

Supporting Information

Fe-Catalyzed hydroxytrifluoromethylation of α -(trifluoromethyl)styrenes with $\text{CF}_3\text{SO}_2\text{Na}$: facile access to α,β -bistrifluoromethyl tertiary alcohols

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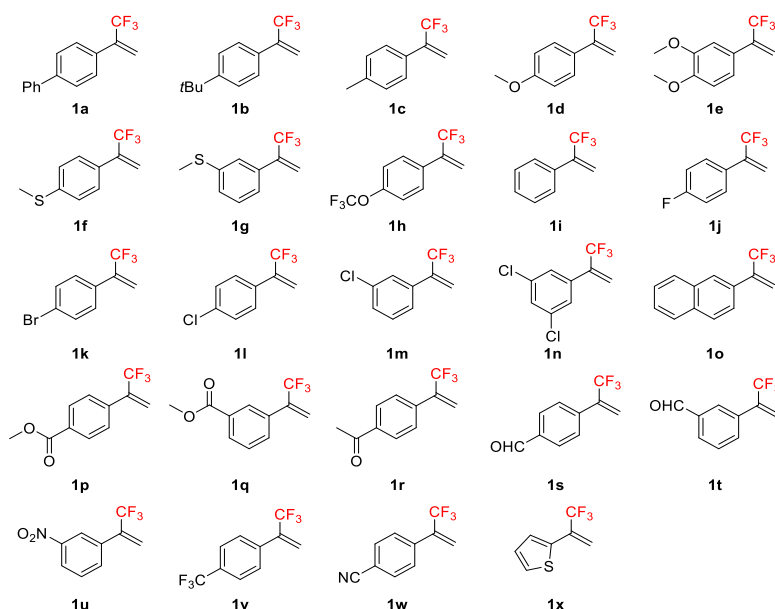
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1. General information

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 Büchi melting point B-540 apparatus and are uncorrected. ^1H NMR and ^{13}C NMR spectra were recorded on a 400 spectrometer (400 MHz for ^1H and 100 MHz for ^{13}C , respectively) using TMS as an internal standard. The ^{19}F NMR spectra were obtained on a 400 or 600 spectrometer (376 MHz) with CF_3COOH as an internal standard. CDCl_3 or $(\text{CD}_3)_2\text{CO}$ was used as the NMR solvents. High resolution mass spectra (HRMS) were acquired in the electron impact mode (EI) 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. α -(Trifluoromethyl)styrenes (**1a–x**) used in this reaction



The α -(trifluoromethyl)styrenes (**1a–x**) were prepared according to the reported procedure.¹

3. General procedure for the synthesis of the target compounds **2a–x**

To a glass tube charged with a stirring bar were added $\text{Fe}(\text{OAc})_2$ (34.79 mg, 0.20 mmol, 20 mol%), $\text{K}_2\text{S}_2\text{O}_8$ (54.06 mg, 0.20 mmol, 0.2 equiv), NaSO_2CF_3 (312.12 mg, 2.0 mmol, 2.0 equiv), α -(trifluoromethyl)styrenes **1** (1.0 mmol, 1.0 equiv), and DMSO (5 mL). Then the reaction mixture was stirred at room temperature under air atmosphere for 12 h (monitored by TLC and GC/MS). After completion of the reaction, the reaction mixture was quenched with saturated aqueous solution of NaCl (10 mL) and extracted with dichloromethane (3×10 mL). The organic layer was separated and dried over Na_2SO_4 , filtered and concentrated in vacuo. The resultant residue was purified by column chromatography on silica gel using *n*-hexane/dichloromethane (20/1~10/1) as eluent to afford the pure target compounds **2a–x**.

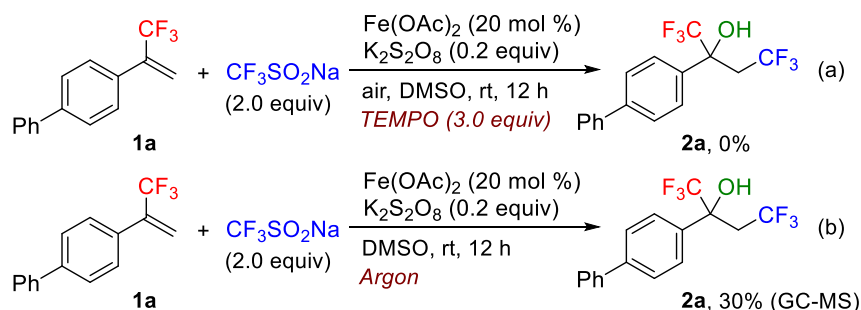
4. General procedure for the synthesis of compound 4a

To a glass tube charged with a stirring bar were added Fe(OAc)₂ (34.79 mg, 0.20 mmol, 20 mol%), K₂S₂O₈ (54.06 mg, 0.20 mmol), NaSO₂CF₃ (312.12 mg, 2.0 mmol), unactivated alkenes **3a–c** (1.0 mmol), and DMSO (5 mL). Then the reaction mixture was stirred at room temperature under air atmosphere for 12 h (monitored by TLC and GC/MS). After completion of the reaction, the reaction mixture was quenched with saturated aqueous solution of NaCl (10 mL) and extracted with dichloromethane (3×10 mL). The organic layer was separated and dried over Na₂SO₄, filtered and concentrated in vacuo. The resultant residue was purified by column chromatography on silica gel using *n*-hexane/dichloromethane (10/1) as eluent to afford compound **4a**.

5. General procedure for the synthesis of compound 5a

A solution of **2a** (334.08 mg, 1.0 mmol), Cs₂CO₃ (651.64 mg, 2.0 mmol) in DMF (5 mL) was stirred at 25 °C for about 30 minutes. Subsequently, iodoethane (187.16 mg, 1.2 mmol) was added to the mixture. Stirring was continued at 25 °C for 4 h (monitored by TLC and GC/MS). After completion of the reaction, the reaction mixture was quenched with saturated aqueous solution of NH₄Cl (10 mL) and extracted with ethyl acetate (3 × 10 mL). The organic layer was separated and dried over Na₂SO₄, filtered and concentrated in vacuo. The resultant residue was purified by column chromatography on silica gel using *n*-hexane/ ethyl acetate (15/1) as eluent to afford **5a**.

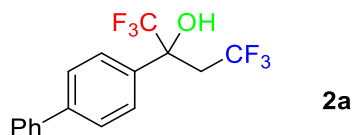
6. Control experiments



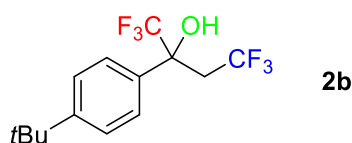
Control experiment (a): To a glass tube charged with a stirring bar were added Fe(OAc)₂ (3.48 mg, 0.02 mmol, 20 mol%), K₂S₂O₈ (5.41 mg, 0.02 mmol), NaSO₂CF₃ (31.21 mg, 0.2 mmol), **1a** (33.41 mg, 0.1 mmol, 1.0 equiv), TEMPO (46.88 mg, 0.3 mmol), and DMSO (1 mL). Then the reaction mixture was stirred at room temperature under air atmosphere for 12 h. Finally, the reaction mixture was analyzed by TLC and GC/MS.

Control experiment (b): To a glass tube charged with a stirring bar were added Fe(OAc)₂ (3.48 mg, 0.02 mmol, 20 mol%), K₂S₂O₈ (5.41 mg, 0.02 mmol), NaSO₂CF₃ (31.21 mg, 0.2 mmol), **1a** (33.41 mg, 0.1 mmol), and DMSO (1 mL). Then the reaction mixture was stirred at room temperature under argon atmosphere for 12 h. Finally, the reaction mixture was analyzed by TLC and GC/MS.

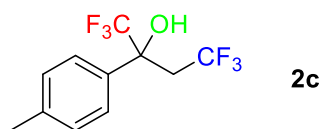
7. Analytical data of the target compounds



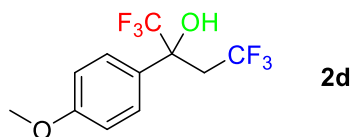
2-([1,1'-Biphenyl]-4-yl)-1,1,1,4,4,4-hexafluorobutan-2-ol (2a). white solid; m.p.: 126.3–129.8 °C, yield 95% (317.4 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.59–7.52 (m, 6H), 7.37 (t, $J = 7.2$ Hz, 2H), 7.29 (t, $J = 7.6$ Hz, 1H), 3.09–2.84 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 141.0, 139.0, 132.4, 127.8, 126.7, 126.1, 125.4, 123.8 (q, $^1J_{\text{CF}} = 276.2$ Hz), 123.4 (q, $^1J_{\text{CF}} = 284.2$ Hz), 73.9 (qd, $^2J_{\text{CF}} = 29.2$ Hz, $^3J_{\text{CF}} = 1.8$ Hz), 38.2 (q, $^2J_{\text{CF}} = 27.9$ Hz); ^{19}F NMR (376 MHz, CDCl_3) δ –58.7 (t, $J = 6.4$ Hz, 3F), –80.6 (s, 3F); HRMS (EI): calcd for $\text{C}_{16}\text{H}_{12}\text{F}_6\text{O}$ $[\text{M}]^+$: 334.0792, found: 334.0795.



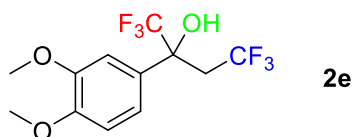
2-(4-(*tert*-Butyl)phenyl)-1,1,1,4,4,4-hexafluorobutan-2-ol (2b). colorless oil; yield 93% (292.1 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.40 (d, $J = 8.4$ Hz, 2H), 7.35 (d, $J = 8.8$ Hz, 2H), 3.04–2.81 (m, 2H), 2.79 (s, 1H), 1.25 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 151.2, 130.5, 124.6, 124.4, 123.8 (q, $^1J_{\text{CF}} = 276.1$ Hz), 123.5 (q, $^1J_{\text{CF}} = 284.4$ Hz), 73.9 (qd, $^2J_{\text{CF}} = 29.4$ Hz, $^3J_{\text{CF}} = 2.2$ Hz), 38.2 (q, $^2J_{\text{CF}} = 27.6$ Hz), 33.6, 30.2; ^{19}F NMR (376 MHz, CDCl_3) δ –58.8 (t, $J = 7.1$ Hz, 3F), –80.6 (s, 3F); HRMS (EI): calcd for $\text{C}_{14}\text{H}_{16}\text{F}_6\text{O}$ $[\text{M}]^+$: 314.1105, found: 314.1103.



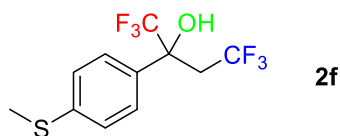
1,1,1,4,4,4-Hexafluoro-2-(*p*-tolyl)butan-2-ol (2c). yellow oil; yield 86% (234.0 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.35 (d, $J = 8.0$ Hz, 2H), 7.13 (d, $J = 8.0$ Hz, 2H), 3.00–2.80 (m, 3H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 138.2, 130.6, 128.2, 124.8, 123.8 (q, $^1J_{\text{CF}} = 276.2$ Hz), 123.5 (q, $^1J_{\text{CF}} = 284.4$ Hz), 73.9 (qd, $^2J_{\text{CF}} = 29.2$ Hz, $^3J_{\text{CF}} = 2.0$ Hz), 38.1 (q, $^2J_{\text{CF}} = 27.5$ Hz), 20.0; ^{19}F NMR (376 MHz, CDCl_3) δ –58.8 (s, 3F), –80.9 (s, 3F); HRMS (EI): calcd for $\text{C}_{11}\text{H}_{10}\text{F}_6\text{O}$ $[\text{M}]^+$: 272.0636, found: 272.0638.



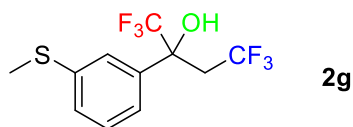
1,1,1,4,4,4-Hexafluoro-2-(4-methoxyphenyl)butan-2-ol (2d). yellow oil; yield 88% (253.5 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.40 (d, $J = 8.4$ Hz, 2H), 6.86 (d, $J = 8.8$ Hz, 2H), 3.73 (s, 3H), 3.02–2.80 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.1, 126.3, 125.4, 123.8 (q, $^1J_{\text{CF}} = 276.1$ Hz), 123.5 (q, $^1J_{\text{CF}} = 284.3$ Hz), 112.8, 73.8 (qd, $^2J_{\text{CF}} = 29.2$ Hz, $^3J_{\text{CF}} = 2.0$ Hz), 54.3, 38.1 (q, $^2J_{\text{CF}} = 27.8$ Hz); ^{19}F NMR (376 MHz, CDCl_3) δ –58.8 (s, 3F), –81.1 (s, 3F); HRMS (EI): calcd for $\text{C}_{11}\text{H}_{10}\text{F}_6\text{O}_2$ $[\text{M}]^+$: 288.0585, found: 288.0581.



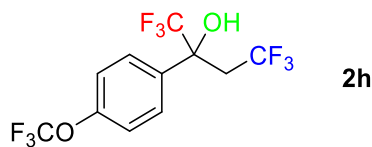
2-(3,4-Dimethoxyphenyl)-1,1,1,4,4,4-hexafluorobutan-2-ol (2e). white solid; m.p.: 126.8–131.2 °C, yield 91% (298.5 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.04 (s, 1H), 7.00 (d, $J = 8.4$ Hz, 1H), 6.82 (d, $J = 8.4$ Hz, 1H), 3.83 (s, 3H), 3.83 (s, 3H), 3.03–2.80 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 148.6, 147.8, 125.8, 123.8 (q, $^1J_{\text{CF}} = 276.3$ Hz), 123.5 (q, $^1J_{\text{CF}} = 283.6$ Hz), 117.7, 109.7, 108.5, 73.7 (qd, $^2J_{\text{CF}} = 29.1$ Hz, $^3J_{\text{CF}} = 2.1$ Hz), 55.0, 54.8, 38.2 (q, $^2J_{\text{CF}} = 27.6$ Hz); ^{19}F NMR (376 MHz, CDCl_3) δ -58.8 (t, $J = 7.1$ Hz, 3F), -80.8 (s, 3F); HRMS (EI): calcd for $\text{C}_{12}\text{H}_{12}\text{F}_6\text{O}_3$ $[\text{M}]^+$: 318.0691, found: 318.0694.



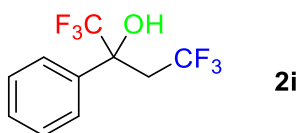
1,1,1,4,4,4-Hexafluoro-2-(4-(methylthio)phenyl)butan-2-ol (2f). colorless oil; yield 90% (273.6 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.39 (d, $J = 8.0$ Hz, 2H), 7.20 (d, $J = 8.8$ Hz, 2H), 3.00–2.82 (m, 3H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 139.4, 129.9, 125.4, 124.9, 123.8 (q, $^1J_{\text{CF}} = 276.5$ Hz), 123.3 (q, $^1J_{\text{CF}} = 284.6$ Hz), 73.8 (qd, $^2J_{\text{CF}} = 29.4$ Hz, $^3J_{\text{CF}} = 2.2$ Hz), 38.0 (q, $^2J_{\text{CF}} = 27.9$ Hz), 14.2; ^{19}F NMR (376 MHz, CDCl_3) δ -58.7 (s, 3F), -80.9 (s, 3F); HRMS (EI): calcd for $\text{C}_{11}\text{H}_{10}\text{F}_6\text{OS}$ $[\text{M}]^+$: 304.0357, found: 304.0359.



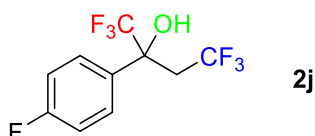
1,1,1,4,4,4-Hexafluoro-2-(3-(methylthio)phenyl)butan-2-ol (2g). colorless oil; yield 92% (279.7 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.42 (s, 1H), 7.27–7.20 (m, 3H), 3.03–2.81 (m, 3H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 138.4, 134.3, 127.9, 126.2, 123.7 (q, $^1J_{\text{CF}} = 276.4$ Hz), 123.3 (q, $^1J_{\text{CF}} = 285.1$ Hz), 123.2, 121.6, 73.8 (qd, $^2J_{\text{CF}} = 29.1$ Hz, $^3J_{\text{CF}} = 2.2$ Hz), 38.3 (q, $^2J_{\text{CF}} = 27.7$ Hz), 14.8; ^{19}F NMR (376 MHz, CDCl_3) δ -58.8 (t, $J = 6.4$ Hz, 3F), -80.5 (s, 3F); HRMS (EI): calcd for $\text{C}_{11}\text{H}_{10}\text{F}_6\text{OS}$ $[\text{M}]^+$: 304.0357, found: 304.0360.



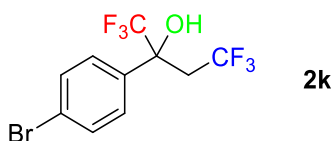
1,1,1,4,4,4-Hexafluoro-2-(4-(trifluoromethoxy)phenyl)butan-2-ol (2h). brown oil; yield 80% (273.6 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.55 (d, $J = 8.8$ Hz, 2H), 7.20 (d, $J = 8.0$ Hz, 2H), 3.05–2.82 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 148.9, 132.0, 126.8, 123.6 (q, $^1J_{\text{CF}} = 276.0$ Hz), 123.2 (q, $^1J_{\text{CF}} = 283.8$ Hz), 119.6, 119.4 (q, $^1J_{\text{CF}} = 256.3$ Hz), 73.6 (qd, $^2J_{\text{CF}} = 29.3$ Hz, $^3J_{\text{CF}} = 2.1$ Hz), 38.2 (q, $^2J_{\text{CF}} = 28.4$ Hz); ^{19}F NMR (376 MHz, CDCl_3) δ -57.9 (s, 3F), -58.9 (t, $J = 7.5$ Hz, 3F), -80.8 (s, 3F); HRMS (EI): calcd for $\text{C}_{11}\text{H}_7\text{F}_9\text{O}_2$ $[\text{M}]^+$: 342.0302, found: 342.0300.



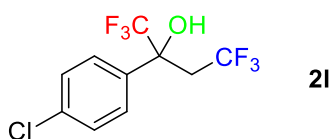
1,1,1,4,4,4-Hexafluoro-2-phenylbutan-2-ol (2i). yellow oil; yield 87% (224.5 mg); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.50 (d, $J = 6.4$ Hz, 2H), 7.39–7.33 (m, 3H), 3.07–2.83 (m, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 133.5, 128.2, 127.5, 124.9, 123.8 (q, $^1J_{\text{CF}} = 276.4$ Hz), 123.4 (q, $^1J_{\text{CF}} = 284.8$ Hz), 73.9 (qd, $^2J_{\text{CF}} = 29.1$ Hz, $^3J_{\text{CF}} = 2.0$ Hz), 38.2 (q, $^2J_{\text{CF}} = 28.0$ Hz); $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -58.8 (t, $J = 6.8$ Hz, 3F), -80.7 (s, 3F); HRMS (EI): calcd for $\text{C}_{10}\text{H}_8\text{F}_6\text{O}$ $[\text{M}]^+$: 258.0479, found: 258.0477.



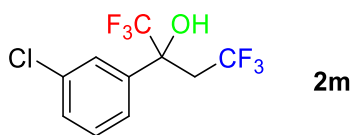
1,1,1,4,4,4-Hexafluoro-2-(4-fluorophenyl)butan-2-ol (2j). yellow oil; yield 87% (240.1 mg); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.51–7.47 (m, 2H), 7.07–7.01 (m, 2H), 3.04–2.80 (m, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 162.2 (d, $^1J_{\text{CF}} = 247.2$ Hz), 129.2 (d, $^4J_{\text{CF}} = 3.2$ Hz), 127.1 (d, $^3J_{\text{CF}} = 8.4$ Hz), 123.7 (q, $^1J_{\text{CF}} = 276.1$ Hz), 123.3 (q, $^1J_{\text{CF}} = 284.6$ Hz), 114.5 (d, $^2J_{\text{CF}} = 21.7$ Hz), 73.7 (qd, $^2J_{\text{CF}} = 29.5$ Hz, $^3J_{\text{CF}} = 2.0$ Hz), 38.2 (q, $^2J_{\text{CF}} = 27.8$ Hz); $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -58.8 (t, $J = 7.1$ Hz, 3F), -81.0 (s, 3F), -112.60–-112.65 (m, 1F); HRMS (EI): calcd for $\text{C}_{10}\text{H}_7\text{F}_7\text{O}$ $[\text{M}]^+$: 276.0385, found: 276.0383.



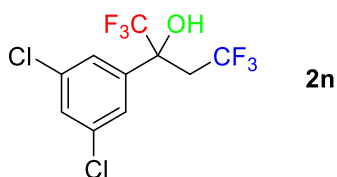
2-(4-Bromophenyl)-1,1,1,4,4,4-hexafluorobutan-2-ol (2k). yellow oil; yield 84% (282.2 mg); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.49 (d, $J = 8.8$ Hz, 2H), 7.38 (d, $J = 8.4$ Hz, 2H), 3.08–2.80 (m, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 132.5, 130.7, 126.8, 123.6 (q, $^1J_{\text{CF}} = 276.3$ Hz), 123.1 (q, $^1J_{\text{CF}} = 284.2$ Hz), 122.7, 73.6 (qd, $^2J_{\text{CF}} = 29.2$ Hz, $^3J_{\text{CF}} = 2.1$ Hz), 38.0 (q, $^2J_{\text{CF}} = 28.0$ Hz); $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -58.8 (t, $J = 6.8$ Hz, 3F), -80.8 (s, 3F); HRMS (EI): calcd for $\text{C}_{10}\text{H}_7\text{BrF}_6\text{O}$ $[\text{M}]^+$: 335.9584, found: 335.9579.



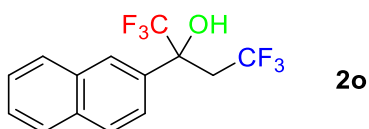
2-(4-Chlorophenyl)-1,1,1,4,4,4-hexafluorobutan-2-ol (2l). colorless oil; yield 83% (242.4 mg); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.45 (d, $J = 8.8$ Hz, 2H), 7.34 (d, $J = 8.8$ Hz, 2H), 3.03–2.80 (m, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 134.5, 132.0, 127.7, 126.5, 123.6 (q, $^1J_{\text{CF}} = 276.2$ Hz), 123.2 (q, $^1J_{\text{CF}} = 284.4$ Hz), 73.6 (qd, $^2J_{\text{CF}} = 29.6$ Hz, $^3J_{\text{CF}} = 2.0$ Hz), 38.1 (q, $^2J_{\text{CF}} = 27.9$ Hz); $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -58.8 (t, $J = 7.1$ Hz, 3F), -80.8 (s, 3F); HRMS (EI): calcd for $\text{C}_{10}\text{H}_7\text{ClF}_6\text{O}$ $[\text{M}]^+$: 292.0090, found: 292.0086.



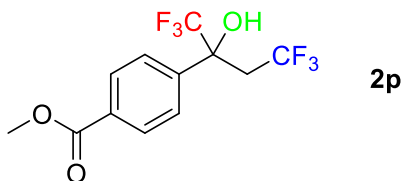
2-(3-Chlorophenyl)-1,1,1,4,4,4-hexafluorobutan-2-ol (2m). yellow oil; yield 86% (251.1 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.54 (s, 1H), 7.38–7.27 (m, 3H), 3.02–2.81 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 135.5, 133.8, 128.7, 128.5, 125.5, 123.6 (q, $^1J_{\text{CF}} = 276.1$ Hz), 123.2, 123.2 (q, $^1J_{\text{CF}} = 284.0$ Hz), 73.6 (qd, $^2J_{\text{CF}} = 29.7$ Hz, $^3J_{\text{CF}} = 2.3$ Hz), 38.2 (q, $^2J_{\text{CF}} = 27.6$ Hz); ^{19}F NMR (376 MHz, CDCl_3) δ –58.9 (t, $J = 7.5$ Hz, 3F), –80.6 (s, 3F); HRMS (EI): calcd for $\text{C}_{10}\text{H}_7\text{ClF}_6\text{O}$ $[\text{M}]^+$: 292.0090, found: 292.0087.



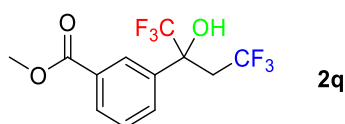
2-(3,5-Dichlorophenyl)-1,1,1,4,4,4-hexafluorobutan-2-ol (2n). colorless oil; yield 85% (277.1 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.41 (s, 2H), 7.35 (t, $J = 2.0$ Hz, 1H), 3.00–2.81 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 136.9, 134.4, 128.6, 123.9, 123.4 (q, $^1J_{\text{CF}} = 276.2$ Hz), 123.0 (q, $^1J_{\text{CF}} = 284.2$ Hz), 73.3 (qd, $^2J_{\text{CF}} = 29.6$ Hz, $^3J_{\text{CF}} = 2.1$ Hz), 38.2 (q, $^2J_{\text{CF}} = 28.0$ Hz); ^{19}F NMR (376 MHz, CDCl_3) δ –58.9 (t, $J = 7.1$ Hz, 3F), –80.5 (s, 3F); HRMS (EI): calcd for $\text{C}_{10}\text{H}_6\text{Cl}_2\text{F}_6\text{O}$ $[\text{M}]^+$: 325.9700, found: 325.9703.



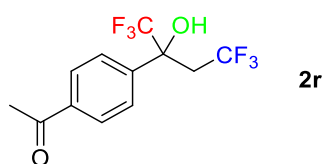
1,1,1,4,4,4-Hexafluoro-2-(naphthalen-2-yl)butan-2-ol (2o). white solid; m.p.: 68.4–72.9 °C, yield 89% (274.2 mg); ^1H NMR (400 MHz, CDCl_3) δ 8.04 (s, 1H), 7.82–7.77 (m, 3H), 7.52 (d, $J = 8.8$ Hz, 1H), 7.48–7.43 (m, 2H), 3.18–2.89 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 133.3, 132.8, 131.8, 128.6, 128.4, 127.6, 127.1, 126.7, 126.1, 124.8 (q, $^1J_{\text{CF}} = 276.3$ Hz), 124.5 (q, $^1J_{\text{CF}} = 276.2$ Hz), 123.0, 75.1 (qd, $^2J_{\text{CF}} = 29.0$ Hz, $^3J_{\text{CF}} = 2.1$ Hz), 39.2 (q, $^2J_{\text{CF}} = 27.1$ Hz); ^{19}F NMR (376 MHz, CDCl_3) δ –58.8 (t, $J = 6.8$ Hz, 3F), –80.3 (s, 3F); HRMS (EI): calcd for $\text{C}_{14}\text{H}_{10}\text{F}_6\text{O}$ $[\text{M}]^+$: 308.0636, found: 308.0639.



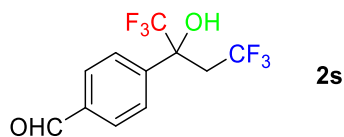
Methyl 4-(1,1,1,4,4,4-hexafluoro-2-hydroxybutan-2-yl)benzoate (2p). white solid; m.p.: 85.3–88.5 °C, yield 92% (290.8 mg); ^1H NMR (400 MHz, CDCl_3) δ 8.01 (d, $J = 8.4$ Hz, 2H), 7.62 (d, $J = 8.4$ Hz, 2H), 3.86 (s, 3H), 3.56 (s, 1H), 3.08–2.85 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 165.7, 138.4, 129.8, 128.6, 125.3, 123.6 (q, $^1J_{\text{CF}} = 276.3$ Hz), 123.3 (q, $^1J_{\text{CF}} = 284.3$ Hz), 73.8 (qd, $^2J_{\text{CF}} = 29.3$ Hz, $^3J_{\text{CF}} = 2.3$ Hz), 51.4, 38.1 (q, $^2J_{\text{CF}} = 27.9$ Hz); ^{19}F NMR (376 MHz, CDCl_3) δ –58.9 (t, $J = 6.4$ Hz, 3F), –80.5 (s, 3F); HRMS (EI): calcd for $\text{C}_{12}\text{H}_{10}\text{F}_6\text{O}_3$ $[\text{M}]^+$: 316.0534, found: 316.0536.



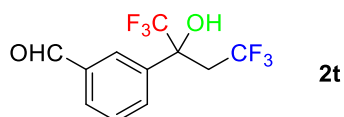
Methyl 3-(1,1,1,4,4,4-hexafluoro-2-hydroxybutan-2-yl)benzoate (2q). white solid; m.p.: 101.3–103.2 °C, yield 93% (293.9 mg); ¹H NMR (400 MHz, CDCl₃) δ 8.29 (s, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 1H), 3.94 (s, 3H), 3.52 (s, 1H), 3.19–2.94 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 166.7, 135.2, 130.7, 130.5, 130.4, 128.7, 127.3, 124.7 (q, ¹*J*_{CF} = 276.1 Hz), 124.3 (q, ¹*J*_{CF} = 285.0 Hz), 74.7 (qd, ²*J*_{CF} = 29.4 Hz, ³*J*_{CF} = 1.8 Hz), 52.4, 39.1 (q, ²*J*_{CF} = 27.6 Hz); ¹⁹F NMR (376 MHz, CDCl₃) δ –58.8 (t, *J* = 6.8 Hz, 3F), –80.7 (s, 3F); HRMS (EI): calcd for C₁₂H₁₀F₆O₃ [M]⁺: 316.0534, found: 316.0532.



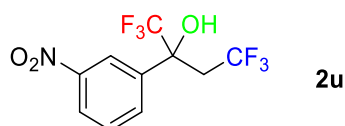
1-(4-(1,1,1,4,4,4-Hexafluoro-2-hydroxybutan-2-yl)phenyl)ethan-1-one (2r). white solid; m.p.: 128.0–133.1 °C, yield 90% (270.0 mg); ¹H NMR (400 MHz, CDCl₃) δ 7.94 (d, *J* = 8.8 Hz, 2H), 7.65 (d, *J* = 8.0 Hz, 2H), 3.66 (s, 1H), 3.10–2.87 (m, 2H), 2.56 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 197.0, 138.6, 136.4, 127.4, 125.5, 123.6 (q, ¹*J*_{CF} = 276.3 Hz), 123.3 (q, ¹*J*_{CF} = 283.5 Hz), 73.8 (qd, ²*J*_{CF} = 29.3 Hz, ³*J*_{CF} = 2.0 Hz), 38.1 (q, ²*J*_{CF} = 27.8 Hz), 25.6; ¹⁹F NMR (376 MHz, CDCl₃) δ –58.8 (t, *J* = 6.4 Hz, 3F), –80.5 (s, 3F); HRMS (EI): calcd for C₁₂H₁₀F₆O₂ [M]⁺: 300.0585, found: 300.0587.



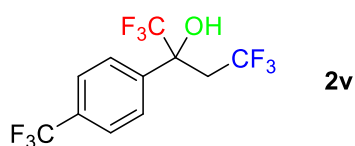
4-(1,1,1,4,4,4-Hexafluoro-2-hydroxybutan-2-yl)benzaldehyde (2s). white solid; m.p.: 137.6–143.4 °C, yield 91% (260.3 mg); ¹H NMR (400 MHz, (CD₃)₂CO) δ 10.11 (s, 1H), 8.03–7.99 (m, 4H), 6.49 (s, 1H), 3.64–3.52 (m, 1H), 3.23–3.12 (m, 1H); ¹³C NMR (100 MHz, (CD₃)₂CO) δ 191.7, 141.7, 136.9, 129.0, 127.5, 125.3 (q, ¹*J*_{CF} = 275.7 Hz), 124.9 (q, ¹*J*_{CF} = 285.2 Hz), 74.6 (qd, ²*J*_{CF} = 28.7 Hz, ³*J*_{CF} = 2.3 Hz), 38.0 (q, ²*J*_{CF} = 27.6 Hz); ¹⁹F NMR (376 MHz, (CD₃)₂CO) δ –59.2 (t, *J* = 7.5 Hz, 3F), –80.9 (s, 3F); HRMS (EI): calcd for C₁₁H₈F₆O₂ [M]⁺: 286.0428, found: 286.0417.



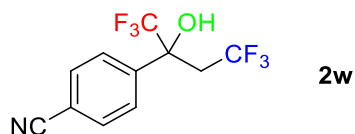
3-(1,1,1,4,4,4-Hexafluoro-2-hydroxybutan-2-yl)benzaldehyde (2t). white solid; m.p.: 98.3–102.1 °C, yield 90% (257.4 mg); ¹H NMR (400 MHz, CDCl₃) δ 9.98 (s, 1H), 8.09 (s, 1H), 7.87 (d, *J* = 7.6 Hz, 1H), 7.82 (d, *J* = 7.6 Hz, 1H), 7.56 (t, *J* = 8.0 Hz, 1H), 3.50 (s, 1H), 3.13–2.89 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 191.1, 135.5, 135.0, 131.1, 129.7, 128.3, 126.4, 123.6 (q, ¹*J*_{CF} = 276.3 Hz), 123.3 (q, ¹*J*_{CF} = 284.2 Hz), 73.6 (qd, ²*J*_{CF} = 29.4 Hz, ³*J*_{CF} = 2.0 Hz), 38.1 (q, ²*J*_{CF} = 27.8 Hz); ¹⁹F NMR (376 MHz, CDCl₃) δ –58.8 (t, *J* = 6.8 Hz, 3F), –80.7 (s, 3F); HRMS (EI): calcd for C₁₁H₈F₆O₂ [M]⁺: 286.0428, found: 286.0424.



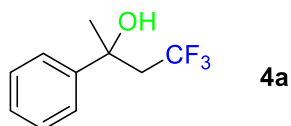
1,1,1,4,4,4-Hexafluoro-2-(3-nitrophenyl)butan-2-ol (2u). white solid; m.p.: 123.8–127.1 °C, yield 91% (275.8 mg); ^1H NMR (400 MHz, CDCl_3) δ 8.45 (s, 1H), 8.24 (d, $J = 8.4$ Hz, 1H), 7.87 (d, $J = 8.0$ Hz, 1H), 7.58 (t, $J = 8.0$ Hz, 1H), 3.13–2.89 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 147.4, 135.7, 131.2, 128.7, 123.4 (q, $^1J_{\text{CF}} = 276.2$ Hz), 123.3, 123.0 (q, $^1J_{\text{CF}} = 284.7$ Hz), 120.6, 73.5 (qd, $^2J_{\text{CF}} = 30.1$ Hz, $^3J_{\text{CF}} = 2.3$ Hz), 38.1 (q, $^2J_{\text{CF}} = 28.1$ Hz); ^{19}F NMR (376 MHz, CDCl_3) δ -58.8 (t, $J = 7.1$ Hz, 3F), -80.7 (s, 3F); HRMS (EI): calcd for $\text{C}_{10}\text{H}_7\text{F}_6\text{NO}_3$ $[\text{M}]^+$: 303.0330, found: 303.0327.



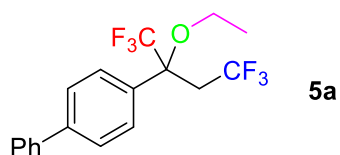
1,1,1,4,4,4-Hexafluoro-2-(4-(trifluoromethyl)phenyl)butan-2-ol (2v). yellow oil; yield 84% (273.9 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.67–7.61 (m, 4H), 3.08–2.84 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 137.4, 130.5 (q, $^2J_{\text{CF}} = 32.7$ Hz), 125.7, 123.5 (q, $^1J_{\text{CF}} = 276.1$ Hz), 124.5 (q, $^3J_{\text{CF}} = 3.7$ Hz), 123.2 (q, $^1J_{\text{CF}} = 284.7$ Hz), 122.8 (q, $^1J_{\text{CF}} = 270.7$ Hz), 73.7 (qd, $^2J_{\text{CF}} = 29.2$ Hz, $^3J_{\text{CF}} = 1.9$ Hz), 38.2 (q, $^2J_{\text{CF}} = 27.9$ Hz); ^{19}F NMR (376 MHz, CDCl_3) δ -58.9 (t, $J = 7.5$ Hz, 3F), -62.9 (s, 3F), -80.6 (s, 3F); HRMS (EI): calcd for $\text{C}_{11}\text{H}_7\text{F}_9\text{O}$ $[\text{M}]^+$: 326.0353, found: 326.0350.



4-(1,1,1,4,4,4-Hexafluoro-2-hydroxybutan-2-yl)benzotrile (2w). white solid; m.p.: 178.7–180.2 °C, yield 88% (249.1 mg); ^1H NMR (400 MHz, $(\text{CD}_3)_2\text{CO}$) δ 7.86 (d, $J = 8.4$ Hz, 2H), 7.75 (d, $J = 8.4$ Hz, 2H), 6.46 (s, 1H), 3.50–3.39 (m, 1H), 3.09–2.98 (m, 1H); ^{13}C NMR (100 MHz, $(\text{CD}_3)_2\text{CO}$) δ 140.7, 131.9, 127.8, 125.2 (q, $^1J_{\text{CF}} = 275.7$ Hz), 124.8 (q, $^1J_{\text{CF}} = 284.9$ Hz), 118.0, 112.8, 74.4 (qd, $^2J_{\text{CF}} = 28.9$ Hz, $^3J_{\text{CF}} = 2.3$ Hz), 37.8 (q, $^2J_{\text{CF}} = 27.7$ Hz); ^{19}F NMR (376 MHz, $(\text{CD}_3)_2\text{CO}$) δ -59.2 (t, $J = 7.1$ Hz, 3F), -80.9 (s, 3F); HRMS (EI): calcd for $\text{C}_{11}\text{H}_7\text{F}_6\text{NO}$ $[\text{M}]^+$: 283.0432, found: 283.0429.



4,4,4-Trifluoro-2-phenylbutan-2-ol (4a, CAS: 1417820-89-3).² colorless oil; yield 74% (151.0 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.38 (d, $J = 8.0$ Hz, 2H), 7.29 (t, $J = 7.6$ Hz, 2H), 7.20 (t, $J = 7.2$ Hz, 1H), 2.63–2.50 (m, 2H), 2.03 (s, 1H), 1.63 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 145.2, 127.4, 126.4, 123.4, 124.8 (q, $^1J_{\text{CF}} = 276.7$ Hz), 70.9 (q, $^3J_{\text{CF}} = 2.0$ Hz), 45.5 (q, $^2J_{\text{CF}} = 25.6$ Hz), 28.6; ^{19}F NMR (376 MHz, CDCl_3) δ -60.2 (t, $J = 7.1$ Hz, 3F).



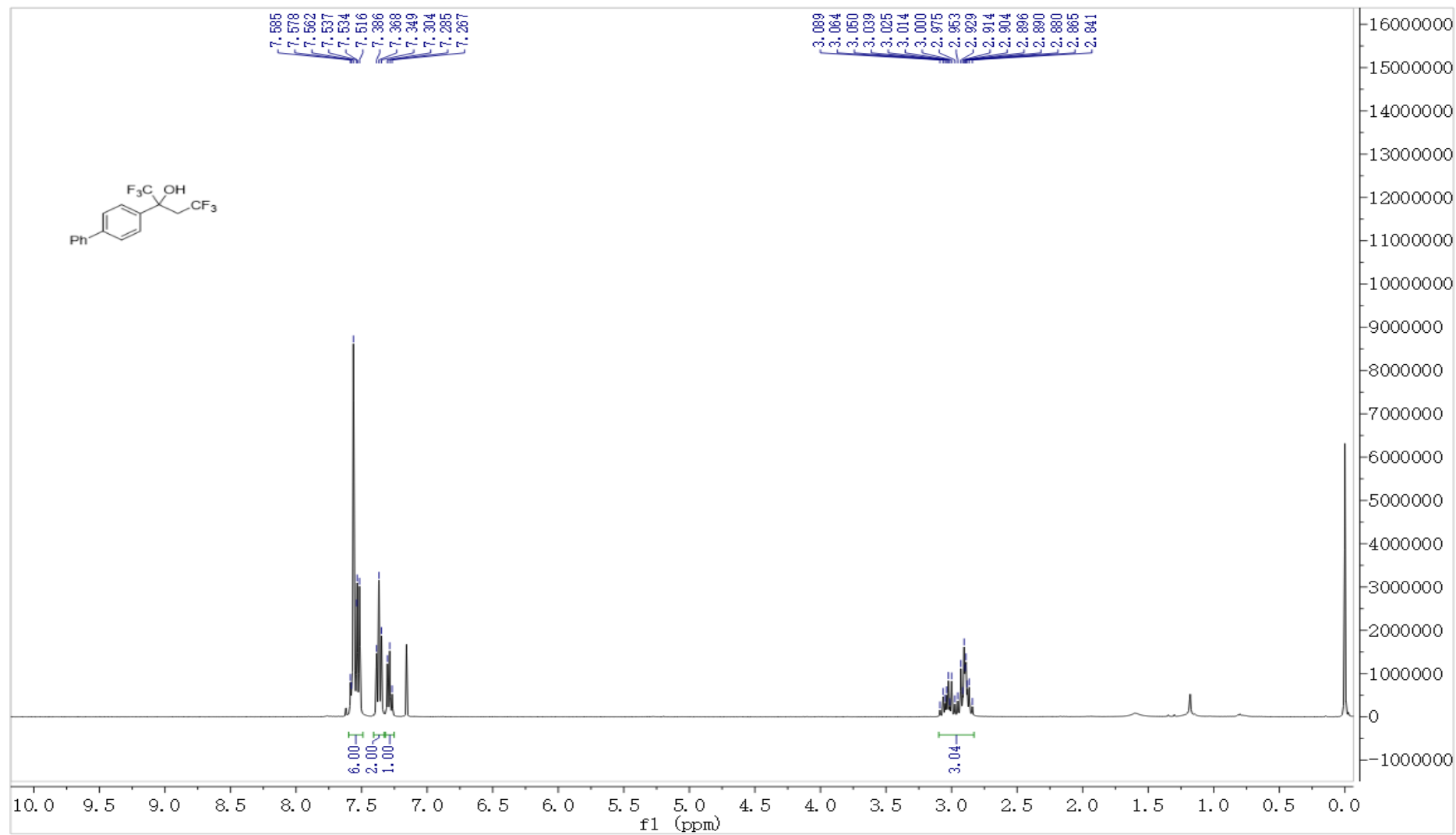
4-(2-Ethoxy-1,1,1,4,4,4-hexafluorobutan-2-yl)-1,1'-biphenyl (5a). colorless oil; yield 92% (333.8 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.56–7.51 (m, 6H), 7.36 (t, $J = 7.6$ Hz, 2H), 7.28 (t, $J = 7.2$ Hz, 1H), 3.62 (q, $J = 6.8$ Hz, 2H), 3.05–2.78 (m, 2H), 1.25 (t, $J = 6.8$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 140.7, 139.1, 132.4, 127.8, 126.7, 126.3, 126.1, 126.0, 123.6 (q, $^1J_{\text{CF}} = 288.5$ Hz), 123.4 (q, $^1J_{\text{CF}} = 276.2$ Hz), 78.2 (qd, $^2J_{\text{CF}} = 27.1$ Hz, $^3J_{\text{CF}} = 1.8$ Hz), 60.1, 36.5 (q, $^2J_{\text{CF}} = 29.1$ Hz), 14.3; ^{19}F NMR (376 MHz, CDCl_3) δ -59.2 (q, $J = 7.1$ Hz, 3F), -72.6 (s, 3F); HRMS (EI): calcd for $\text{C}_{18}\text{H}_{16}\text{F}_6\text{O}$ $[\text{M}]^+$: 362.1105, found: 362.1111.

8. Reference:

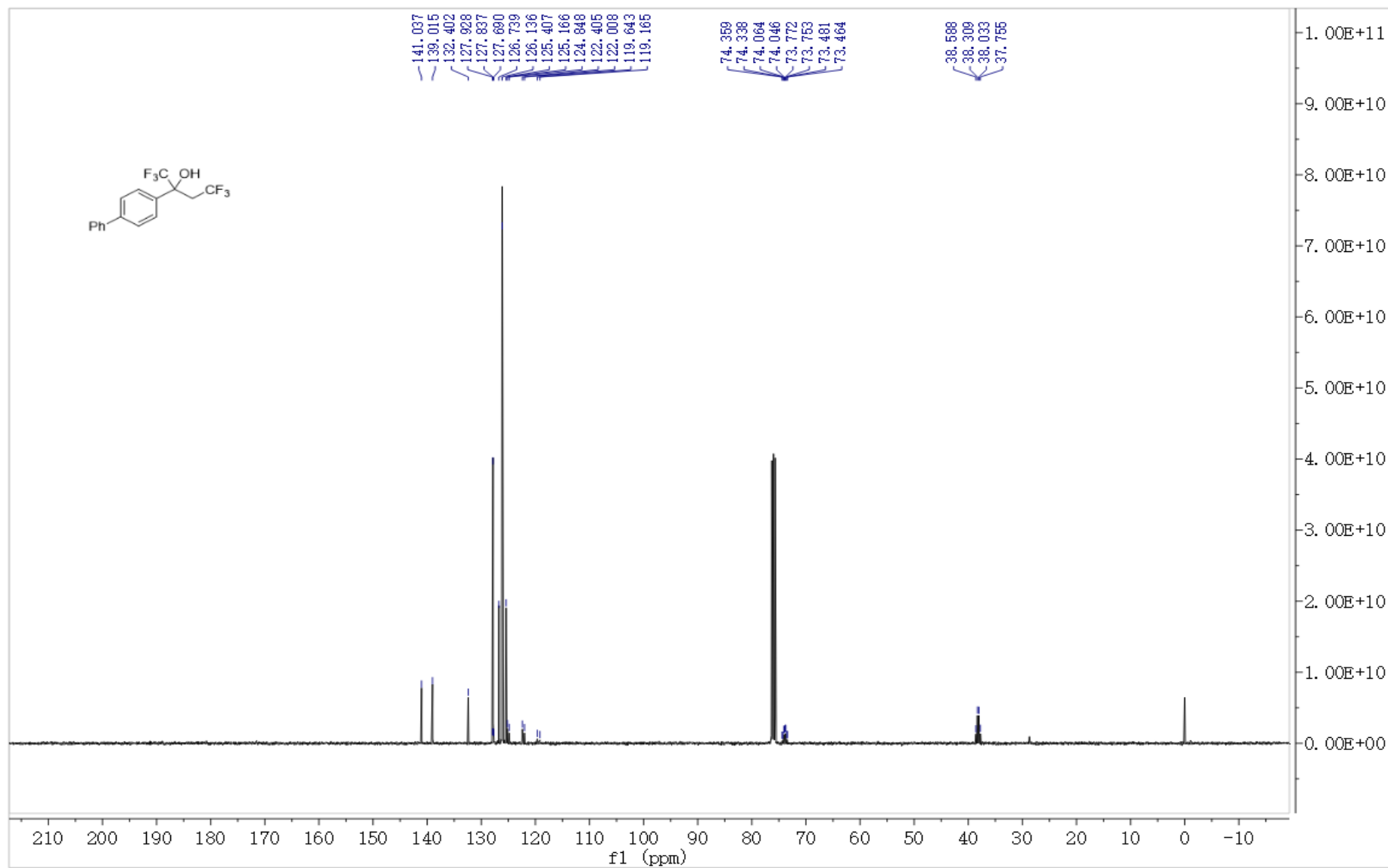
1. Y.-Q., Guo, Y.-P. Cao, H.-J. Song, Y.-X. Liu and Q.-M. Wang, *Chem. Commun.*, 2021, **57**, 9768–9771.
2. W.-G. Shen, Q.-Y. Wu, X.-Y. Gong, G.-Z. Ao and F. Liu, *Green Chem.*, 2019, **21**, 2983–2987.

9. ^1H , ^{13}C , ^{19}F NMR and HRMS (EI) spectra of the target compounds

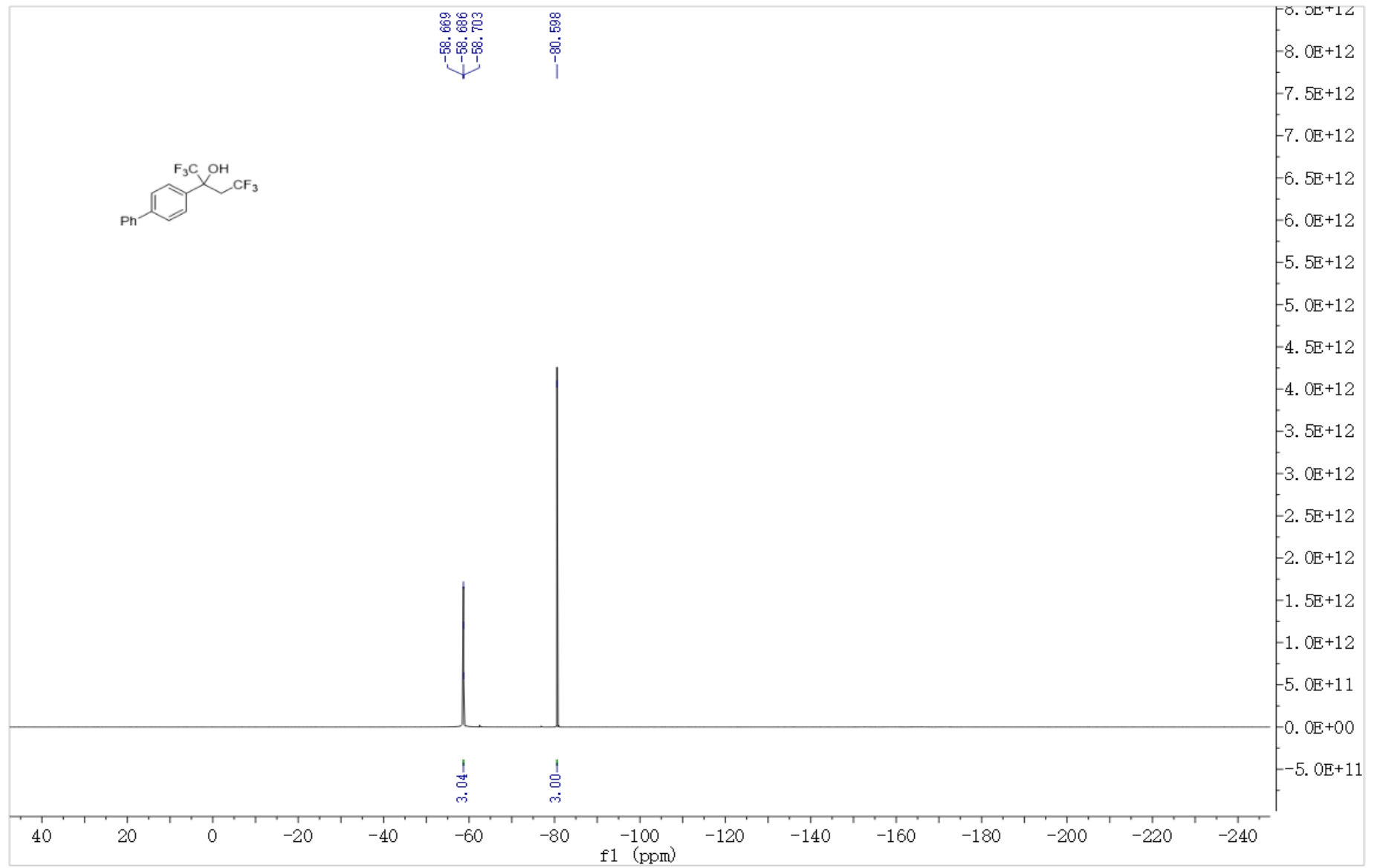
^1H NMR spectrum of 2a



¹³C NMR spectrum of 2a



¹⁹F NMR spectrum of 2a



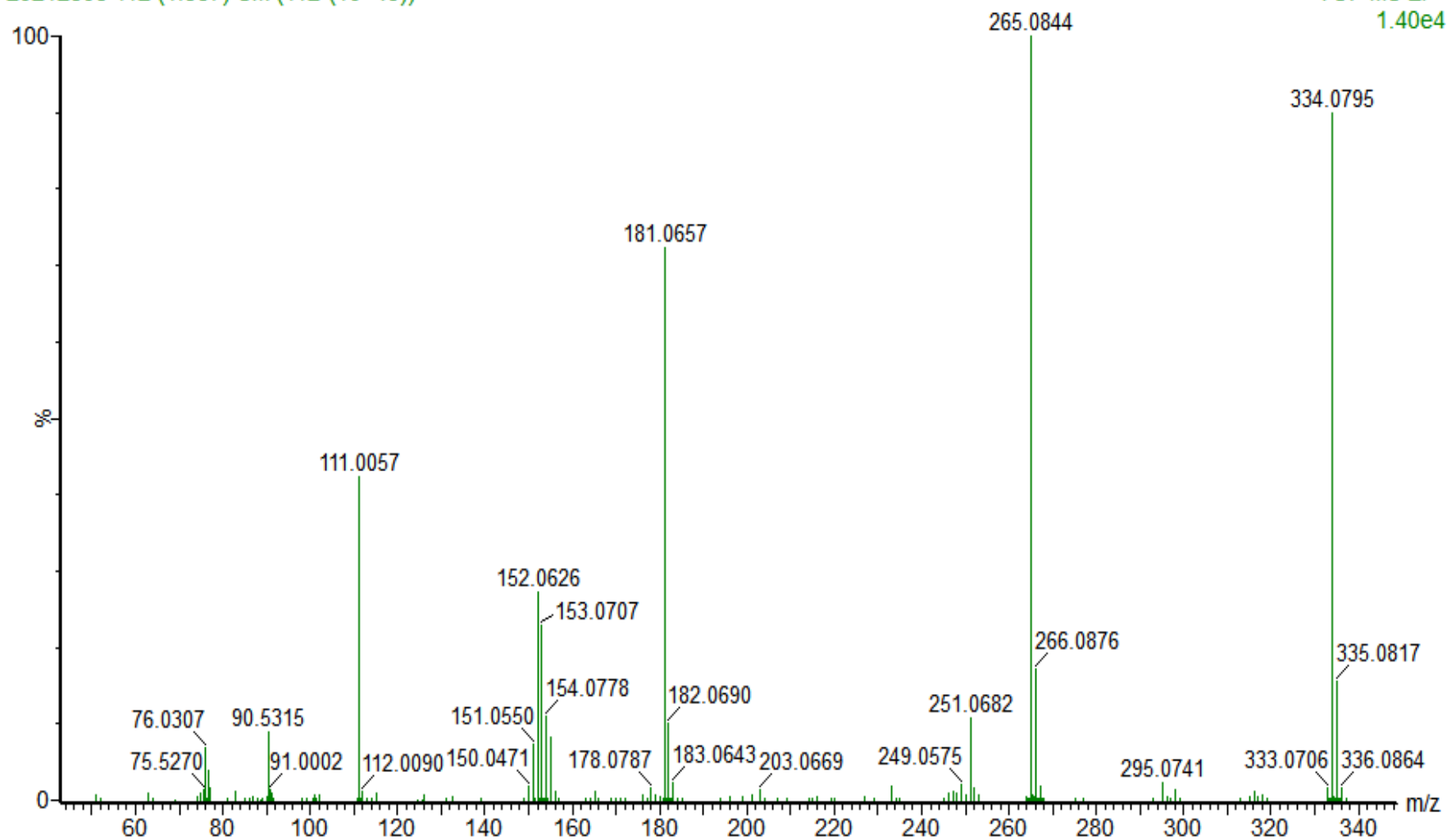
HRMS (EI) spectrum of 2a

CS-LC-P-334

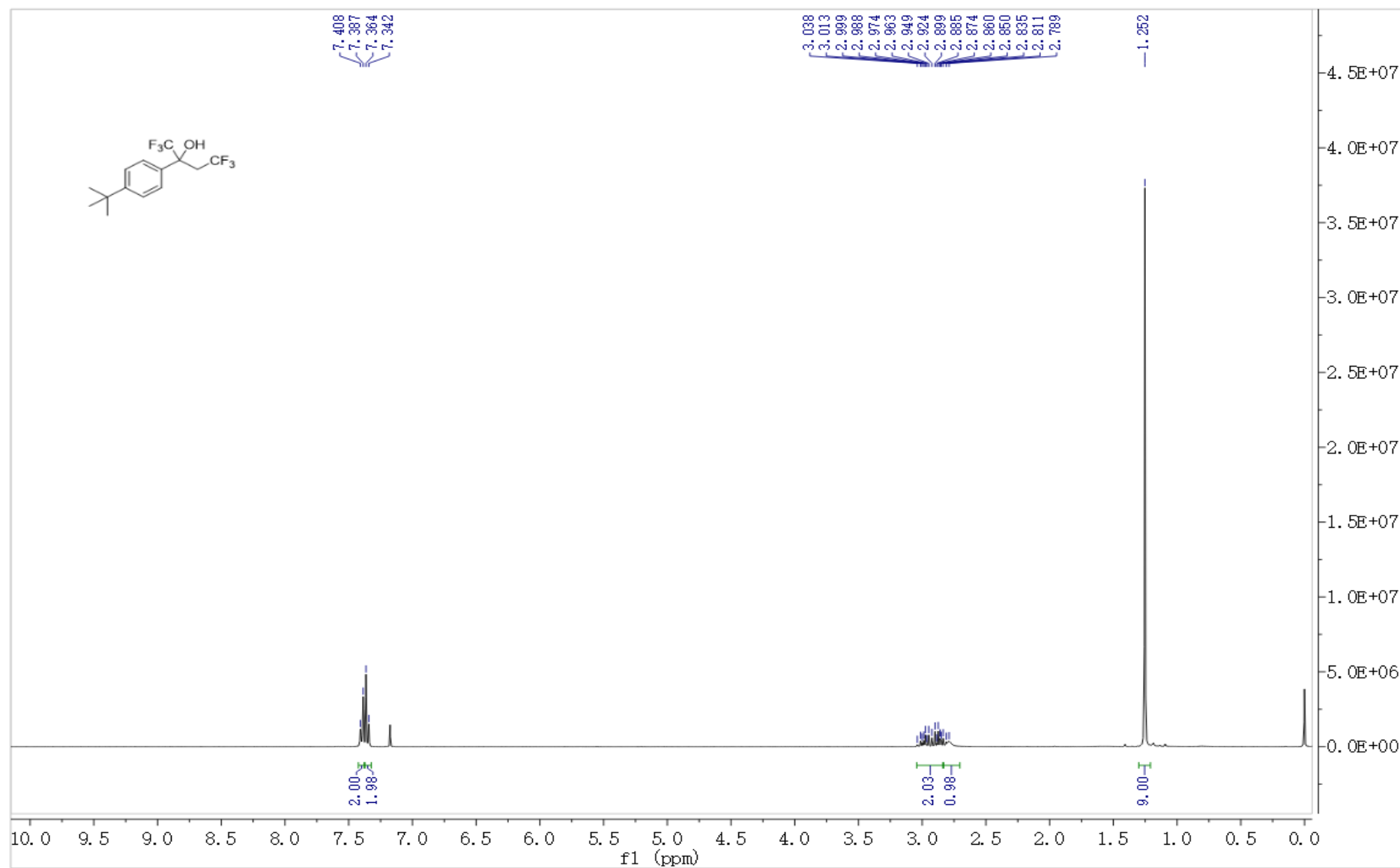
Waters GCT Premier

20212808 112 (1.867) Cm (112-(10+43))

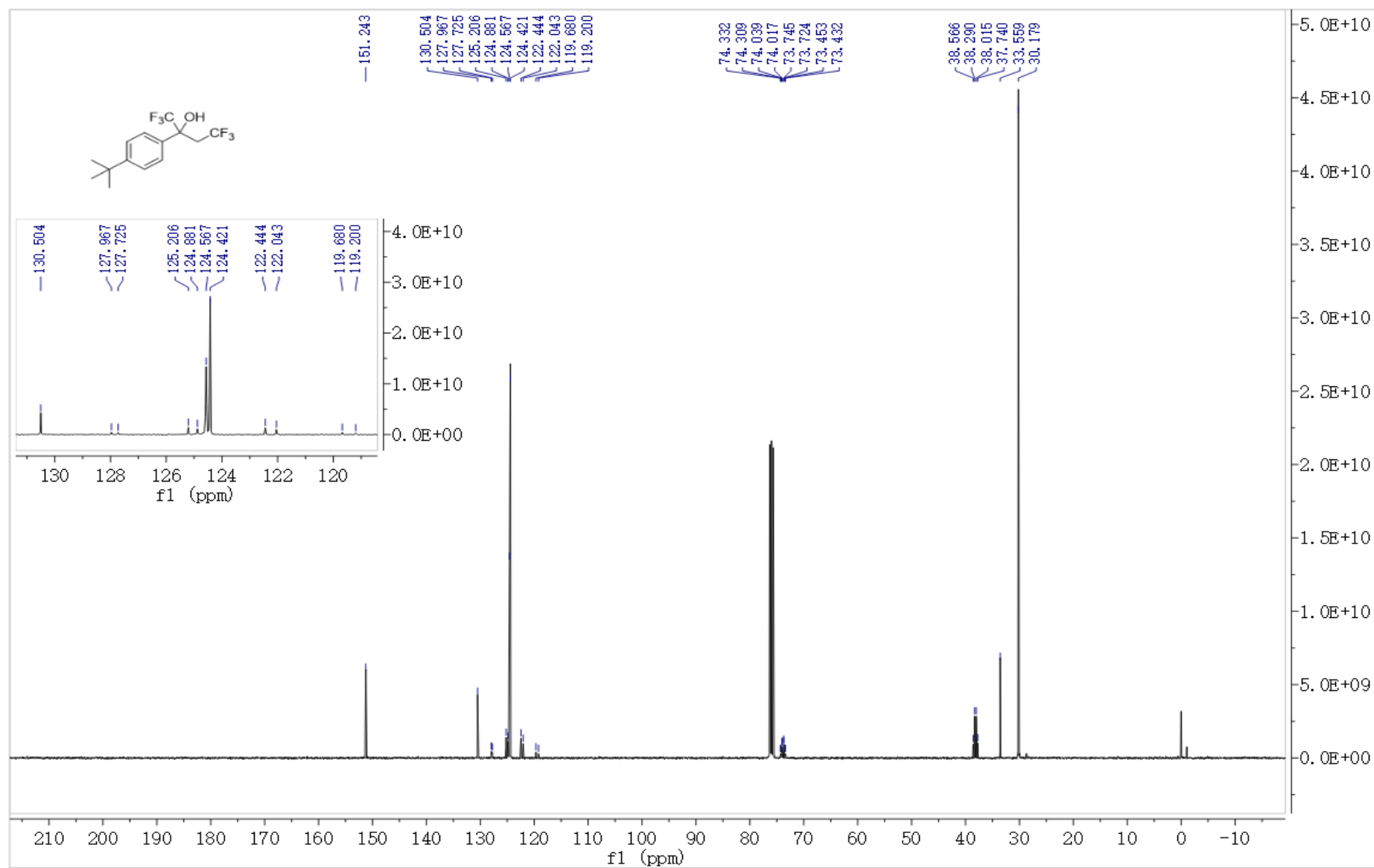
TOF MS EI+
1.40e4



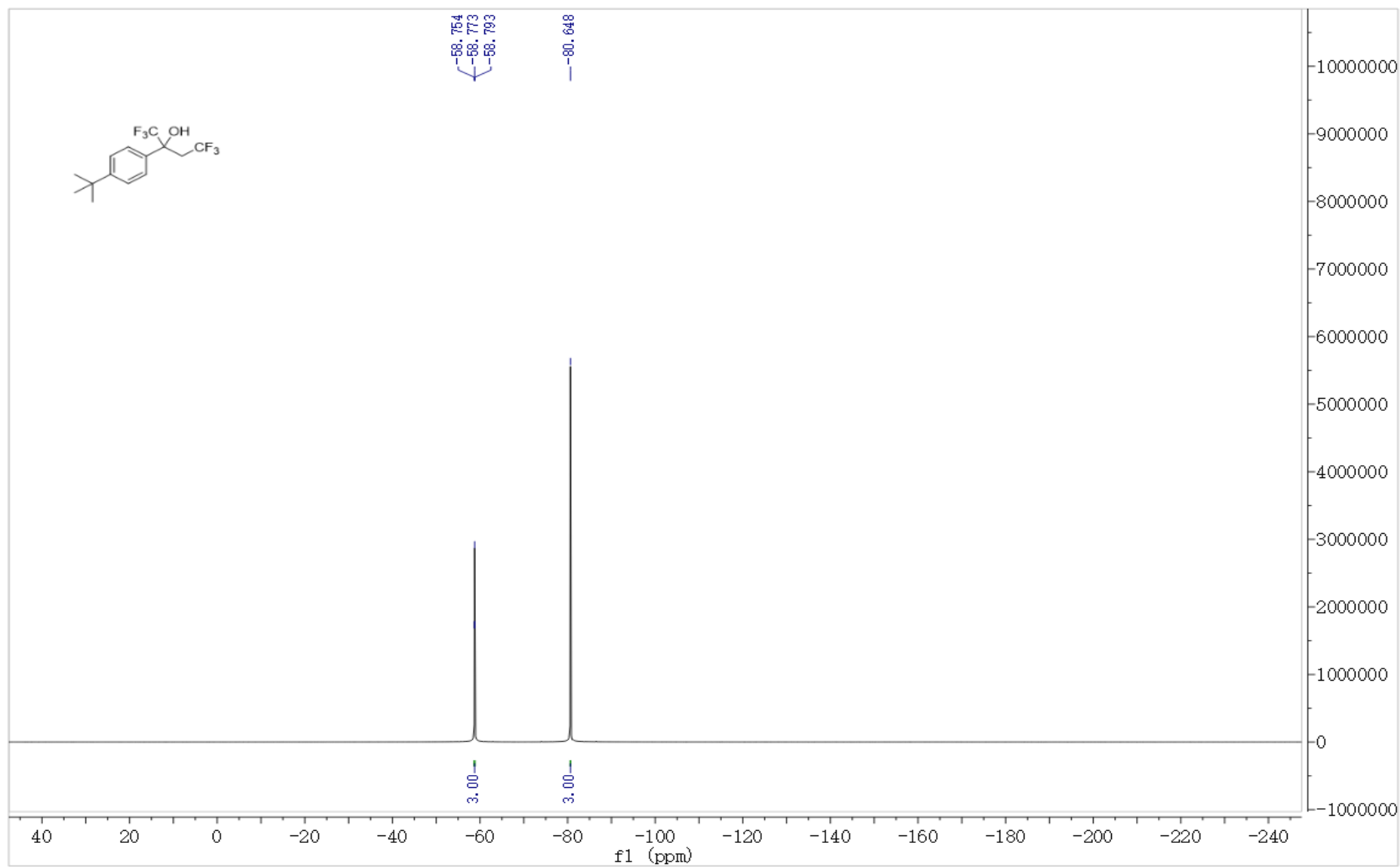
¹H NMR spectrum of 2b



¹³C NMR spectrum of 2b



¹⁹F NMR spectrum of 2b



HRMS (EI) spectrum of 2b

CS-LC-P-314

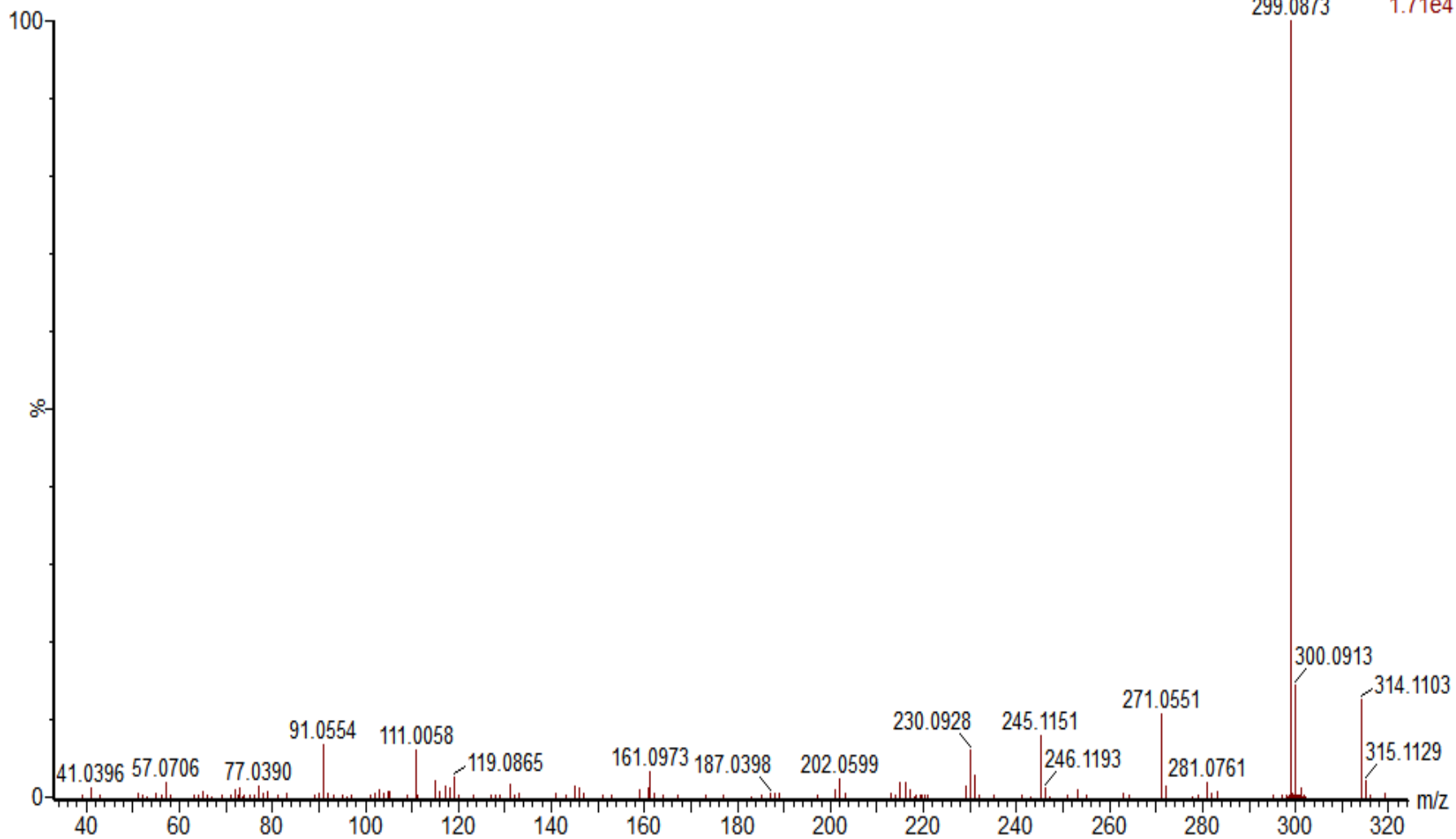
Waters GCT Premier

2022030 258 (4.300) Cm (258-(41+392))

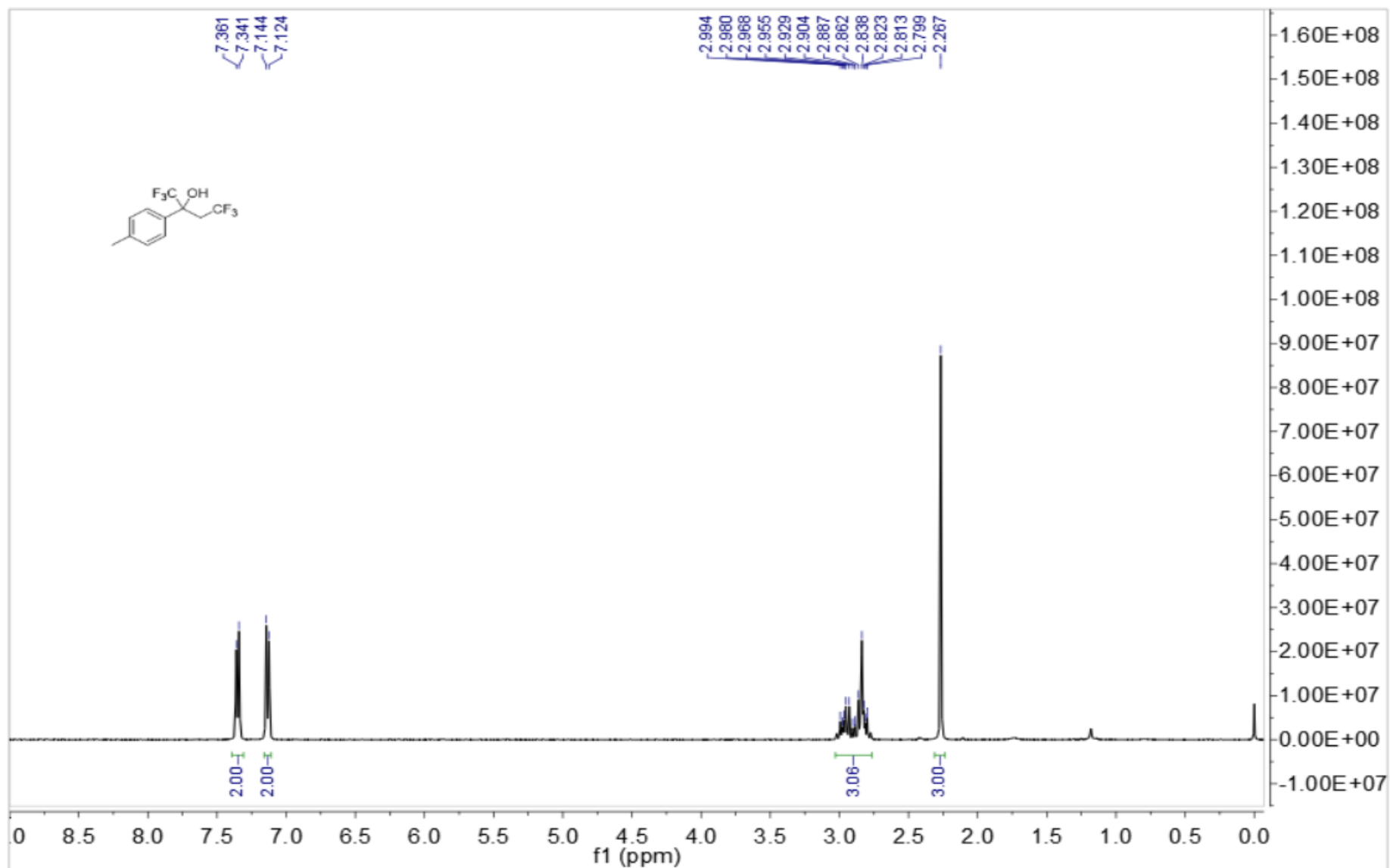
TOF MS EI+

299.0873

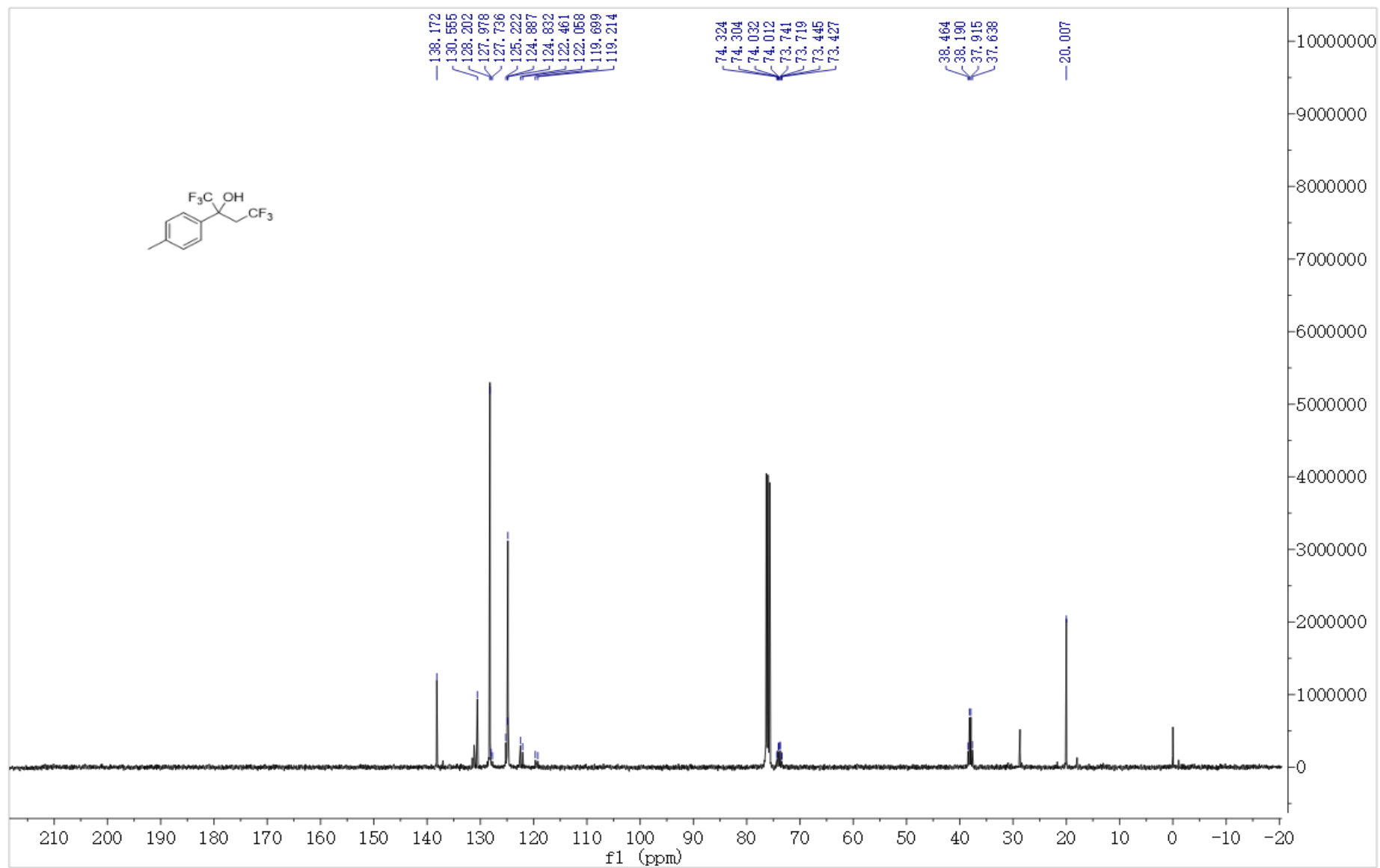
1.71e4



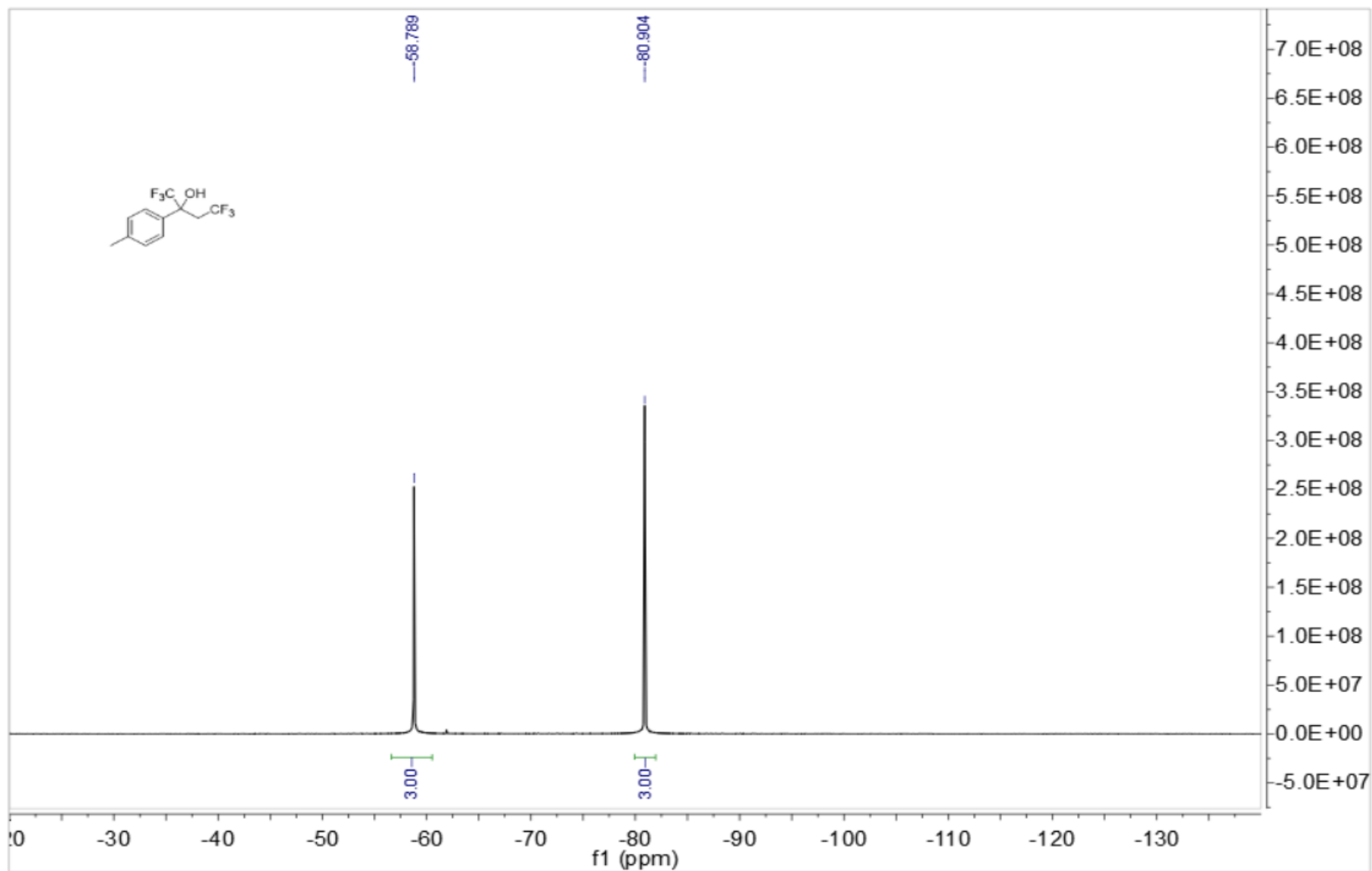
¹H NMR spectrum of 2c



¹³C NMR spectrum of 2c



¹⁹F NMR spectrum of 2c



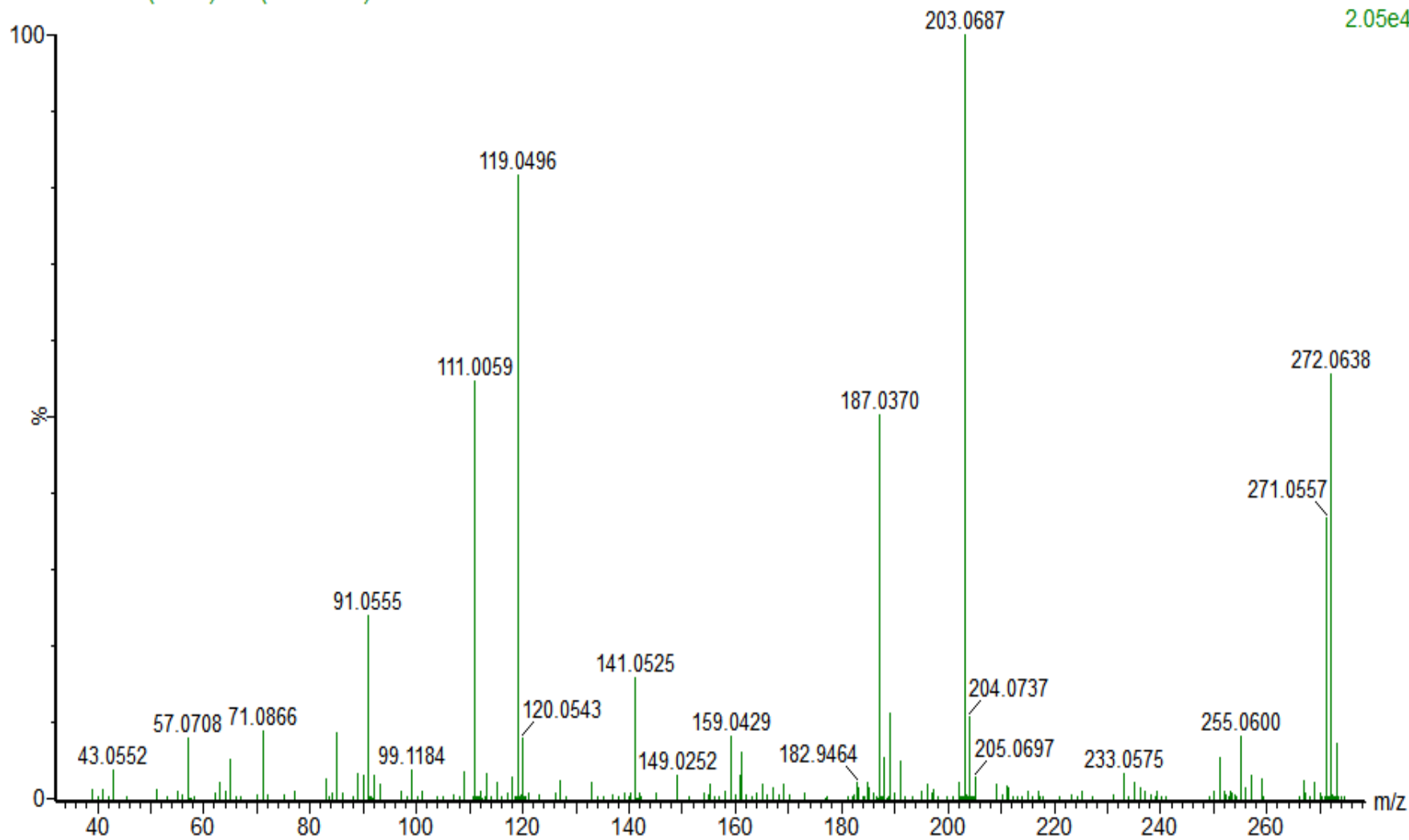
HRMS (EI) spectrum of 2c

CS-LC-P-272

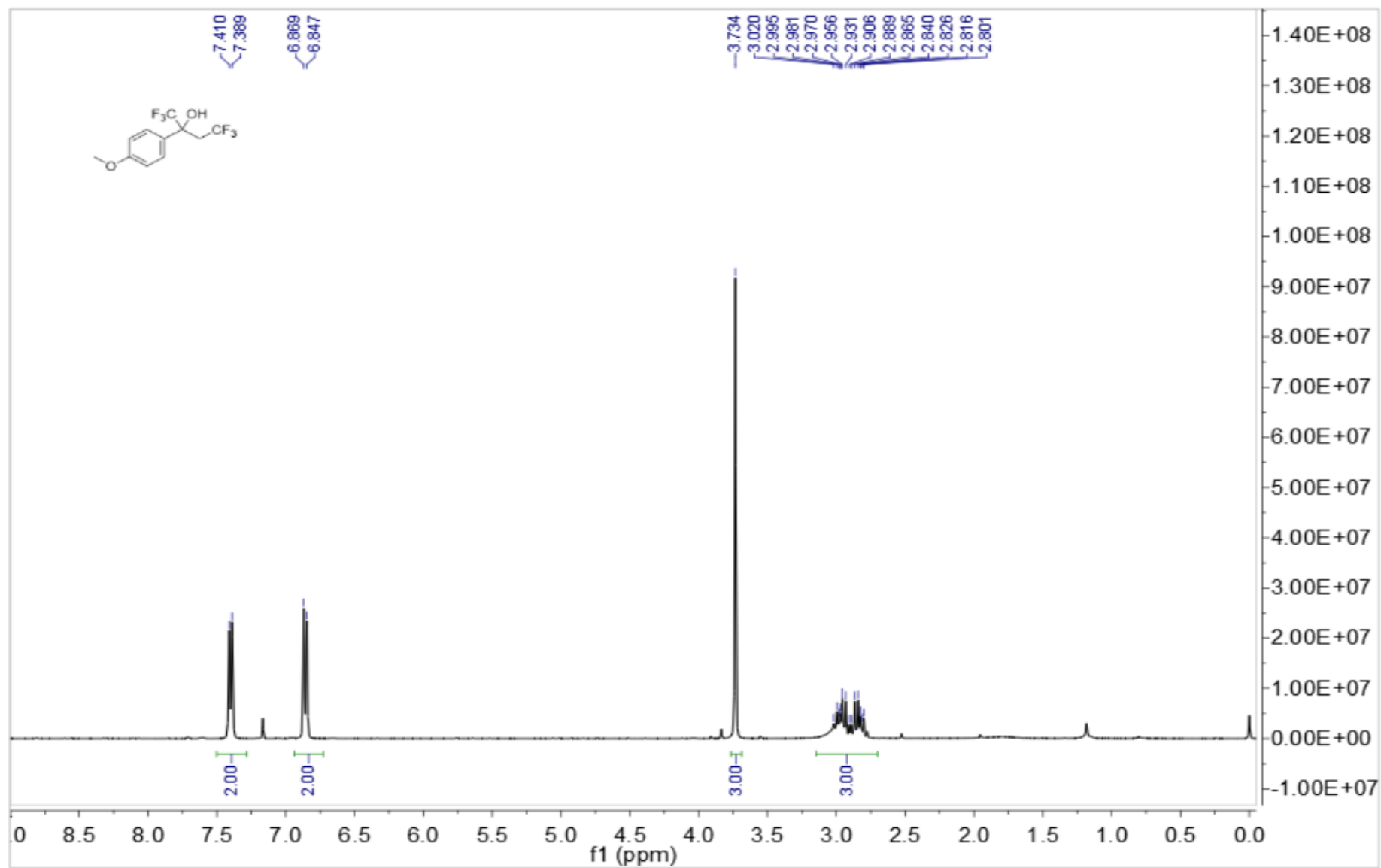
20220484 311 (5.185) Cm (311-22:26)

Waters GCT Premier

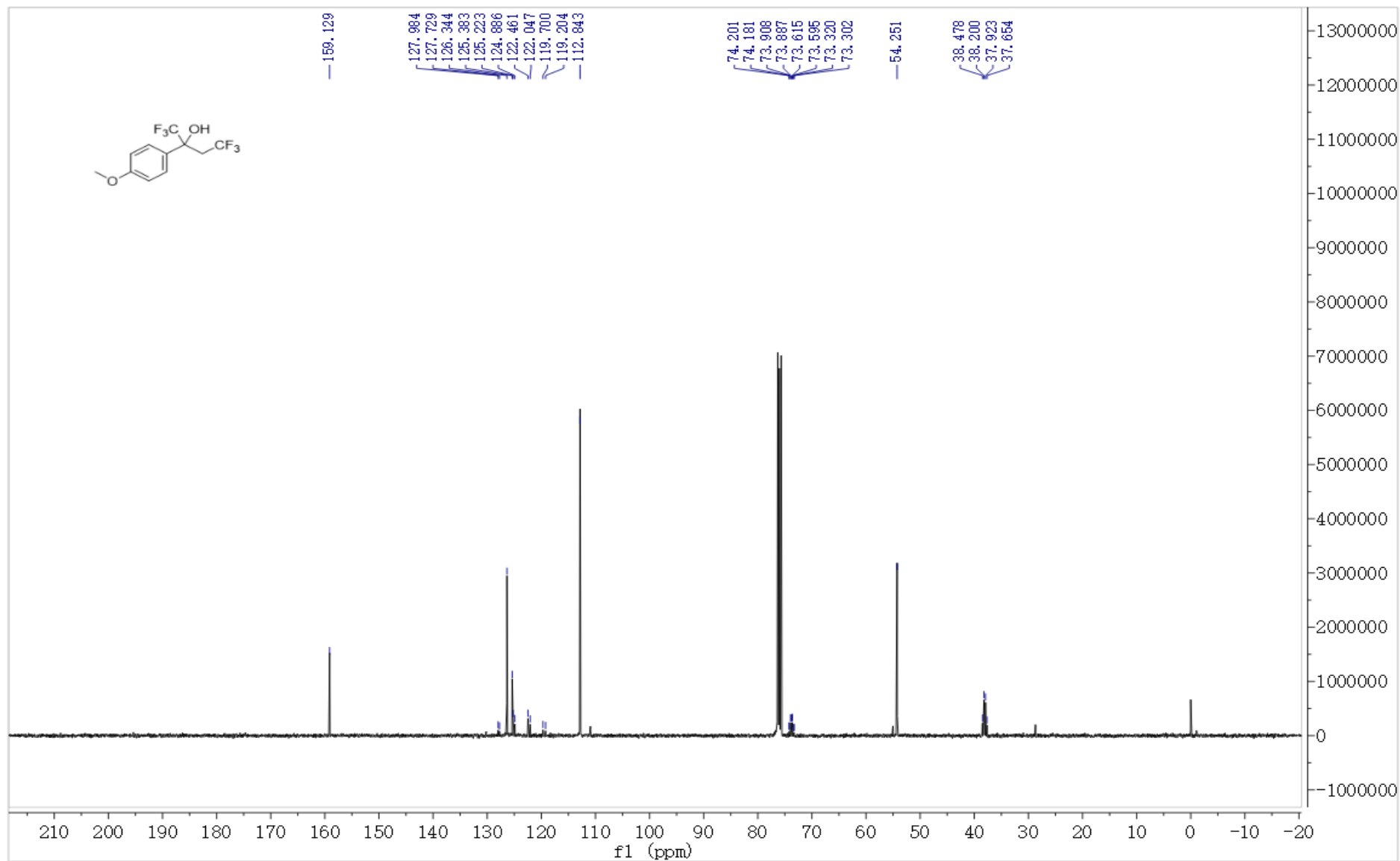
TOF MS EI+
2.05e4



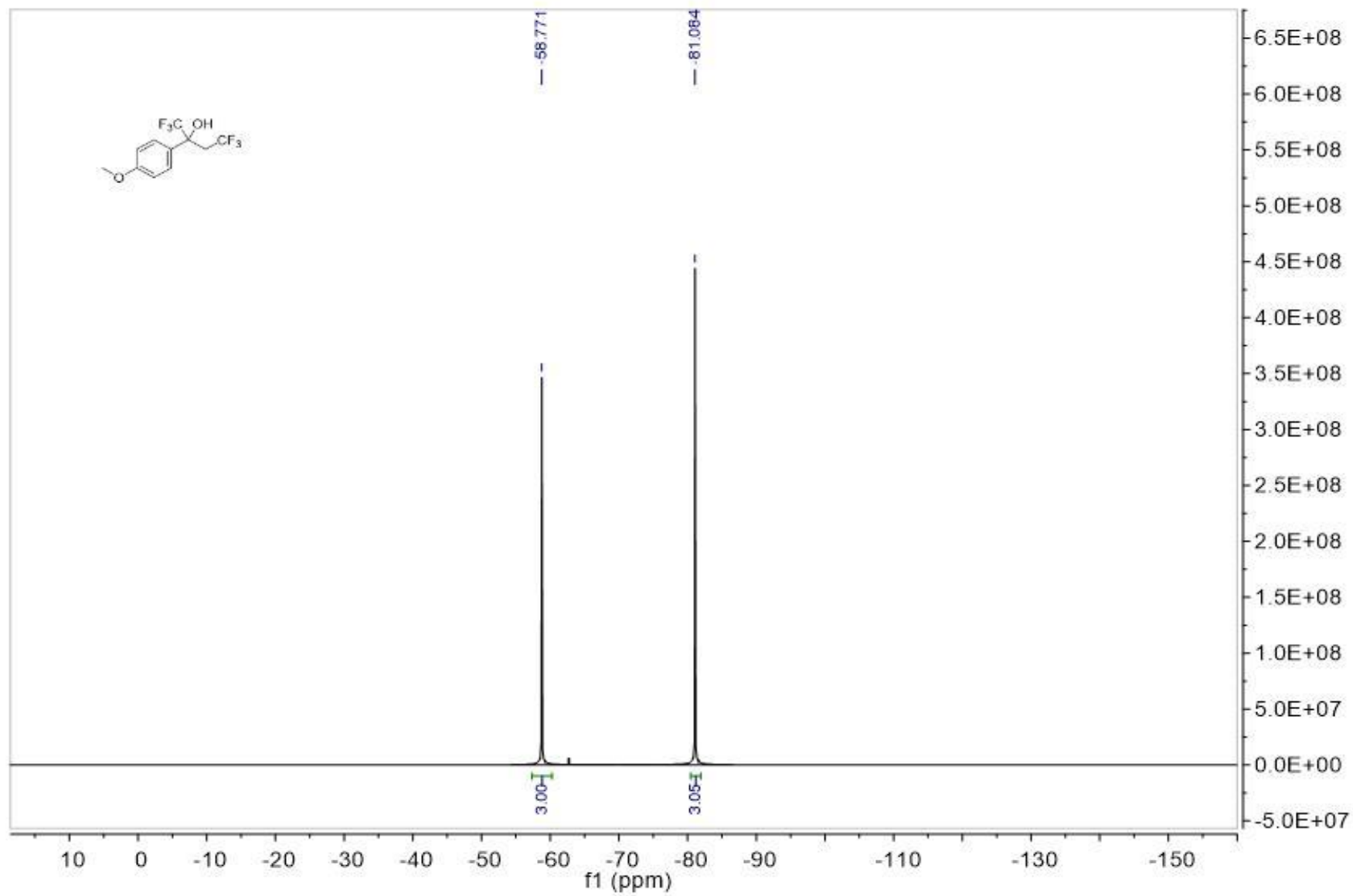
¹H NMR spectrum of 2d



¹³C NMR spectrum of 2d



¹⁹F NMR spectrum of 2d



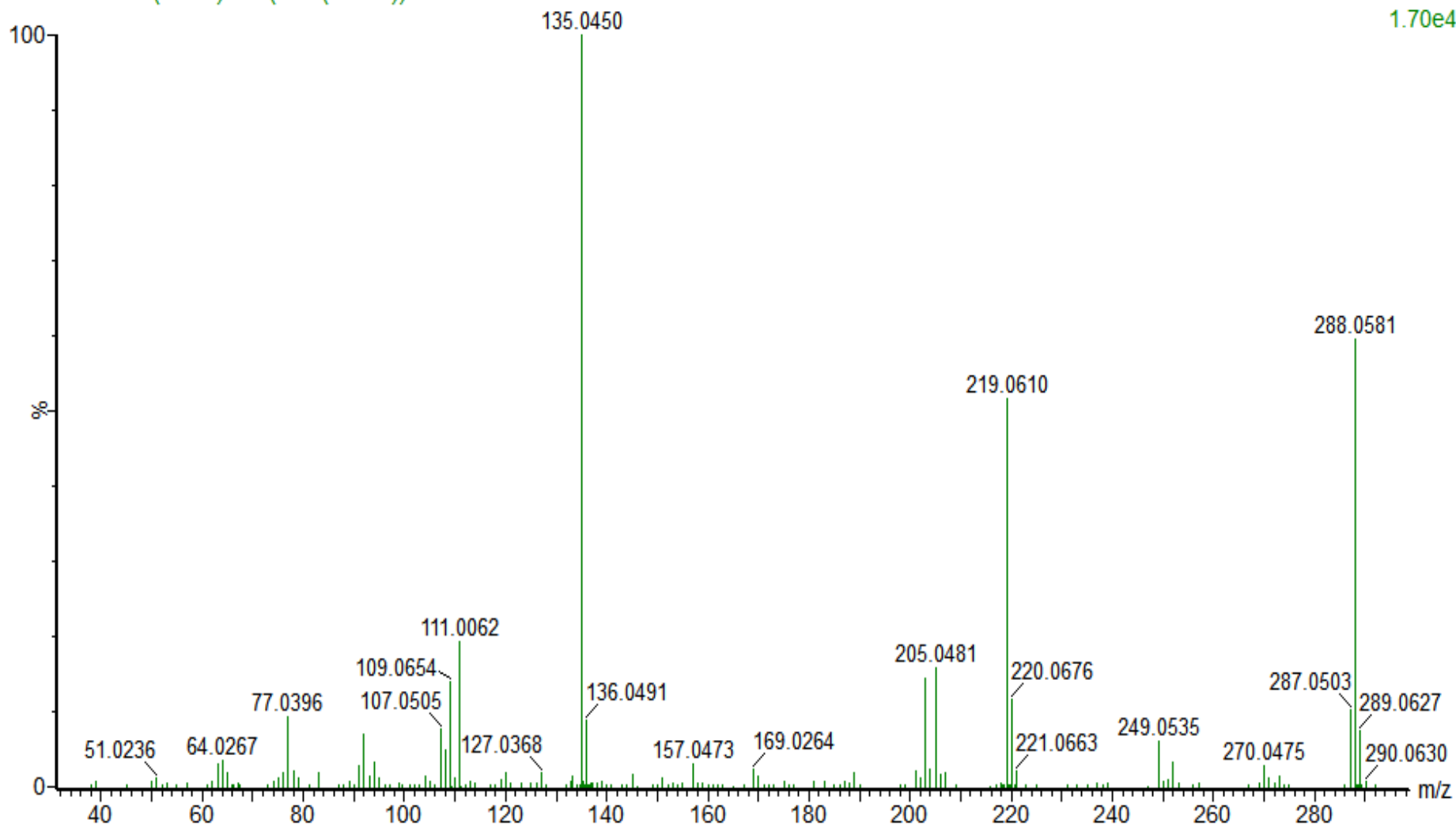
HRMS (EI) spectrum of 2d

CS-LC-P-288

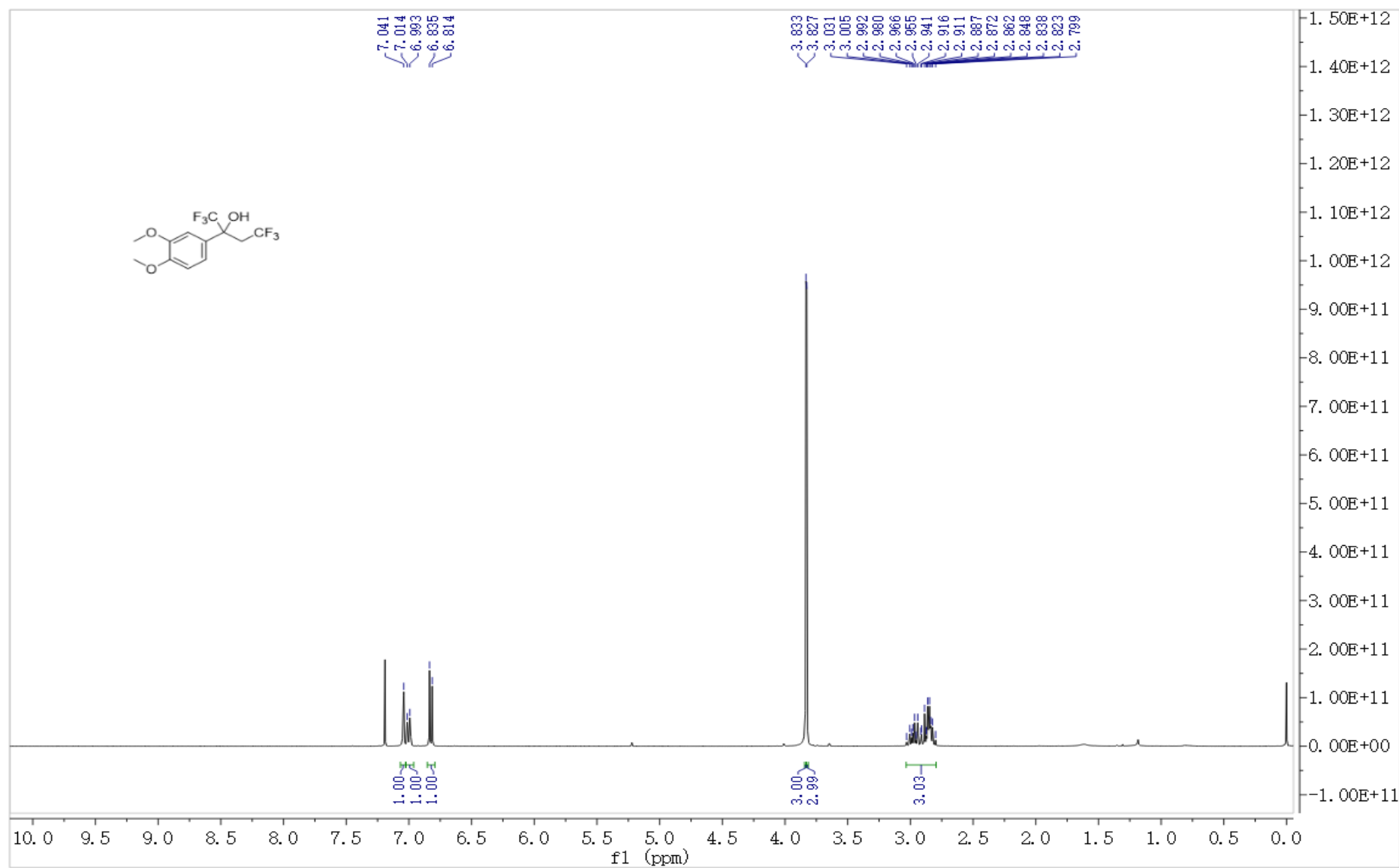
Waters GCT Premier

20220310 121 (2.017) Cm (121-(33+34))

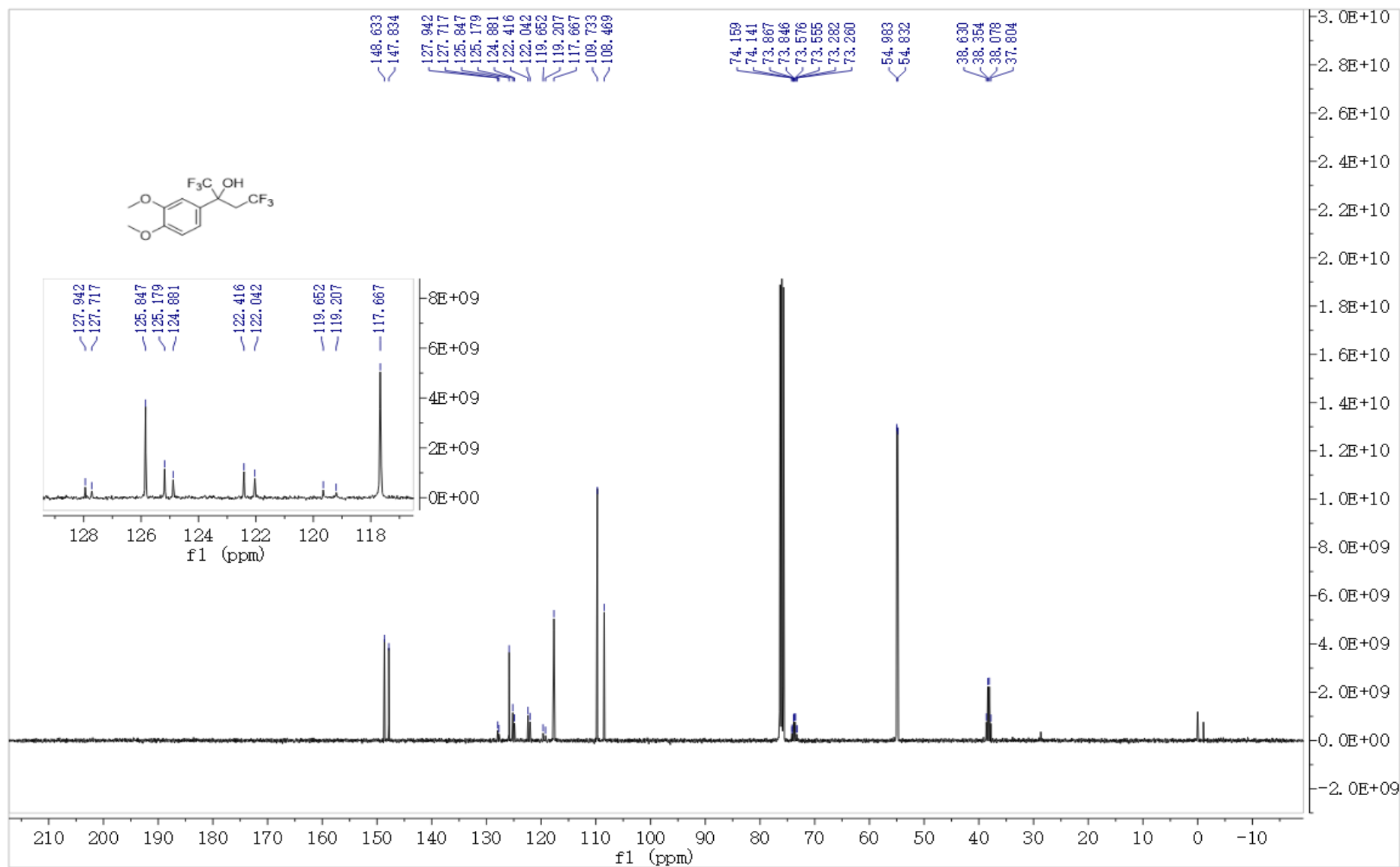
TOF MS EI+
1.70e4



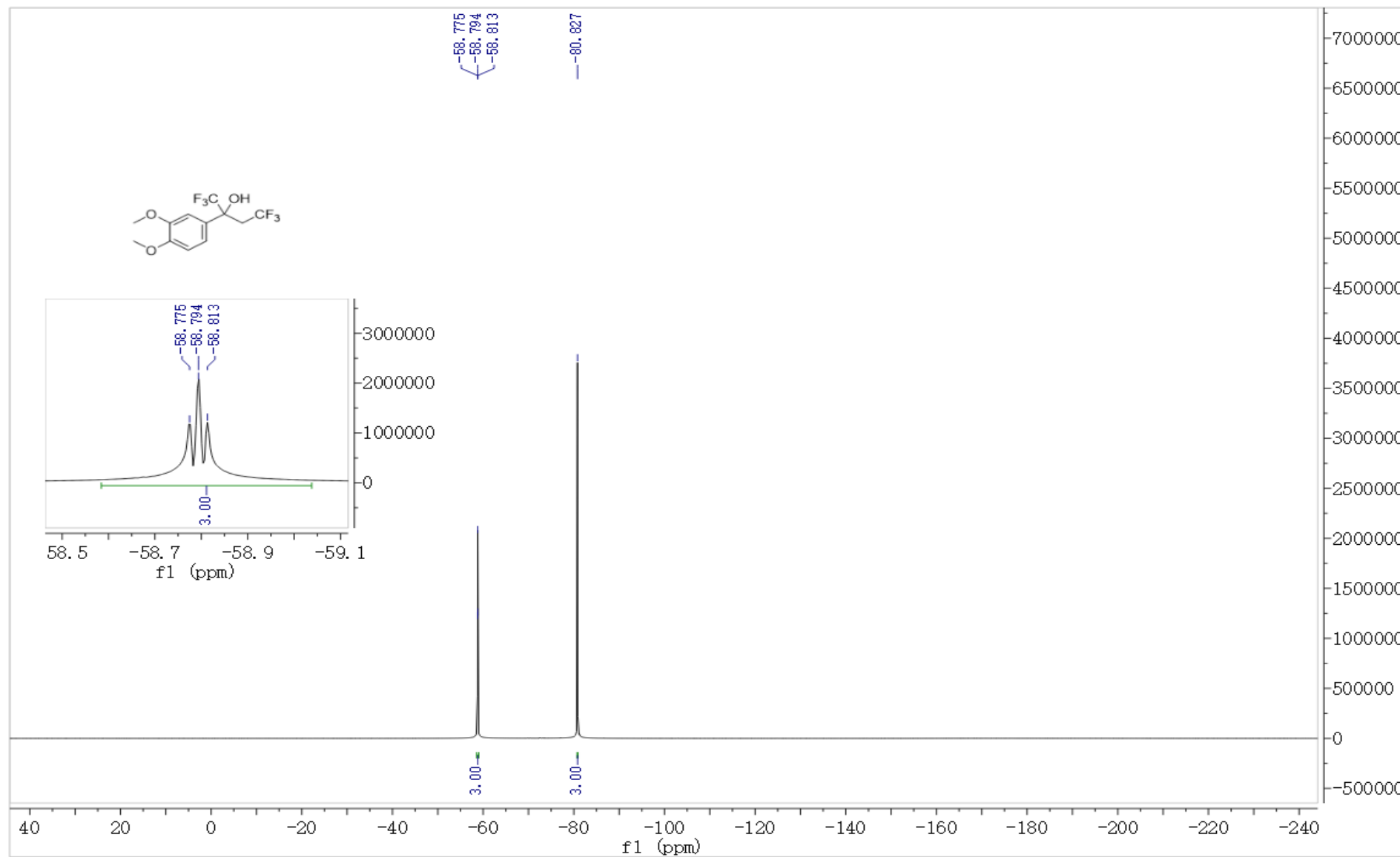
¹H NMR spectrum of 2e



¹³C NMR spectrum of 2e



¹⁹F NMR spectrum of 2e

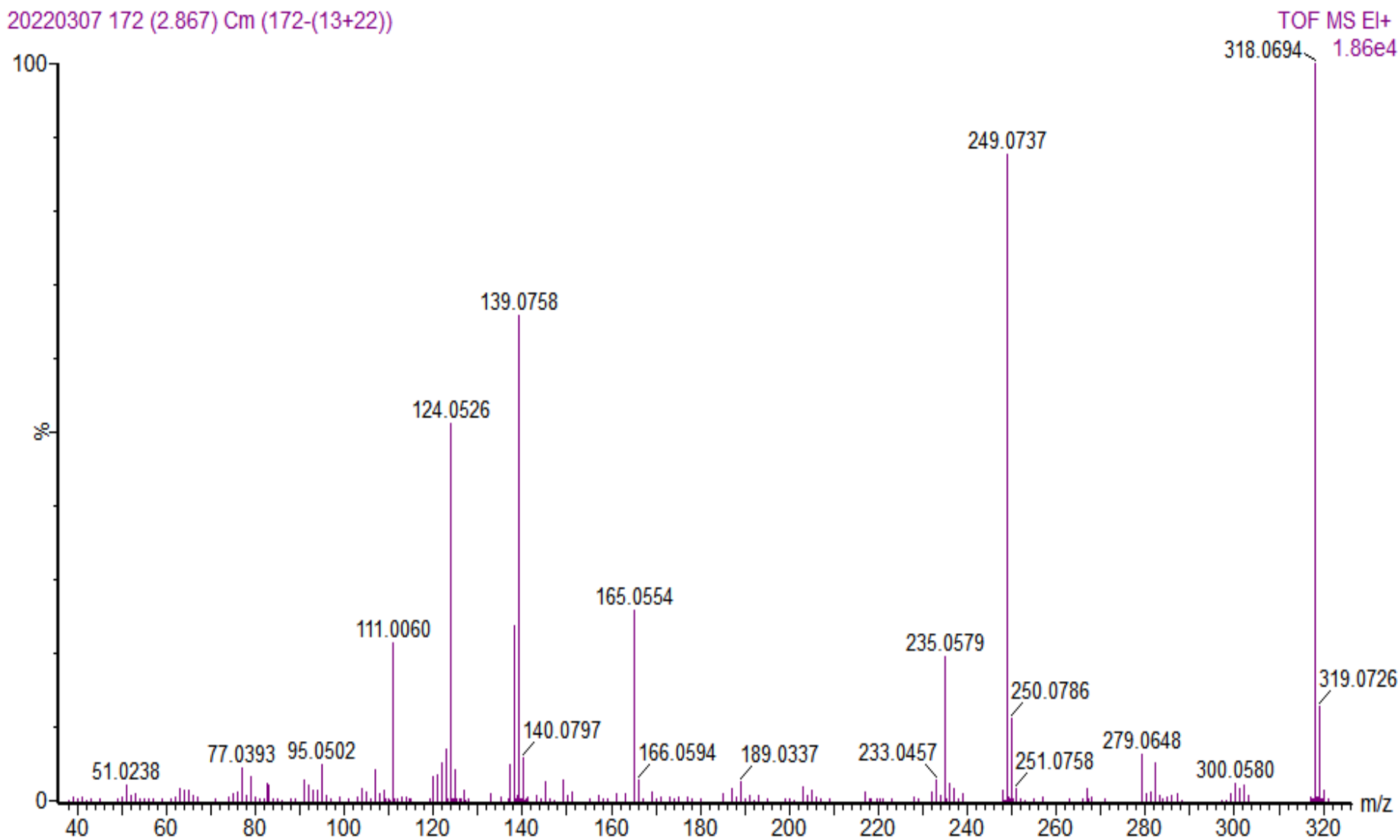


HRMS (EI) spectrum of 2e

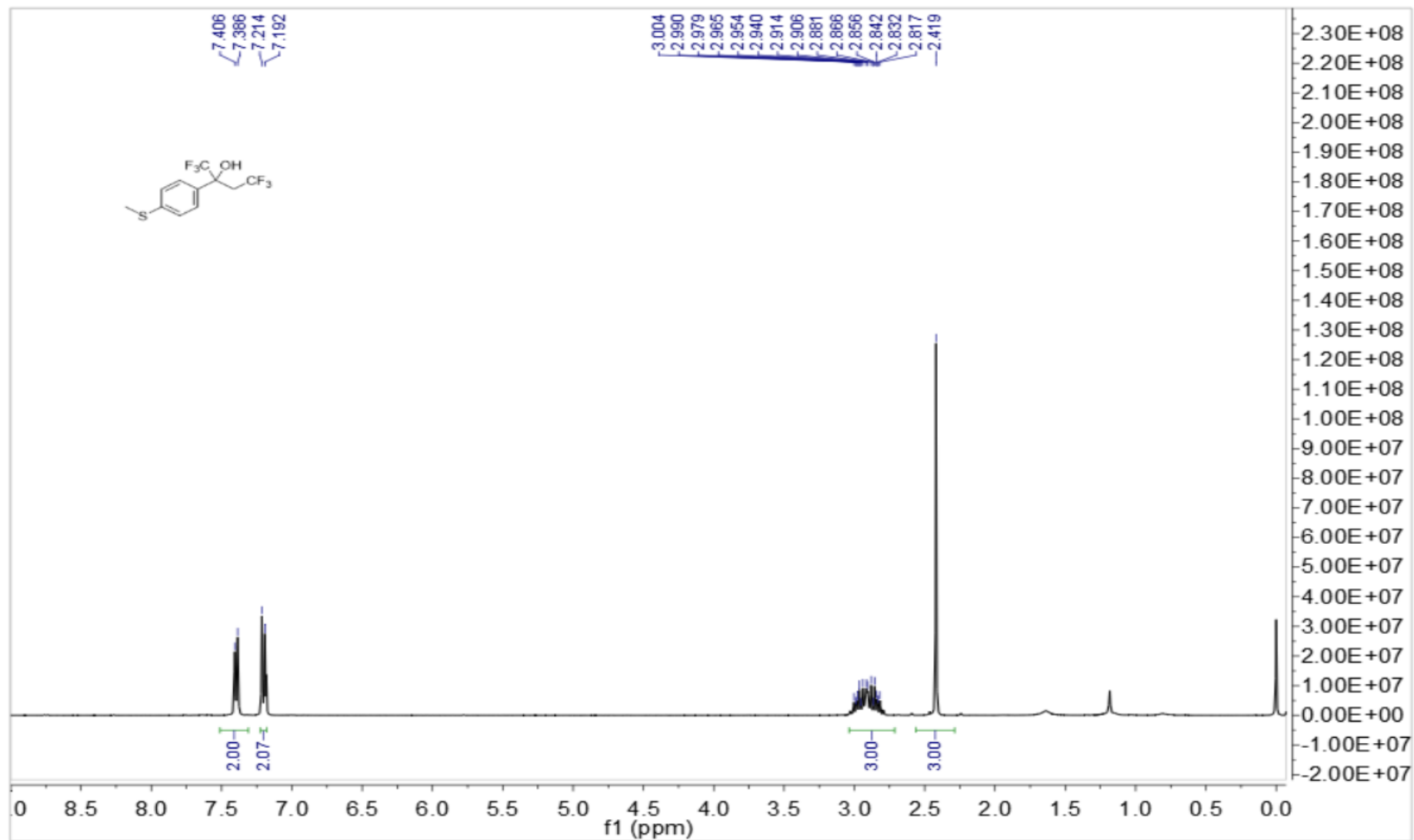
CS-LC-318

20220307 172 (2.867) Cm (172-(13+22))

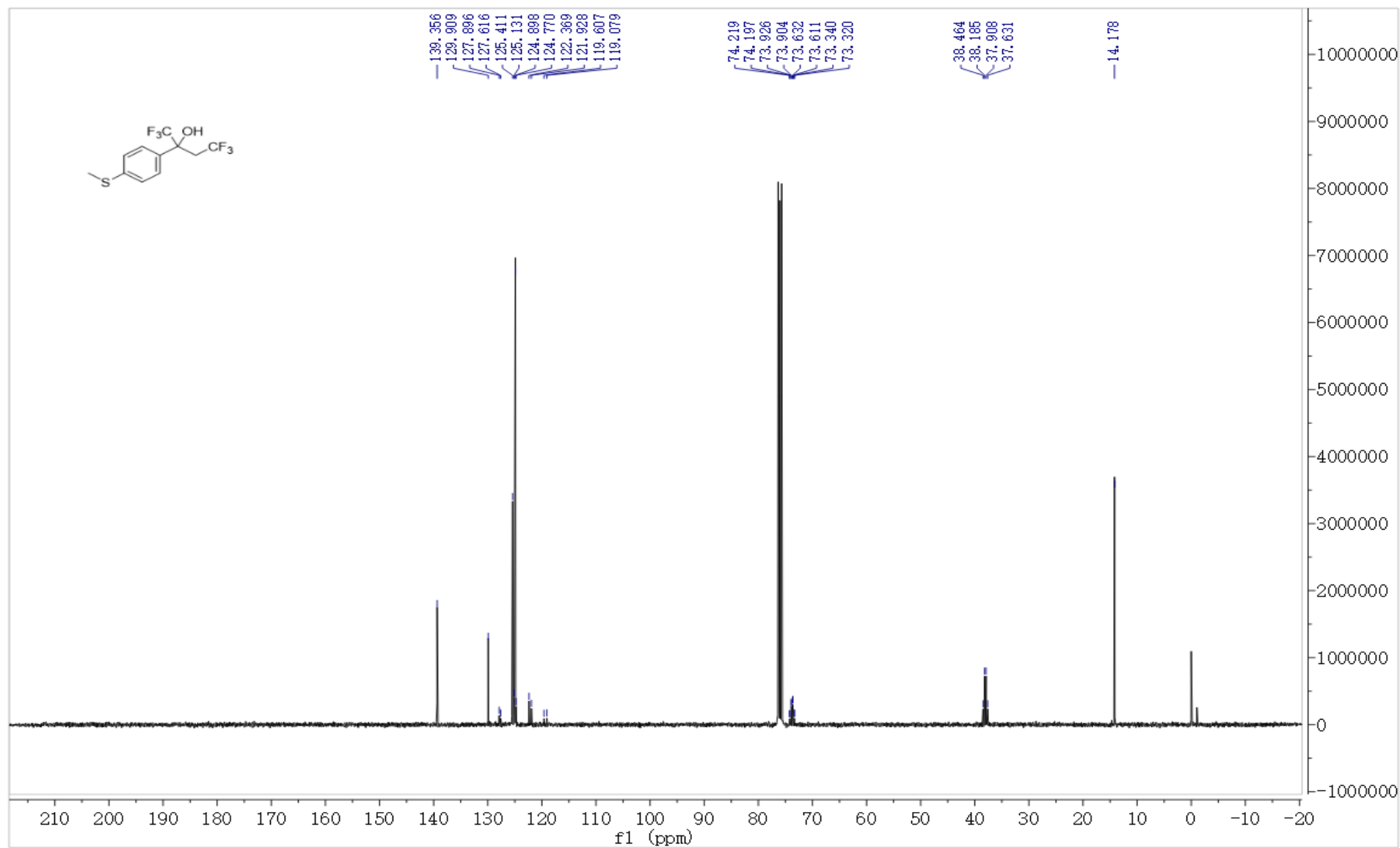
Waters GCT Premier



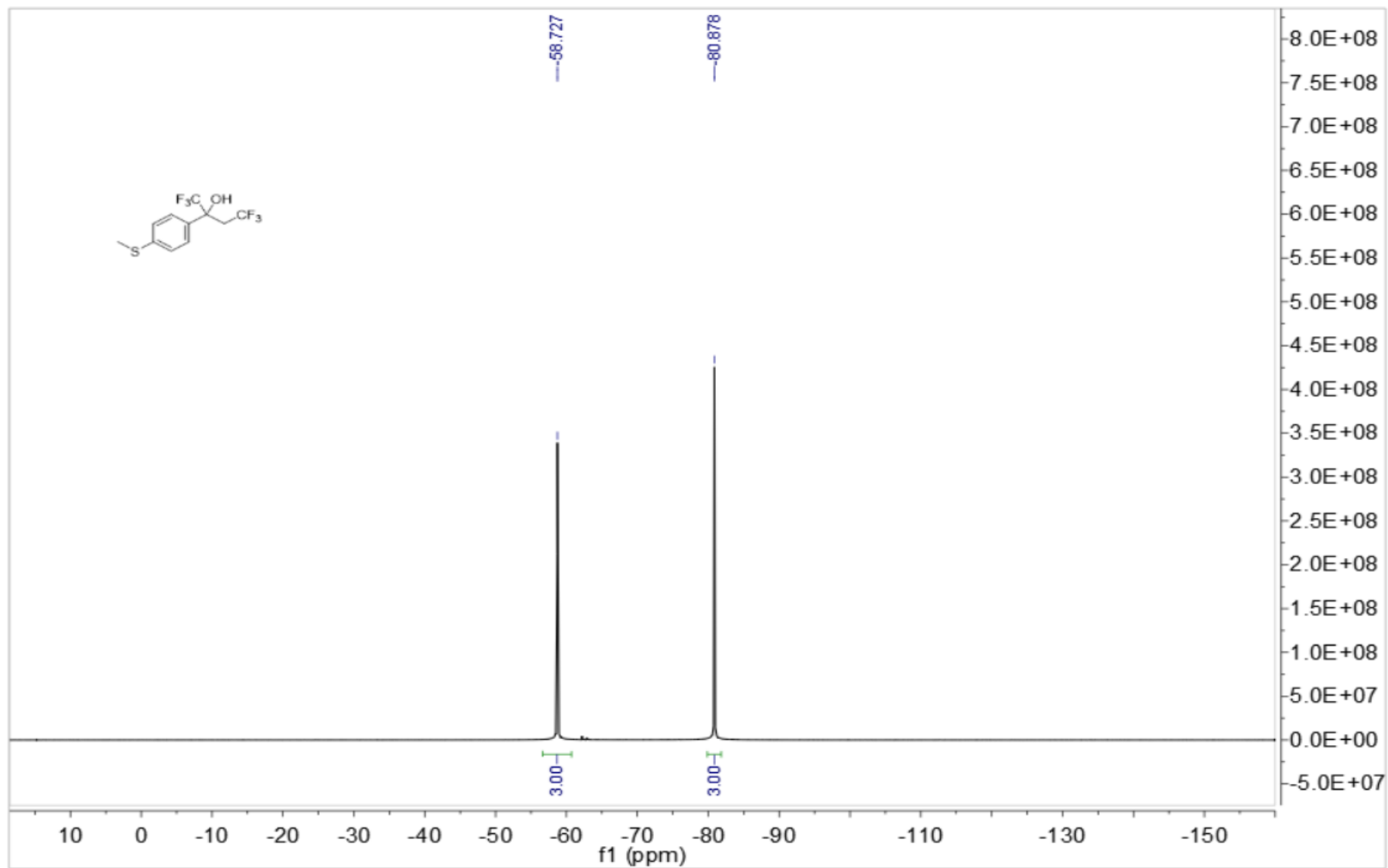
¹H NMR spectrum of 2f



¹³C NMR spectrum of 2f



¹⁹F NMR spectrum of 2f



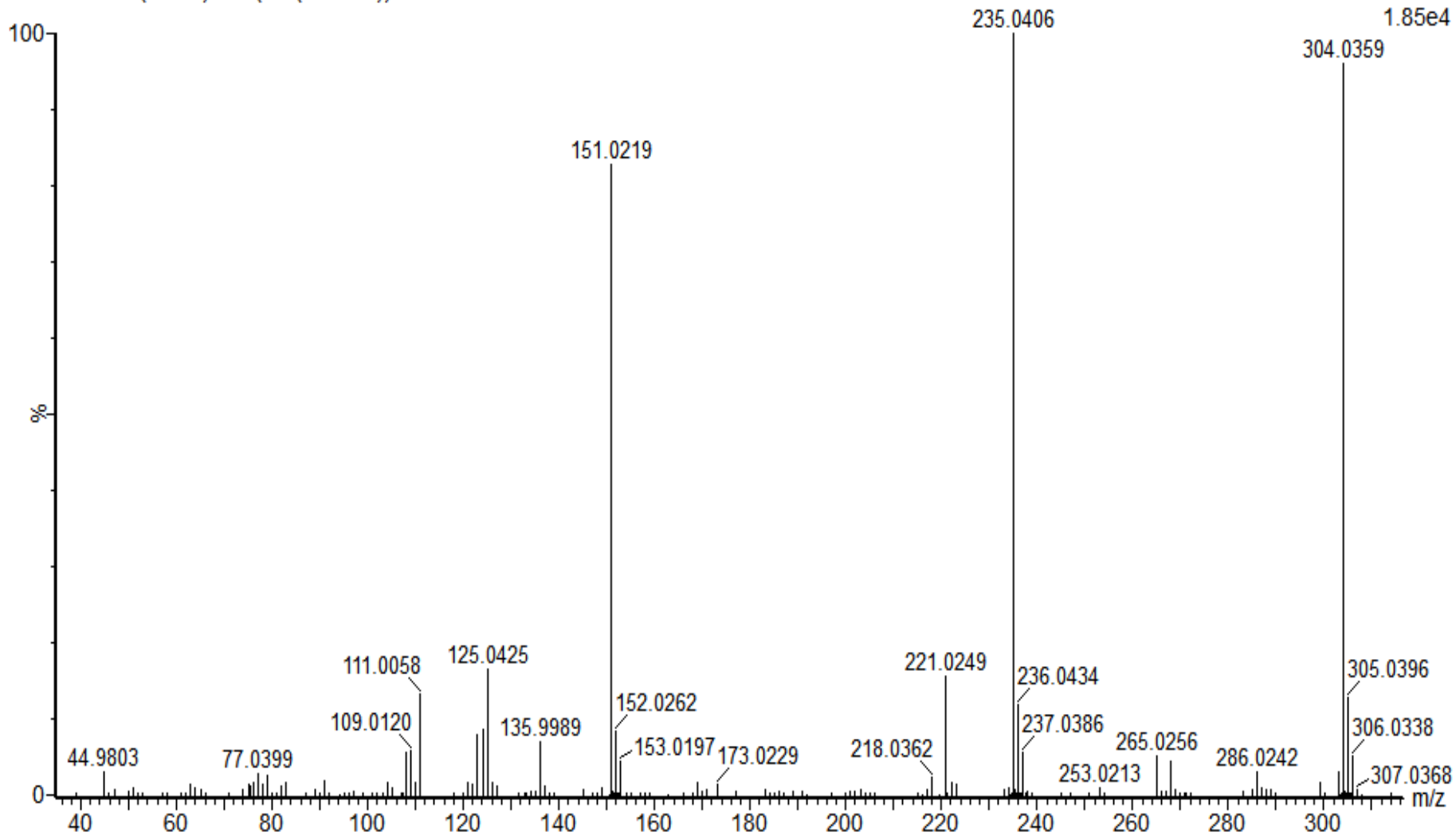
HRMS (EI) spectrum of 2f

CS-LC-P-304

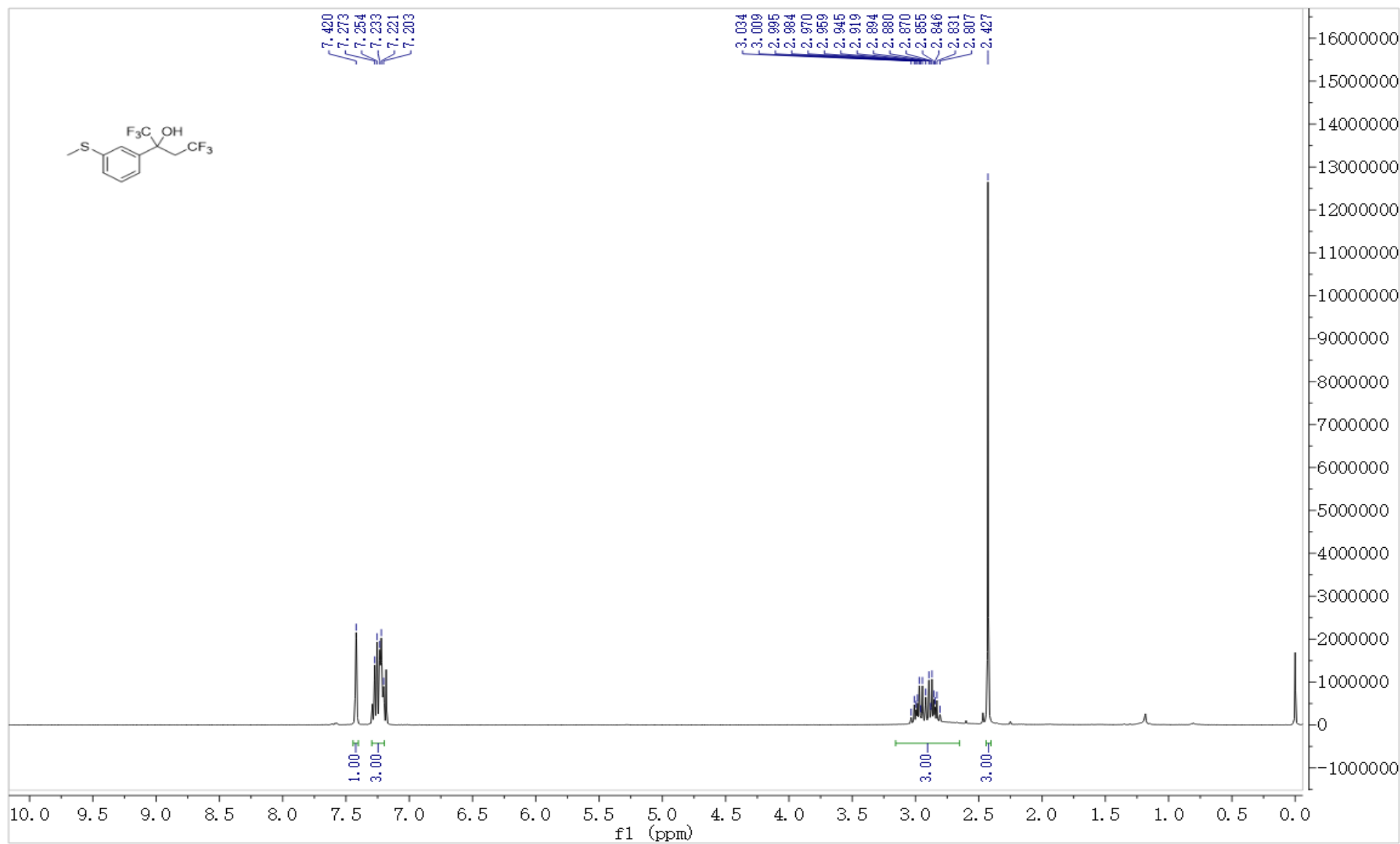
Waters GCT Premier

20220301 76 (1.267) Cm (76-(14+151))

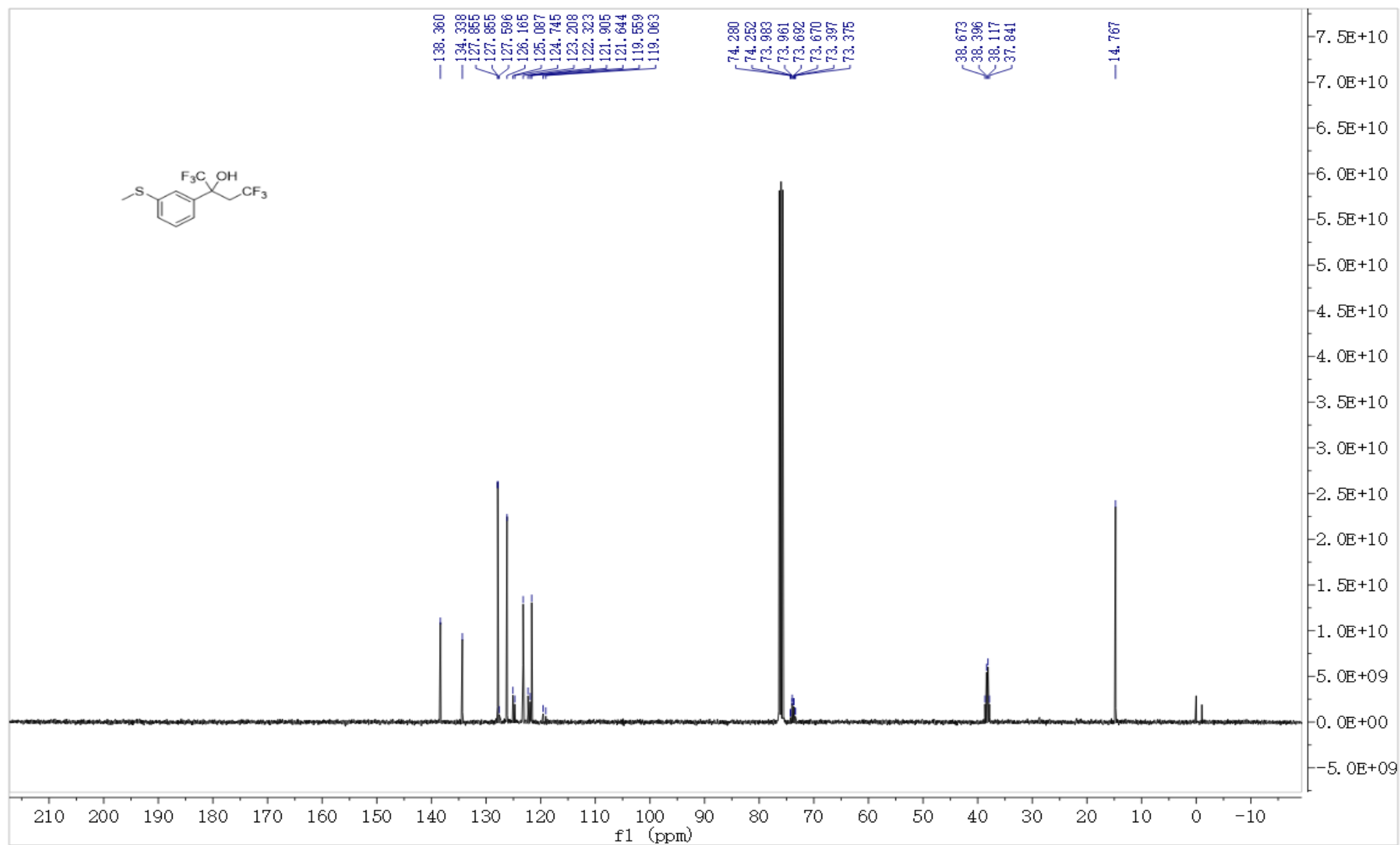
TOF MS EI+
1.85e4



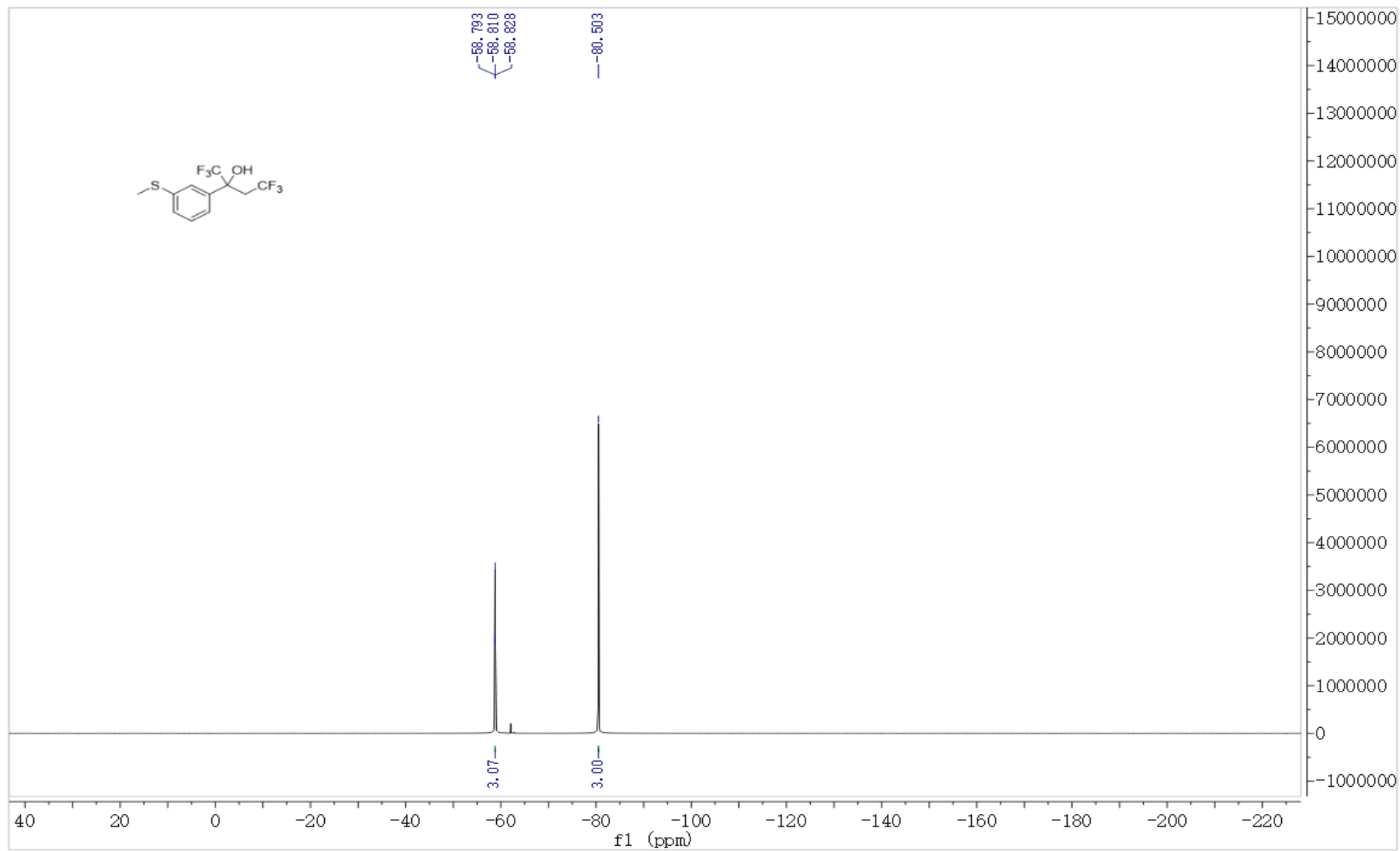
¹H NMR spectrum of 2g



¹³C NMR spectrum of 2g



¹⁹F NMR spectrum of 2g

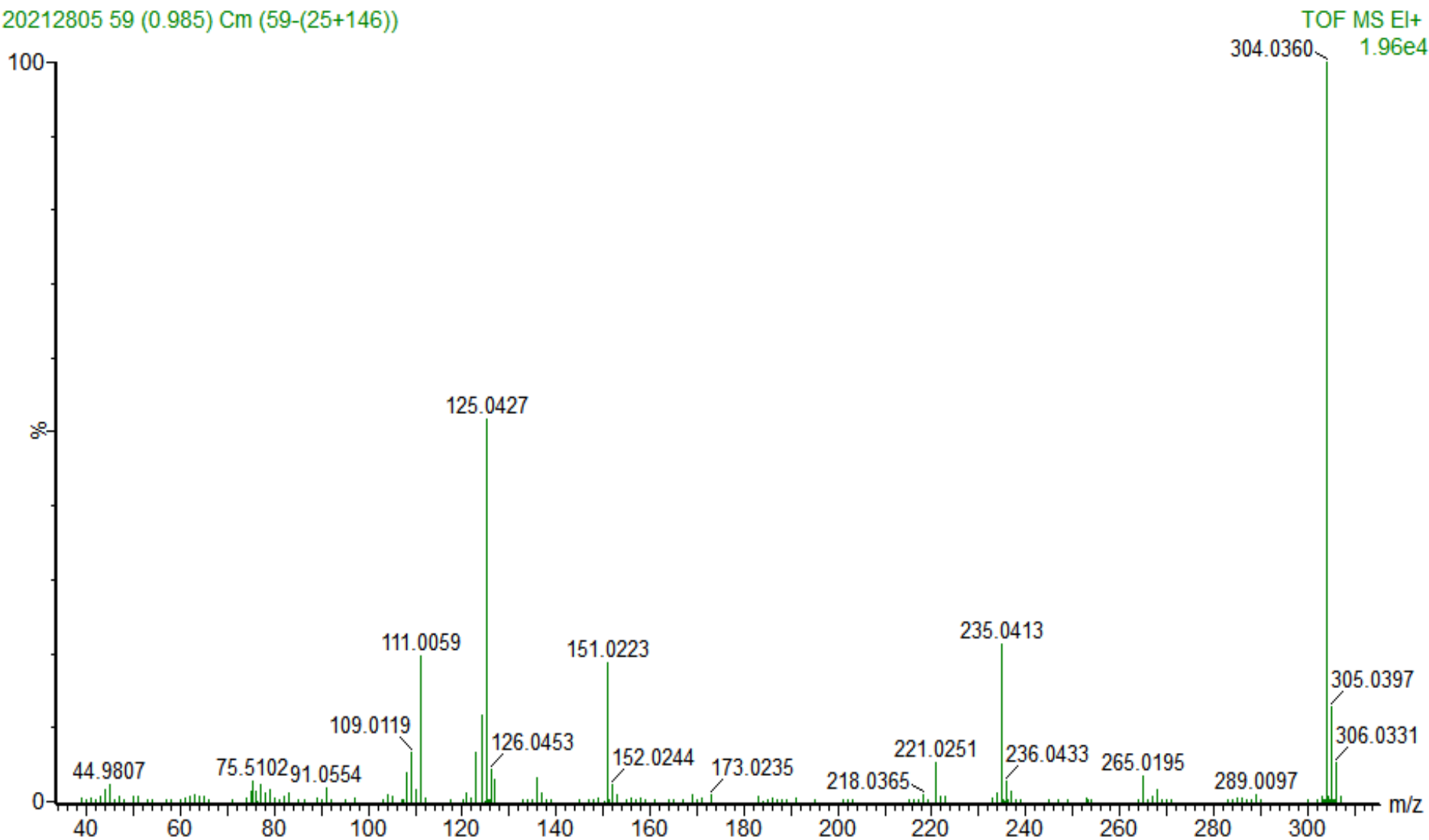


HRMS (EI) spectrum of 2g

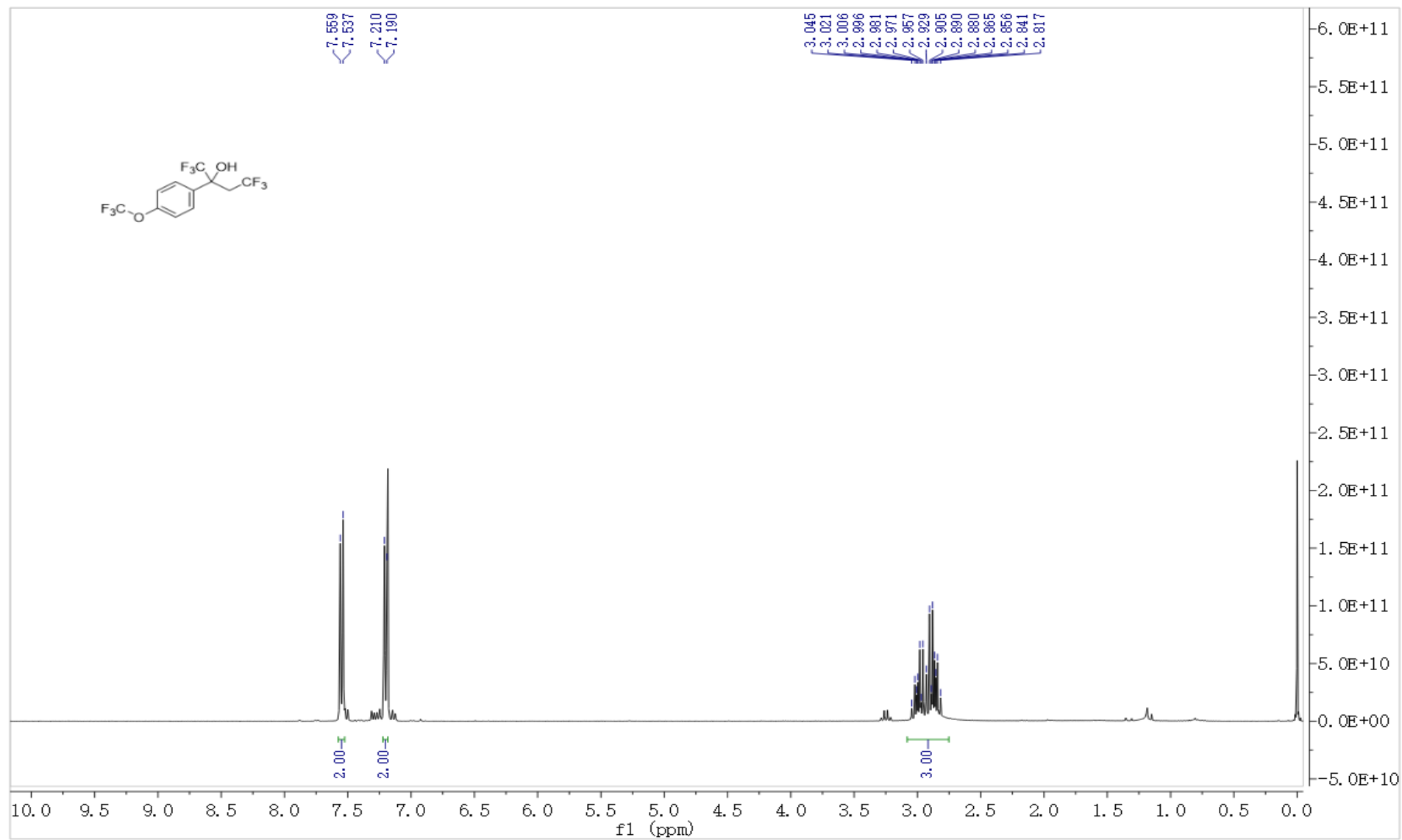
CS-LC-M-304

20212805 59 (0.985) Cm (59-(25+146))

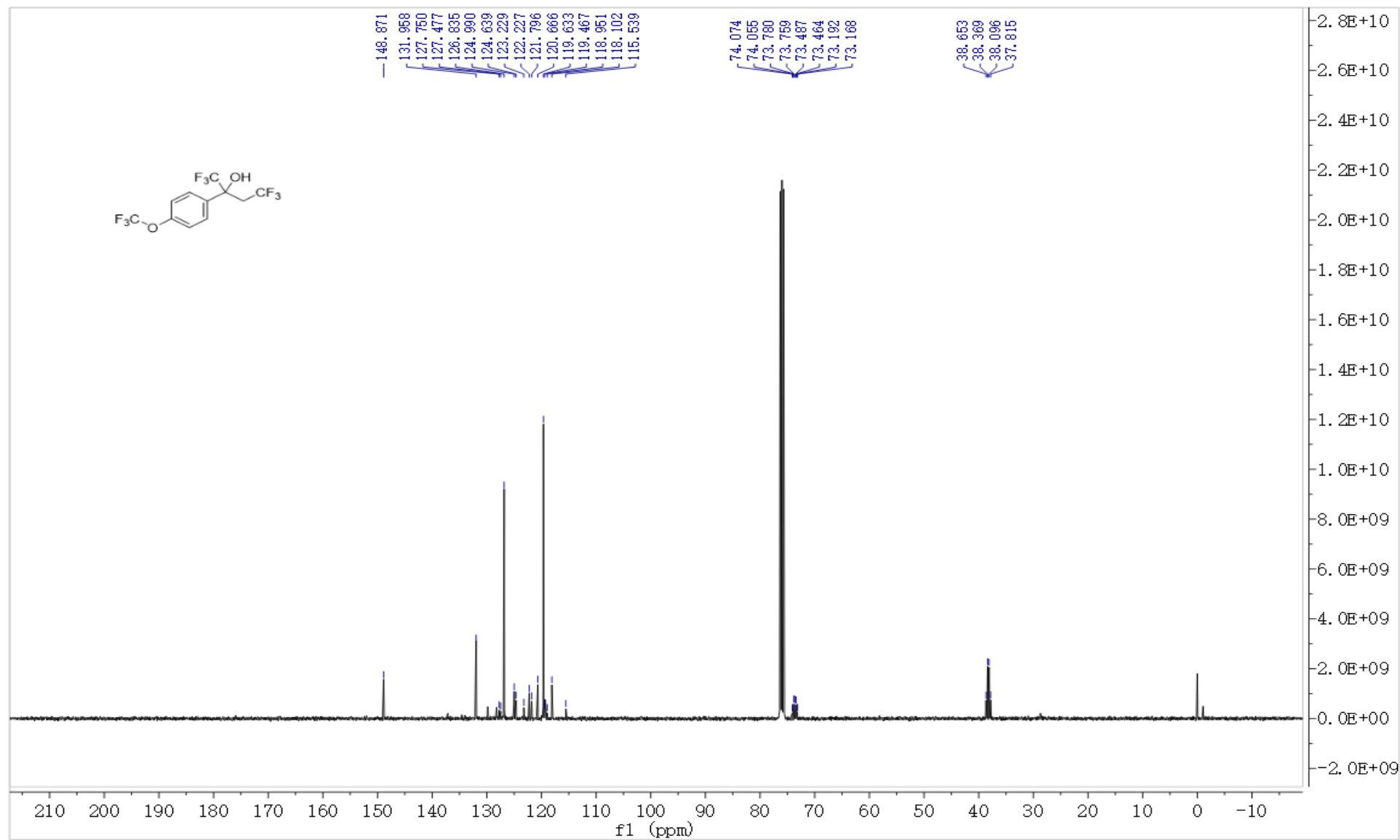
Waters GCT Premier



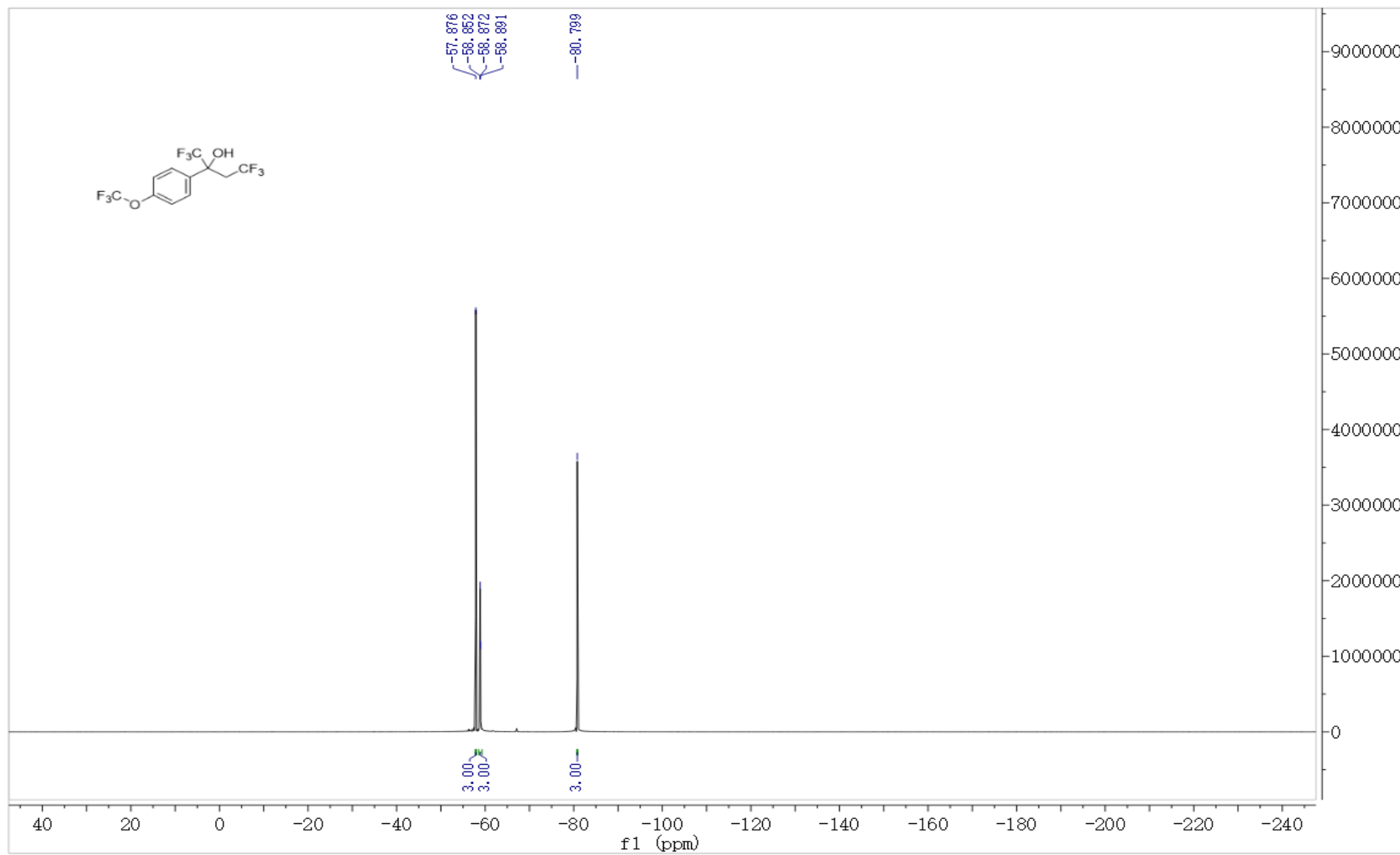
¹H NMR spectrum of 2h



¹³C NMR spectrum of 2h



^{19}F NMR spectrum of 2h



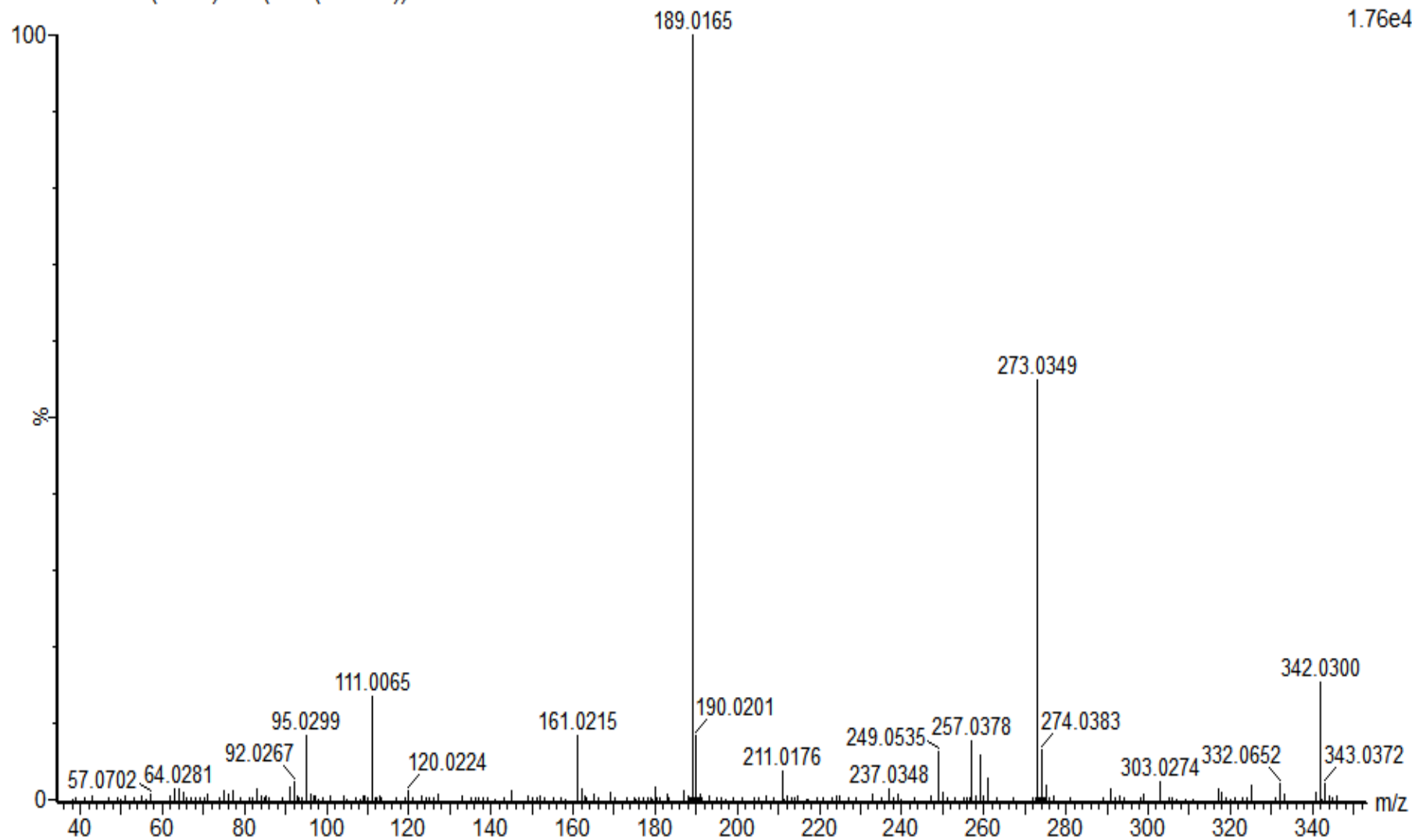
HRMS (EI) spectrum of 2h

CS-LC-P-342

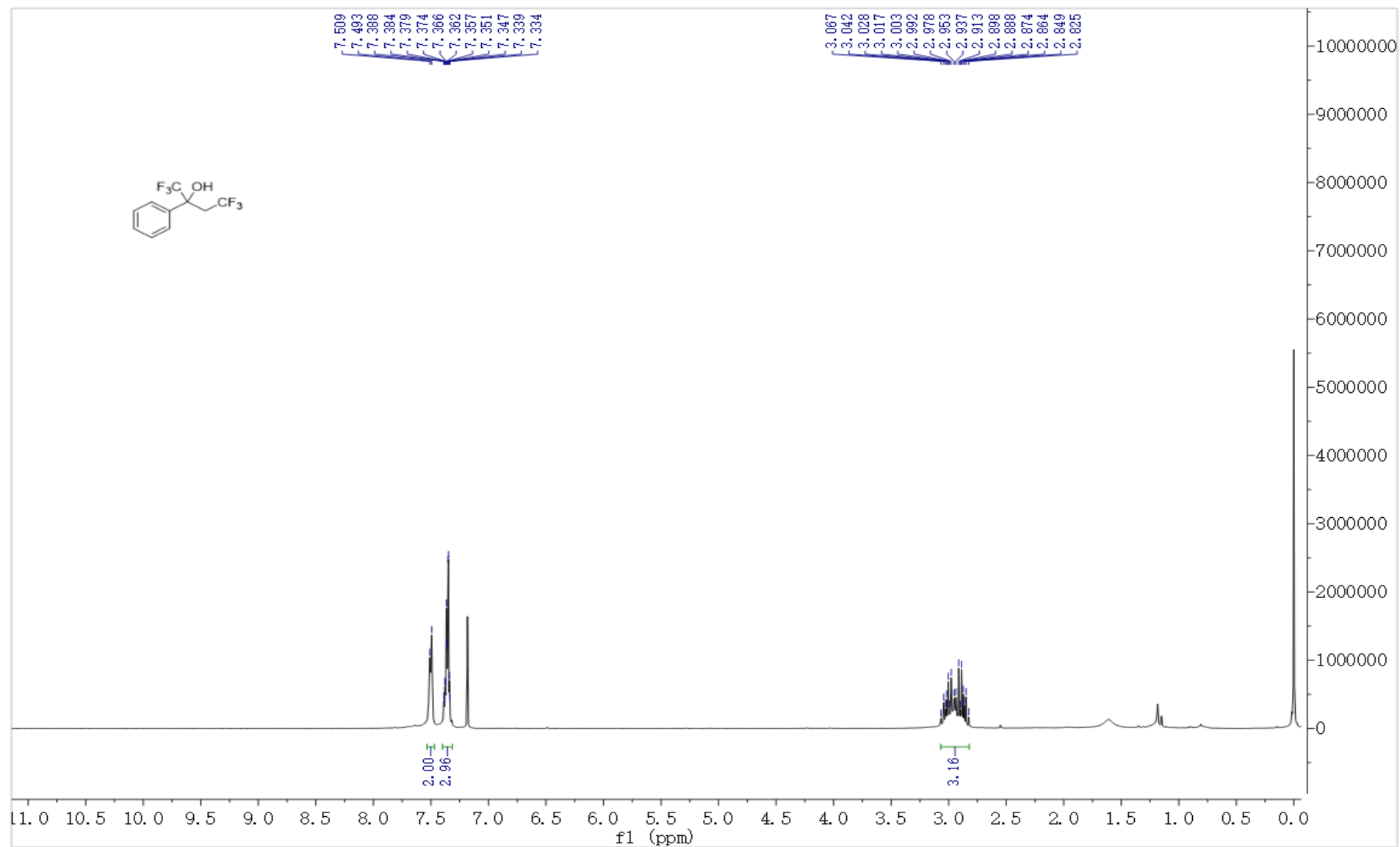
20220306 251 (3.020) Cm (251-(83+122))

Waters GCT Premier

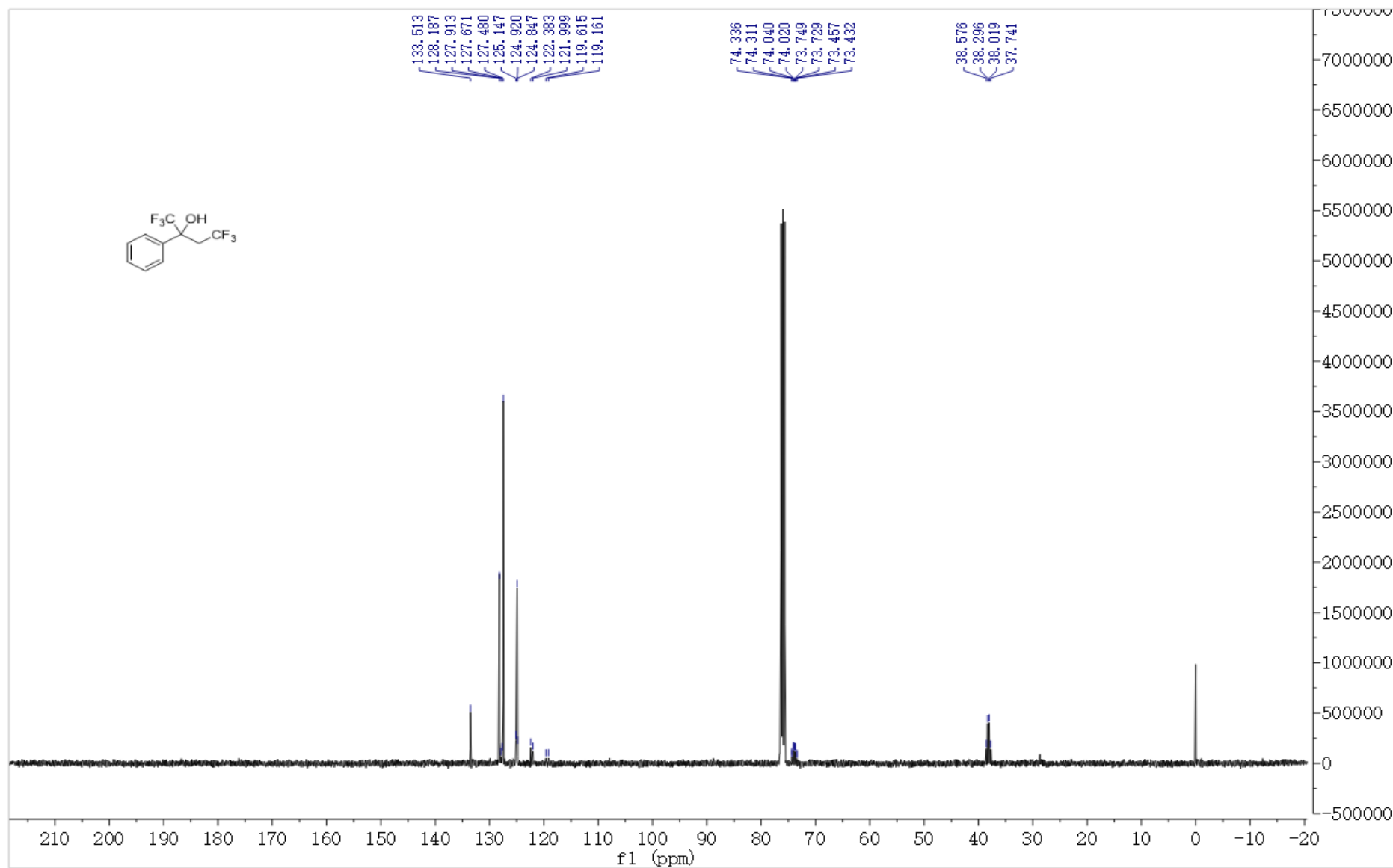
TOF MS EI+
1.76e4



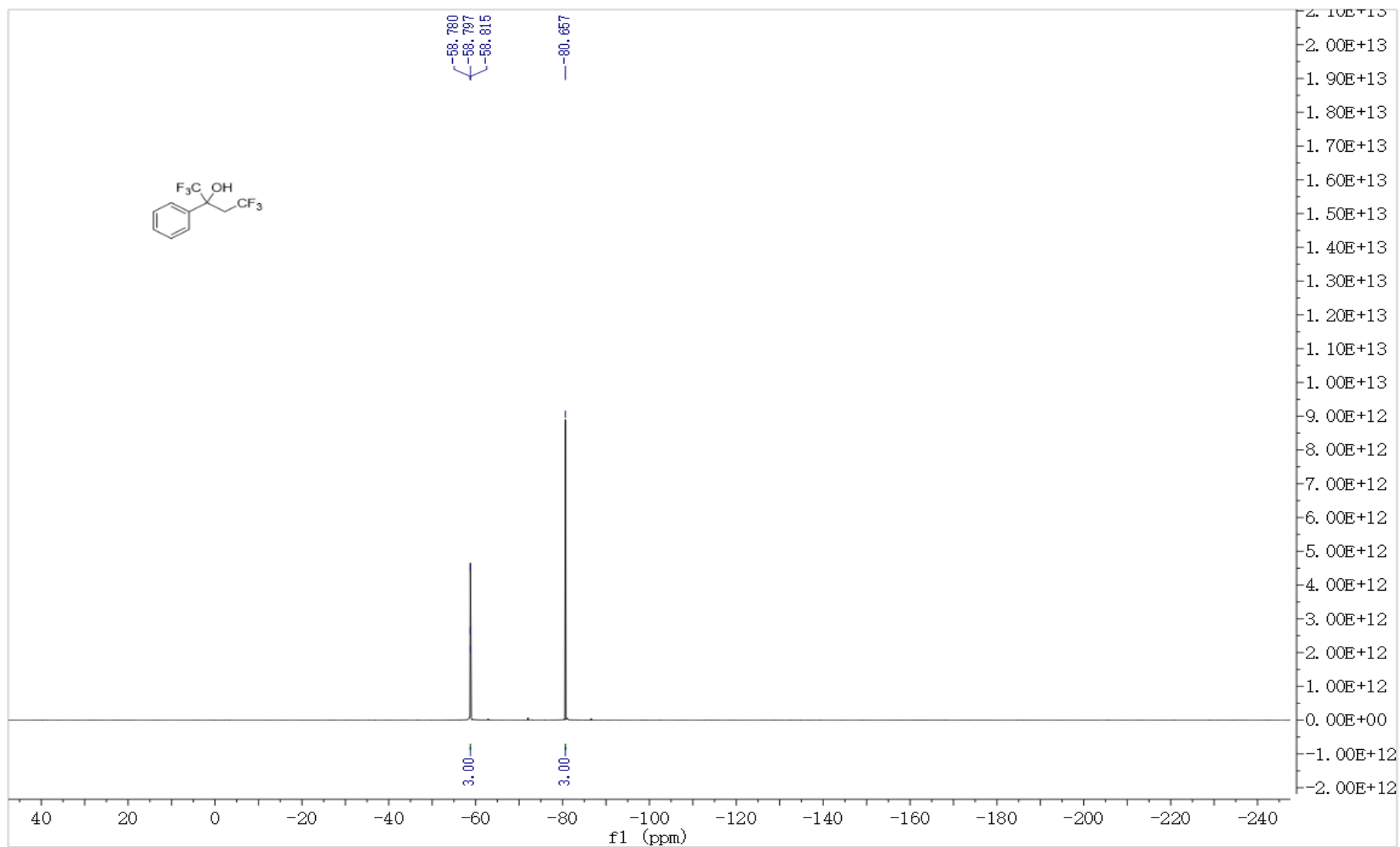
¹H NMR spectrum of 2i



¹³C NMR spectrum of 2i



¹⁹F NMR spectrum of 2i



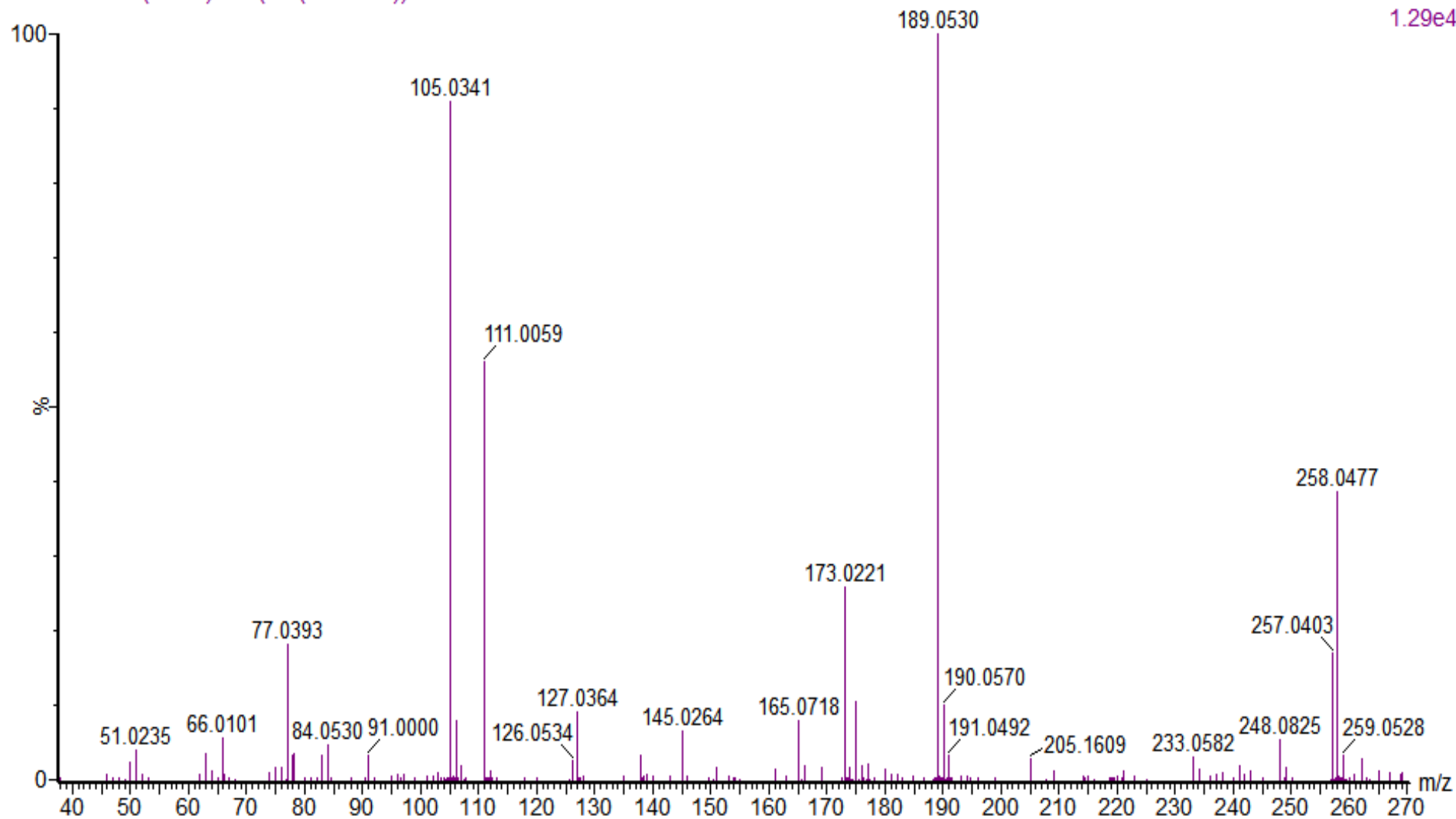
HRMS (EI) spectrum of 2i

CS-LC-P-258

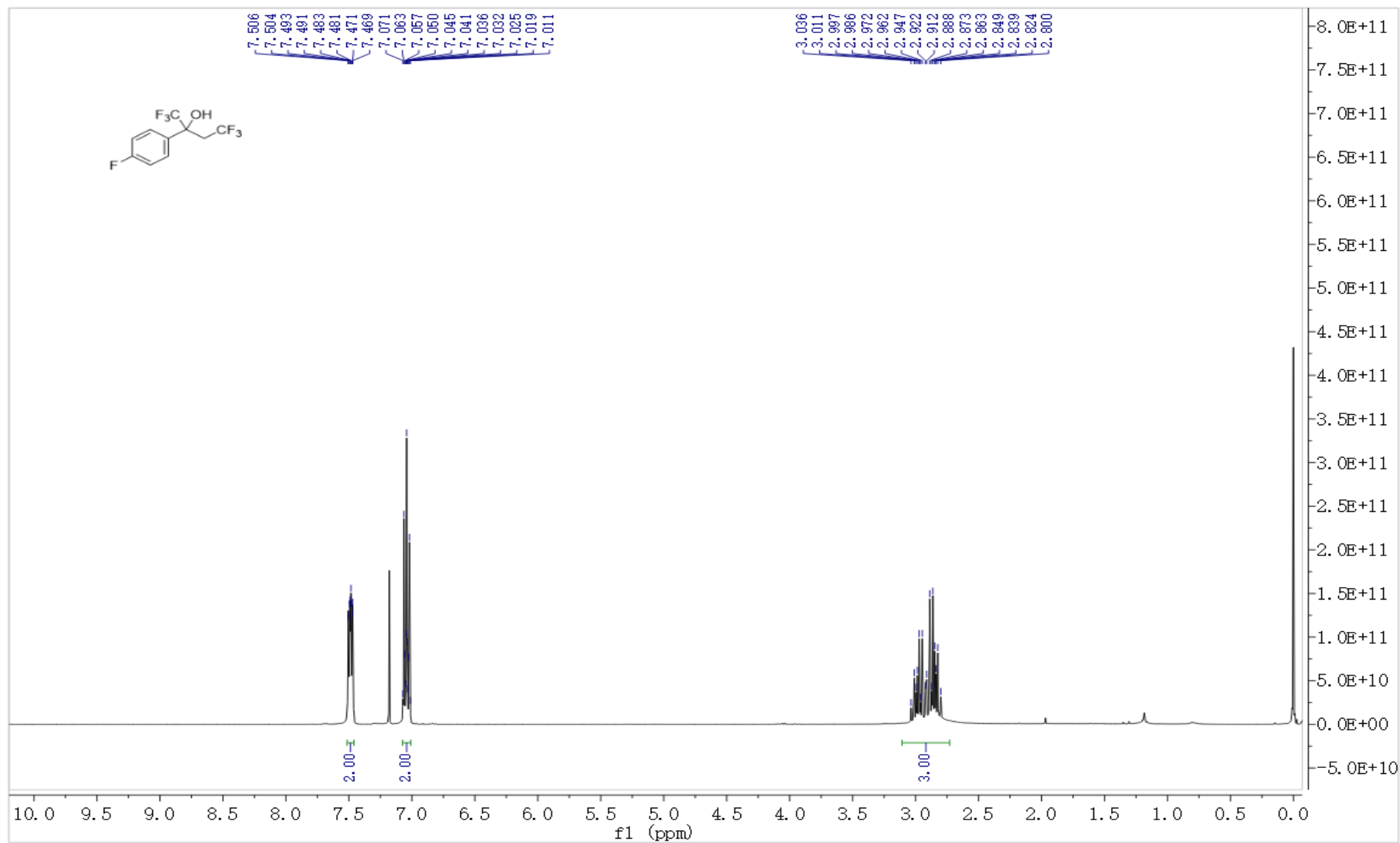
Waters GCT Premier

20220486 69 (1.150) Cm (69-(160+508))

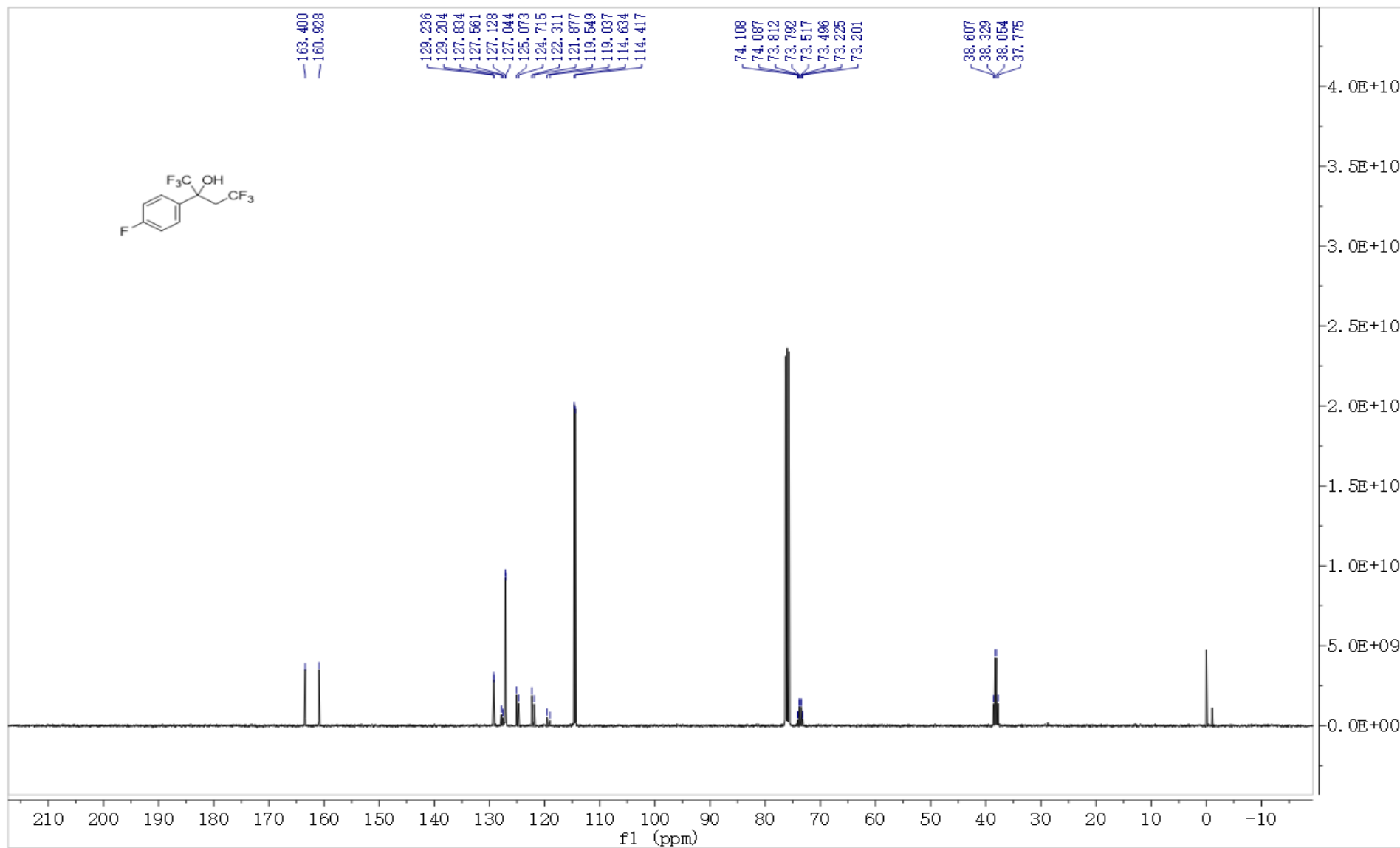
TOF MS EI+
1.29e4



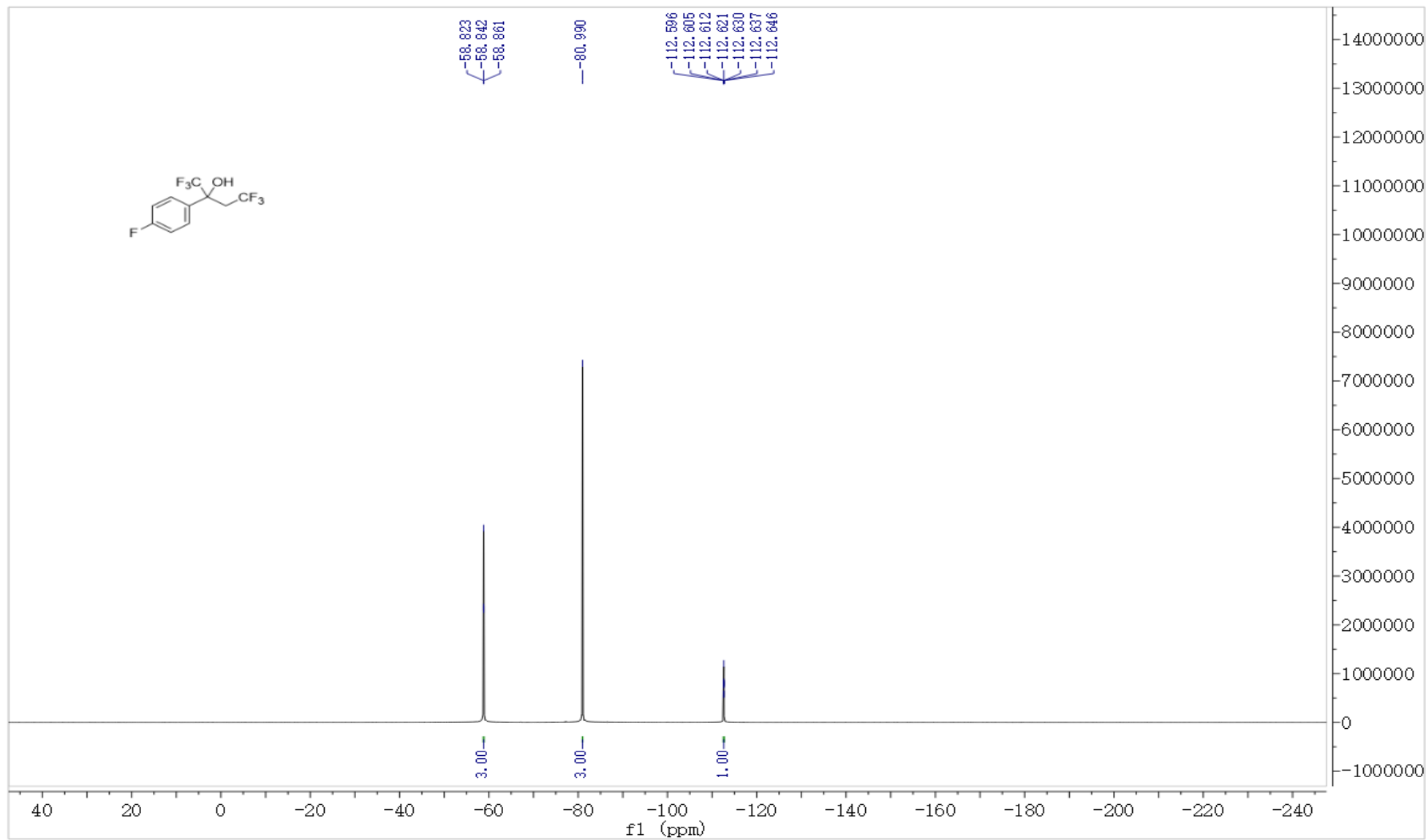
¹H NMR spectrum of 2j



¹³C NMR spectrum of 2j



¹⁹F NMR spectrum of 2j



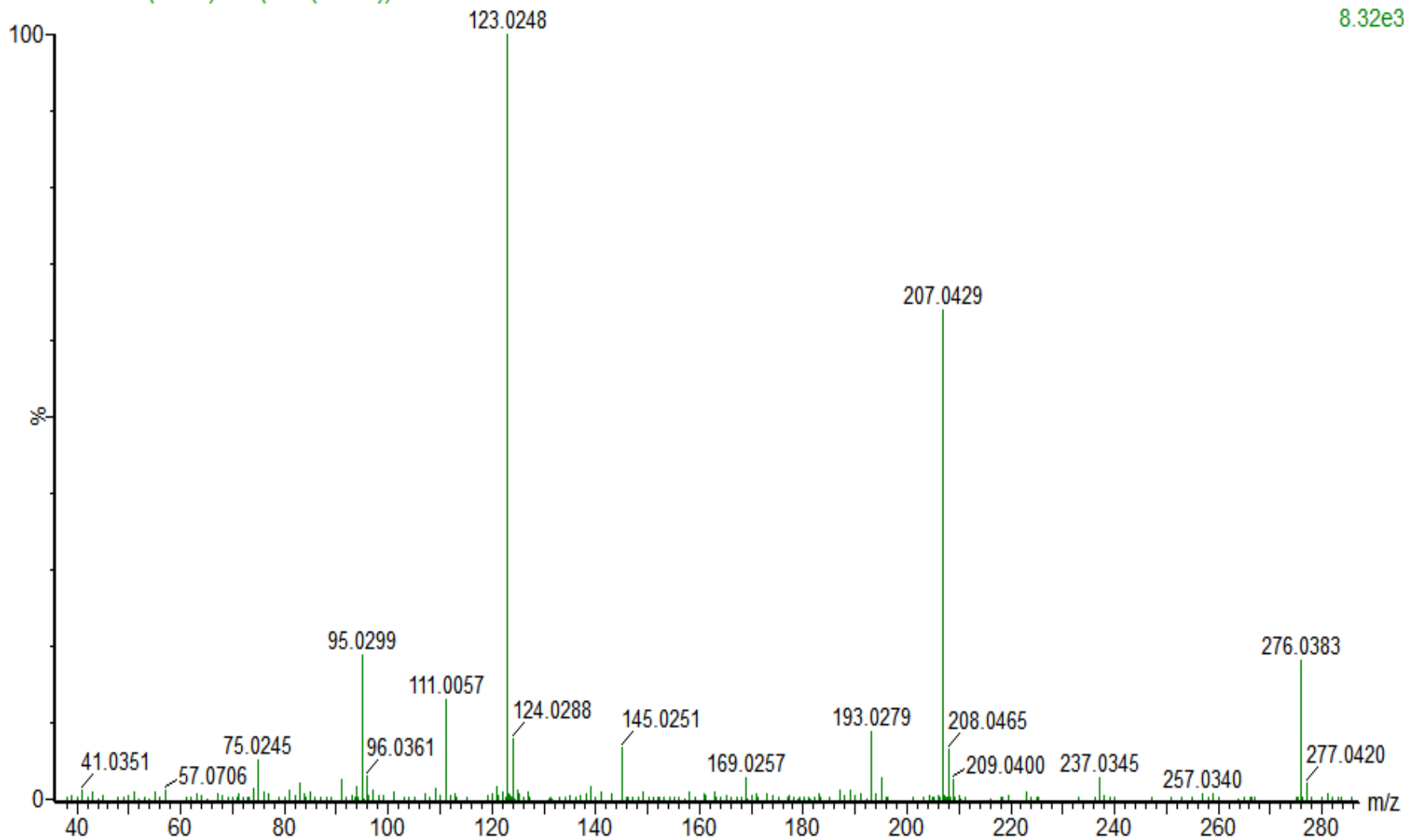
HRMS (EI) spectrum of 2j

CS-LC-P-276

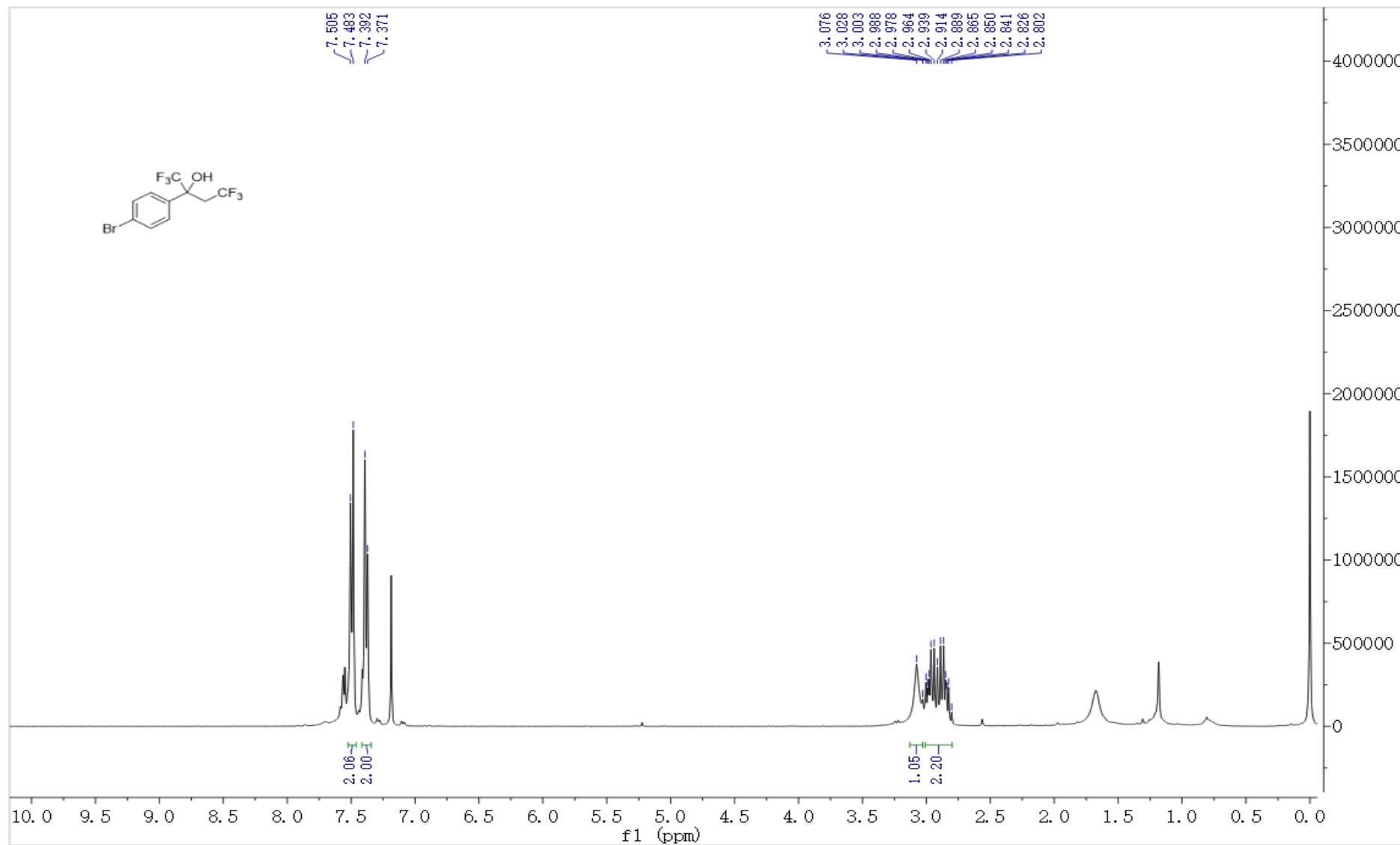
Waters GCT Premier

20220305 175 (2.917) Cm (175-(25+60))

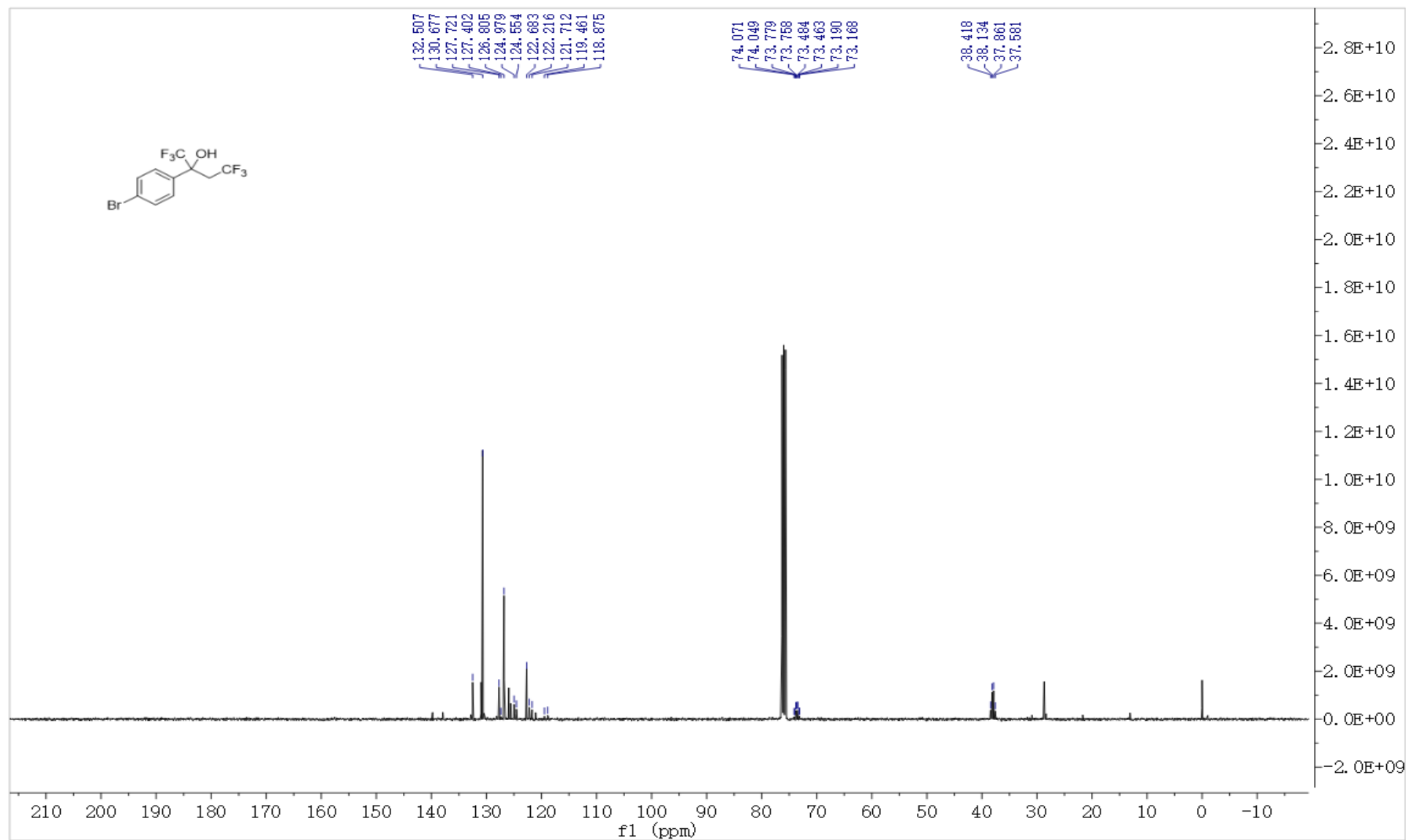
TOF MS EI+
8.32e3



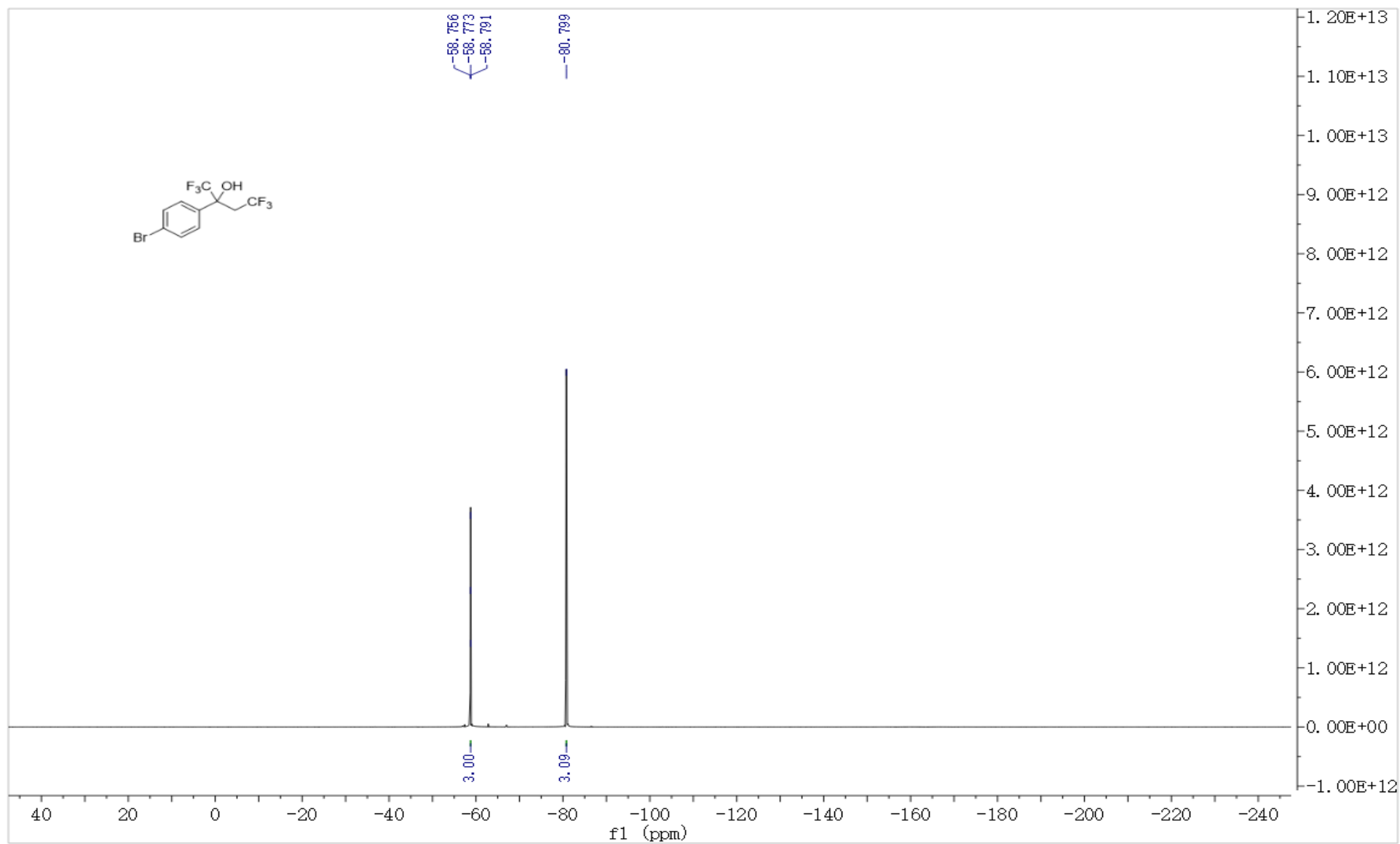
¹H NMR spectrum of 2k



¹³C NMR spectrum of 2k



¹⁹F NMR spectrum of 2k



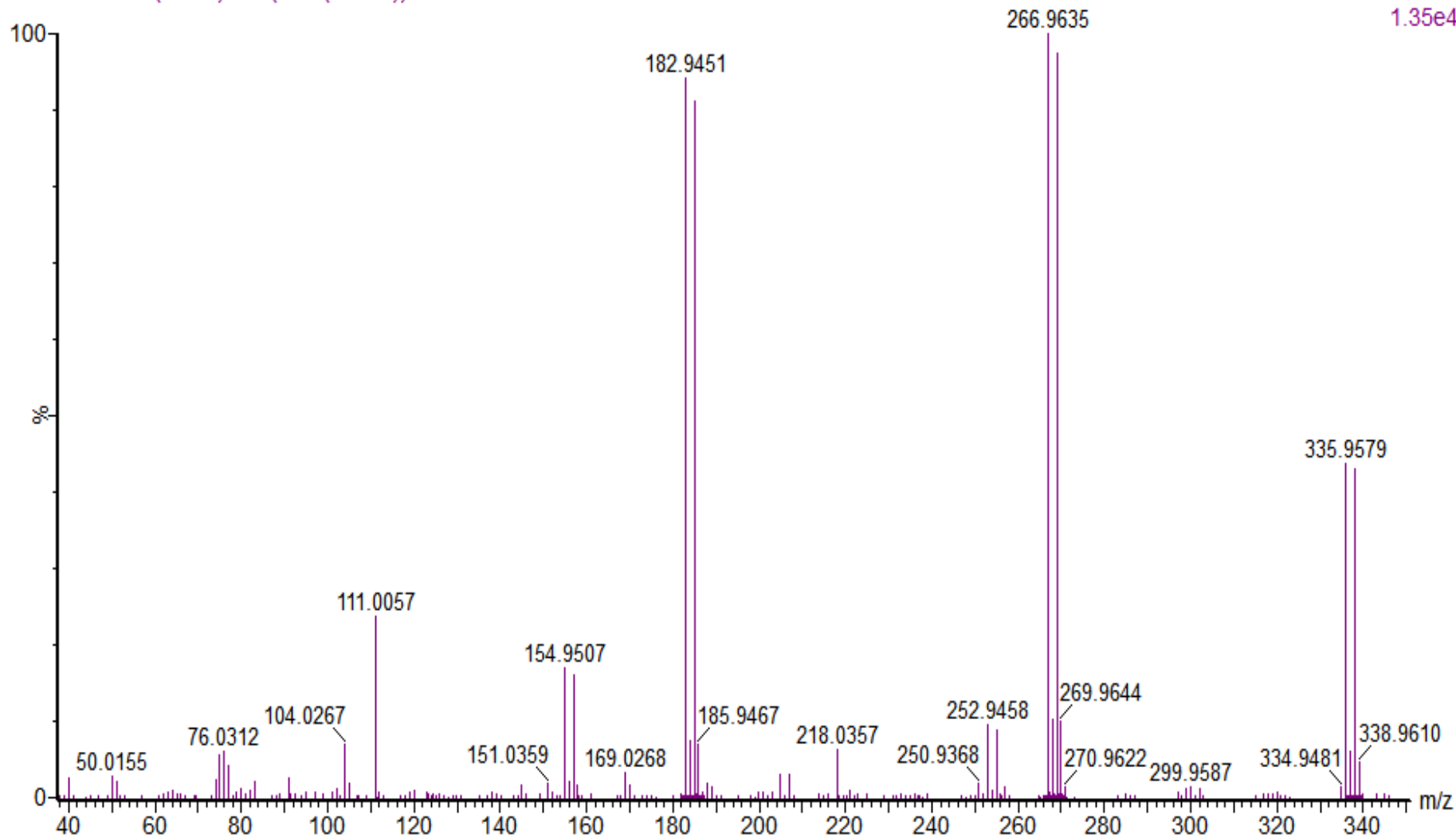
HRMS (EI) spectrum of 2k

CS-LC-P-337

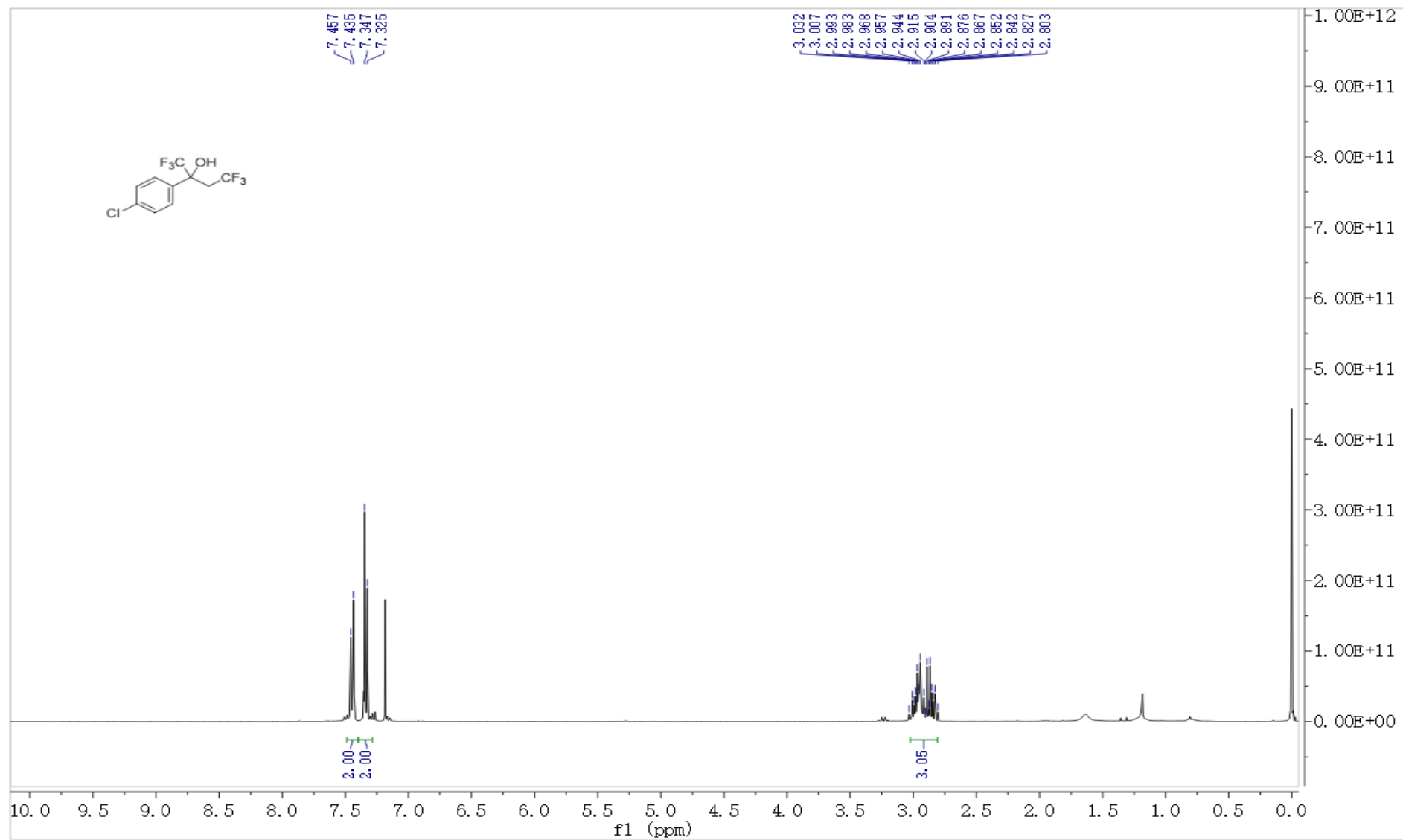
20220483 105 (1.750) Cm (105-(14+23))

Waters GCT Premier

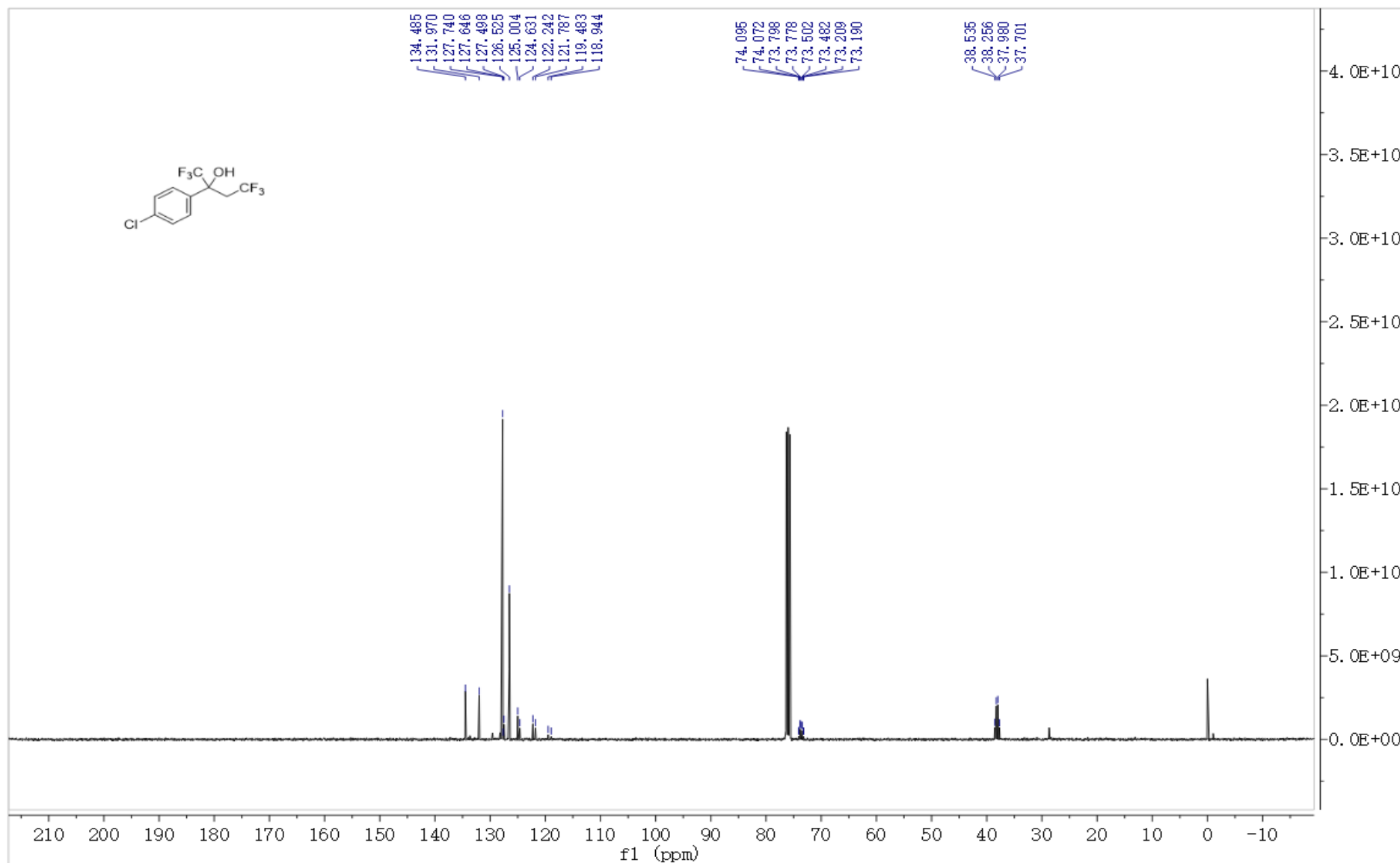
TOF MS EI+
1.35e4



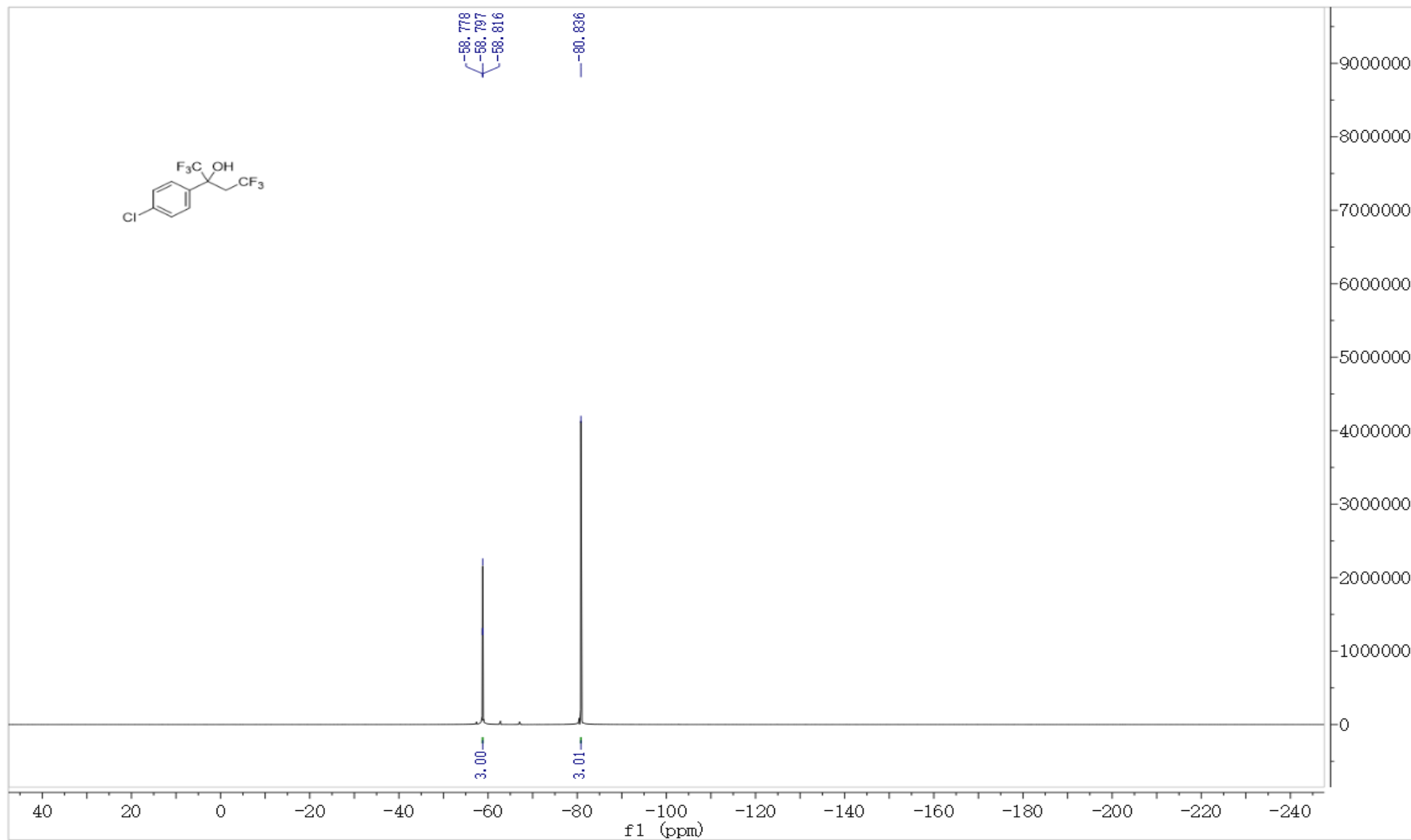
¹H NMR spectrum of 2l



¹³C NMR spectrum of 2l



¹⁹F NMR spectrum of 2l



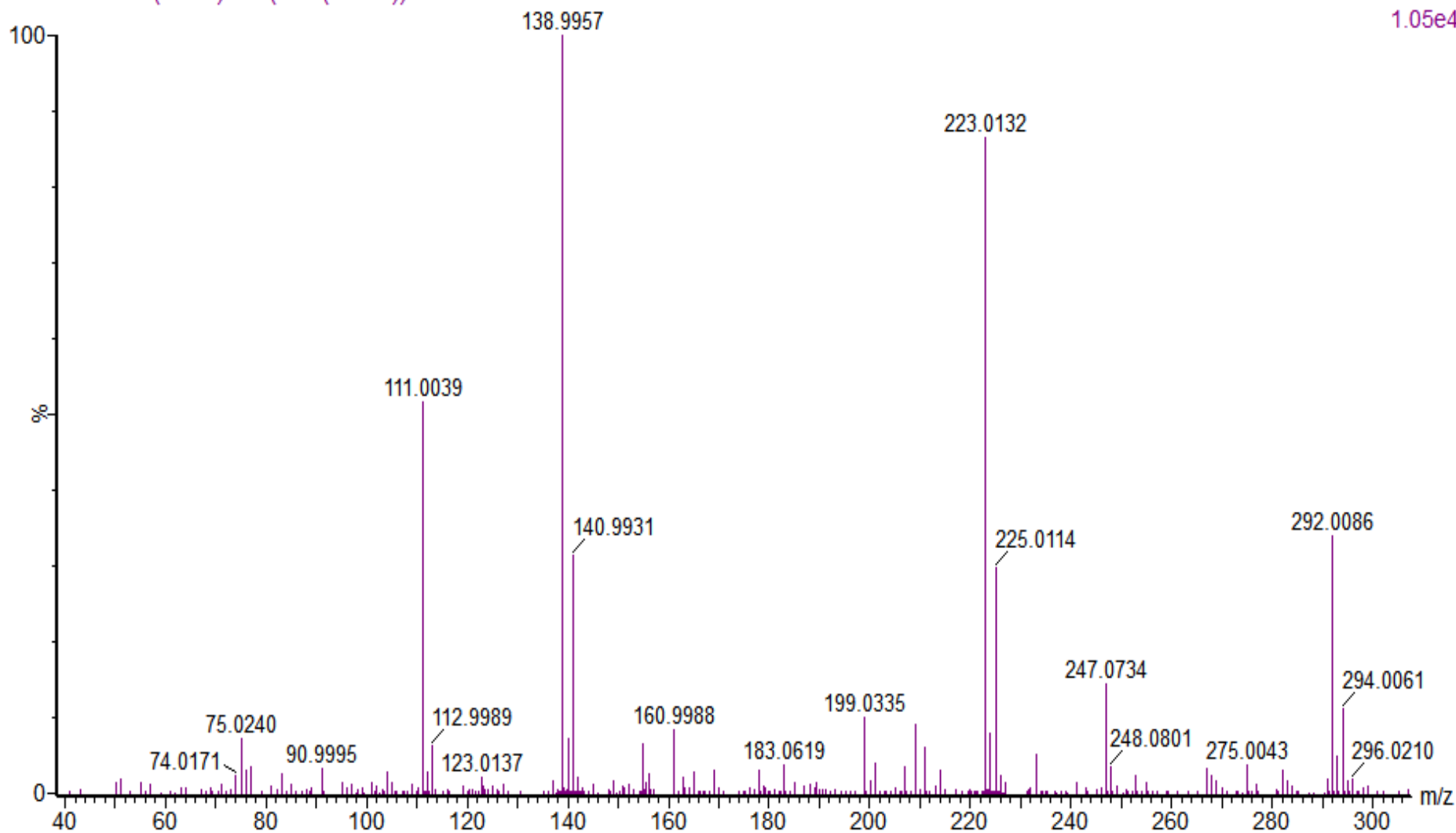
HRMS (EI) spectrum of 2l

CS-LC-P-292

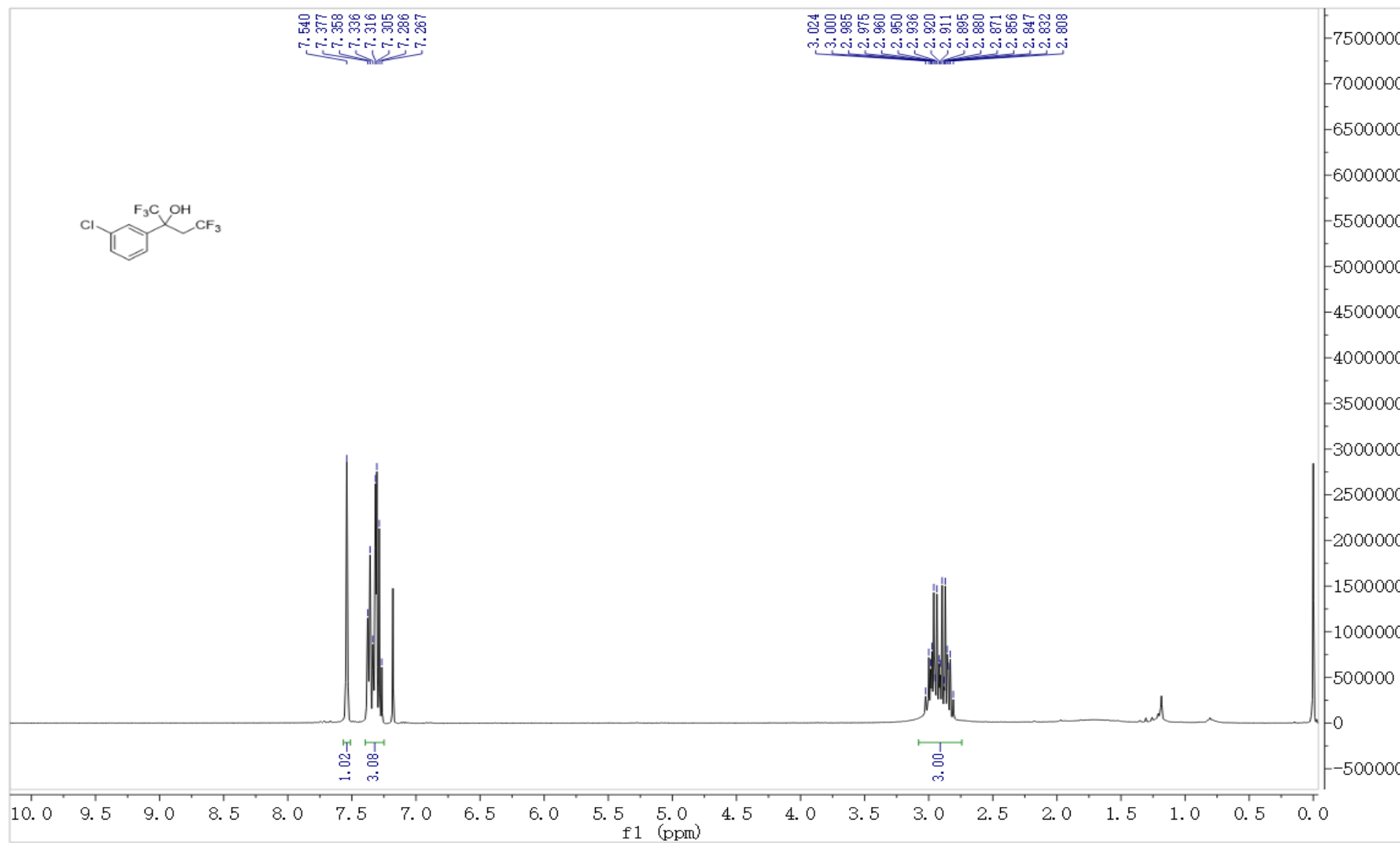
Waters GCT Premier

20220309 256 (4.267) Cm (256-(14+41))

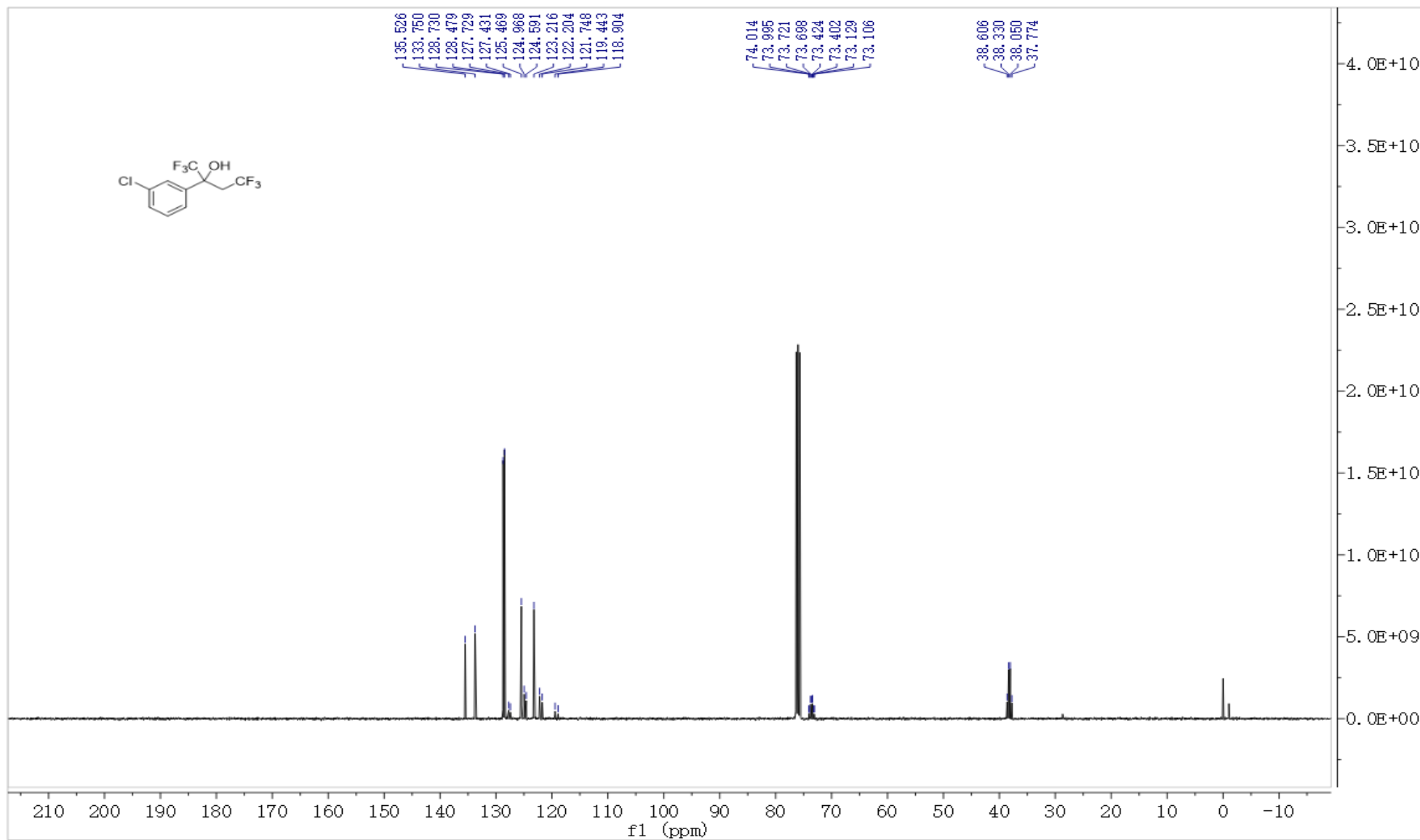
TOF MS EI+
1.05e4



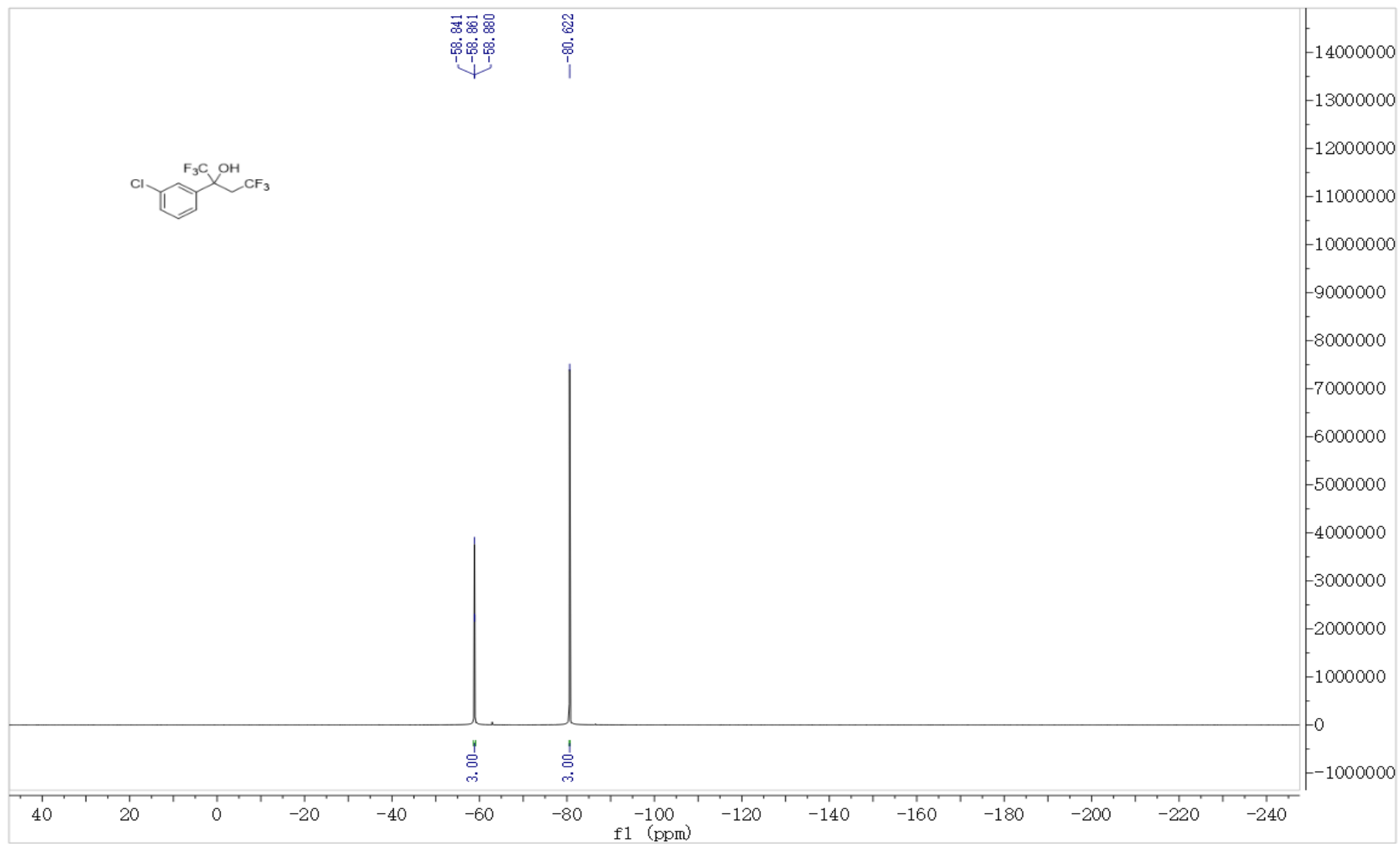
¹H NMR spectrum of 2m



¹³C NMR spectrum of 2m



¹⁹F NMR spectrum of 2m



HRMS (EI) spectrum of 2m

CS-LC-M-292

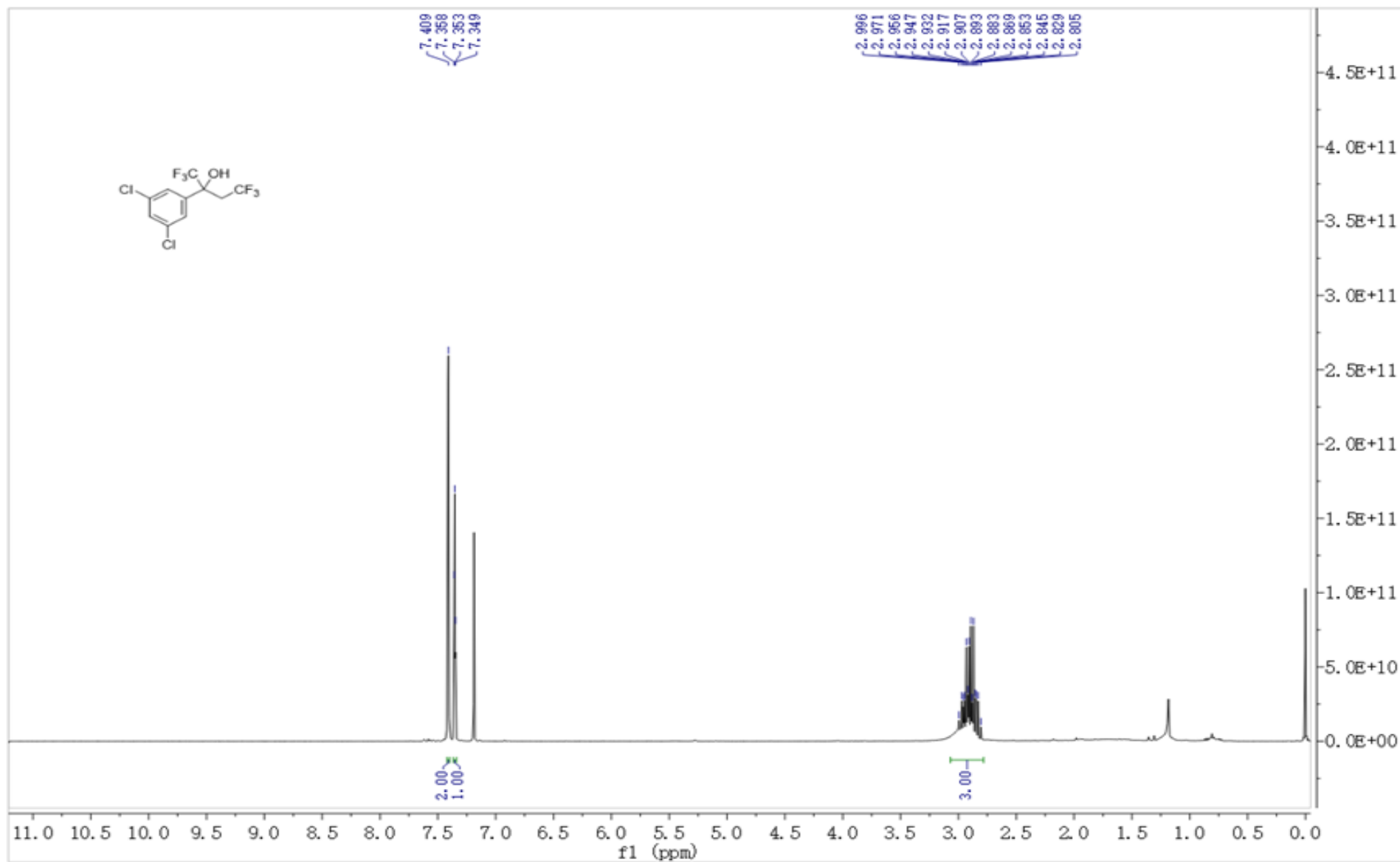
20220304 74 (1.233) Cm (74-(4+5))

Waters GCT Premier

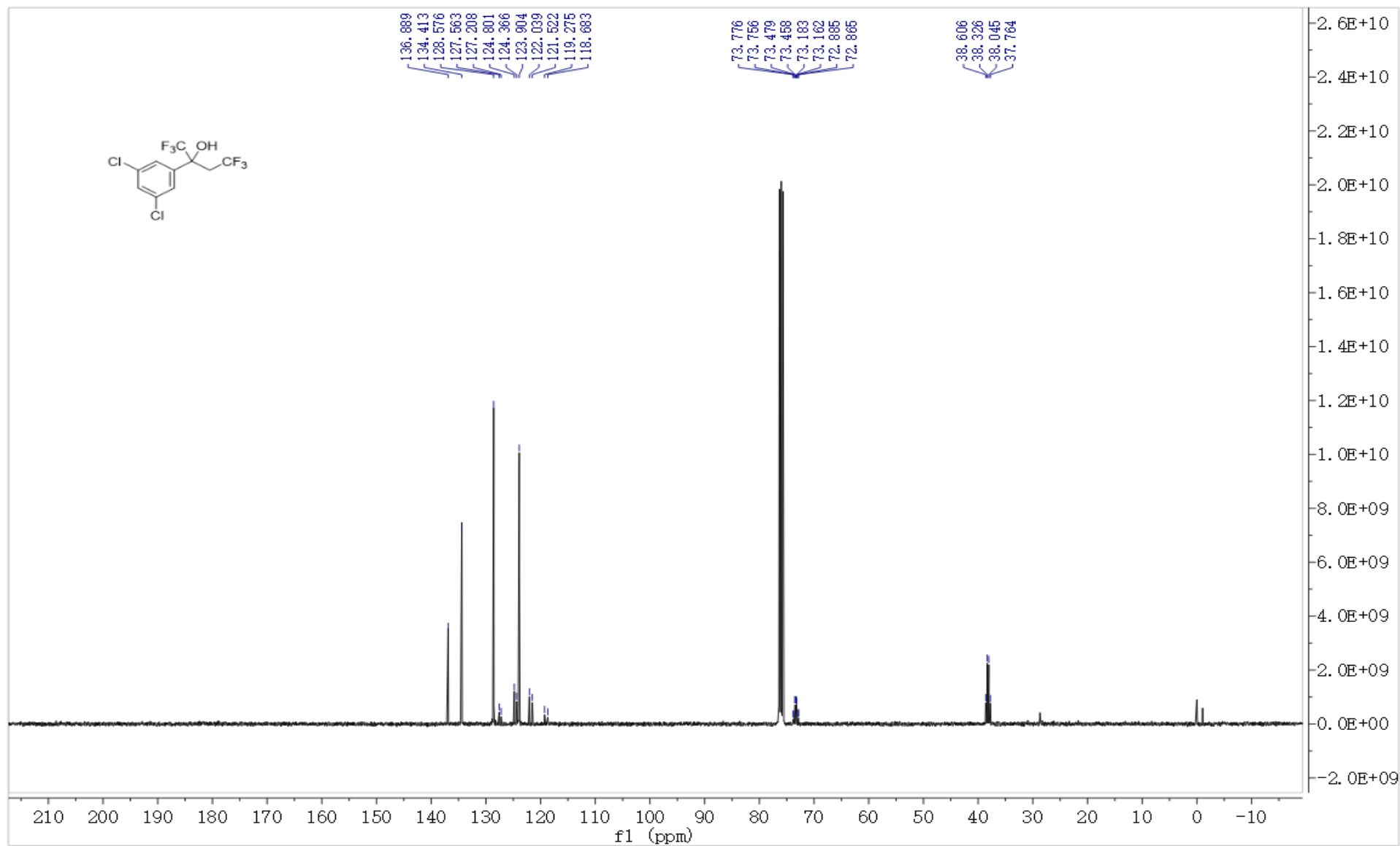
TOF MS EI+
1.43e4



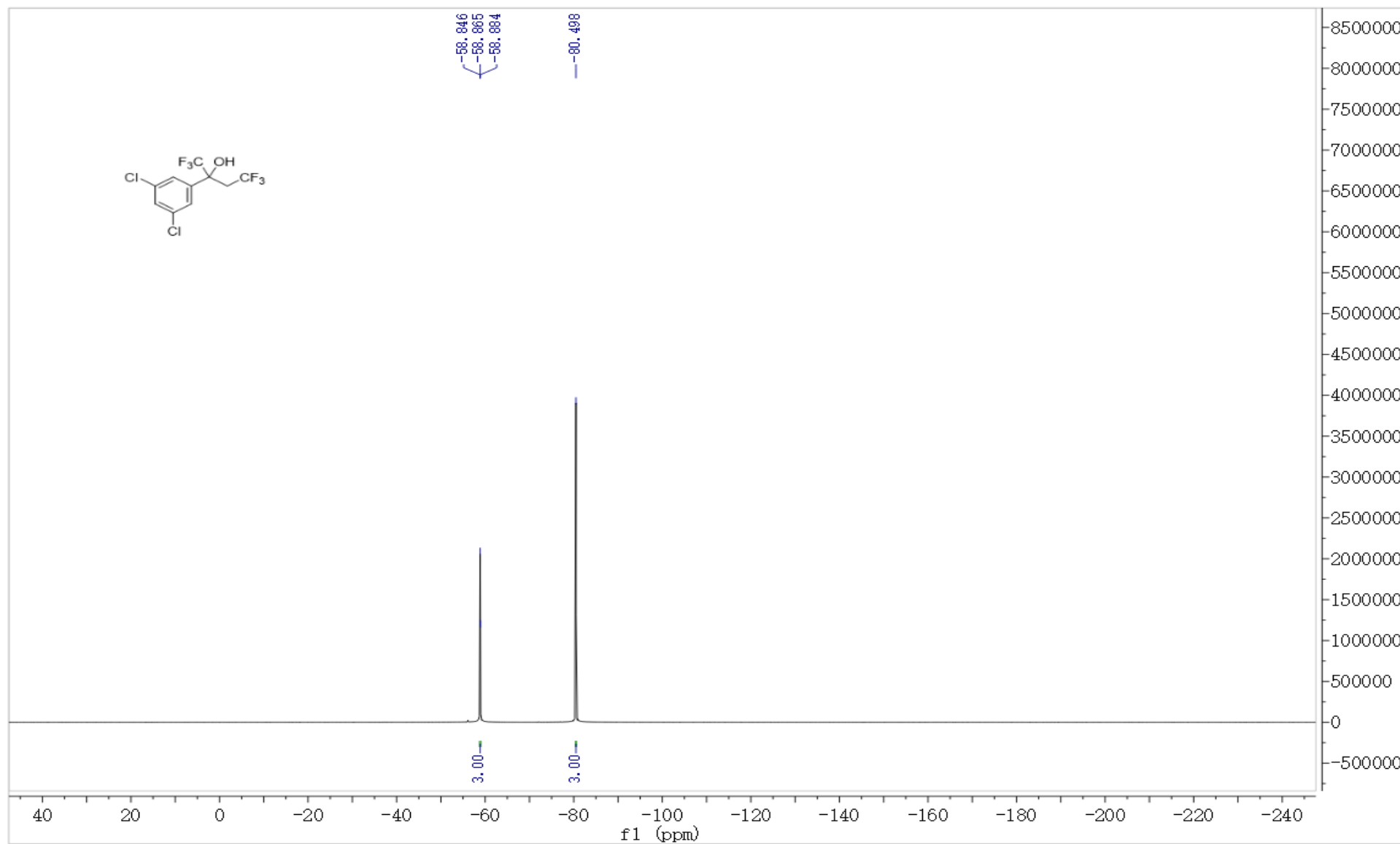
¹H NMR spectrum of 2n



¹³C NMR spectrum of 2n



¹⁹F NMR spectrum of 2n



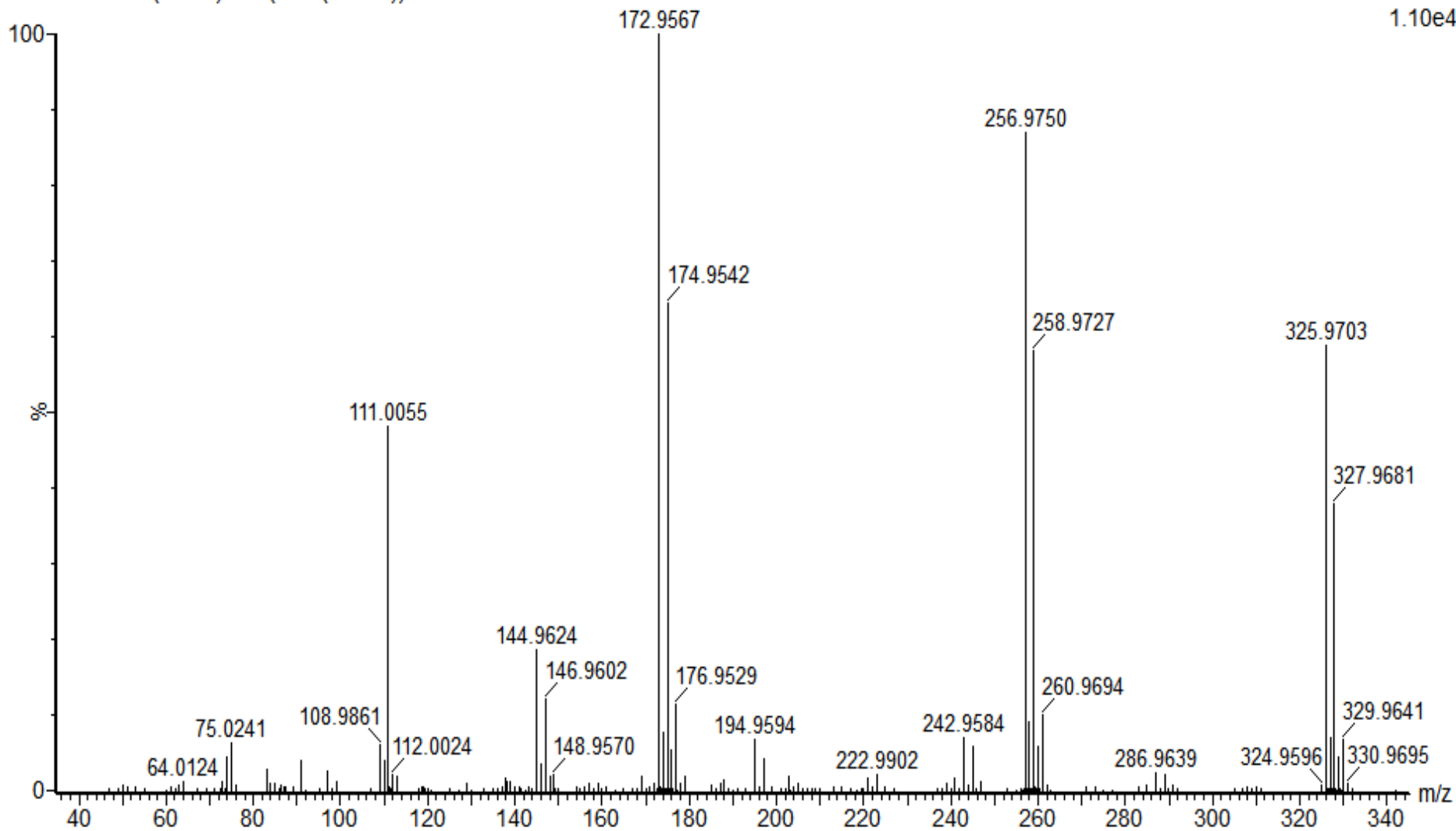
HRMS (EI) spectrum of 2n

CS-LC-P-327

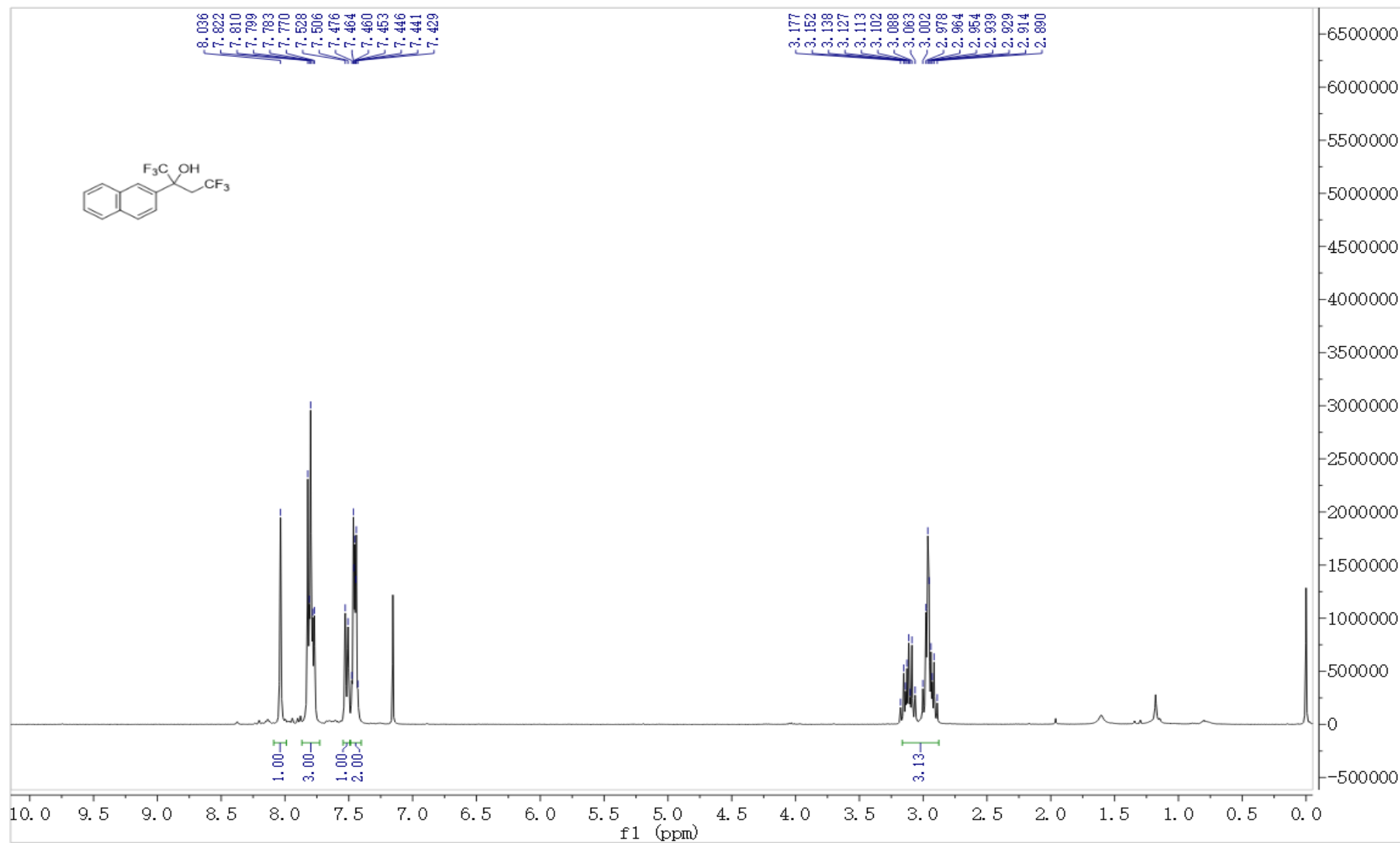
20220303 160 (2.667) Cm (160-(26+52))

Waters GCT Premier

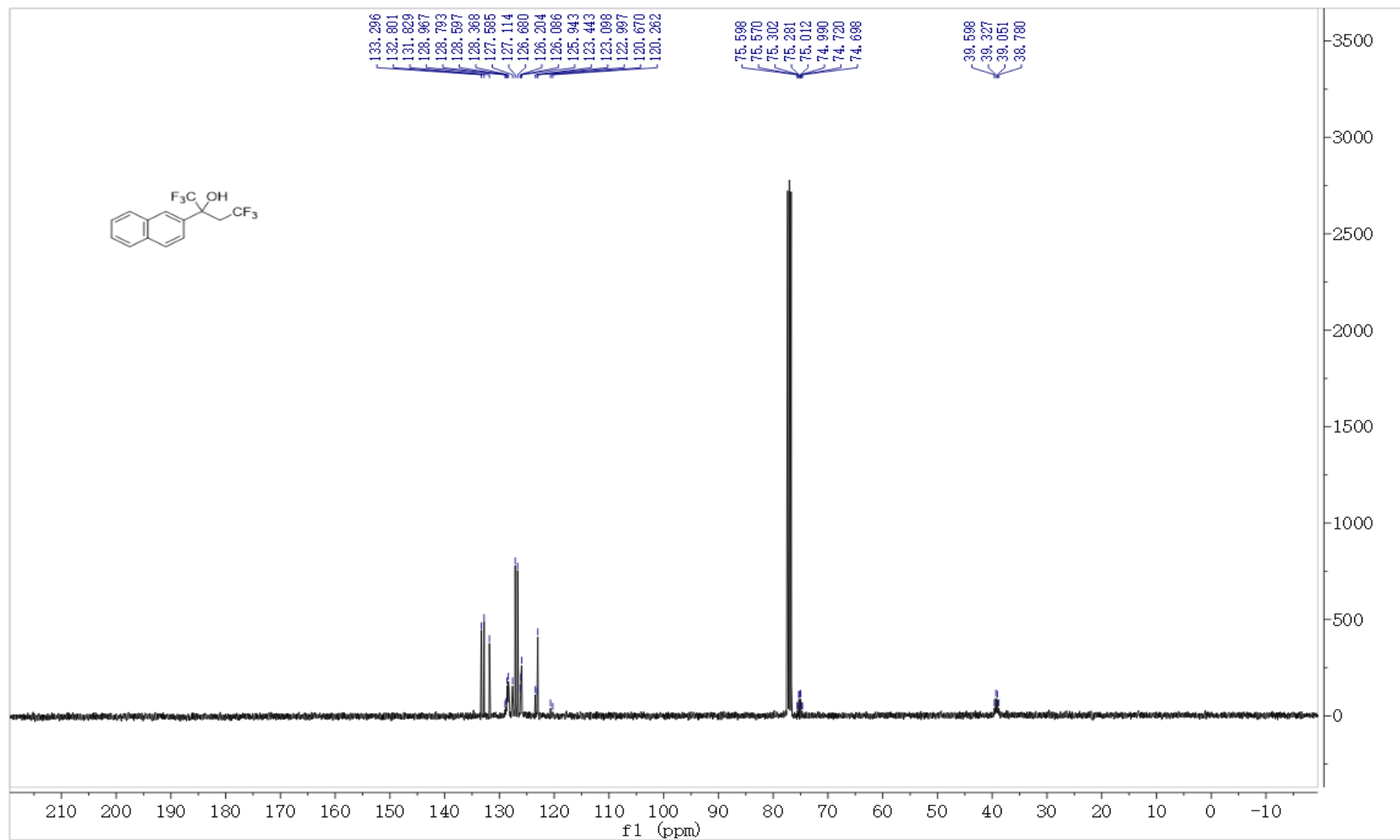
TOF MS EI+
1.10e4



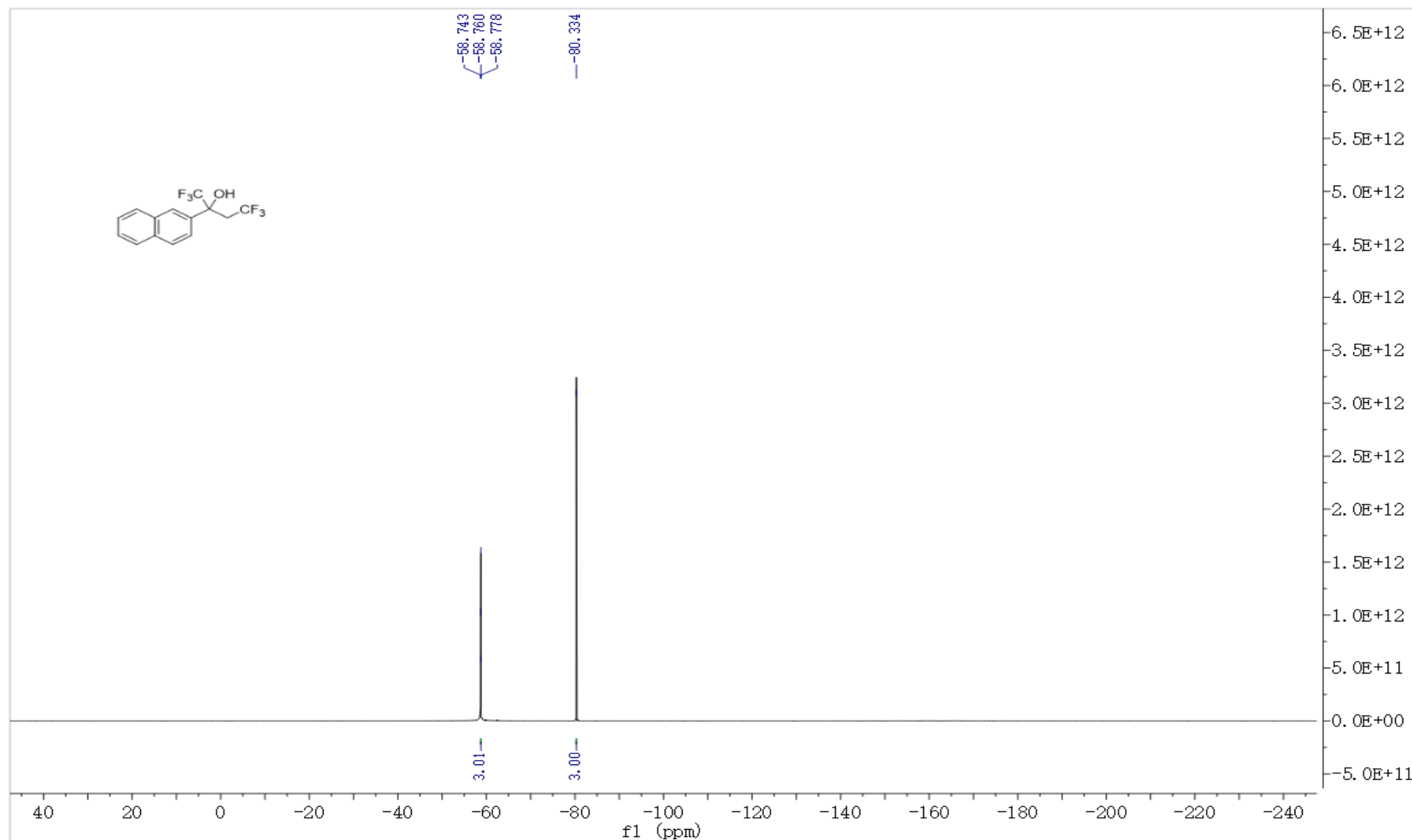
¹H NMR spectrum of 2o



¹³C NMR spectrum of 2o



¹⁹F NMR spectrum of 2o



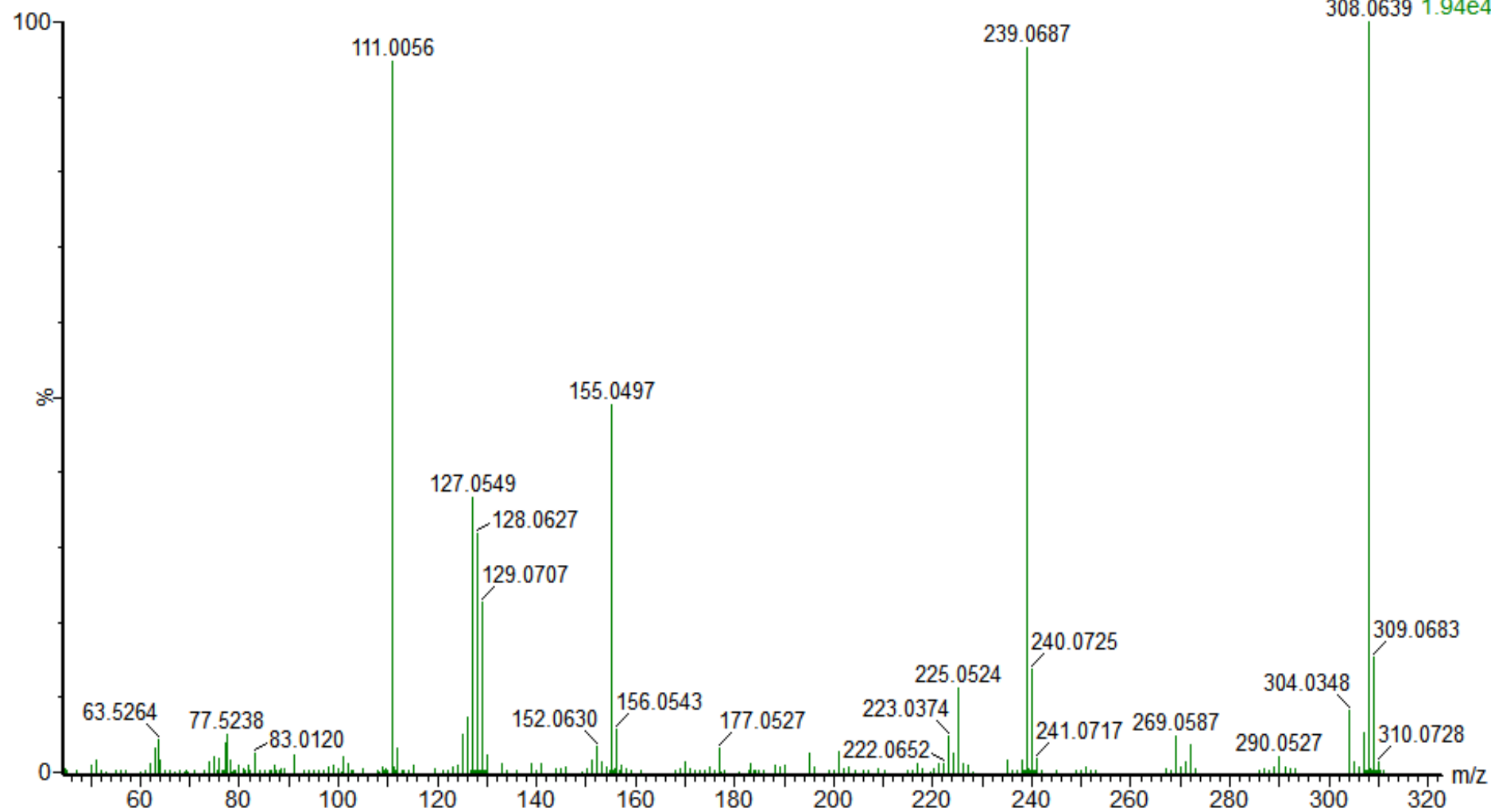
HRMS (EI) spectrum of 2o

CS-LC-M-308

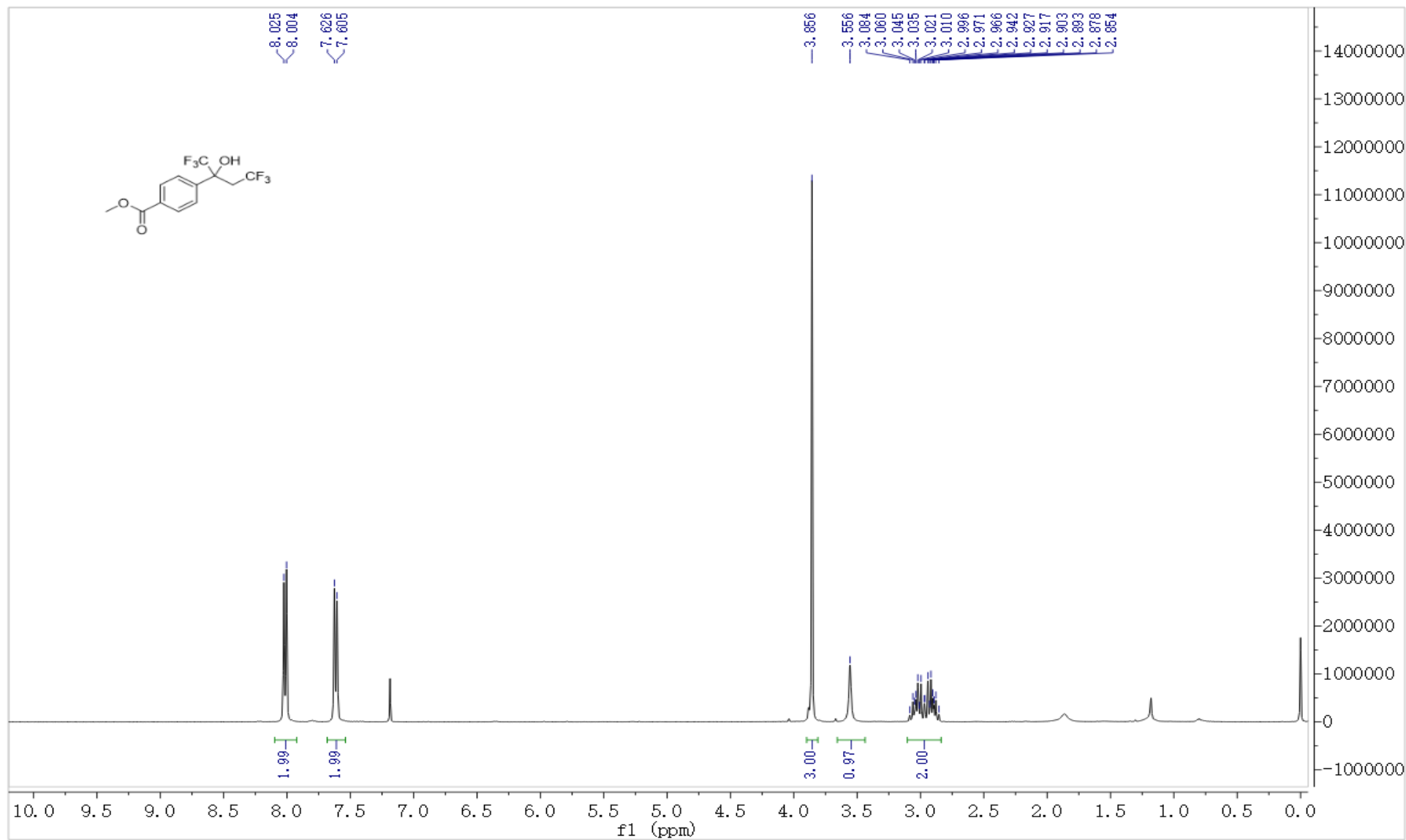
Waters GCT Premier

20212807 61 (1.017) Cm (61-(23+29))

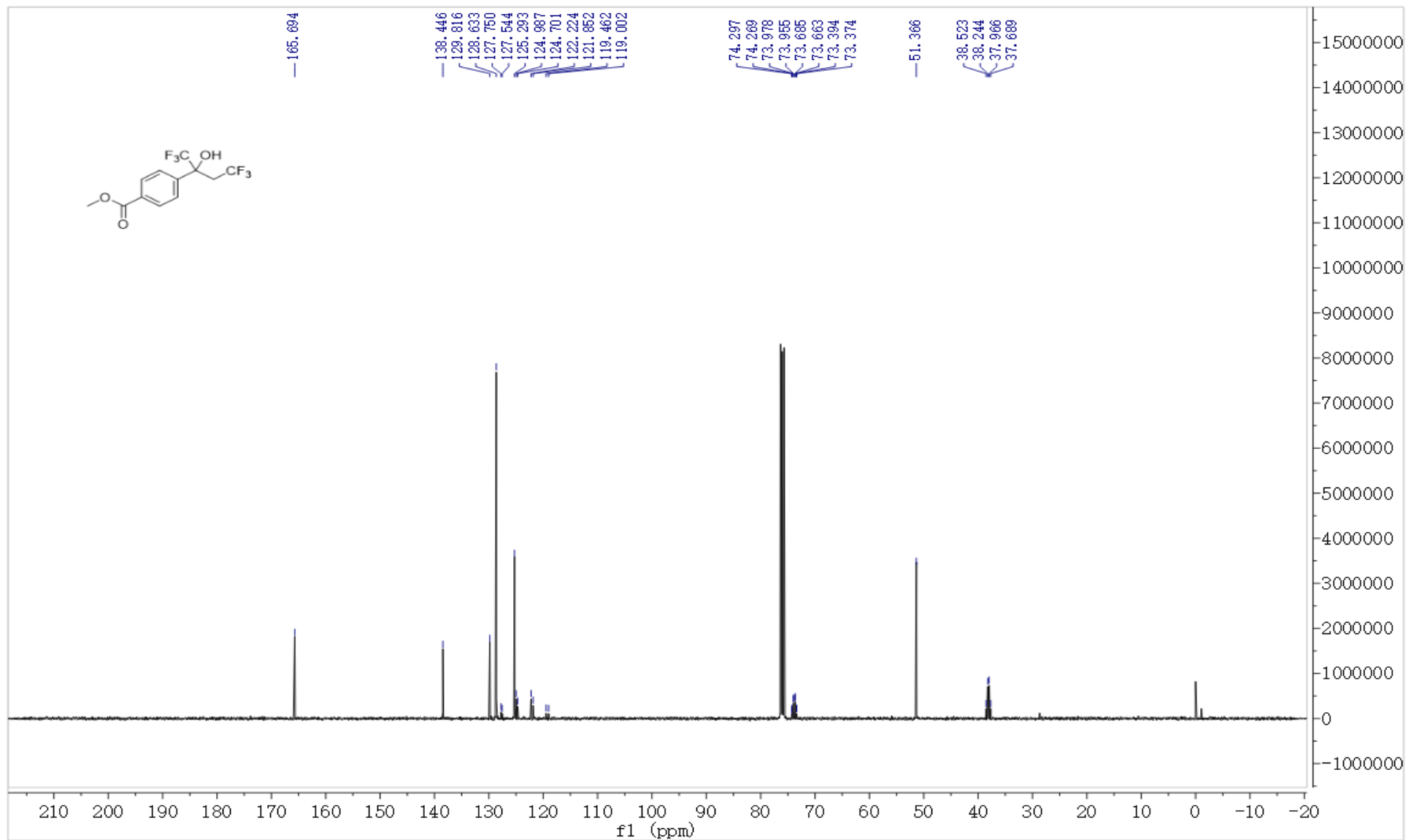
TOF MS EI+
308.0639 1.94e4



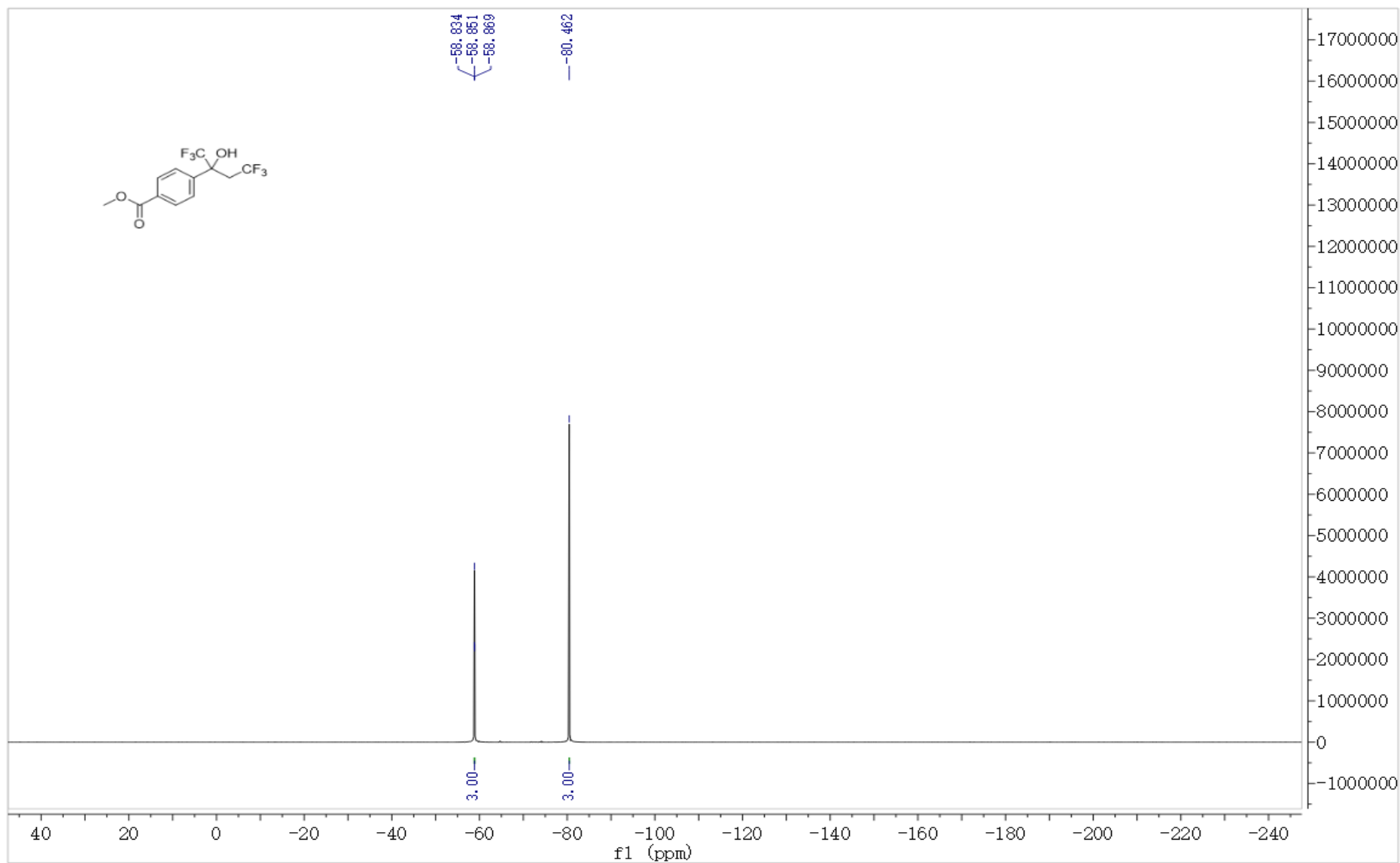
¹H NMR spectrum of 2p



¹³C NMR spectrum of 2p



¹⁹F NMR spectrum of 2p



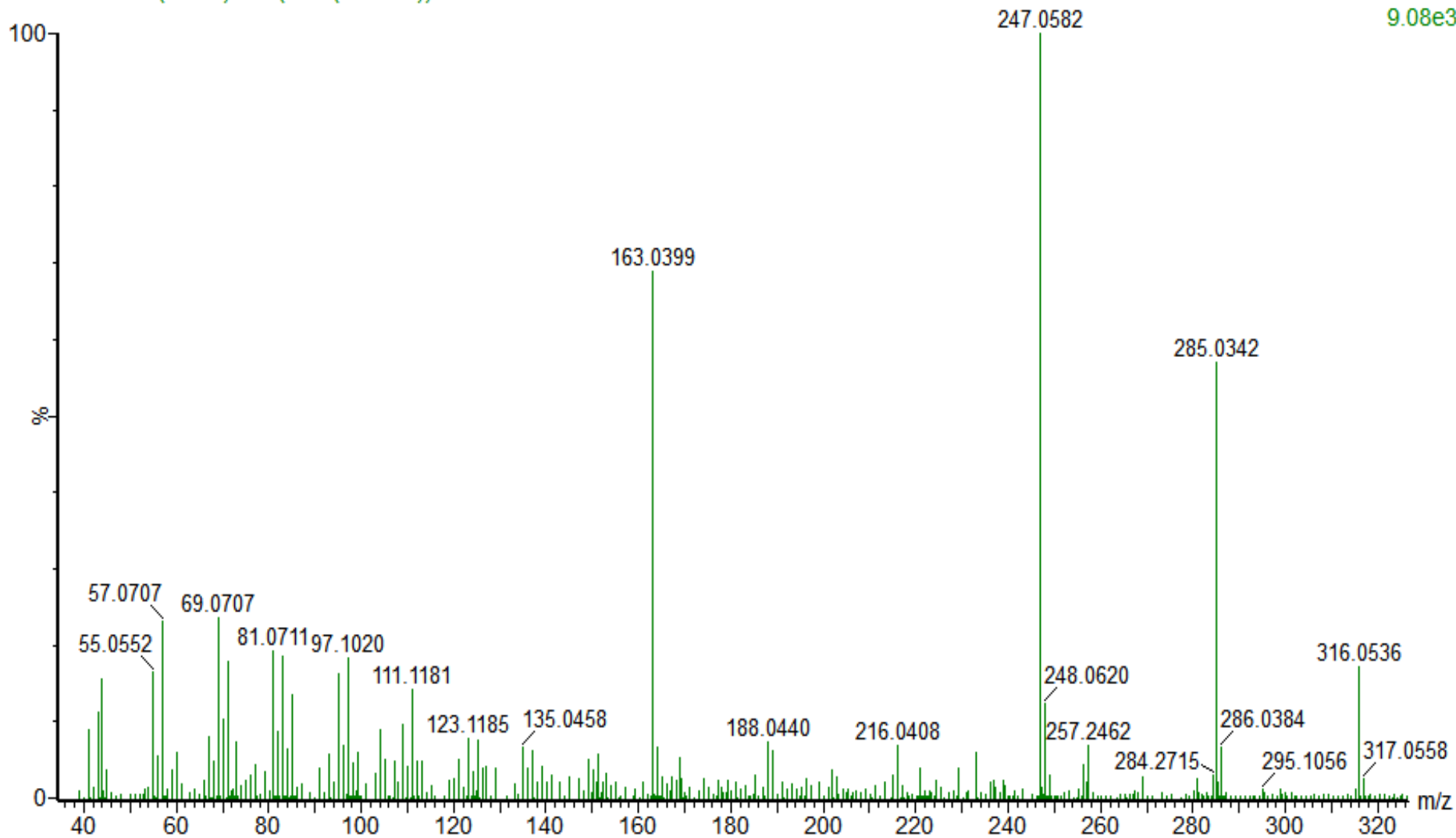
HRMS (EI) spectrum of 2p

CS-LC-P-316

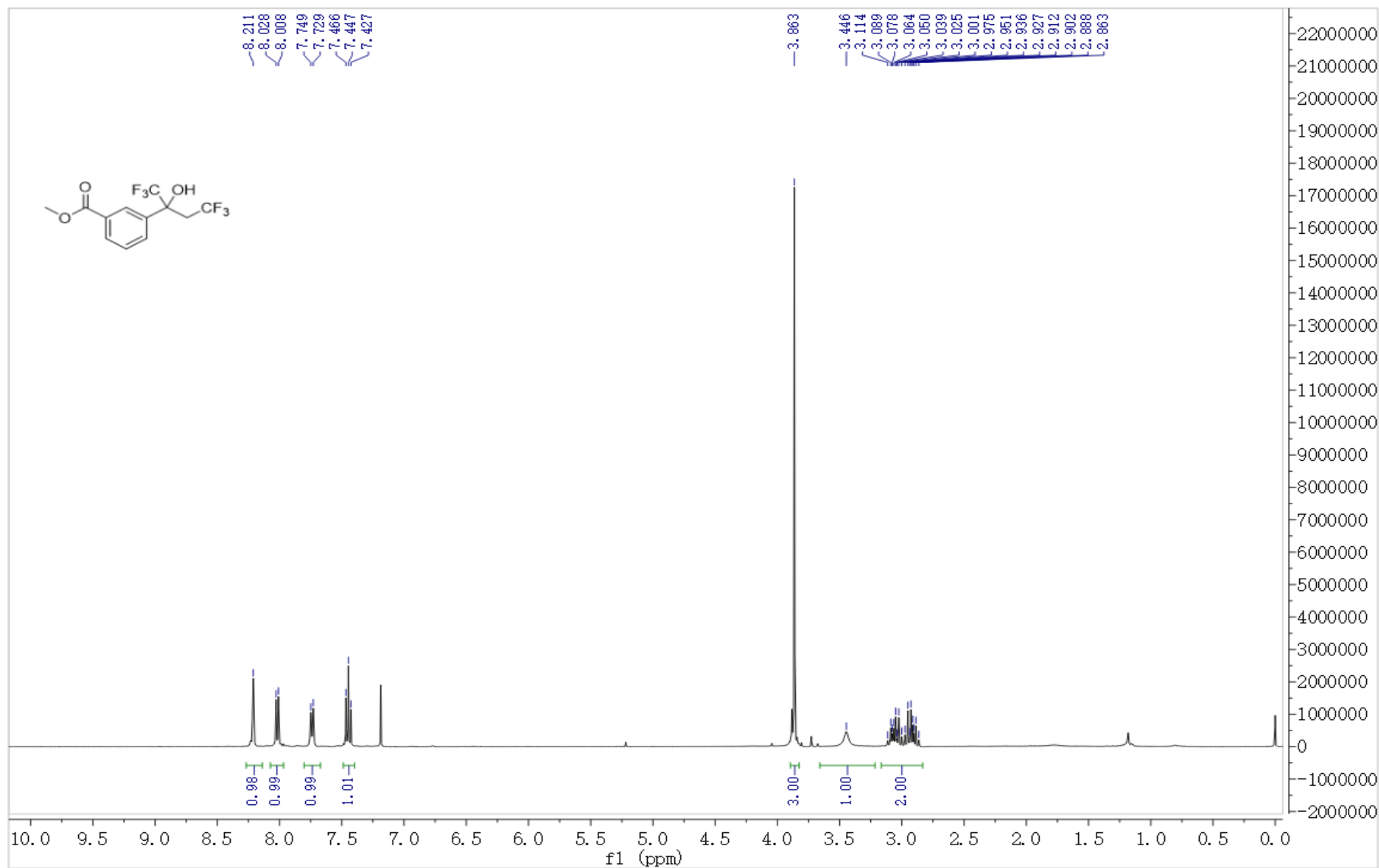
20212803 199 (3.317) Cm (199-(99+319))

Waters GCT Premier

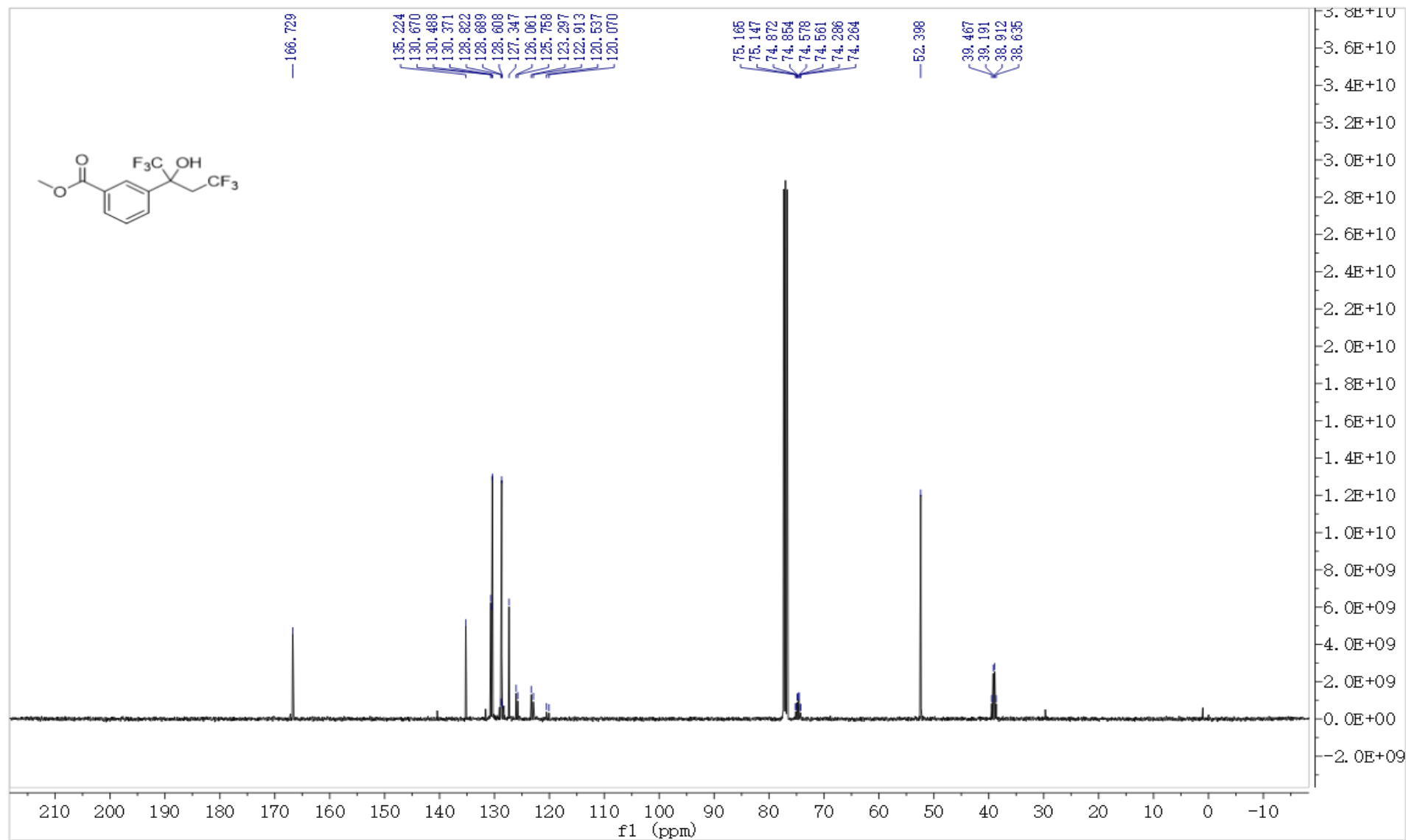
TOF MS EI+
9.08e3



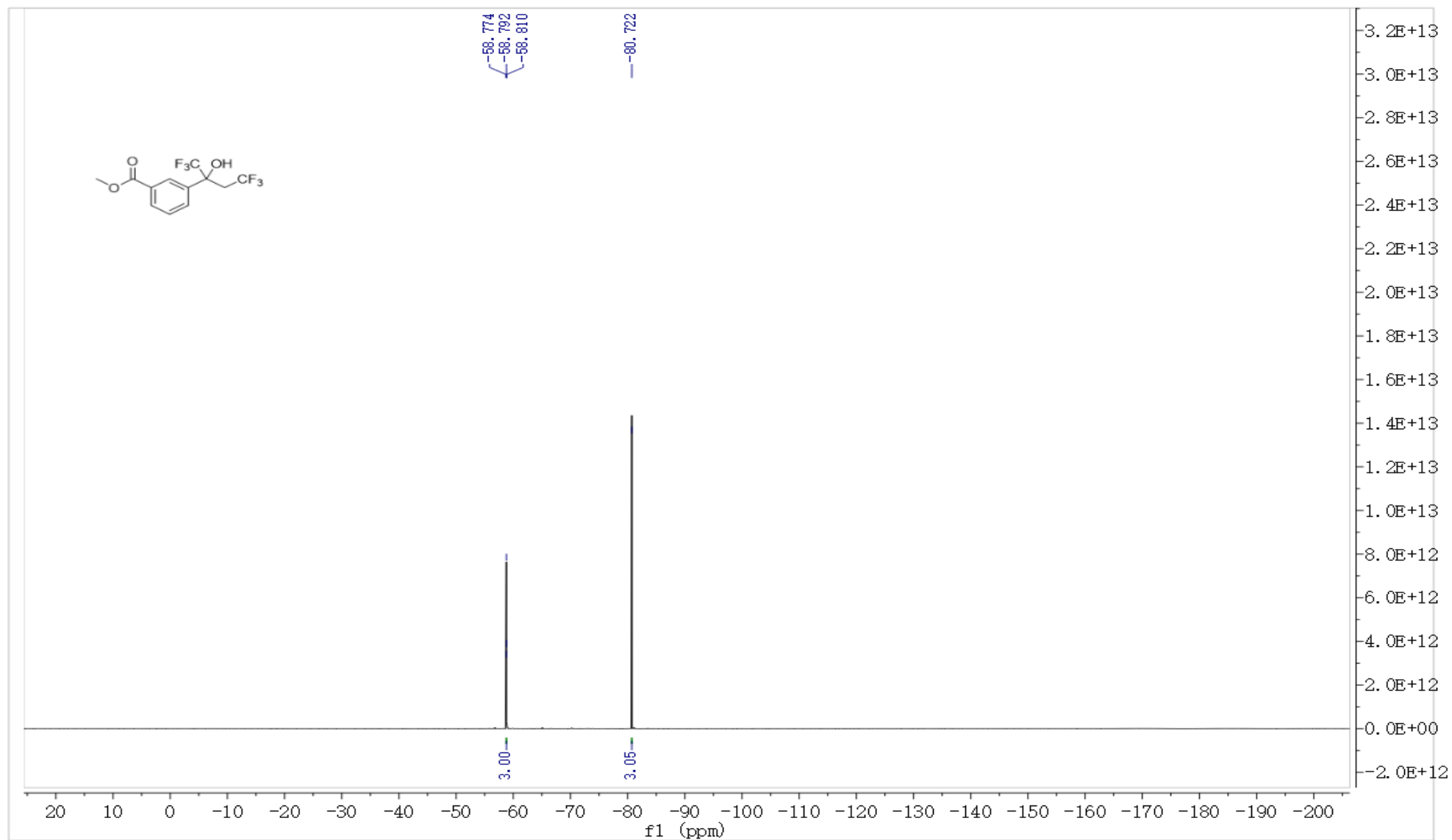
¹H NMR spectrum of 2q



¹³C NMR spectrum of 2q



¹⁹F NMR spectrum of 2q



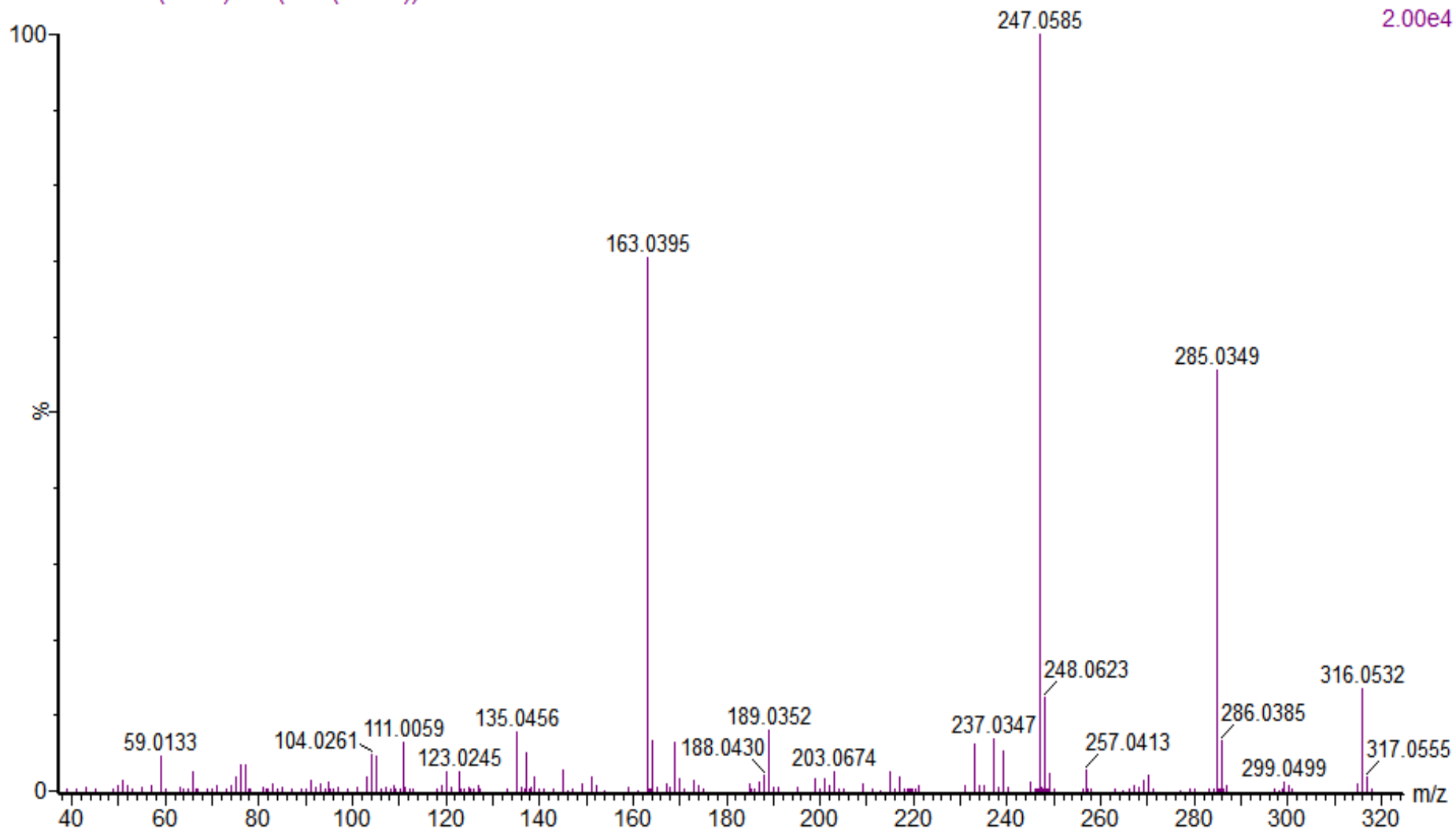
HRMS (EI) spectrum of 2q

CS-LC-M-316

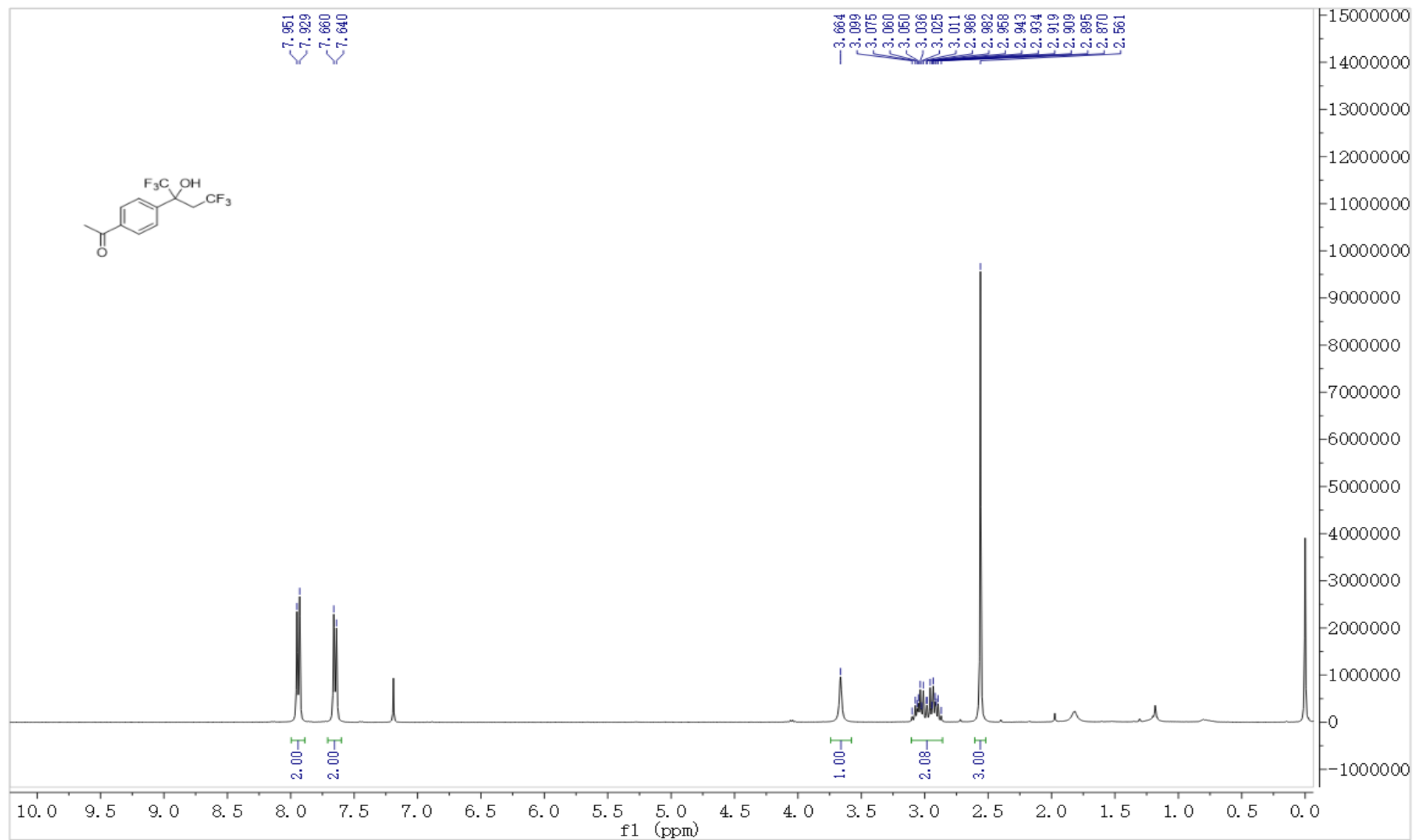
20212804 101 (1.683) Cm (101-(21+58))

Waters GCT Premier

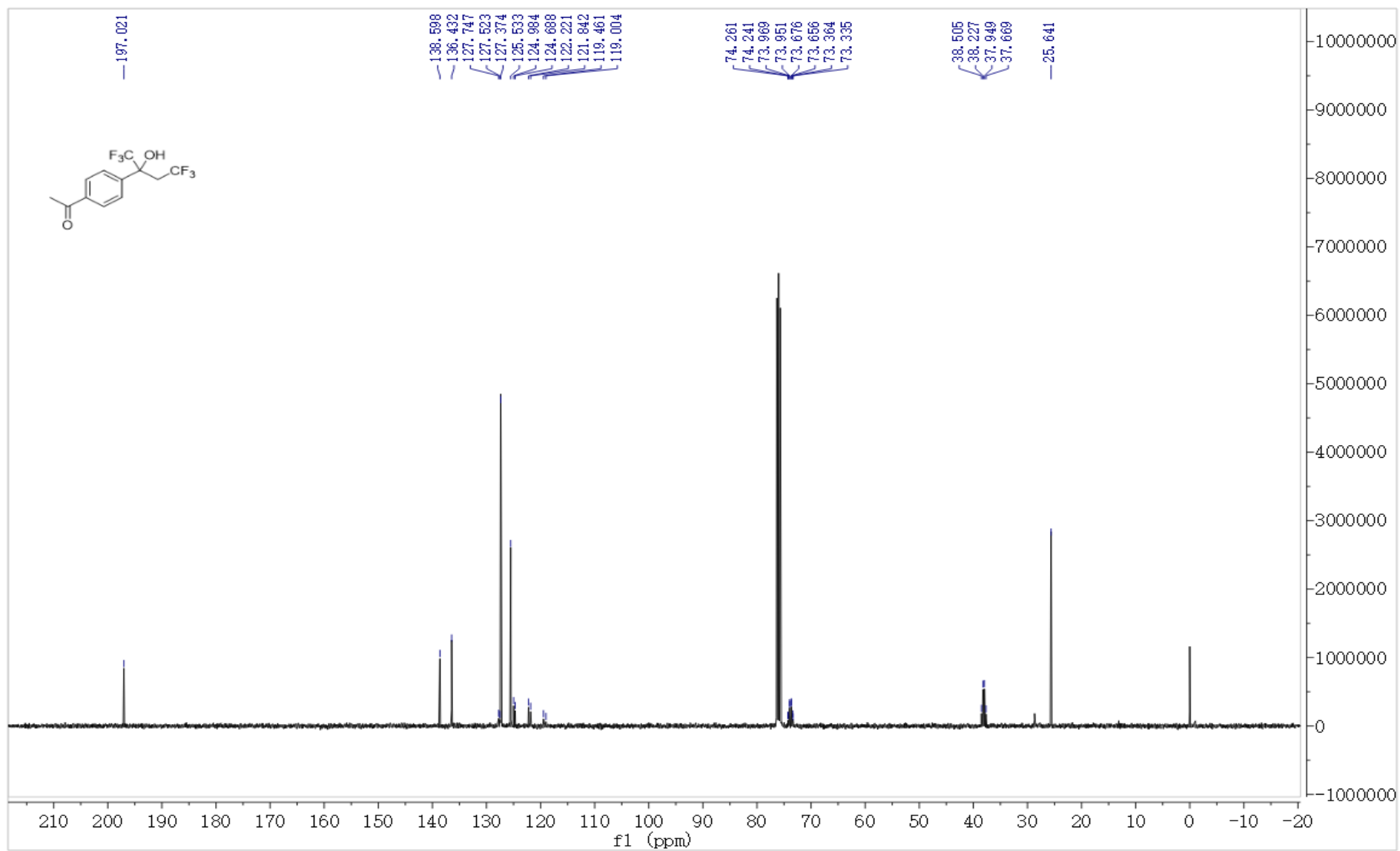
TOF MS EI+
2.00e4



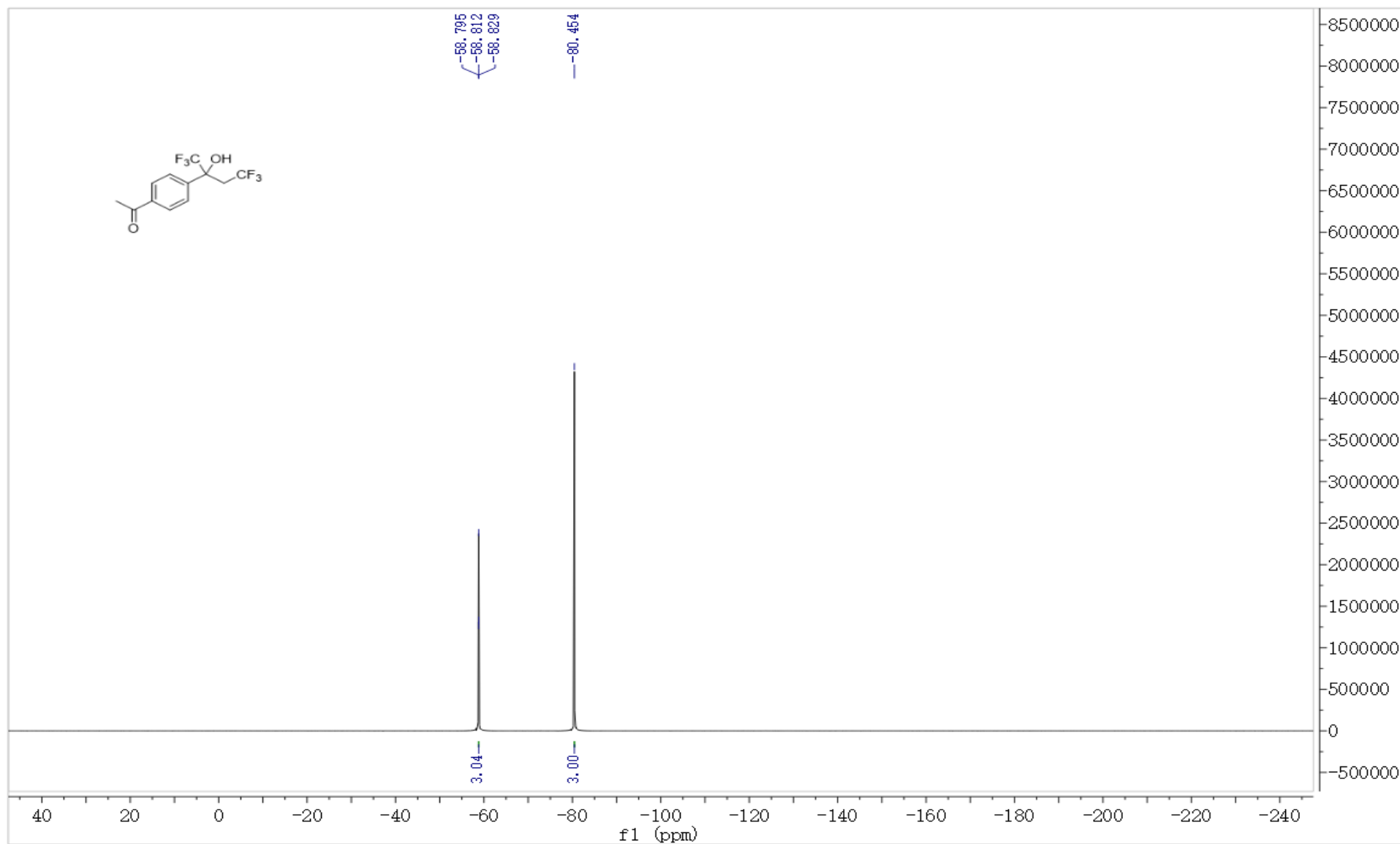
¹H NMR spectrum of 2r



¹³C NMR spectrum of 2r



¹⁹F NMR spectrum of 2r



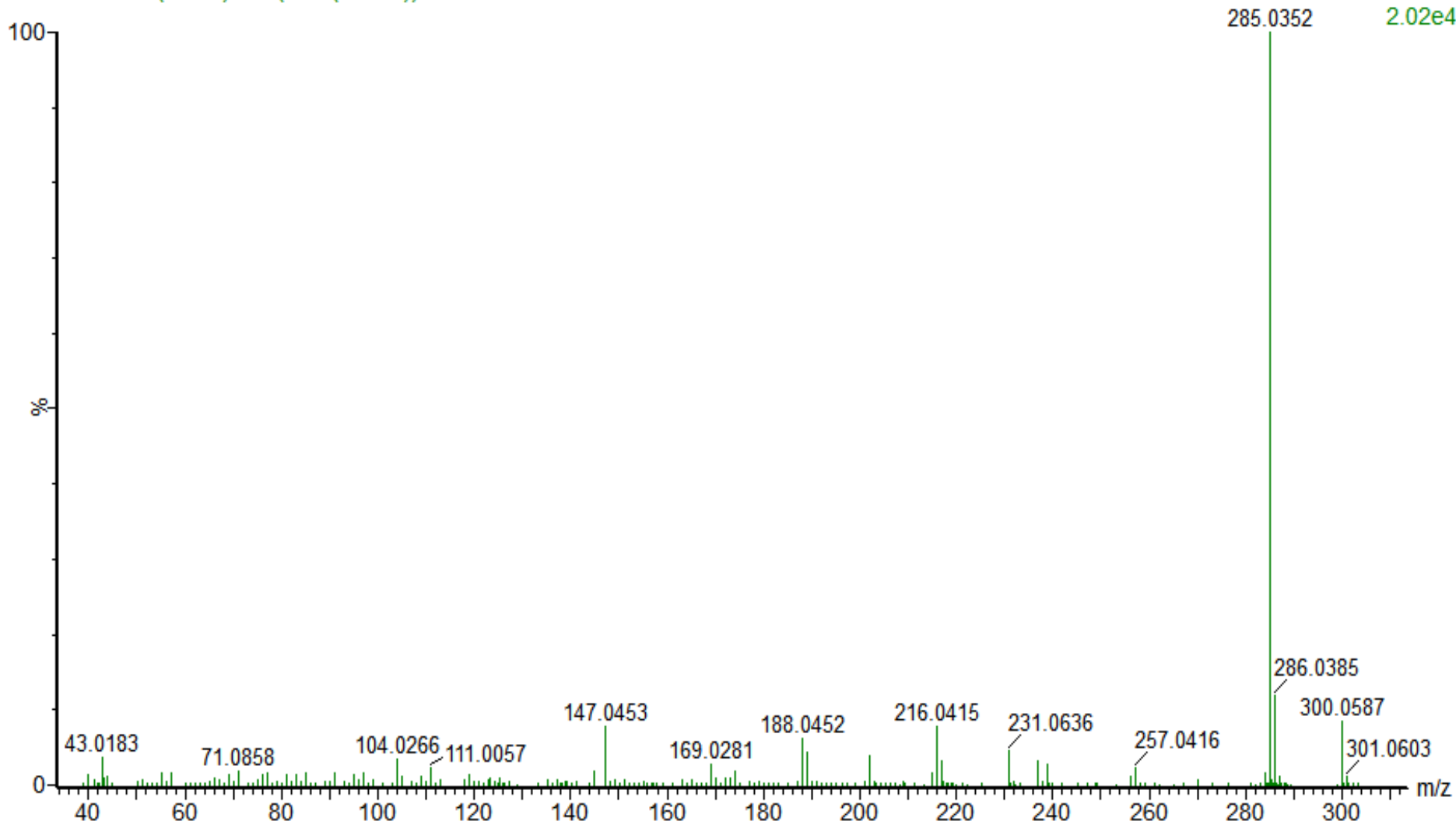
HRMS (EI) spectrum of 2r

CS-LC-P-300

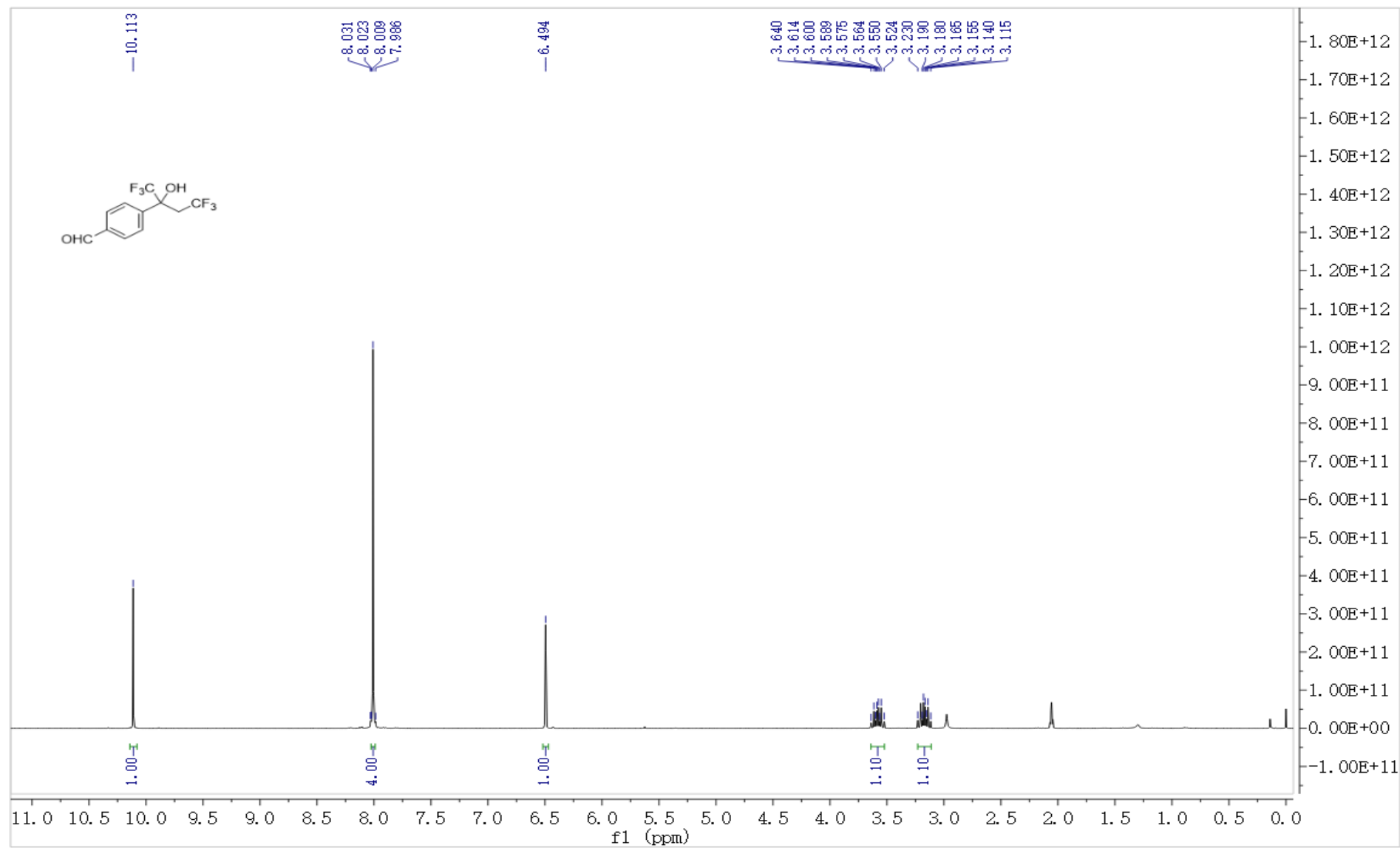
20212802 303 (5.050) Cm (303-(41+44))

Waters GCT Premier

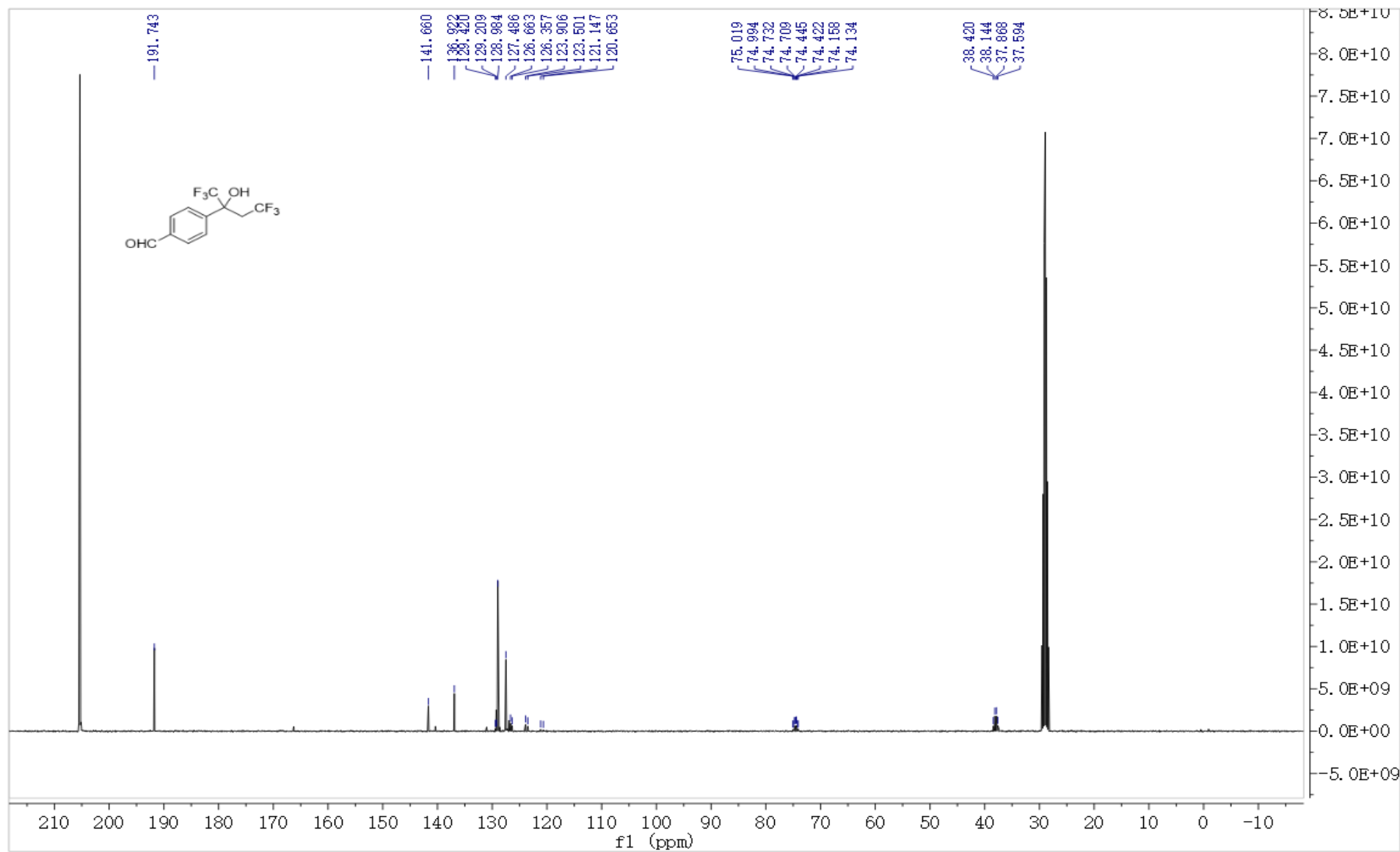
TOF MS EI+
2.02e4



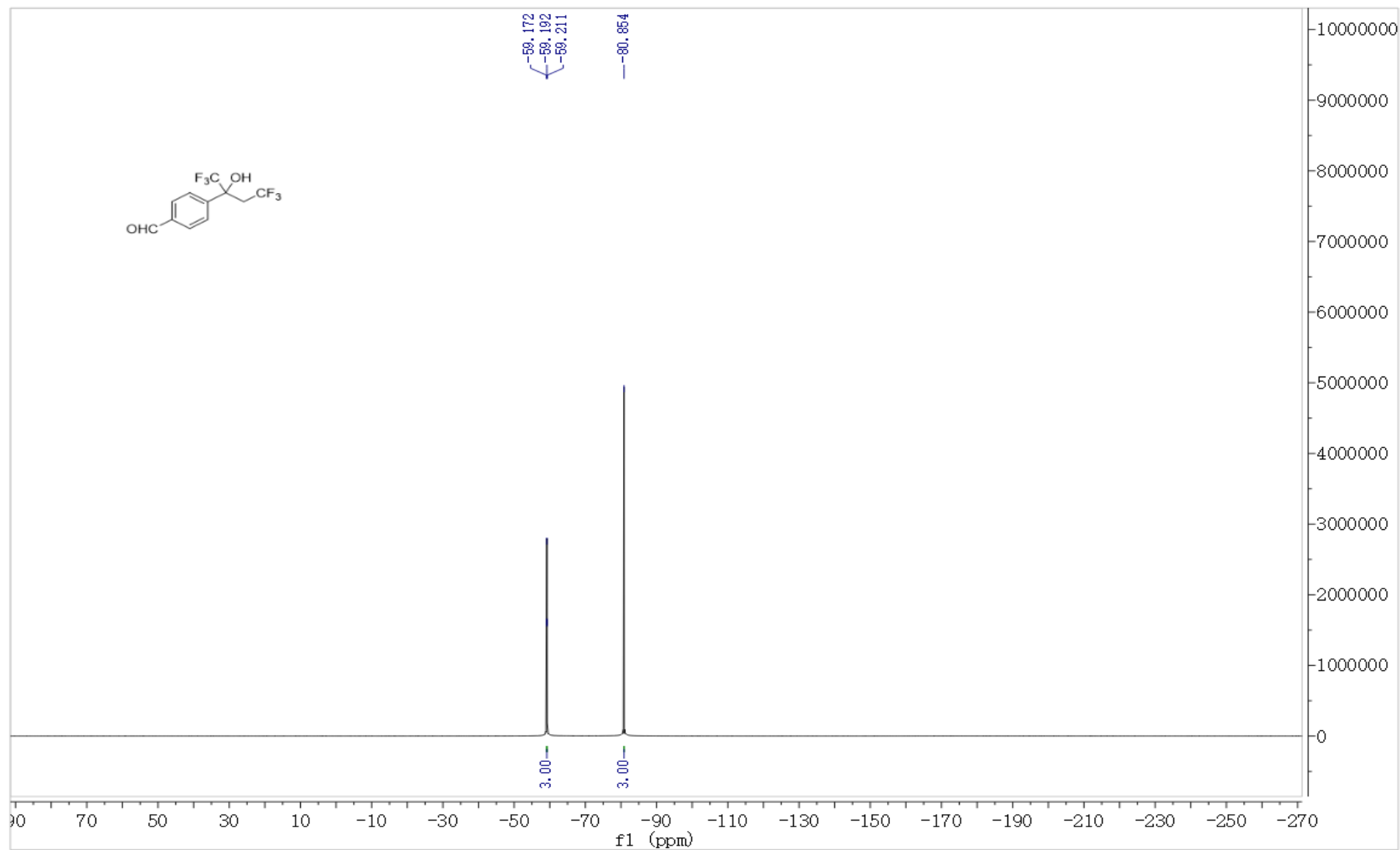
¹H NMR spectrum of 2s



¹³C NMR spectrum of 2s



¹⁹F NMR spectrum of 2s



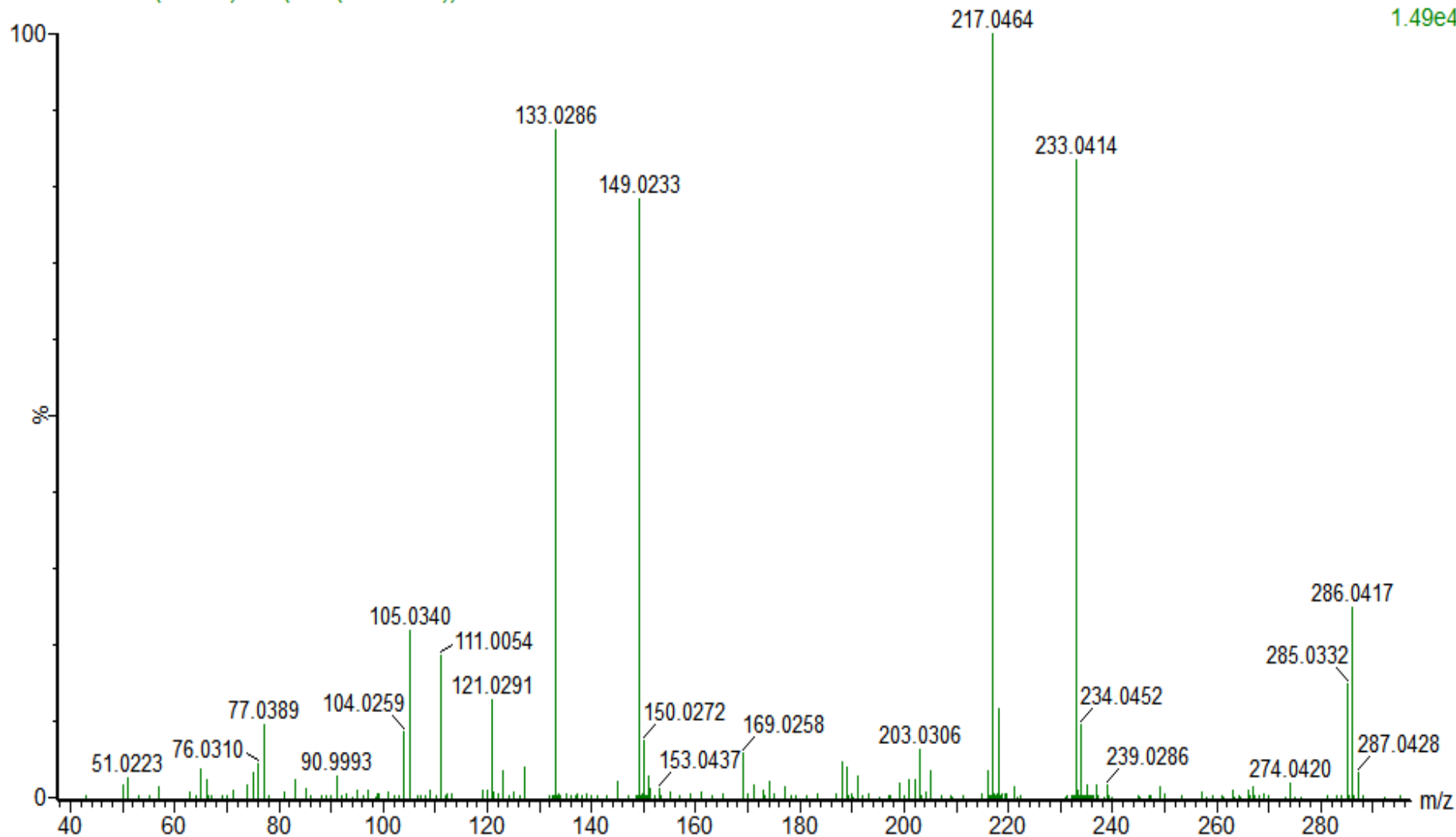
HRMS (EI) spectrum of 2s

CS-LC-P-286

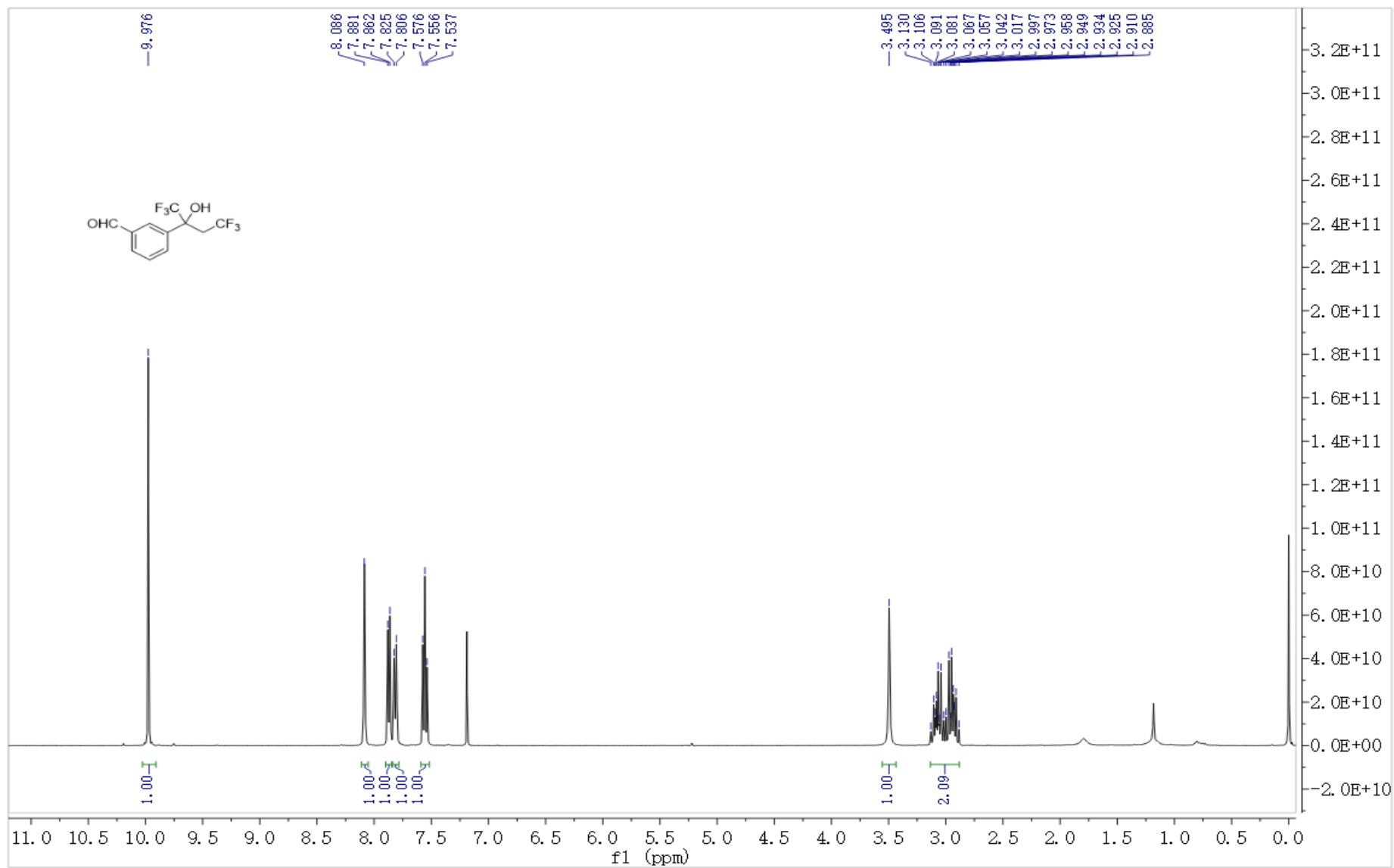
Waters GCT Premier

20220481 738 (12.304) Cm (738-(1571+275))

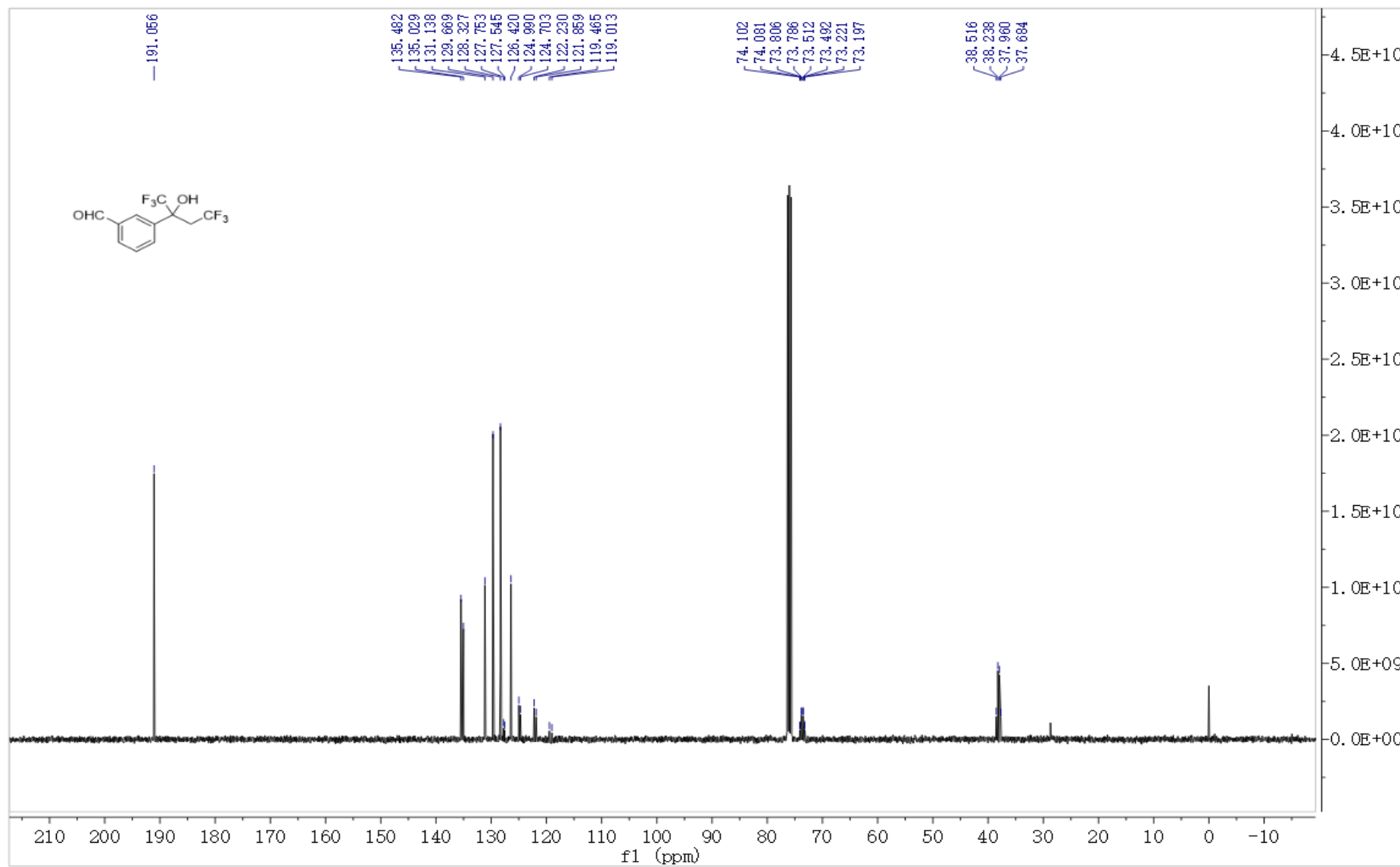
TOF MS EI+
1.49e4



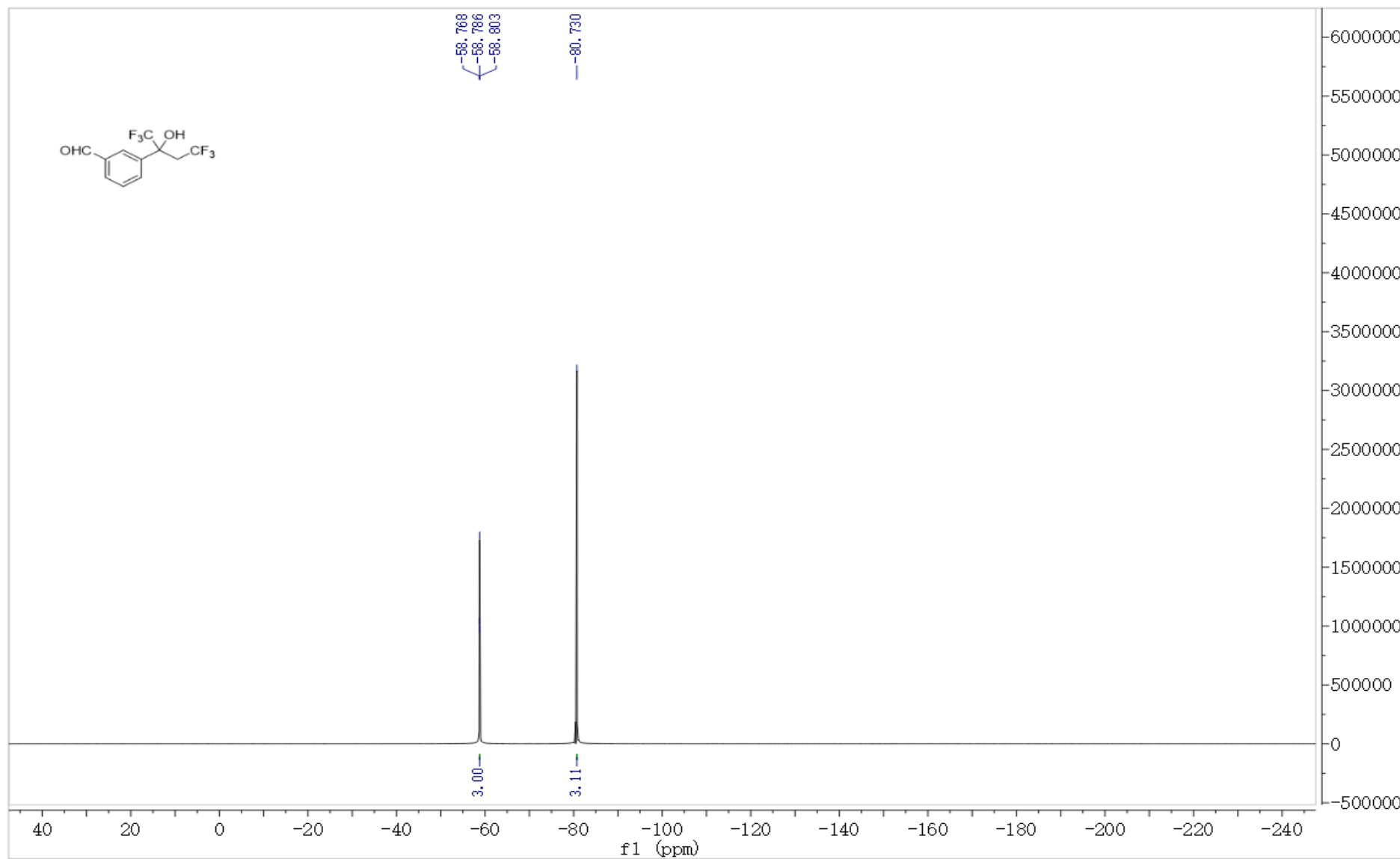
¹H NMR spectrum of 2t



¹³C NMR spectrum of 2t



¹⁹F NMR spectrum of 2t



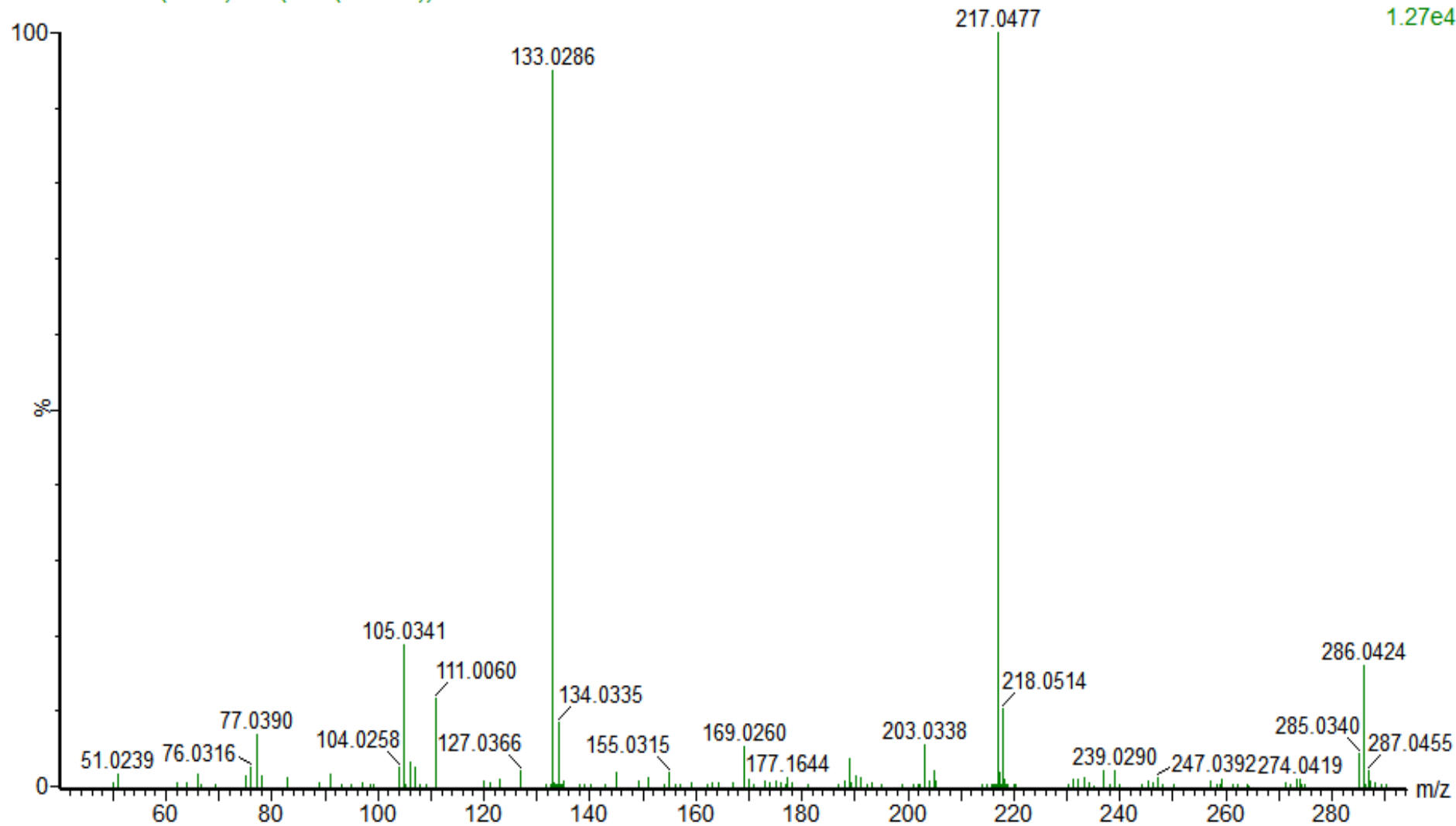
HRMS (EI) spectrum of 2t

CS-LC-M-286

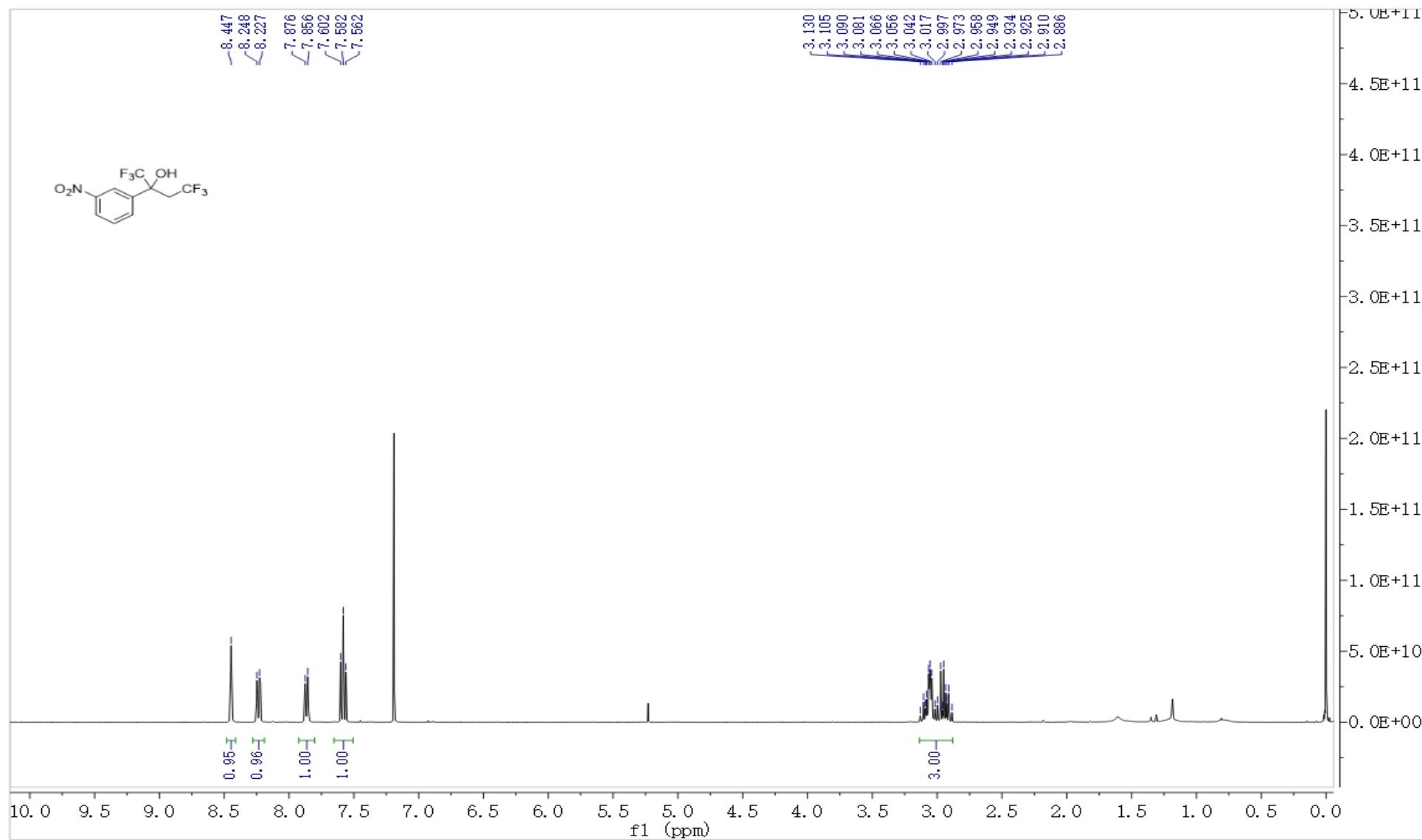
Waters GCT Premier

20212806 143 (2.383) Cm (143-(33+432))

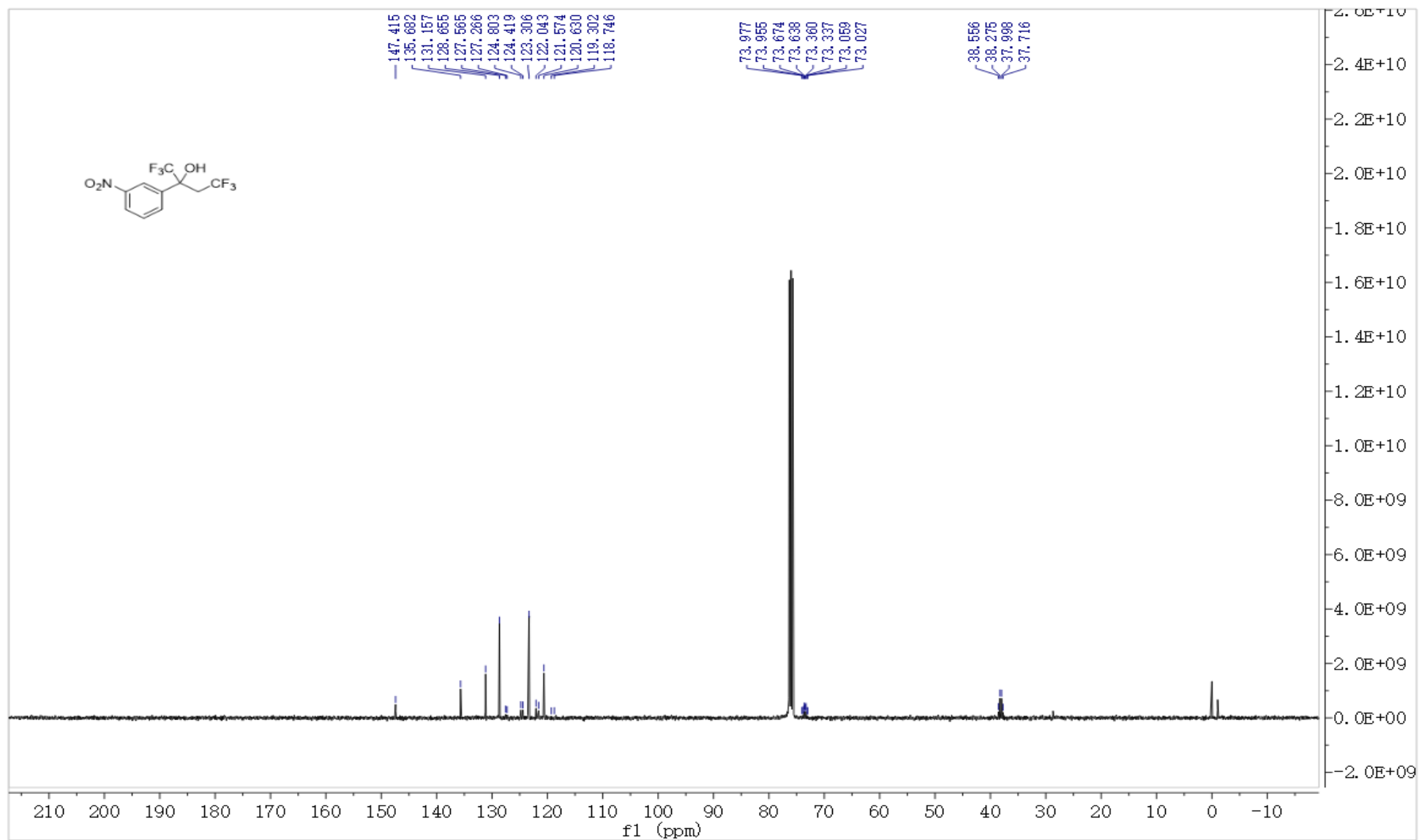
TOF MS EI+
1.27e4



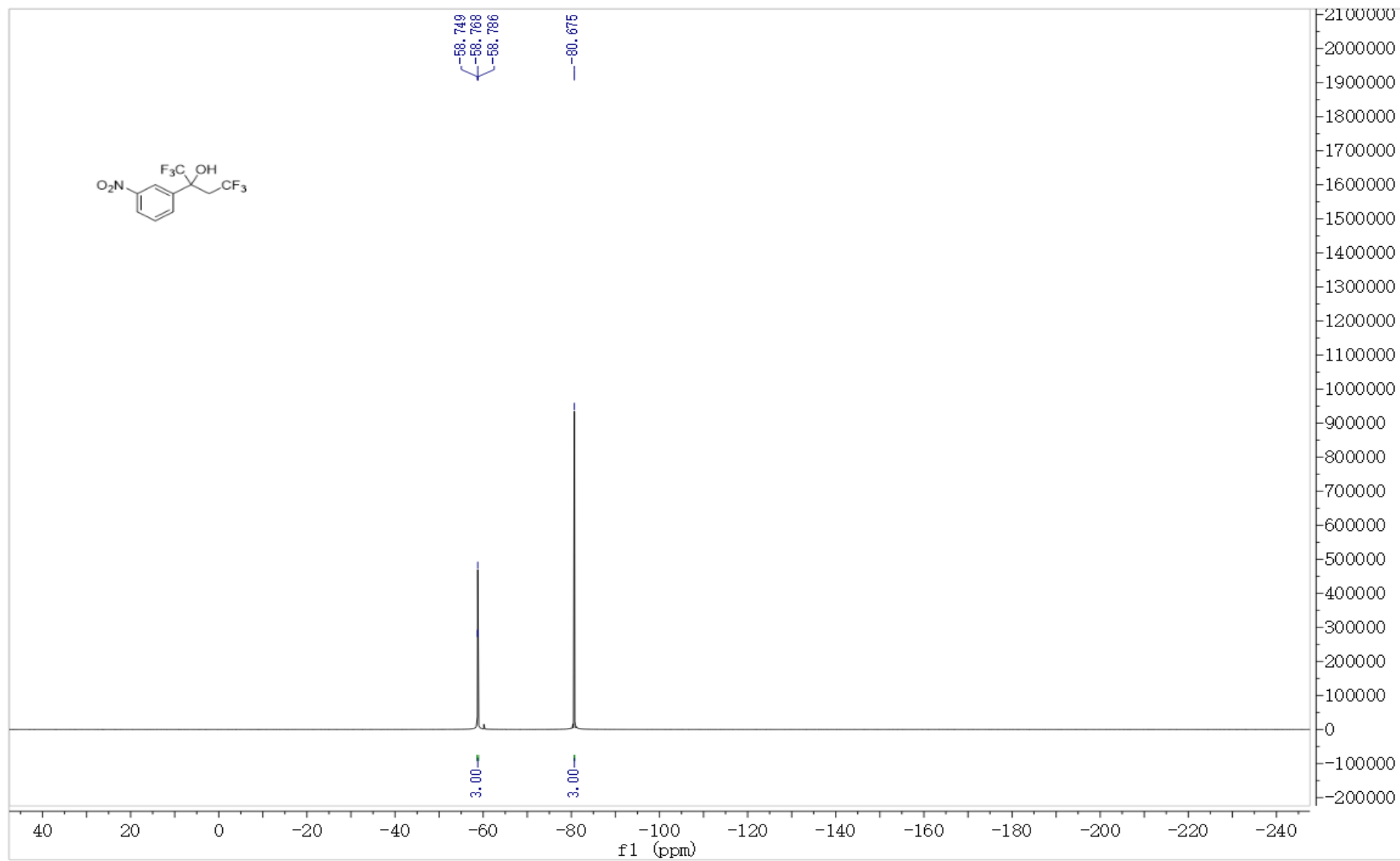
¹H NMR spectrum of 2u



¹³C NMR spectrum of 2u



¹⁹F NMR spectrum of 2u



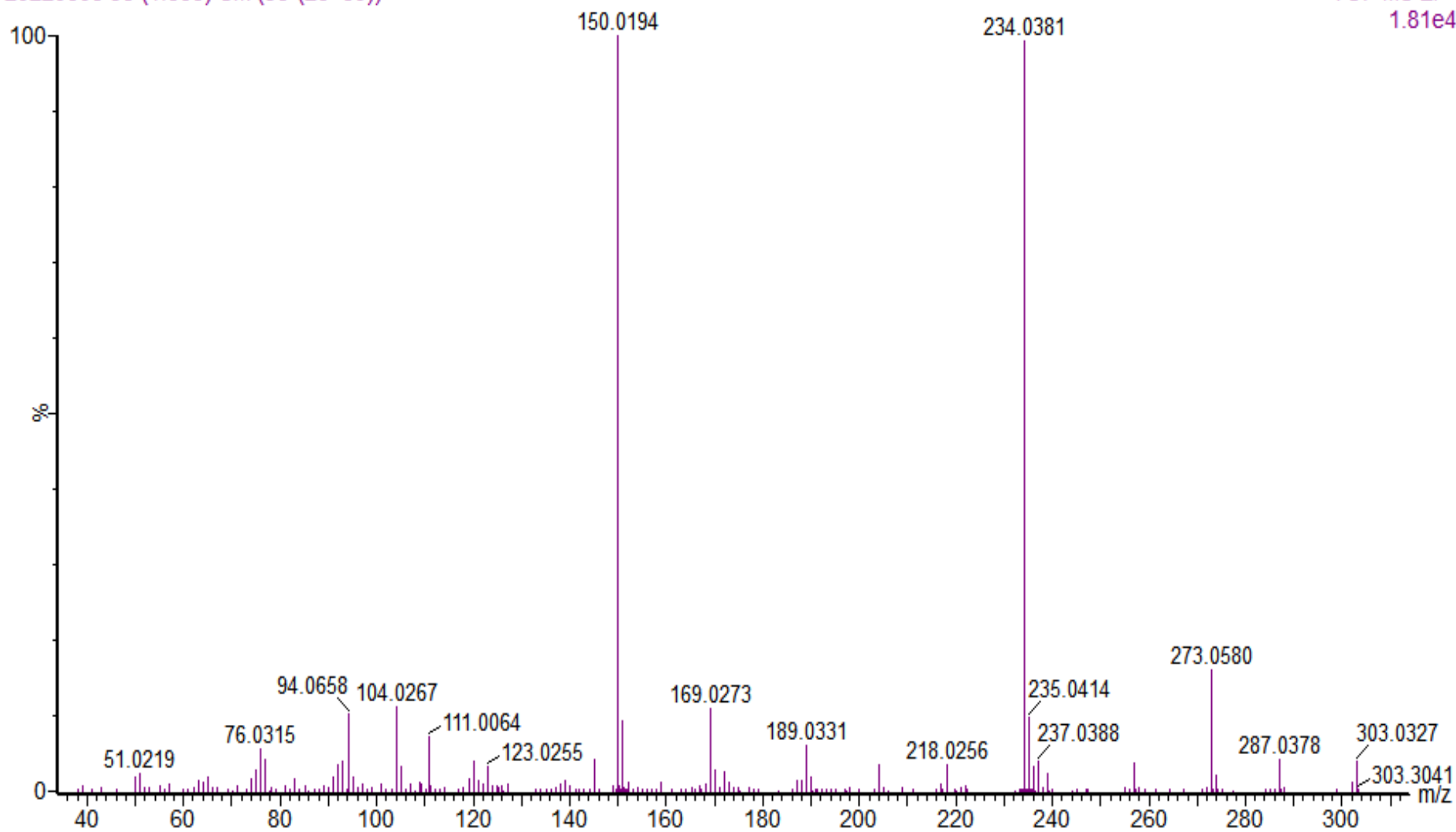
HRMS (EI) spectrum of 2u

CS-LC-M-303

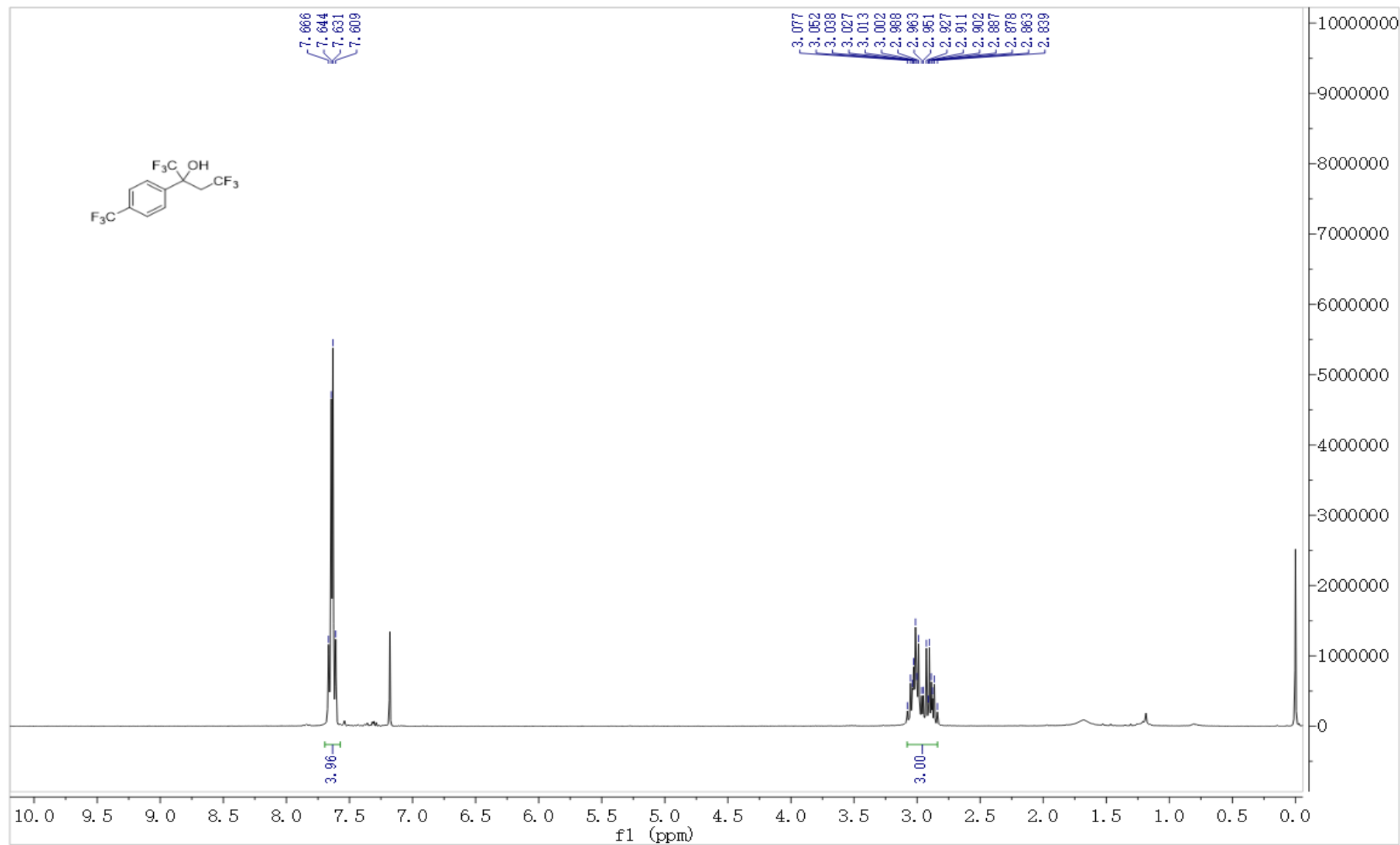
20220308 98 (1.633) Cm (98-(23+60))

Waters GCT Premier

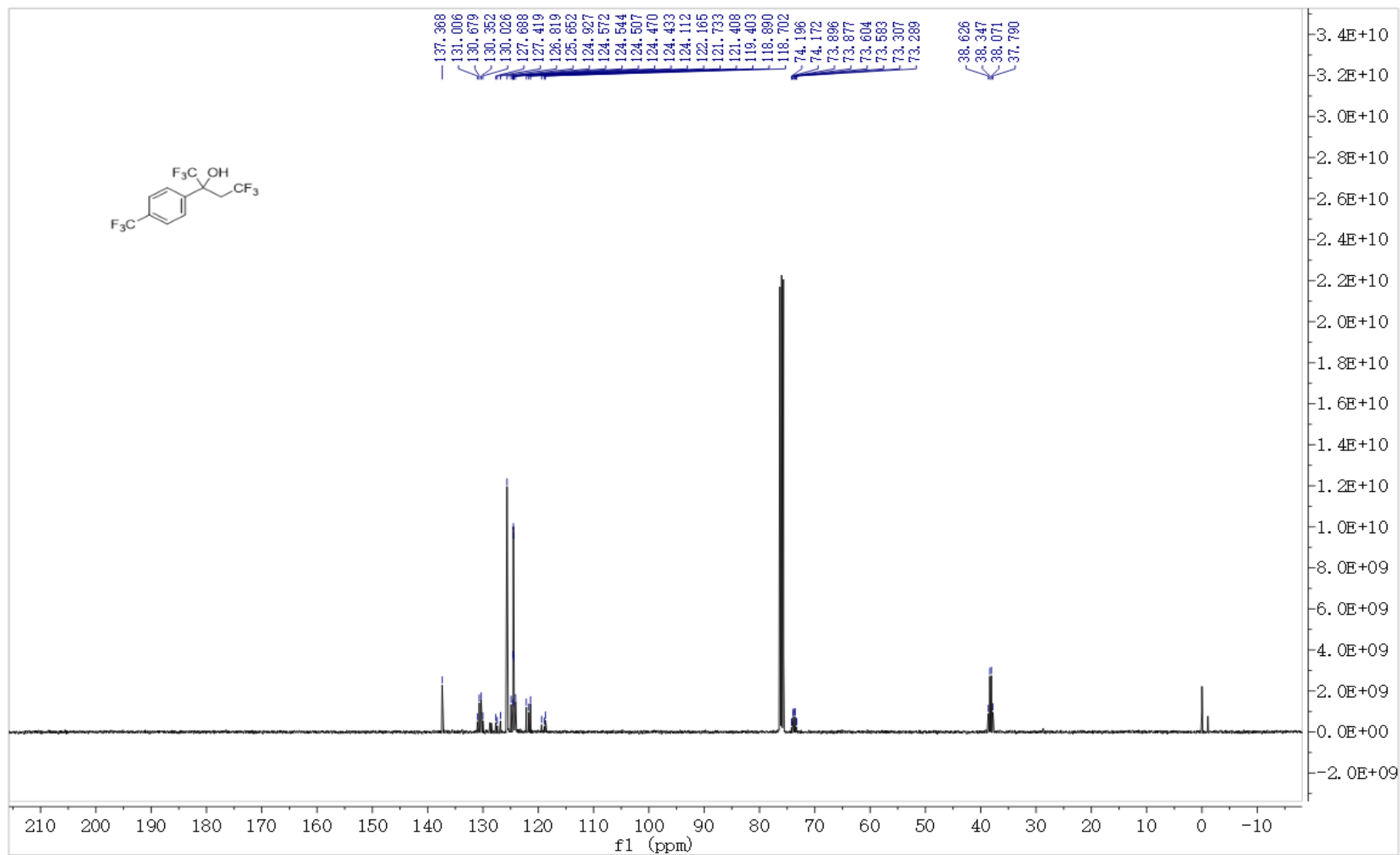
TOF MS EI+
1.81e4



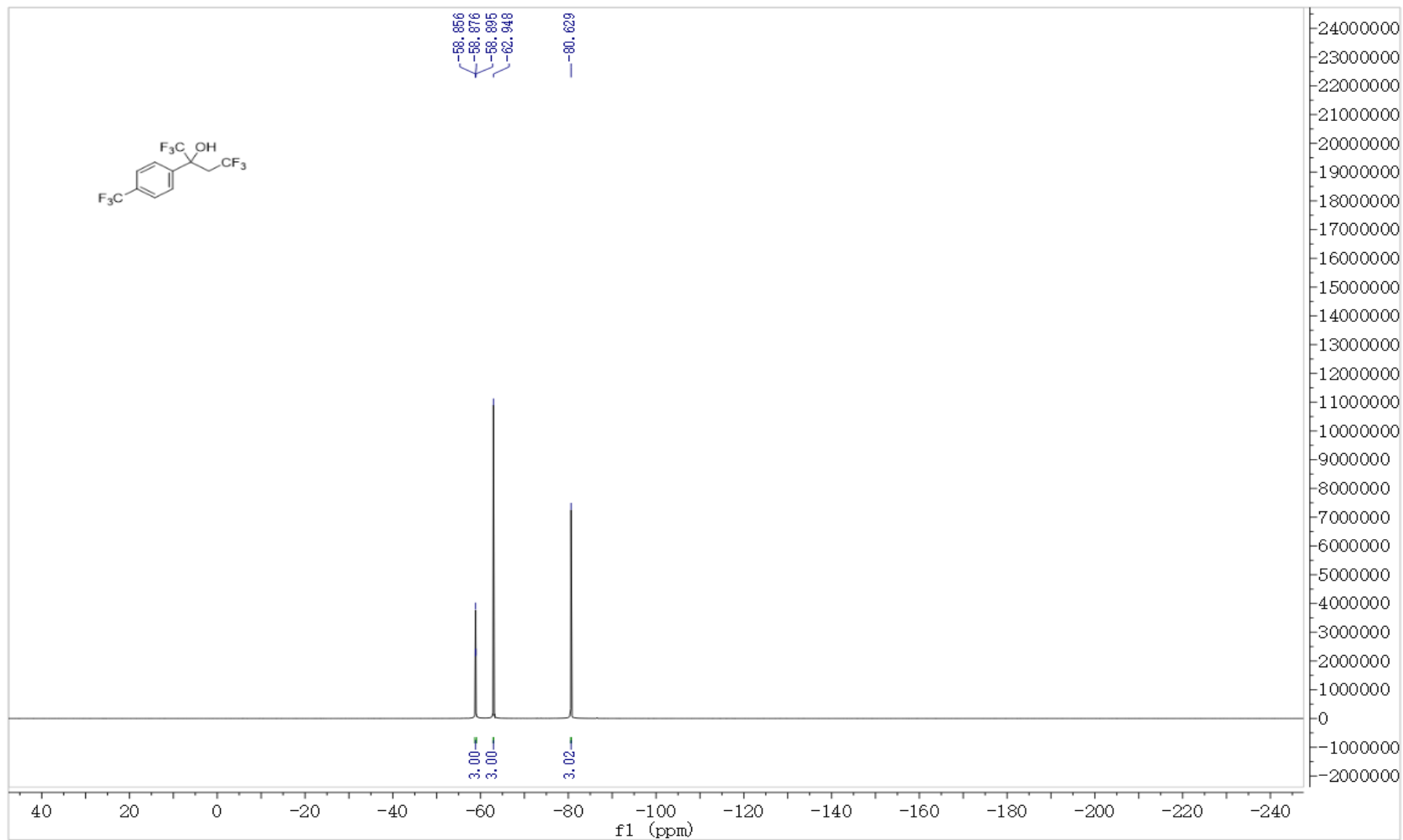
¹H NMR spectrum of 2v



¹³C NMR spectrum of 2v



¹⁹F NMR spectrum of 2v



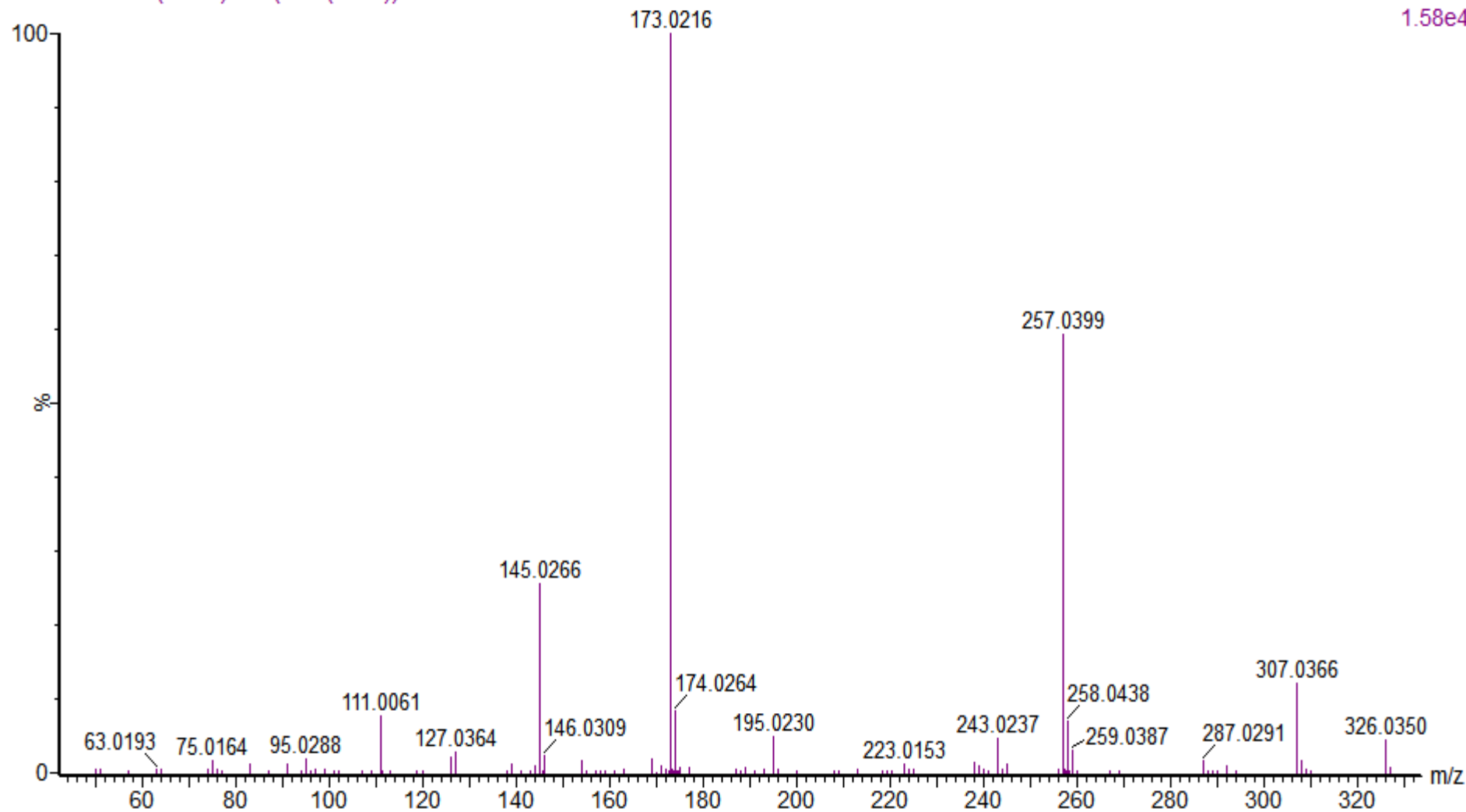
HRMS (EI) spectrum of 2v

CS-LC-P-326

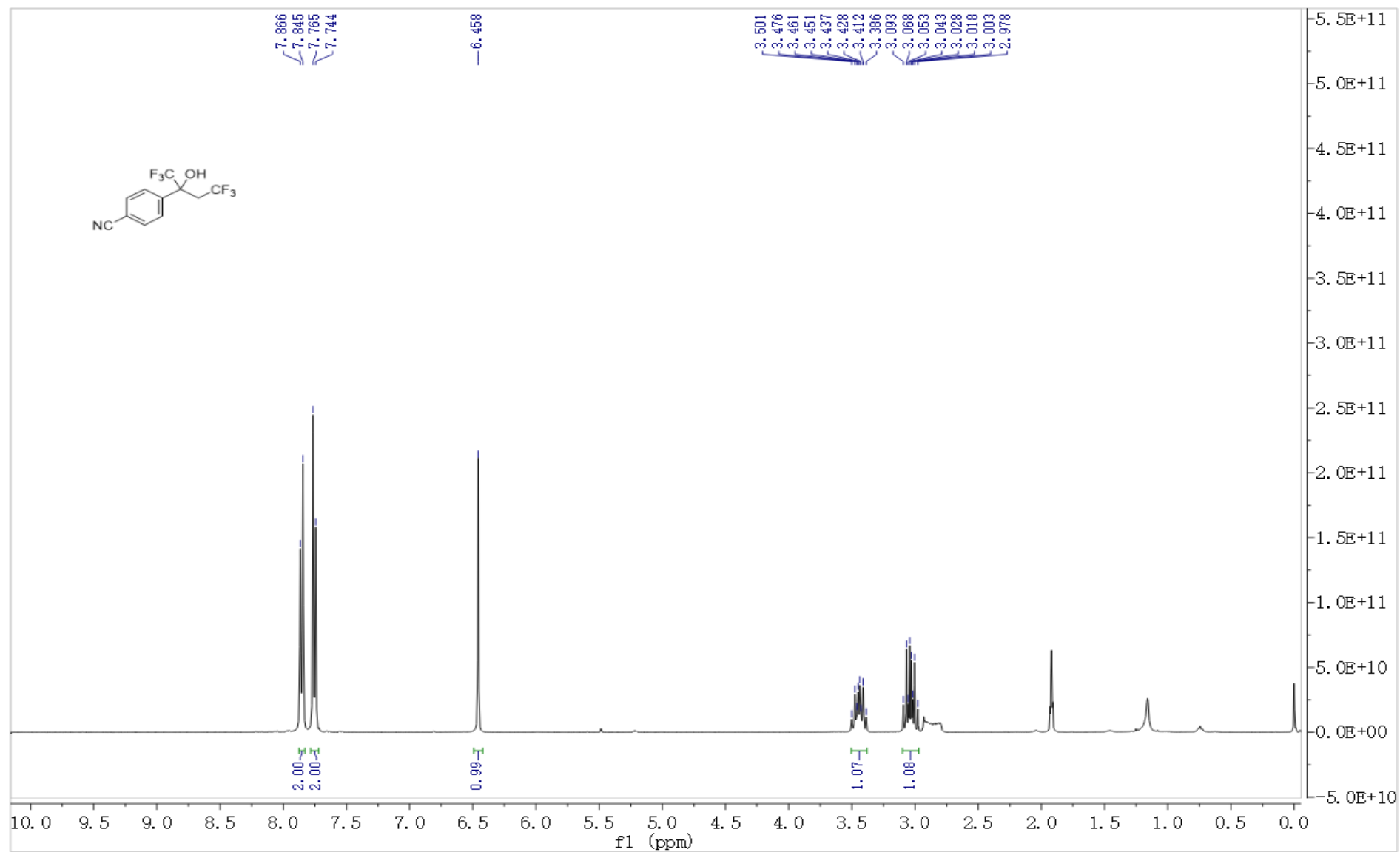
20220302 132 (2.200) Cm (132-(1+21))

Waters GCT Premier

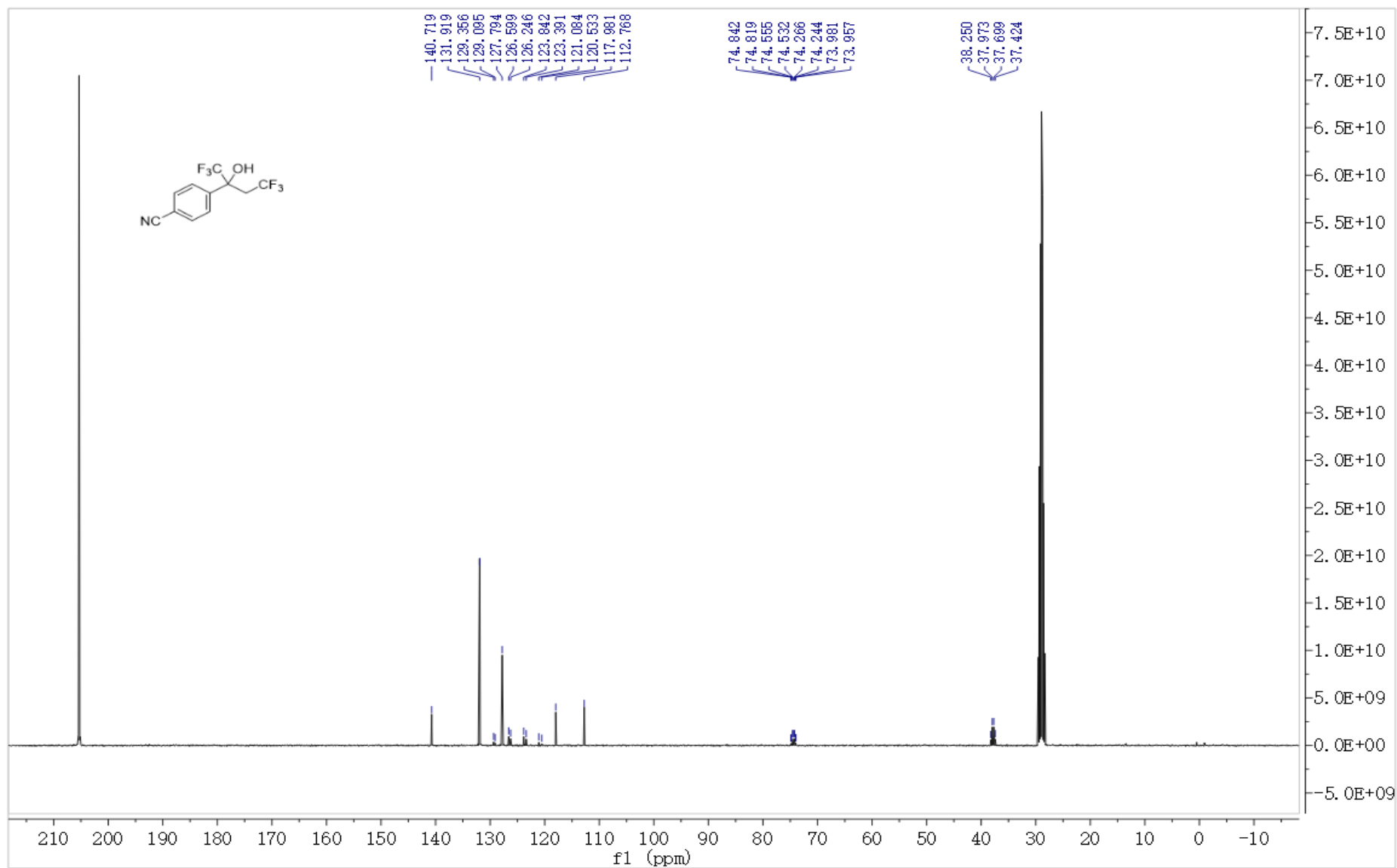
TOF MS EI+
1.58e4



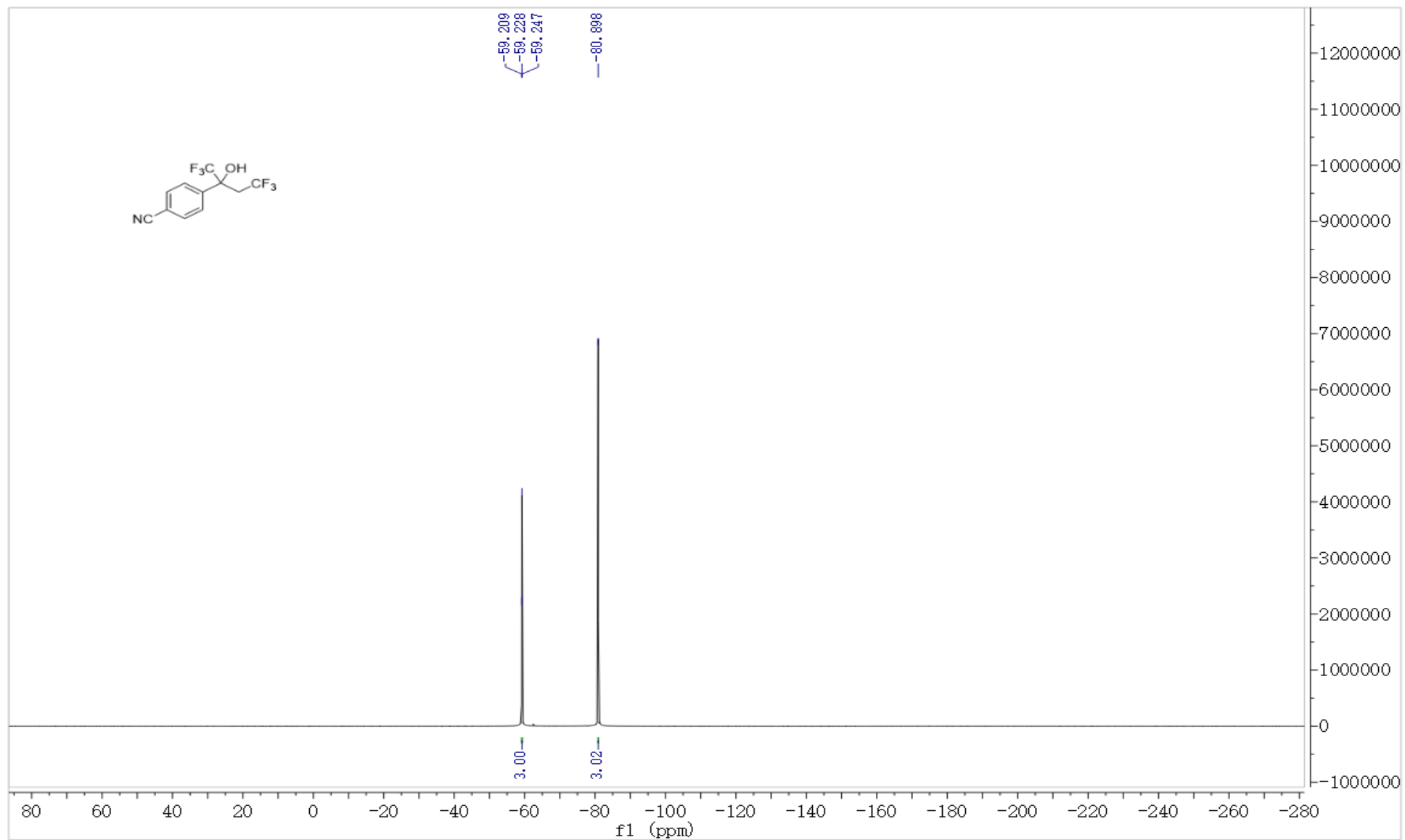
¹H NMR spectrum of 2w



¹³C NMR spectrum of 2w



^{19}F NMR spectrum of 2w



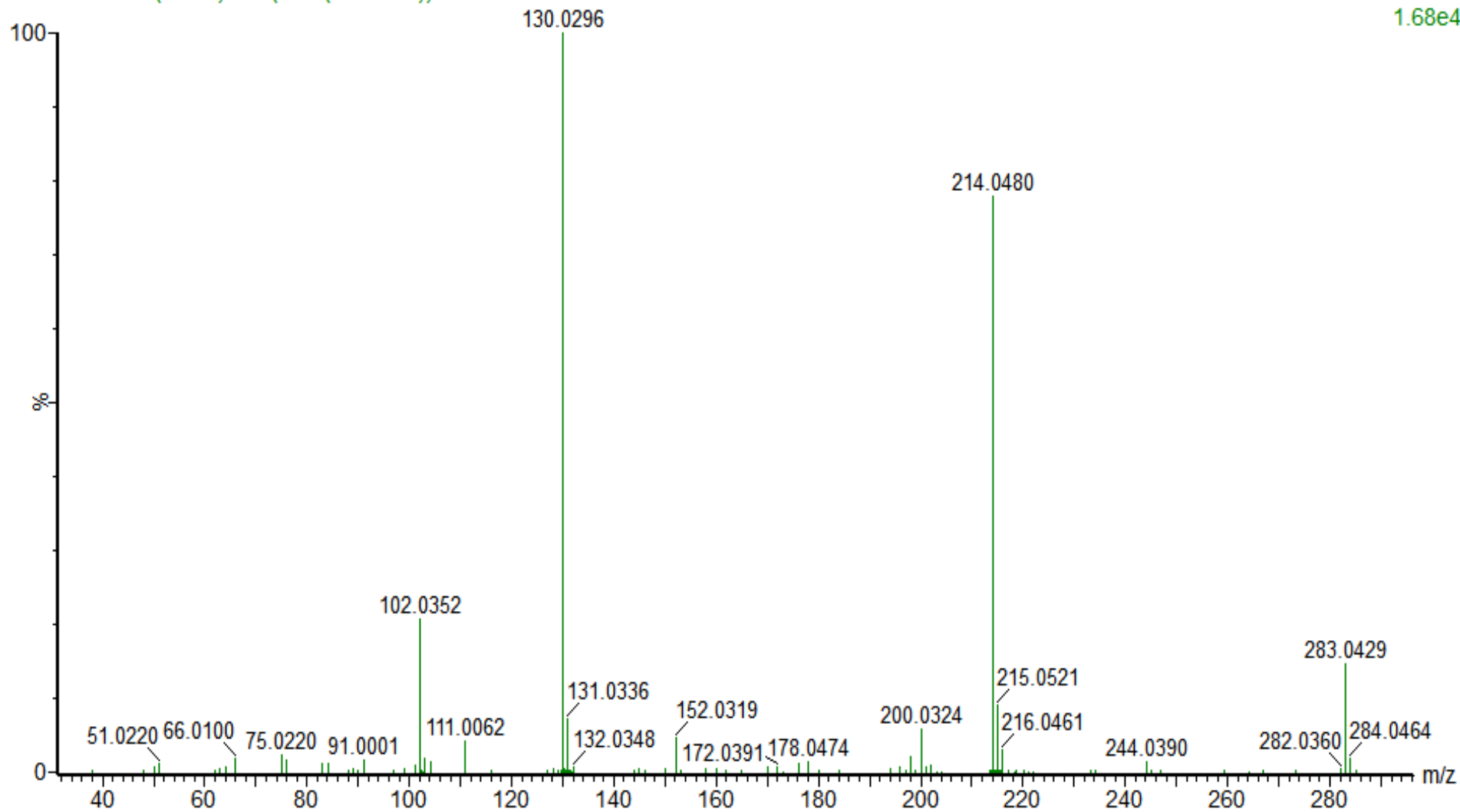
HRMS (EI) spectrum of 2w

CS-LC-P-283

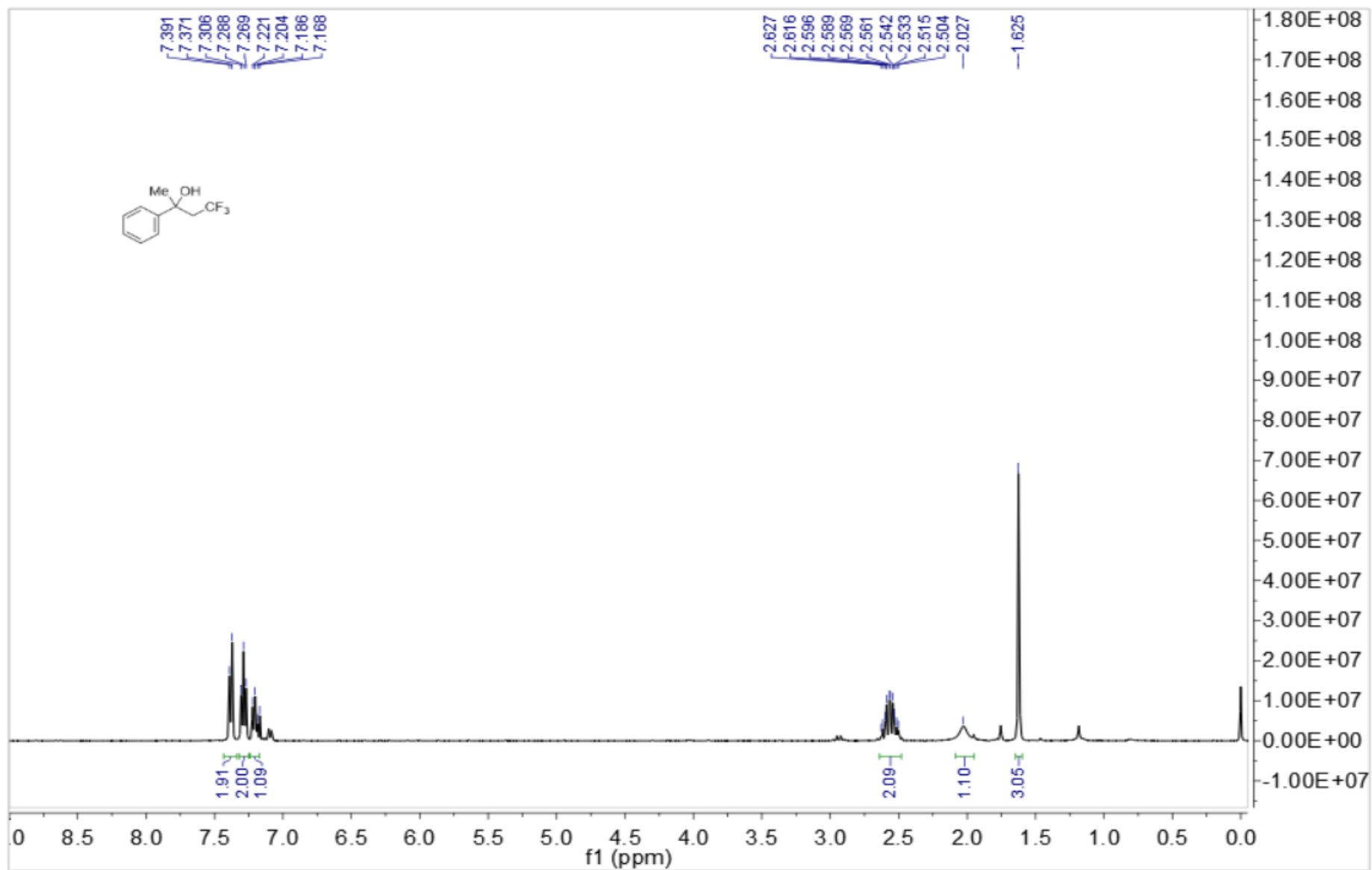
Waters GCT Premier

20220482 239 (3.985) Cm (239-(758+760))

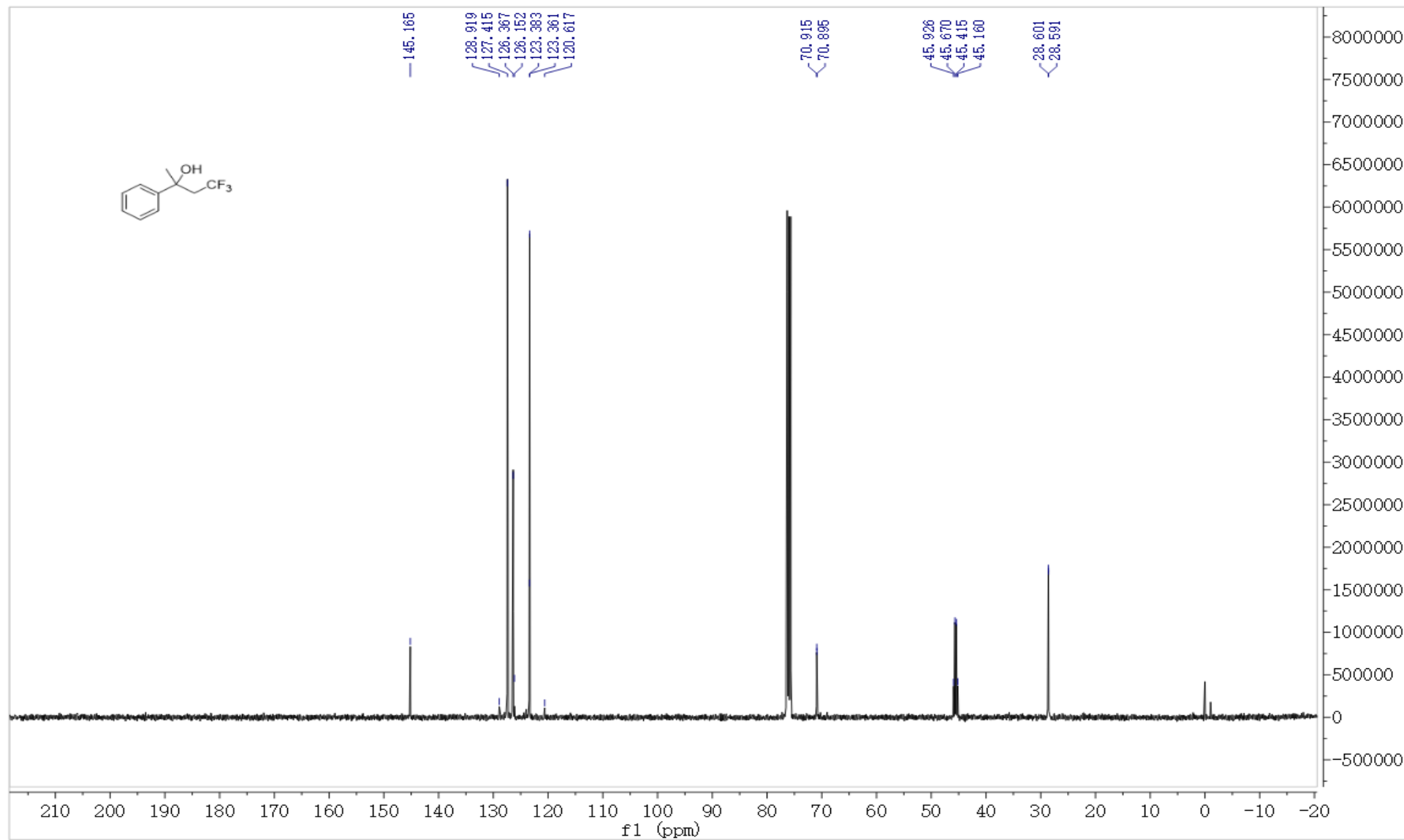
TOF MS EI+
1.68e4



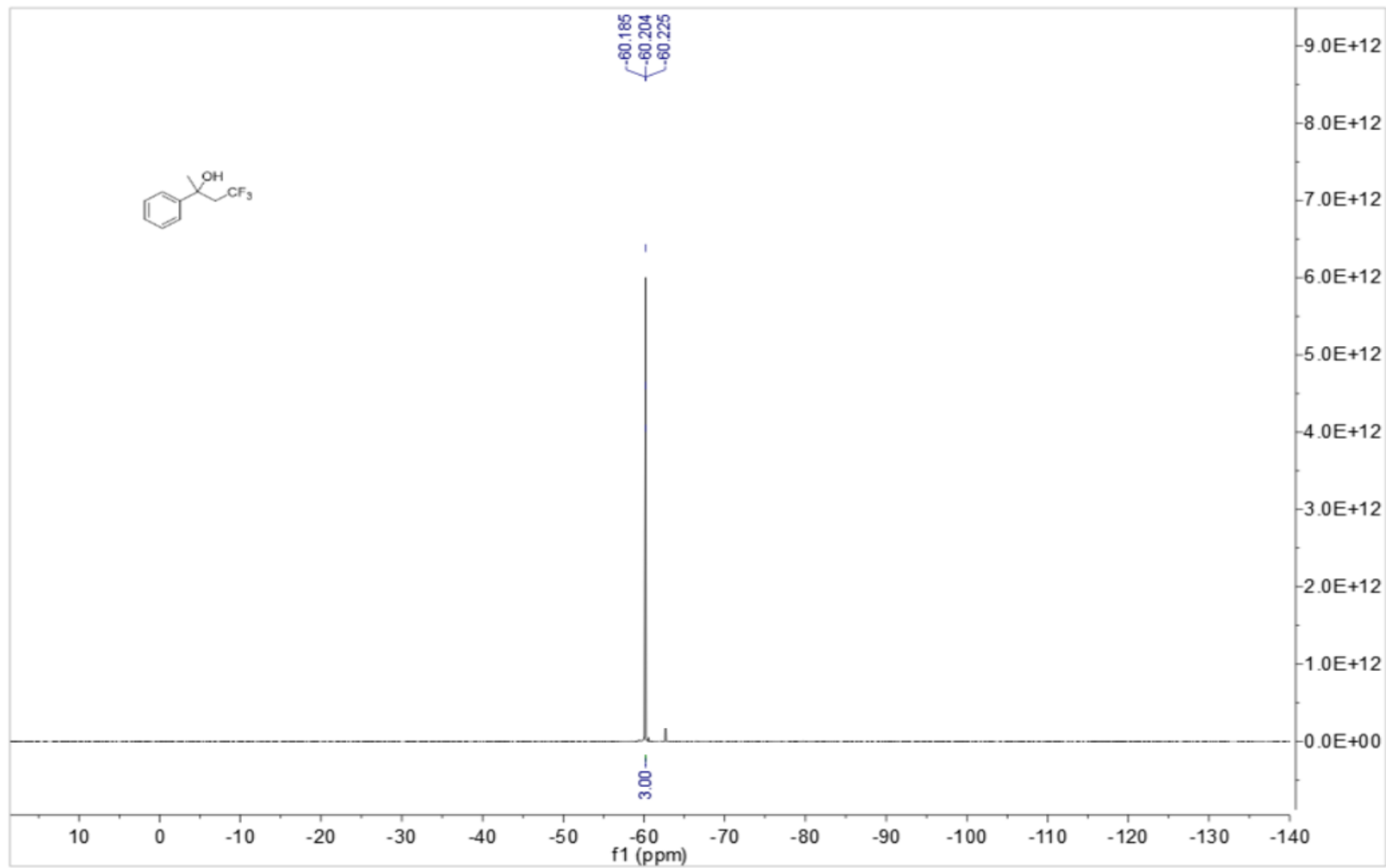
¹H NMR spectrum of 4a



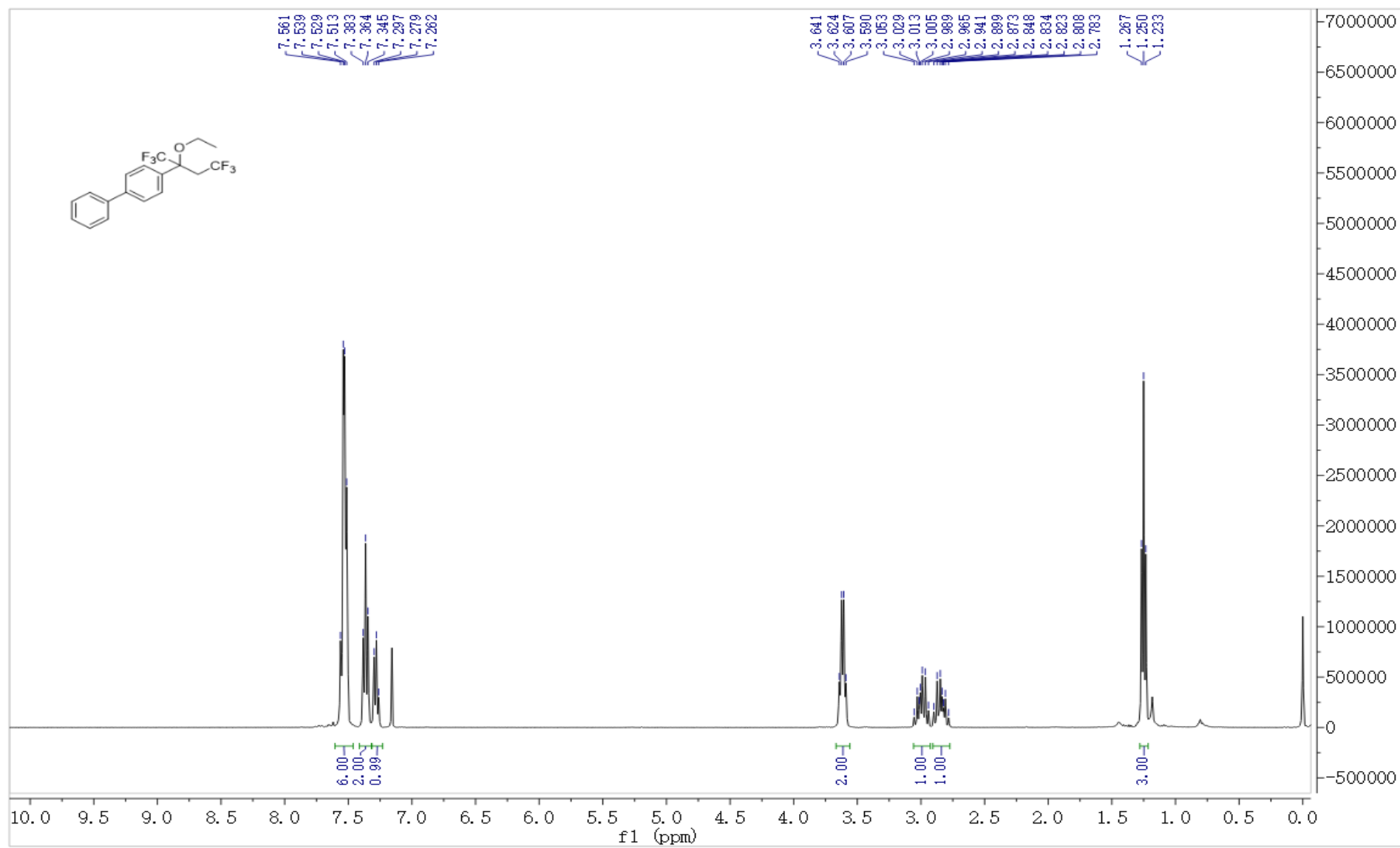
¹³C NMR spectrum of 4a



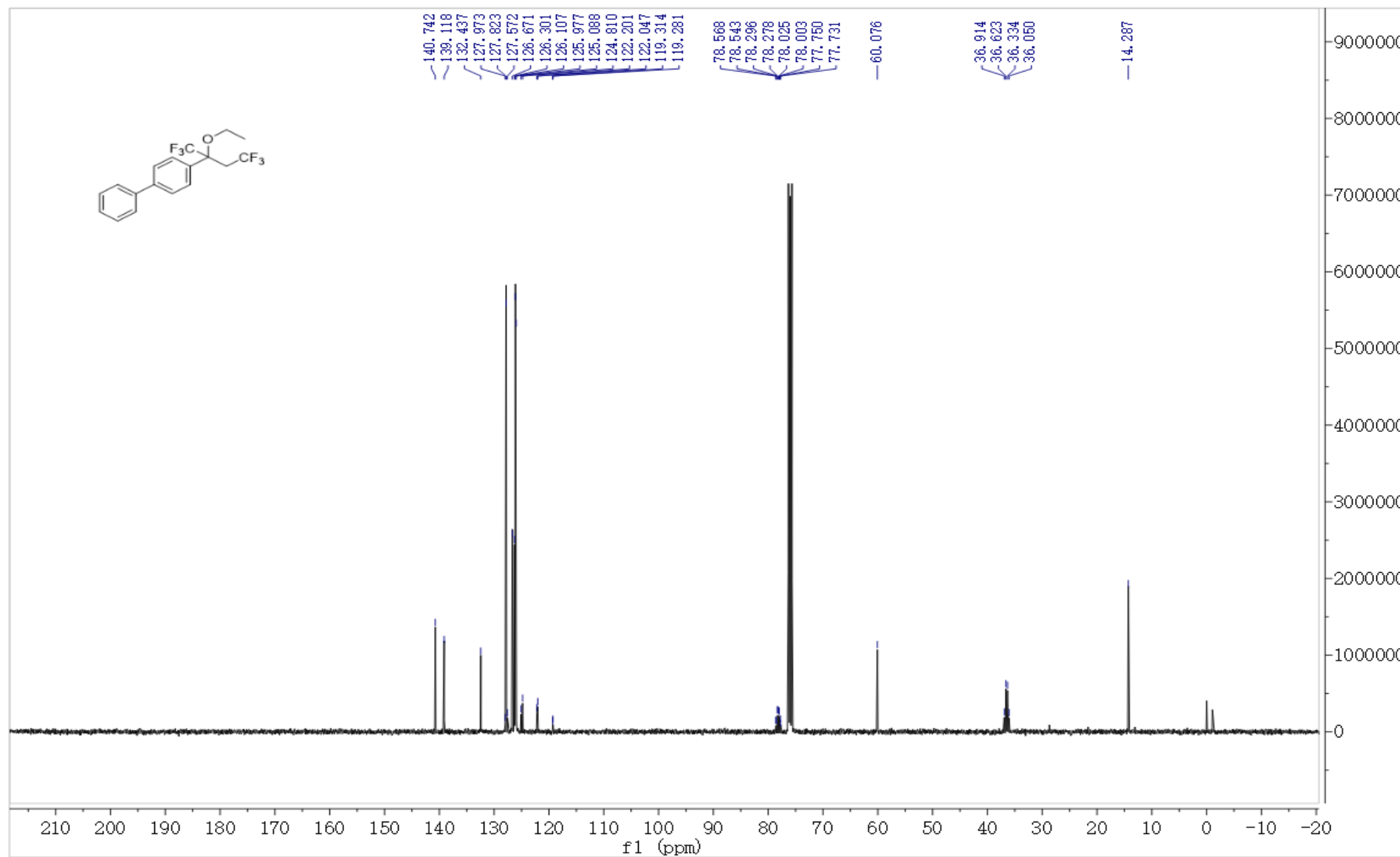
¹⁹F NMR spectrum of 4a



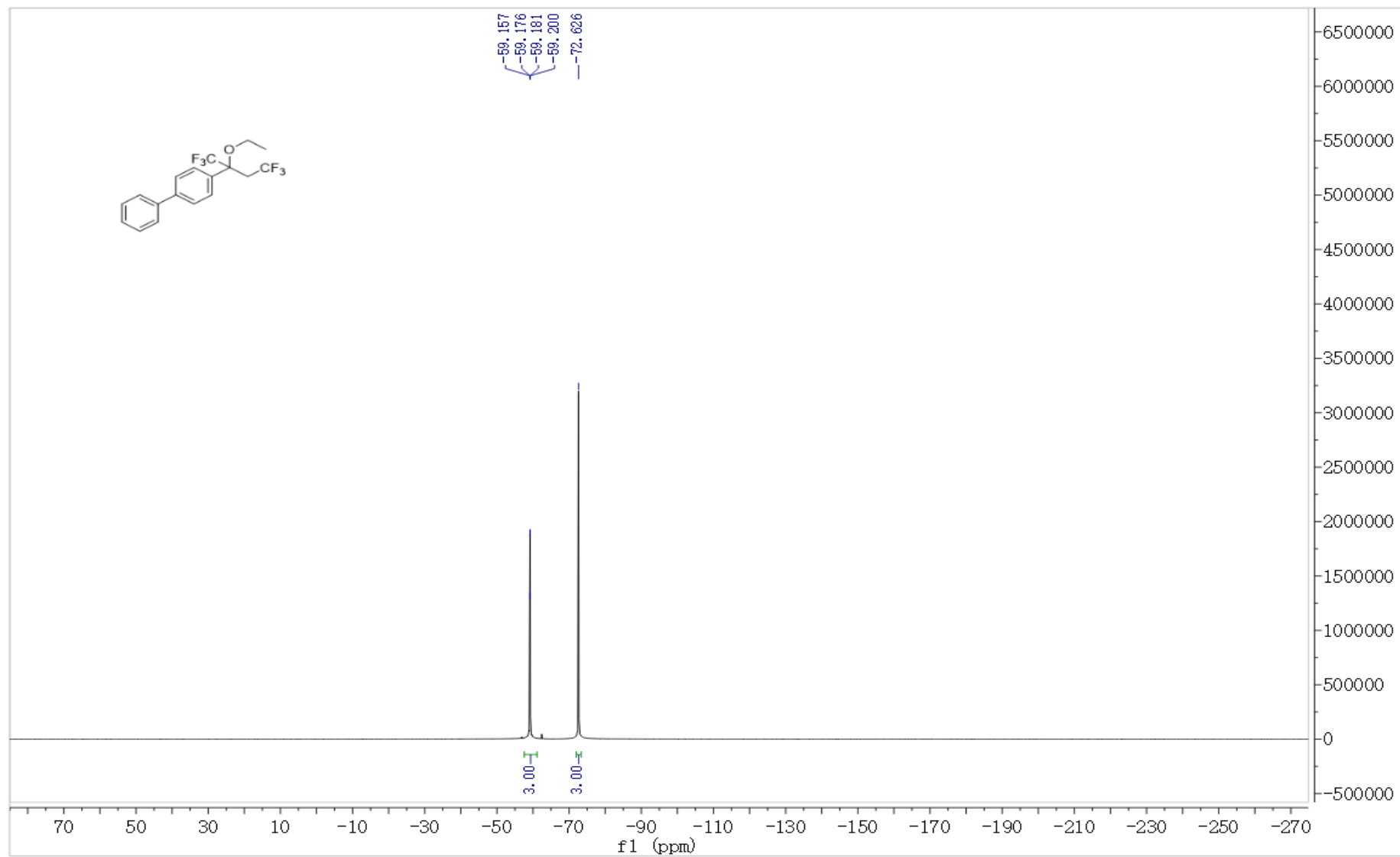
¹H NMR spectrum of 5a



¹³C NMR spectrum of 5a



¹⁹F NMR spectrum of 5a



HRMS (EI) spectrum of 5a

CS-LC-P-362

Waters GCT Premier

20220311 171 (2.850) Cm (171-(33+41))

TOF MS EI+
1.47e4

