

# Supporting Information

## Synthesis and Functional Characterization of 2-(2,5-Dimethoxyphenyl)-N-(2-fluorobenzyl)ethanamine (25H-NBF) Positional Isomers

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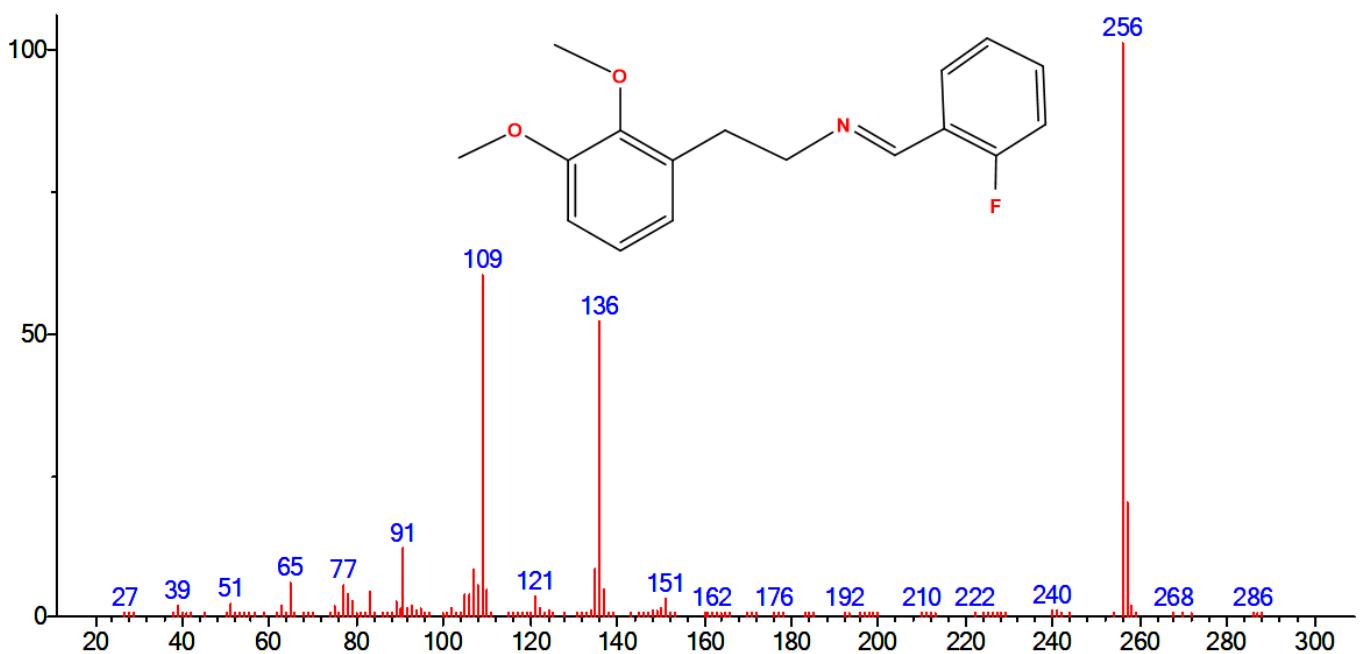
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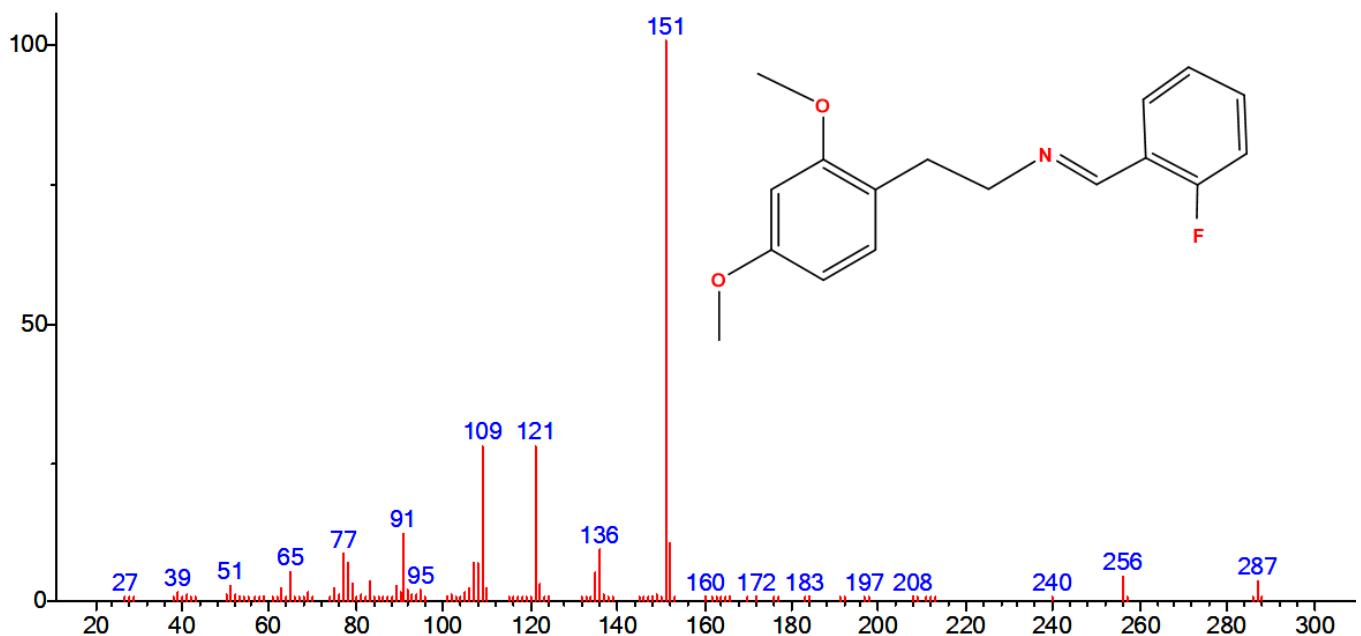
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**23H-NBF imine (10a).**



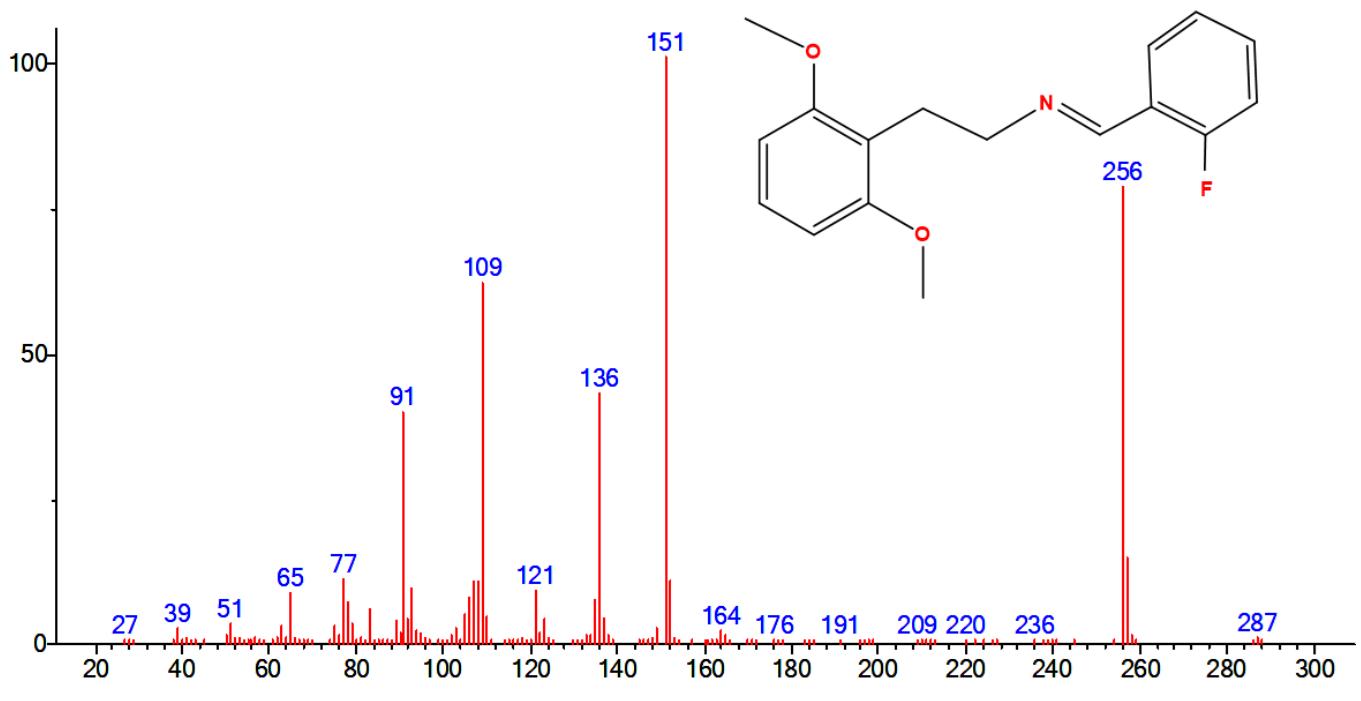
**Figure S1.** EI mass spectrum of **10a**

**24H-NBF imine (10b).**



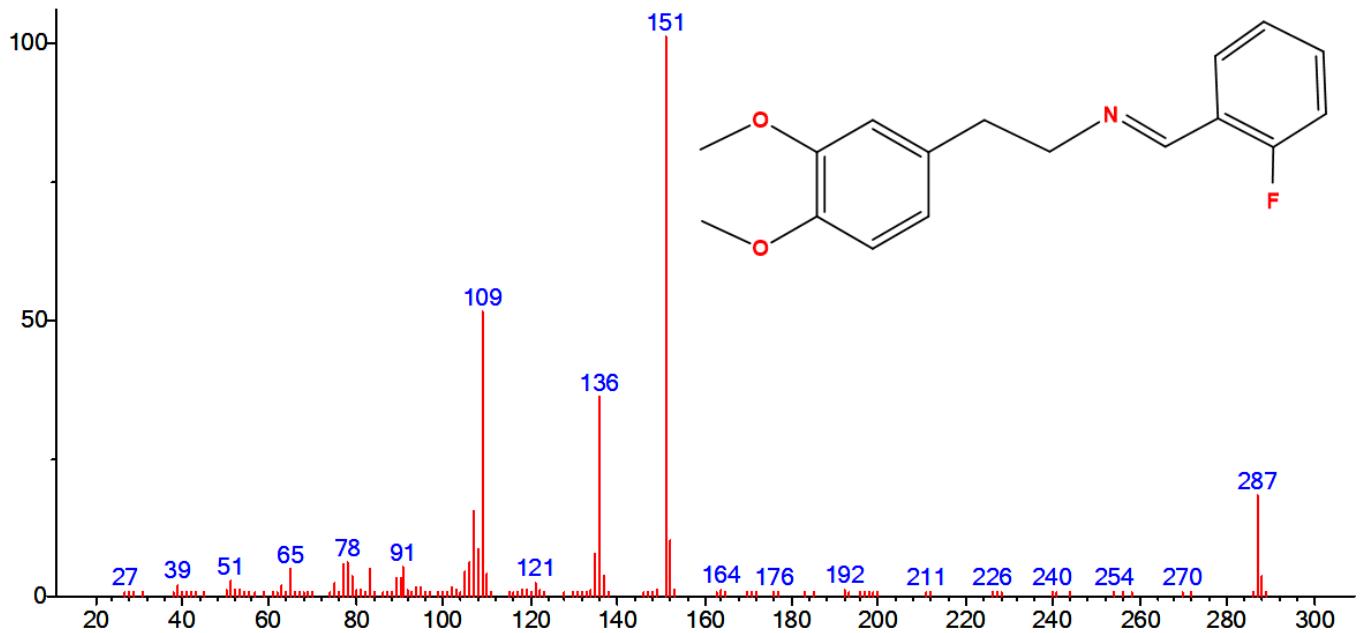
**Figure S2.** EI mass spectrum of **10b**

**26H-NBF imine (10c).**



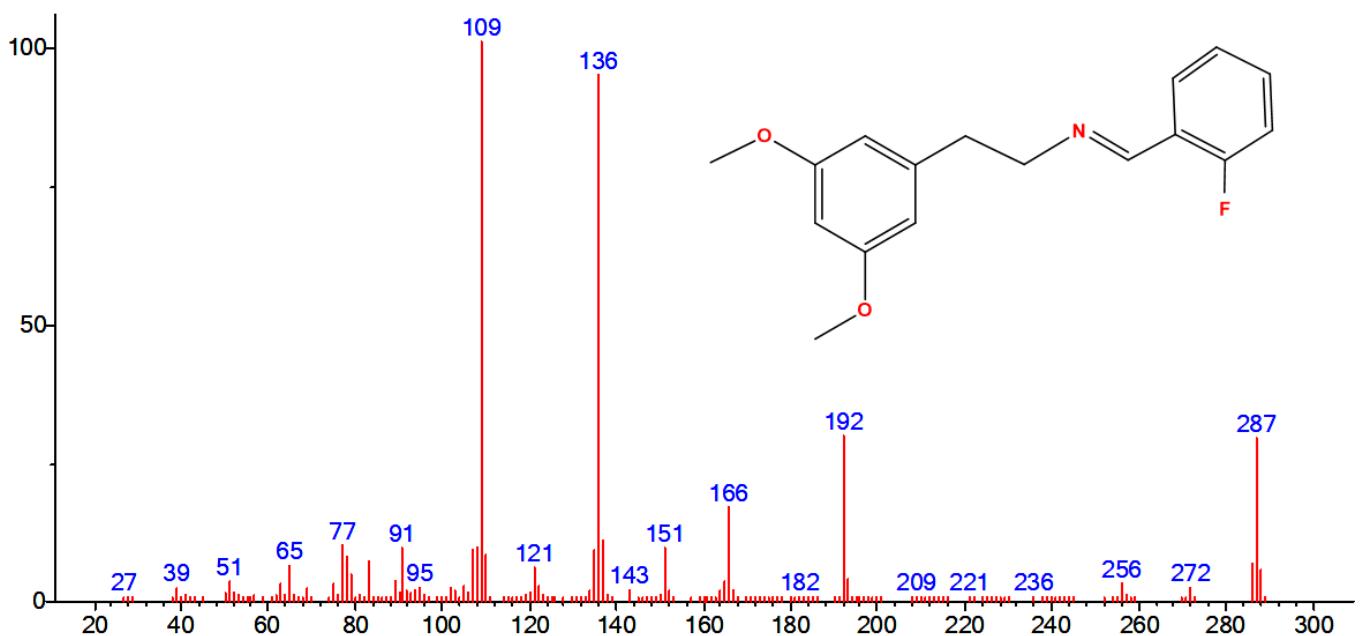
**Figure S3.** EI mass spectrum of **10c**

**34H-NBF imine (10d).**



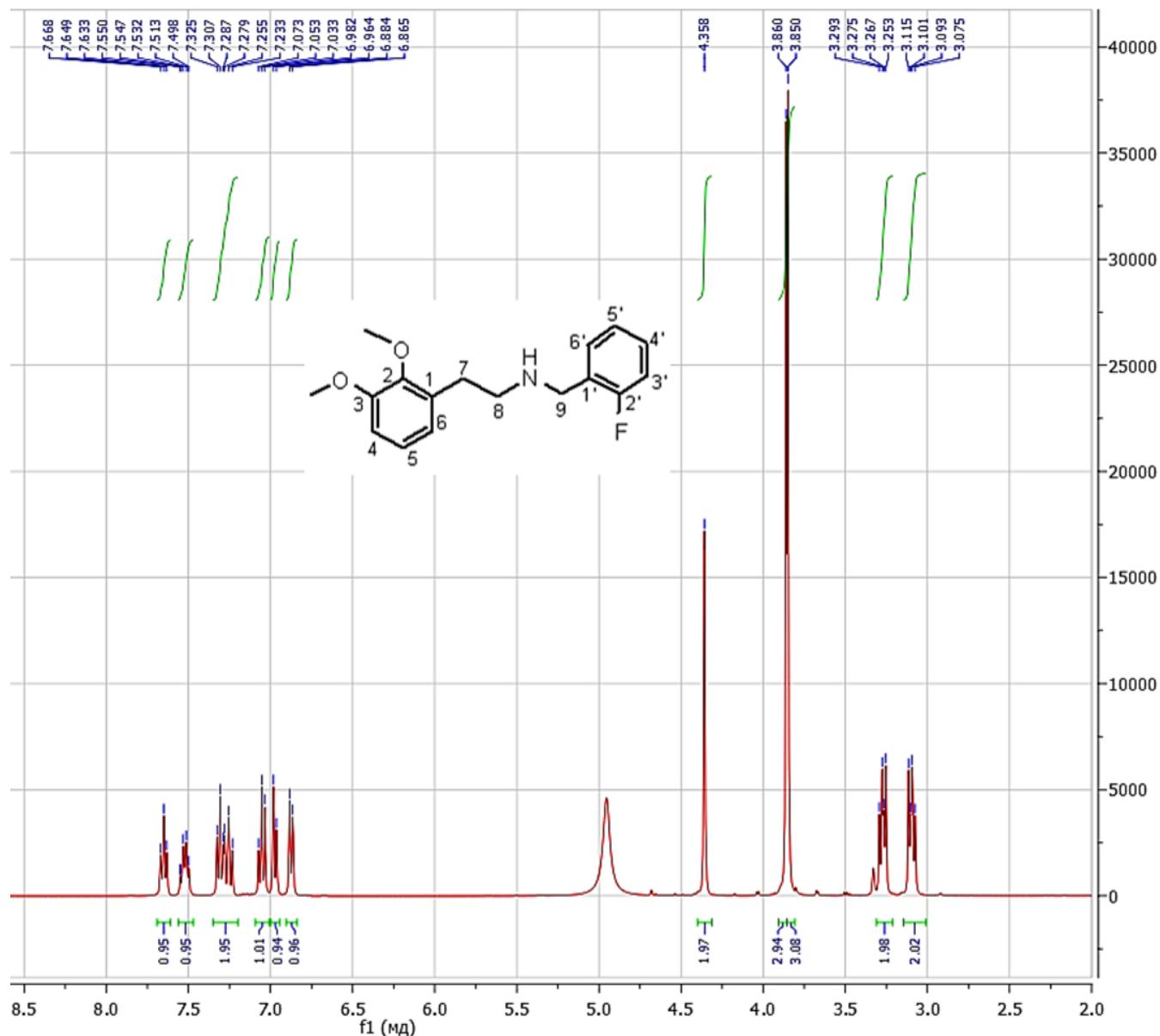
**Figure S4.** EI mass spectrum of **10d**

**35H-NBF imine (10e).**

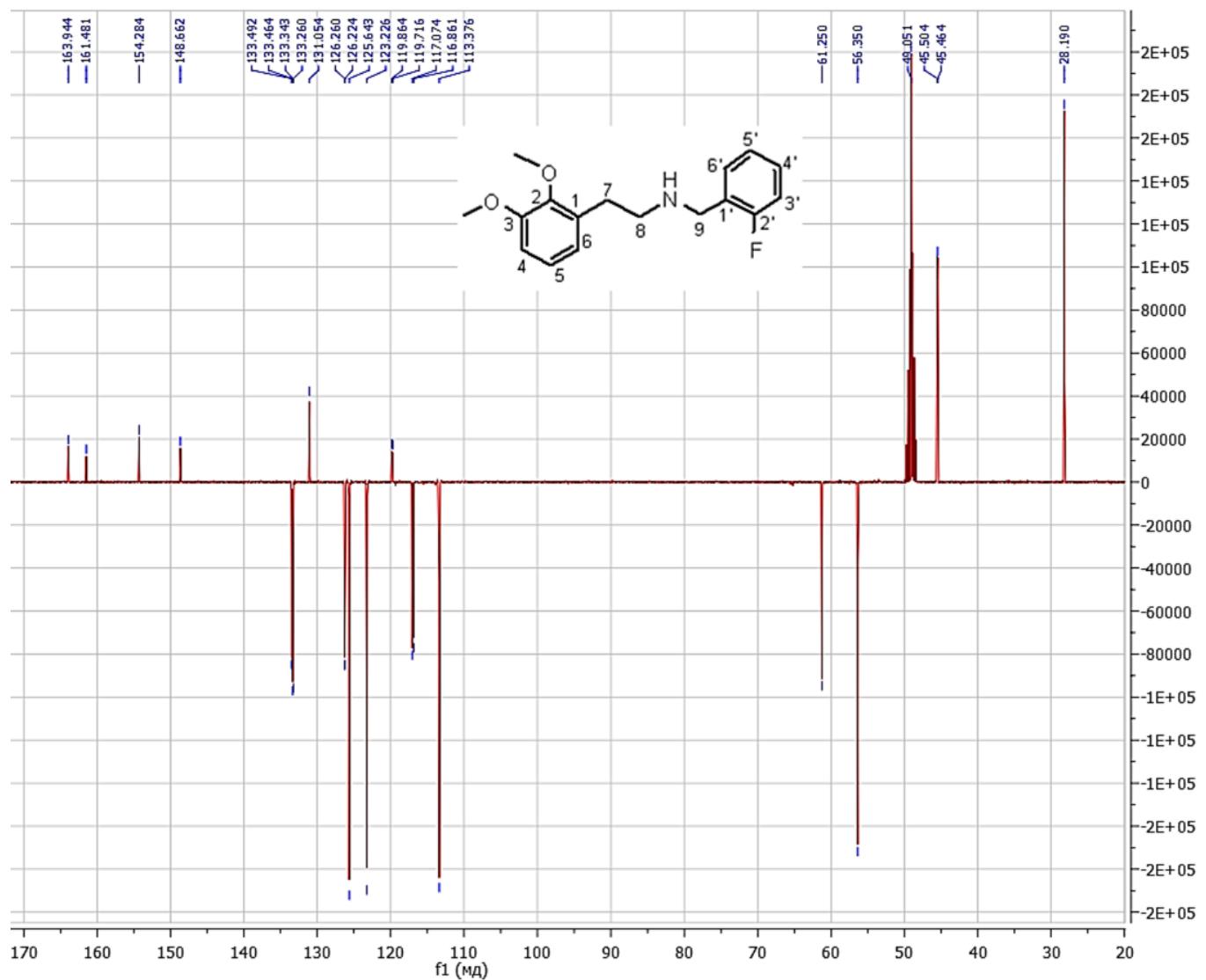


**Figure S5.** EI mass spectrum of **10e**

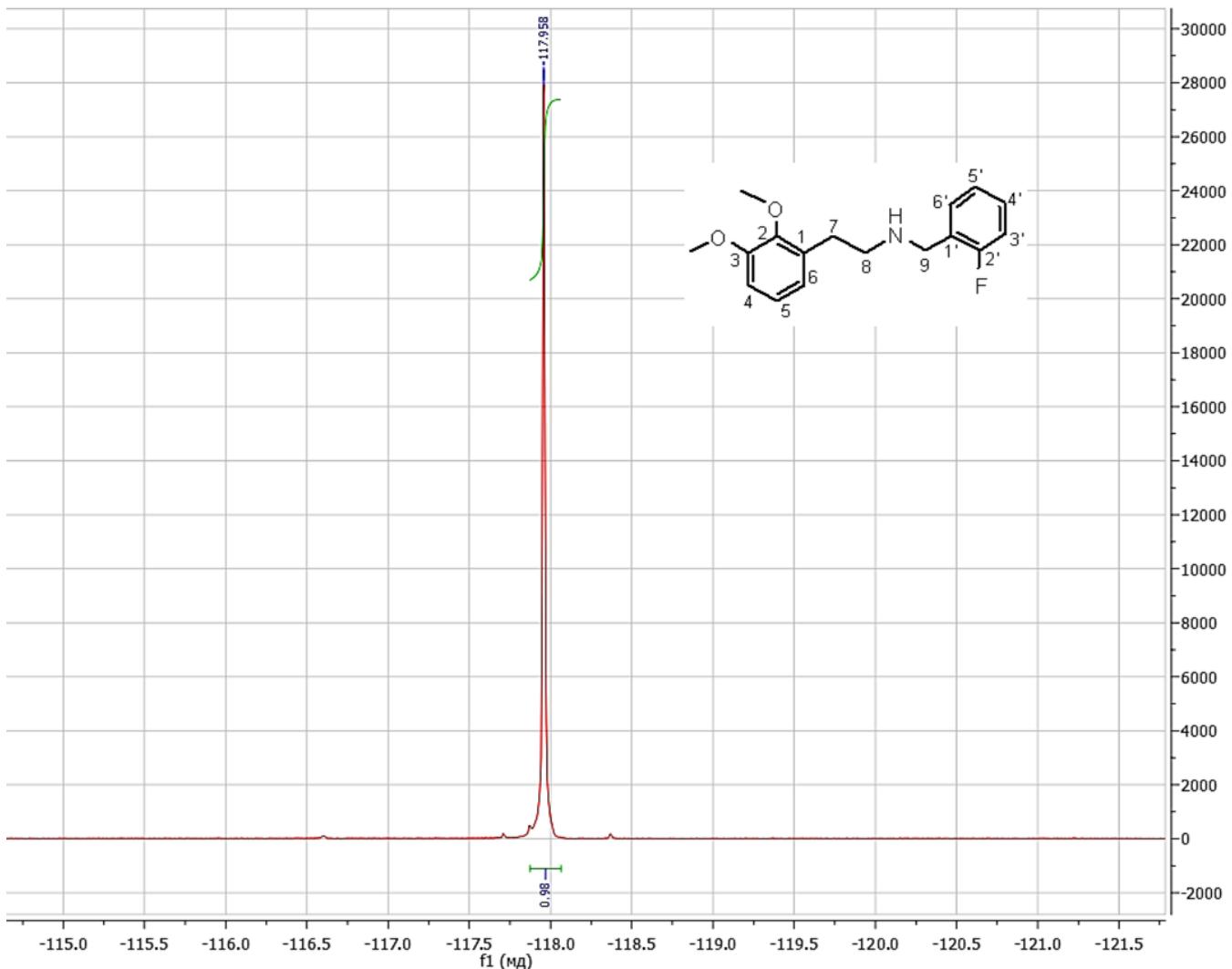
**2-(2,3-Dimethoxyphenyl)-N-(2-fluorobenzyl)ethanamine hydrochloride (23H-NBF, (2))**



**Figure S6.**  $^1\text{H}$  NMR spectrum of **2** (400 MHz,  $\text{CD}_3\text{OD}$ )

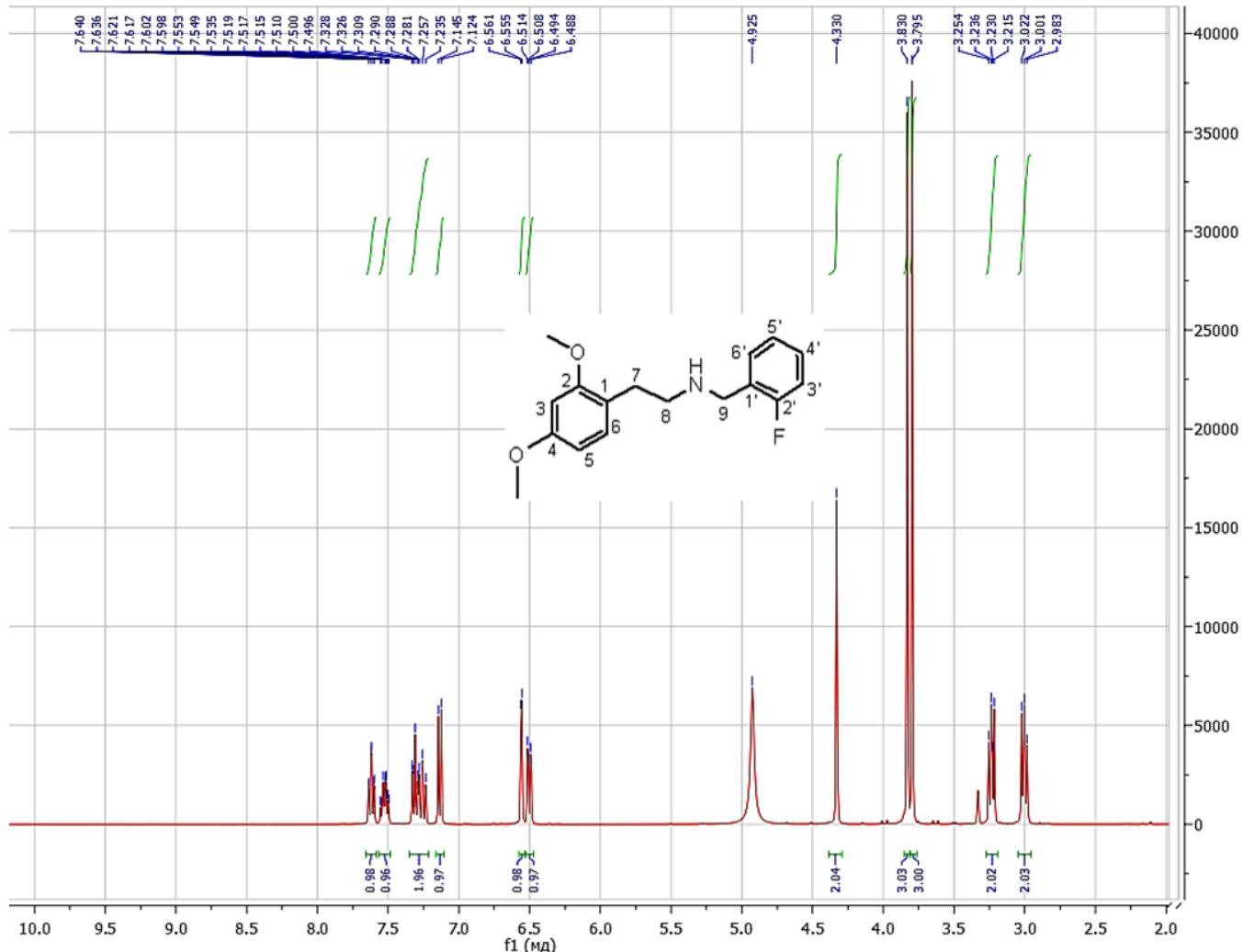


**Figure S7.**  $^{13}\text{C}$  NMR spectrum of **2** (101 MHz,  $\text{CD}_3\text{OD}$ )

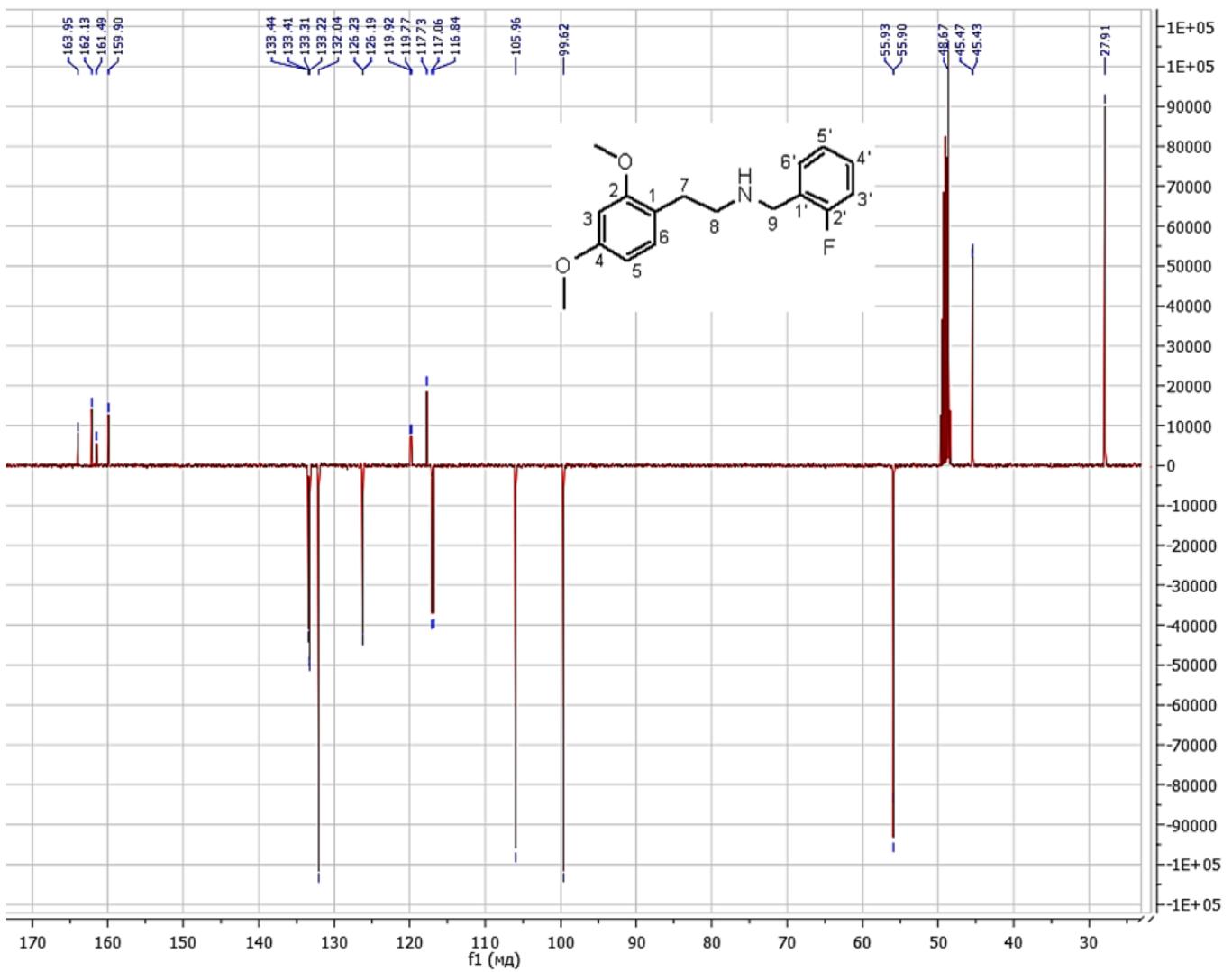


**Figure S8.**  $^{19}\text{F}$  NMR spectrum of **2** (376 MHz,  $\text{CD}_3\text{OD}$ )

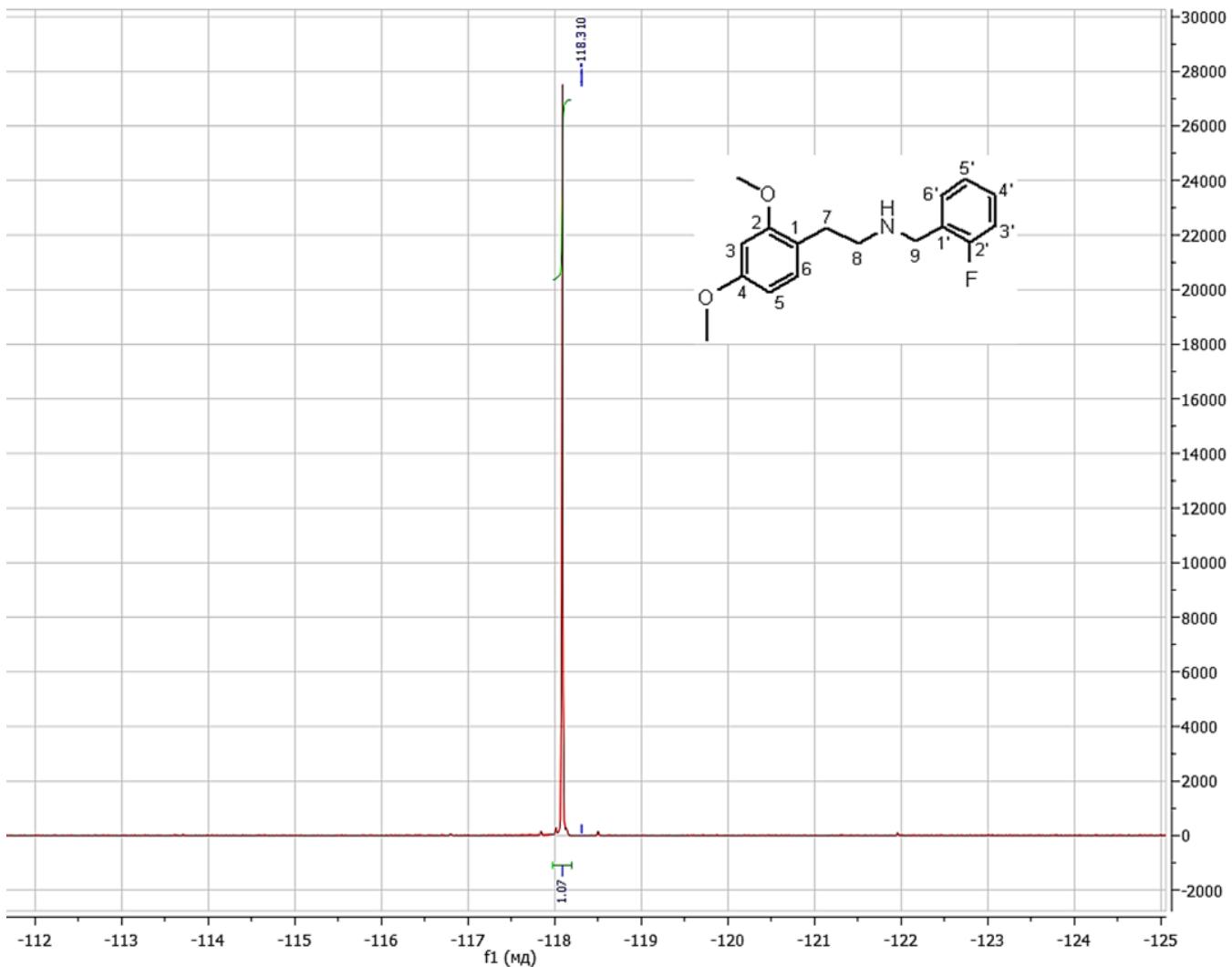
**2-(2,4-Dimethoxyphenyl)-N-(2-fluorobenzyl)ethanamine hydrochloride (24H-NBF, (3))**



**Figure S9.**  $^1\text{H}$  NMR spectrum of 3 (400 MHz,  $\text{CD}_3\text{OD}$ )

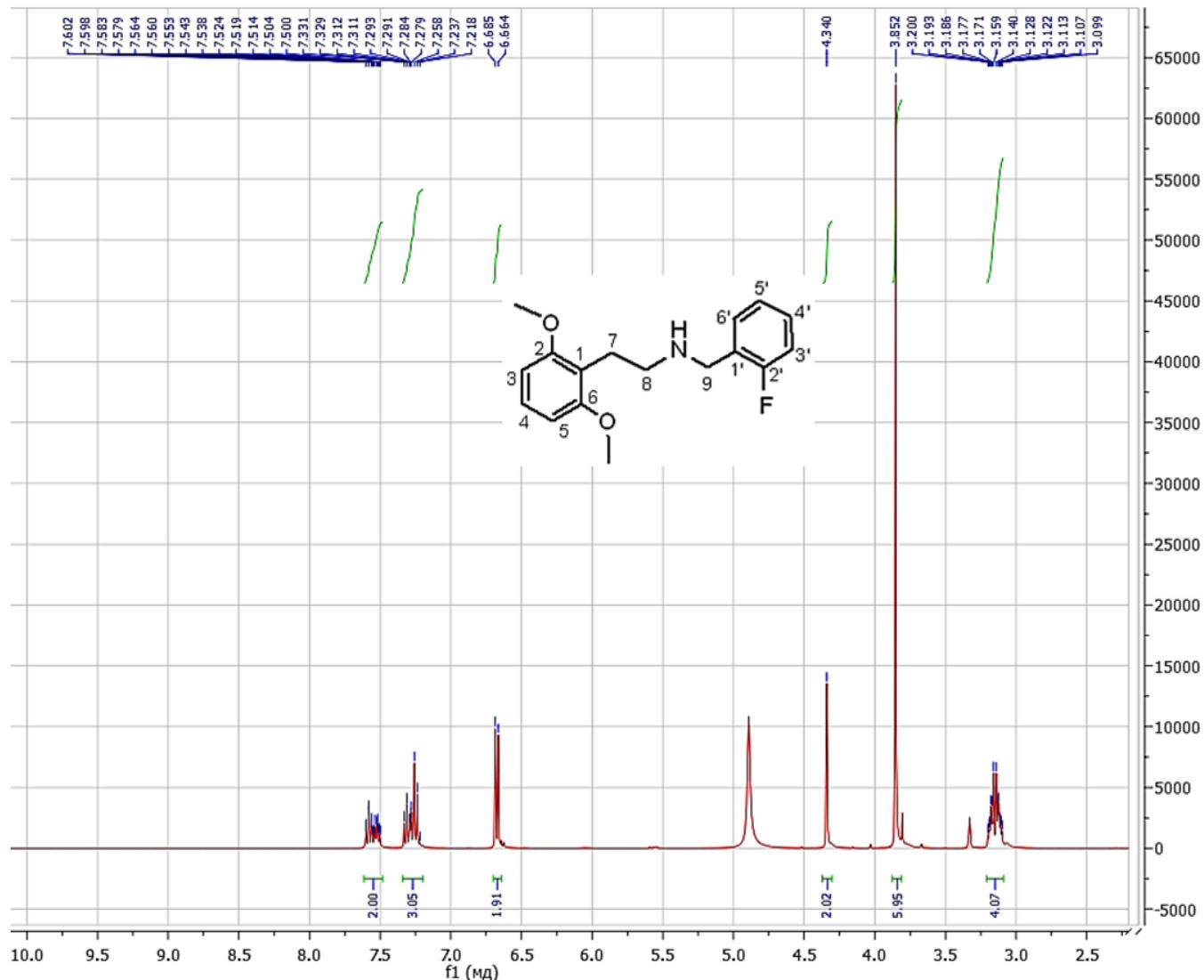


**Figure S10.**  $^{13}\text{C}$  NMR spectrum of **3** (101 MHz,  $\text{CD}_3\text{OD}$ )

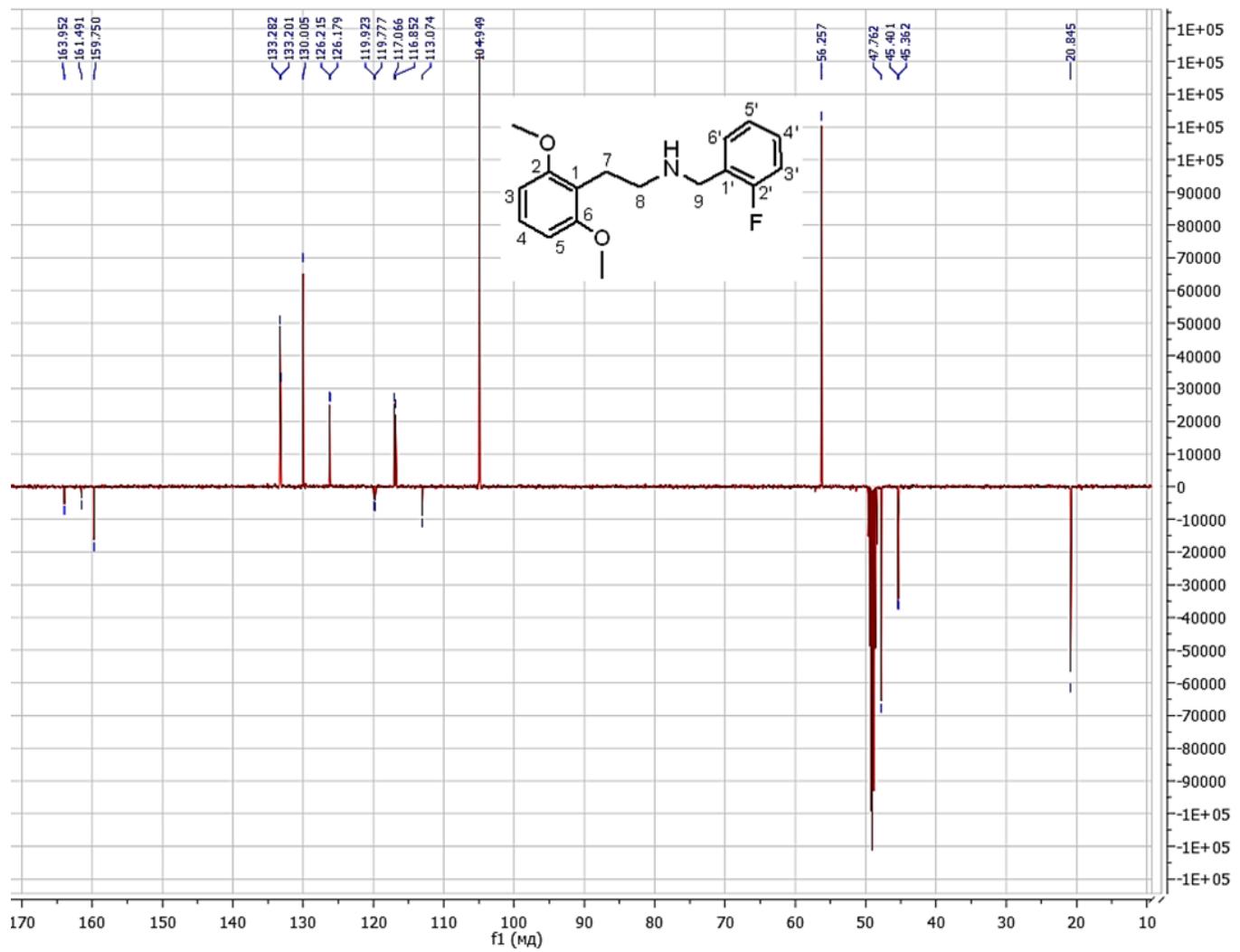


**Figure S11.**  $^{19}\text{F}$  NMR spectrum of **3** (376 MHz,  $\text{CD}_3\text{OD}$ )

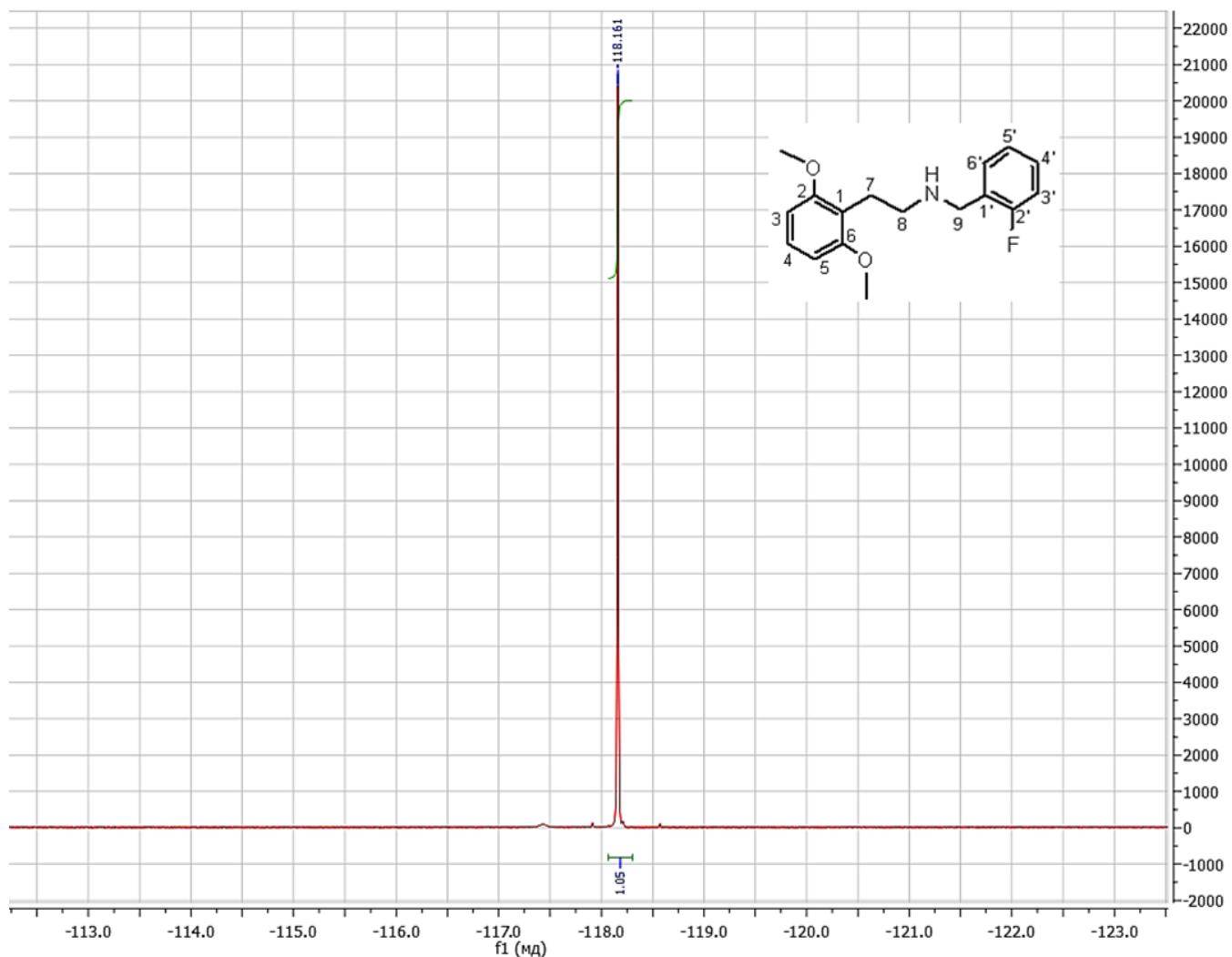
**2-(2,6-Dimethoxyphenyl)-N-(2-fluorobenzyl)ethanamine hydrochloride (26H-NBF, (4))**



**Figure S12.** <sup>1</sup>H NMR spectrum of **4** (400 MHz, CD<sub>3</sub>OD)

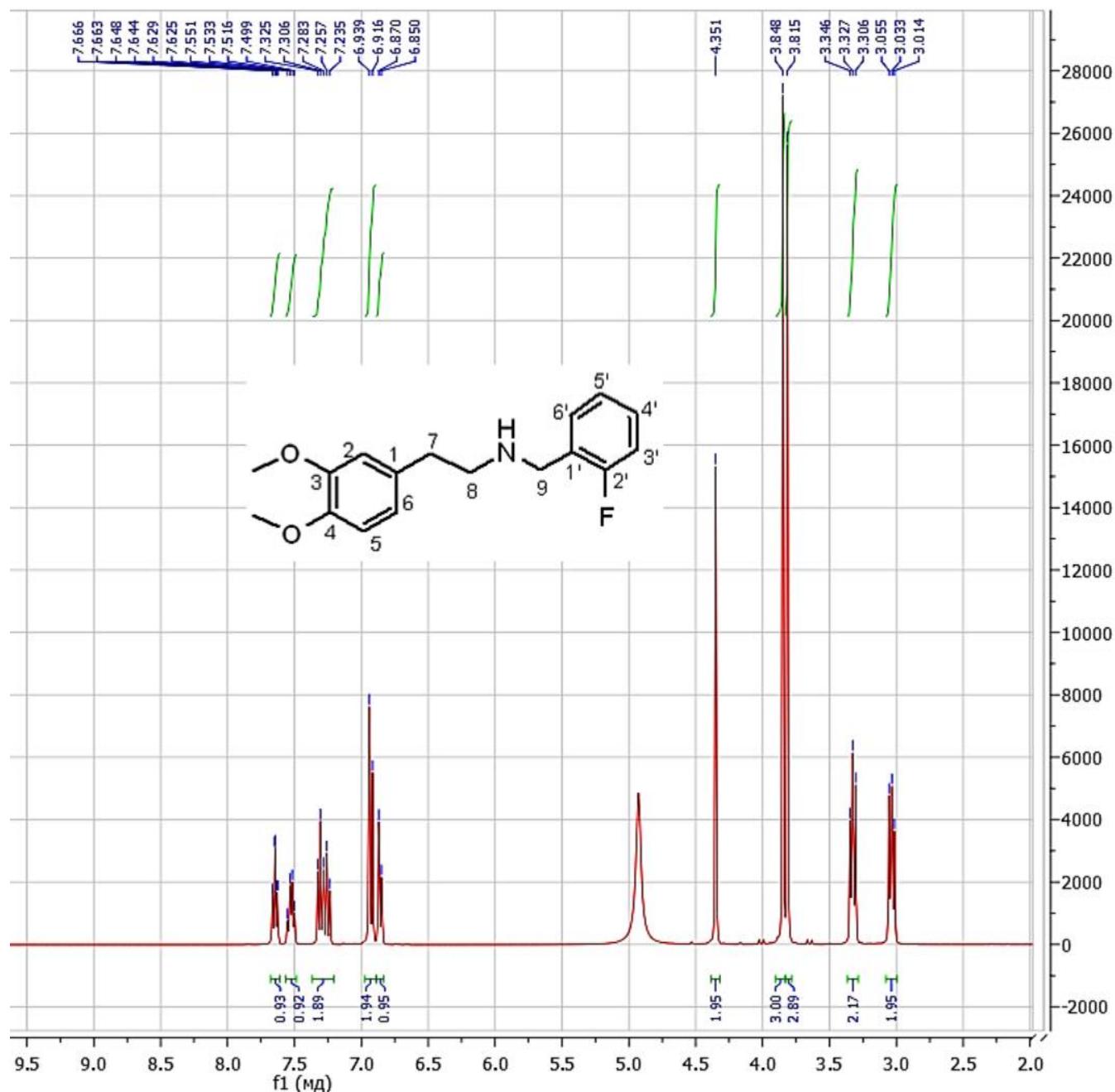


**Figure S13.**  $^{13}\text{C}$  NMR spectrum of **4** (101 MHz,  $\text{CD}_3\text{OD}$ )

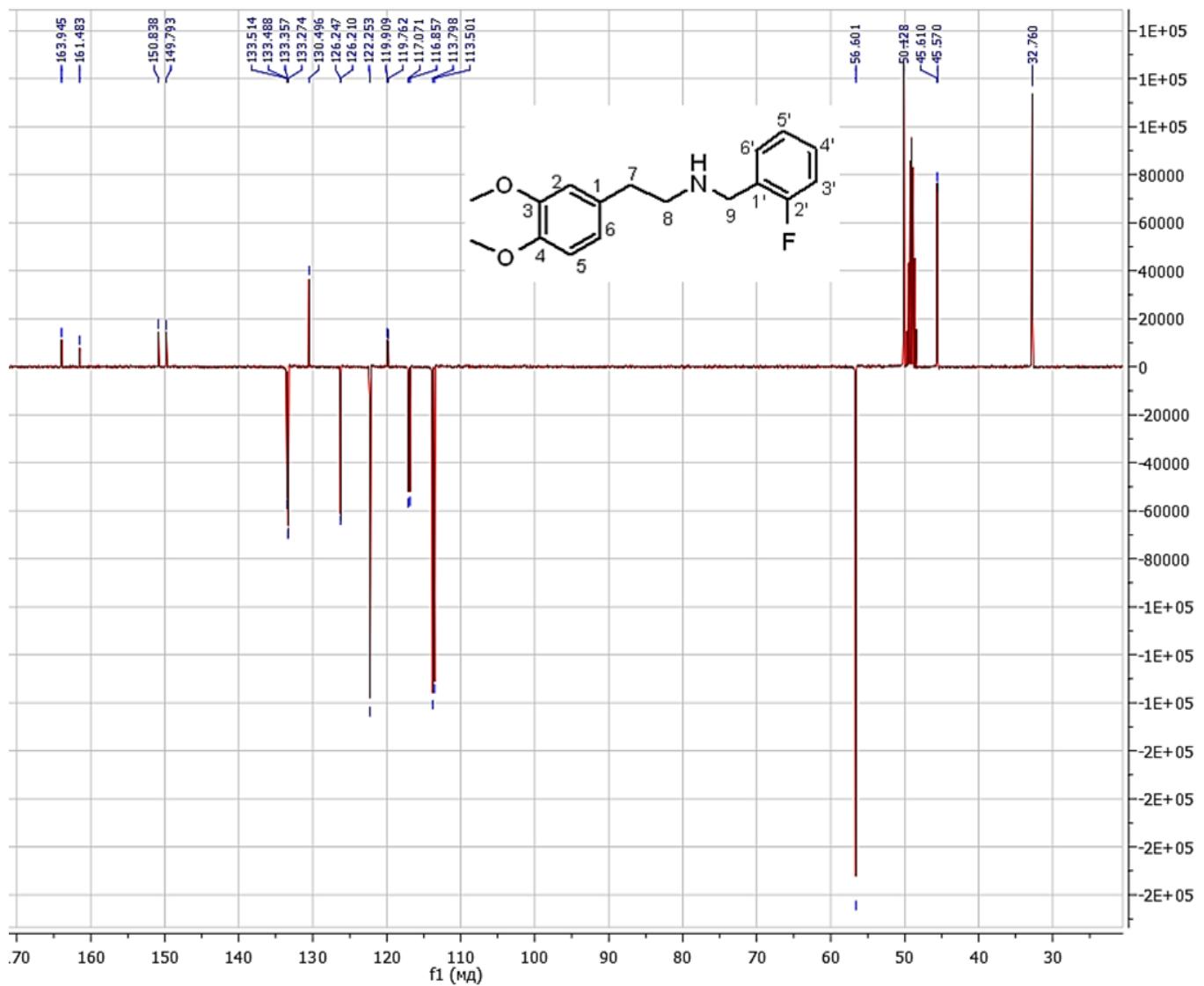


**Figure S14.**  ${}^{19}\text{F}$  NMR spectrum of **4** (376 MHz,  $\text{CD}_3\text{OD}$ )

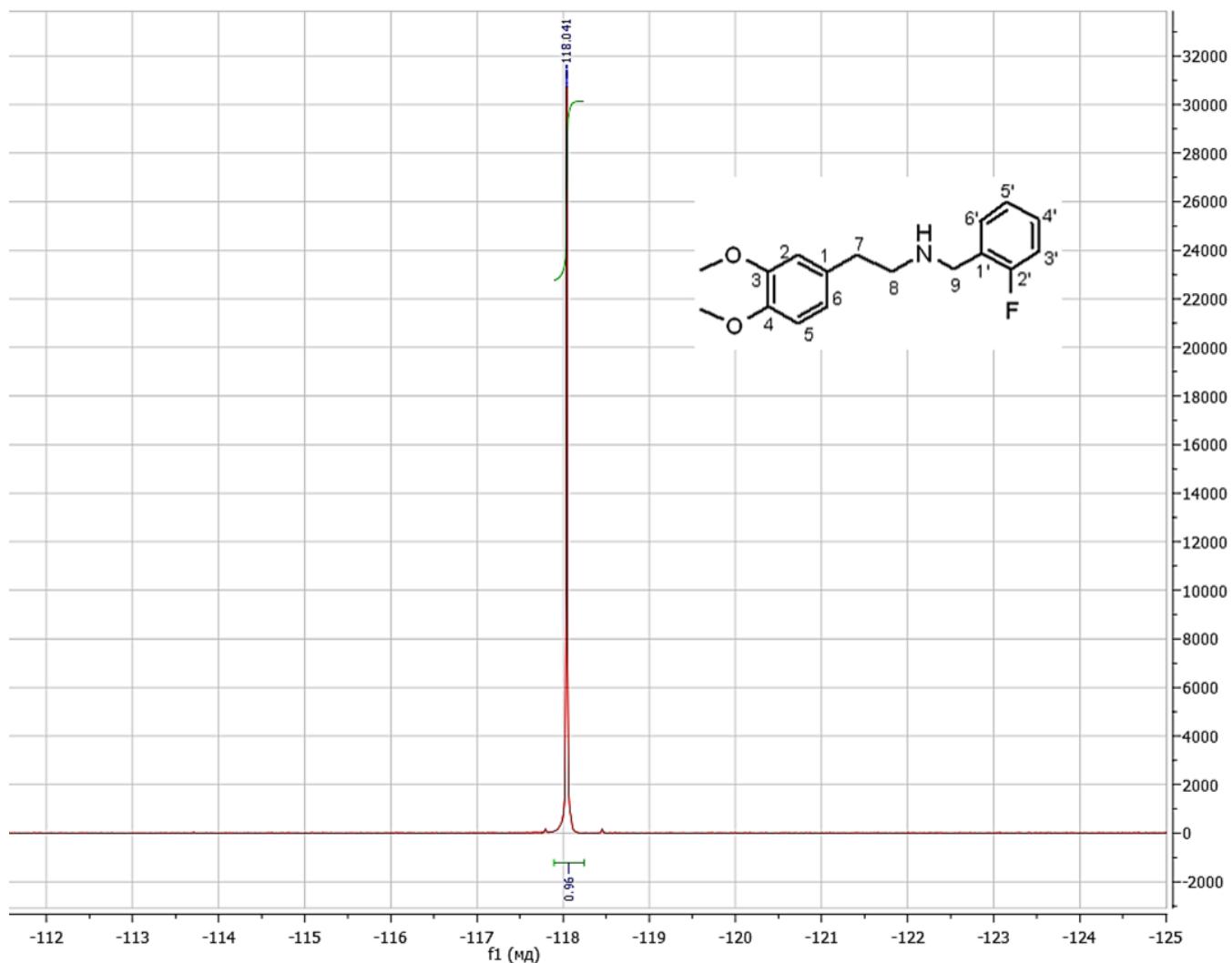
**2-(3,4-Dimethoxyphenyl)-N-(2-fluorobenzyl)ethanamine hydrochloride (34H-NBF, (5))**



**Figure S15.**  $^1\text{H}$  NMR spectrum of **5** (400 MHz,  $\text{CD}_3\text{OD}$ )

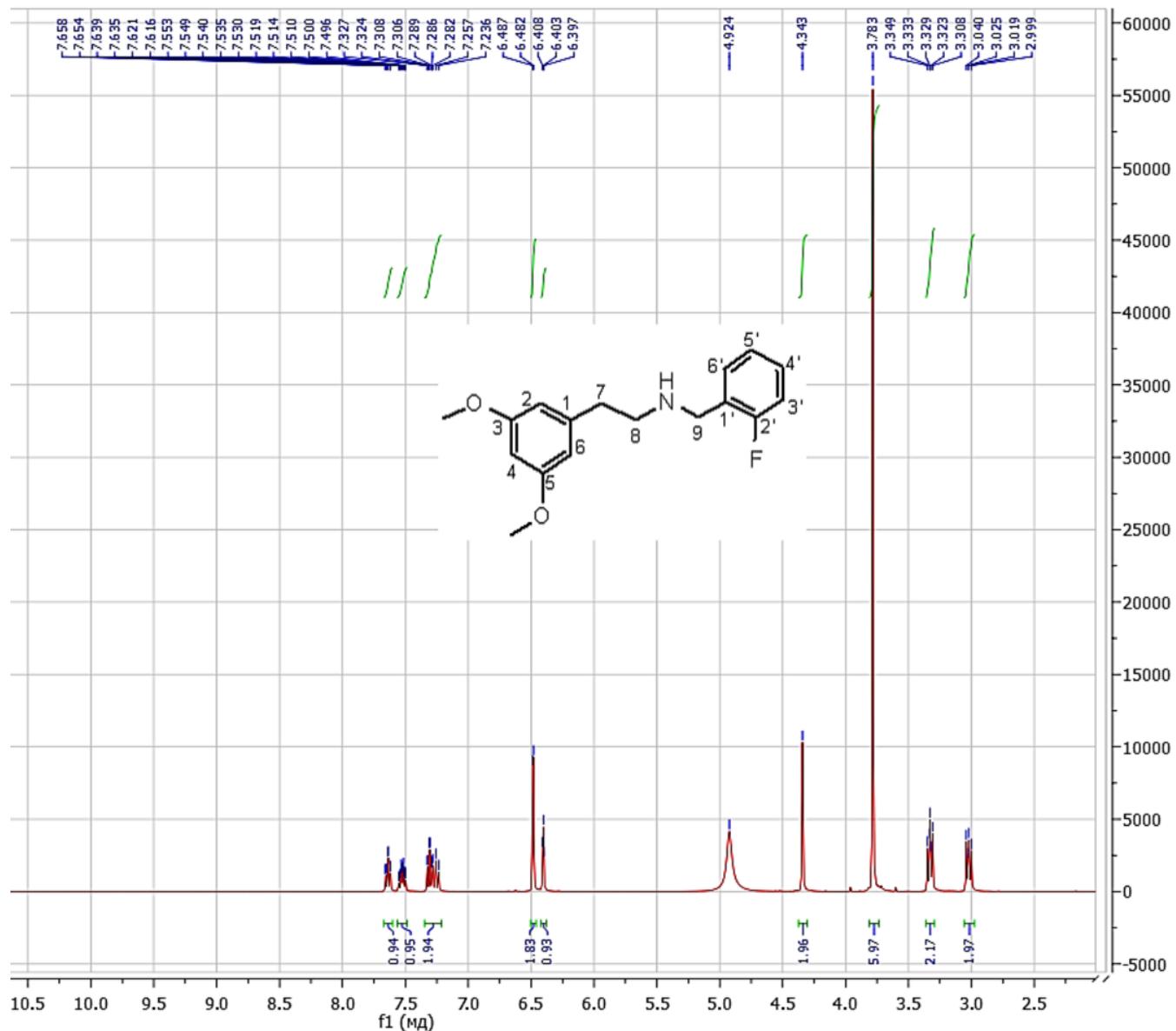


**Figure S16.**  $^{13}\text{C}$  NMR spectrum of **5** (101 MHz,  $\text{CD}_3\text{OD}$ )

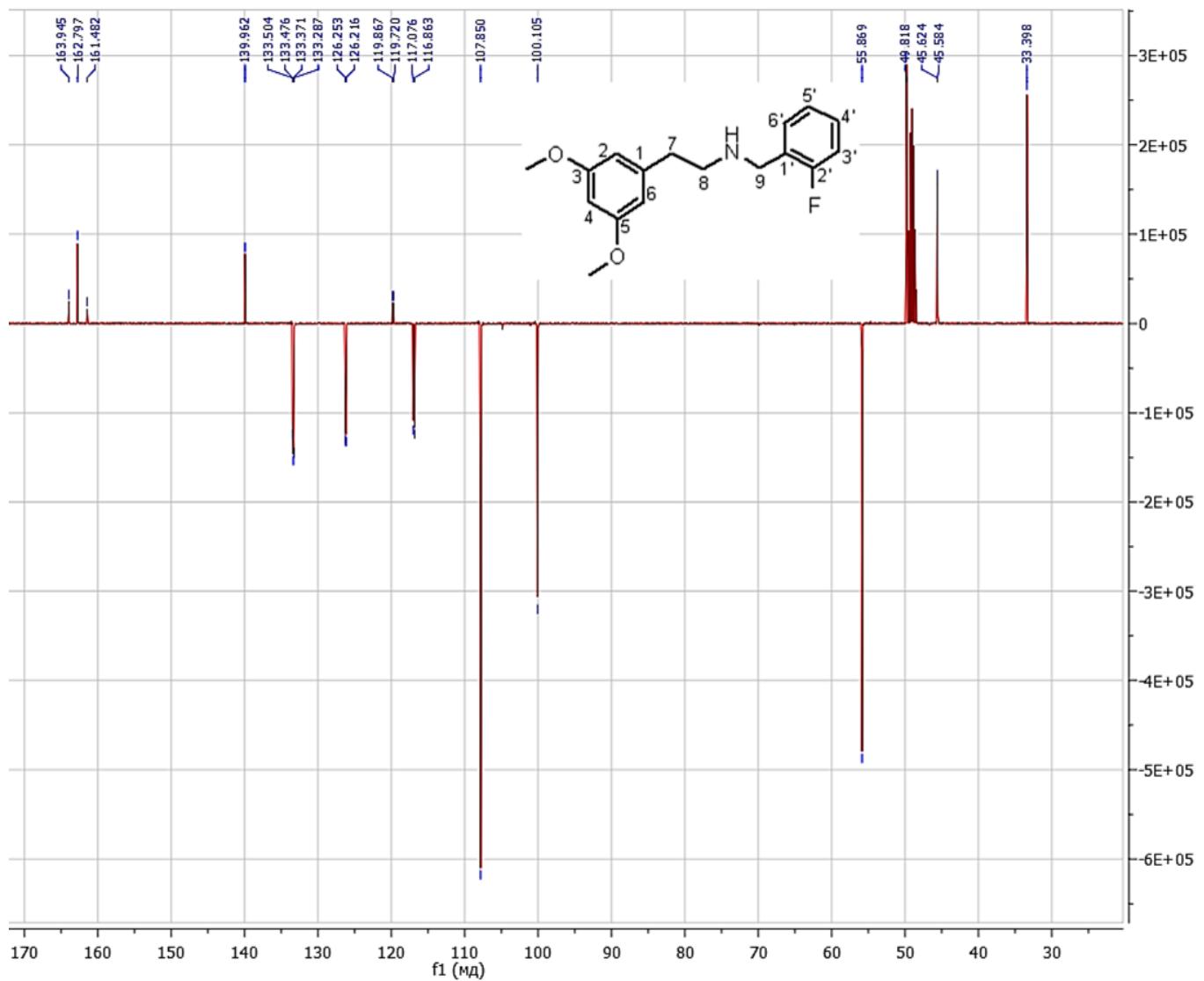


**Figure S17.**  $^{19}\text{F}$  NMR spectrum of **5** (376 MHz,  $\text{CD}_3\text{OD}$ )

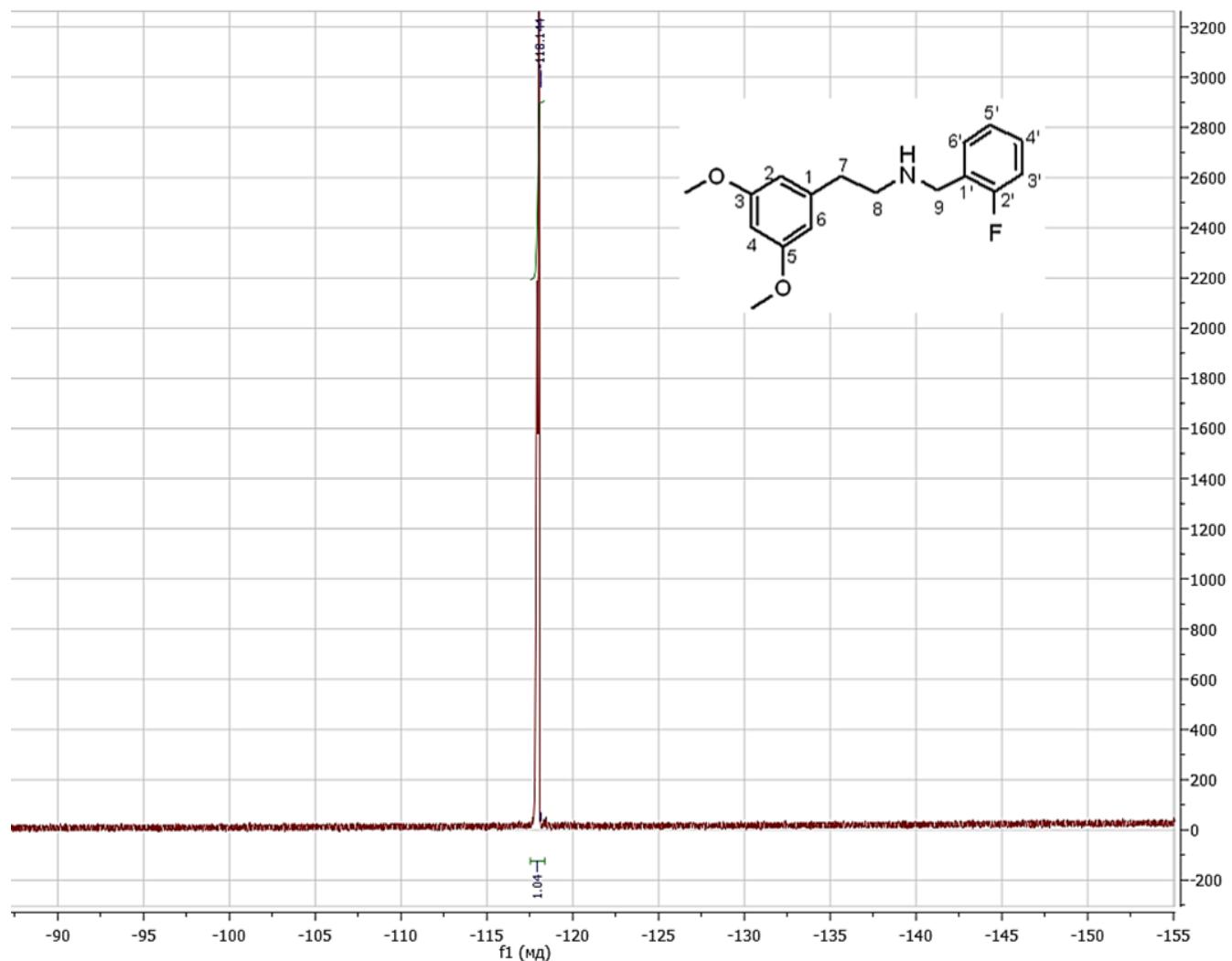
**2-(3,5-Dimethoxyphenyl)-N-(2-fluorobenzyl)ethanamine hydrochloride (35H-NBF, (6))**



**Figure S18.**  $^1\text{H}$  NMR spectrum of **6** (400 MHz,  $\text{CD}_3\text{OD}$ )



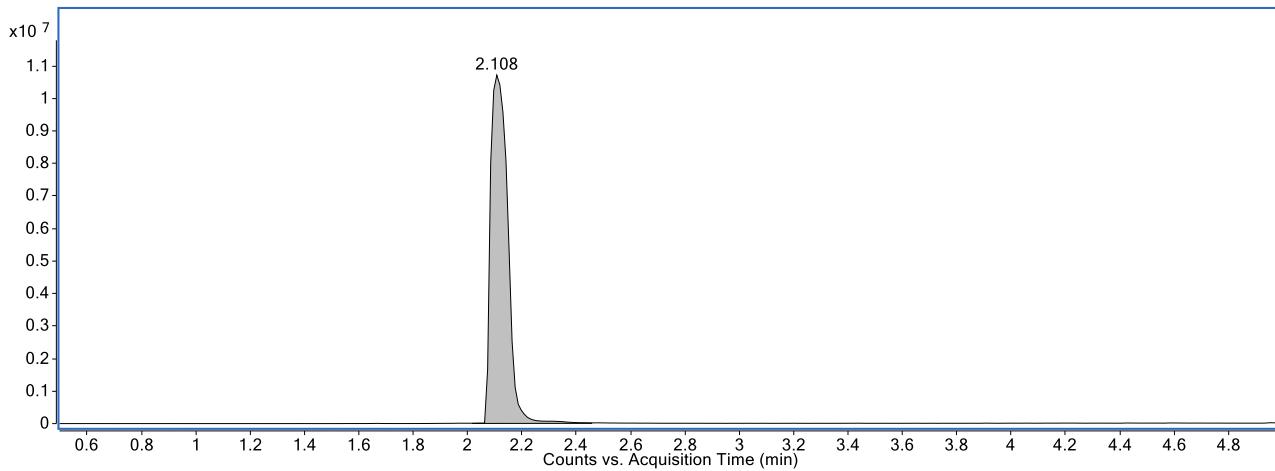
**Figure S19.**  $^{13}\text{C}$  NMR spectrum of **6** (101 MHz,  $\text{CD}_3\text{OD}$ )



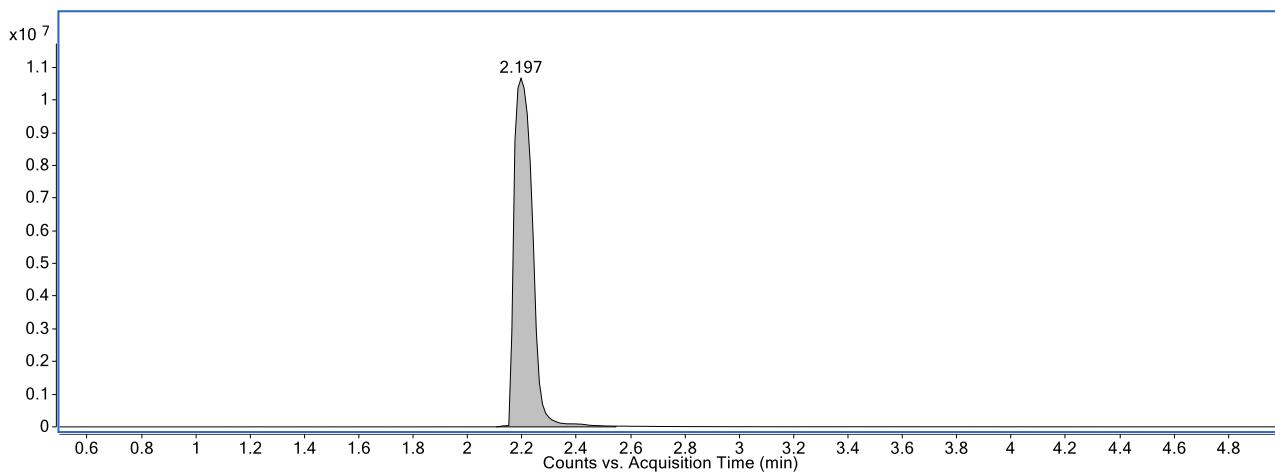
**Figure S20.**  ${}^{19}\text{F}$  NMR spectrum of **6** (376 MHz,  $\text{CD}_3\text{OD}$ )

**Table S1.** Data of elemental analysis for compounds **2–6**

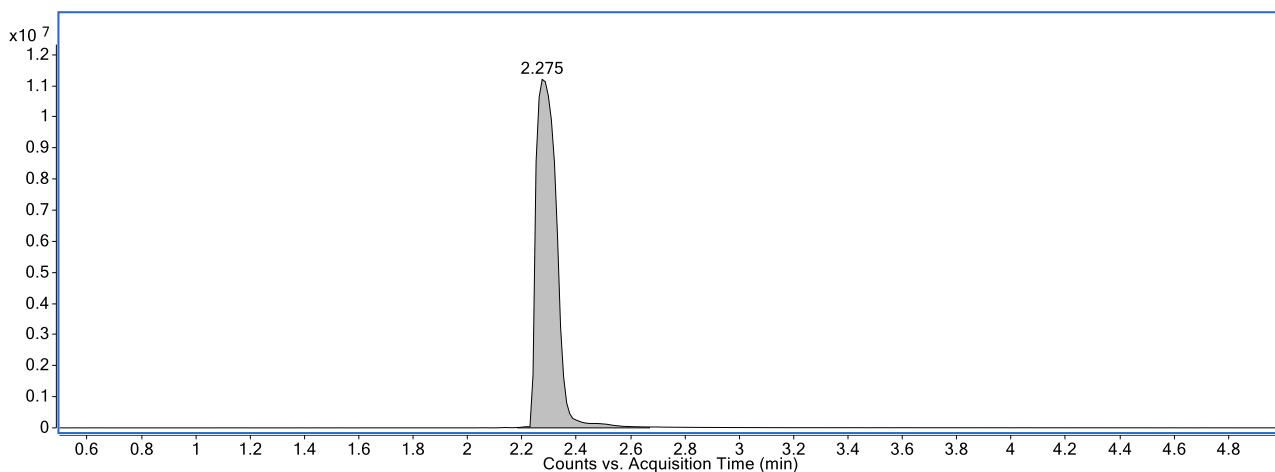
Compound	Calculated, %	Found, %
<b>23H-NBF hydrochloride (2)</b> (C <sub>17</sub> H <sub>20</sub> NO <sub>2</sub> F·HCl)	C - 62.67 H - 6.50 N - 4.30 Cl - 10.88	C - 62.18 H - 6.37 N - 4.25 Cl - 10.85
<b>24H-NBF hydrochloride (3)</b> (C <sub>17</sub> H <sub>20</sub> NO <sub>2</sub> F·HCl)	C - 62.67 H - 6.50 N - 4.30 Cl - 10.88	C - 62.29 H - 6.27 N - 4.22 Cl - 10.80
<b>26H-NBF hydrochloride (4)</b> (C <sub>17</sub> H <sub>20</sub> NO <sub>2</sub> F·HCl)	C - 62.67 H - 6.50 N - 4.30 Cl - 10.88	C - 62.15 H - 6.33 N - 4.24 Cl - 10.83
<b>34H-NBF hydrochloride (5)</b> (C <sub>17</sub> H <sub>20</sub> NO <sub>2</sub> F·HCl)	C - 62.67 H - 6.50 N - 4.30 Cl - 10.88	C - 62.21 H - 6.27 N - 4.20 Cl - 10.80
<b>35H-NBF hydrochloride (6)</b> (C <sub>17</sub> H <sub>20</sub> NO <sub>2</sub> F·HCl)	C - 62.67 H - 6.50 N - 4.30 Cl - 10.88	C - 62.25 H - 6.33 N - 4.22 Cl - 10.85



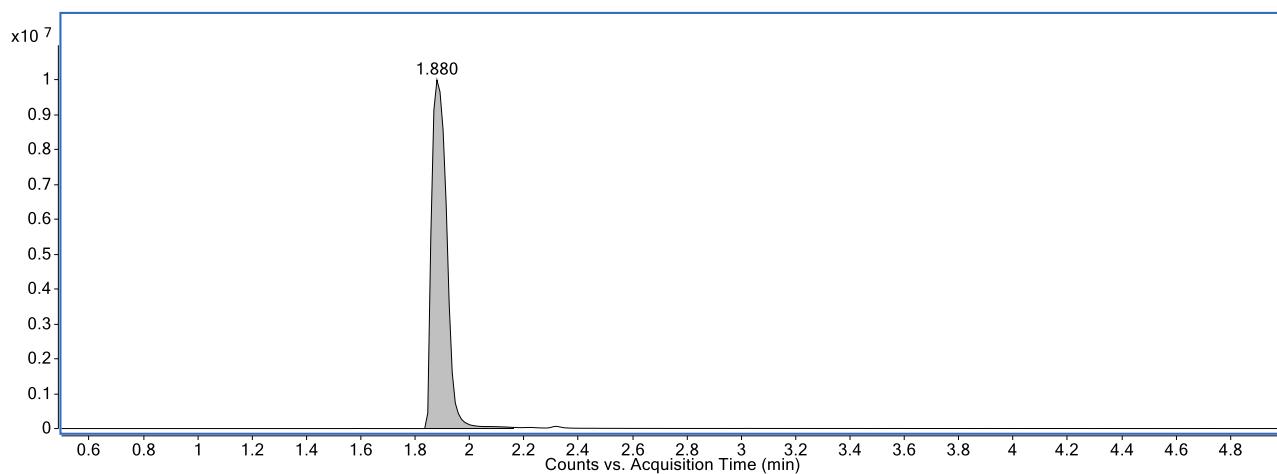
**Figure S21.** LC-MS chromatogram of 23H-NBF (**2**)



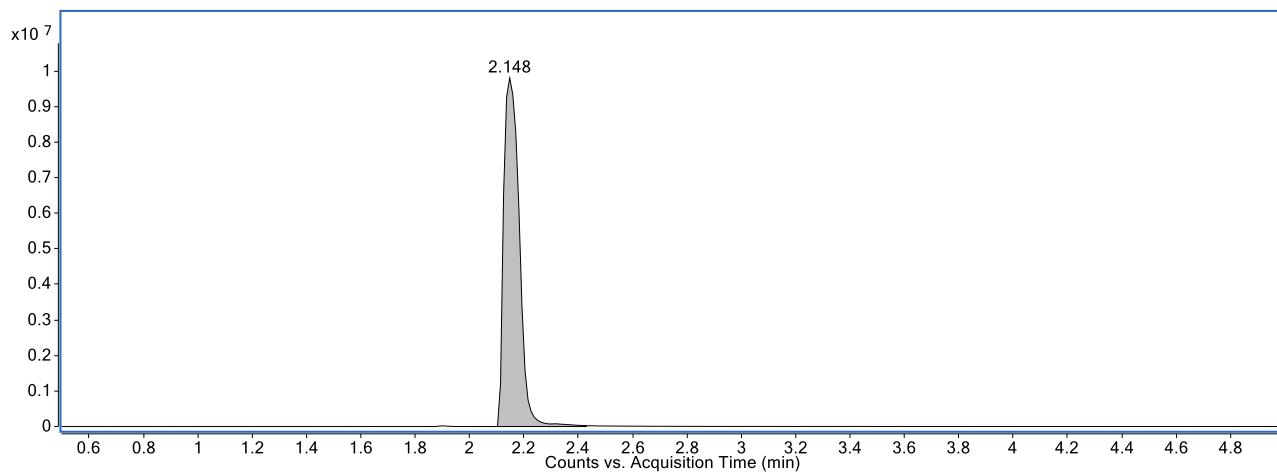
**Figure S22.** LC-MS chromatogram of 24H-NBF (**3**)



**Figure S23.** LC-MS chromatogram of 26H-NBF (**4**)



**Figure S24.** LC-MS chromatogram of 34H-NBF (**5**)



**Figure S25.** LC-MS chromatogram of 35H-NBF (**6**)