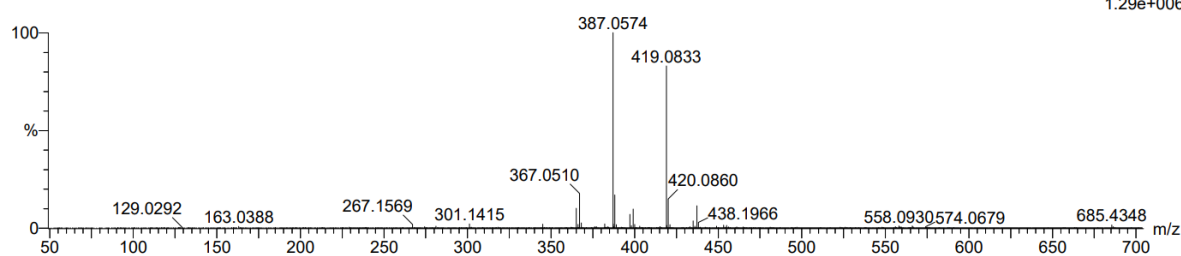
**HRMS (ESI) spectrum of 3r**

Monoisotopic Mass, Even Electron Ions  
 2126 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)  
 Elements Used:

C: 17-17 H: 11-11 N: 0-100 O: 0-100 F: 3-6 Na: 0-2

37  
 240511-2-2 11 (0.094)

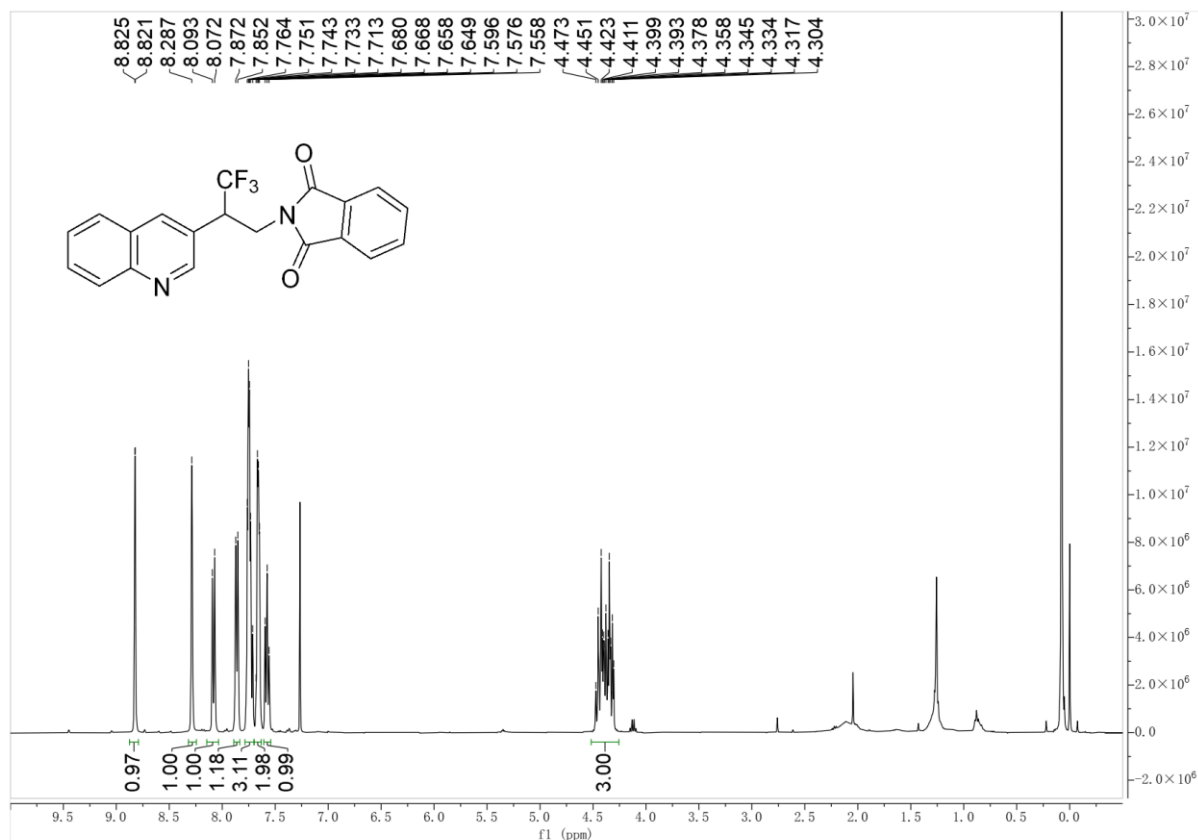
1: TOF MS ES+  
 1.29e+006



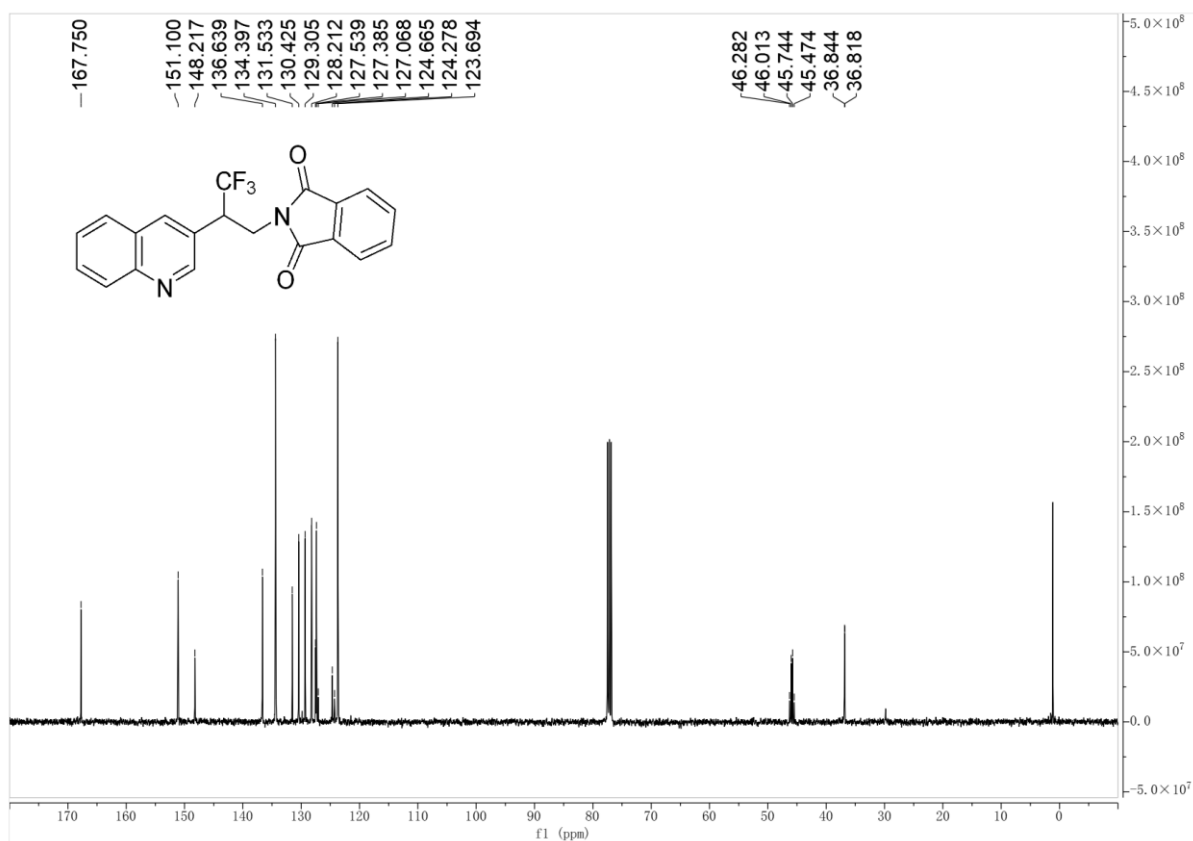
Minimum: -1.5  
 Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
387.0574	387.0569	0.5	1.3	11.5	737.1	n/a	n/a	C17 H11 N2 O4 F3 Na

**<sup>1</sup>H NMR spectrum of 3s (400 MHz, CDCl<sub>3</sub>)**



**<sup>13</sup>C NMR spectrum of 3s (100 MHz, CDCl<sub>3</sub>)**



## HRMS (ESI) spectrum of 3s

Monoisotopic Mass, Even Electron Ions

2021 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

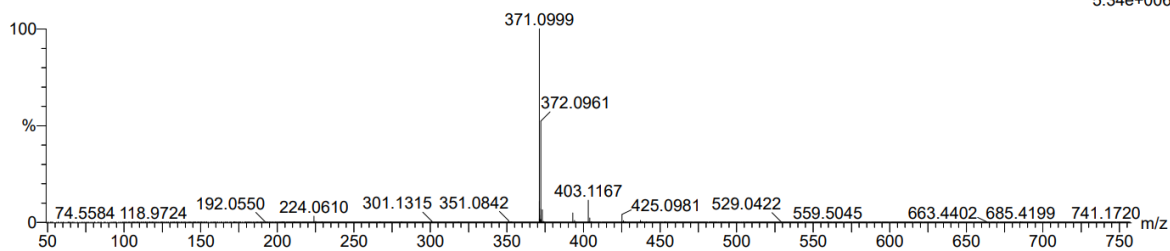
Elements Used:

C: 20-20 H: 14-14 N: 0-100 O: 0-100 F: 3-6 Na: 0-2

32

240511-2-4 10 (0.089)

1: TOF MS ES+  
5.34e+006

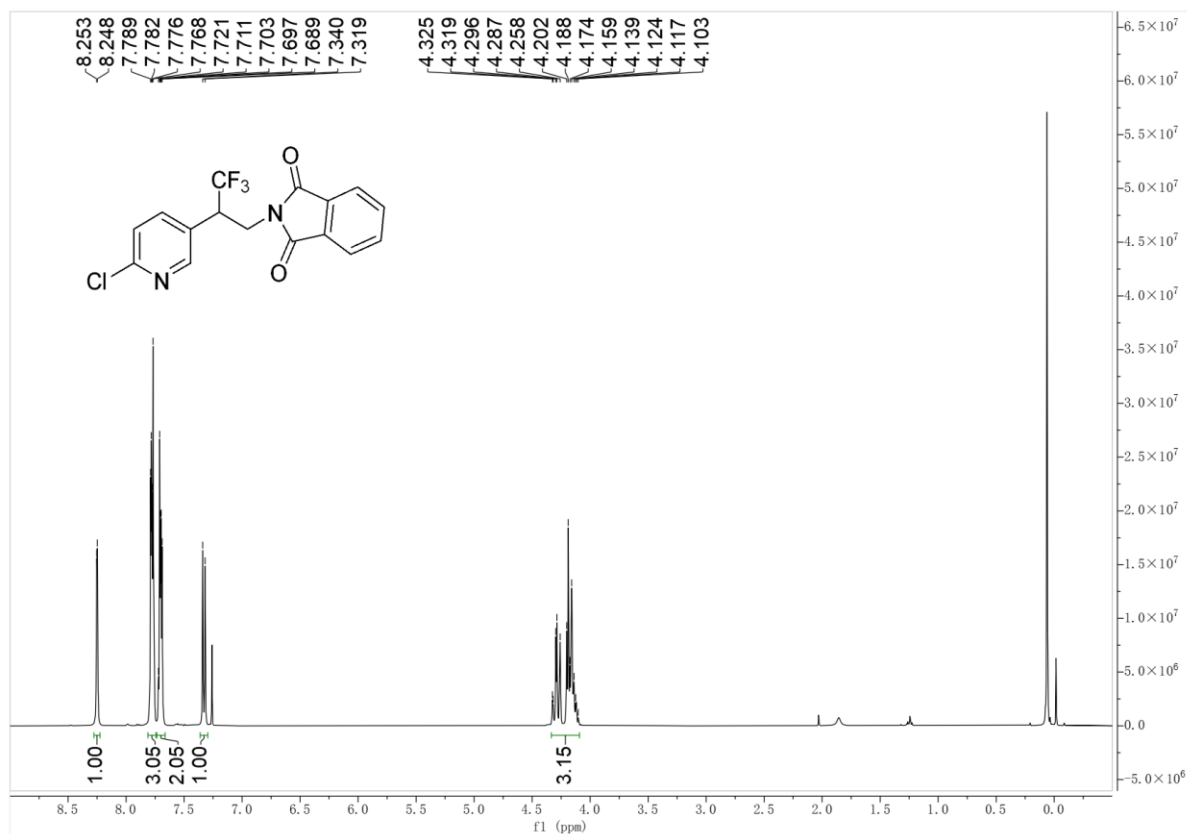


Minimum: -1.5

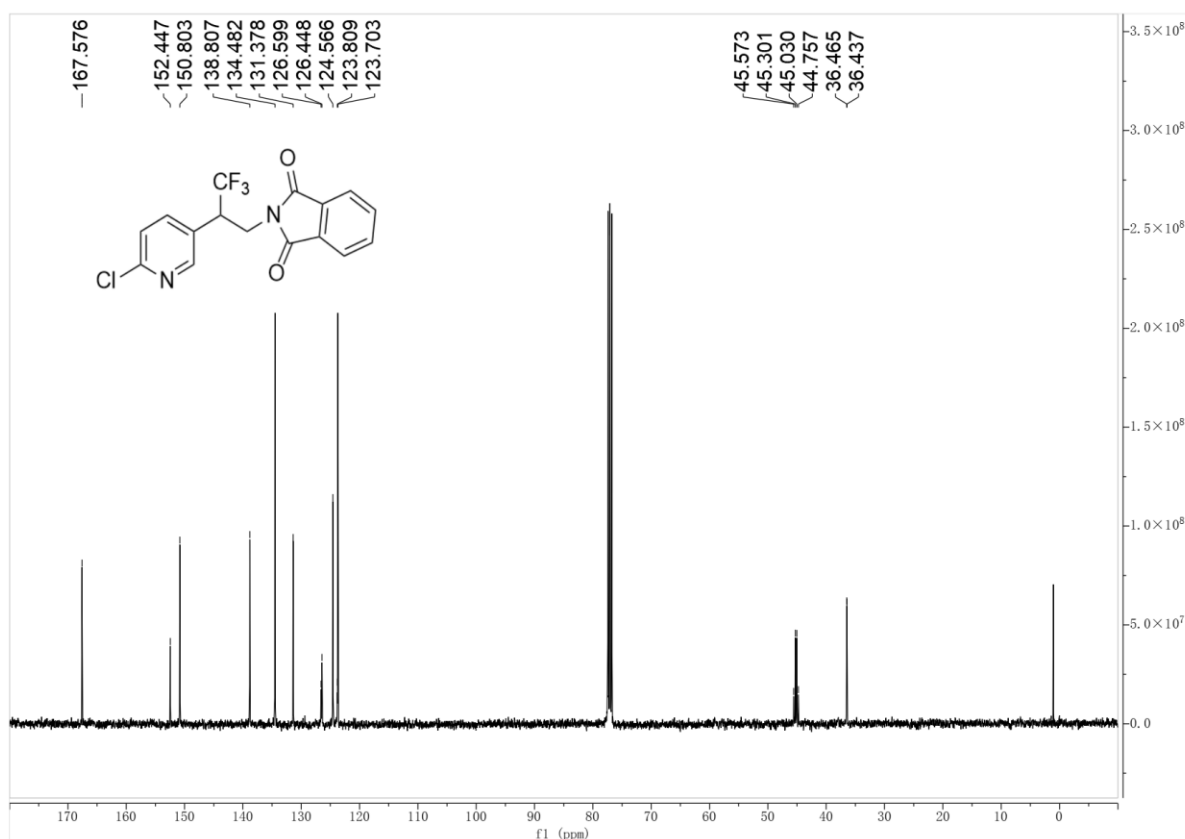
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
371.0999	371.1007	-0.8	-2.2	13.5	1044.7	n/a	n/a	C20 H14 N2 O2 F3

## <sup>1</sup>H NMR spectrum of 3t (400 MHz, CDCl<sub>3</sub>)



**<sup>13</sup>C NMR spectrum of 3t (100 MHz, CDCl<sub>3</sub>)**



**HRMS (ESI) spectrum of 3t**

Monoisotopic Mass, Even Electron Ions  
 3436 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

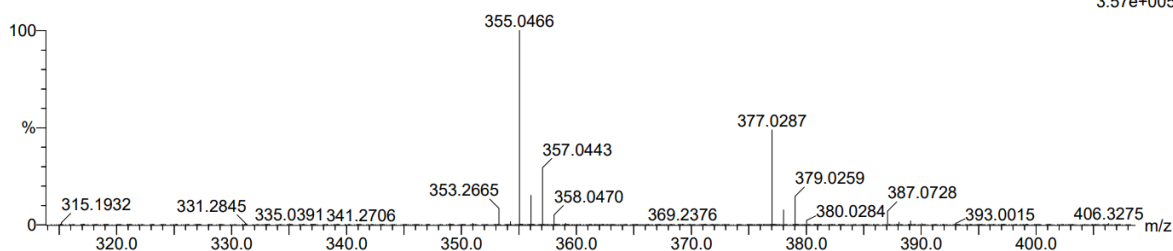
Elements Used:

C: 16-16 H: 11-11 N: 0-100 O: 0-100 F: 3-6 Na: 0-2 Cl: 1-4

32

240511-2-11 18 (0.131)

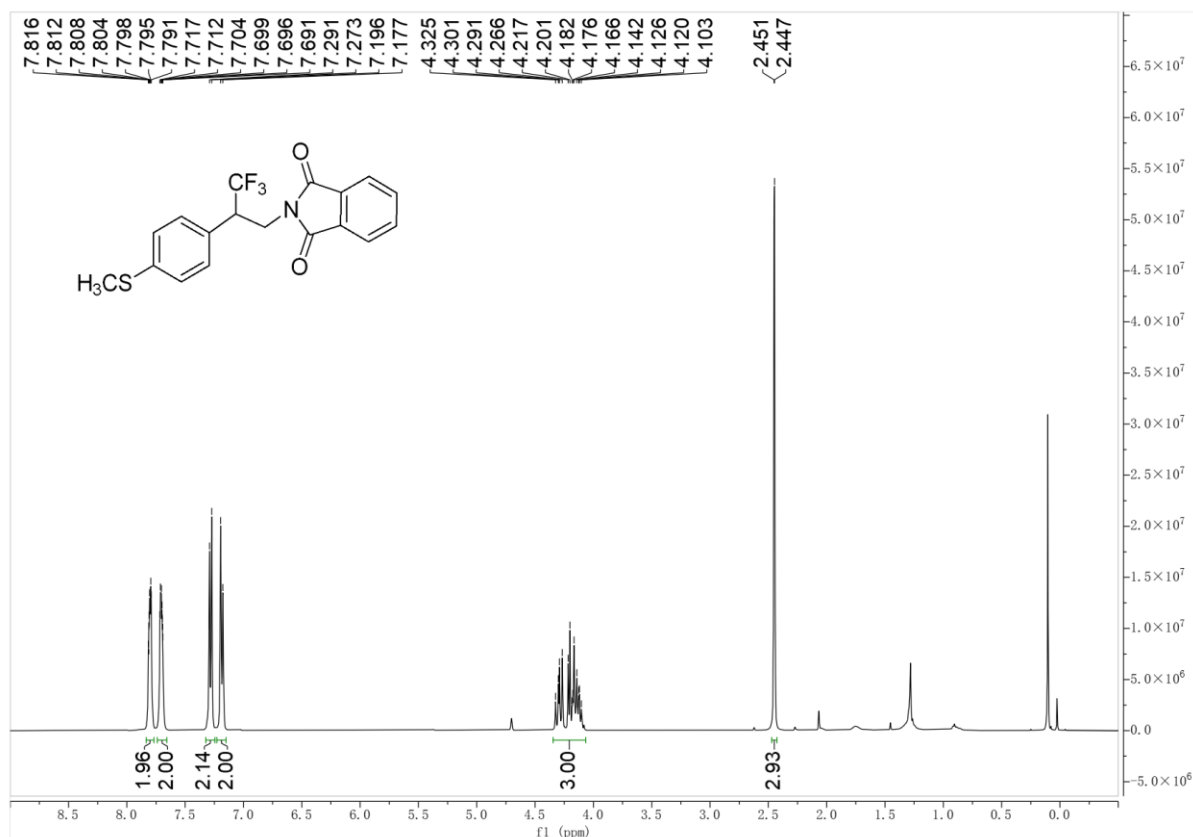
1: TOF MS ES+  
 3.57e+005



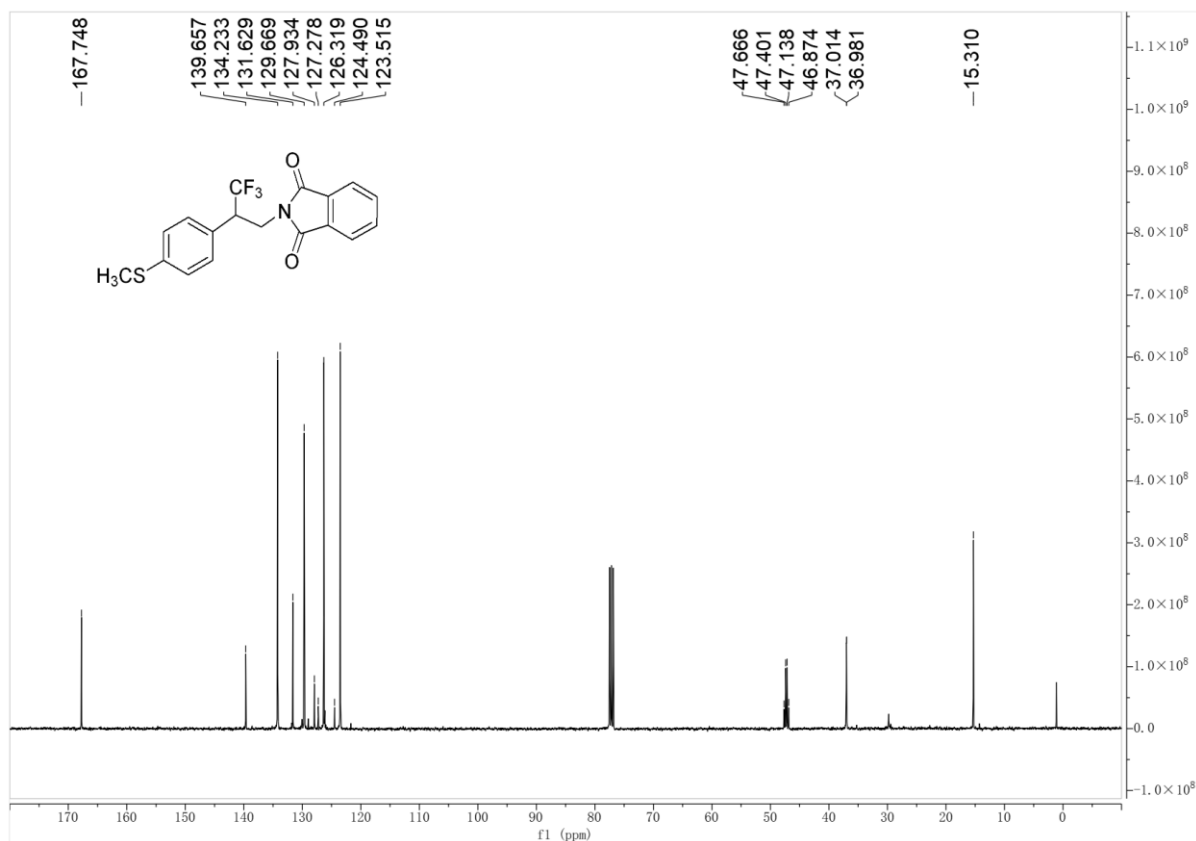
Minimum: -1.5  
 Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
355.0466	355.0461	0.5	1.4	10.5	571.5	n/a	n/a	C16 H11 N2 O2 F3 Cl

**<sup>1</sup>H NMR spectrum of 3u (400 MHz, CDCl<sub>3</sub>)**



**<sup>13</sup>C NMR spectrum of 3u (100 MHz, CDCl<sub>3</sub>)**



## HRMS (ESI) spectrum of 3u

Monoisotopic Mass, Even Electron Ions

1783 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

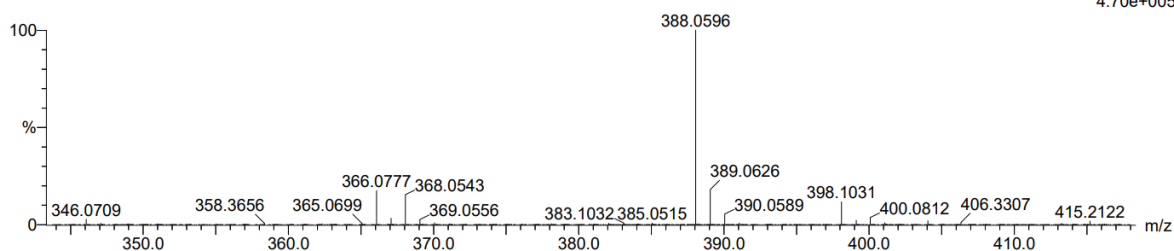
Elements Used:

C: 18-18 H: 14-14 N: 0-100 O: 0-100 F: 3-6 Na: 0-2 S: 1-1

32

240511-2-15 12 (0.100)

1: TOF MS ES+  
4.70e+005



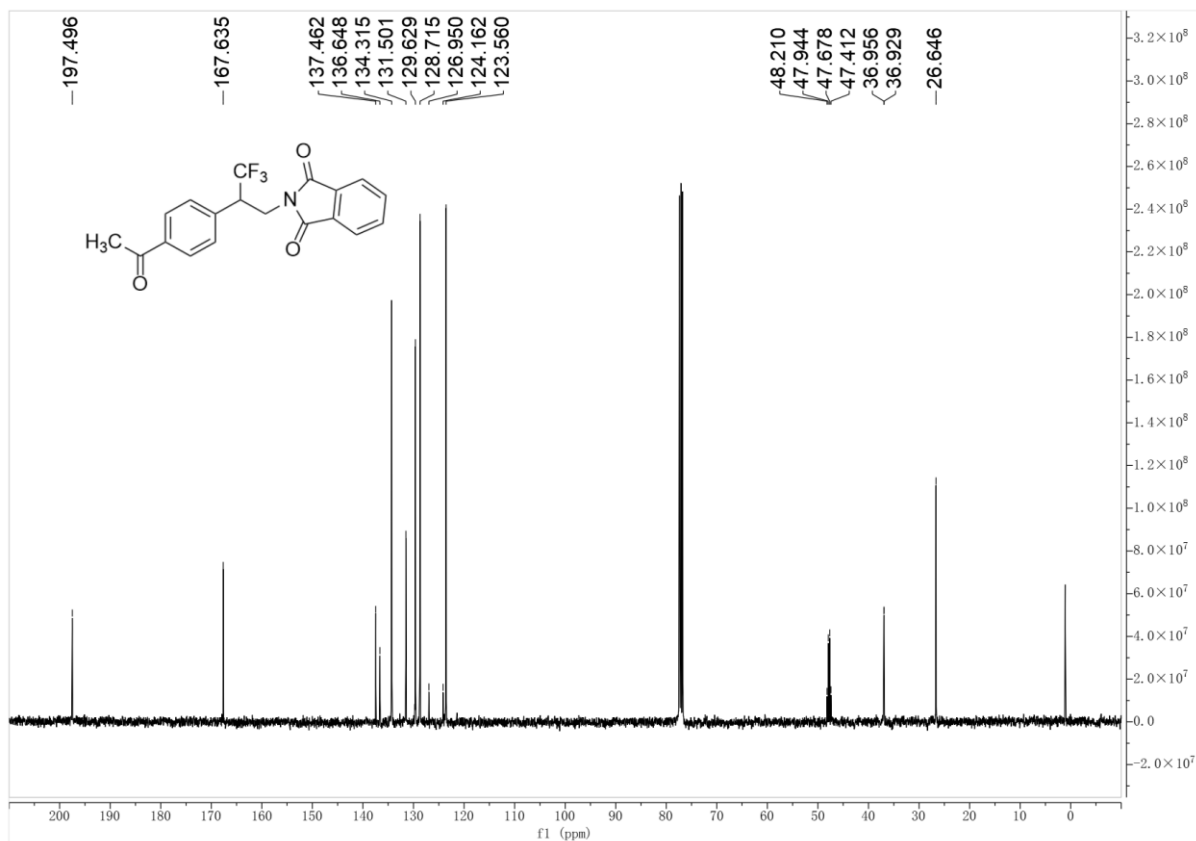
Minimum: -1.5  
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
388.0596	388.0595	0.1	0.3	10.5	561.3	n/a	n/a	C18 H14 N O2 F3 Na S

## <sup>1</sup>H NMR spectrum of 3v (400 MHz, CDCl<sub>3</sub>)



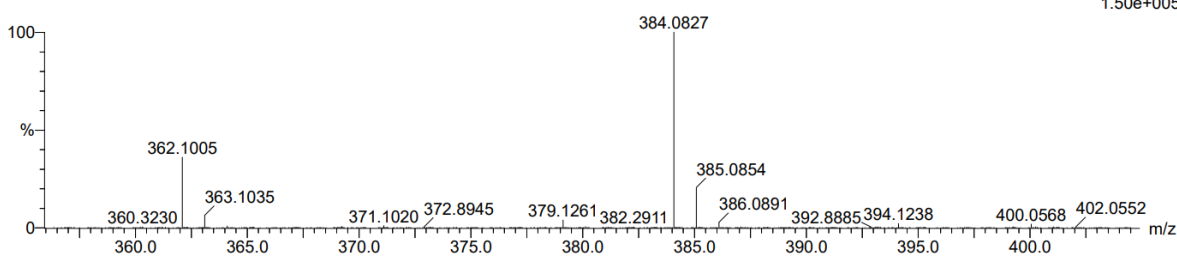
**<sup>13</sup>C NMR spectrum of 3v (100 MHz, CDCl<sub>3</sub>)**



**HRMS (ESI) spectrum of 3v**

Monoisotopic Mass, Even Electron Ions  
 2157 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)  
 Elements Used:  
 C: 19-19 H: 14-14 N: 0-100 O: 0-100 F: 3-6 Na: 0-2  
 32  
 240511-2-5 22 (0.152)

1: TOF MS ES+  
 1.50e+005

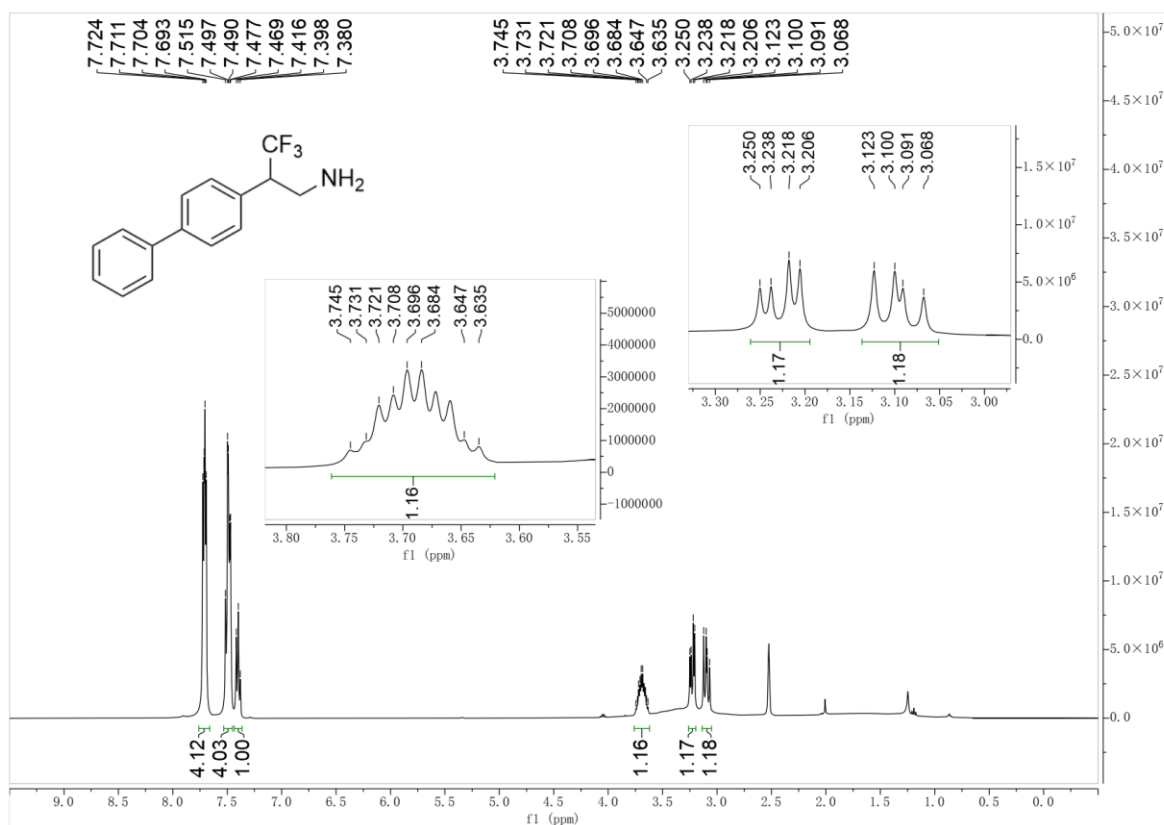


Minimum: -1.5  
 Maximum: 5.0 10.0 50.0

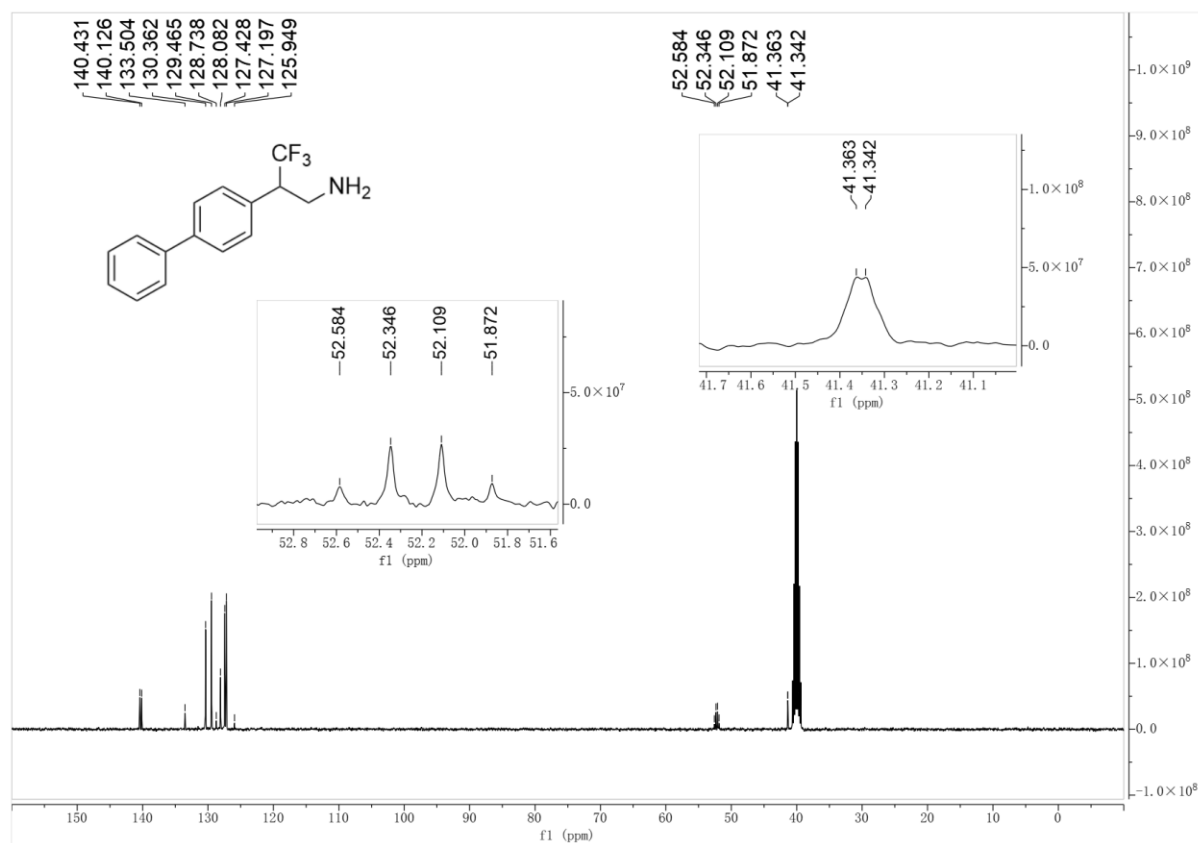
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
384.0827	384.0823	0.4	1.0	11.5	411.2	n/a	n/a	C19 H14 N O3 F3 Na



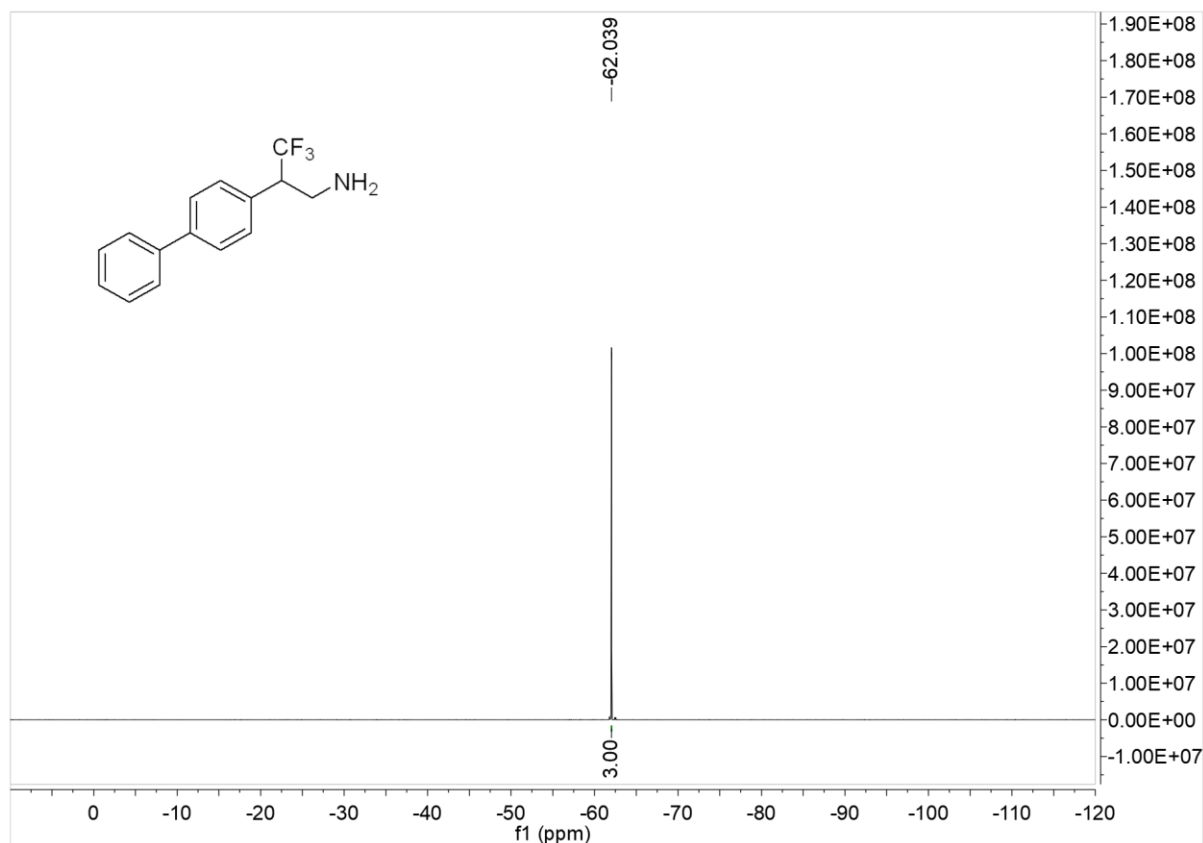
**<sup>1</sup>H NMR spectrum of 4a (400 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4a (100 MHz, DMSO-*d*<sub>6</sub>)**



### <sup>19</sup>F NMR spectrum of 4a (376 MHz, DMSO-d<sub>6</sub>)



### HRMS (ESI) spectrum of 4a

Monoisotopic Mass, Even Electron Ions

322 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

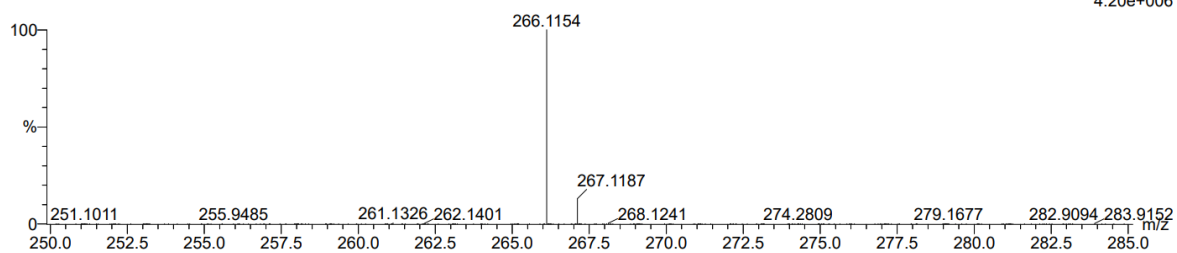
Elements Used:

C: 15-15 H: 15-15 N: 0-20 O: 0-20 F: 3-3 Na: 0-3

6

230410-1-25 6 (0.085)

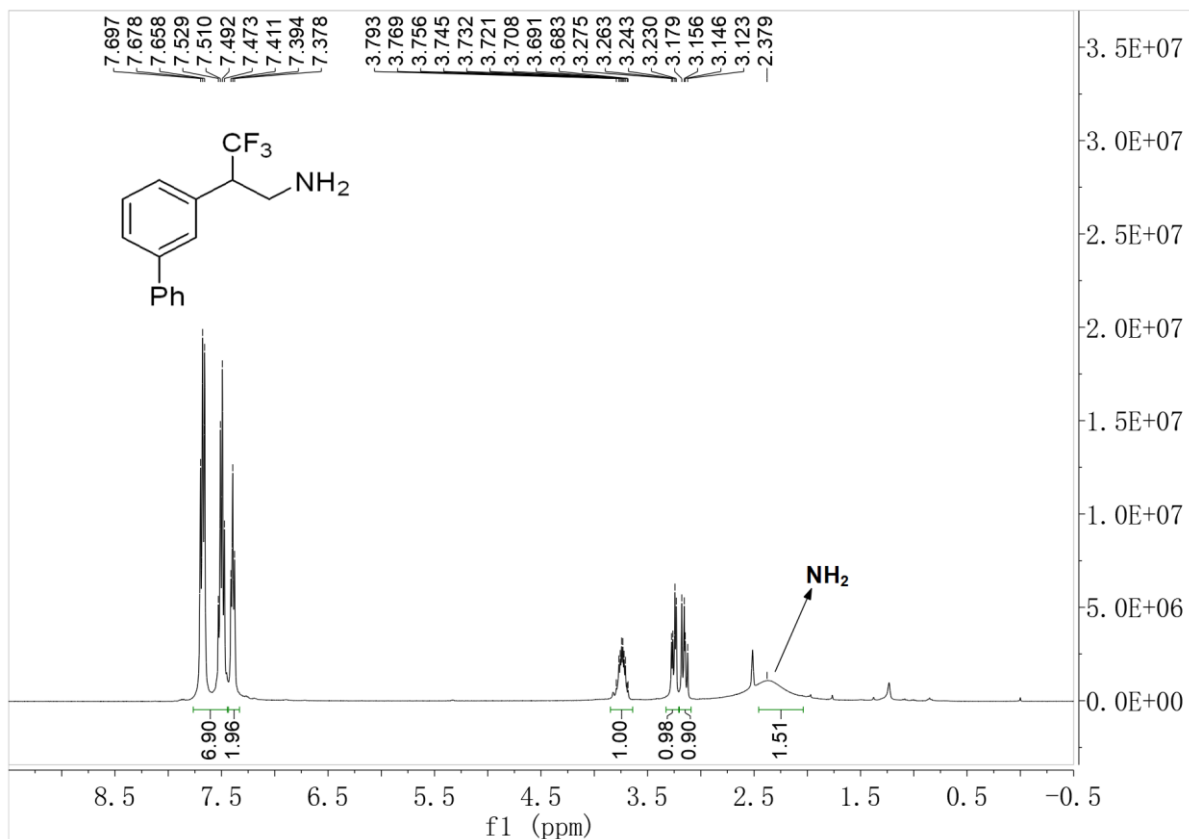
1: TOF MS ES+  
4.20e+006



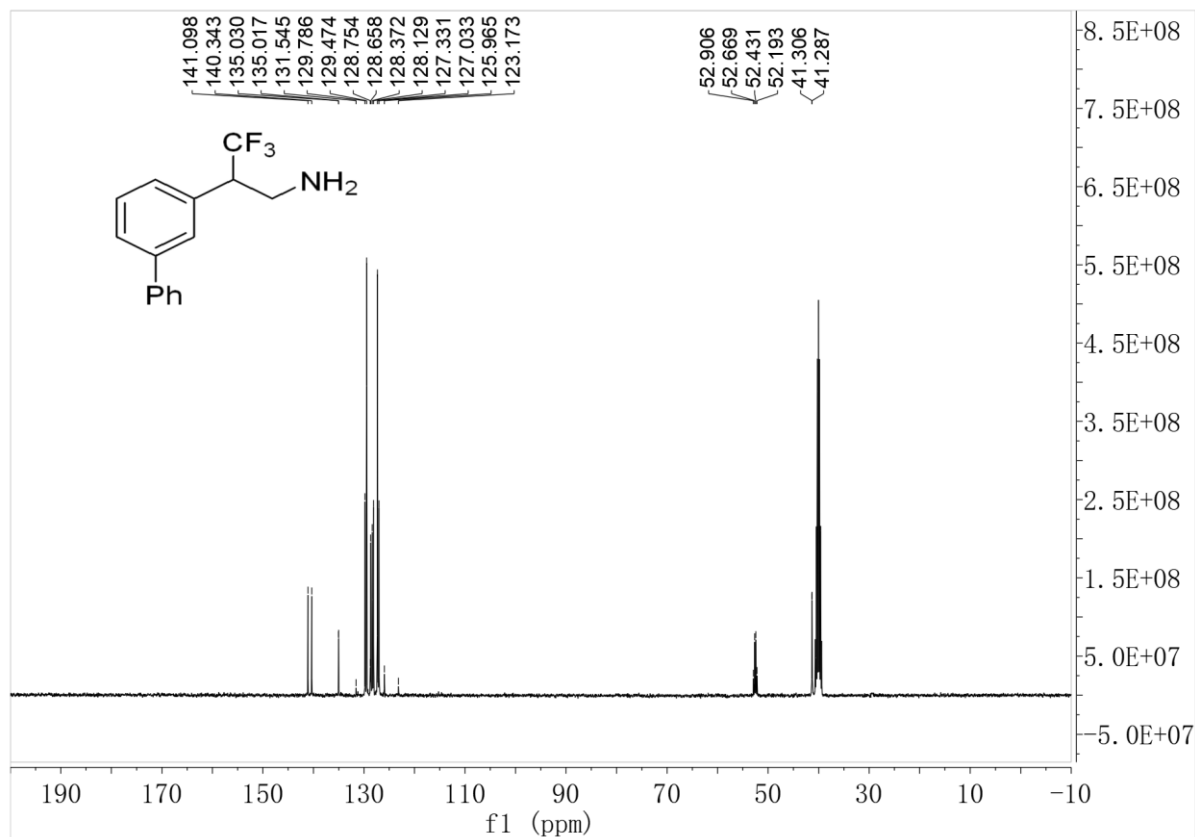
Minimum: -1.5  
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
266.1154	266.1157	-0.3	-1.1	7.5	250.5	n/a	n/a	C15 H15 N F3

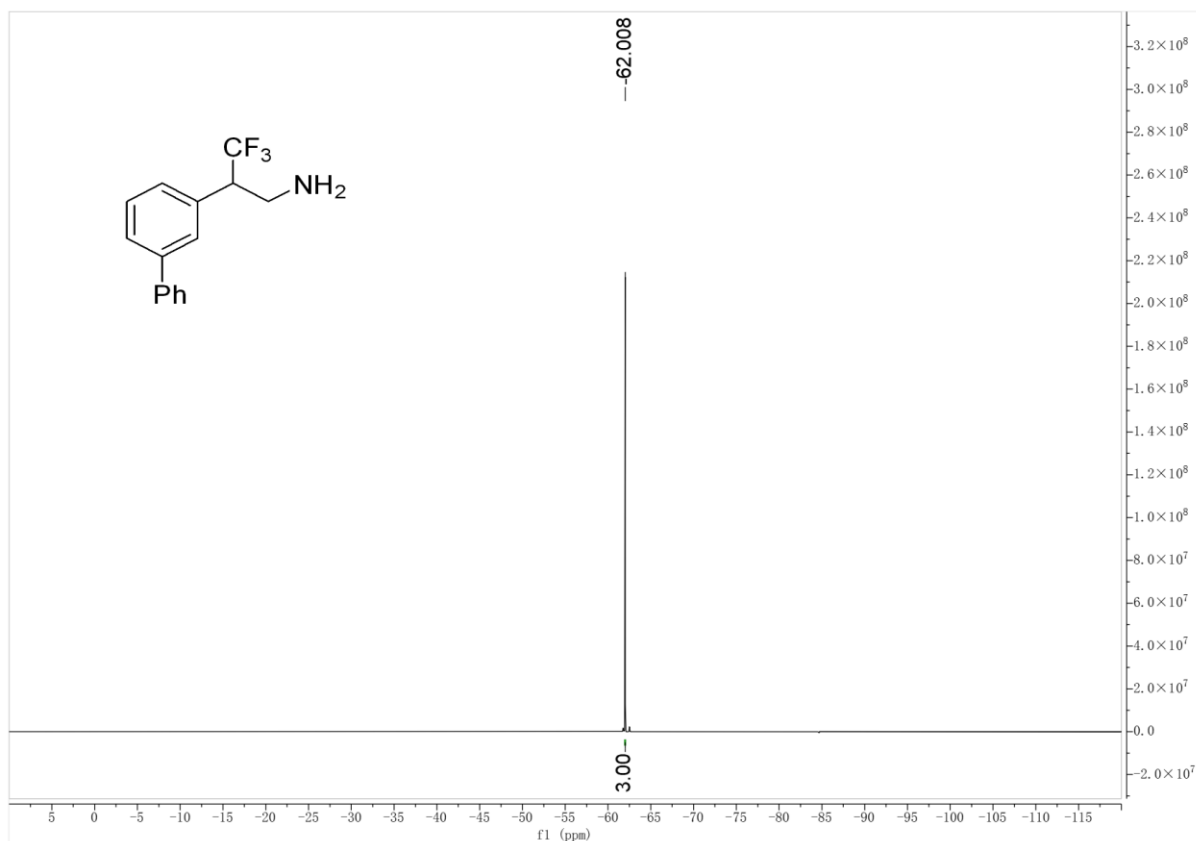
**<sup>1</sup>H NMR spectrum of 4b (400 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4b (100 MHz, DMSO-*d*<sub>6</sub>)**



### <sup>19</sup>F NMR spectrum of 4b (376 MHz, DMSO-*d*<sub>6</sub>)



### HRMS (ESI) spectrum of 4b

Monoisotopic Mass, Even Electron Ions  
268 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

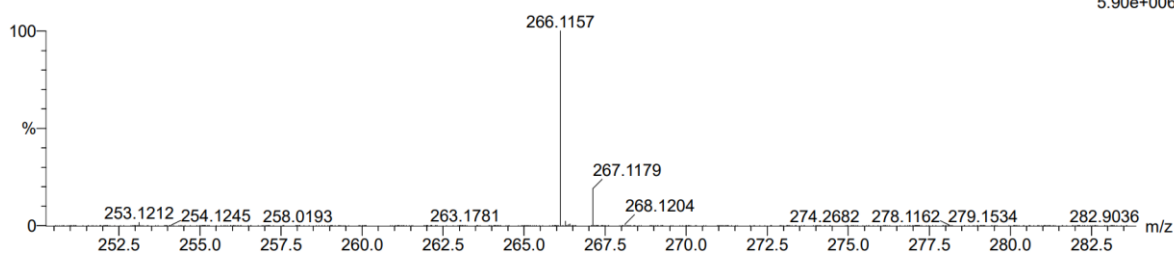
Elements Used:

C: 15-15 H: 15-15 N: 0-200 O: 0-200 F: 3-3 Na: 0-2

25

231109-3-2-3-2-- 14 (0.157)

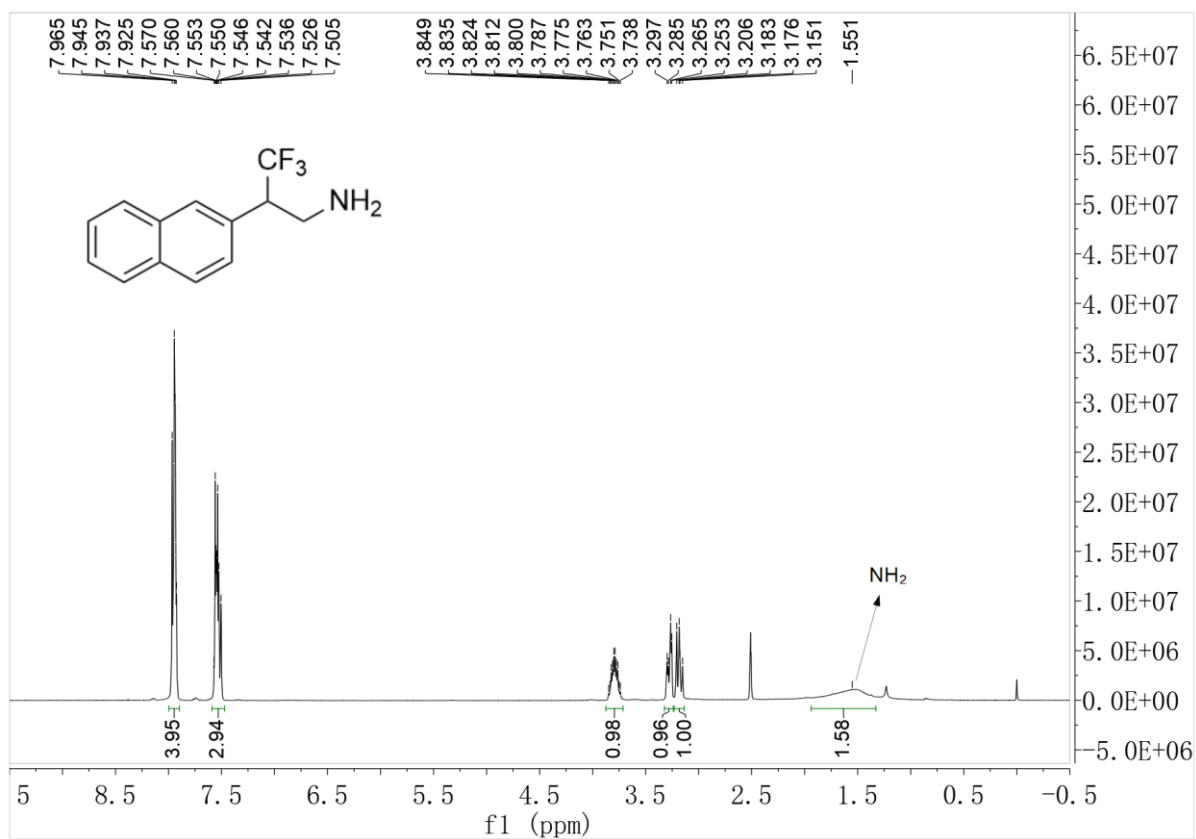
1: TOF MS ES+  
5.90e+006



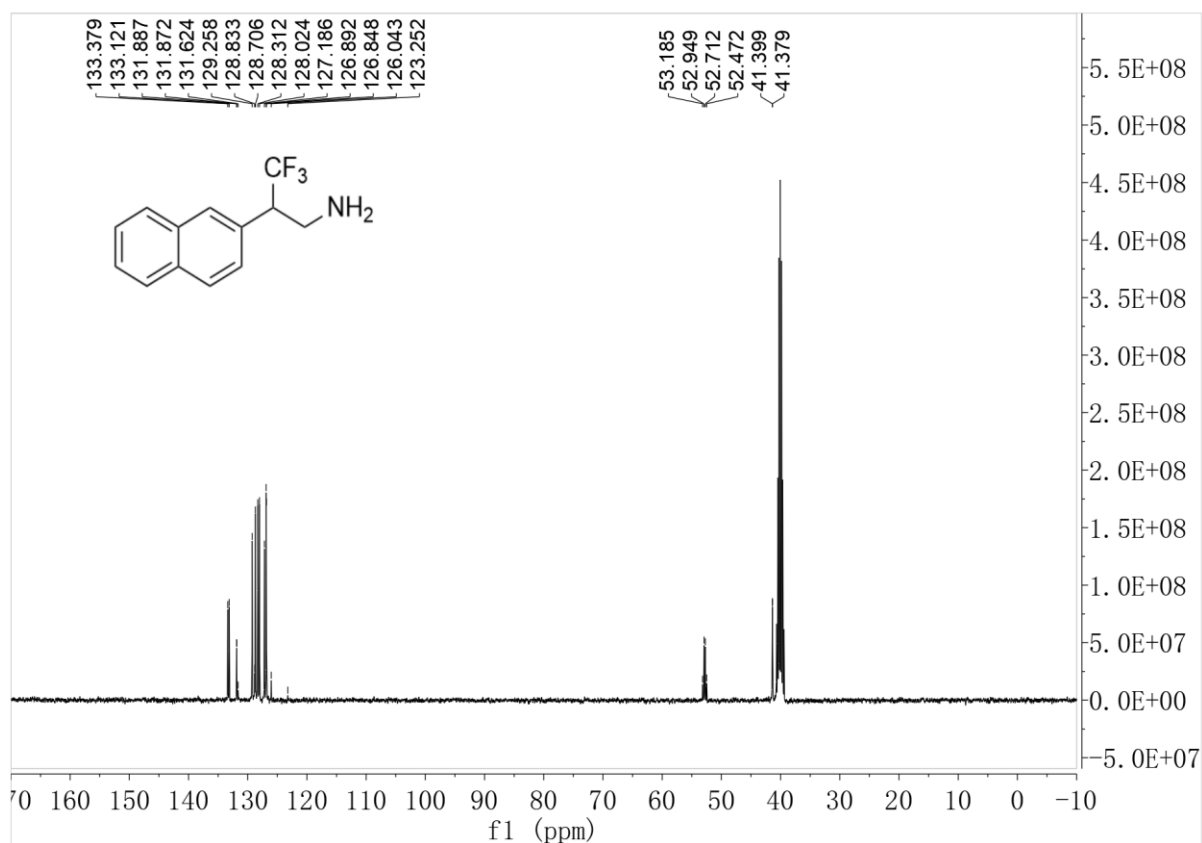
Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
266.1157	266.1157	0.0	0.0	7.5	420.1	n/a	n/a	C15 H15 N F3

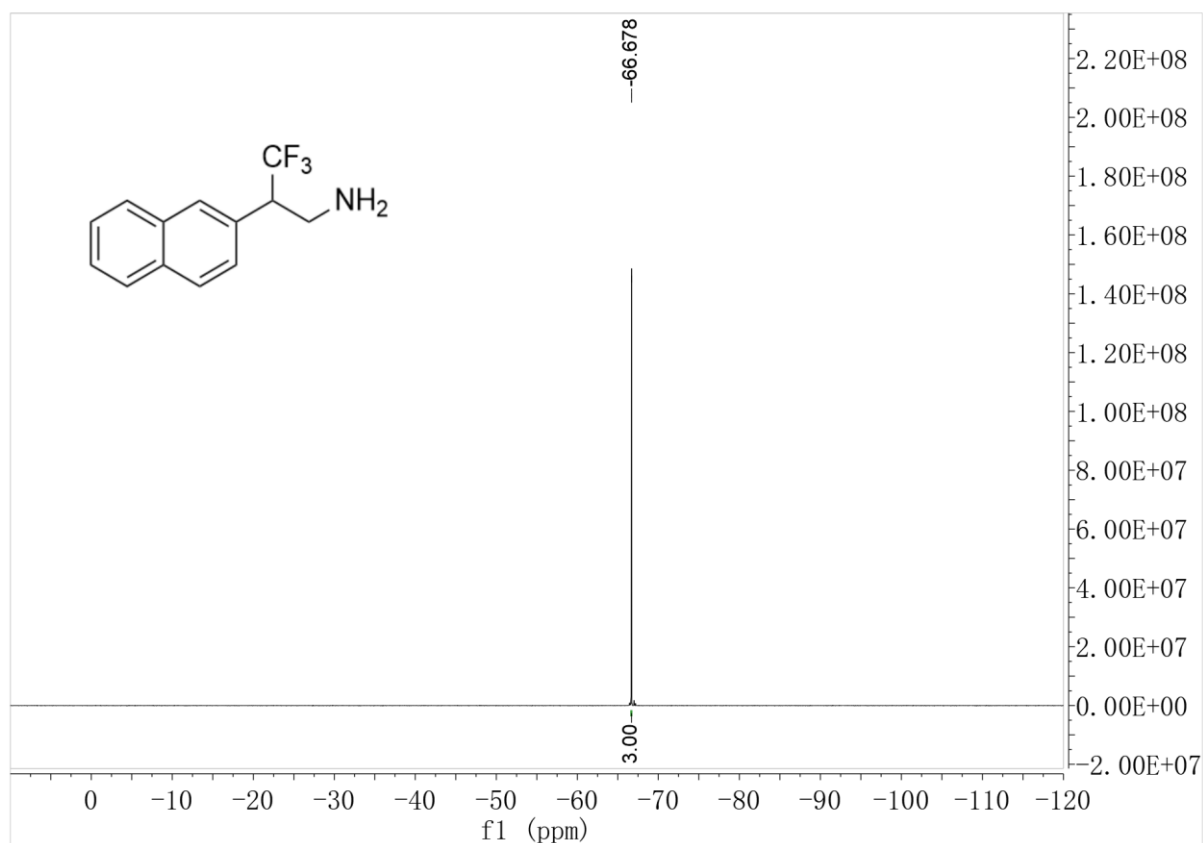
**<sup>1</sup>H NMR spectrum of 4c (400 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4c (100 MHz, DMSO-*d*<sub>6</sub>)**



### <sup>19</sup>F NMR spectrum of 4c (376 MHz, DMSO-d<sub>6</sub>)



### HRMS (ESI) spectrum of 4c

Monoisotopic Mass, Even Electron Ions

151 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

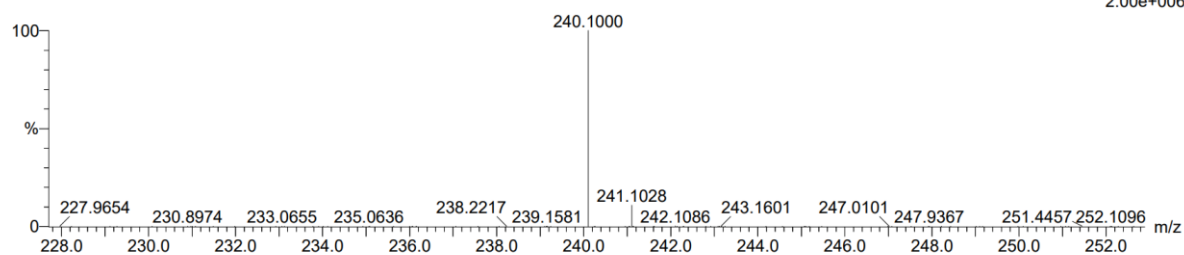
Elements Used:

C: 13-13 H: 13-13 N: 0-30 O: 0-100 F: 3-3 Na: 0-1

3

230512-2-20 11 (0.136)

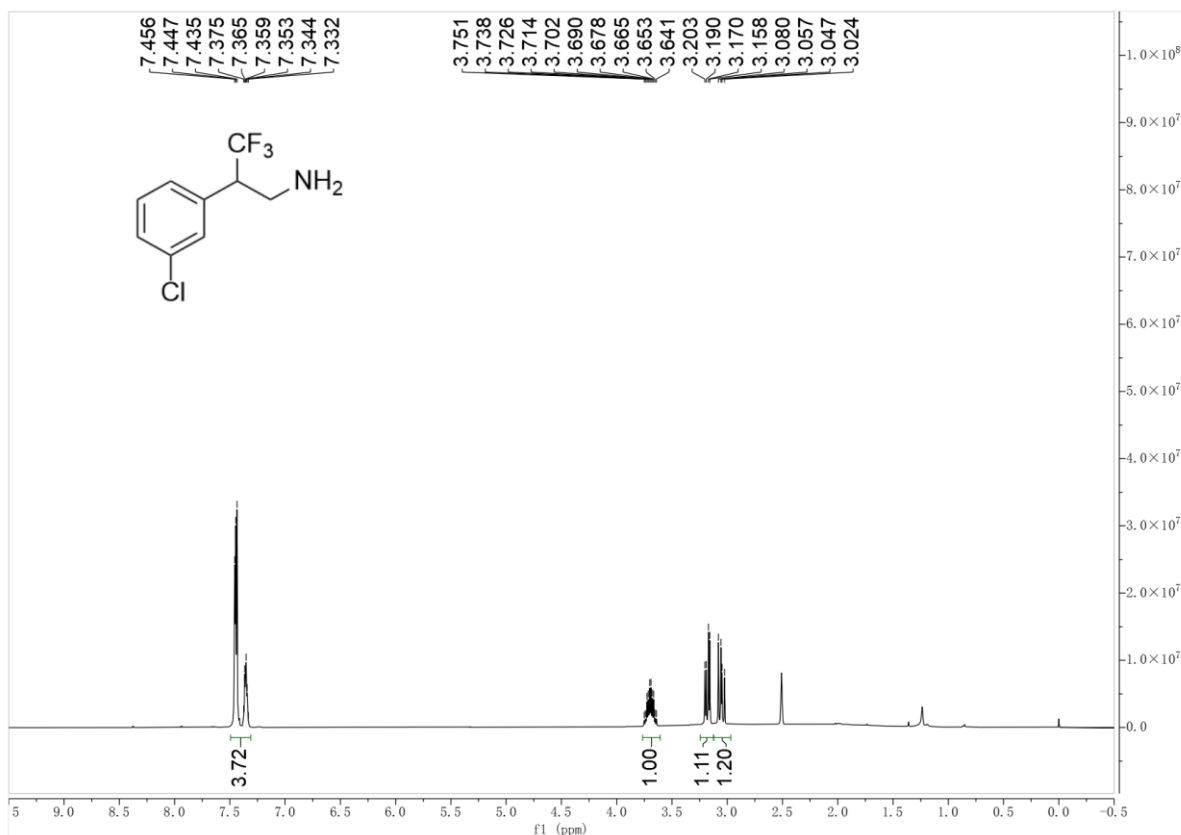
1: TOF MS ES+  
2.00e+006



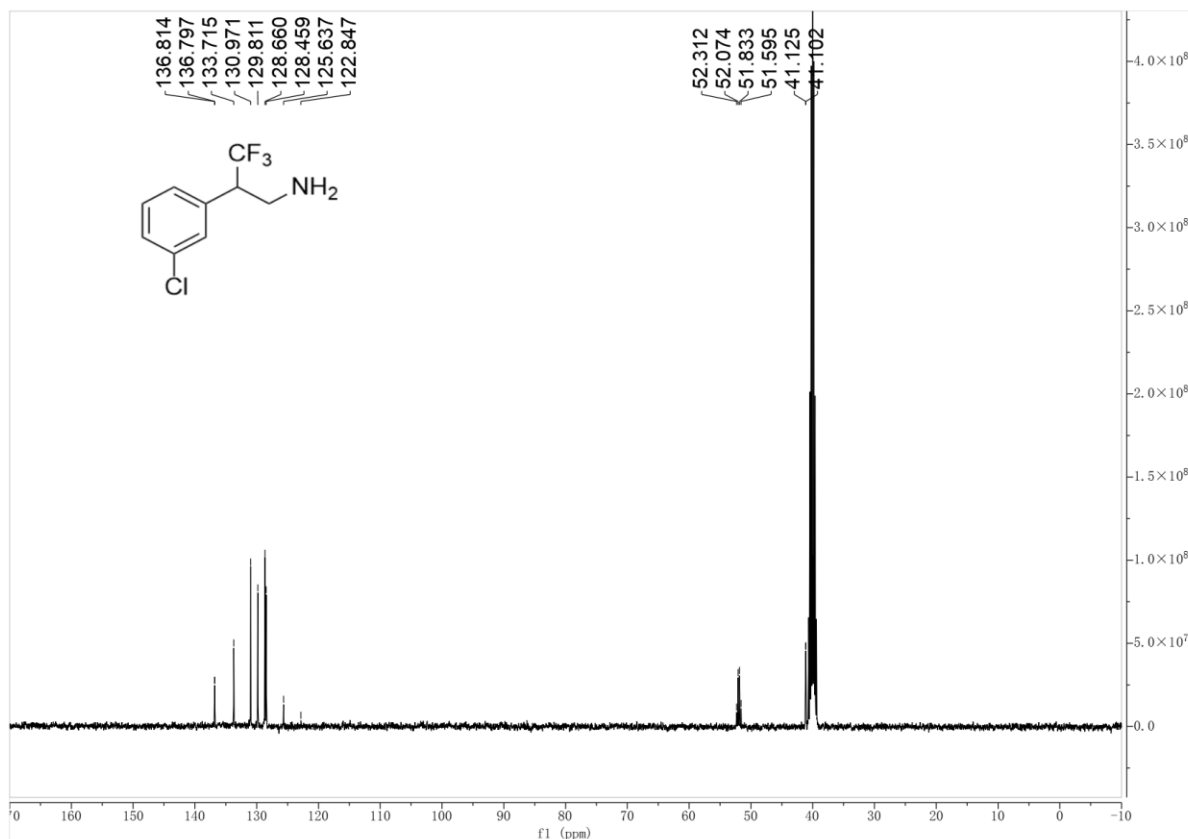
Minimum: -1.5  
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
240.1000	240.1000	0.0	0.0	6.5	122.0	n/a	n/a	C13 H13 N F3

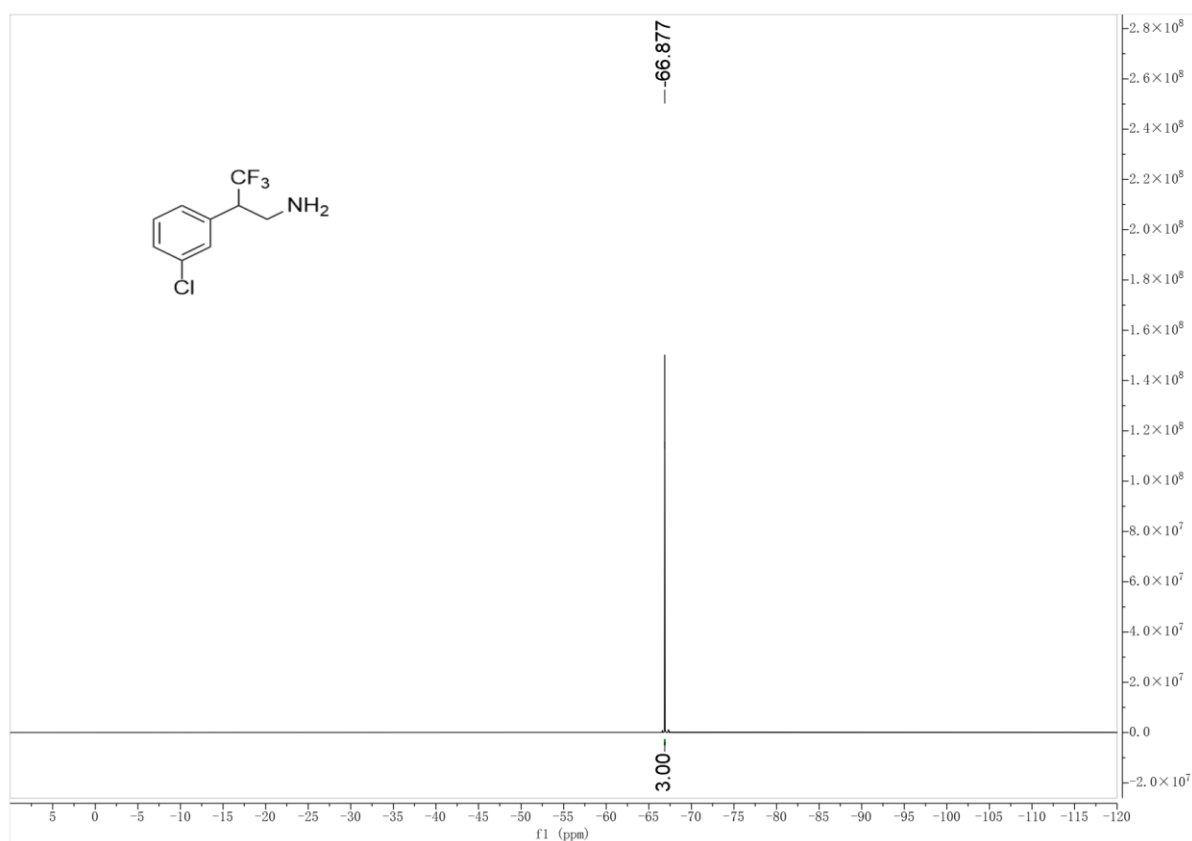
**<sup>1</sup>H NMR spectrum of 4d (400 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4d (100 MHz, DMSO-*d*<sub>6</sub>)**



### <sup>19</sup>F NMR spectrum of 4d (376 MHz, DMSO-*d*<sub>6</sub>)



### HRMS (ESI) spectrum of 4d

Monoisotopic Mass, Even Electron Ions

313 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

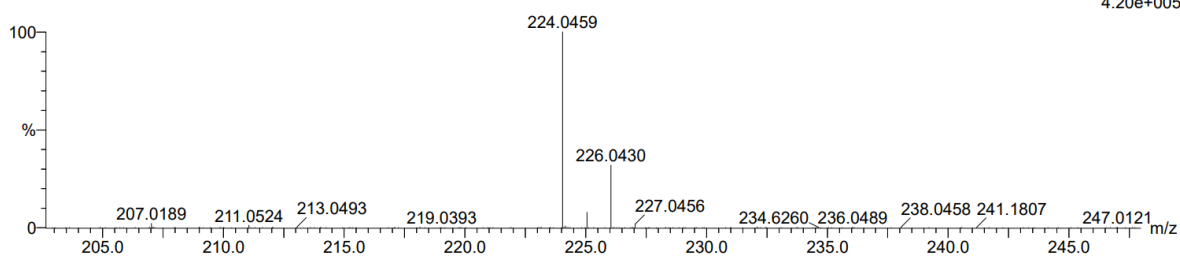
Elements Used:

C: 9-9 H: 10-10 N: 0-100 O: 0-100 F: 3-6 Na: 0-1 Cl: 1-2

25

240117-7-37 20 (0.108)

1: TOF MS ES+  
4.20e+005

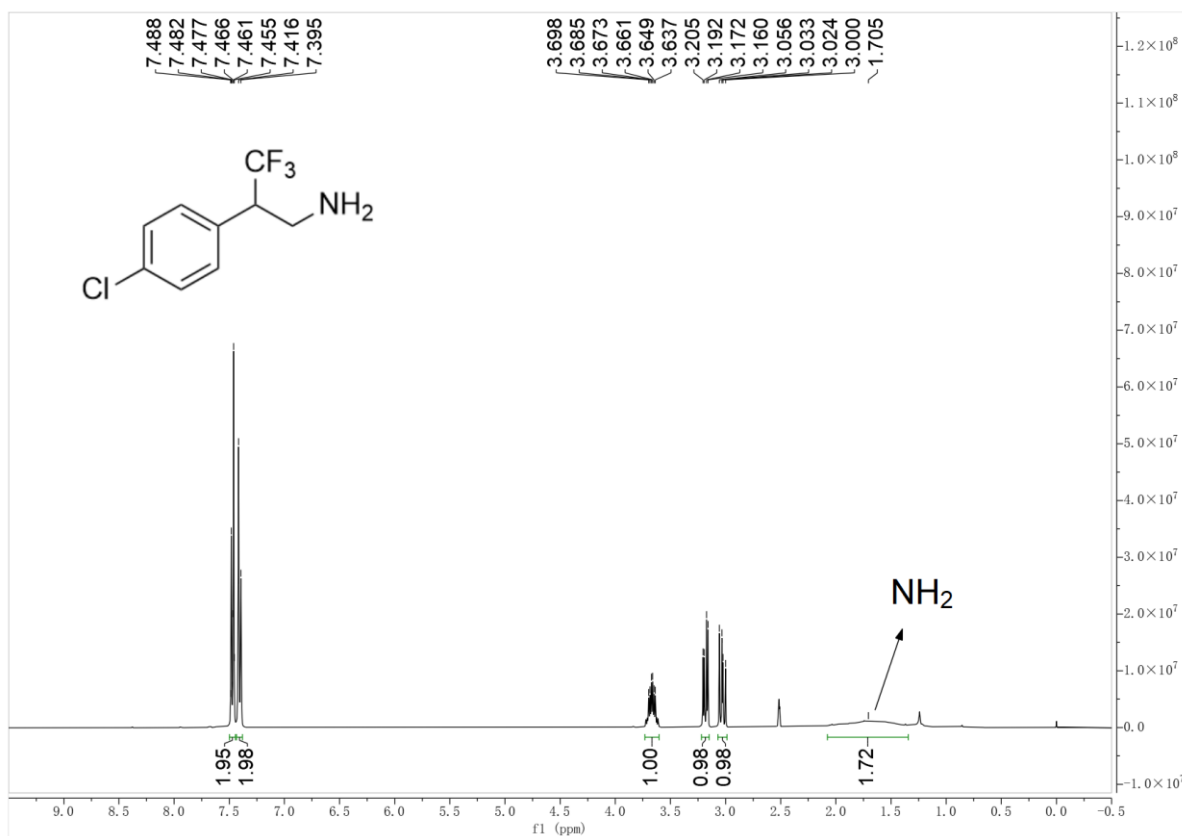


Minimum: -1.5  
Maximum: 5.0 10.0 50.0

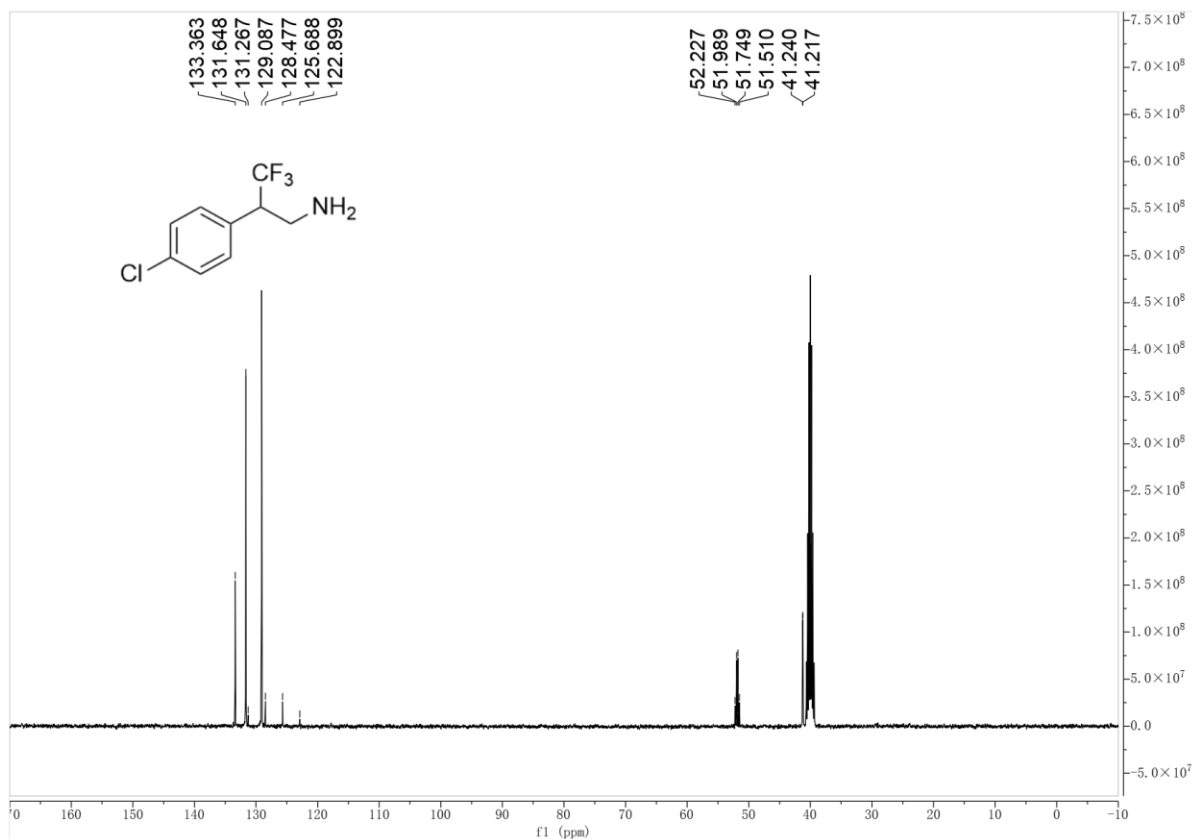
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
224.0459	224.0454	0.5	2.2	3.5	126.3	n/a	n/a	C9 H10 N F3 Cl



**<sup>1</sup>H NMR spectrum of 4e (400 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4e (100 MHz, DMSO-*d*<sub>6</sub>)**



### <sup>19</sup>F NMR spectrum of 4e (376 MHz, DMSO-d<sub>6</sub>)



### HRMS (ESI) spectrum of 4e

Monoisotopic Mass, Even Electron Ions

283 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

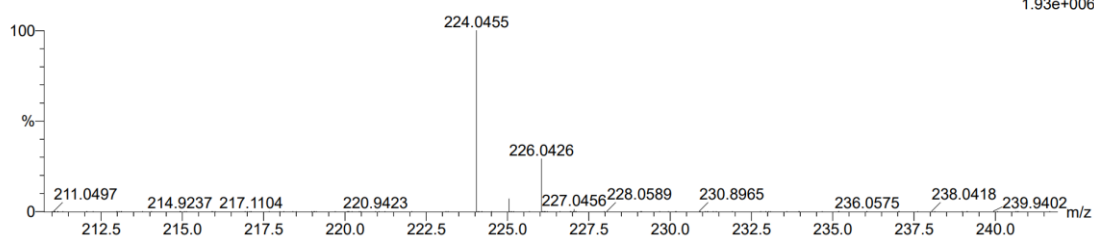
Elements Used:

C: 9-9 H: 10-10 N: 0-30 O: 0-100 F: 2-3 Na: 0-1 Cl: 1-2

3

230512-2-16 13 (0.161)

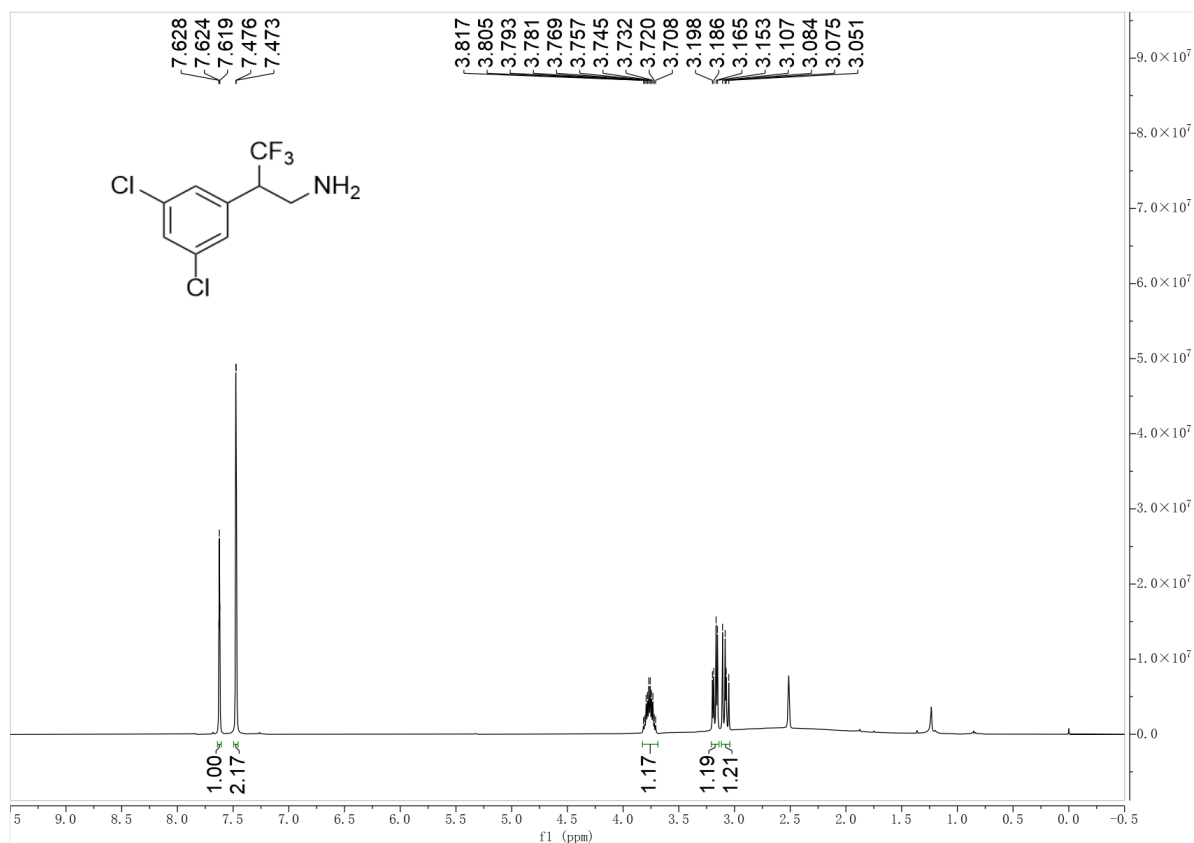
1: TOF MS ES+  
1.93e+006



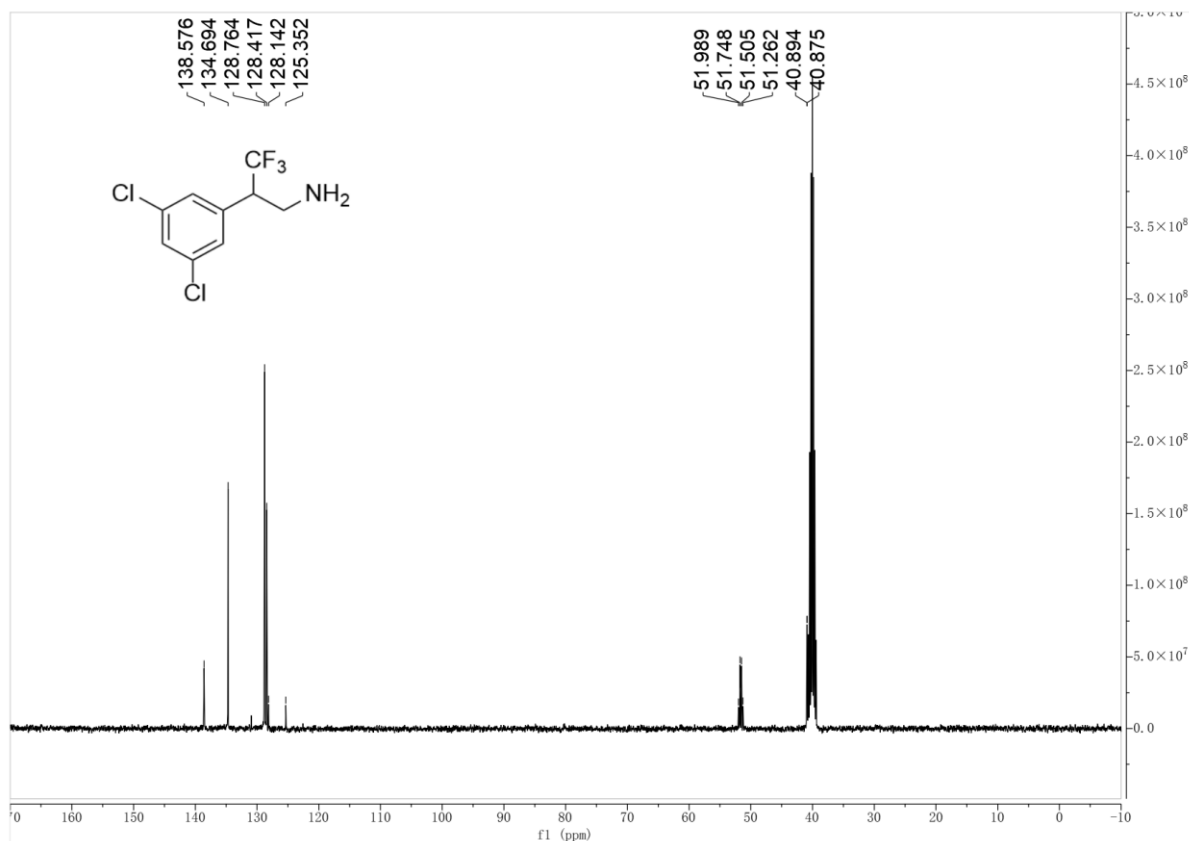
Minimum: -1.5  
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
224.0455	224.0454	0.1	0.4	3.5	119.0	n/a	n/a	C9 H10 N F3 Cl

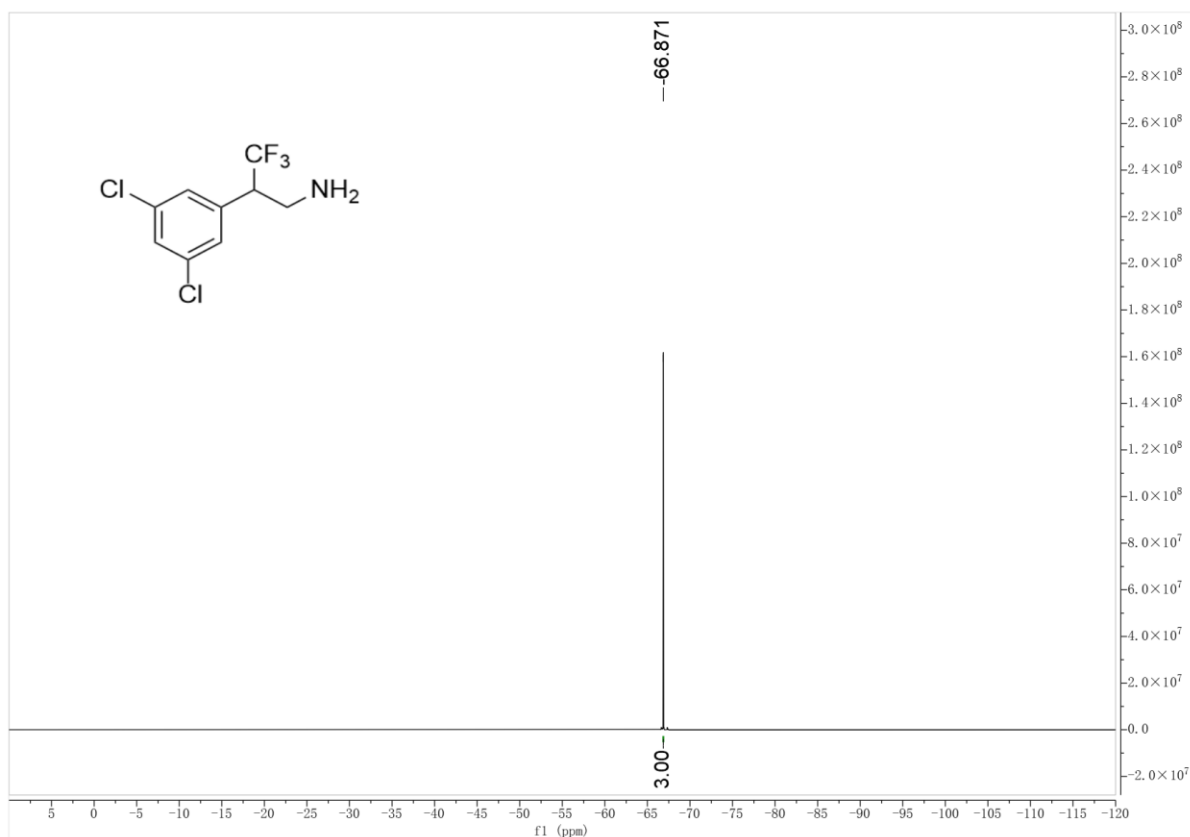
**<sup>1</sup>H NMR spectrum of 4f (400 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4f (100 MHz, DMSO-*d*<sub>6</sub>)**



### <sup>19</sup>F NMR spectrum of 4f (376 MHz, DMSO-*d*<sub>6</sub>)



### HRMS (ESI) spectrum of 4f

Monoisotopic Mass, Even Electron Ions

544 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

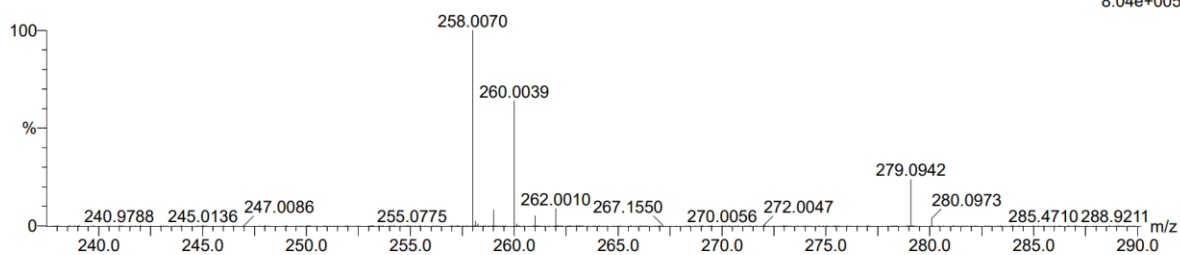
Elements Used:

C: 9-9 H: 9-9 N: 0-100 O: 0-100 F: 3-6 Na: 0-1 Cl: 1-2

25

240117-7-38 16 (0.094)

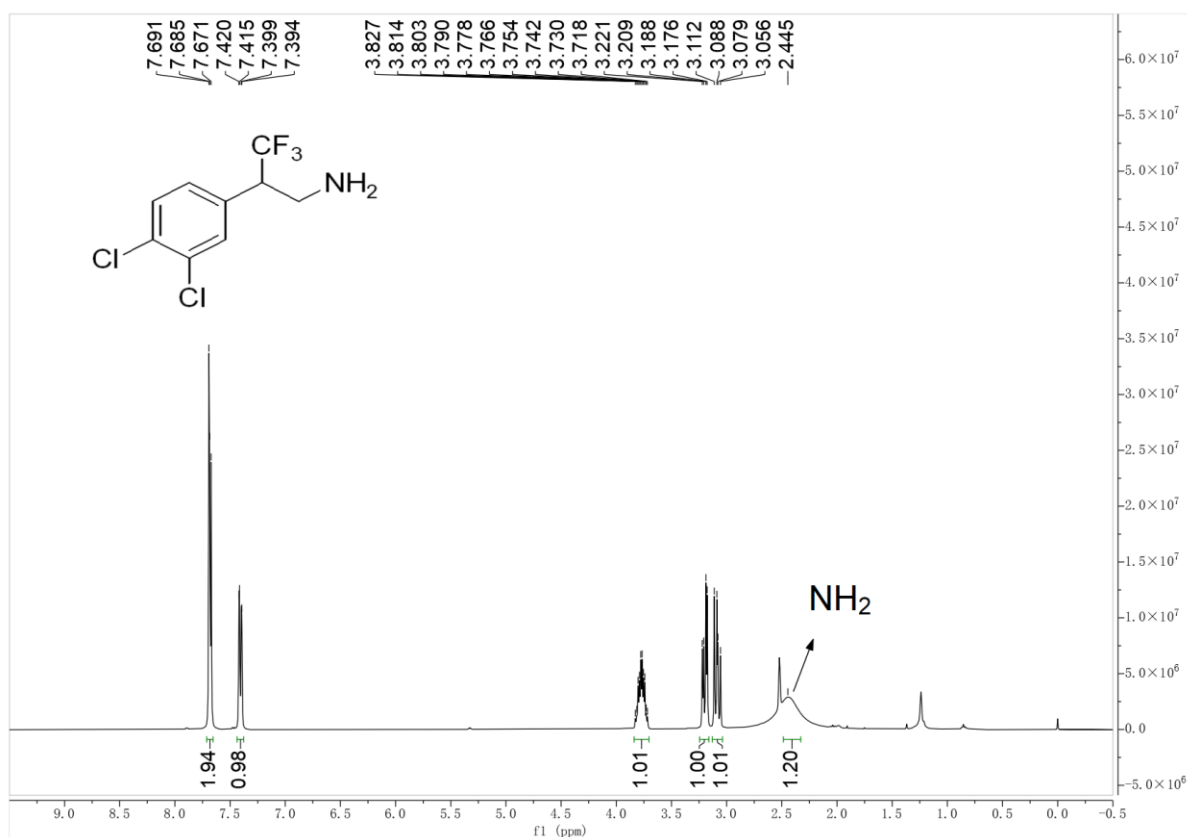
1: TOF MS ES+  
8.04e+005



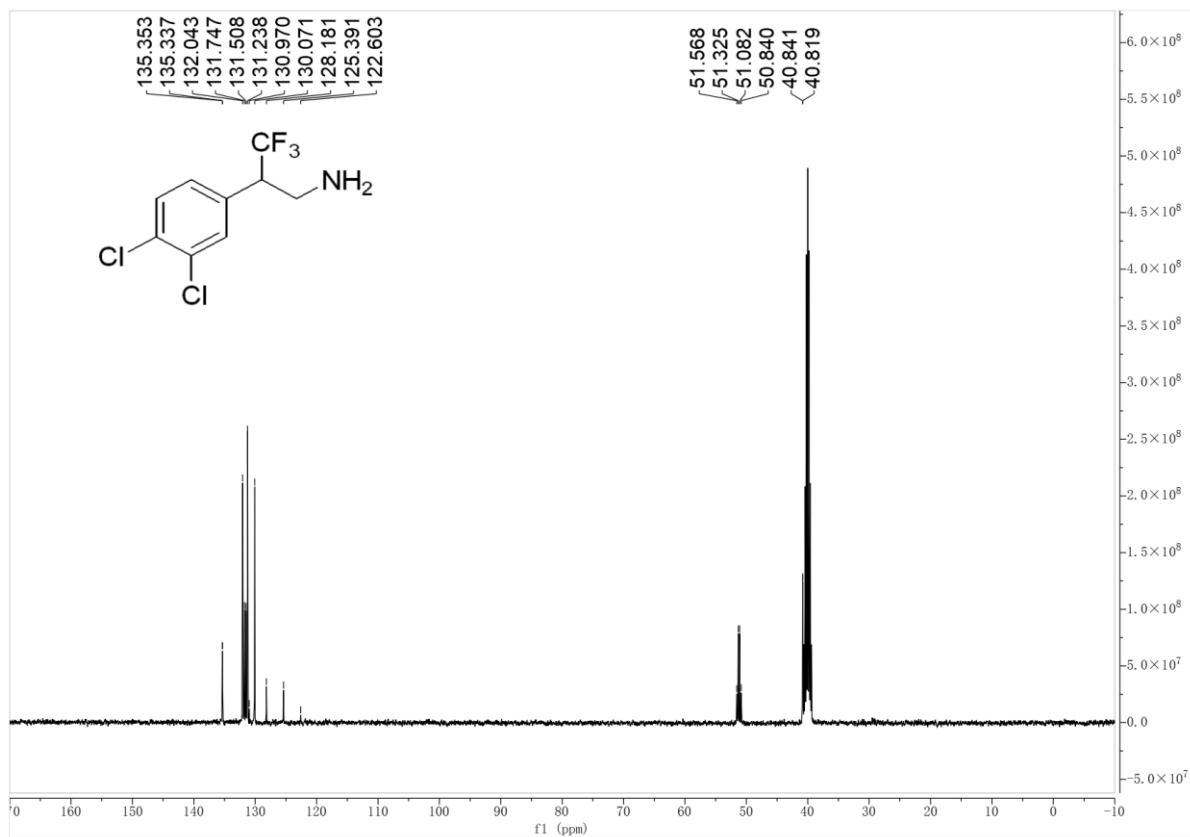
Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
258.0070	258.0064	0.6	2.3	3.5	266.7	n/a	n/a	C9 H9 N F3 Cl2

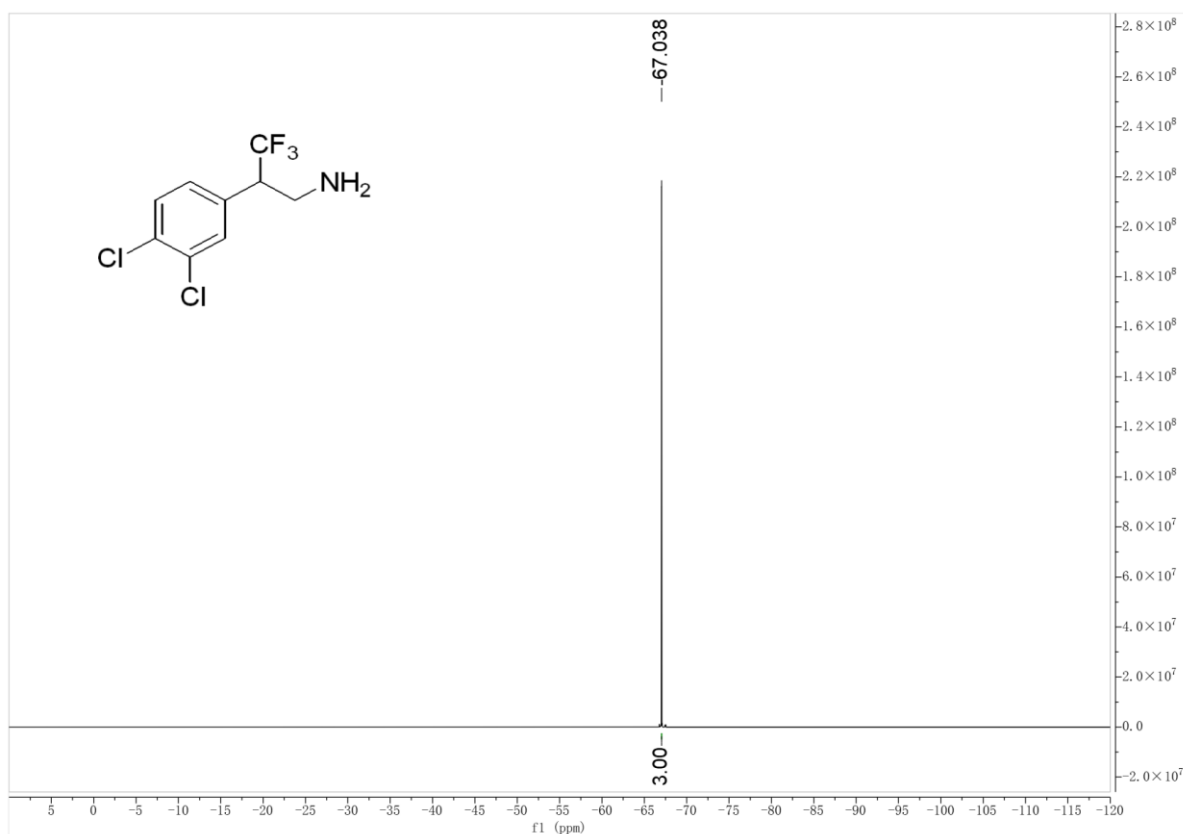
**<sup>1</sup>H NMR spectrum of 4g (400 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4g (100 MHz, DMSO-*d*<sub>6</sub>)**



### <sup>19</sup>F NMR spectrum of 4g (376 MHz, DMSO-*d*<sub>6</sub>)



### HRMS (ESI) spectrum of 4g

Monoisotopic Mass, Even Electron Ions

250 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

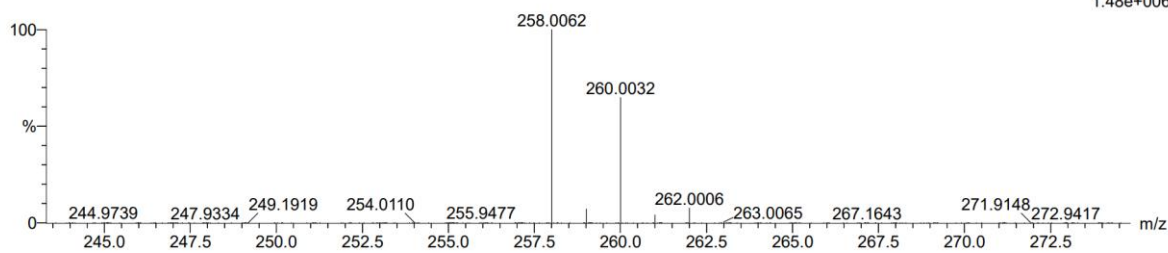
Elements Used:

C: 9-9 H: 9-9 N: 0-200 O: 0-200 F: 3-3 Na: 0-2 Cl: 1-2

25

231109-3-2-3-1- 6 (0.088)

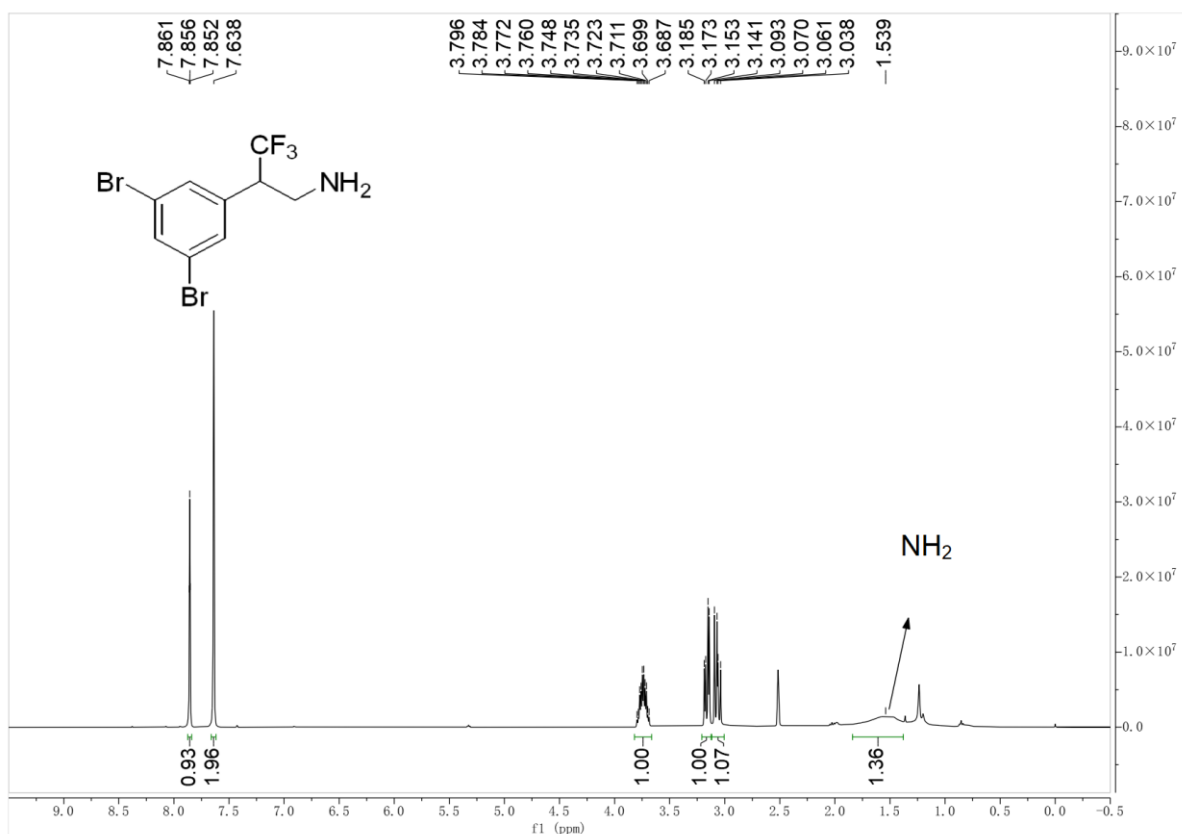
1: TOF MS ES+  
1.48e+006



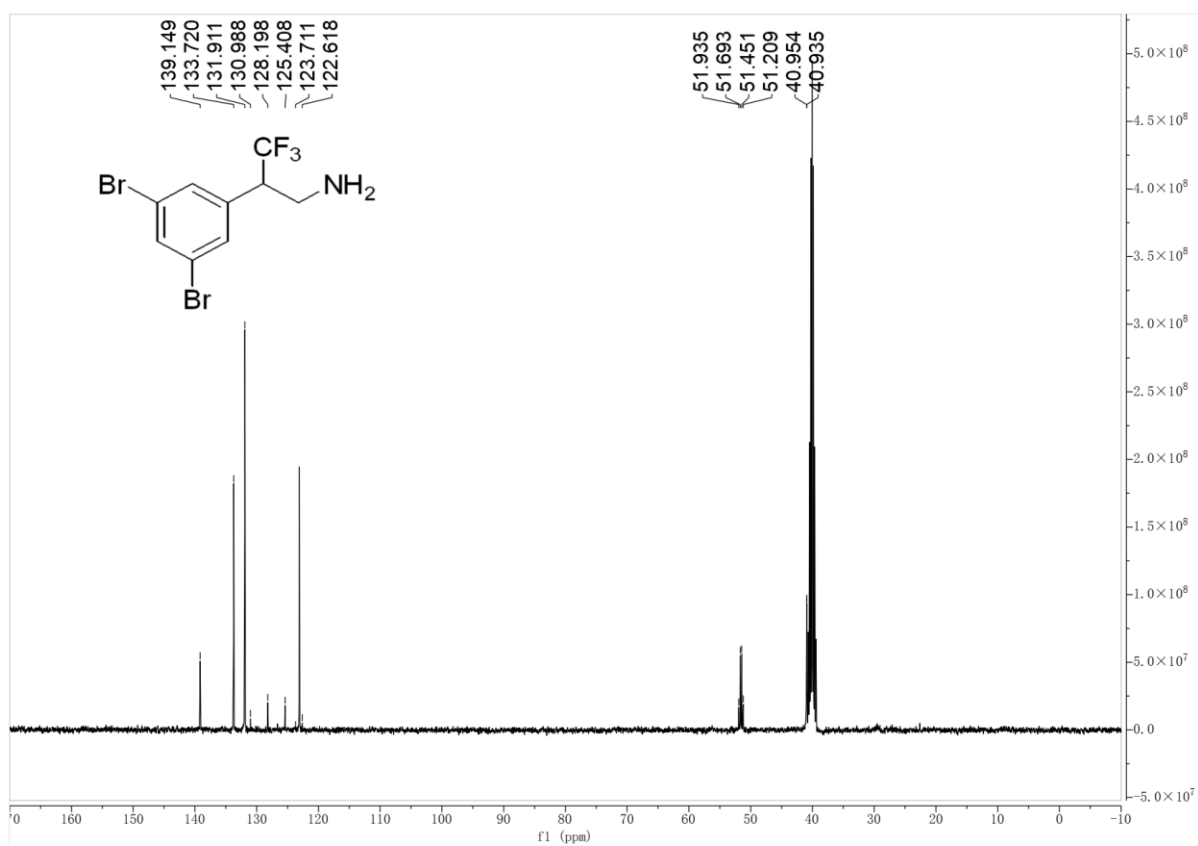
Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
258.0062	258.0064	-0.2	-0.8	3.5	220.3	n/a	n/a	C9 H9 N F3 Cl2

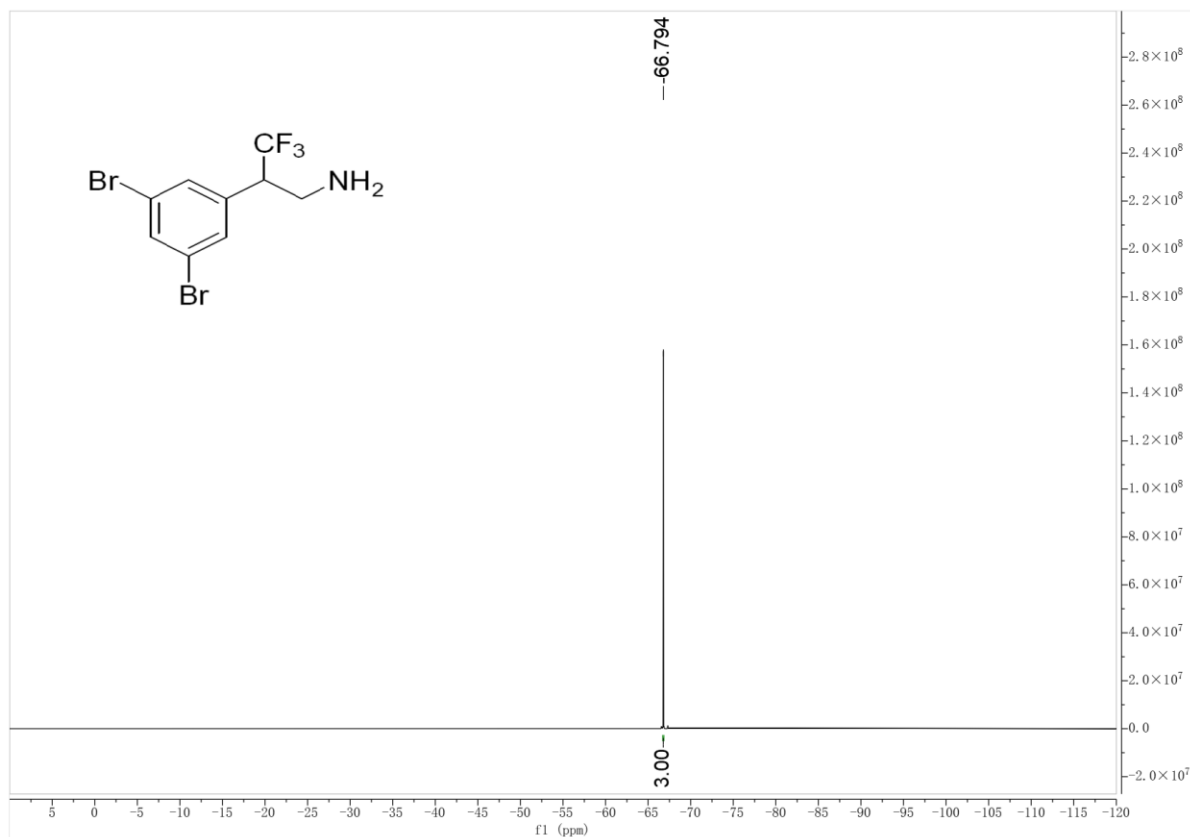
**<sup>1</sup>H NMR spectrum of 4h (400 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4h (100 MHz, DMSO-*d*<sub>6</sub>)**



### <sup>19</sup>F NMR spectrum of 4h (376 MHz, DMSO-*d*<sub>6</sub>)

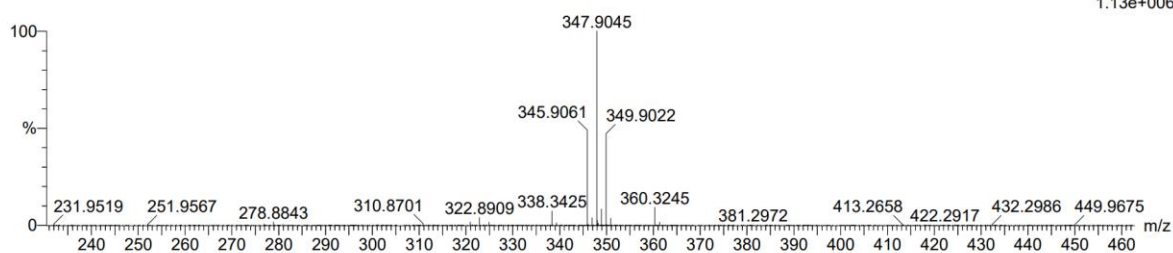


### HRMS (ESI) spectrum of 4h

Monoisotopic Mass, Even Electron Ions  
764 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)  
Elements Used:  
C: 9-9 H: 9-9 N: 0-100 O: 0-100 F: 3-6 Na: 0-1 Br: 1-4

25  
240117-7-39 17 (0.097)

1: TOF MS ES+  
1.13e+006

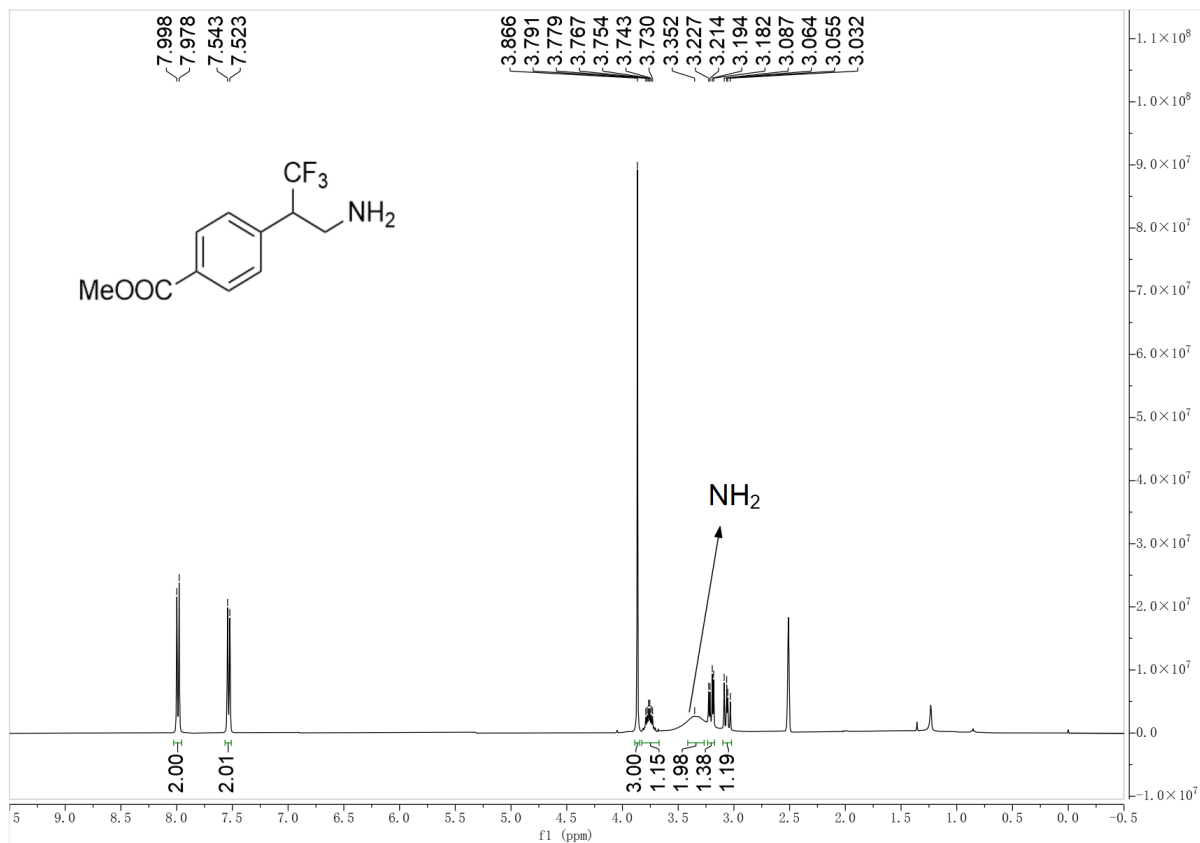


Minimum: -1.5  
Maximum: 5.0 10.0 50.0

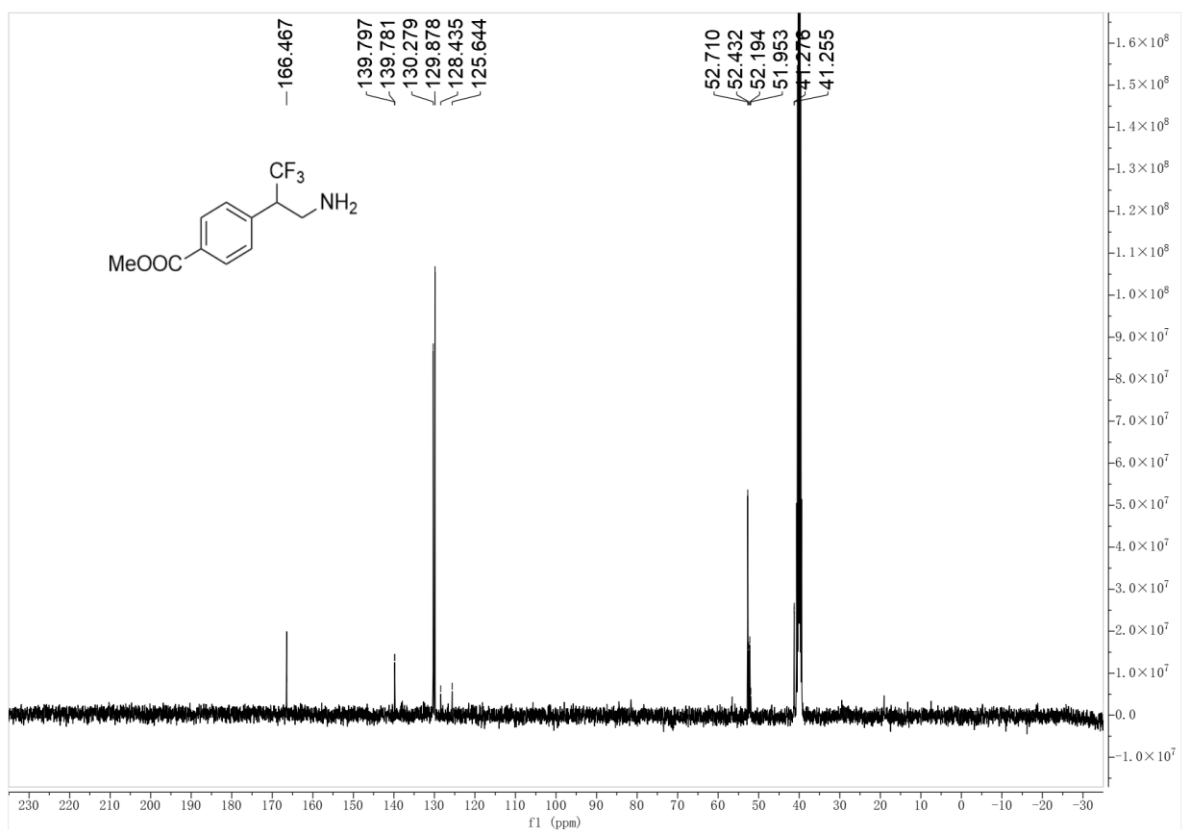
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
345.9061	345.9054	0.7	2.0	3.5	264.8	n/a	n/a	C9 H9 N F3 Br2



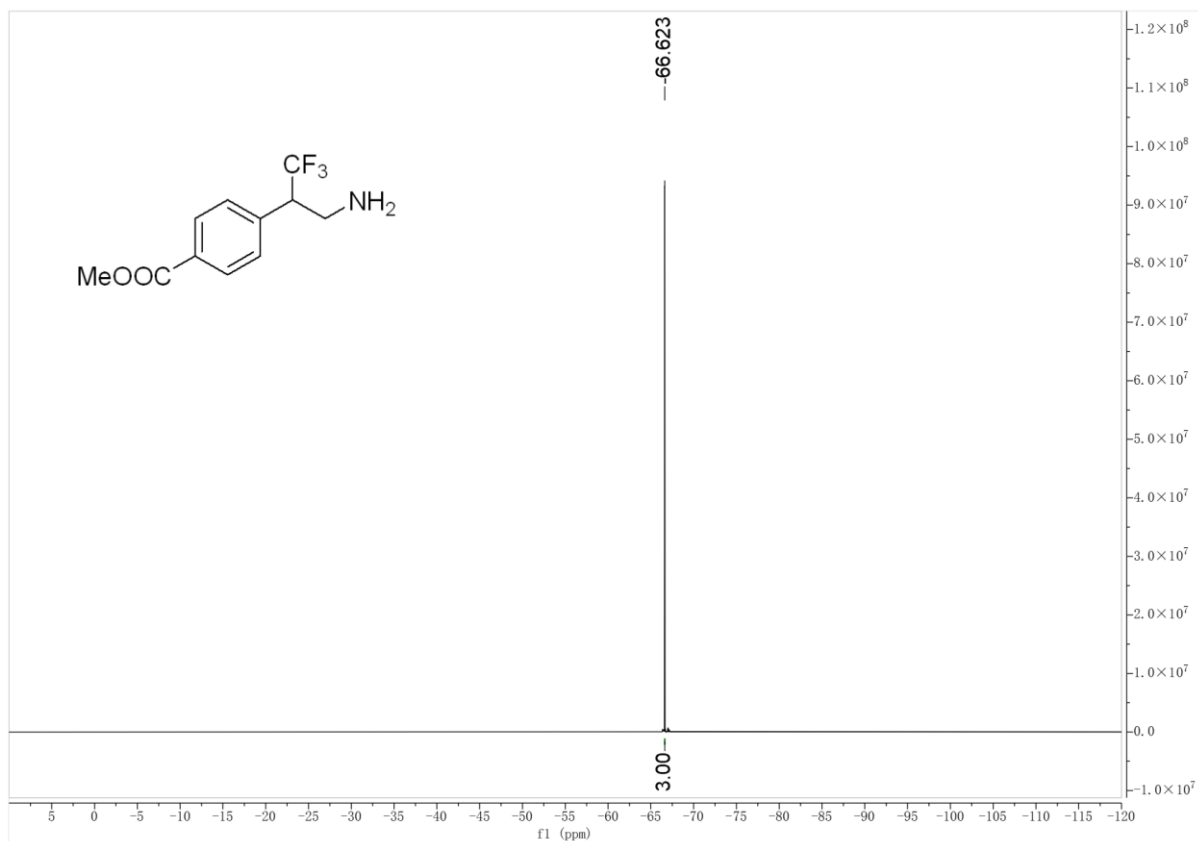
**<sup>1</sup>H NMR spectrum of 4i (400 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4i (100 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>19</sup>F NMR spectrum of 4i (376 MHz, DMSO-d<sub>6</sub>)**



**HRMS (ESI) spectrum of 4i**

Monoisotopic Mass, Even Electron Ions

250 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

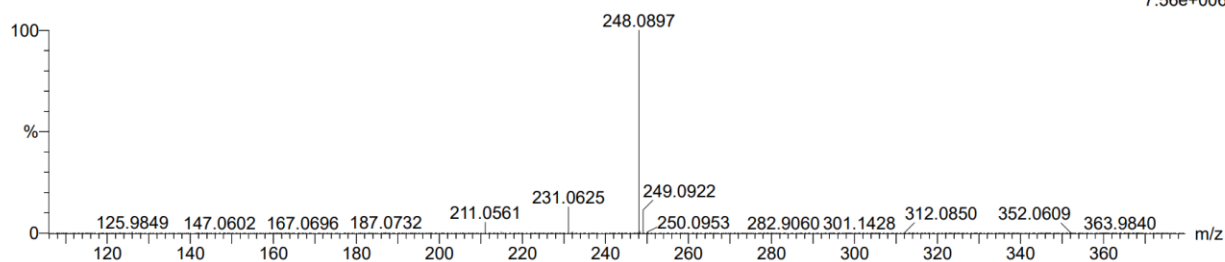
Elements Used:

C: 11-11 H: 13-13 N: 0-20 O: 0-20 F: 3-3 Na: 0-3

6

230410-1-23 7 (0.093)

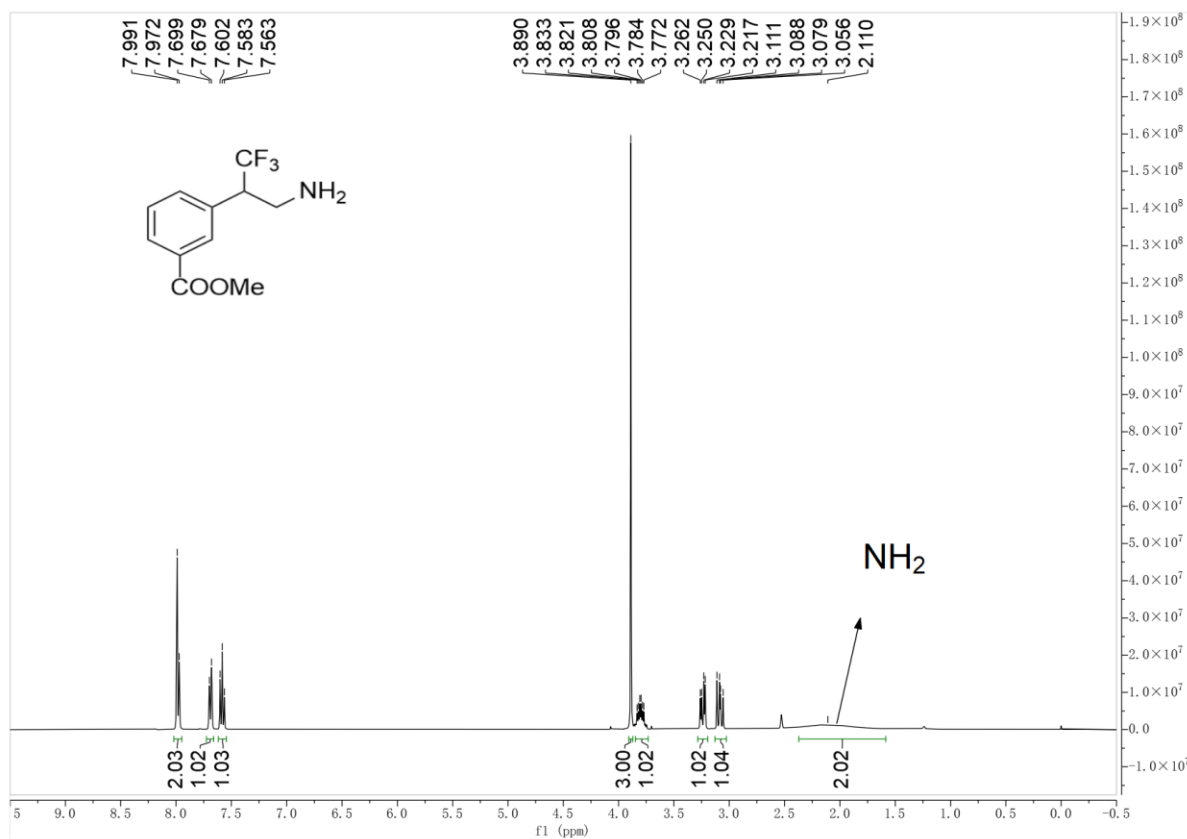
1: TOF MS ES+  
7.56e+006



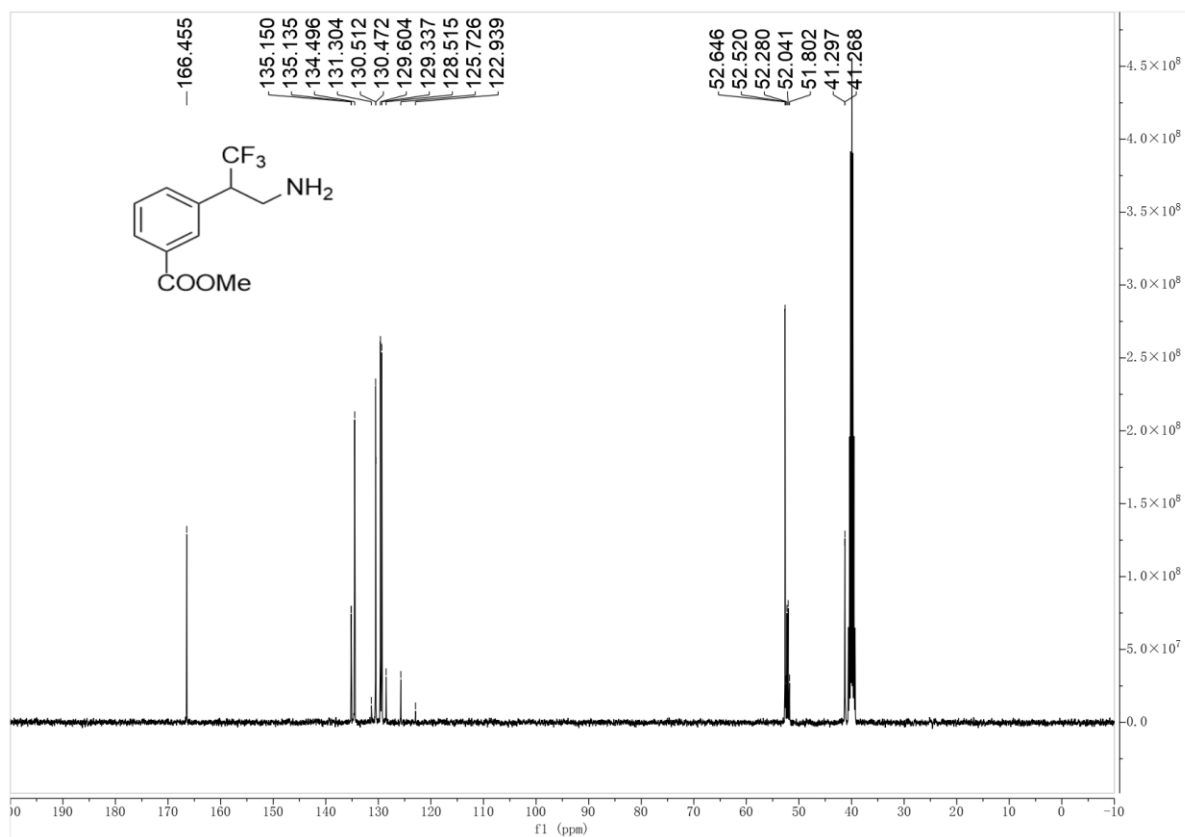
Minimum: -1.5  
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
248.0897	248.0898	-0.1	-0.4	4.5	212.1	n/a	n/a	C11 H13 N O2 F3

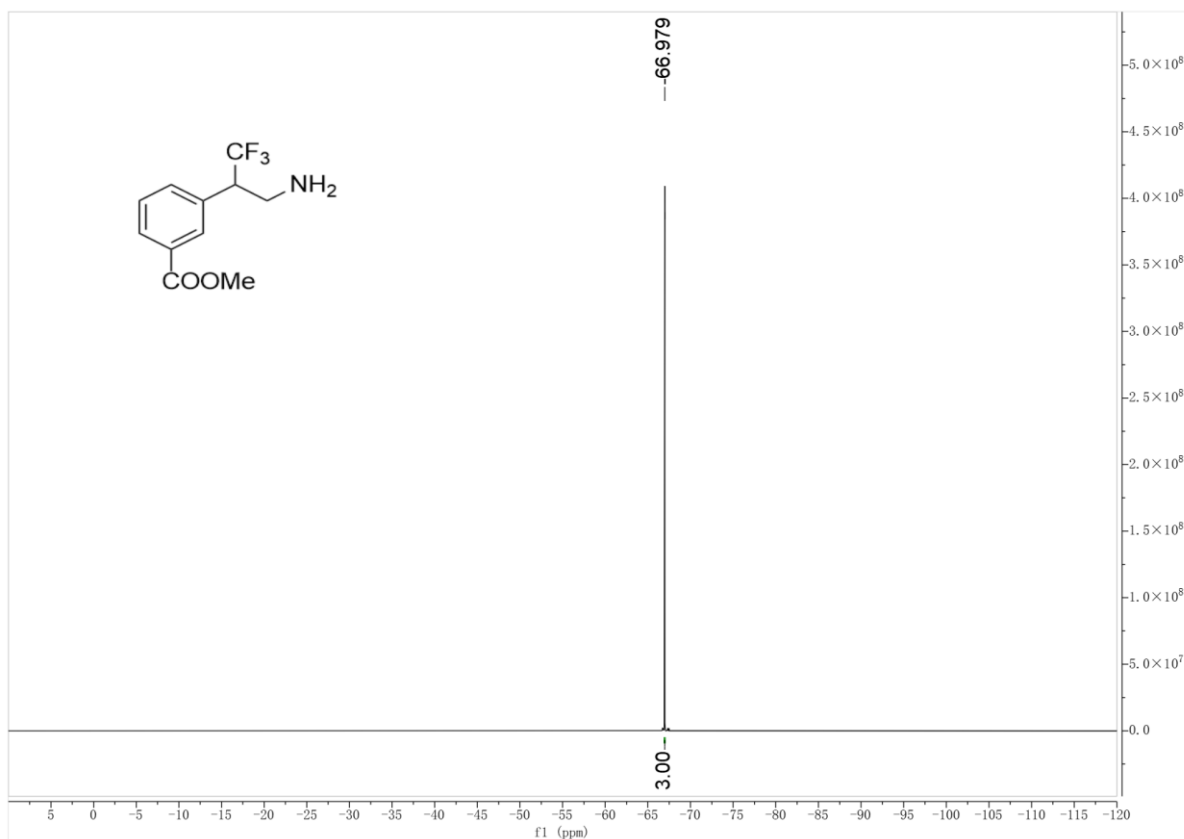
**<sup>1</sup>H NMR spectrum of 4j (400 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4j (100 MHz, DMSO-*d*<sub>6</sub>)**



### <sup>19</sup>F NMR spectrum of 4j (376 MHz, DMSO-d<sub>6</sub>)



### HRMS (ESI) spectrum of 4j

Monoisotopic Mass, Even Electron Ions

469 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

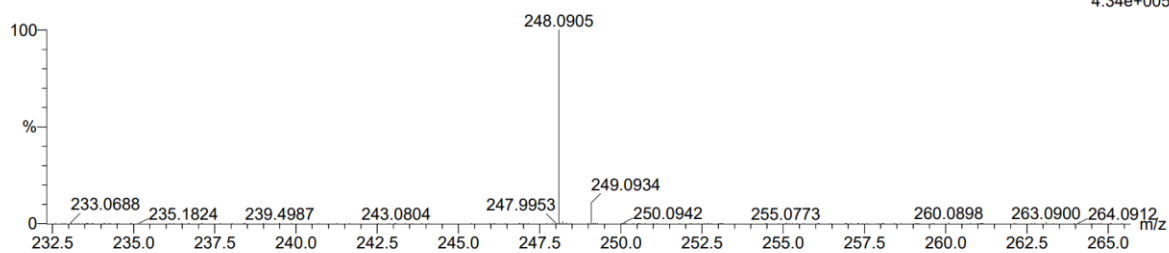
Elements Used:

C: 11-11 H: 13-13 N: 0-100 O: 0-100 F: 3-6 Na: 0-1

25

240117-7-40 11 (0.076)

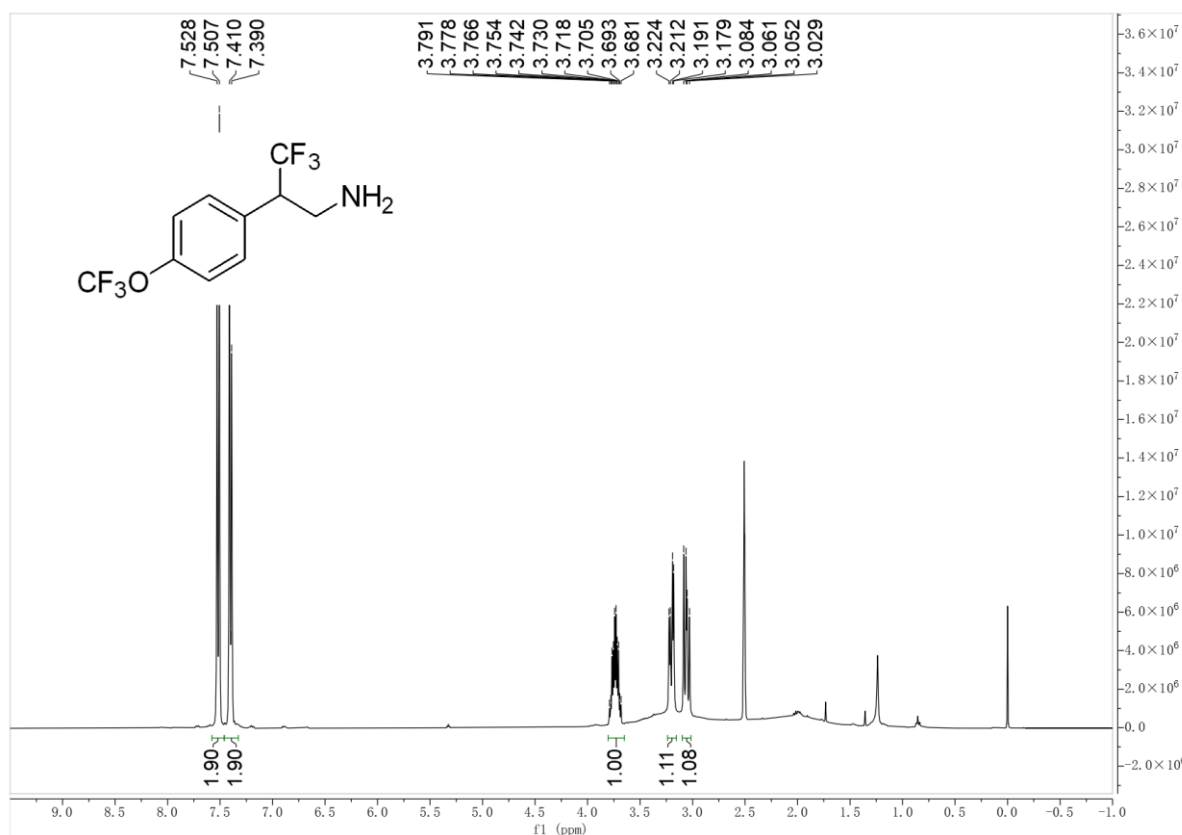
1: TOF MS ES+  
4.34e+005



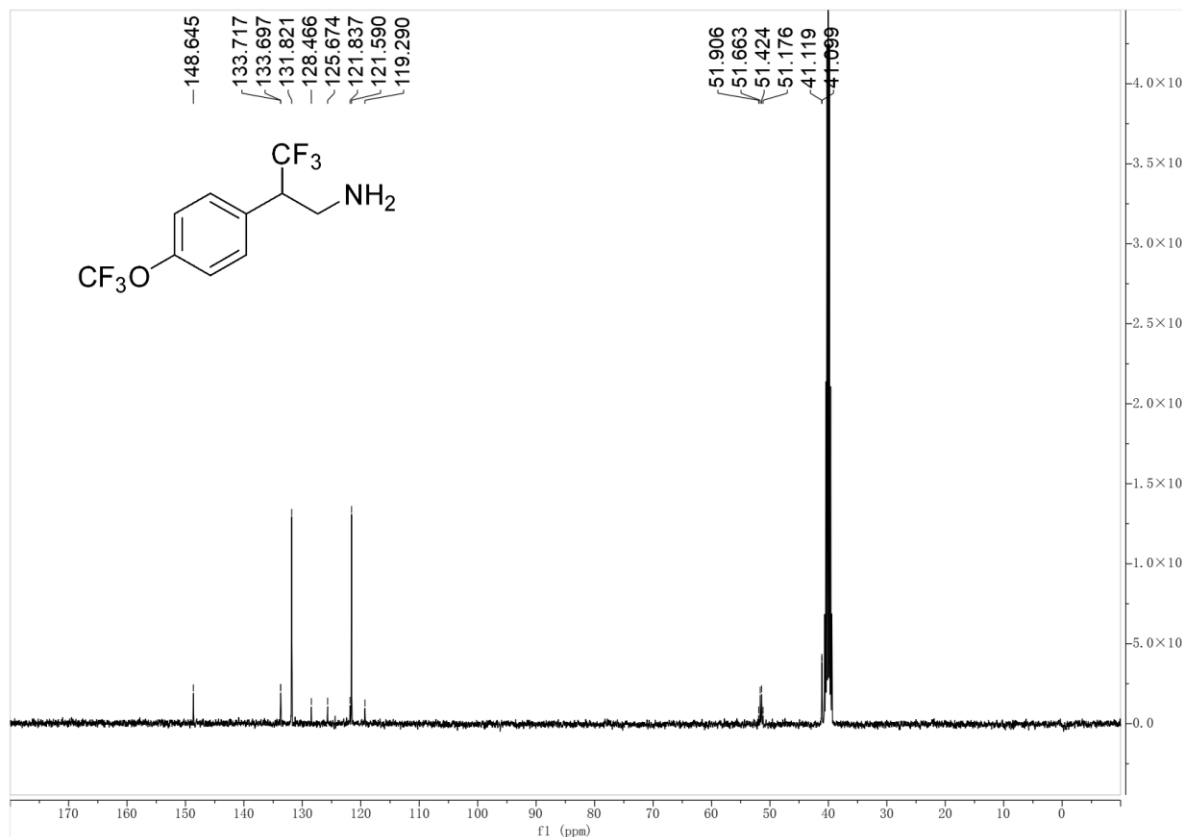
Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
248.0905	248.0898	0.7	2.8	4.5	169.2	n/a	n/a	C11 H13 N O2 F3

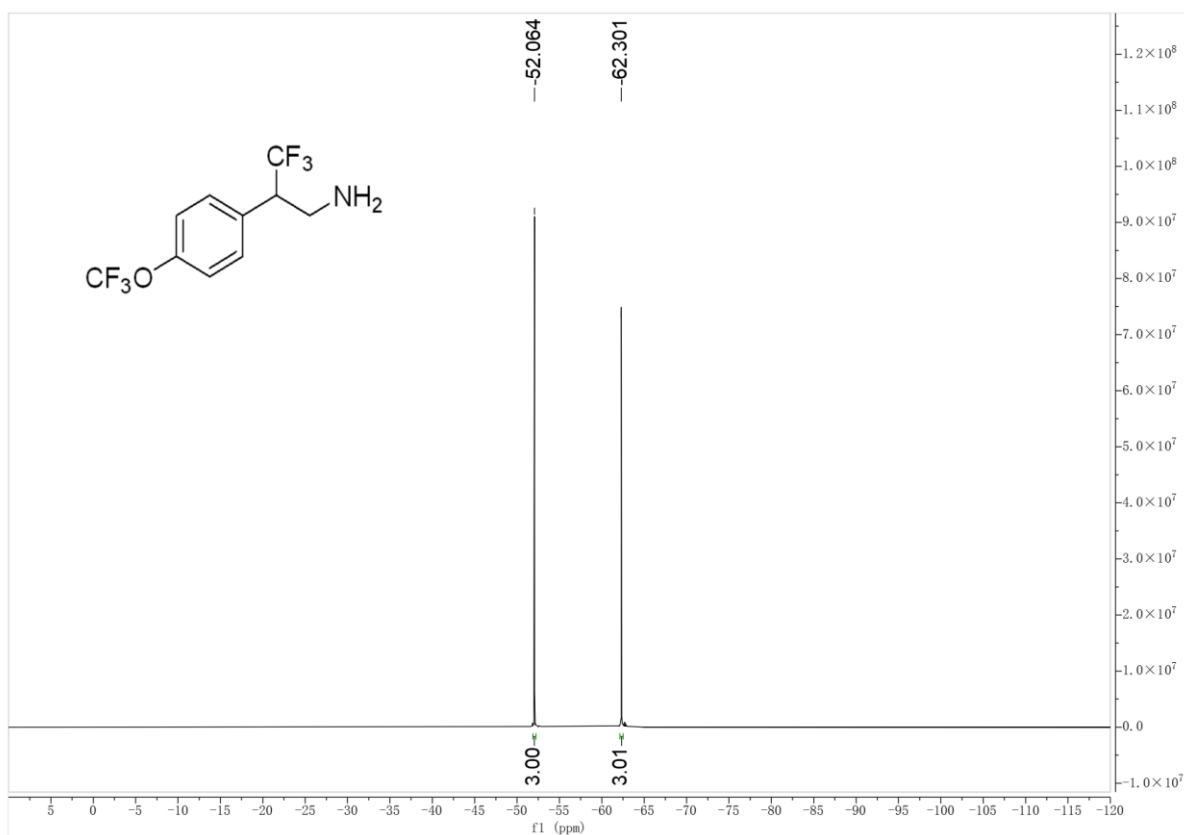
**<sup>1</sup>H NMR spectrum of 4k (400 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4k (100 MHz, DMSO-*d*<sub>6</sub>)**



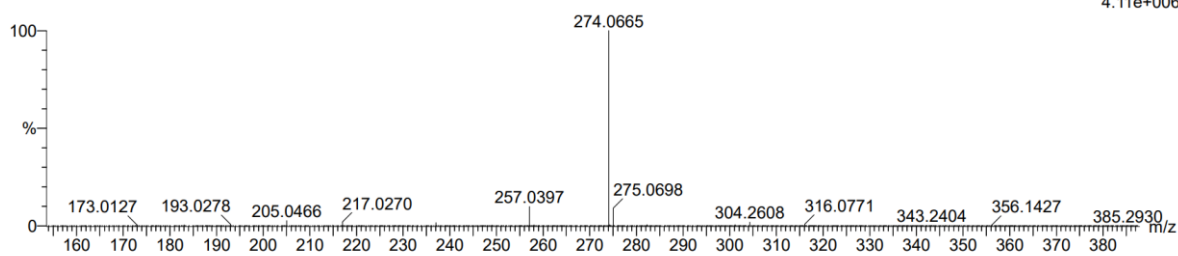
**<sup>19</sup>F NMR spectrum of 4k (376 MHz, DMSO-*d*<sub>6</sub>)**



**HRMS (ESI) spectrum of 4k**

Monoisotopic Mass, Even Electron Ions  
 148 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)  
 Elements Used:  
 C: 10-10 H: 10-10 N: 0-200 O: 0-200 F: 6-6 Na: 0-2  
 25  
 231109-3-2-3-3-- 17 (0.183)

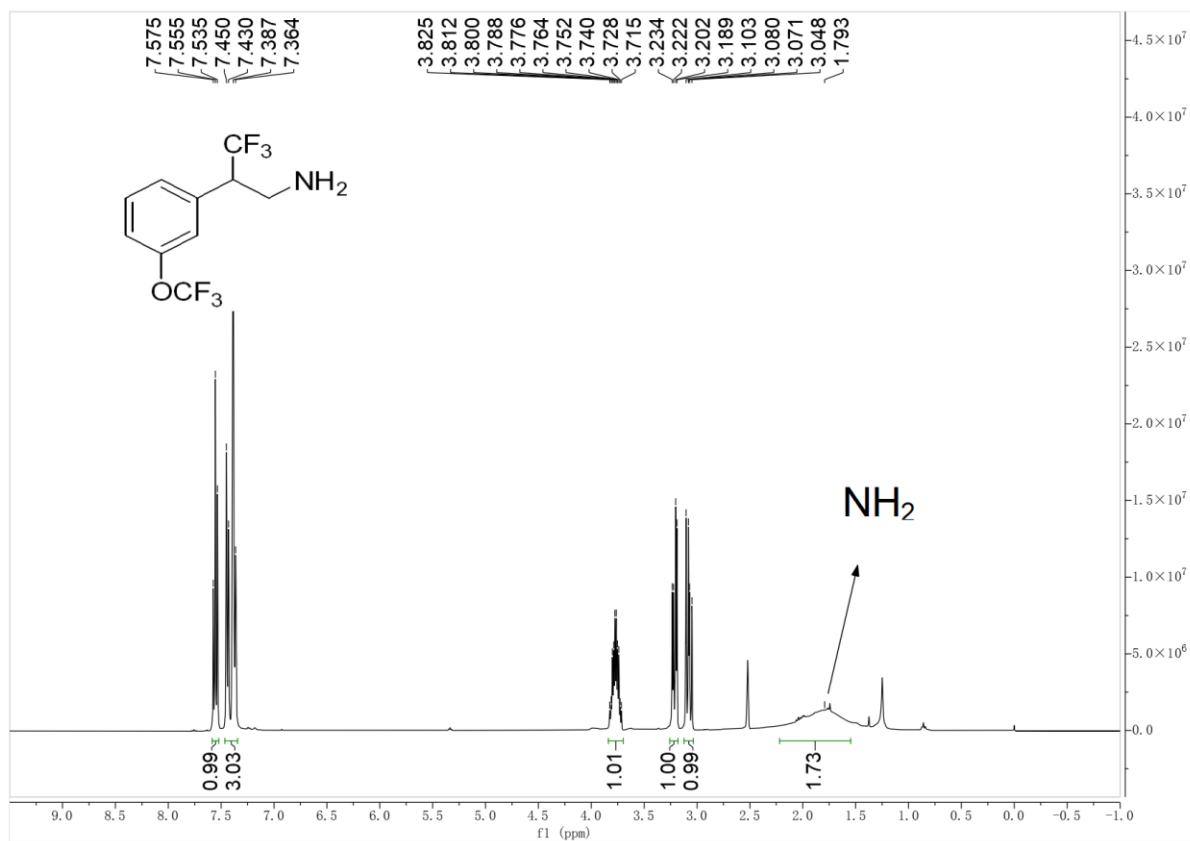
1: TOF MS ES+  
 4.11e+006



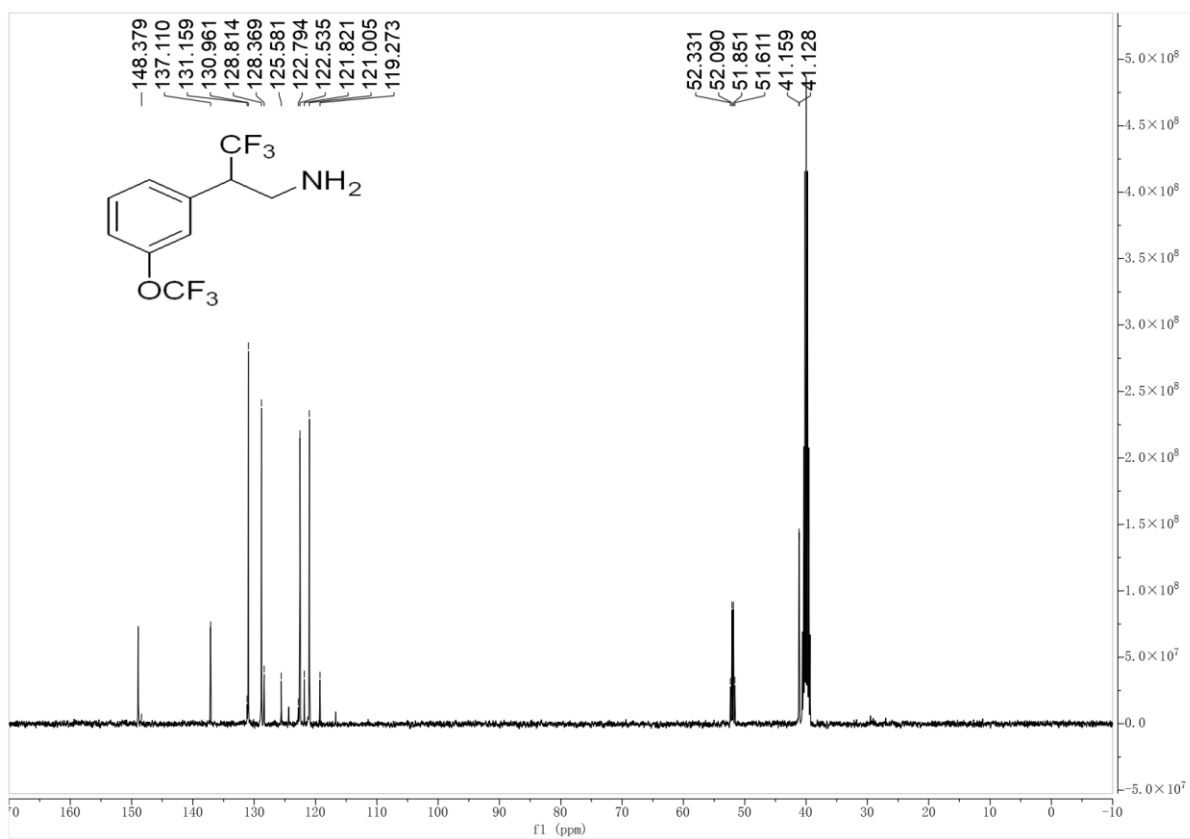
Minimum: -1.5  
 Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
274.0665	274.0667	-0.2	-0.7	3.5	354.8	n/a	n/a	C10 H10 N O F6

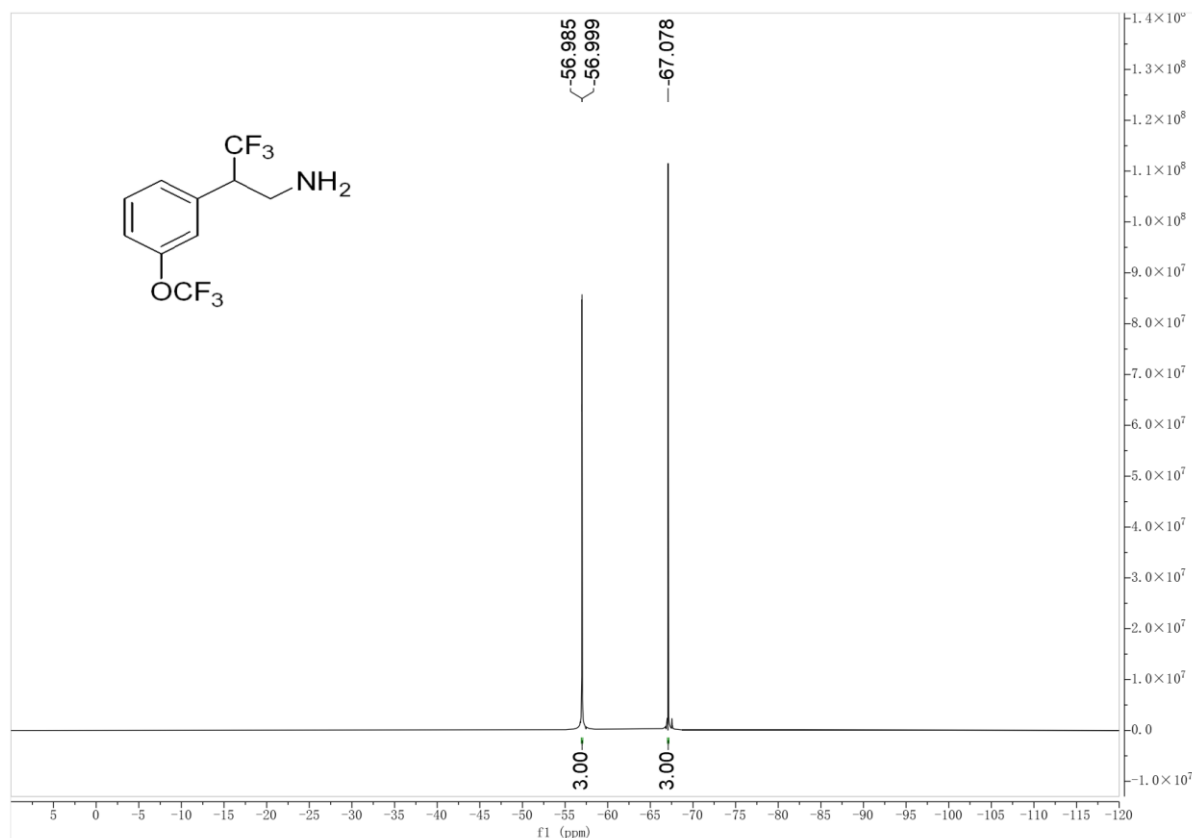
**<sup>1</sup>H NMR spectrum of 4l (400 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4l (100 MHz, DMSO-*d*<sub>6</sub>)**



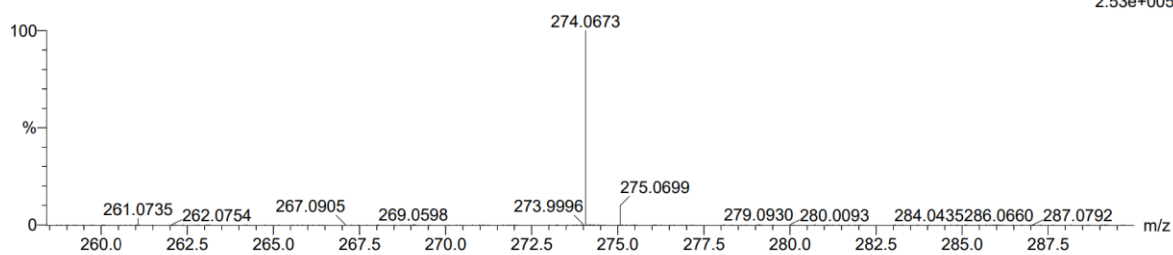
**<sup>19</sup>F NMR spectrum of 4l (376 MHz, DMSO-d<sub>6</sub>)**



**HRMS (ESI) spectrum of 4l**

Monoisotopic Mass, Even Electron Ions  
 584 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)  
 Elements Used:  
 C: 10-10 H: 10-10 N: 0-100 O: 0-100 F: 3-6 Na: 0-1  
 25  
 240117-7-41 8 (0.065)

1: TOF MS ES+  
 2.53e+005

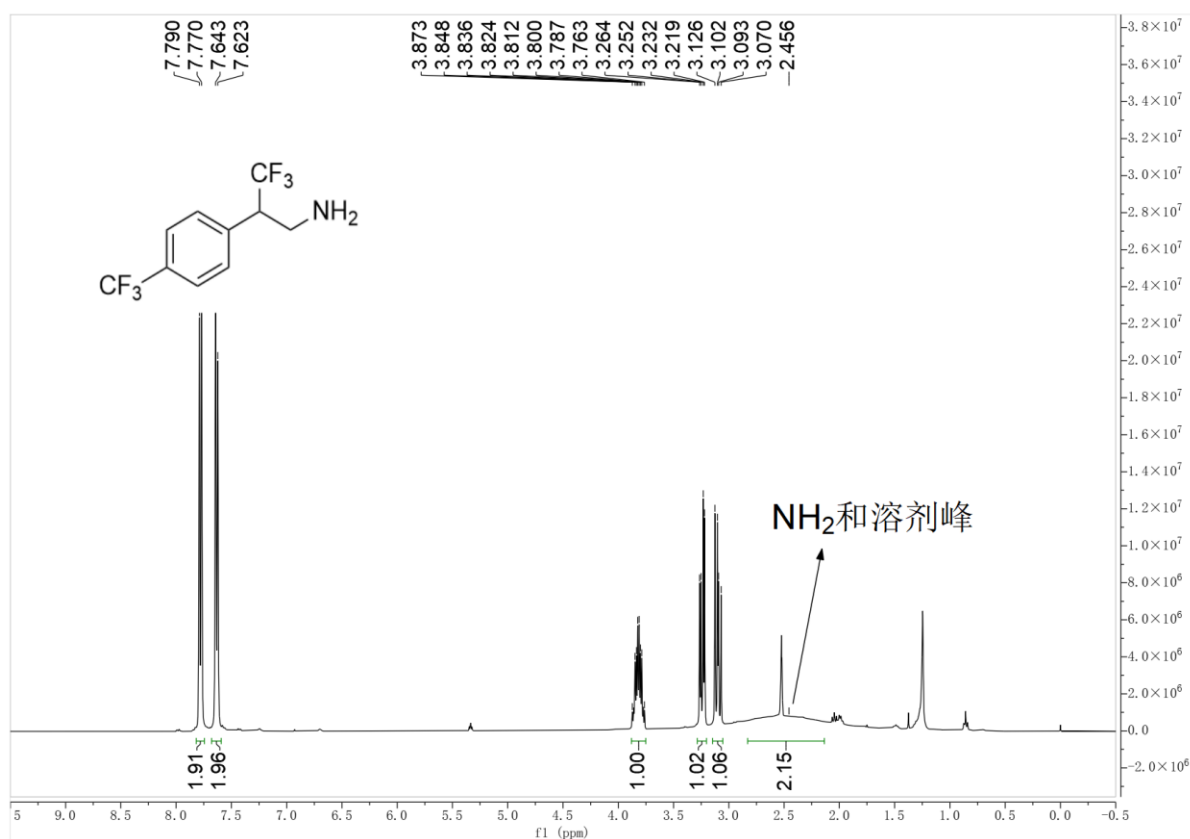


Minimum: -1.5  
 Maximum: 5.0 10.0 50.0

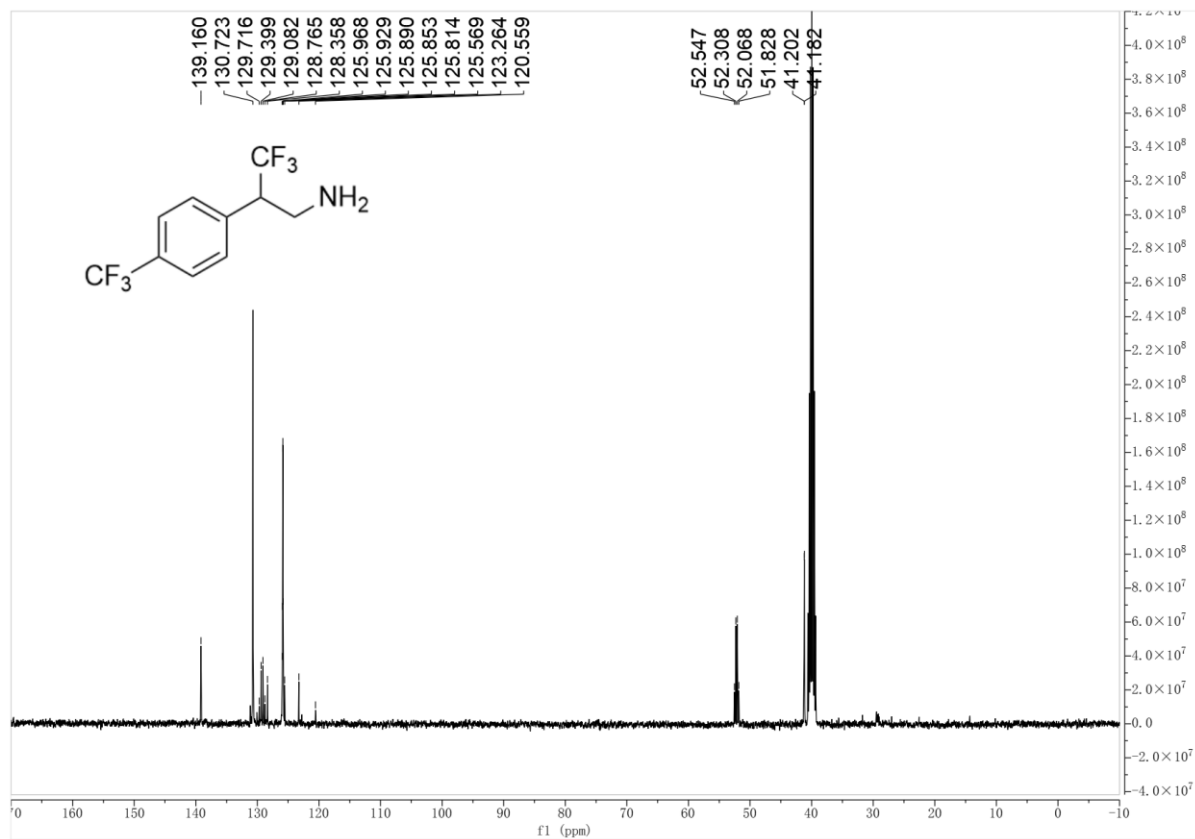
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
274.0673	274.0667	0.6	2.2	3.5	194.3	n/a	n/a	C10 H10 N O F6



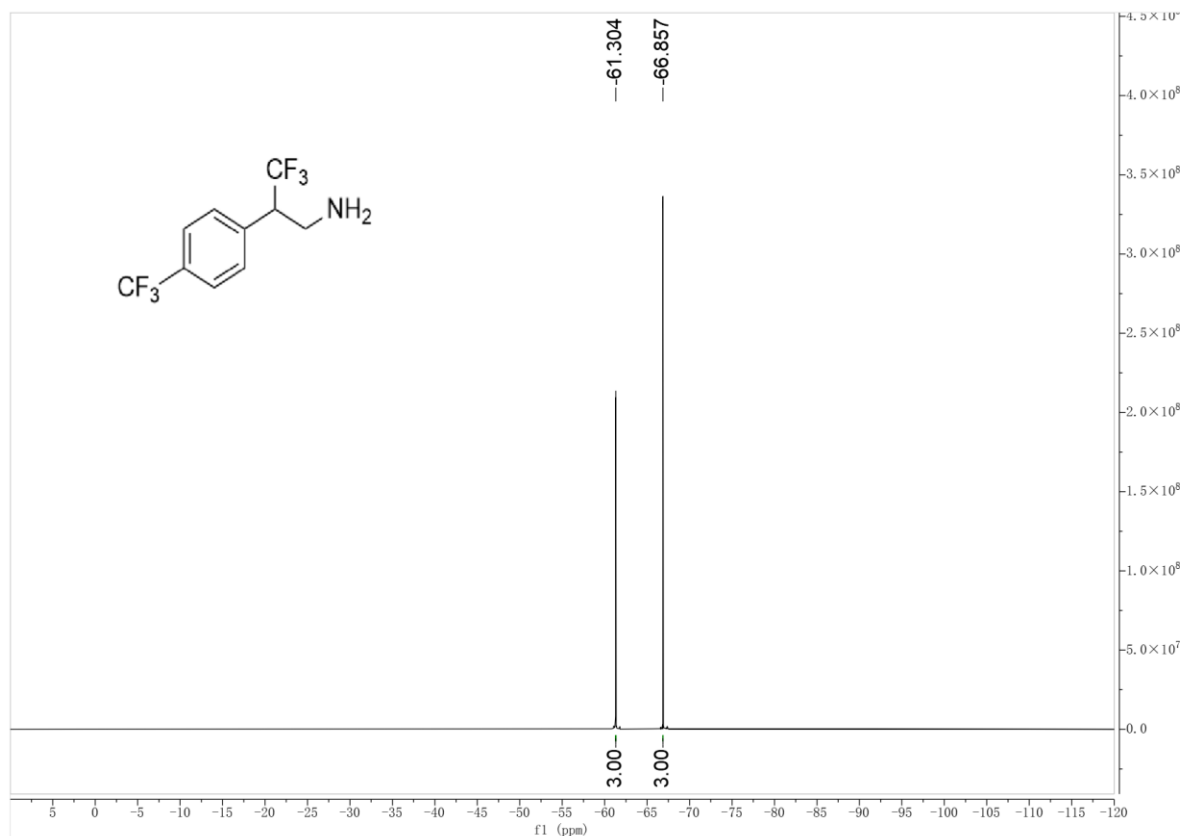
<sup>1</sup>H NMR spectrum of 4m (400 MHz, DMSO-d<sub>6</sub>)



<sup>13</sup>C NMR spectrum of 4m (100 MHz, DMSO-d<sub>6</sub>)



**<sup>19</sup>F NMR spectrum of 4m (376 MHz, DMSO-d<sub>6</sub>)**



**HRMS (ESI) spectrum of 4m**

Monoisotopic Mass, Even Electron Ions

94 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

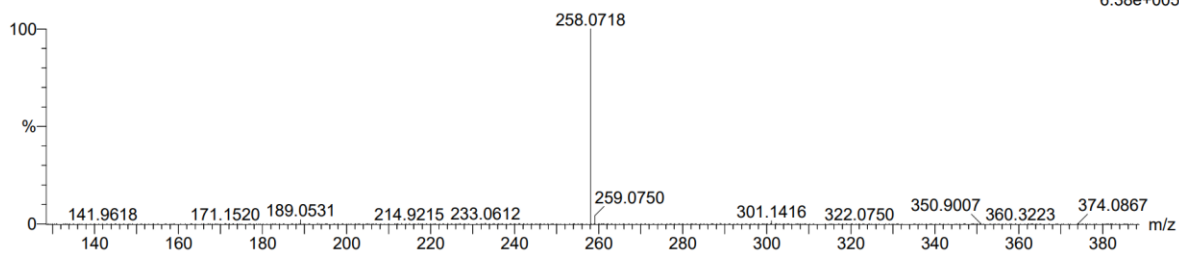
Elements Used:

C: 10-10 H: 10-10 N: 0-30 O: 0-100 F: 6-6 Na: 0-1

3

230512-2-19 29 (0.331)

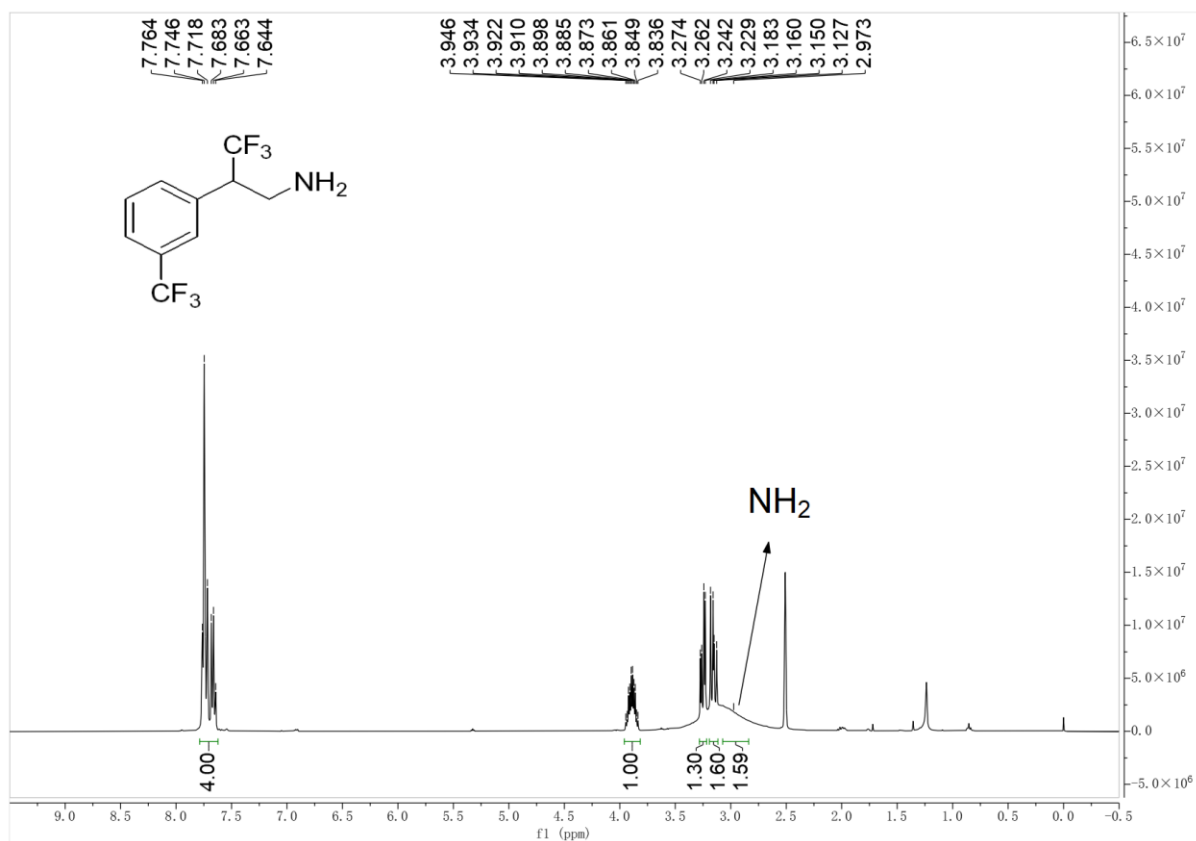
1: TOF MS ES+  
6.38e+005



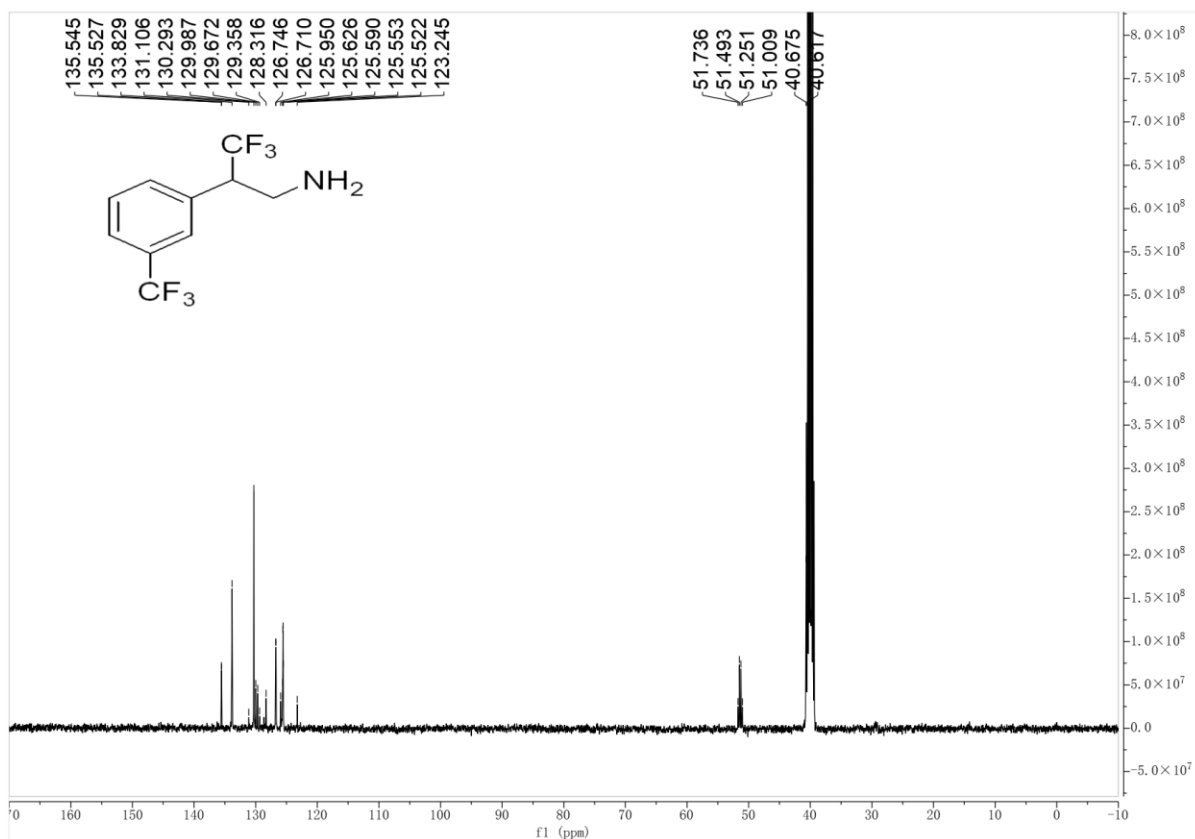
Minimum: -1.5  
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
258.0718	258.0717	0.1	0.4	3.5	85.8	n/a	n/a	C10 H10 N F6

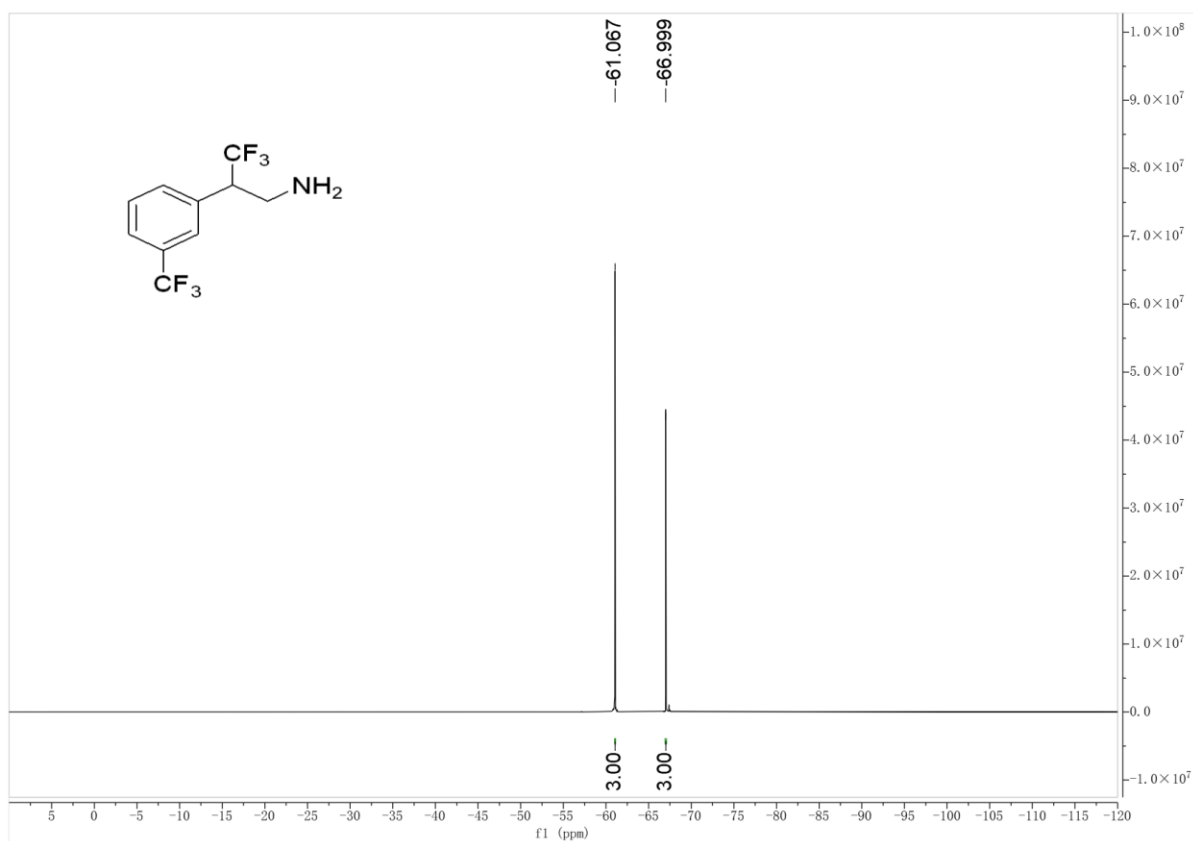
**<sup>1</sup>H NMR spectrum of 4n (400 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4n (100 MHz, DMSO-*d*<sub>6</sub>)**



### <sup>19</sup>F NMR spectrum of 4n (376 MHz, DMSO-d<sub>6</sub>)



### HRMS (ESI) spectrum of 4n

Monoisotopic Mass, Even Electron Ions

504 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

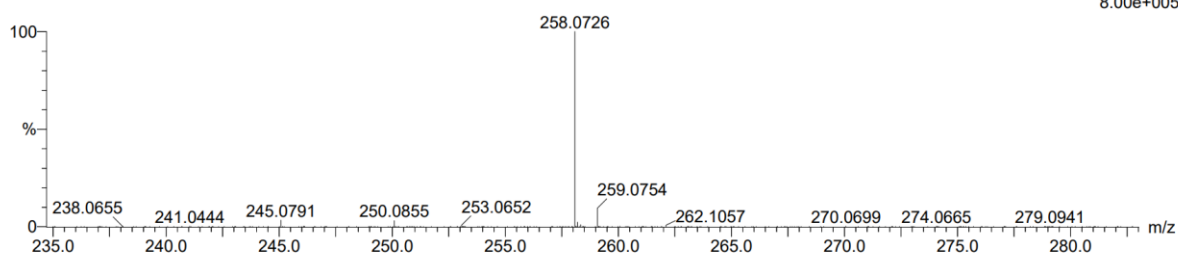
Elements Used:

C: 10-10 H: 10-10 N: 0-100 O: 0-100 F: 3-6 Na: 0-1

25

240117-7-42 11 (0.076)

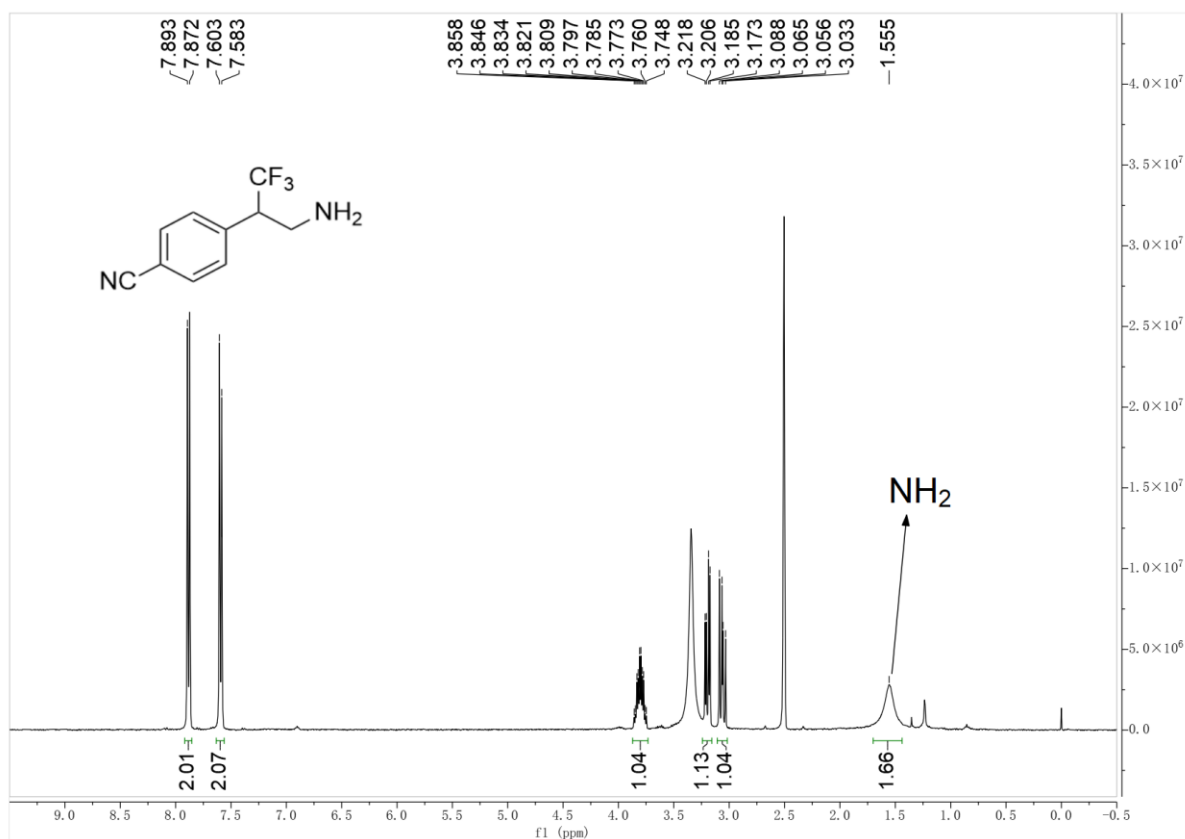
1: TOF MS ES+  
8.00e+005



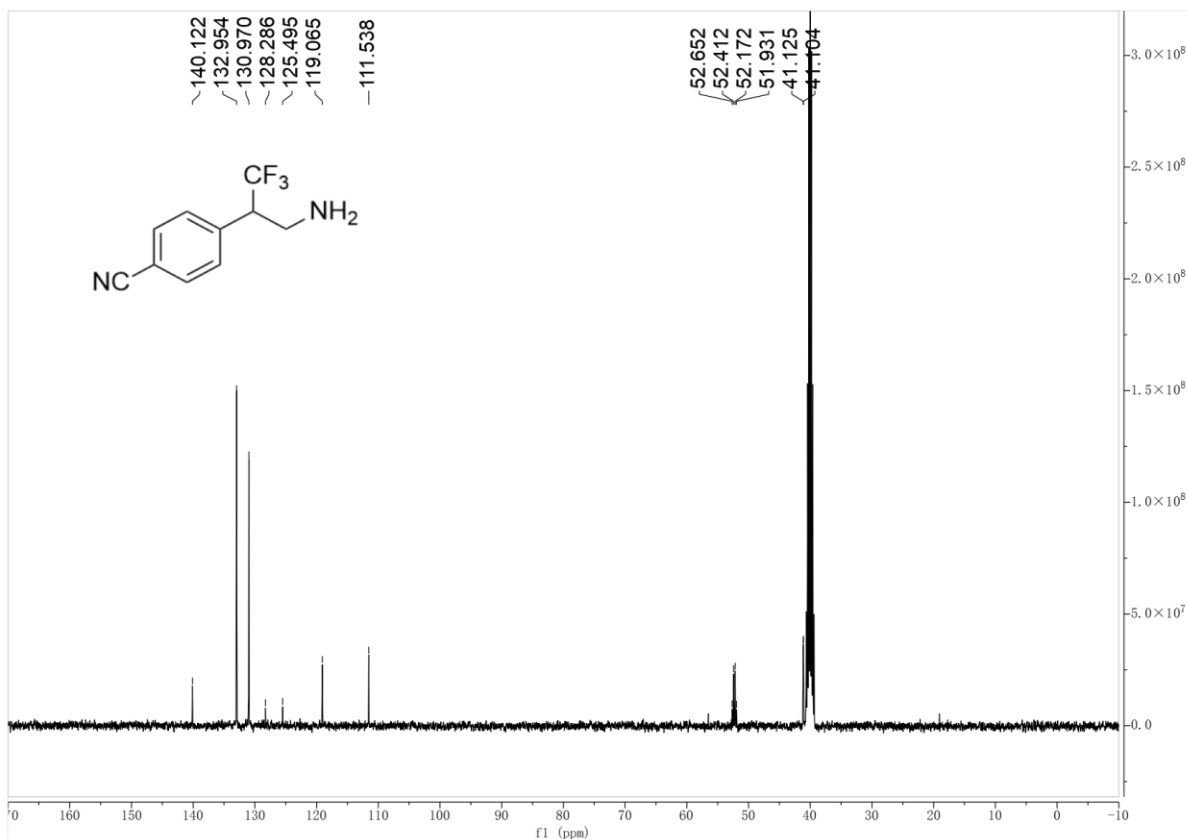
Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
258.0726	258.0717	0.9	3.5	3.5	217.6	n/a	n/a	C10 H10 N F6

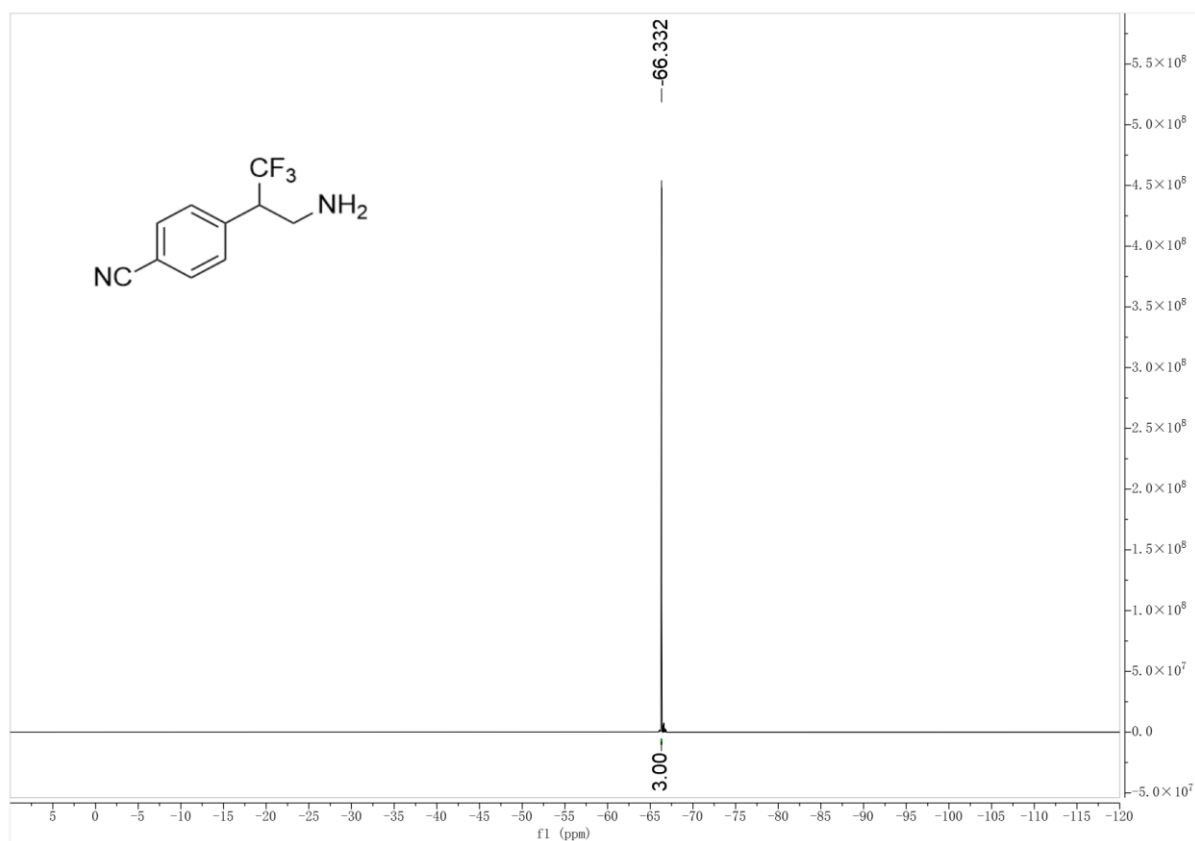
**<sup>1</sup>H NMR spectrum of 4o (400 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4o (100 MHz, DMSO-*d*<sub>6</sub>)**



### <sup>19</sup>F NMR spectrum of 4o (376 MHz, DMSO-d<sub>6</sub>)



### HRMS (ESI) spectrum of 4o

Monoisotopic Mass, Even Electron Ions

170 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

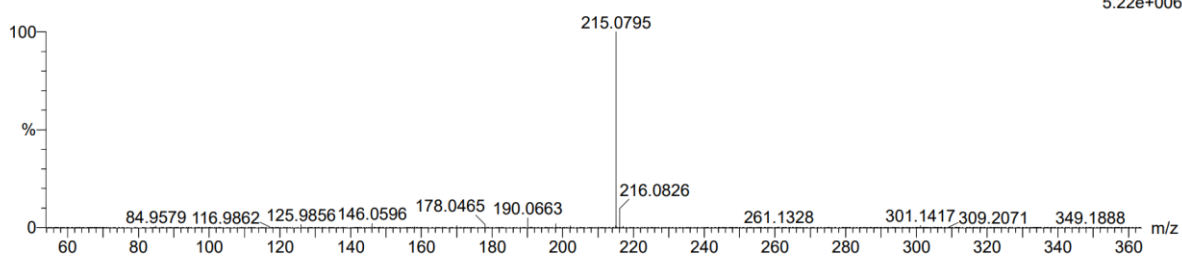
Elements Used:

C: 10-10 H: 10-10 N: 0-20 O: 0-20 F: 3-3 Na: 0-3

6

230410-1-22 7 (0.093)

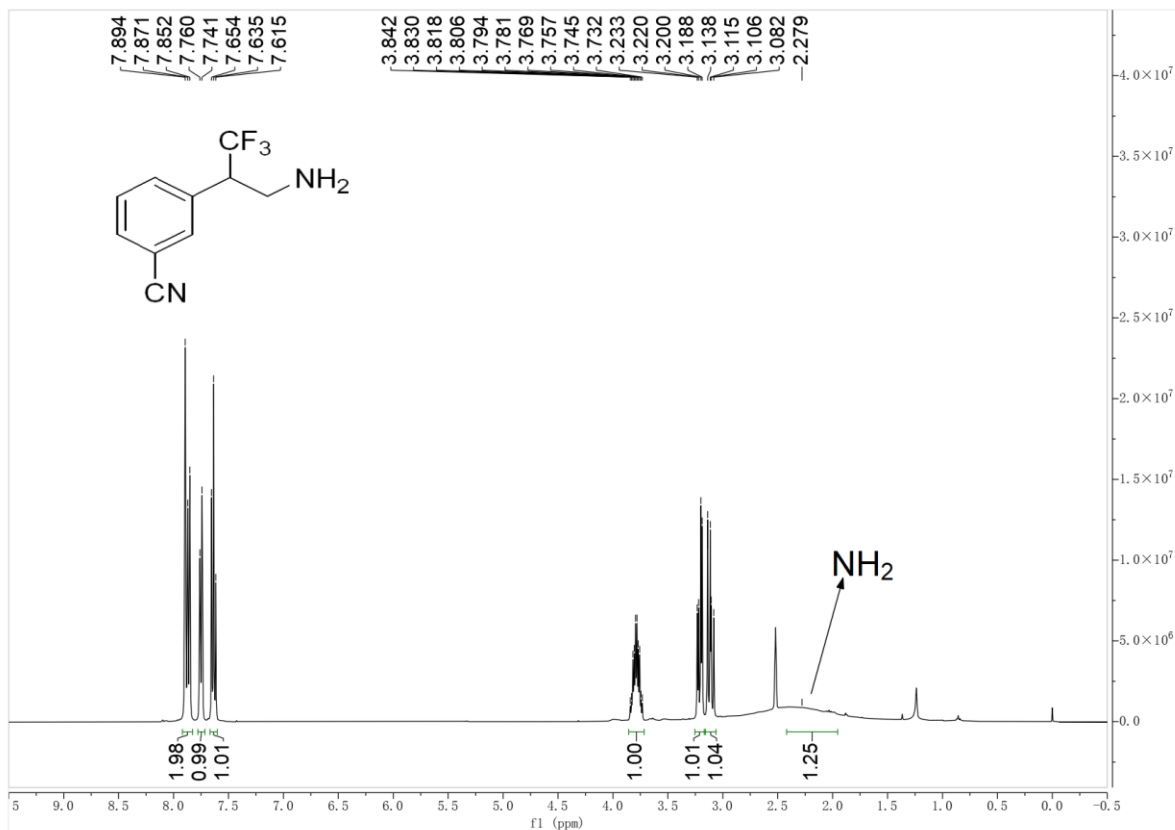
1: TOF MS ES+  
5.22e+006



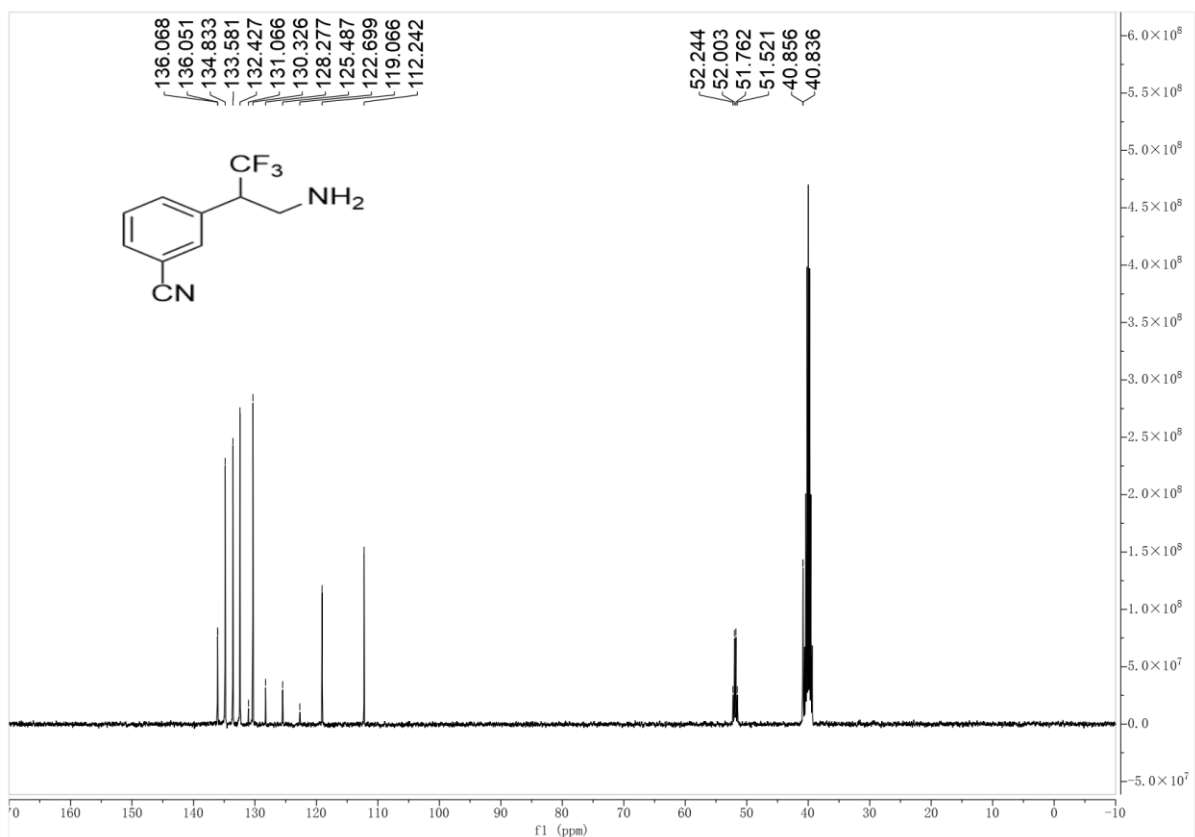
Minimum: -1.5  
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
215.0795	215.0796	-0.1	-0.5	5.5	254.7	n/a	n/a	C10 H10 N2 F3

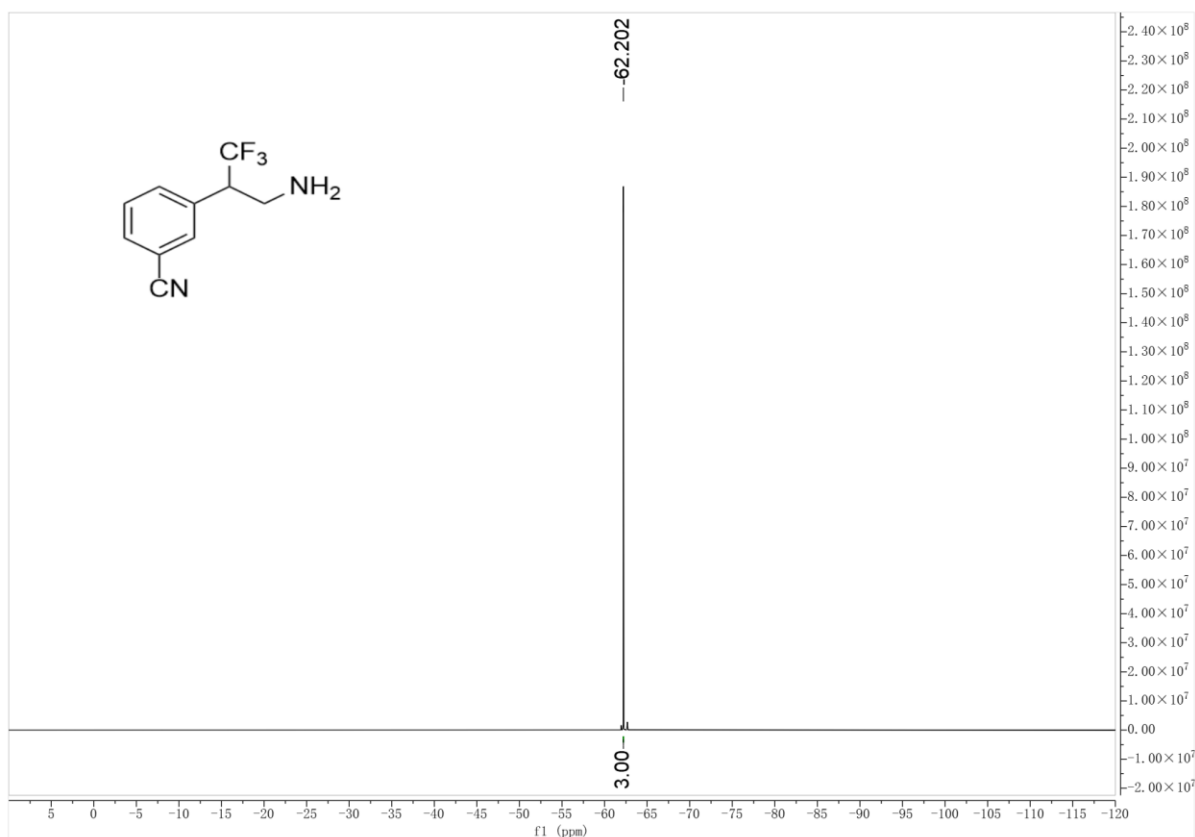
**<sup>1</sup>H NMR spectrum of 4p (400 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4p (100 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>19</sup>F NMR spectrum of 4p (376 MHz, DMSO-*d*<sub>6</sub>)**



**HRMS (ESI) spectrum of 4p**

Monoisotopic Mass, Even Electron Ions

170 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

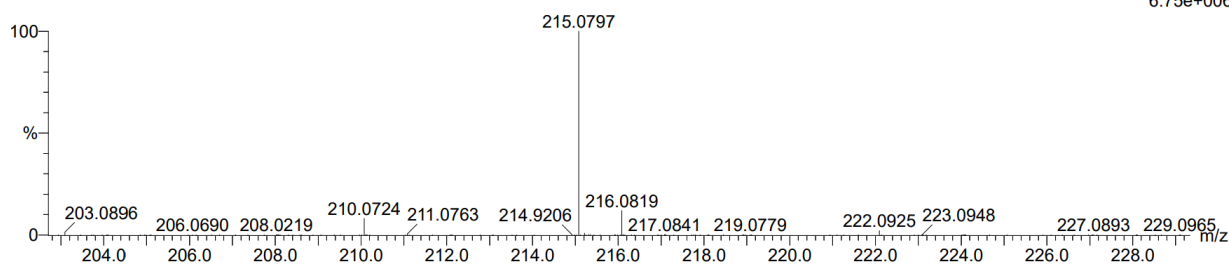
Elements Used:

C: 10-10 H: 10-10 N: 0-20 O: 0-20 F: 3-3 Na: 0-3

6

230410-1-24 5 (0.076)

1: TOF MS ES+  
6.75e+006

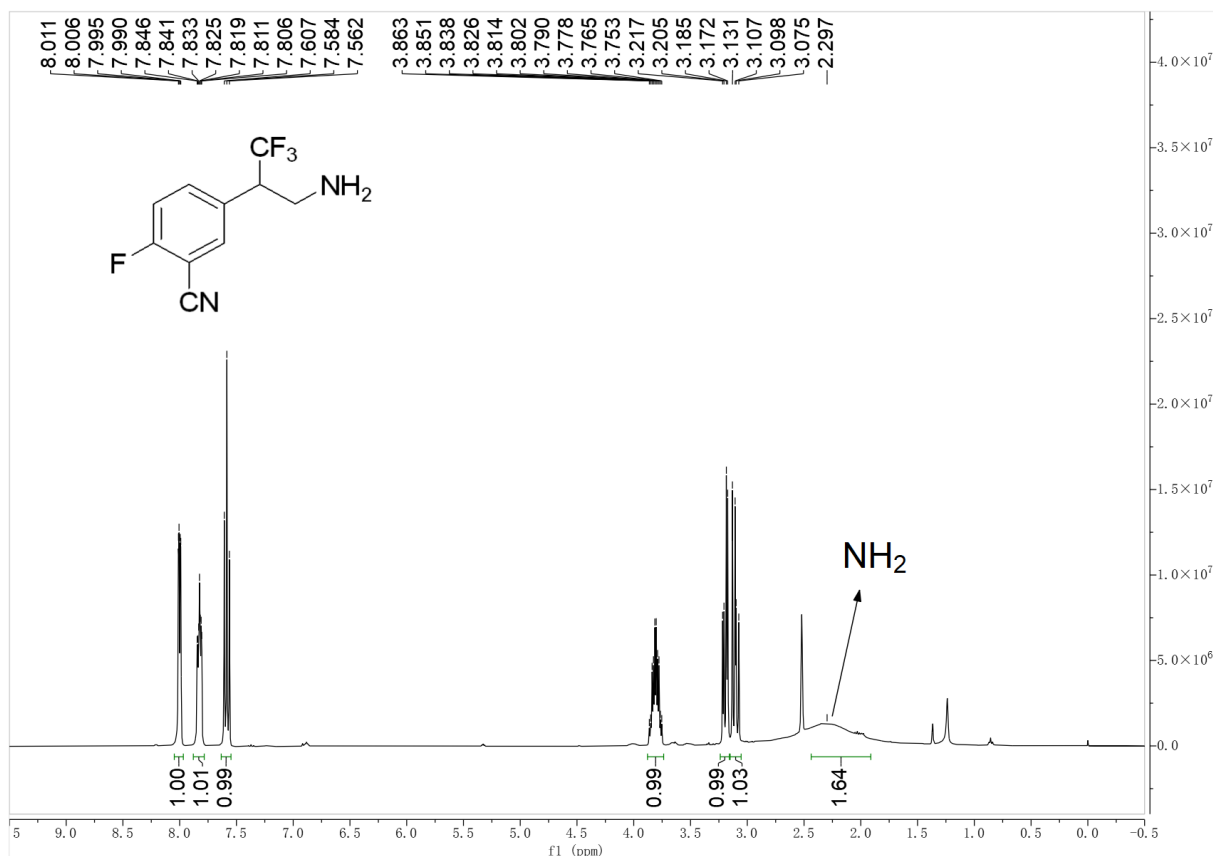


Minimum: -1.5  
Maximum: 50.0

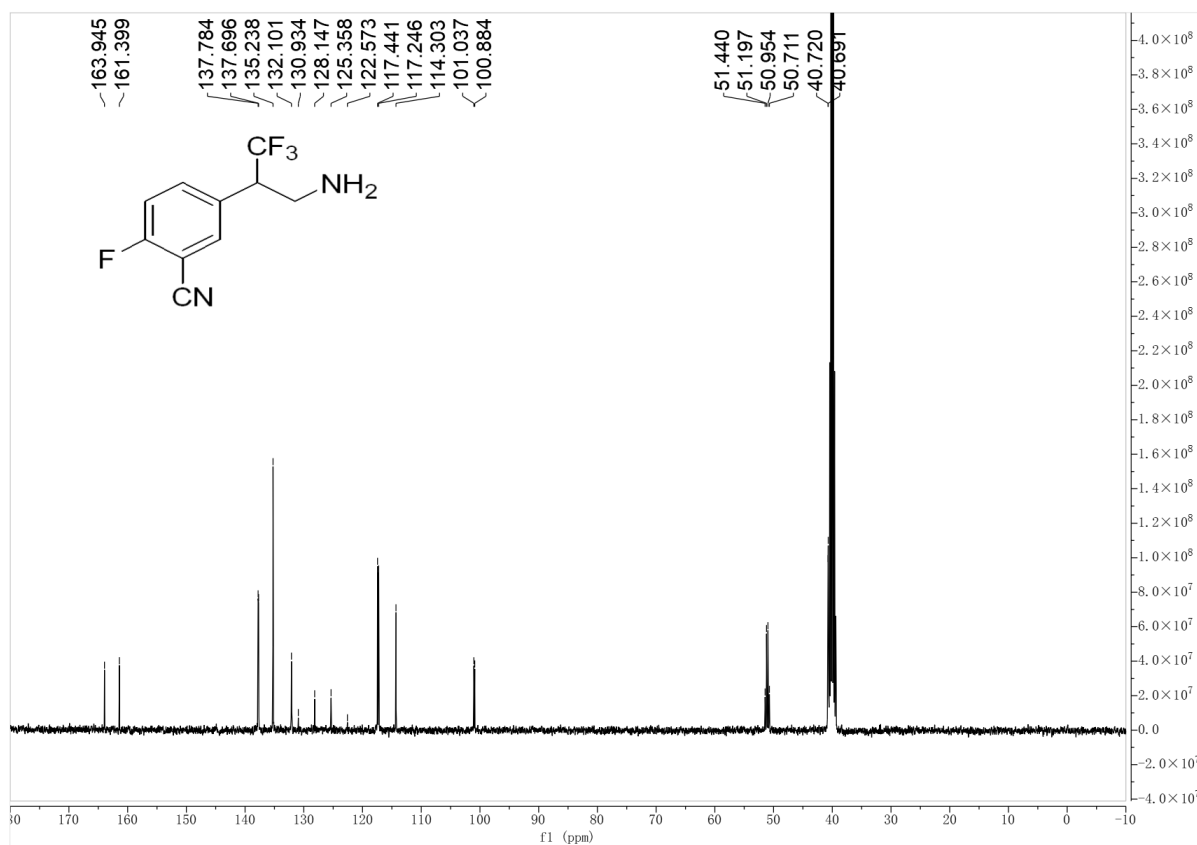
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
215.0797	215.0796	0.1	0.5	5.5	254.8	n/a	n/a	C10 H10 N2 F3



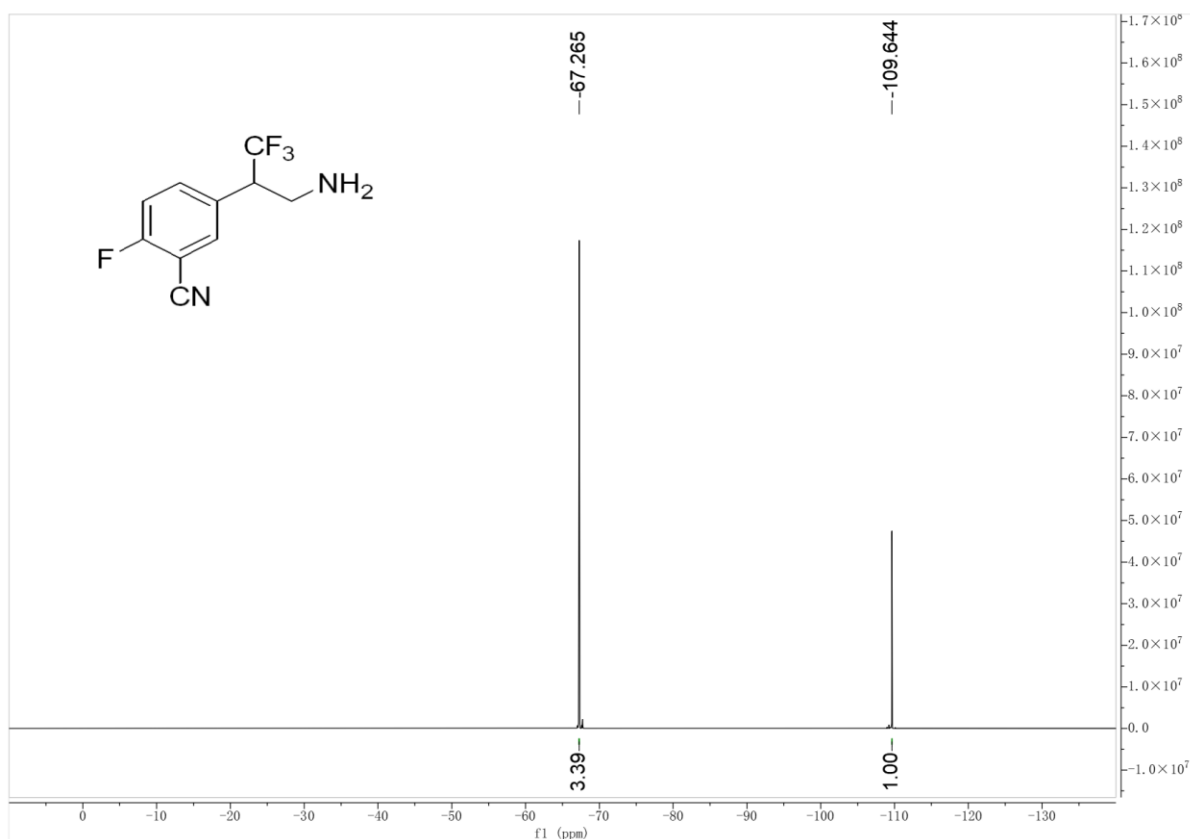
**<sup>1</sup>H NMR spectrum of 4q (400 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4q (100 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>19</sup>F NMR spectrum of 4q (376 MHz, DMSO-*d*<sub>6</sub>)**



**HRMS (ESI) spectrum of 4q**

Monoisotopic Mass, Even Electron Ions

389 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

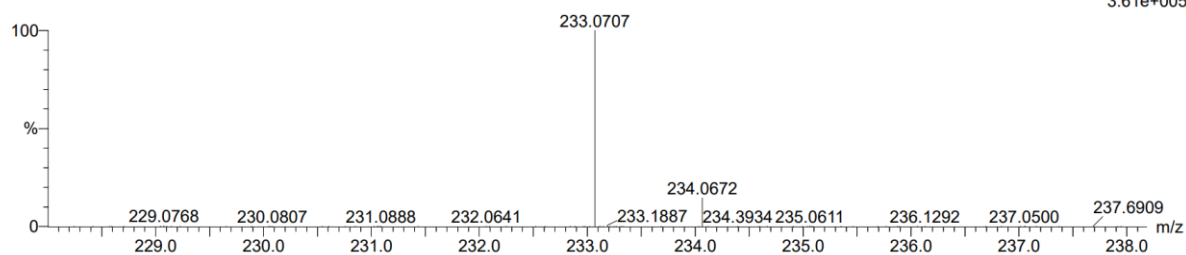
Elements Used:

C: 10-10 H: 9-9 N: 0-100 O: 0-100 F: 3-6 Na: 0-1

25

240117-7-43 6 (0.058)

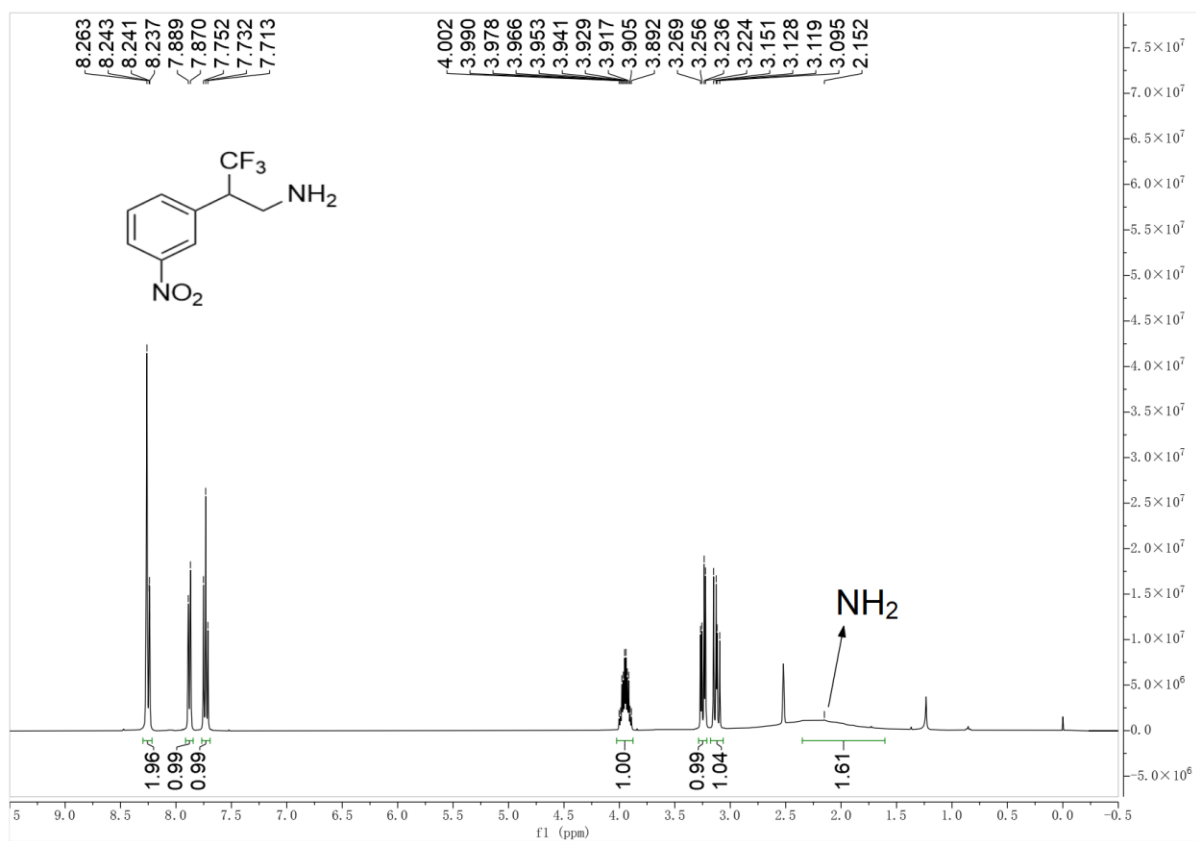
1: TOF MS ES+  
3.61e+005



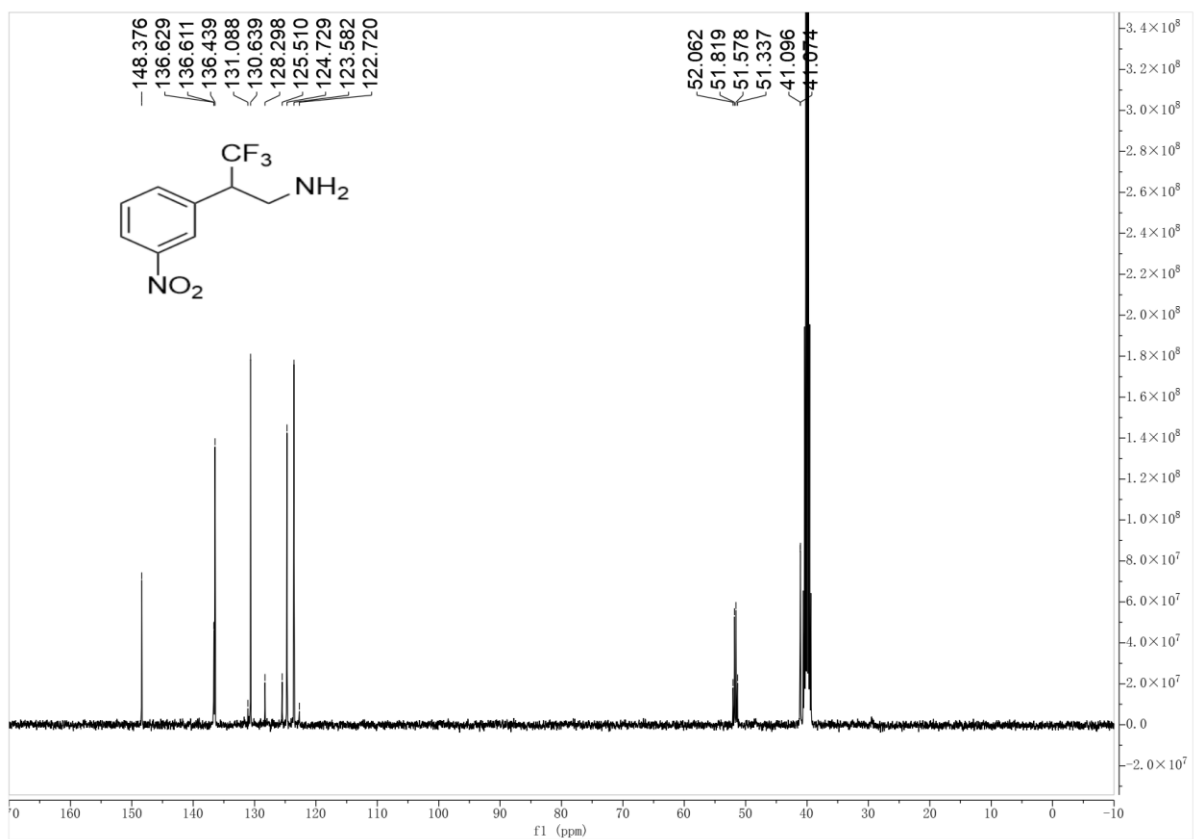
Minimum: -1.5  
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
233.0707	233.0702	0.5	2.1	5.5	179.7	n/a	n/a	C10 H9 N2 F4

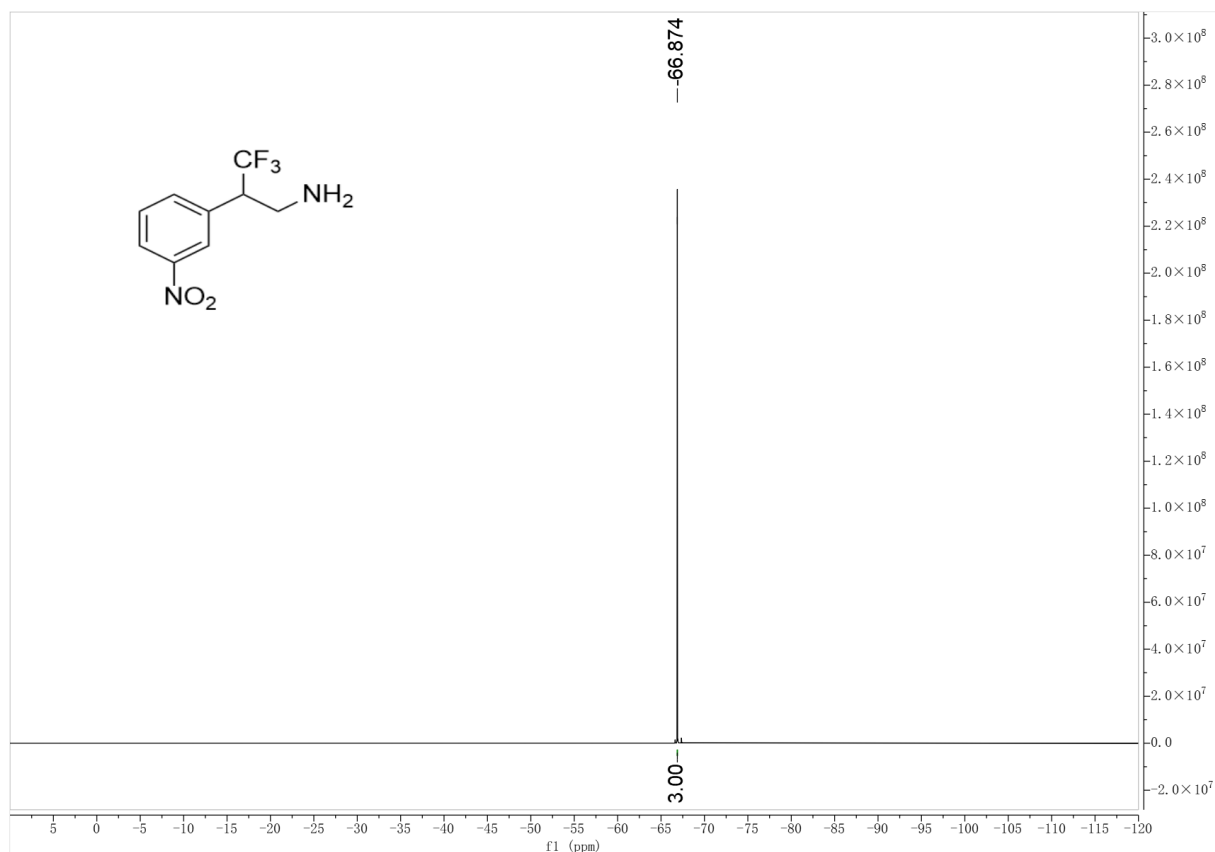
**<sup>1</sup>H NMR spectrum of 4r (400 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4r (100 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>19</sup>F NMR spectrum of 4r (376 MHz, DMSO-*d*<sub>6</sub>)**



**HRMS (ESI) spectrum of 4r**

Monoisotopic Mass, Even Electron Ions

280 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

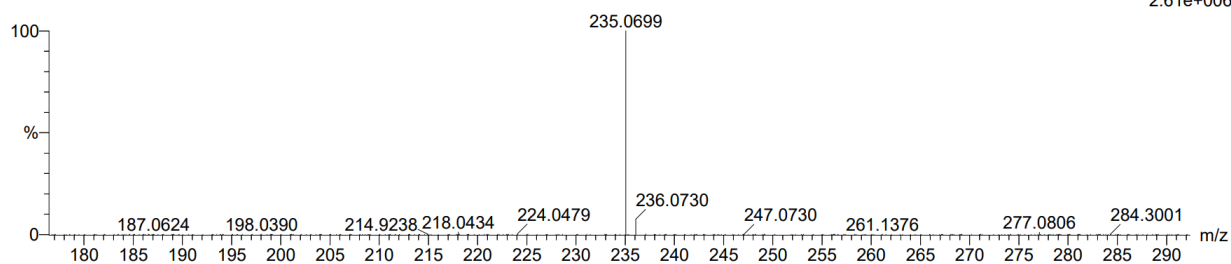
Elements Used:

C: 9-9 H: 10-10 N: 0-30 O: 0-100 F: 2-3 Na: 0-1

3

230512-2-18 10 (0.127)

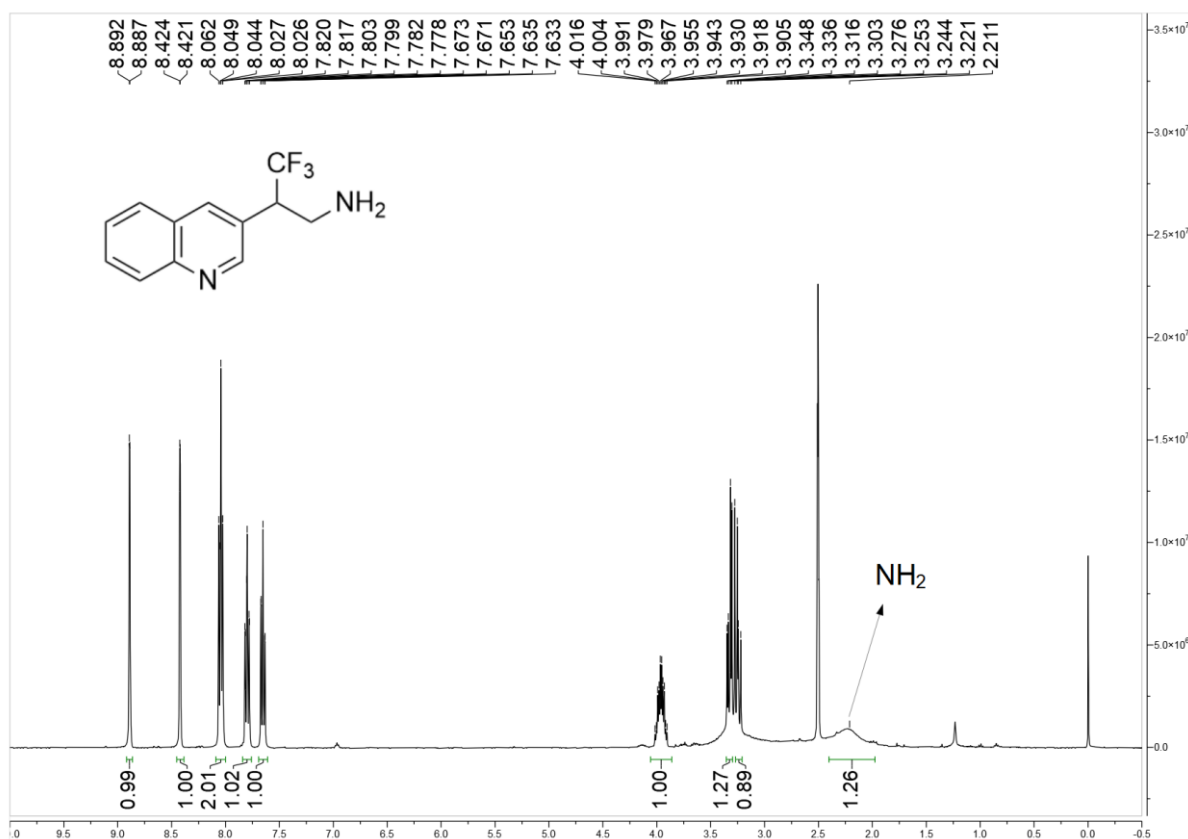
1: TOF MS ES+  
2.61e+006



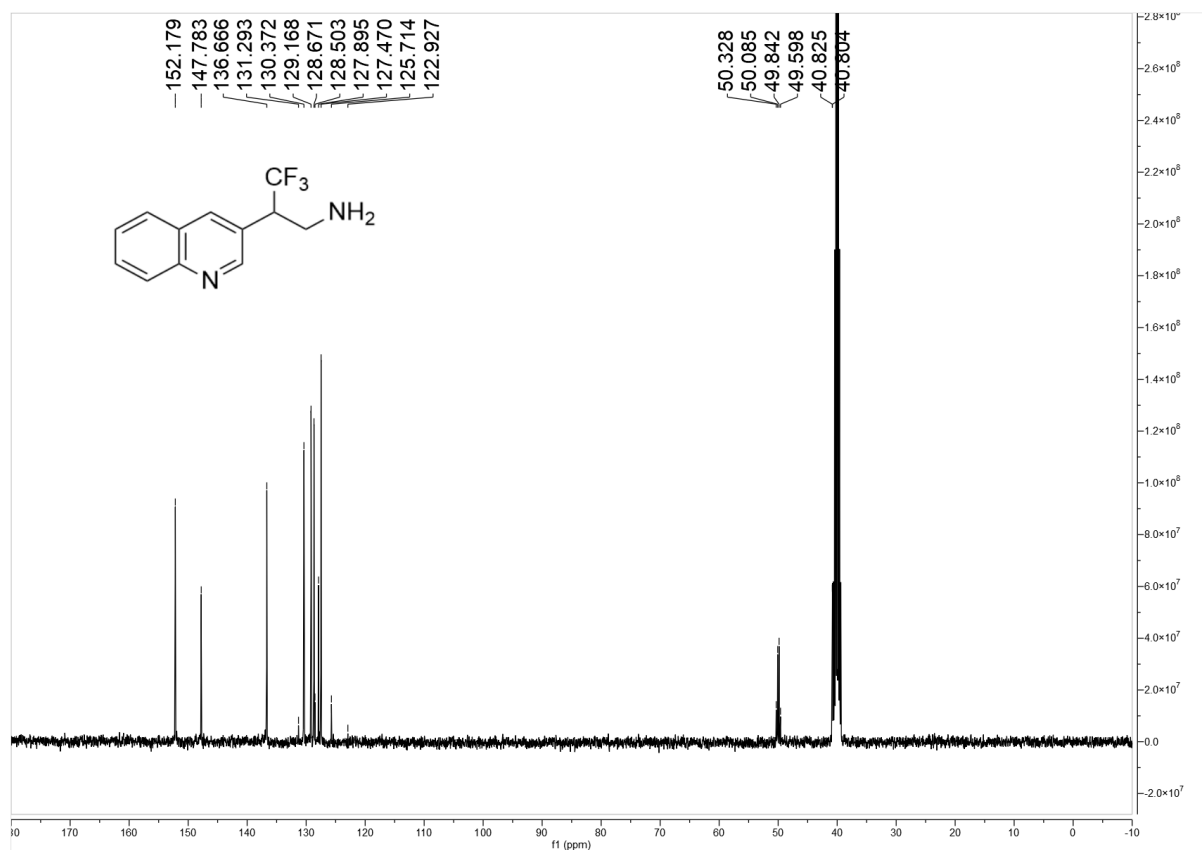
Minimum: -1.5  
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
235.0699	235.0694	0.5	2.1	4.5	59.2	n/a	n/a	C9 H10 N2 O2 F3

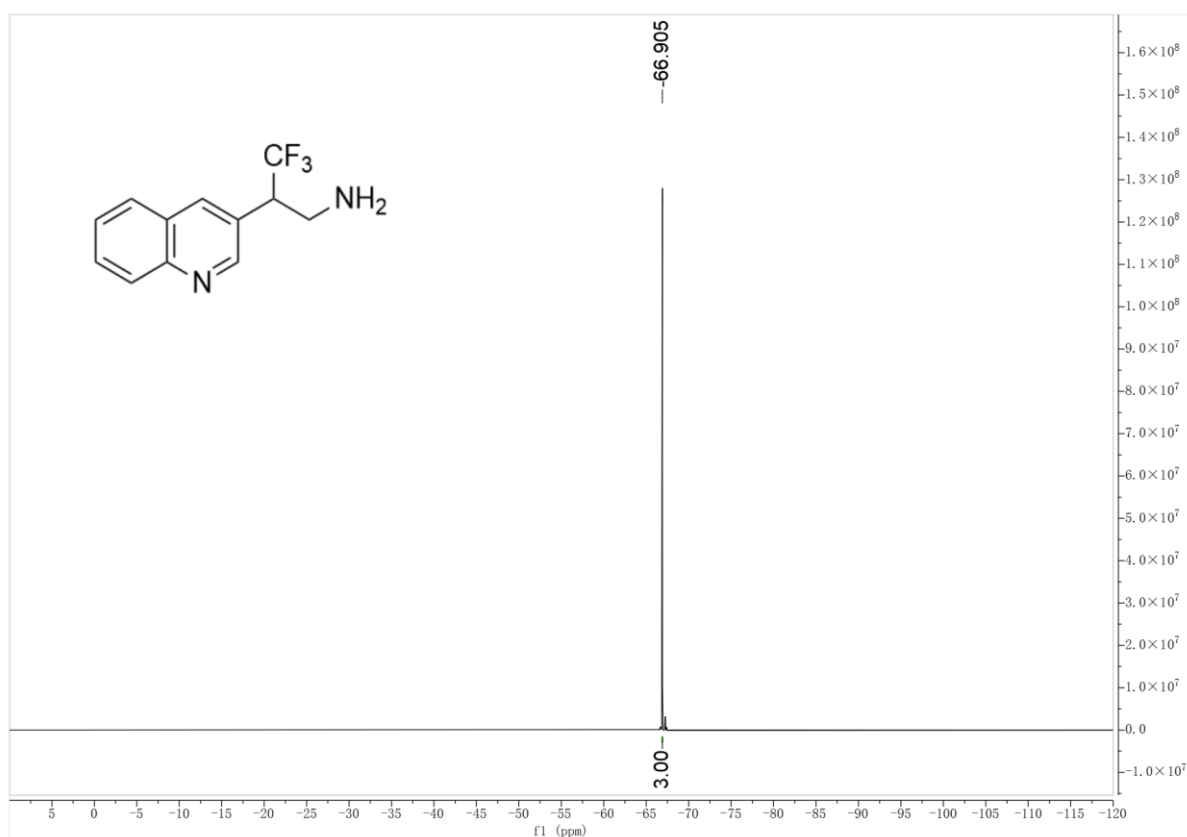
**<sup>1</sup>H NMR spectrum of 4s (400 MHz, DMSO-d<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4s (100 MHz, DMSO-d<sub>6</sub>)**



### <sup>19</sup>F NMR spectrum of 4s (376 MHz, DMSO-d<sub>6</sub>)



### HRMS (ESI) spectrum of 4s

Monoisotopic Mass, Even Electron Ions

319 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

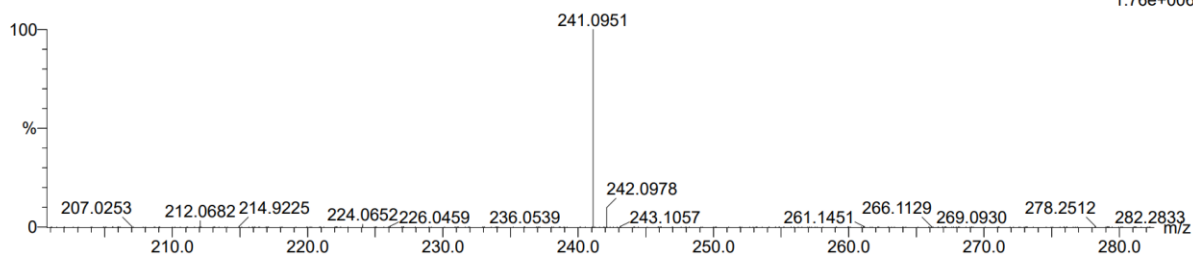
Elements Used:

C: 12-12 H: 12-12 N: 0-30 O: 0-100 F: 2-3 Na: 0-1

3

230512-2-17 9 (0.118)

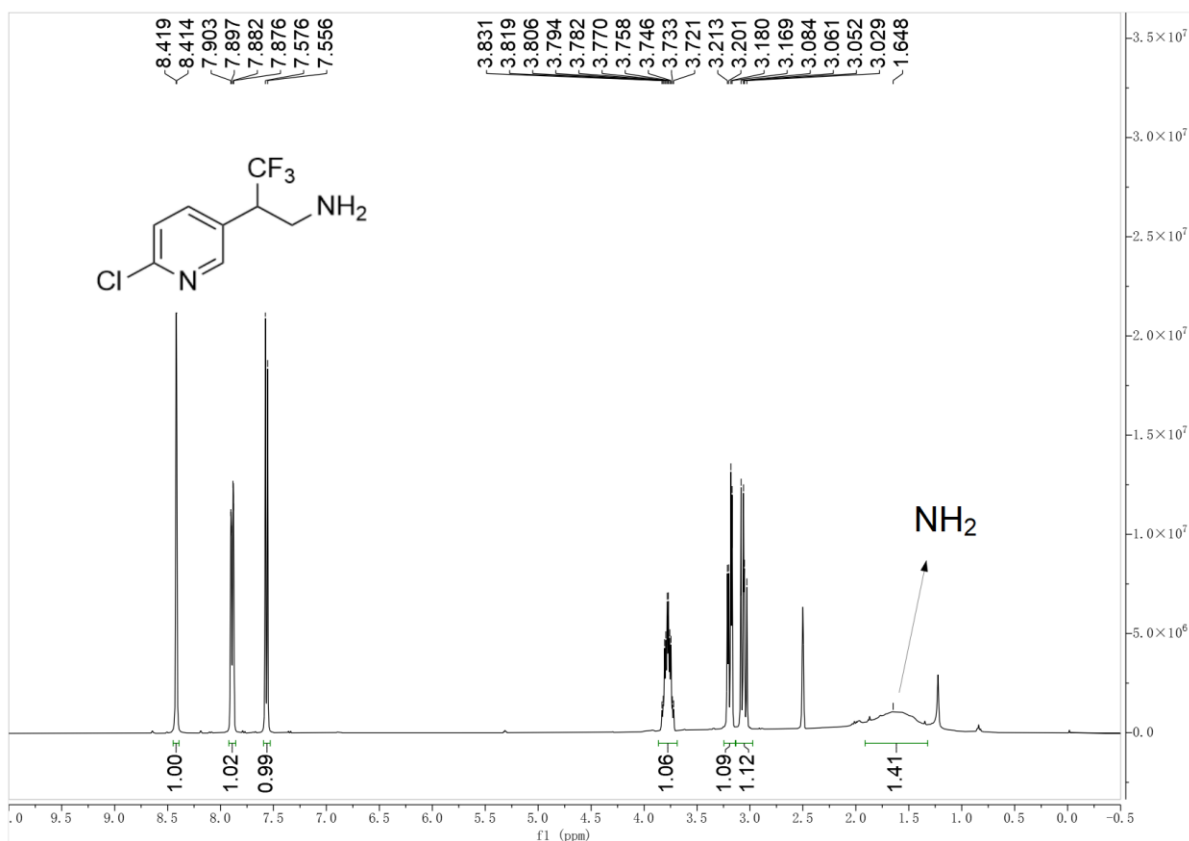
1: TOF MS ES+  
1.76e+006



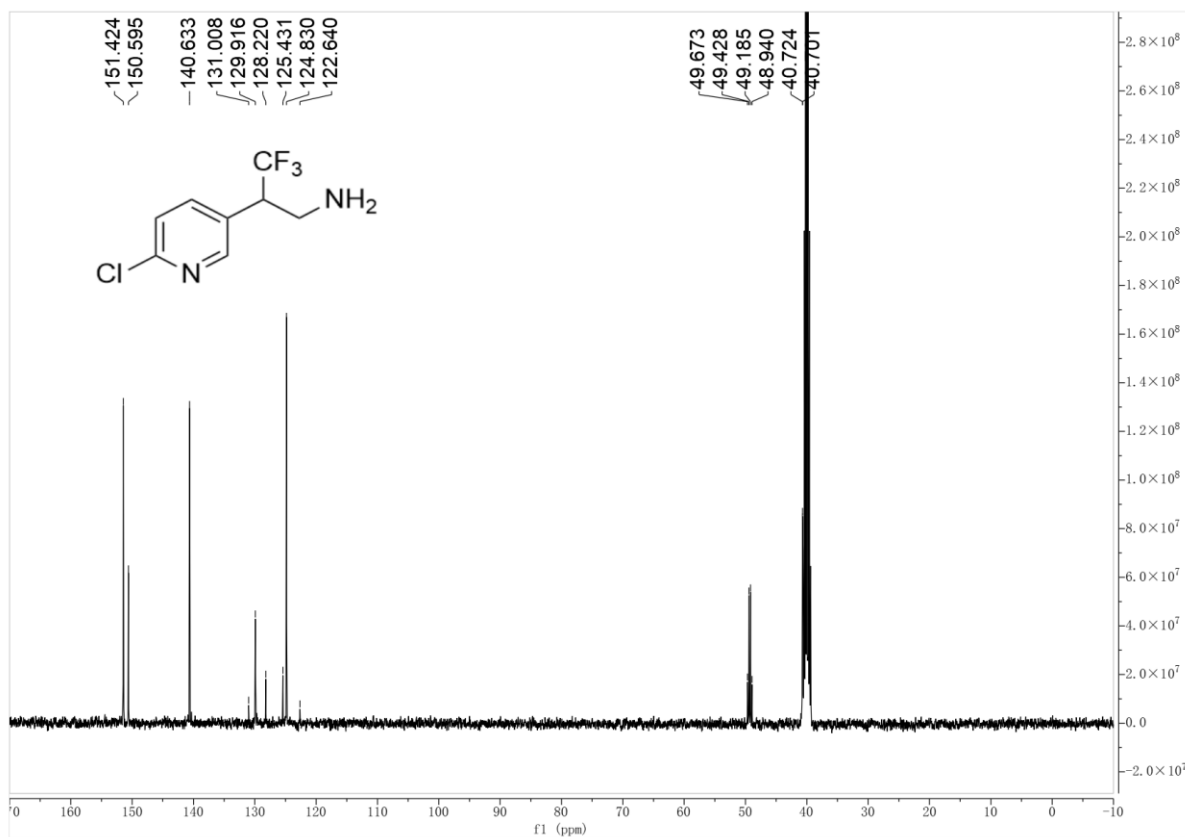
Minimum: -1.5  
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
241.0951	241.0953	-0.2	-0.8	6.5	103.4	n/a	n/a	C12 H12 N2 F3

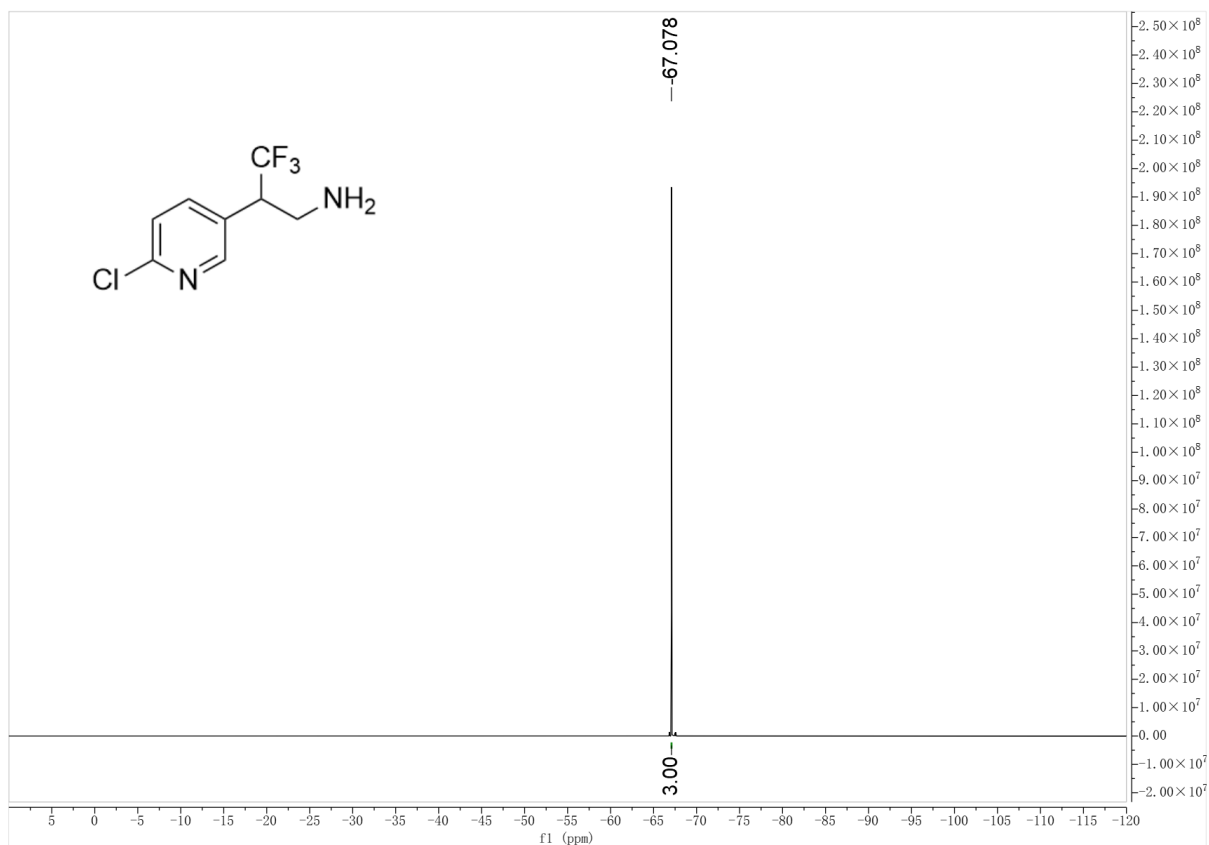
**<sup>1</sup>H NMR spectrum of 4t (400 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4t (100 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>19</sup>F NMR spectrum of 4t (376 MHz, DMSO-d<sub>6</sub>)**



**HRMS (ESI) spectrum of 4t**

Monoisotopic Mass, Even Electron Ions

202 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

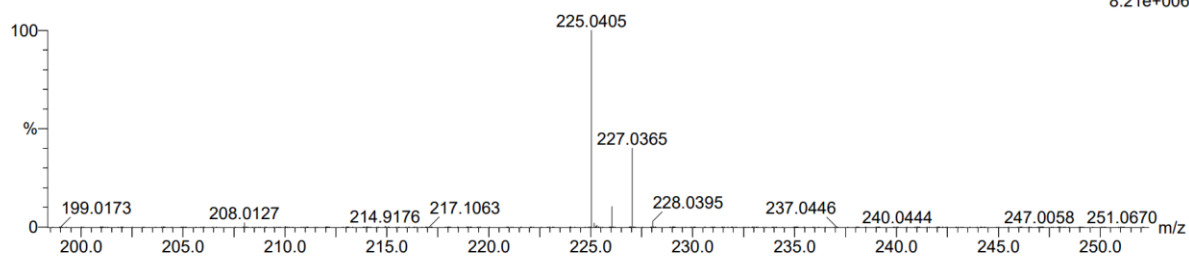
Elements Used:

C: 8-8 H: 9-9 N: 0-20 O: 0-20 F: 3-3 Na: 0-3 Cl: 1-4

6

230410-1-26 8 (0.102)

1: TOF MS ES+  
8.21e+006

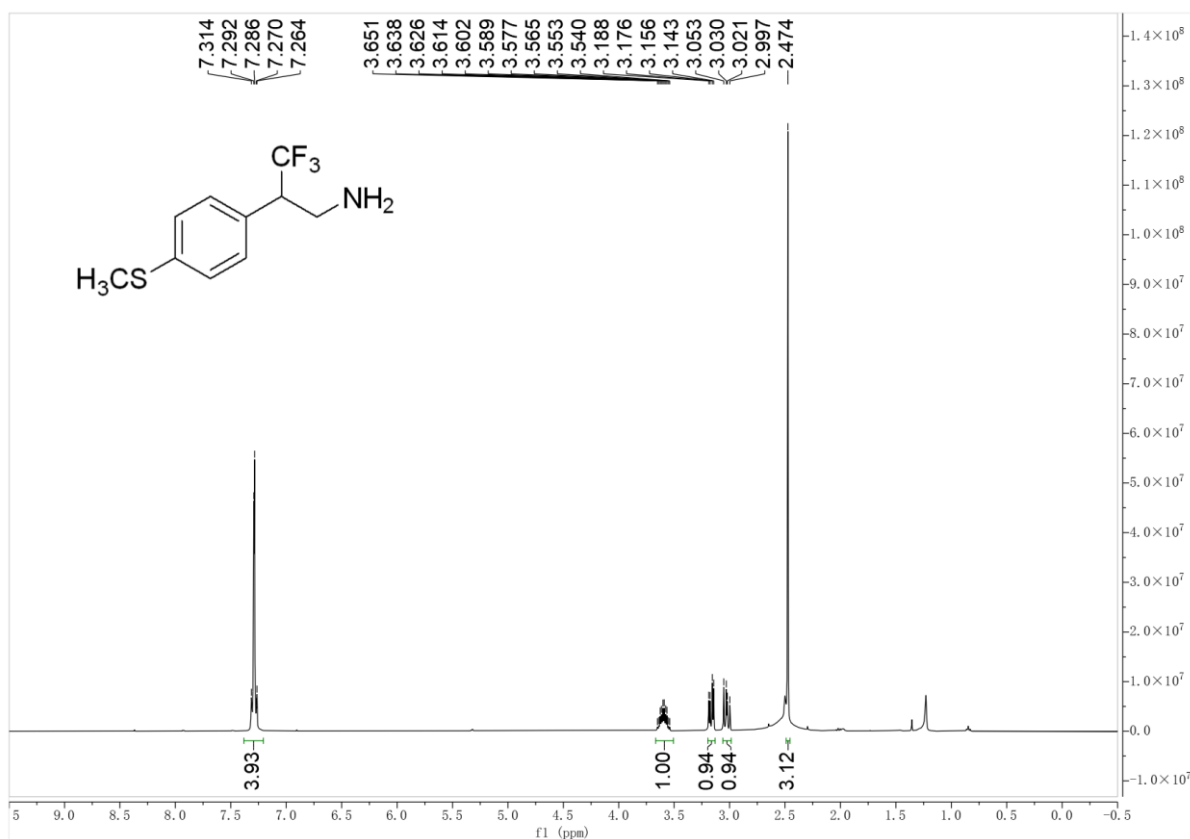


Minimum: -1.5  
Maximum: 5.0 20.0 50.0

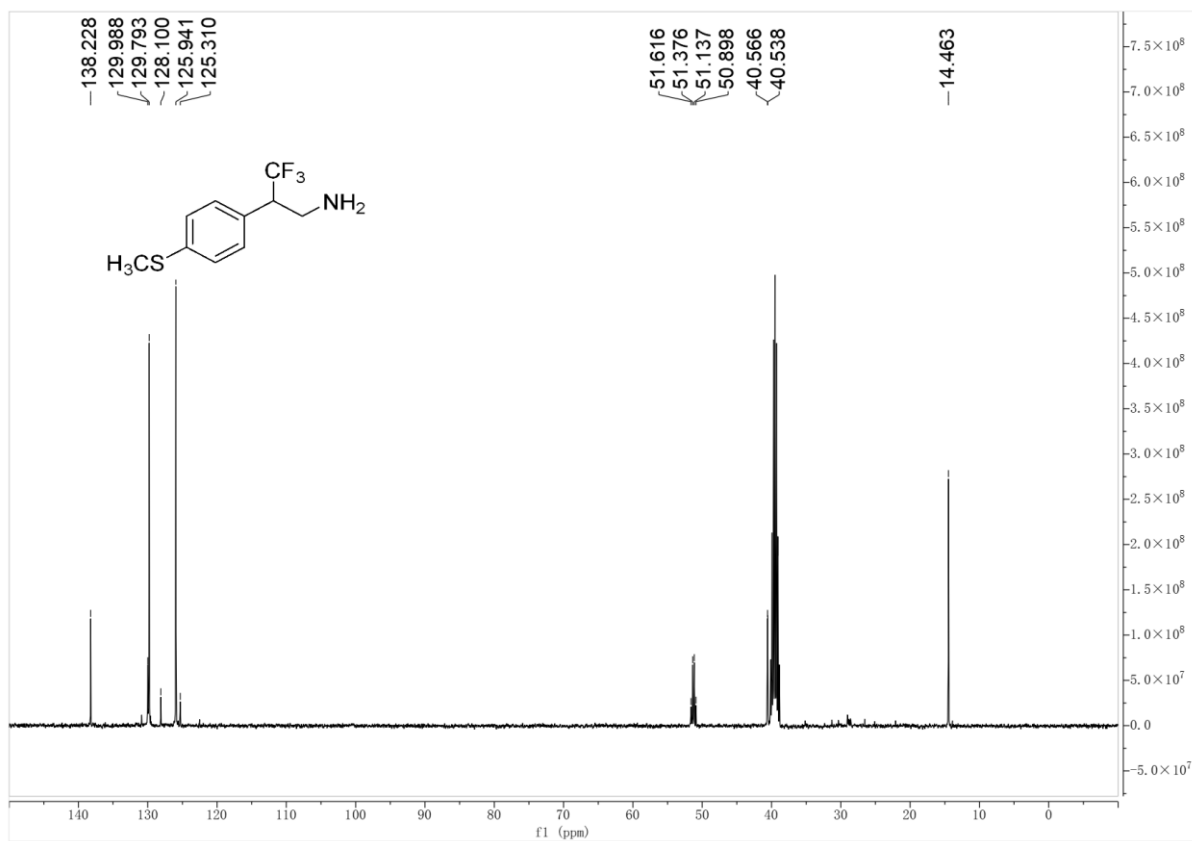
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
225.0405	225.0406	-0.1	-0.4	3.5	295.5	n/a	n/a	C8 H9 N2 F3 Cl



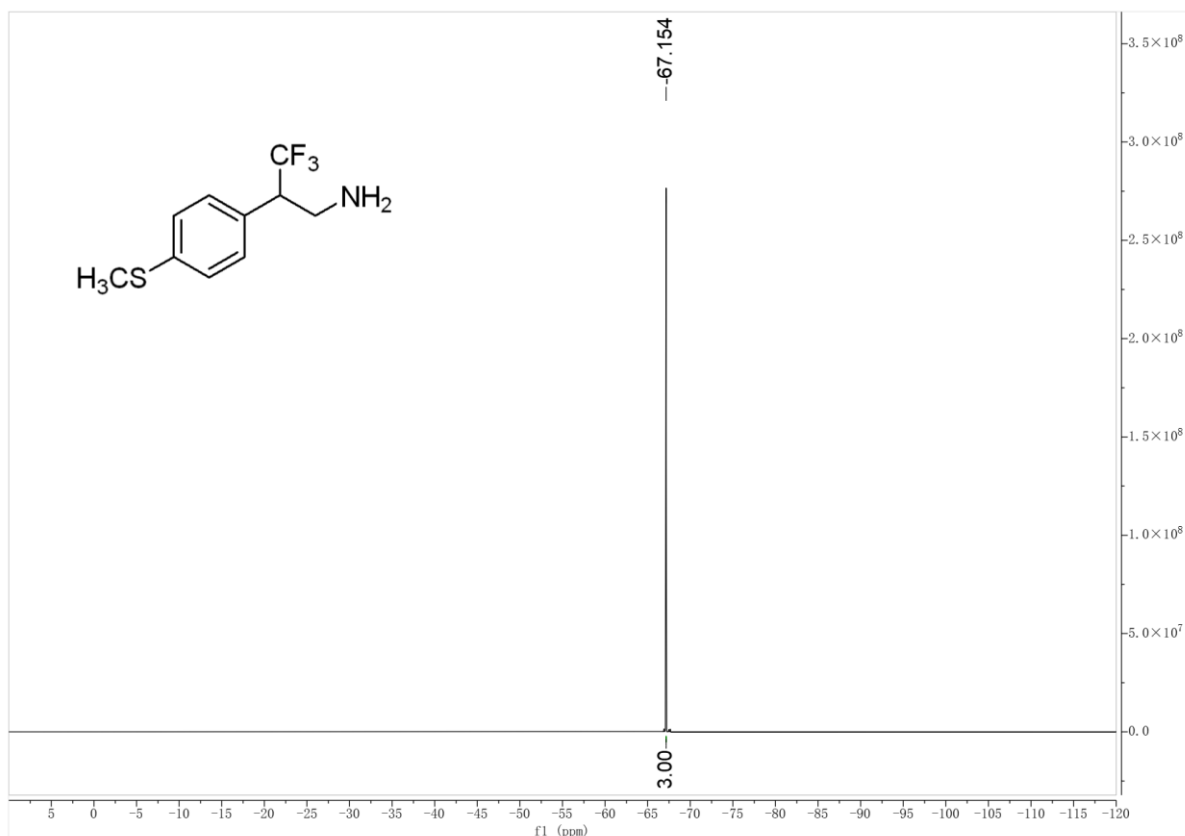
**<sup>1</sup>H NMR spectrum of 4u (400 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>13</sup>C NMR spectrum of 4u (100 MHz, DMSO-*d*<sub>6</sub>)**



**<sup>19</sup>F NMR spectrum of 4u (376 MHz, DMSO-*d*<sub>6</sub>)**



**HRMS (ESI) spectrum of 4u**

Monoisotopic Mass, Even Electron Ions

425 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

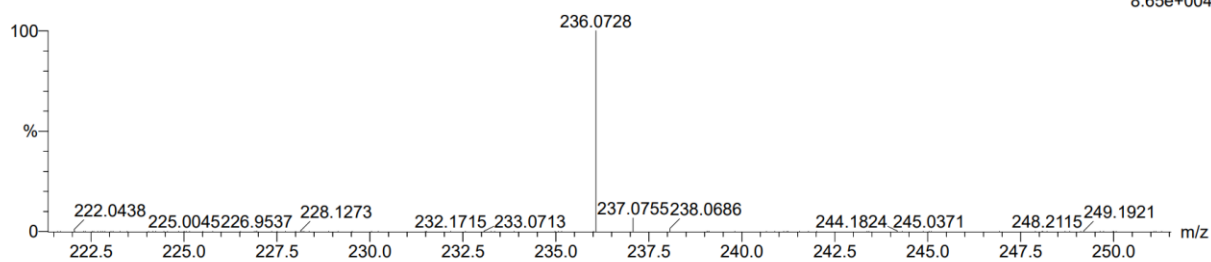
Elements Used:

C: 10-10 H: 13-13 N: 0-100 O: 0-100 F: 3-6 Na: 0-1 S: 1-2

25

240117-7-44 5 (0.055)

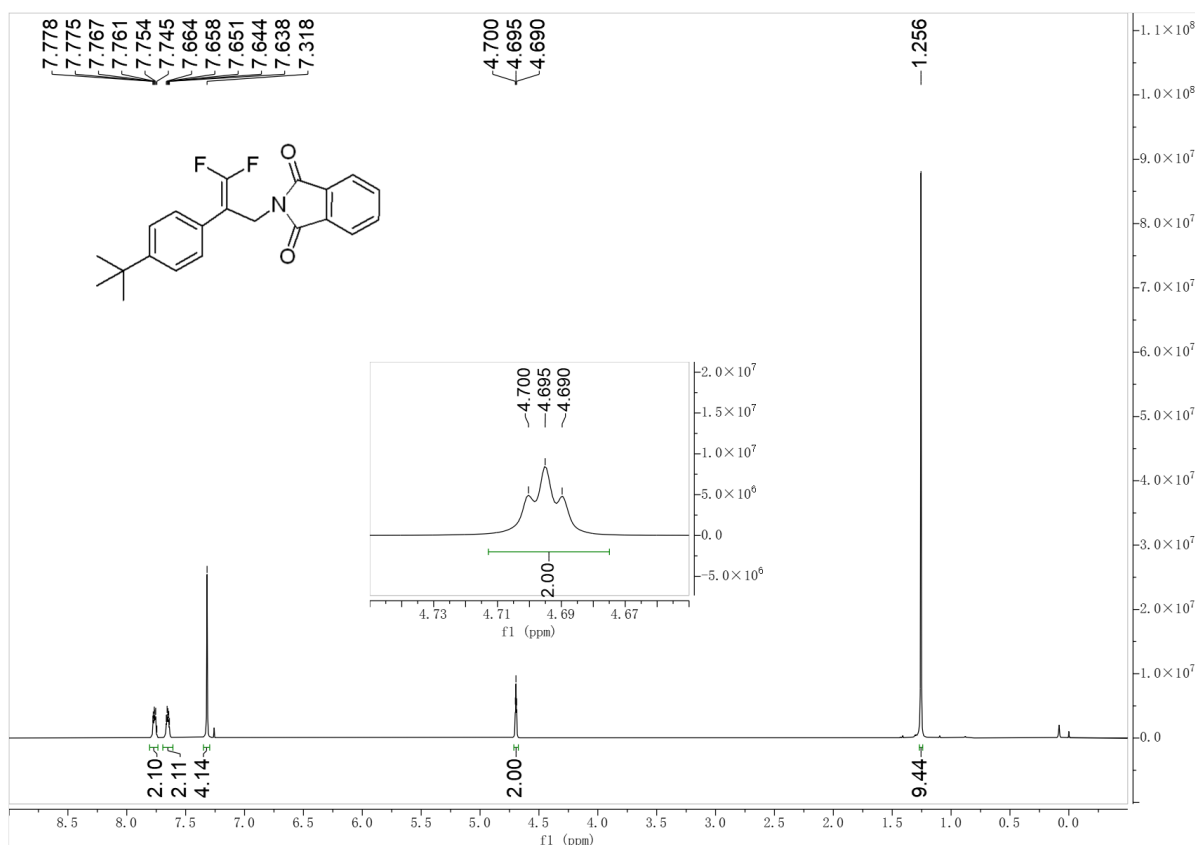
1: TOF MS ES+  
8.65e+004



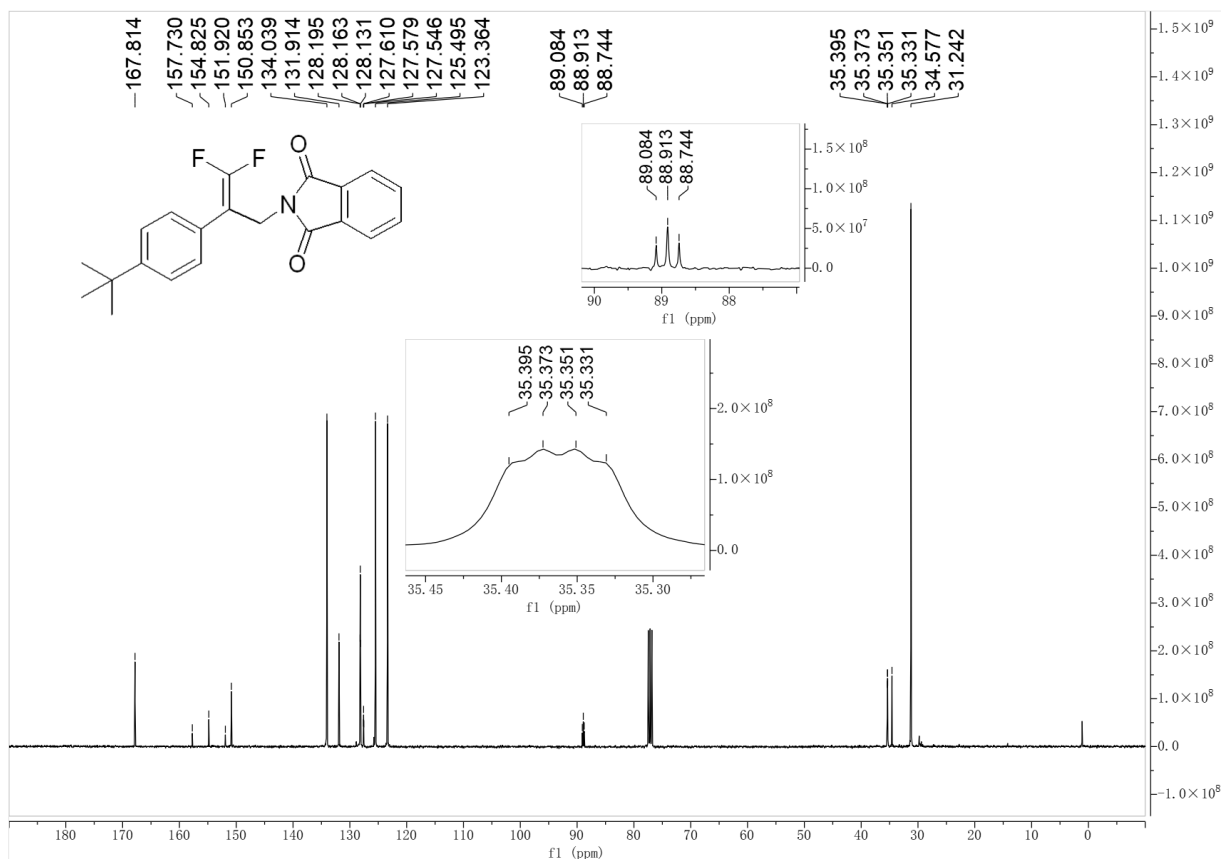
Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
236.0728	236.0721	0.7	3.0	3.5	24.5	n/a	n/a	C10 H13 N F3 S

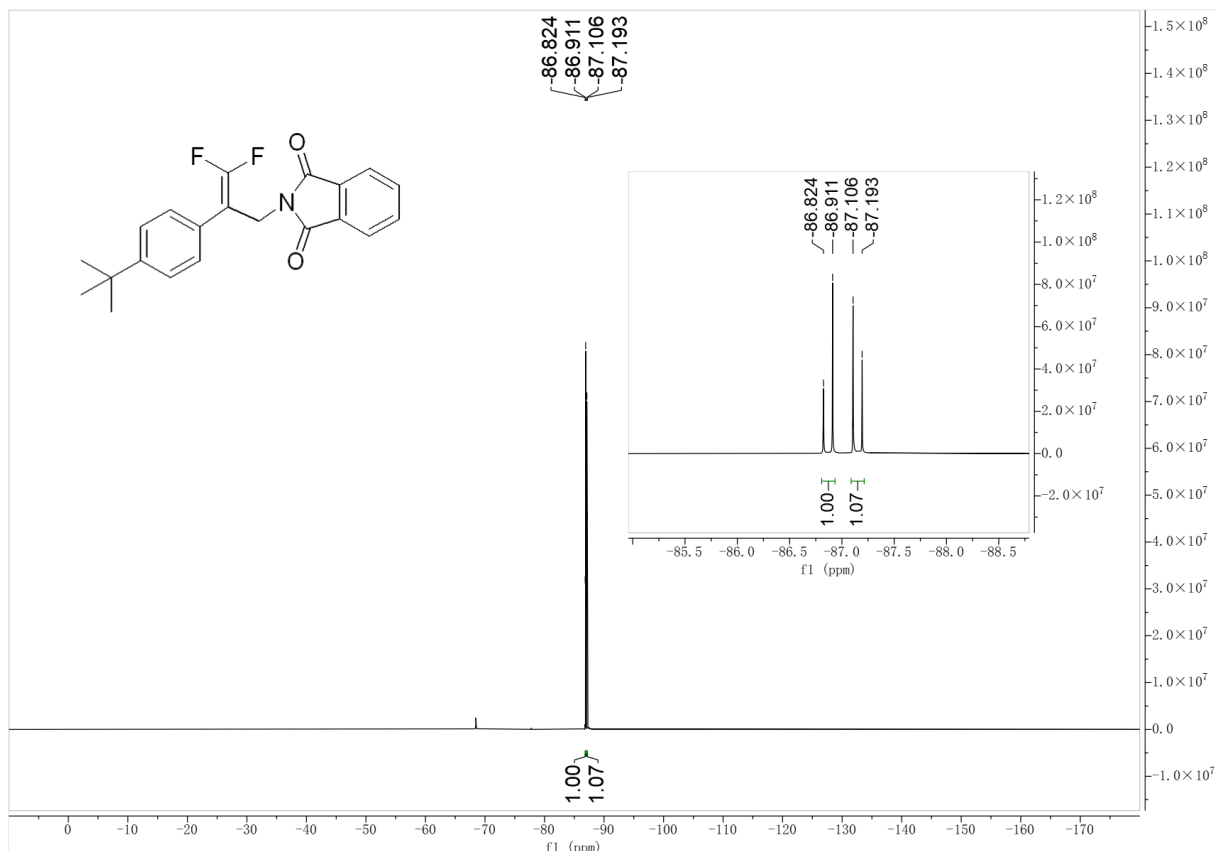
**<sup>1</sup>H NMR spectrum of 5a (400 MHz, CDCl<sub>3</sub>)**



**<sup>13</sup>C NMR spectrum of 5a (100 MHz, CDCl<sub>3</sub>)**



**<sup>19</sup>F NMR spectrum of 5a (376 MHz, CDCl<sub>3</sub>)**

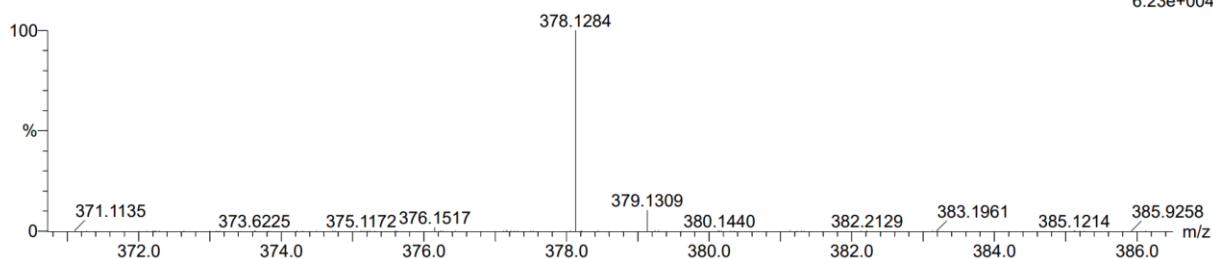


**HRMS (ESI) spectrum of 5a**

Monoisotopic Mass, Even Electron Ions  
 3794 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)  
 Elements Used:  
 C: 21-21 H: 19-19 N: 0-100 O: 0-100 Na: 0-6 F: 1-3

10  
 240301-4-1 11 (0.076)

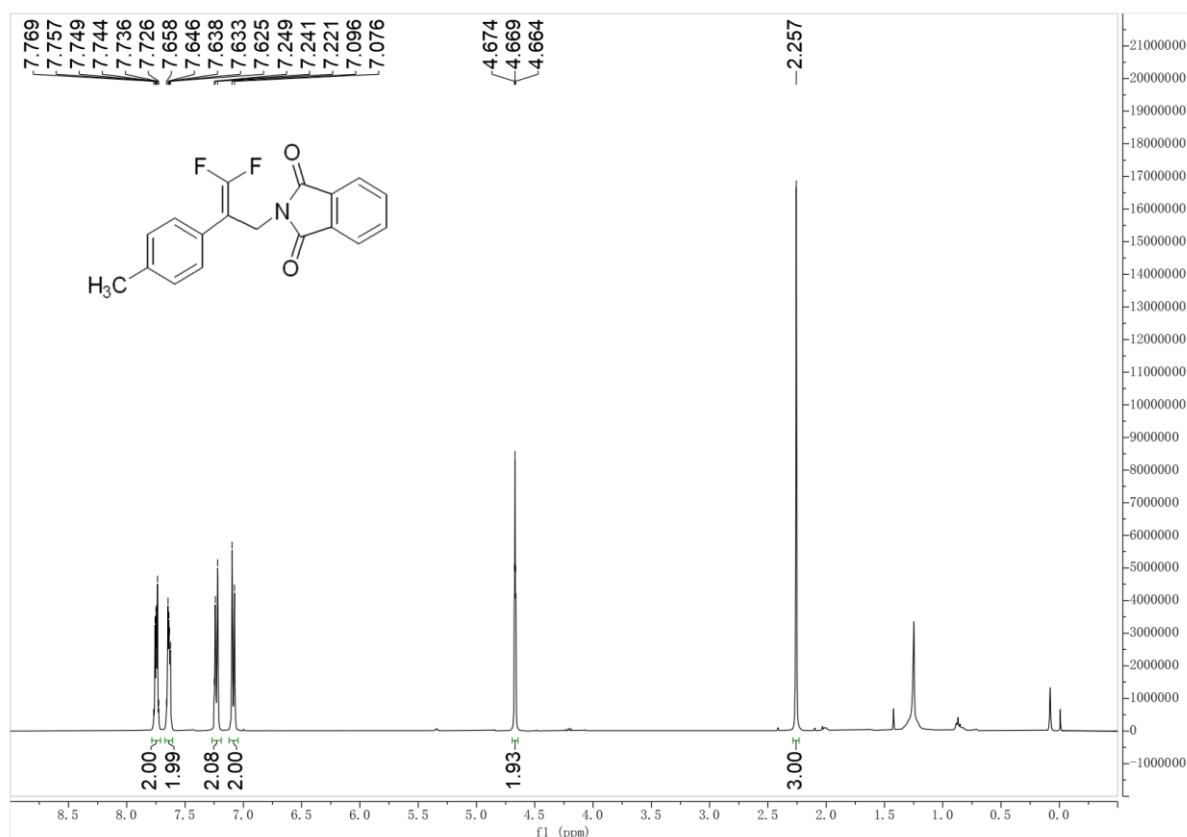
1: TOF MS ES+  
 6.23e+004



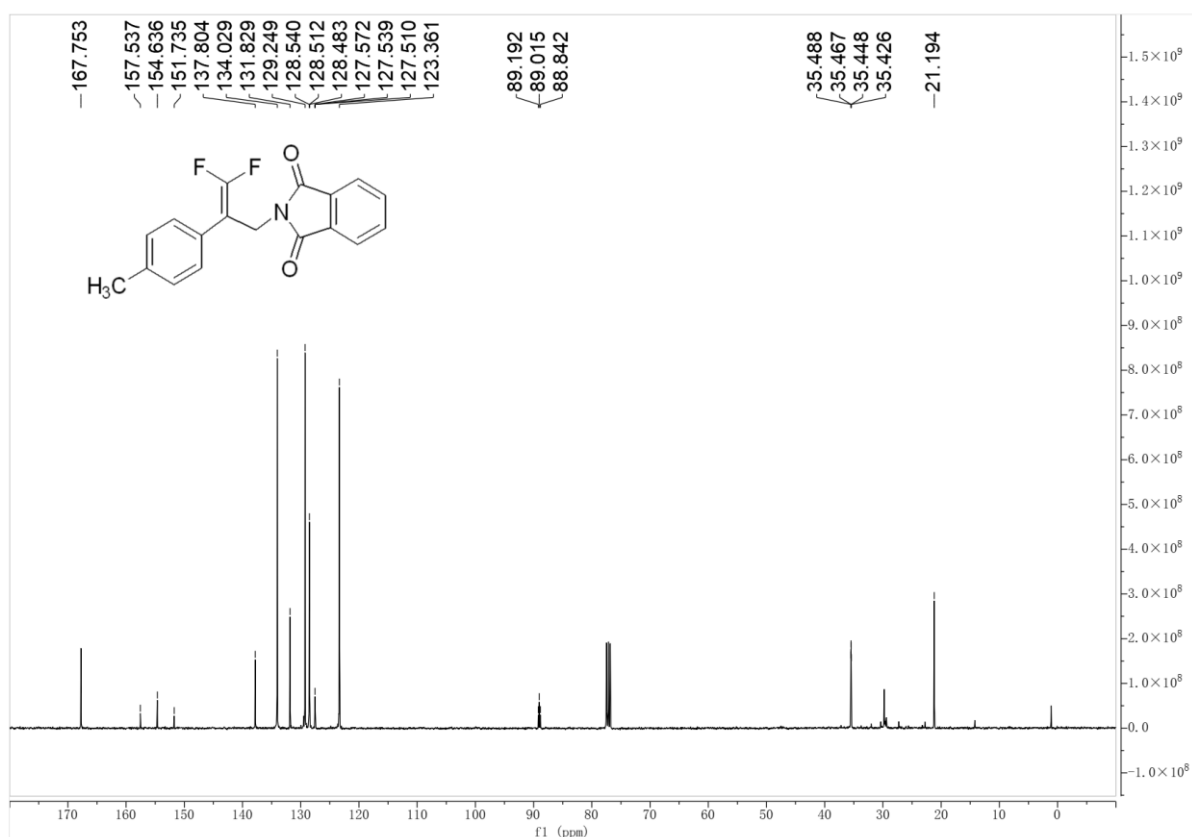
Minimum: -1.5  
 Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
378.1284	378.1282	0.2	0.5	11.5	89.6	n/a	n/a	C <sub>21</sub> H <sub>19</sub> N <sub>02</sub> Na F <sub>2</sub>

**<sup>1</sup>H NMR spectrum of 5b (400 MHz, CDCl<sub>3</sub>)**



**<sup>13</sup>C NMR spectrum of 5b (100 MHz, CDCl<sub>3</sub>)**



**<sup>19</sup>F NMR spectrum of 5b (376 MHz, CDCl<sub>3</sub>)**



**HRMS (ESI) spectrum of 5b**

Monoisotopic Mass, Even Electron Ions

2778 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

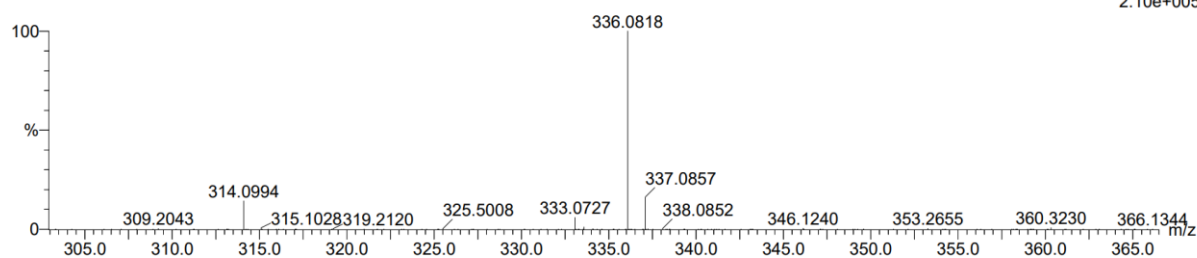
Elements Used:

C: 18-18 H: 13-13 N: 0-100 O: 0-100 F: 1-3 Na: 0-6

10

240301-4-2 12 (0.080)

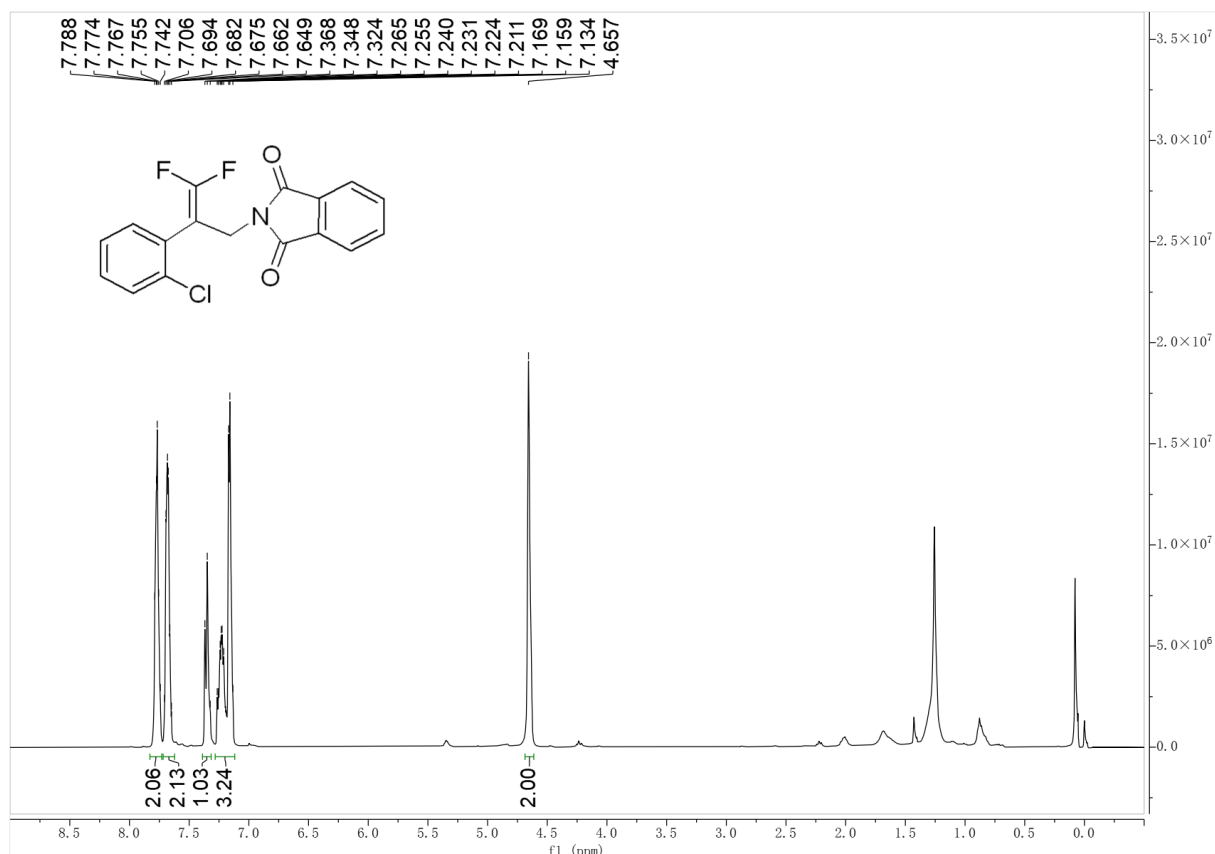
1: TOF MS ES+  
2.10e+005



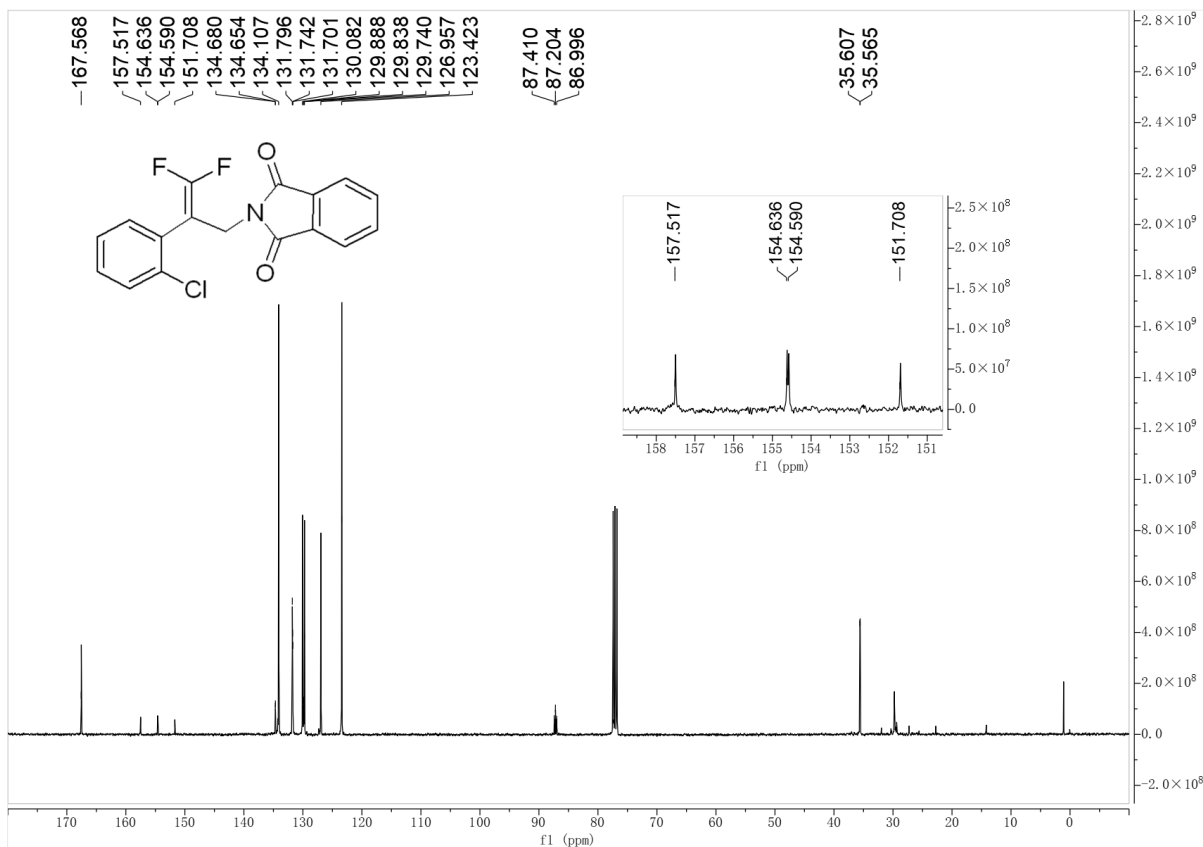
Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
336.0818	336.0812	0.6	1.8	11.5	127.4	n/a	n/a	C18 H13 N O2 F2 Na

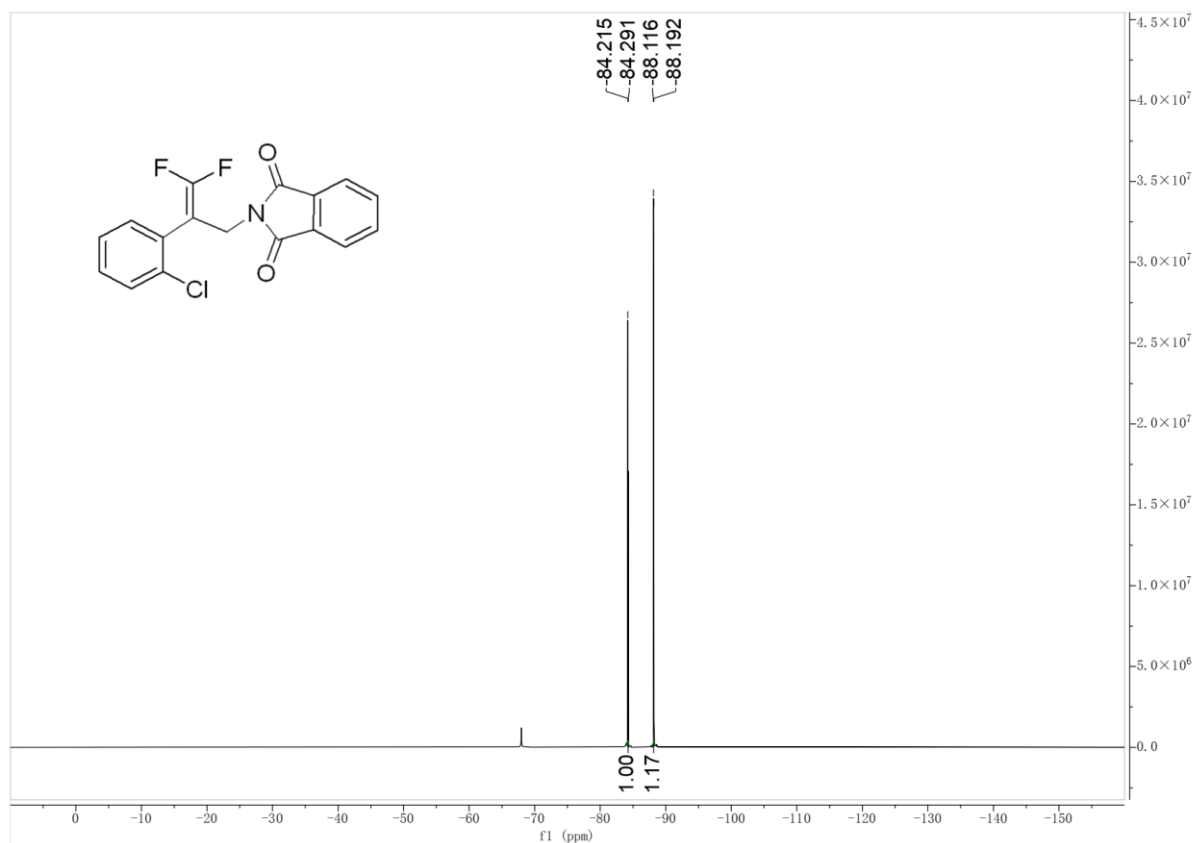
**<sup>1</sup>H NMR spectrum of 5c (400 MHz, CDCl<sub>3</sub>)**



**<sup>13</sup>C NMR spectrum of 5c (100 MHz, CDCl<sub>3</sub>)**



**<sup>19</sup>F NMR spectrum of 5c (376 MHz, CDCl<sub>3</sub>)**



**HRMS (ESI) spectrum of 5c**

Monoisotopic Mass, Even Electron Ions

6421 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

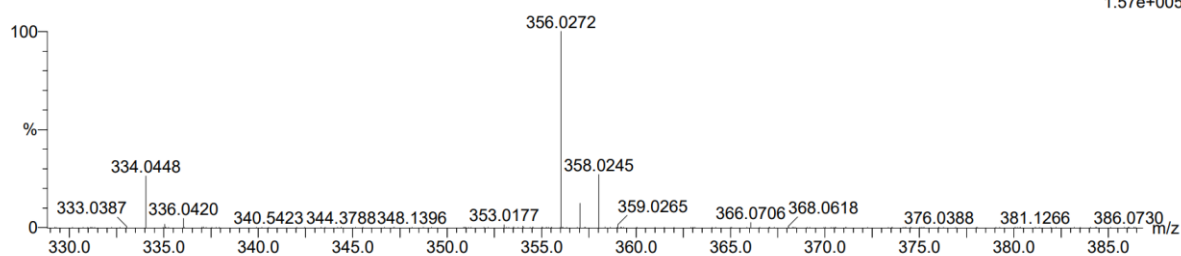
Elements Used:

C: 17-17 H: 10-10 N: 0-100 O: 0-100 F: 1-3 Na: 0-6 Cl: 1-4

10

240301-4-3 9 (0.069)

1: TOF MS ES+  
1.57e+005

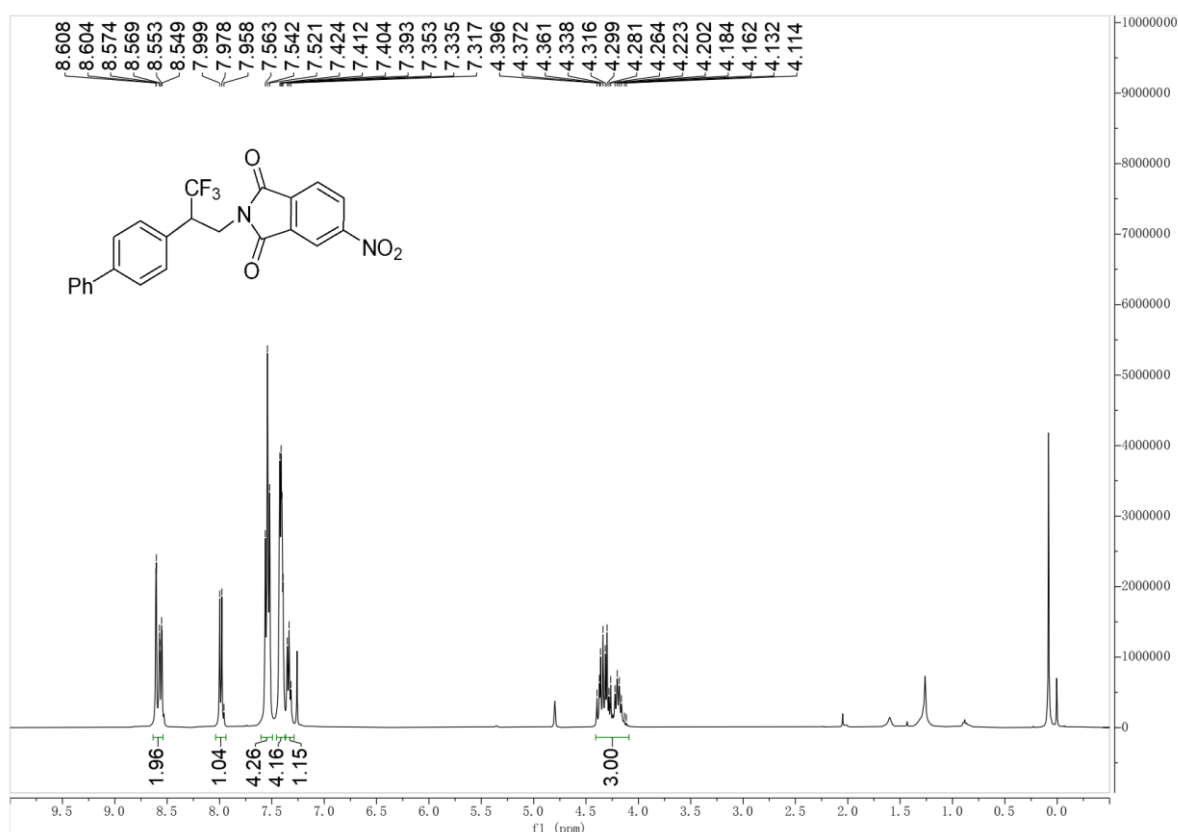


Minimum: -1.5  
Maximum: 5.0 10.0 50.0

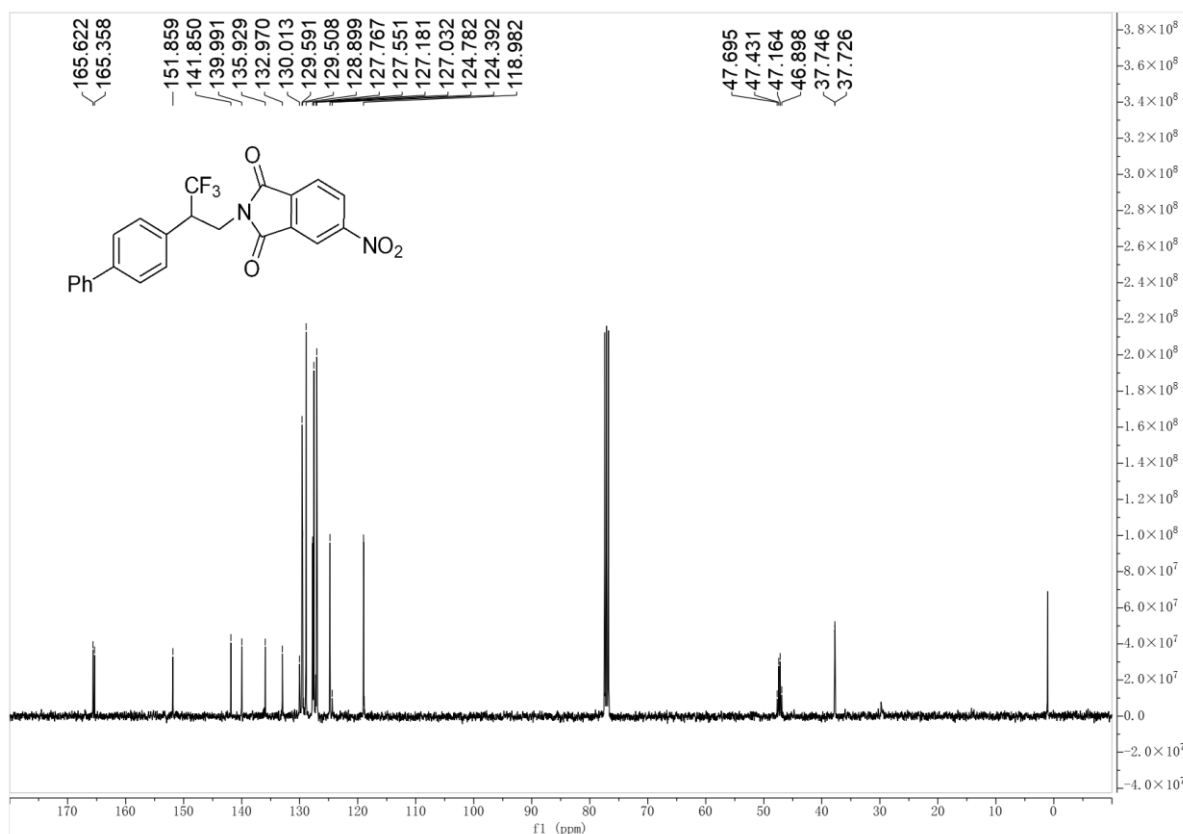
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
356.0272	356.0266	0.6	1.7	11.5	69.3	n/a	n/a	C17 H10 N 02 F2 Na Cl



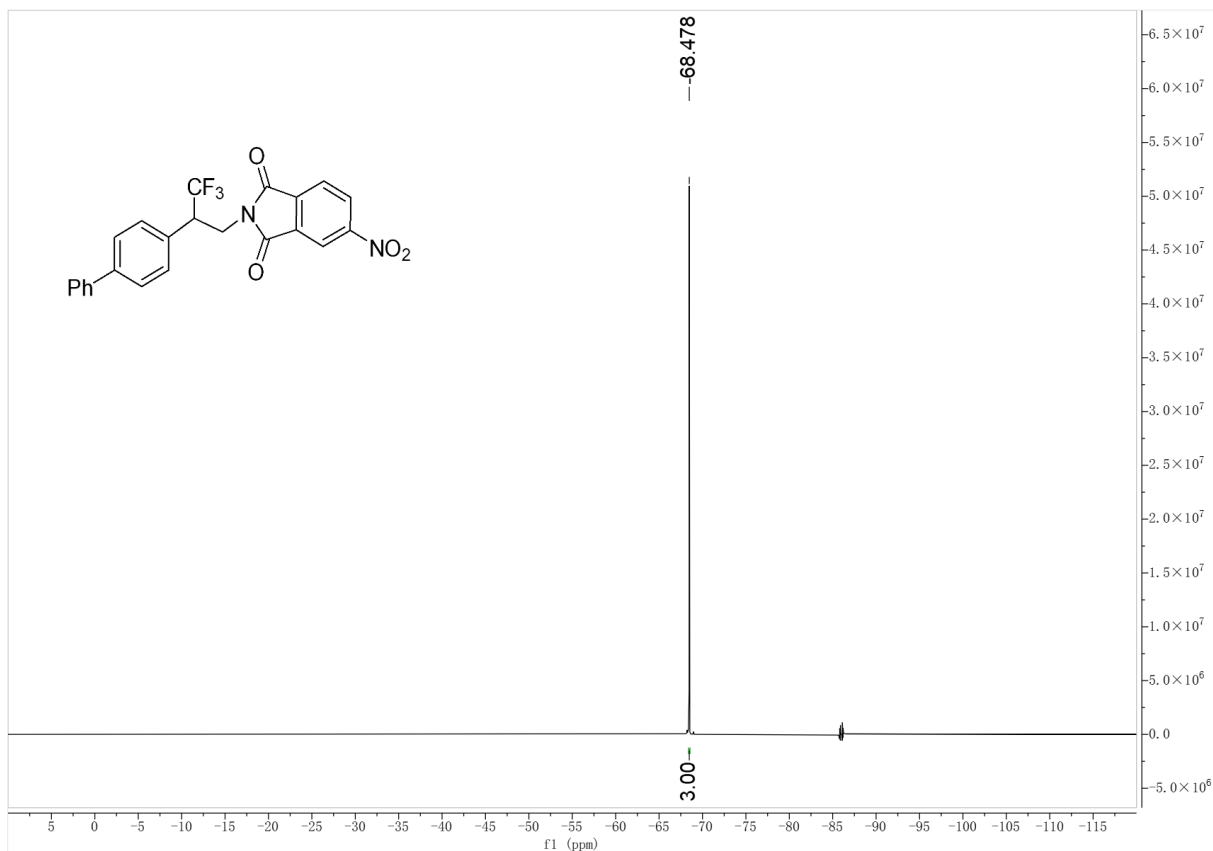
### <sup>1</sup>H NMR spectrum of 7a (400 MHz, CDCl<sub>3</sub>)



### <sup>13</sup>C NMR spectrum of 7a (100 MHz, CDCl<sub>3</sub>)



### <sup>19</sup>F NMR spectrum of 7a (376 MHz, CDCl<sub>3</sub>)



### HRMS (ESI) spectrum of 7a

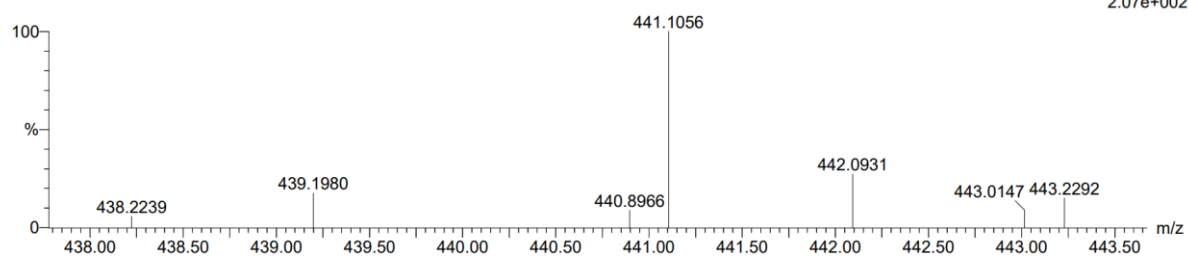
Monoisotopic Mass, Even Electron Ions  
2178 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)  
Elements Used:

C: 23-23 H: 16-16 N: 0-100 O: 0-100 F: 3-6 Na: 0-1

31

240308-3-21 8 (0.065)

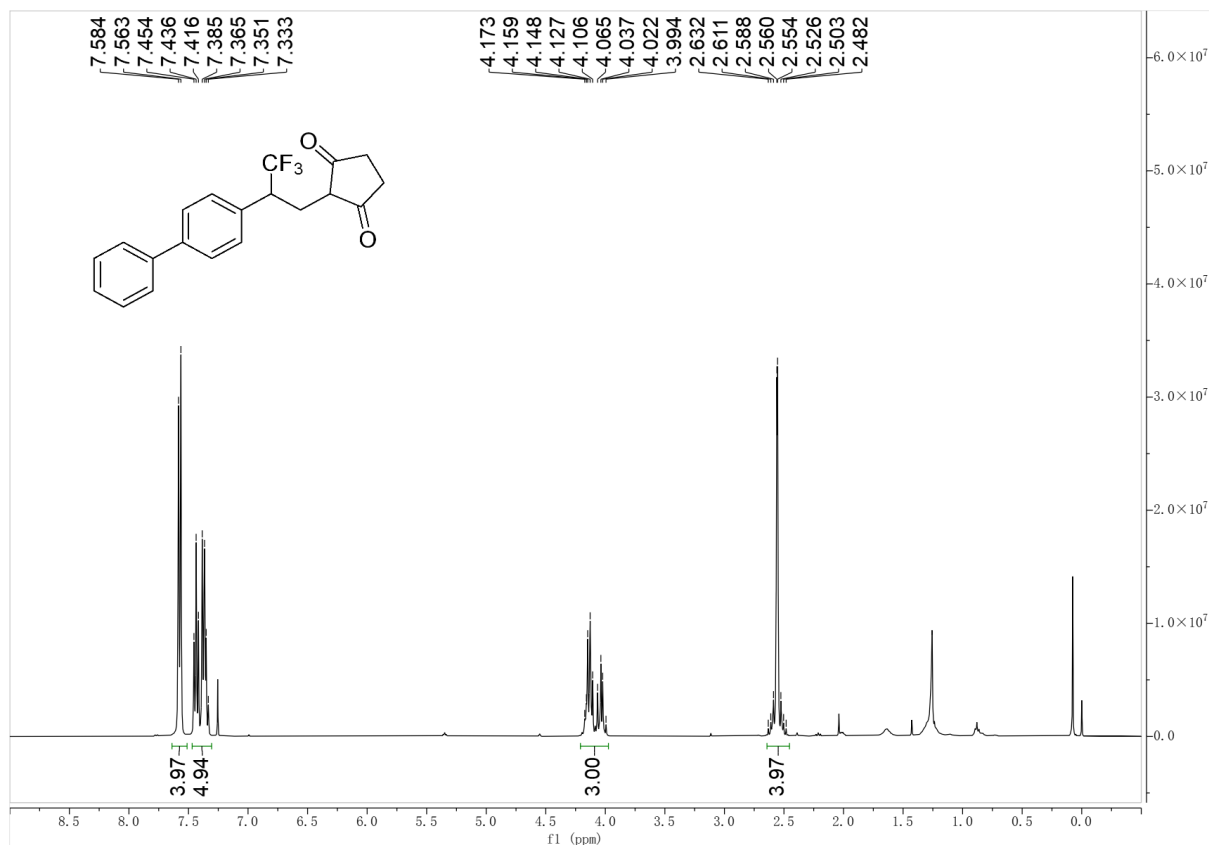
1: TOF MS ES+  
2.07e+002



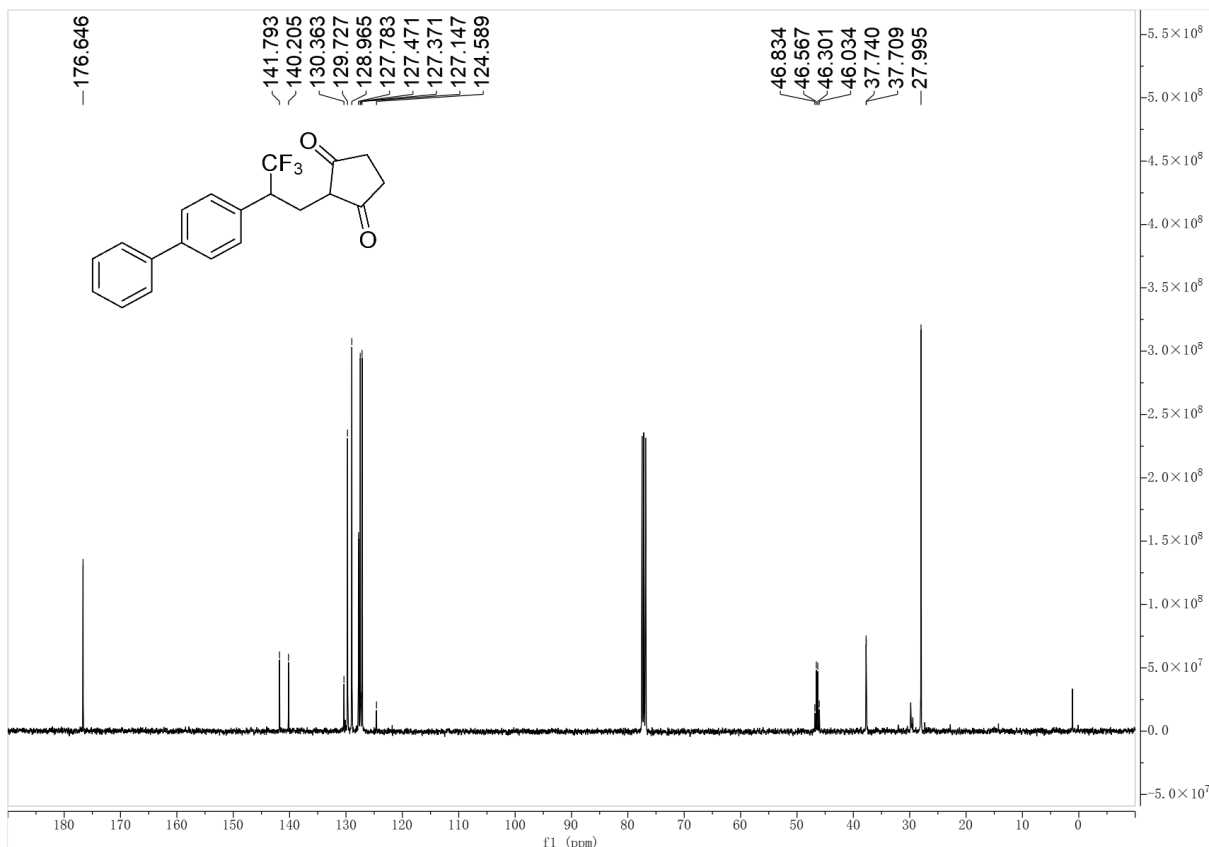
Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
441.1056	441.1062	-0.6	-1.4	15.5	25.9	n/a	n/a	C23 H16 N2 O4 F3

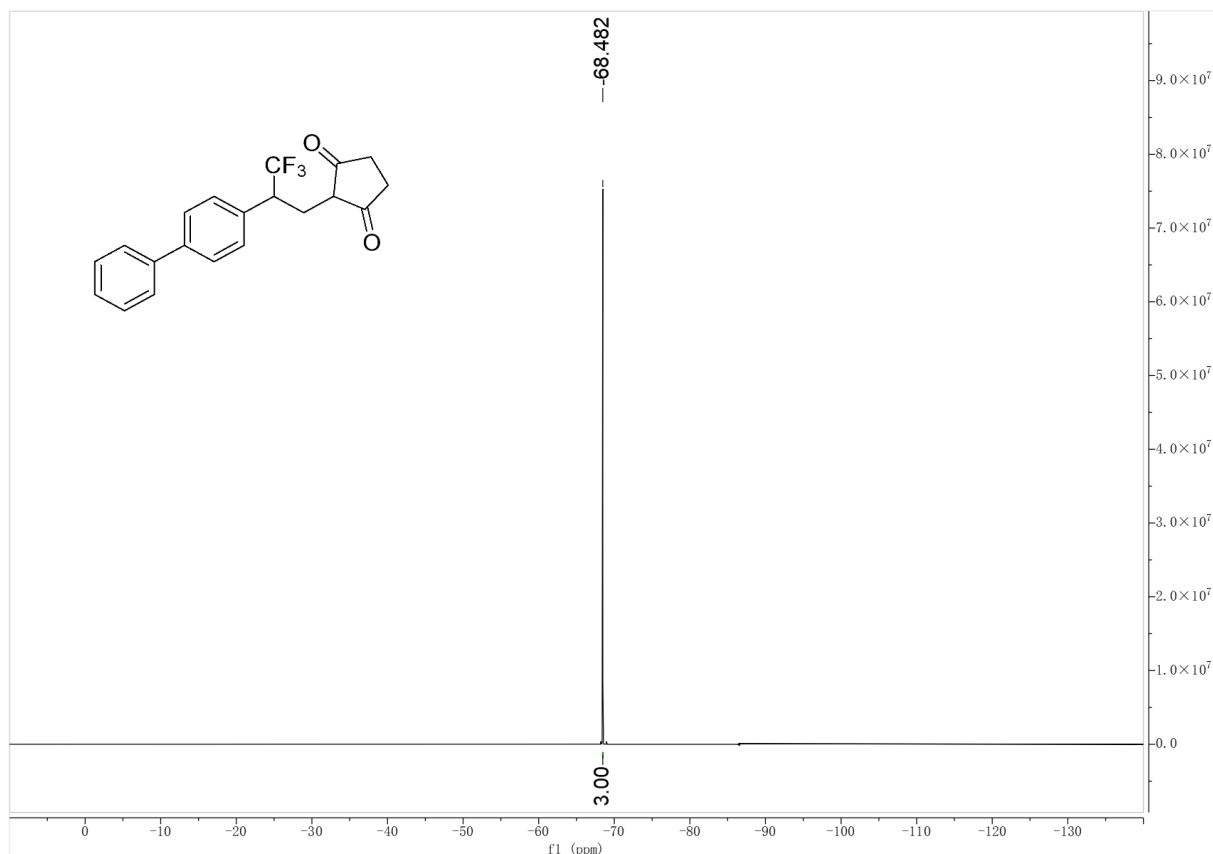
**<sup>1</sup>H NMR spectrum of 7b (400 MHz, CDCl<sub>3</sub>)**



**<sup>13</sup>C NMR spectrum of 7b (100 MHz, CDCl<sub>3</sub>)**



### <sup>19</sup>F NMR spectrum of 7b (376 MHz, CDCl<sub>3</sub>)



### HRMS (ESI) spectrum of 7b

Monoisotopic Mass, Even Electron Ions

3529 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

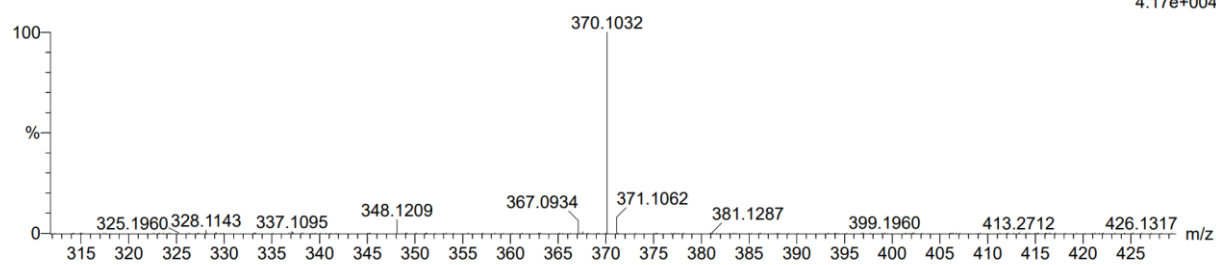
Elements Used:

C: 19-19 H: 16-16 N: 0-100 O: 0-100 F: 1-3 Na: 0-6

10

240301-4-5 10 (0.072)

1: TOF MS ES+  
4.17e+004



Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
370.1032	370.1031	0.1	0.3	10.5	47.0	n/a	n/a	C19 H16 N 02 F3 Na