Supporting Information

Investigations into the flexibility of the 3D structure and rigid backbone of quinoline by fluorine addition to enhance its blue emission

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Experimental section

Materials and Methods

All NMR spectra were recorded on Bruker AVANCE III 400 or 600 MHz instruments. Chemical shifts are quoted in parts per million (ppm) downfield from TMS as the internal standard and the coupling constants are reported in Hertz. Multiplicities of the NMR resonances are abbreviated as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet) and br (broad). Assignments of ^{1}H NMR, ^{13}C NMR and ^{19}F NMR resonances were made with the aid of COSY, NOESY, HMBC and HSQC experiments. A Waters Synapt G2 quadrupole time-of-flight mass spectrometer fitted with a Waters Ultra pressure liquid chromatograph was used for HRMS analysis. The instrument was operated with an electrospray ionization probe in the positive mode and data was acquired in MS scan mode from *m/z* 100-2000. Infra-red spectra were recorded in the range 4000-600 cm^{-1} on a Perkin Elmer Spectrum as neat films onto a NaCl window. Abbreviations used in the description of IR spectra are: w (weak), m (medium), s (strong) and br (broad).

Computational Section

The structural energy minimization calculation was carried out using GAUSSIAN 09.[1] The Density Functional Theory (DFT) calculation was selected for simulation of the compounds in gas phase.[1] The structures were fully optimized by DFT calculations with a hybrid functional B3LYP at 6-311++G** basis set. To account for the solvent effect, Polarized Continuum Model (PCM) was used.[2] The theoretical UV absorption spectrum of all the molecules in a solvent (acetonitrile) was calculated using CAM-B3LYP/6-311++G** method.

Reagents and solvents were purchased from Sigma Aldrich and used as received. Commercially available Merck Kieselgel 60 F_{254} aluminium backed plates were used for TLC analysis. Visualisation of TLC plates was achieved by UV fluorescence and iodine vapour. Compounds were purified by column chromatography packed with 60-200 mesh silica gel.

4.2. Synthetic procedure

Compounds **1** and **2** were prepared according to standard procedures reported in the literature.[3]

Preparation of 4-alkyne quinoline (**4**):

A mixture of 4-chloroquinoline, **2** (0.5 mmol), acetylenes, **3** (1 mmol), xantphos (10 mmol %), triethylamine (2.0 equiv.), water (0.5 mL) and tetrahydrofuran (5 mL) was degassed twice using argon gas. $Pd(OAc)_2$ (2.5 mmol %) was then added, again degassed twice and heated at 70 °C in a sealed tube under argon for 12 hours. After completion of the reaction, the resulting solution was filtered off using celite pad (to remove catalyst) and the filtrate concentrated in vacuo. The crude products were subjected to silica-gel column chromatography using hexane/ethyl acetate (90:10) eluent to afford the pure products.

4-(phenylethynyl)-2,8-bis(trifluoromethyl)quinoline (**4A**). ν_{max} /cm^{-1} (film) 3062 (w), 2220 (m), 1601 (m), 1591 (m), 1309, (s), 1130 (s), 1143 (s). ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 7.45 (3H, m), 7.68 (2H, m), 7.78 (1H, t, *J*=7.6 Hz), 7.96 (1H, s), 8.19 (1H, d, *J*=7.3 Hz), 8.62 (1H, d, *J*=8.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ_C 83.9, 101.3, 120.0, 121.3, 122.1, 124.8, 127.7, 128.7, 128.8, 129.0, 129.5 (q, *J*=5.3 Hz), 130.1, 130.3, 132.2, 132.5, 143.7, 148.0 (q, *J*=36.5 Hz). HRMS–ES$^+$: *m/z* [M+H] calcd. for $C_{19}H_{10}F_6N$: 366.0712, found: 366.0722.

4-(p-tolylethynyl)-2,8-bis(trifluoromethyl)quinoline (**4B**). ν_{max} /cm^{-1} (film) 2927 (w), 2198 (m), 1590 (s), 1309 (s), 1132 (s). ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 2.40 (3H, s), 7.22 (2H, d, *J*=8.1), 7.52 (2H, d, *J*=8.1), 7.74 (1H, t, *J*=7.8), 7.91 (1H, s), 8.15 (1H, d, *J*=7.2), 8.57 (1H, d, *J*=8.4); ^{13}C NMR (100 MHz, $CDCl_3$) δ_C 21.6, 83.5, 101.9, 117.0, 118.2, 119.8, 122.2, 122.5, 124.9, 127.6, 128.7, 129.4 (q, *J*=5.4), 130.3, 132.1, 132.7, 141.0, 143.7, 148.3 (q, *J*=35.5). HRMS–ES$^+$: *m/z* [M+H] calcd. for $C_{20}H_{12}F_6N$: 380.0868, found: 380.0873.

4-((4-(tert-butyl)phenyl)ethynyl)-2,8-bis(trifluoromethyl) quinoline (**4C**). ν_{max} /cm^{-1} (film) 2963 (m), 2213 (m), 1590 (s), 1517 (w), 1312 (s), 1136 (s), 922 (m), 321 (m), 771 (m), 560 (m). ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 1.36 (9H, s), 7.47 (2H, d, *J*=8.4 Hz), 7.61 (2H, d, *J*=8.4 Hz), 7.76 (1H, t, *J*=7.8 Hz), 7.94 (1H, s), 8.17 (1H, d, *J*=7.2 Hz), 8.60 (1H, d, *J*=8.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ_C 29.7, 35.1, 83.5, 101.8, 118.3, 119.9 (q, *J*=5.3 Hz), 122.1, 122.4, 124.9, 125.8, 127.6, 129.5, 130.4, 131.9, 132.8, 143.7, 148.2 (q, *J*=35.2 Hz), 153.8. The signal of an aromatic quaternary carbon was not observed in the ^{13}C NMR spectrum. HRMS–ES$^+$: *m/z* [M+H] calcd. for $C_{23}H_{18}F_6N$: 422.1338, found: 422.1335.

2,8-bis(trifluoromethyl)-4-((4-(trifluoromethyl)phenyl) ethynyl) quinoline (**4D**). ν_{max} /cm^{-1} (film) 3118 (w), 2220 (m), 1593 (m), 1310 (s), 1066 (s). ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 7.72 (2H, d, *J*=8.3 Hz), 7.82 (3H, m), 8.01 (1H, m), 8.20 (1H, d, *J*=8.2 Hz), 8.60 (1H, d, *J*=8.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ_C 85.8, 99.1, 120.4, 122.0, 122.5, 125.7 (q, *J*=3.6 Hz), 126.8, 128.0, 128.5, 129.7 (q, *J*=5.5 Hz), 130.1, 131.7, 132.4. The signals for the five aromatic quaternary carbons were not observed in the ^{13}C NMR spectrum. HRMS–ES$^+$: *m/z* [M+H] calcd. for $C_{20}H_9F_9N$: 434.0586, found: 434.0580.

2,8-bis(trifluoromethyl)-4-((2-(trifluoromethyl)phenyl)ethynyl) quinoline (**4E**). ν_{max} /cm^{-1} (film) 2965 (w), 2218 (w), 1589 (m), 1310 (m), 1127 (s). ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 7.59 (2H, m), 7.79 (3H, m), 7.97 (1H, s), 8.20 (1H, d, *J*=7.2 Hz), 8.61 (1H, d, *J*=8.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ_C 88.9, 96.3, 119.4 (q, *J*=10.3 Hz), 120.4, 122.0, 122.3, 124.8, 126.3 (q, *J*=5.1 Hz), 128.0, 129.6 (q, *J*=5.3 Hz), 129.8, 130.2, 131.8, 132.1, 134.5, 143.7, 148.0, 148.3. The signals for two aromatic quaternary carbons were not observed in the ^{13}C NMR spectrum. HRMS–ES$^+$: *m/z* [M+H] calcd. for $C_{20}H_9F_9N$: 434.0586, found: 434.0585.

4-((4-fluorophenyl)ethynyl)-2,8-bis(trifluoromethyl)quinoline (**4F**). ν_{max} /cm^{-1} (film) 2953 (w), 2222 (m), 1589 (s), 1505 (s), 1307 (s), 1103 (s). ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 7.16 (2H, m), 7.67 (2H, m), 7.79 (1H, t, *J*=7.9 Hz), 7.96 (1H, s), 8.20 (1H, d, *J*=7.2 Hz), 8.60 (1H, d, *J*=8.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$); δ_C 83.7, 100.1, 116.2 (d, $^2J_{C-F}$=22.6 Hz), 117.5 (q, *J*=3.6 Hz), 120.1, 123.5 (d, $^1J_{C-F}$=273.2 Hz), 127.7, 128.6, 129.6 (q, *J*=5.3 Hz), 130.2, 132.3, 134.2 (d, $^3J_{C-F}$=8.7 Hz), 162.3, 164.8. The signals for three aromatic quaternary carbons were not observed in the ^{13}C NMR spectrum. HRMS–ES$^+$: *m/z* [M+H] calcd. for $C_{19}H_9F_7N$: 384.0623, found: 384.0612.

4-((3,5-difluorophenyl)ethynyl)-2,8-bis(trifluoromethyl) quinoline (**4G**). ν_{max} /cm^{-1} (film) 3087 (w), 2954 (m), 1616 (m), 1590 (s), 1320 (m), 1303 (m), 1136 (s). ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 6.95 (1H, m), 7.20 (2H, m), 7.82 (1H, t, *J*=8.0 Hz), 7.99 (1H, s), 8.23 (1H, d, *J*=7.3 Hz), 8.56 (1H, d, *J*=8.5 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ_C 85.3, 98.1, 106.3 (t, $^2J_{C-F}$=25.4 Hz), 115.1 (d, $^2J_{C-F}$=27.3 Hz), 120.5, 122.0, 123.8, 124.8, 125.9, 128.1, 129.8 (d, $^3J_{C-F}$ =5.3 Hz), 130.0, 131.4, 139.0, 148.2, 163.0 (d, *J* = 253.6 Hz). HRMS–ES$^+$: *m/z* [M+H] calcd. for $C_{19}H_7F_8N$: 402.0524, found: 402.0540.

4-((4-(tert-butyl)phenyl)ethynyl)-2-(trifluoromethyl)quinoline (**4H**). ν_{max} /cm^{-1} (film) 3085 (w), 2926 (m), 2219 (w), 1591 (s), 1312 (m), 1138 (s). ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 7.20 (2H, m), 7.45 (1H, m), 7.62 (1H, td, *J*=7.4, 1.7 Hz), 7.78 (1H, t, *J*=7.8 Hz), 7.96 (1H, s), 8.18 (1H, d, *J*=7.2 Hz), 8.62 (1H, d, *J*=7.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ_C 88.8 (d, *J*=3.4 Hz), 94.5, 110.2 (d, $^2J_{C-F}$ =15.5 Hz), 115.9 (d, $^2J_{C-F}$ =20.5 Hz), 119.9, 122.1, 124.4 (d, $^4J_{C-F}$ =3.7 Hz), 128.0, 129.6 (q, *J*=5.3 Hz), 130.3, 132.0, 134.5 (d, $^3J_{C-F}$=8.2 Hz), 133.6, 143.7, 148.2 (m), 163.2 (d, $^1J_{C-F}$=253.2 Hz). The signals for three aromatic quaternary carbons were not observed in the ^{13}C NMR spectrum. HRMS–ES$^+$: *m/z* [M+H] calcd. for $C_{19}H_9F_7N$: 384.0618, found: 384.0609.

4-(cyclopropylethynyl)-2,8-bis(trifluoromethyl)quinolone (**4I**). ν_{max} /cm^{-1} (film) 3025 (w), 2226 (m), 1585 (m), 1424 (m), 1308 (m), 1160 (m), 1122 (s), 1055 (s). ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 0.99 (m, 2H), 1.06 (m, 2H), 1.63 (1H, m), 7.66 (1H, t, *J*=7.8 Hz), 7.76 (1H, s), 8.10 (1H, d, *J*=7.4 Hz), 8.40 (1H, d, *J*=8.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ_C 0.0, 8.9, 70.5, 107.0, 118.9, 119.4, 121.6, 121.9, 124.4, 126.7, 128.7 (q, *J*=5.3 Hz), 129.8, 132.9, 143.0, 147.5 (q, *J*=35.1 Hz). HRMS–ES$^+$: *m/z* [M+H] calcd. for $C_{16}H_{10}F_6N$: 330.0712, found: 330.0715.

8-methyl-4-(phenylethynyl)-2-(trifluoromethyl)quinoline (**4J**). ν_{max} /cm^{-1} (film) 3055 (m), 2921 (m), 2222 (m), 1608 (m), 1559 (m), 1363 (s), 1267 (s), 1150 (s). ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 2.87 (s, 3H), 7.41 (3H, m), 7.56 (1H, m), 7.68 (3H, m), 7.68 (1H, m), 7.89 (1H, s), 7.96 (1H, d, *J*=8.5 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ_C 18.6, 89.1, 90.8, 121.5 (q, *J*=5.3 Hz), 121.7 (q, *J*=2.1 Hz), 128.5, 129.4, 130.8, 132.3, 138.4, 142.0, 148.4. The signals for the four aromatic quaternary carbons were not observed in the ^{13}C NMR spectrum. HRMS–ES$^+$: *m/z* [M+H] calcd. for $C_{19}H_{13}F_3N$: 312.0995, found: 312.0992.

8-methyl-4-(p-tolylethynyl)-2-(trifluoromethyl)quinoline (**4K**). ν_{max} /cm^{-1} (film) 2925 (m), 2200 (m), 2217 (m), 1588 (m), 1514 (m), 1281 (s), 1104 (s). ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 2.41 (3H, s), 2.84 (3H, s), 7.24 (2H, d, *J*=8.1), 7.56 (2H, d, *J*=8.1), 7.64 (2H, m), 7.86 (1H, s), 8.26 (1H, d, *J*=8.2); ^{13}C NMR (100 MHz, $CDCl_3$) δ_C 17.8, 21.7, 84.4, 100.1, 118.8 (q, *J*=5.2), 123.8, 128.4, 128.7, 129.4, 131.0, 132.0, 132.1, 139.0, 140.1, 146.0, 146.4. The signals of two aromatic quaternary carbons were not observed in the ^{13}C NMR spectrum. HRMS–ES$^+$: *m/z* [M+H] calcd. for $C_{20}H_{15}F_3N$: 326.1151, found: 326.1148.

4-((4-(tert-butyl)phenyl)ethynyl)-8-methyl-2-(trifluoromethyl)quinoline (**4L**). ν_{max} /cm^{-1} (film) 2965 (m), 2201 (m), 1589 (m), 1392 (m), 1311 (m), 1281 (s), 1190 (s), 1129 (s), 1067 (s). ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 1.35 (9H, s), 2.84 (3H, s), 7.45 (2H, m), 7.60 (3H, m), 7.66 (1H, d, *J*=6.9 Hz), 7.86 (1H, s), 8.25 (1H, d, *J*=8.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ_C 17.8, 31.1, 35.0, 84.4, 100.1, 118.9 (q, *J*=2.0 Hz), 123.8, 125.4, 125.6, 128.4, 128.7, 130.9, 131.8, 132.1, 132.3, 138.9, 146.4, 146.4, 153.2. HRMS–ES$^+$: *m/z* [M+H] calcd. for $C_{23}H_{21}F_3N$: 368.1621, found: 368.1619.

8-methyl-2-(trifluoromethyl)-4-((4-(trifluoromethyl)phenyl)ethynyl)quinoline (**4M**). ν_{max} /cm^{-1} (film) 2927 (m), 2222 (w), 1613 (m), 1392 (m), 1319 (s), 1159 (m), 1103 (s), 1063 (s). ^{1}H

NMR (400 MHz, $CDCl_3$) δ_H 2.85 (3H, s), 7.63 (1H, t, *J*=7.5 Hz), 7.70 (3H, m), 7.77 (2H, d, *J*=8.2 Hz), 7.90 (1H, s), 8.23 (1H, d, *J*=8.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ_C 17.8, 86.8, 97.6, 119.3 (q, *J*=2.0 Hz), 123.5, 125.6 (q, *J*=3.8 Hz), 128.3, 129.1, 131.0, 131.2, 131.5, 132.3, 135.7, 139.1, 146.1, 146.4. The signals for the two aromatic quaternary carbons were not observed in the ^{13}C NMR spectrum. HRMS–ES$^+$: *m/z* [M+H] calcd. for $C_{20}H_{12}F_6N$: 380.0868, found: 380.0868.

4-(cyclopropylethynyl)-8-methyl-2-(trifluoromethyl)quinoline (**4N**). ν_{max} /cm^{-1} (film) 3022 (w), 2226 (m), 1592 (m), 1421 (m), 1309 (m), 1174 (m), 1126 (s), 1055 (s). ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 1.00 (m, 4H), 1.62 (1H, m), 2.80 (3H, s), 7.53 (1H, t, *J*=8.0 Hz), 7.61 (1H, d, *J*=7.0 Hz), 7.70 (1H, s), 8.09 (1H, d, *J*=8.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ_C 0.0, 8.8, 17.2, 71.3, 104.8, 118.4, 119.6, 122.4, 123.2, 127.9, 128.3, 130.2, 132.2, 138.1, 145.6 (q, *J*=34.8 Hz). HRMS–ES$^+$: *m/z* [M+H] calcd. for $C_{16}H_{13}F_3N$: 276.0995, found: 276.0991.

4-(phenylethynyl)-2-(trifluoromethyl)quinoline (**4O**). ν_{max}/cm^{-1} (film) 3054 (m), 2922 (m), 2224 (s), 1606 (m), 1549 (m), 1374 (m), 1250 (m), 1147 (s). ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 7.42 (4H, m), 7.69 (2H, m), 7.83 (1H, t, *J*=7.6 Hz), 7.90 (1H, s), 8.13 (1H, d, *J*=8.4 Hz), 8.24 (1H, d, *J*=8.5 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ_C 88.4, 91.5, 121.4, 121.8, 123.9, 124.5, 128.5, 128.7, 129.6, 130.2, 130.8, 132.3, 134.4, 134.7, 143.0, 149.0. The signal for an aromatic quaternary carbon was not observed in the ^{13}C NMR spectrum. HRMS–ES$^+$: *m/z* [M+H] calcd. for $C_{18}H_{11}F_3N$: 298.0838, found: 298.0840.

4-(p-tolylethynyl)-2-(trifluoromethyl)quinoline (**4P**). ν_{max} /cm^{-1} (film) 3059 (m), 2922 (m), 2213 (s), 2197 (m), 1580 (m), 1514 (m), 1394 (m), 1280 (m), 1173 (s), 1143 (s), 1097 (m). ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 2.42 (3H, s), 7.24 (2H, d, *J*=7.8 Hz), 7.57 (2H, d, *J*=8.0 Hz), 7.74 (1H, t, *J*=7.6 Hz), 7.84 (1H, t, *J*=7.3 Hz), 7.88 (1H, s), 8.24 (1H, d, *J*=8.4 Hz), 8.42 (1H, d, *J*=8.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ_C 21.7, 84.0, 100.9, 118.6, 119.1, 126.0, 128.4, 129.0, 129.5, 130.5, 131.1, 132.0, 132.3, 140.3, 147.2. The signals for the two aromatic quaternary carbons were not observed in the ^{13}C NMR spectrum. HRMS–ES$^+$: *m/z* [M+H] calcd. for $C_{19}H_{13}F_3N$: 312.0995, found: 312.0994.

4-((4-(tert-butyl)phenyl)ethynyl)-2-(trifluoromethyl)quinoline (**4Q**). ν_{max} /cm^{-1} (film) 2960 (m), 2221 (s), 1603 (m), 1592 (m), 1310 (s), 1280 (m), 1149 (s). ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 1.33 (9H, s), 7.42 (2H, d, *J*=8.4 Hz), 7.63 (3H, m), 7.80 (1H, m), 7.88 (1H, s), 8.10 (1H, d, *J*=8.6 Hz), 8.22 (1H, d, *J*=8.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ_C 31.1, 88.1, 92.0, 118.5, 121.6, 123.8, 124.5, 125.5, 127.3, 128.6, 130.2, 130.7, 132.2, 134.5 (q, *J*=32.2

Hz), 143.3, 149.0, 153.2. The signal for an aromatic quaternary carbon was not observed in the ^{13}C NMR spectrum. HRMS–ES^{+}: *m/z* [M+H] calcd. for $C_{22}H_{19}F_3N$: 354.1464, found: 354.1463.

4-(hex-1-yn-1-yl)-2-(trifluoromethyl)quinoline (**4R**). ν_{max} /cm^{-1} (film) 3015 (w), 2225 (m), 1583 (m), 1387 (m), 1175 (s), 1096 (s). ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 1.00 (3H, t, *J*=7.3 Hz), 1.56 (2H, m), 1.71 (2H, m), 2.60 (2H, t, *J*=7.1 Hz), 7.68 (1H, td, *J*=7.7, 1.0 Hz), 7.75 (1H, s), 7.80 (1H, td, *J*=7.7, 1.4 Hz), 7.19 (1H, d, *J*=8.5 Hz), 8.30 (1H, d, *J*=8.3 Hz), ^{13}C NMR (100 MHz, $CDCl_3$) δ_C 13.6, 19.5, 22.1, 30.4, 76.2, 102.9, 119.3, 120.1, 122.8, 125.6, 129.6, 131.6, 133.0, 147.2 (q, *J*=34.2 Hz), 148.0. The signal for an aromatic quaternary carbon was not observed in the ^{13}C NMR spectrum. HRMS–ES^{+}: *m/z* [M+H] calcd. for $C_{16}H_{15}F_3N$: 278.1151, found: 278.1151.

4-(cyclopropylethynyl)-2-(trifluoromethyl)quinoline (**4S**). ν_{max} /cm^{-1} (film) 3090 (w), 3018 (w), 2927 (w), 2221 (m), 1584 (m), 1997 (m), 1198 (s), 1104 (s). ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 1.02 (4H, m), 1.64 (1H, m), 7.68 (1H, t, *J*=7.5 Hz), 7.80 (1H, td, *J*=7.2, 1.2 Hz), 8.18 (1H, d, *J*=8.5 Hz), 7.88 (1H, d, *J*=8.3 Hz), 8.26 (1H, d, *J*=8.4 Hz), ^{13}C NMR (100 MHz, $CDCl_3$) δ_C 0.6, 9.4, 71.5, 106.3, 119.2, 126.0, 126.5, 127.4 (q, *J*=5.3 Hz), 128.8, 130.4, 130.9, 133.0, 138.7. The signal for an aromatic quaternary carbon was not observed in the ^{13}C NMR spectrum. HRMS–ES^{+}: *m/z* [M+H] calcd. for $C_{15}H_{11}F_3N$: 262.0838, found: 262.0841.

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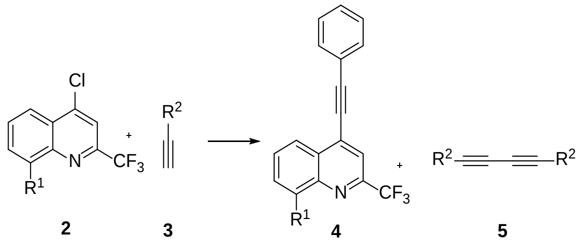
Table S1. Optimization of conditions for the final step in the synthesis of 4-alkynyl quinolines **4**



2 3 4 5

Entry	Catalyst	Ligand	Solvent	Base	Co-catalyst	Yield[a, b] 4	Yield[a, b] 5
1	**$PdCl_2$**	xantphos	THF:Water	TEA	None	58	5
2	$Pd(OAc)_2$	**$P(Ph)_3$**	THF:Water	TEA	None	52	10
3	**$Pd(OAc)_2$**	**xantphos**	**THF:Water**	**TEA**	**None**	**80**	**7**
4	$Pd(OAc)_2$	xantphos	**DMSO**	TEA	None	15	7
5	$Pd(OAc)_2$	xantphos	**DMF**	TEA	None	27	6
6	$Pd(OAc)_2$	xantphos	**THF**	TEA	None	31	8
7	$Pd(OAc)_2$	xantphos	THF:Water	**Pyrrolidine**	None	56	10
8	$Pd(OAc)_2$	xantphos	THF:Water	**Piperidine**	None	62	28
9	$Pd(OAc)_2$	xantphos	THF:Water	**$NH(ipr)_2$**	None	21	9
10	$Pd(OAc)_2$	xantphos	THF:Water	**None**	None	NR	NR
11	$Pd(OAc)_2$	xantphos	THF:Water	TEA	**CuI**	12	80
12	$Pd(OAc)_2$	xantphos	THF:Water	TEA	**$Cu(OAc)_2$**	10	70
13	$Pd(OAc)_2$	xantphos	THF:Water	TEA	**TBAB[c]**	18	20

[a] Reaction conditions: **2** (1 mmol), **3** (1.5 mmol), base (2 equiv), $Pd(OAc)_2$ (2.5 mol %), ligand (10 mol %) and solvent (10 mL) at 70 °C for 12 hrs.

[b] Isolated yield

[c] TBAB : Tetra-*n*-butylammonium bromide

Table S2. Selected bond parameters in compounds **4A, 4B, 4E, 4I, 4K, 4L, 4M, 4N, 4P** and **4S**

Compound	**Bond lengths/Å**			**Bond angles/°**	
	$C_{quinolyl}$-$C_{ethylyl}$	$C_{ethylyl}$-$C_{ethylyl}$	$C_{ethylyl}$-C_{phenyl}	$C_{quinolyl}$-$C_{ethylyl}$-$C_{ethylyl}$	C_{phenyl}-$C_{ethylyl}$-$C_{ethylyl}$
4A	1.426(2)	1.198(2)	1.432(2)	177.4(2)	177.6(2)
4B	1.428(2) 1.432(2)	1.198(2) 1.198(2)	1.431(2) 1.437(2)	176.6(2) 176.8(2)	174.0(2) 175.8(2)
4E	1.433(2) 1.431(2)	1.196(2) 1.197(2)	1.436(2) 1.435(2)	179.1(2) 175.7(1)	178.7(1) 177.0(1)
4I	1.434(2) 1.429(2)	1.194(2) 1.182(2)	1.434(2) 1.433(2)	176.2(2) 178.8(2)	177.8(2) 178.5(2)
4K	1.428(2)	1.201(2)	1.432(2)	179.1(2)	178.2(2)
4L	1.434(3) 1.435(3) 1.433(3) 1.434(3)	1.194(3) 1.194(3) 1.194(3) 1.198(3)	1.434(3) 1.438(3) 1.436(3) 1.441(3)	176.3(2) 178.2(2) 178.1(2) 178.8(2)	176.6(2) 178.1(2) 175.9(2) 178.9(2)
4M	1.430(2) 1.430(3)	1.200(2) 1.201(3)	1.432(2) 1.432(2)	176.5(2) 178.2(2)	178.3(2) 177.9(2)
4N	1.434(3) 1.435(3)	1.196(3) 1.199(3)	1.439(3) 1.439(3)	177.7(2) 175.5(2)	177.9(2) 176.4(2)
4P	1.431(2)	1.197(2)	1.435(2)	178.9(1)	178.5(1)
4S	1.436(3) 1.432(3)	1.185(3) 1.209(6) 1.226(7)	1.446(3) 1.460(7) 1.445(9)	176.6(2) 164.9(3) 175.4(6)	175.5(2) 164.4(3) 171.2(7)

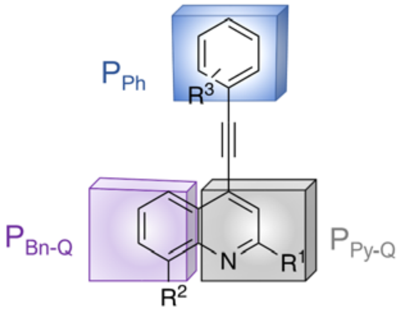


Table S3. Angles between the benzene ($P_{Bn\text{-}Q}$), pyridine ($P_{Py\text{-}Q}$) and phenyl (P_{Ph}) planes.

Compound	Dihedral angle between planes/°		
	$P_{Bn\text{-}Q}$ - $P_{Py\text{-}Q}$	$P_{Py\text{-}Q}$ - P_{Ph}	$P_{Bn\text{-}Q}$ - P_{Ph}
4A	0.85(3)	4.74(4)	5.48(4)
4B	2.59(4)*	7.38(4)*	8.13(4)*
4E	2.8(2)*	14.96(3)*	14.79(2)*
4I	1.69(6)*	N/A	N/A
4K	1.78(9)	4.31(9)	5.11(9)
4L	1.0(1)*	10.1(1)*	9.9(1)*
4M	1.4(1)*	9.5(1)*	10.8(1)*
4N	0.8(9)*	N/A	N/A
4P	0.4(1)	21.23(8)	21.62(8)
4S	1.11(2)*	N/A	N/A

*The mean dihedral angle and standard deviation observed in the molecules in the asymmetric unit

Table S4: Analysis of Short Ring-Interactions with Cg-Cg Distances < 4.0 Å, Alpha < 20.000° and Beta < 60.0°

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)
- Slippage = Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang).
- P,Q,R,S = J-Plane Parameters for Carth. Coord. (Xo, Yo, Zo)

<u>COMPOUND 4A</u>

Cg(I)	Res(I)		Cg(J)	[ARU(J)]	Cg-Cg	Transformed J-Plane P	Q	R	S	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg(1)	[1]	->	Cg(3)	[3566.01]	3.6087(8)	-0.9562	0.2292	0.1822	5.6975	4.73(7)	18.3	20.5	-3.3806(5)	-3.4258(6)	1.134
Cg(1)	[1]	->	Cg(3)	[3666.01]	3.8204(8)	-0.9562	0.2292	0.1822	-1.0744	4.73(7)	23.9	27.4	3.3913(5)	3.4941(6)	1.545
Cg(2)	[1]	->	Cg(3)	[3566.01]	3.7377(8)	-0.9562	0.2292	0.1822	5.6975	5.47(7)	23.2	26.6	-3.3423(6)	-3.4355(6)	1.472
Cg(2)	[1]	->	Cg(3)	[3666.01]	3.8119(8)	-0.9562	0.2292	0.1822	-1.0744	5.47(7)	23.2	25.9	3.4295(6)	3.5027(6)	1.504

[3566] = -X,1-Y,1-Z
[3666] = 1-X,1-Y,1-Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

Cg(I)	x	y	z	Xo	Yo	Zo
Cg(1)	0.42202(8)	0.61259(4)	0.69044(4)	1.7736(5)	9.6043(6)	9.9434(5)
Cg(2)	0.40395(8)	0.72504(4)	0.57713(4)	1.8451(6)	11.3673(6)	8.3115(6)
Cg(3)	0.07301(8)	0.32785(4)	0.35267(4)	-0.1037(6)	5.1401(6)	5.0790(6)

COMPOUND 4B

Cg(I)	Res(I)	Cg(J)	[ARU(J)]	Cg-Cg	Transformed J-Plane P	Q	R	S	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg(1)	[1] ->	Cg(7)	[1556.02]	3.8772(9)	-0.1222	0.0444	0.9915	15.9199	2.10(8)	20.0	19.9	-3.6451(6)	3.6432(7)	1.327
Cg(1)	[1] ->	Cg(7)	[4565.02]	3.7541(9)	-0.1222	-0.0444	0.9915	7.7511	7.16(8)	17.6	24.0	3.4304(6)	-3.5775(7)	1.138
Cg(2)	[1] ->	Cg(7)	[4565.02]	3.7910(9)	-0.1222	-0.0444	0.9915	7.7511	7.95(8)	18.9	16.8	3.6291(6)	-3.5868(7)	1.227
Cg(3)	[1] ->	Cg(3)	[3677.01]	3.7231(10)	0.1874	-0.0296	-0.9818	-15.1659	0.00(8)	26.3	26.3	3.3368(7)	3.3368(7)	1.651
Cg(3)	[1] ->	Cg(5)	[4565.02]	3.5882(9)	-0.1729	0.1159	0.9781	9.7476	5.02(8)	18.1	13.7	3.4867(7)	-3.4104(6)	1.115
Cg(3)	[1] ->	Cg(6)	[4565.02]	3.8035(9)	-0.1202	0.1157	0.9860	9.9270	6.27(8)	23.0	22.9	3.5040(7)	-3.5022(6)	1.484
Cg(5)	[2] ->	Cg(3)	[4564.01]	3.5882(9)	-0.1874	-0.0296	0.9818	3.9031	5.02(8)	13.7	18.1	-3.4104(6)	3.4867(7)	0.848
Cg(6)	[2] ->	Cg(3)	[4564.01]	3.8035(9)	-0.1874	-0.0296	0.9818	3.9031	6.27(8)	22.9	23.0	-3.5022(6)	3.5040(7)	1.479

[1556] = X,Y,1+Z
[4565] = X,3/2-Y,1/2+Z
[3677] = 1-X,2-Y,2-Z
[4564] = X,3/2-Y,-1/2+Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

Cg(I)	x	y	z	Xo	Yo	Zo
Cg(1)	0.07008(4)	0.77688(4)	0.83348(4)	-3.4294(7)	12.3180(6)	11.4060(6)
Cg(2)	0.17980(4)	0.66181(4)	0.85600(5)	-1.8915(7)	10.4935(6)	11.7142(6)
Cg(3)	0.44279(5)	1.03826(4)	0.87204(5)	1.9992(8)	16.4624(7)	11.9337(7)
Cg(5)	0.41840(4)	0.53604(4)	0.13358(4)	5.6079(7)	8.4994(6)	1.8280(6)
Cg(6)	0.30636(4)	0.42200(4)	0.10155(5)	4.0861(7)	6.6911(6)	1.3897(6)
Cg(7)	0.04533(5)	0.80336(4)	0.08517(5)	0.2268(8)	12.7378(7)	1.1656(7)

COMPOUND 4E

Cg(I)	Res(I)	Cg(J)	[ARU(J)]	Cg-Cg	Transformed J-Plane P	Q	R	S	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg(2)	[1] ->	Cg(7)	[1555.02]	3.8667(8)	0.0297	0.3141	0.9489	6.8387	16.52(6)	15.6	17.4	3.6899(5)	-3.7237(6)	1.042
Cg(3)	[1] ->	Cg(5)	[1555.02]	3.8555(8)	0.1233	-0.1164	0.9855	0.9650	11.66(6)	29.5	17.8	3.6708(5)	-3.3570(5)	1.896
Cg(3)	[1] ->	Cg(5)	[4565.02]	3.7681(8)	0.1233	0.1164	0.9855	10.6191	3.13(6)	22.2	25.0	-3.4141(5)	3.4894(5)	1.422
Cg(3)	[1] ->	Cg(6)	[1555.02]	3.9137(8)	0.0770	-0.1375	0.9875	0.6625	12.62(6)	14.9	19.5	3.6897(5)	-3.7824(5)	1.005
Cg(3)	[1] ->	Cg(6)	[4565.02]	3.7253(8)	0.0770	0.1375	0.9875	10.8435	3.19(6)	25.0	21.9	-3.4572(5)	3.3753(5)	1.576
Cg(5)	[2] ->	Cg(3)	[1555.01]	3.8555(8)	0.0814	0.0823	0.9933	6.8167	11.66(6)	17.8	29.5	-3.3570(5)	3.6708(5)	1.179

[1555] = X,Y,Z
[4565] = X,3/2-Y,1/2+Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

Cg(I)	x	y	z	Xo	Yo	Zo
Cg(2)	0.35446(3)	1.10004(3)	0.36927(4)	5.1528(5)	17.2925(5)	5.2096(5)
Cg(3)	0.10757(3)	0.70193(4)	0.41381(4)	1.3538(5)	11.0342(6)	5.8380(5)
Cg(5)	0.04770(3)	0.80099(3)	0.16943(4)	0.6102(5)	12.5914(5)	2.3903(5)
Cg(6)	0.14063(4)	0.68061(3)	0.14183(4)	2.0475(5)	10.6991(5)	2.0009(5)
Cg(7)	0.39311(4)	1.07068(4)	0.10275(4)	5.9279(5)	16.8310(6)	1.4496(6)

COMPOUND 4I

Cg(I)	Res(I)	Cg(J)	[ARU(J)]	Cg-Cg	Transformed J-Plane P	Q	R	S	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg(3)	[1] ->	Cg(5)	[6555.02]	3.9301(10)	-0.9829	0.0070	-0.1839	-5.2039	4.24(7)	20.2	23.3	3.6104(7)	3.6887(6)	1.356
Cg(5)	[2] ->	Cg(5)	[2555.02]	3.8102(9)	-0.9829	0.0070	-0.1839	2.5317	0.80(7)	16.2	16.2	-3.6596(6)	-3.6596(6)	1.061

[6555] = 1/2-X,1/2+Y,1/2-Z
[2555] = -X,Y,1/2-Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

Cg(I)	x	y	z	Xo	Yo	Zo
Cg(2)	0.12697(4)	0.81645(4)	0.07907(2)	1.4572(6)	12.4582(6)	1.8154(5)
Cg(3)	0.13666(4)	0.90324(4)	0.16407(2)	1.0139(7)	13.7826(6)	3.7668(6)
Cg(5)	0.12389(4)	0.30444(4)	0.28736(2)	-0.0540(6)	4.6455(5)	6.5973(5)

COMPOUND 4K

Cg(I)	Res(I)	Cg(J)	[ARU(J)]	Cg-Cg	Transformed J-Plane P	Q, R	S	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg(1)	[1] ->	Cg(1)	[2765.01]	3.5527(8)	-0.4973	0.5341-0.6837	-4.9453	0.03(7)	16.0	16.0	3.4146(6)	3.4146(6)	0.981
Cg(1)	[1] ->	Cg(2)	[2765.01]	3.8328(8)	-0.4807	0.5203-0.7059	-4.8378	1.78(7)	27.6	26.3	3.4356(6)	3.3959(6)	1.777
Cg(1)	[1] ->	Cg(3)	[2675.01]	3.6269(8)	-0.5568	0.4899-0.6708	1.0265	4.31(7)	17.3	21.2	-3.3819(6)	-3.4621(6)	1.081
Cg(2)	[1] ->	Cg(3)	[2675.01]	3.8859(10)	-0.5568	0.4899-0.6708	1.0265	5.11(7)	27.8	23.0	-3.5773(6)	-3.4373(6)	1.812
Cg(3)	[1] ->	Cg(1)	[2675.01]	3.6268(8)	-0.4973	0.5341-0.6837	2.0128	4.31(7)	21.2	17.3	-3.4621(6)	-3.3819(6)	1.310

[2765] = 2-X,1-Y,-Z
[2675] = 1-X,2-Y,-Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

Cg(I)	x	y	z	Xo	Yo	Zo
Cg(1)	0.86855(7)	0.59605(6)	-0.12581(5)	10.0141(7)	4.8177(5)	-1.2823(5)
Cg(2)	1.04998(7)	0.73582(7)	-0.18970(6)	12.0692(7)	5.8627(6)	-1.9336(6)
Cg(3)	0.37192(7)	1.02844(7)	0.33359(6)	8.6236(7)	9.6689(6)	3.4001(6)

COMPOUND 4L

Cg(I)	Res(I)	Cg(J)	[ARU(J)]	Cg-Cg	Transformed J-Plane P	Q, R	S	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg(1)	[1] ->	Cg(8)	[1555.03]	3.4828(13)	0.8764	0.0592-0.4780	-2.9853	2.53(10)	16.5	15.2	3.3606(9)	-3.3390(9)	0.990
Cg(2)	[1] ->	Cg(7)	[1555.03]	3.4566(13)	0.8722	0.0648-0.4848	-3.0424	1.70(10)	15.2	14.9	3.3396(9)	-3.3353(9)	0.908
Cg(2)	[1] ->	Cg(8)	[1555.03]	3.6605(13)	0.8764	0.0592-0.4780	-2.9853	1.86(10)	24.2	24.4	3.3339(9)	-3.3383(9)	1.502

Cg(4) [2] -> Cg(11) [1555.04] 3.5278(12) 0.9134-0.0559 0.4032   9.9070 3.10(10) 18.6 16.6 -3.3813(9)   3.3428(9)   1.128
Cg(5) [2] -> Cg(10) [1555.04] 3.5277(12) 0.9169-0.0698 0.3930   9.7959 3.27(10) 15.7 18.1 -3.3528(9)   3.3961(8)   0.955
Cg(5) [2] -> Cg(11) [1555.04] 3.6455(12) 0.9134-0.0559 0.4032   9.9070 2.28(10) 23.8 23.0 -3.3546(9)   3.3354(9)   1.471

[1555] = X,Y,Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

Cg(I)	x	y	z	Xo	Yo	Zo
Cg(1)	0.19155(8)	0.00827(5)	0.13292(4)	2.0547(9)	-0.8980(9)	2.8712(9)
Cg(2)	0.29610(8)	0.06208(6)	0.23118(4)	3.1737(9)	-0.7758(10)	4.9939(9)
Cg(4)	0.53736(8)	0.41921(5)	0.17941(4)	5.7712(9)	5.5118(10)	3.8756(9)
Cg(5)	0.45157(8)	0.41828(5)	0.27521(4)	4.8405(9)	4.7511(10)	5.9451(9)
Cg(7)	0.06557(8)	0.08029(5)	0.33924(4)	0.6824(9)	-1.3164(10)	7.3282(9)
Cg(8)	-0.04248(8)	0.06116(6)	0.24373(5)	-0.4750(9)	-0.8885(11)	5.2649(10)
Cg(10)	0.70251(8)	0.47749(5)	0.38030(4)	7.5362(8)	4.9092(9)	8.2153(8)
Cg(11)	0.78985(8)	0.42318(5)	0.27852(4)	8.4848(9)	4.8061(9)	6.0166(9)

COMPOUND 4M

Cg(I) Res(I)   Cg(J) [ARU(J)]   Cg-Cg Transformed J-Plane P, Q, R, S   Alpha Beta Gamma   CgI_Perp   CgJ_Perp Slippage

Cg(1) [1] -> Cg(2) [2777.01] 3.7588(12) -0.3211-0.6788 0.6604   4.5579   1.18(9) 24.0 23.4   3.4485(8)   3.4324(8)   1.532
Cg(1) [1] -> Cg(3) [2767.01] 3.8255(12) -0.5445-0.6803 0.4907   6.5571 14.97(9) 18.5 25.5 -3.4541(8) -3.6276(8)   1.214
Cg(2) [1] -> Cg(2) [2777.01] 3.5640(12) -0.3211-0.6788 0.6604   4.5579 0.00(10) 15.5 15.5   3.4343(8)   3.4343(8)   0.953
Cg(4) [2] -> Cg(5) [2666.02] 3.6991(11) 0.6756-0.2589-0.6903 -6.6448   1.69(9) 23.4 22.3   3.4215(8) -3.3957(8)   1.467
Cg(4) [2] -> Cg(6) [2766.02] 3.7600(11) -0.7060 0.3268 0.6283 -0.5495   4.07(9) 23.5 25.5   3.3946(8)   3.4484(8)   1.499
Cg(5) [2] -> Cg(5) [2666.02] 3.6163(12) 0.6756-0.2589-0.6903 -6.6448   0.00(9) 20.1 20.1   3.3954(8)   3.3954(8)   1.245
Cg(5) [2] -> Cg(6) [2766.02] 3.8745(12) -0.7060 0.3268 0.6283 -0.5495   5.55(9) 26.6 31.9   3.2884(8) -3.4656(8)   1.732

[2777] = 2-X,2-Y,2-Z
[2767] = 2-X,1-Y,2-Z
[2666] = 1-X,1-Y,1-Z
[2766] = 2-X,1-Y,1-Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

Cg(I)	x	y	z	Xo	Yo	Zo
Cg(1)	1.14919(8)	0.82149(8)	1.06414(5)	7.2466(8)	3.5764(8)	19.3221(8)
Cg(2)	0.91632(8)	0.91363(8)	1.05609(5)	5.0374(8)	4.5000(8)	19.1758(8)
Cg(3)	0.94785(8)	0.27083(8)	0.76423(5)	6.3845(8)	-0.5158(8)	13.8764(8)
Cg(4)	0.68424(8)	0.60294(8)	0.44333(4)	4.9902(8)	4.0095(8)	8.0497(8)
Cg(5)	0.59960(8)	0.37185(8)	0.44740(5)	4.1650(8)	1.7595(8)	8.1236(8)
Cg(6)	1.24975(8)	0.64070(8)	0.72964(4)	9.4038(8)	3.2006(8)	13.2484(8)

COMPOUND 4N

Cg(I)	Res(I)		Cg(J)	[ARU(J)]	Cg-Cg	Transformed J-Plane P, Q, R, S				Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg(2)	[1]	->	Cg(6)	[2666.02]	3.7146(7)	-0.9078	-0.0987	-0.4077	-2.9187	0.71(6)	22.6	21.9	-3.4470(5)	-3.4301(5)	1.426
Cg(2)	[1]	->	Cg(7)	[2666.02]	3.8786(8)	-0.9064	-0.1147	-0.4065	-2.8932	0.27(6)	27.4	27.7	-3.4354(5)	-3.4421(5)	1.788
Cg(2)	[1]	->	Cg(7)	[2766.02]	3.7189(8)	-0.9064	-0.1147	-0.4065	-9.7601	0.27(6)	22.5	22.7	3.4315(5)	3.4355(5)	1.424
Cg(3)	[1]	->	Cg(6)	[2666.02]	3.8470(8)	-0.9078	-0.0987	-0.4077	-2.9187	1.30(6)	26.8	27.4	-3.4148(5)	-3.4335(5)	1.735
Cg(3)	[1]	->	Cg(6)	[2766.02]	3.7488(8)	-0.9078	-0.0987	-0.4077	-9.7958	1.30(6)	21.6	22.5	3.4623(5)	3.4845(5)	1.383
Cg(3)	[1]	->	Cg(7)	[2766.02]	3.6435(8)	-0.9064	-0.1147	-0.4065	-9.7601	0.95(6)	19.3	18.6	3.4524(5)	3.4380(5)	1.206
Cg(7)	[2]	->	Cg(3)	[2766.01]	3.6435(8)	-0.9132	-0.1137	-0.3914	-8.7055	0.95(6)	18.6	19.3	3.4380(5)	3.4524(5)	1.164

[2666] = 1-X,1-Y,1-Z
[2766] = 2-X,1-Y,1-Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

Cg(I)	x	y	z	Xo	Yo	Zo
Cg(2)	0.64853(6)	0.25319(4)	0.81009(3)	1.4877(5)	-1.2822(5)	12.6125(5)
Cg(3)	0.69989(7)	0.24728(5)	0.67202(3)	2.3499(5)	-0.6584(6)	10.4627(5)
Cg(6)	0.79323(6)	0.72621(5)	0.32117(3)	2.7896(5)	6.3017(5)	5.0003(5)
Cg(7)	0.84846(7)	0.71917(5)	0.18362(3)	3.6826(6)	6.9106(6)	2.8588(5)

COMPOUND 4P

Cg(I) Res(I) Cg(J) [ARU(J)] Cg-Cg Transformed J-Plane P, Q, R, S Alpha Beta Gamma CgI_Perp CgJ_Perp Slippage

Cg(1) [1] -> Cg(1) [3655.01] 3.6793(7) -0.6187 0.4241-0.6614 -1.5653 0.00(6) 21.9 21.9 -3.4134(5) -3.4134(5) 1.373
Cg(2) [1] -> Cg(3) [1545.01] 3.8666(8) 0.3487-0.3098 0.8846 6.3017 21.61(7) 17.8 17.2 -3.6939(6) 3.6824(6)

[3655] = 1-X,-Y,-Z
[1545] = X,-1+Y,Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

Cg(I)	x	y	z	Xo	Yo	Zo
Cg(1)	0.57819(5)	-0.14372(6)	0.07259(3)	5.9420(5)	-1.2794(5)	1.1493(5)
Cg(2)	0.69562(6)	-0.20595(6)	-0.03992(4)	7.4540(6)	-1.8333(6)	-0.6321(6)
Cg(3)	0.86903(6)	0.54661(6)	0.14018(4)	8.8564(6)	4.8658(6)	2.2196(6)

COMPOUND 4S

Cg(I) Res(I) Cg(J) [ARU(J)] Cg-Cg Transformed J-Plane P, Q, R, S Alpha Beta Gamma CgI_Perp CgJ_Perp Slippage

Cg(4) [1] -> Cg(6) [1555.02] 3.6143(11) -0.0618-0.0840 0.9945 3.2463 8.51(9) 24.1 15.9 3.4760(8) -3.2989(8) 1.477

[1555] = X,Y,Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

Cg(I)	x	y	z	Xo	Yo	Zo
Cg(4)	0.63088(8)	0.80260(5)	0.59694(6)	6.4137(8)	13.8537(8)	8.3277(8)
Cg(6)	0.65842(7)	0.87639(4)	0.35549(6)	6.7217(7)	15.1273(7)	4.9593(8)

==

Table S5. Hydrogen bonding parameters in compounds **4A, 4B, 4E, 4I, 4K, 4L, 4M, 4N, 4P** and **4S**

Compound	**D—H…A**	**Bond distance/ Å**			**Bond angle/°**
		D—H	**H…A**	**D…A**	**D—H…A**
4A	C7—H7…F4	0.95	2.31	2.6704(17)	102
	C19—H19..F4^{i}	0.95	2.52	3.2663(17)	135
4B	C2—H2…F4^{i}	0.95	2.50	3.2733(18)	138
	C7—H7…F6	0.95	2.34	2.691(2)	101
	C7—H7…F8^{ii}	0.95	2.52	3.228(2)	131
	C20—H20C…F10^{iii}	0.98	2.48	3.185(2)	128
	C27—H27…F12	0.95	2.31	2.671(2)	102
	C27—H27…F1^{iv}	0.95	2.55	3.081(2)	116
4E	C7—H7…F6	0.95	2.33	2.6844(16)	102
	C7—H7…F12^{i}	0.95	2.53	3.1609(17)	124
	C16—H16…F8	0.95	2.35	2.6962(15)	101
	C16—H16…F10^{ii}	0.95	2.49	3.2006(16)	131
	C17—H17…F16^{ii}	0.95	2.50	3.3428(16)	148
	C22—H22…F14^{i}	0.95	2.46	3.2784(15)	145
	C27—H27…F15	0.95	2.35	2.6964(16)	101
	C36—H36…F17	0.95	2.35	2.7004(17)	101
	C36—H36…F1^{iii}	0.95	2.53	3.1718(18)	125
	C37—H37…F7^{iii}	0.95	2.49	3.3219(16)	146
4I	C3A—H3A…F1A	0.95	2.38	2.7075(17)	100
	C3B—H3B…F1B	0.95	2.34	2.6889(18)	101
	C8A—H8A…F6A	0.95	2.34	2.6877(18)	101
	C15A---H15A…F3B^{i}	0.95	2.55	3.502(2)	162
4K	---	---	---	---	---
4L	C11—H11A…N1	0.96	2.36	2.836(3)	110
	C36—H36A…N2	0.96	2.35	2.825(3)	110
	C57—H57A…N3	0.96	2.36	2.891(3)	110
	C82---H82A…N4	0.96	2.33	2.809(3)	110
4M	C16—H16…F7^{i}	0.95	2.55	3.496(3)	175
4N	C11-H11…N1	0.96	2.36	2.831(2)	110
	C14—H14…F1^{i}	0.98	2.46	3.362(3)	152
	C29—H29A…N2	0.96	2.34	2.812(3)	110
	C29—H29B..F1^{ii}	0.96	2.46	3.295(2)	145
	C33—H33A…F3^{iii}	0.97	2.51	3.479(3)	178
4P	C17—H17…F3^{i}	0.95	2.53	3.3822(18)	150
4S	---	---	---	---	---

Symmetry codes: **1** (i) -1/2+*x*,3/2-*y*,-1/2+z; **2** (i) *x*,1/2+*y*,3/2-*z*, (ii) 1-*x*,1-*y*,1-*z*, (iii) *x*,3/2-*y*,1/2+*z*, (iv) -*x*,1-*y*,1-*z*; **3** (i) -*x*,1/2+*y*,1/2-*z*, (ii) -*x*,-1/2+*y*,1/2-*z*, (iii) 1-*x*,1/2+*y*,1/2-*z*; **4** (i) -*x*,*y*,1/2-*z*; **7** (i) 3-*x*,2-*y*,2-*z* **8** (i)1-*x*,1-*y*,2-*z*, (ii) *x*,*y*,*z*-1, (iii) 1-*x*,1-*y*,1-*z*; **9** (i) 1+*x*,1+*y*,*z*;

Table S6. Various types of intermolecular interactions in compounds **4A-B, 4E, 4I, 4K-N, 4P** and **4S** (Summary of π stacking and H bonding from **figure S1**and **table S3**, respectively).

Compound	Intermolecular interactions	
	Number of π stacking	Number of Non-Conventional HB
4A	2	2
4B	5	6
4E	2	10
4I	1	4
4K	2	None
4L	4	4
4M	5	1
4N	4	5
4P	1	1
4S	1	None

Table S7. FMOs values computed by DFT method. The values are reported on eV.

	E.G. vaccum	E.G. solvent	Vacuum		Solvent	
			HOMO	LUMO	HOMO	LUMO
4A	3.76	3.69	-6.82	-3.06	-6.65	-2.95
4B	**3.67**	**3.57**	-6.67	-2.99	-6.50	-2.92
4E	3.82	3.76	-7.06	-3.23	-6.83	-3.07
4I	4.08	4.00	-6.95	-2.86	-6.78	-2.77
4K	3.72	3.67	-6.33	-2.61	-6.34	-2.67
4L	3.72	3.67	-6.32	-2.60	-6.34	-2.67
4M	3.73	3.73	-6.72	-2.98	-6.57	-2.85
4N	4.05	4.00	-6.47	-2.42	-6.49	-2.48
4P	3.75	3.68	-6.42	-2.66	-6.39	-2.71
4S	**4.22**	**4.18**	-6.76	-2.53	-6.77	-2.58

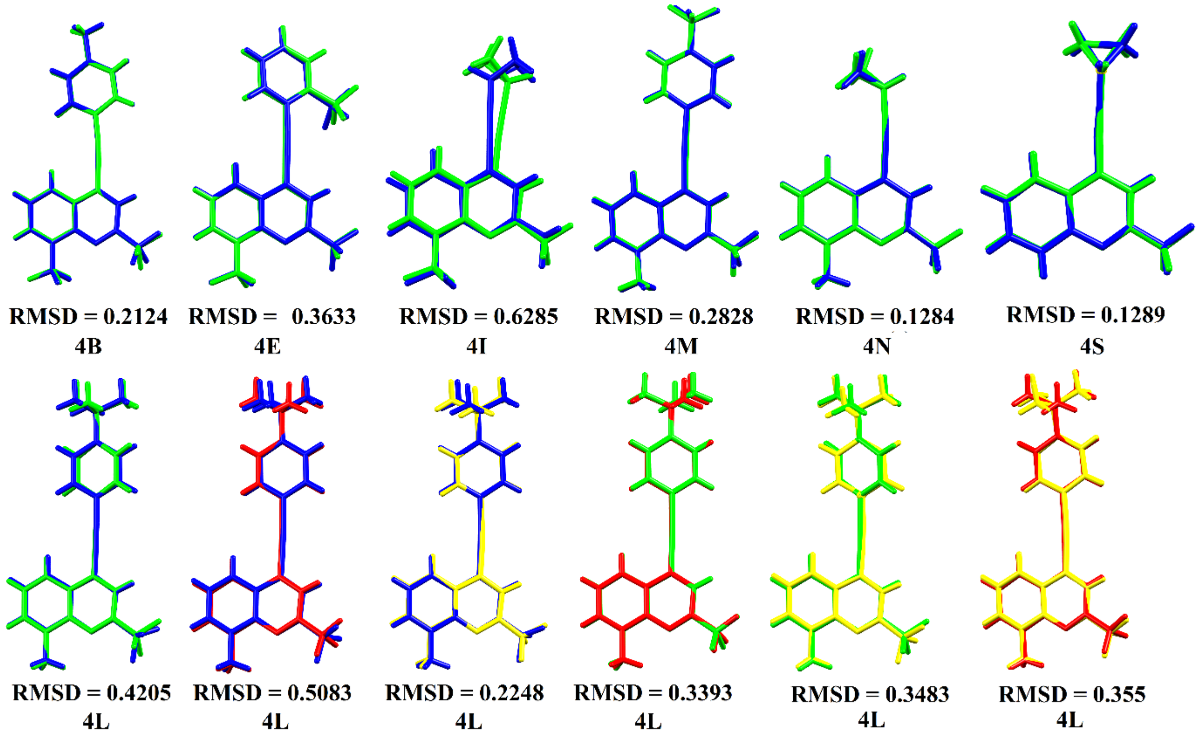


Figure S1: Molecular overlay diagrams with their respective RMSD values.

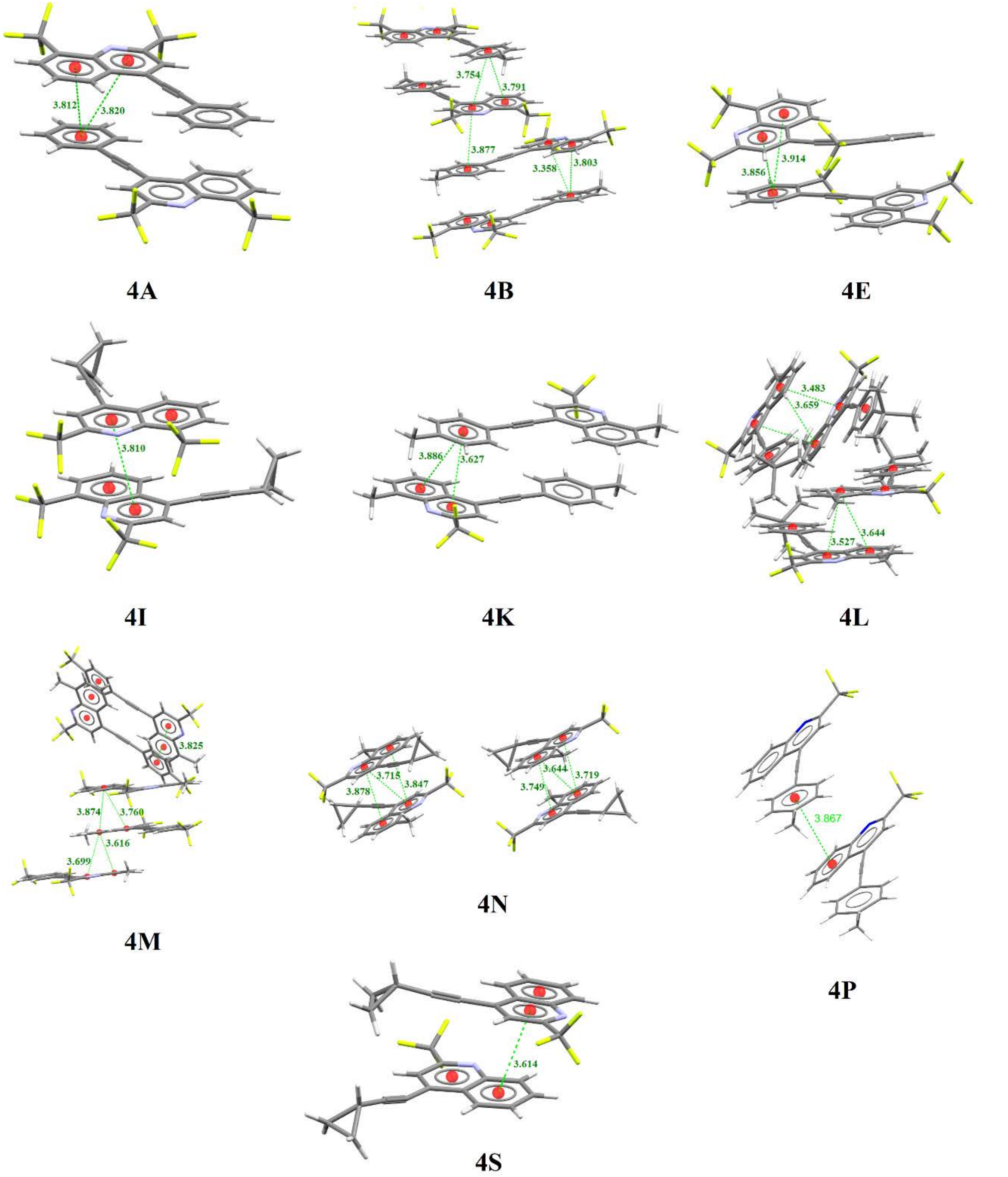


Figure S2. Visual interpretation of the various types of π stacking in compounds **4A-4B, 4E, 4I, 4K, 4L, 4M, 4N, 4P** and **4S**.

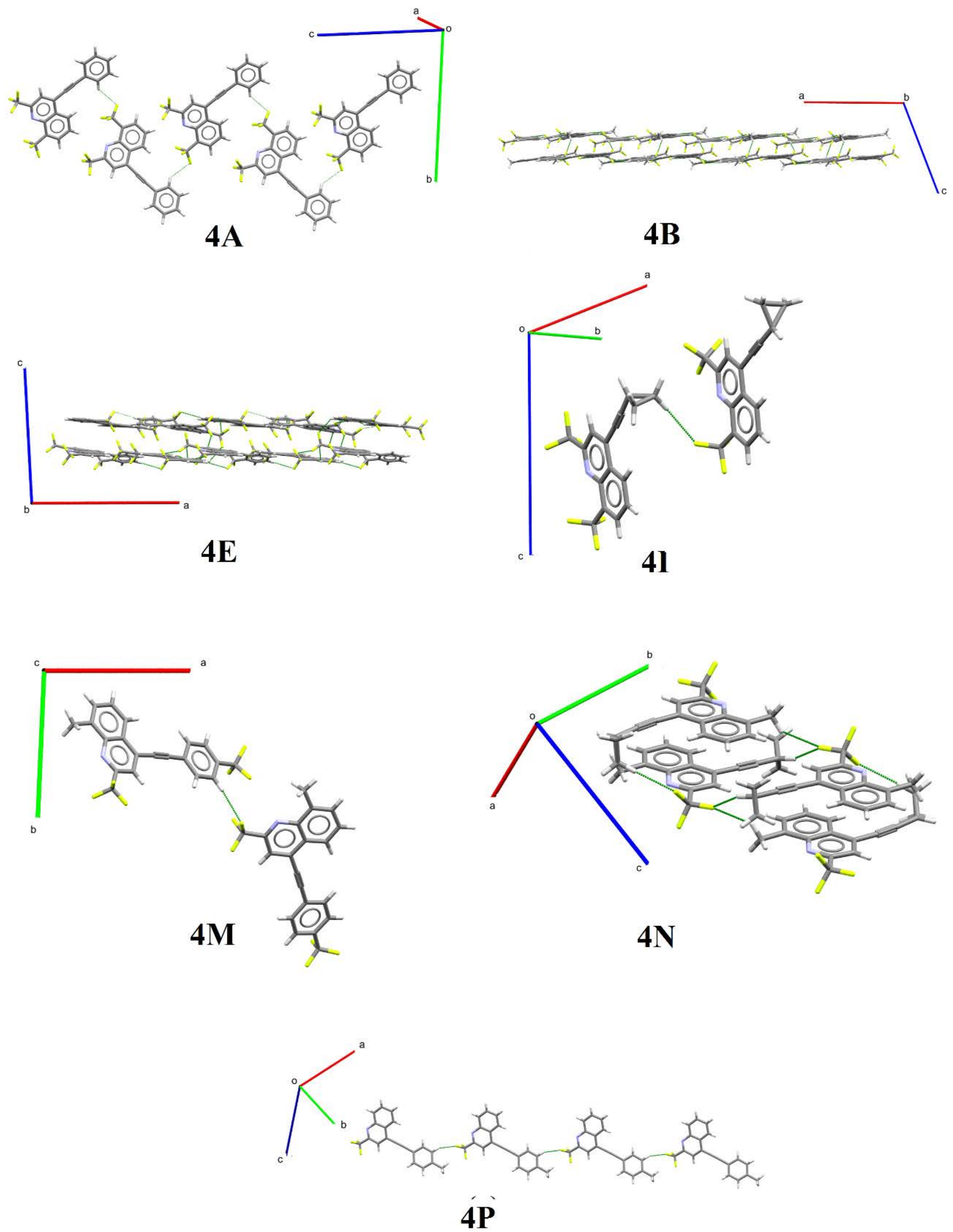


Figure S3. Visual interpretation of hydrogen bonding networks

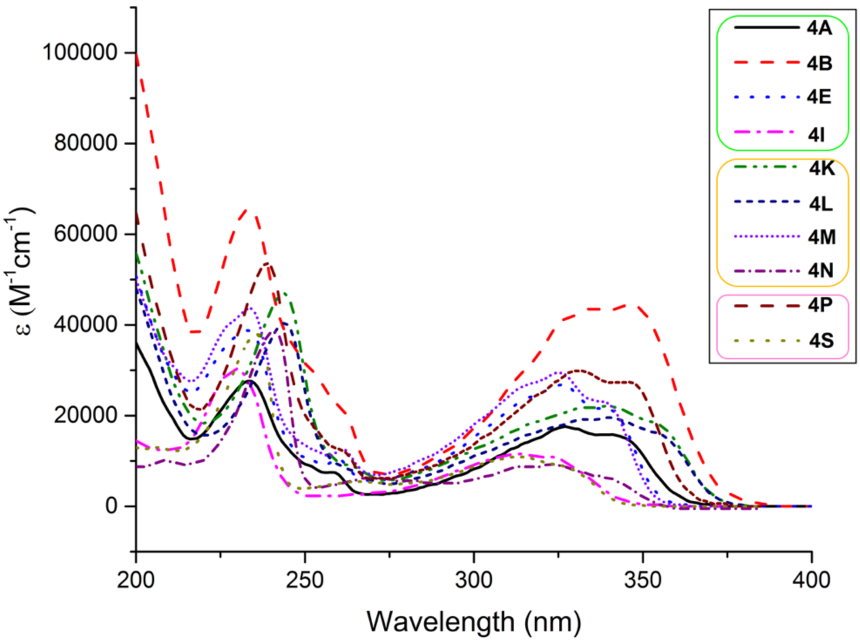


Figure S4: Absorption spectra of compounds **4A, 4B, 4E, 4I, 4K, 4L, 4M, 4N, 4P** and **4S** in acetonitrile

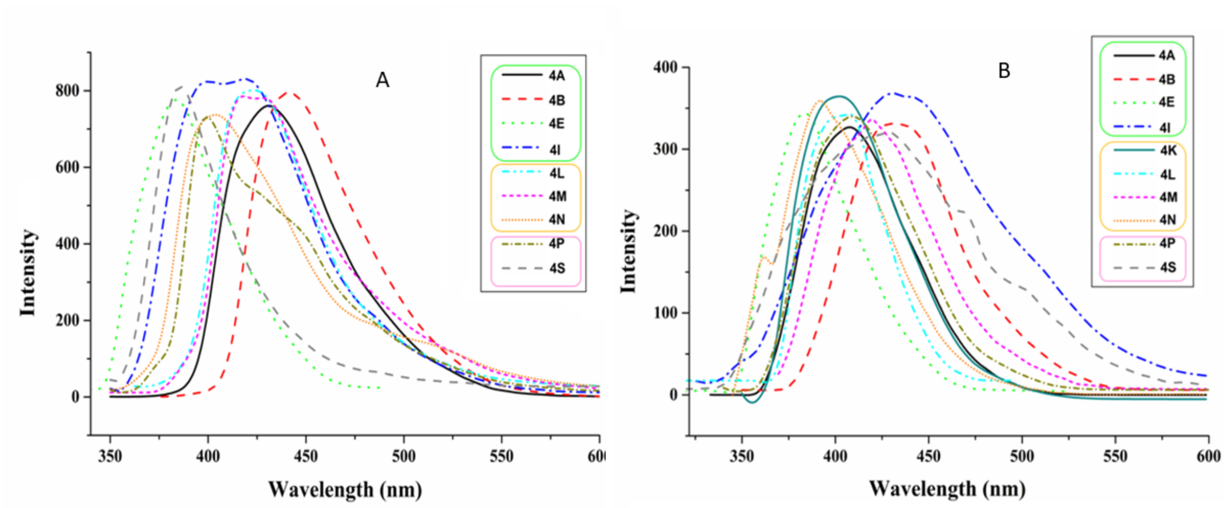
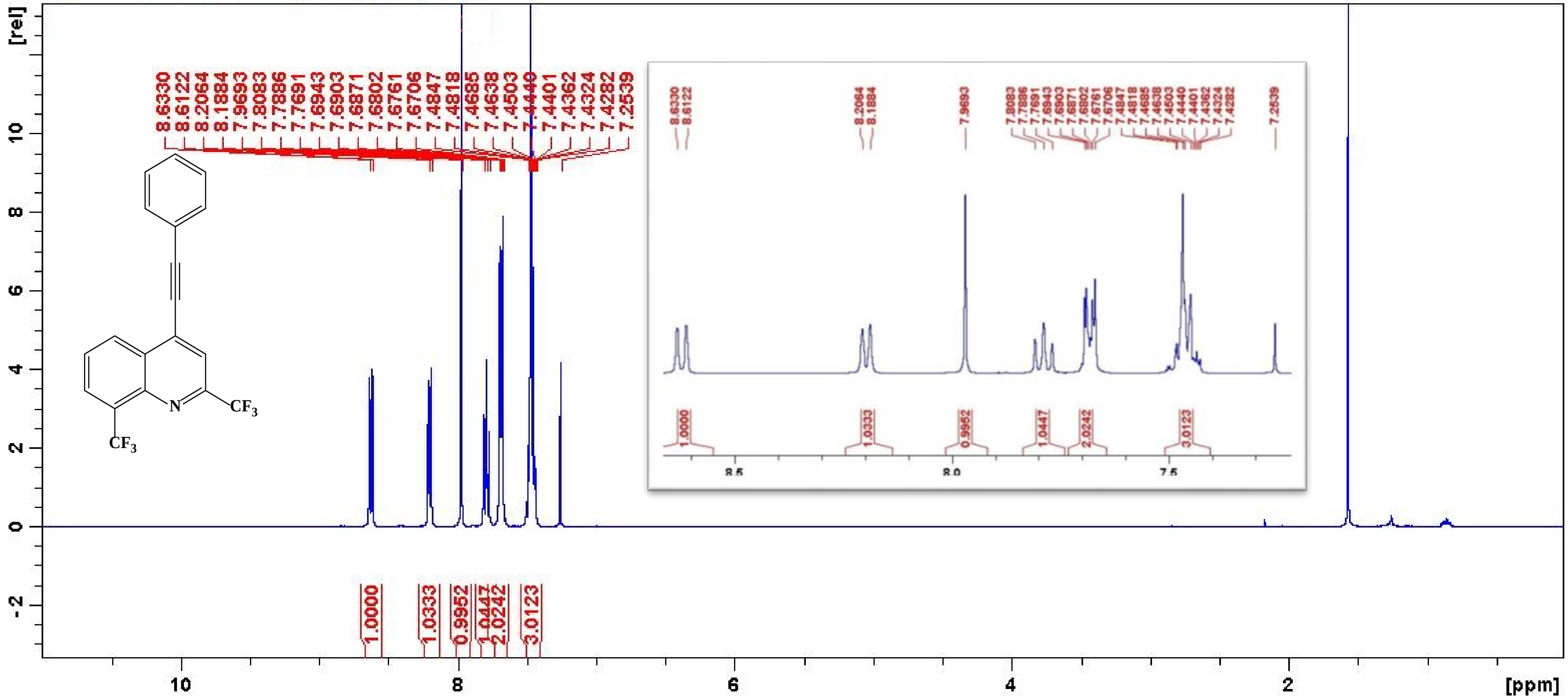


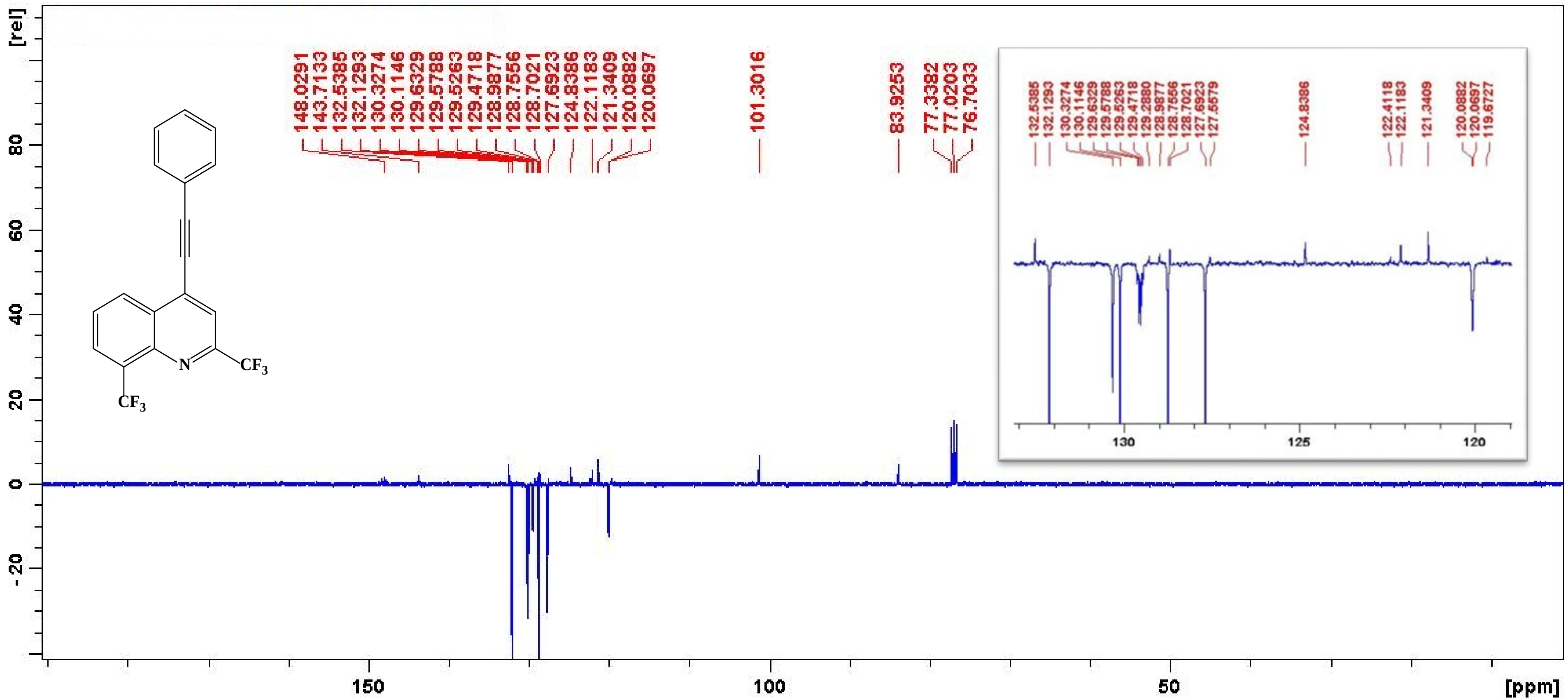
Figure S5. Emission spectra of compounds **4A, 4B, 4E, 4I, 4K, 4L, 4M, 4N, 4P** and **4S** in acetonitrile (A) and solid state(B).

NMR spectra

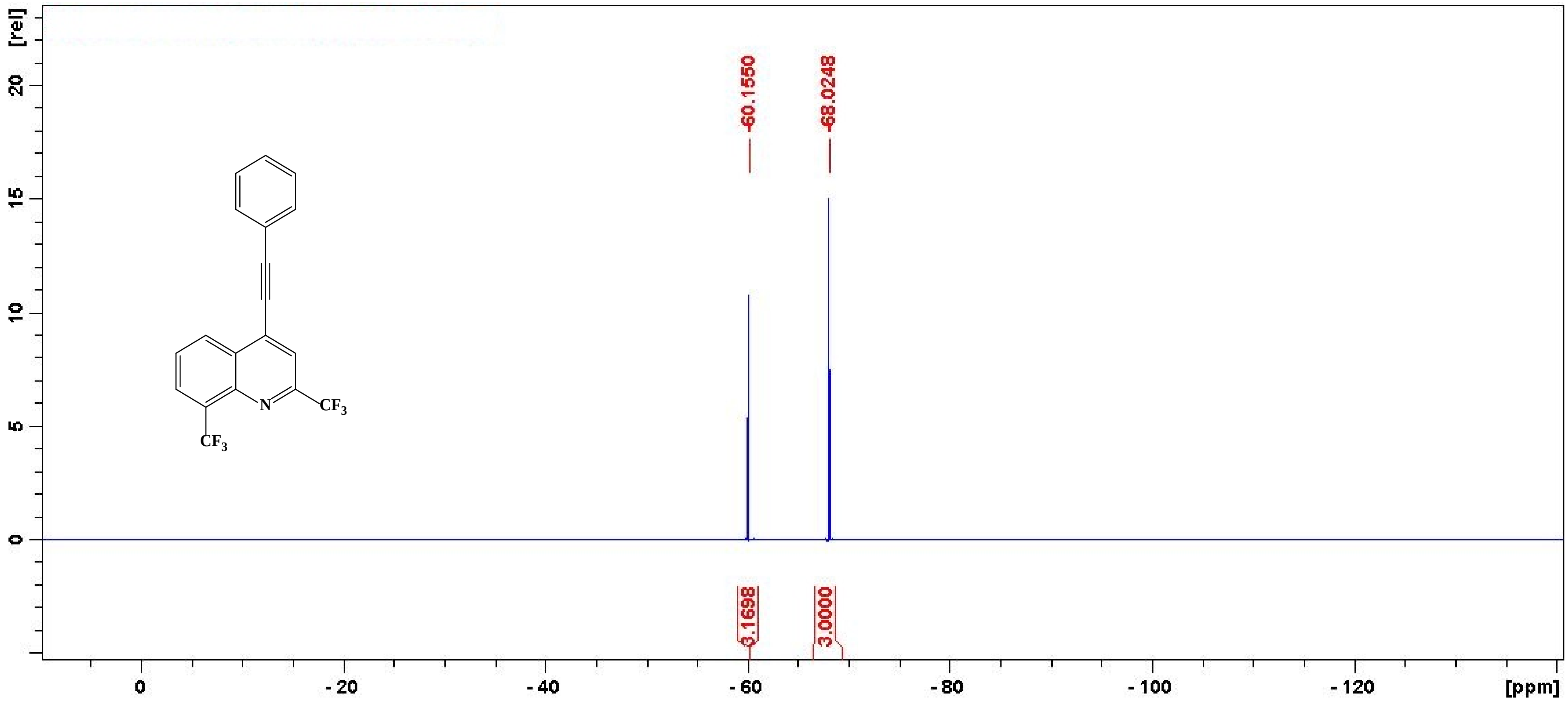
[1]H NMR spectrum of **4A (CDCl₃, 400 MHz)**



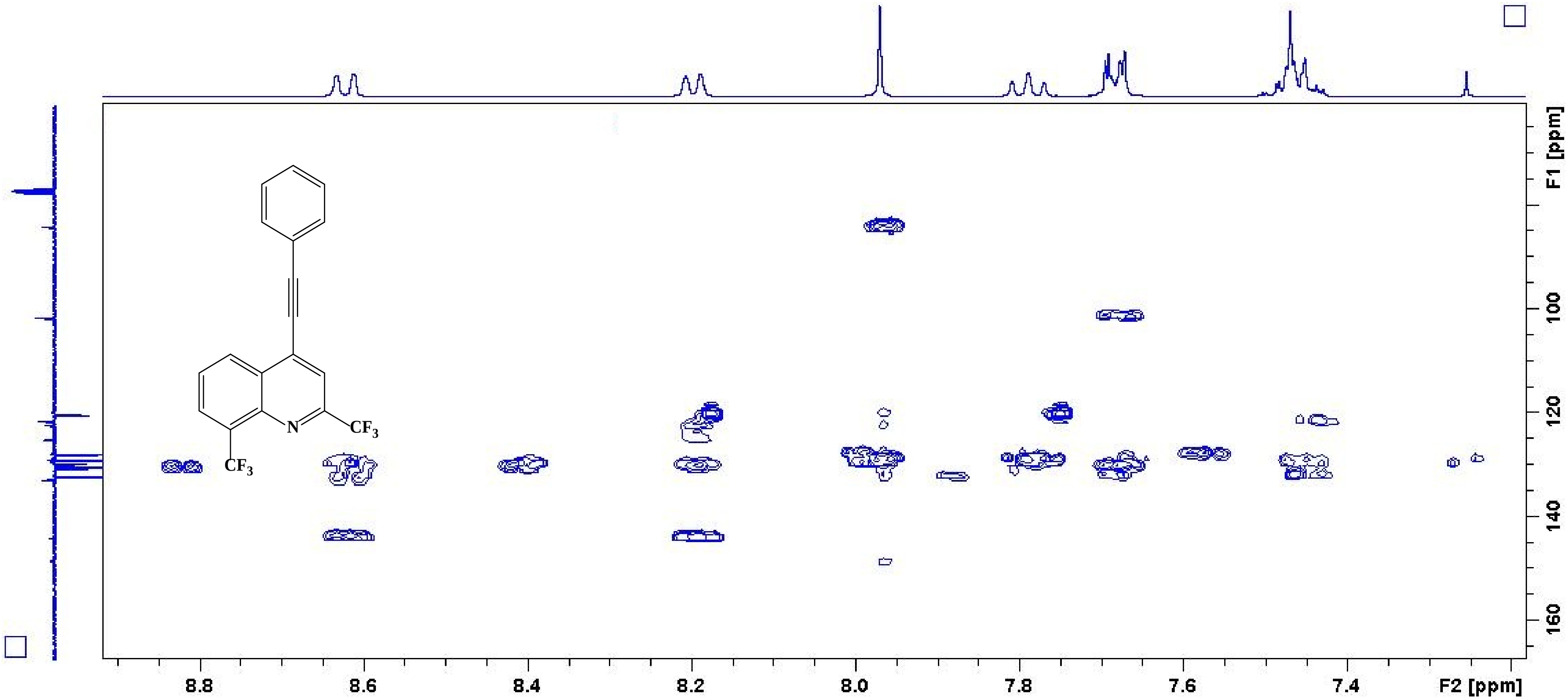
^{13}C NMR spectrum of **4A ($CDCl_3$, 100 MHz)**



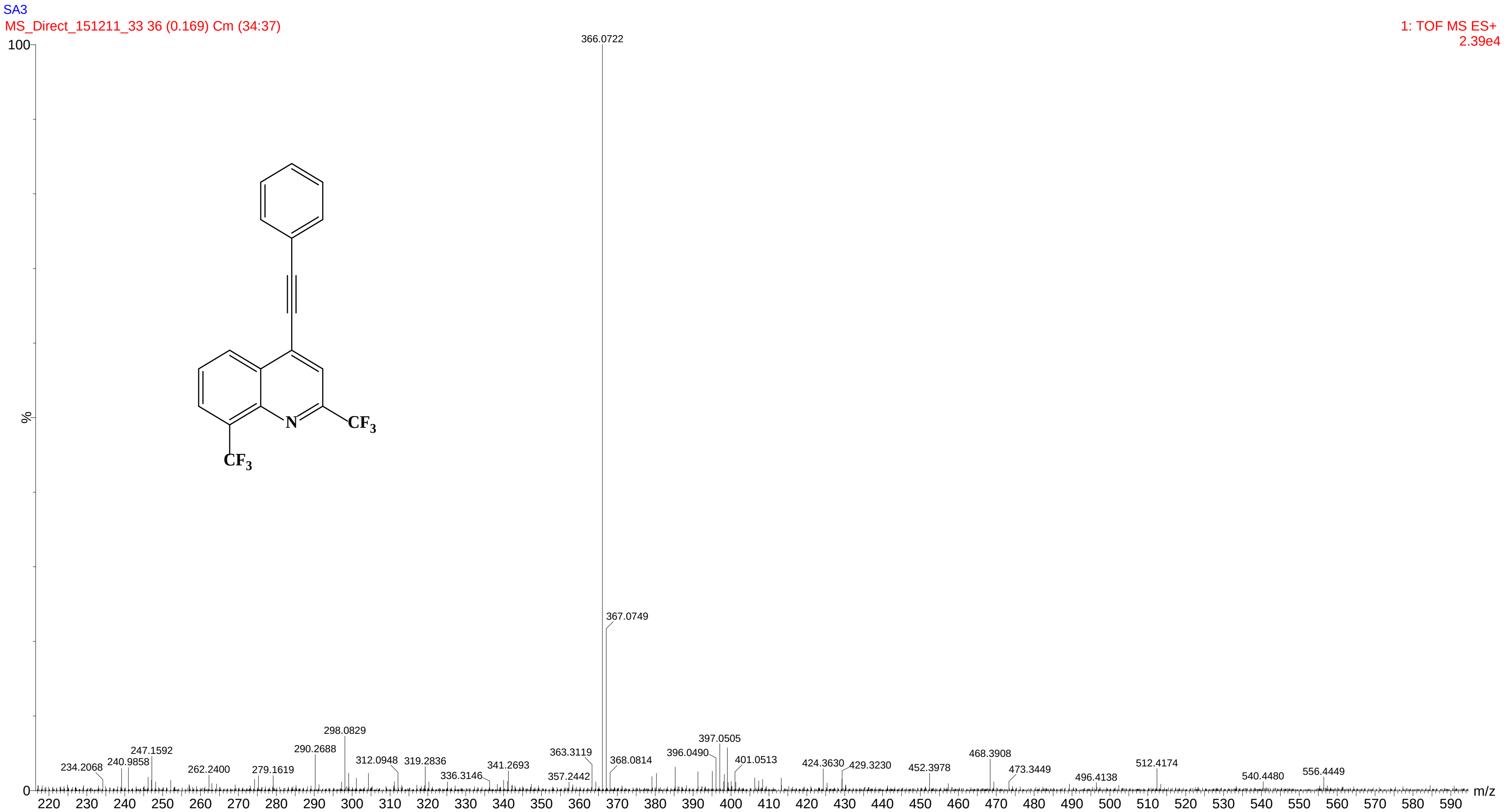
^{19}F NMR spectrum of **4A (CDCl$_3$, 376 MHz)**



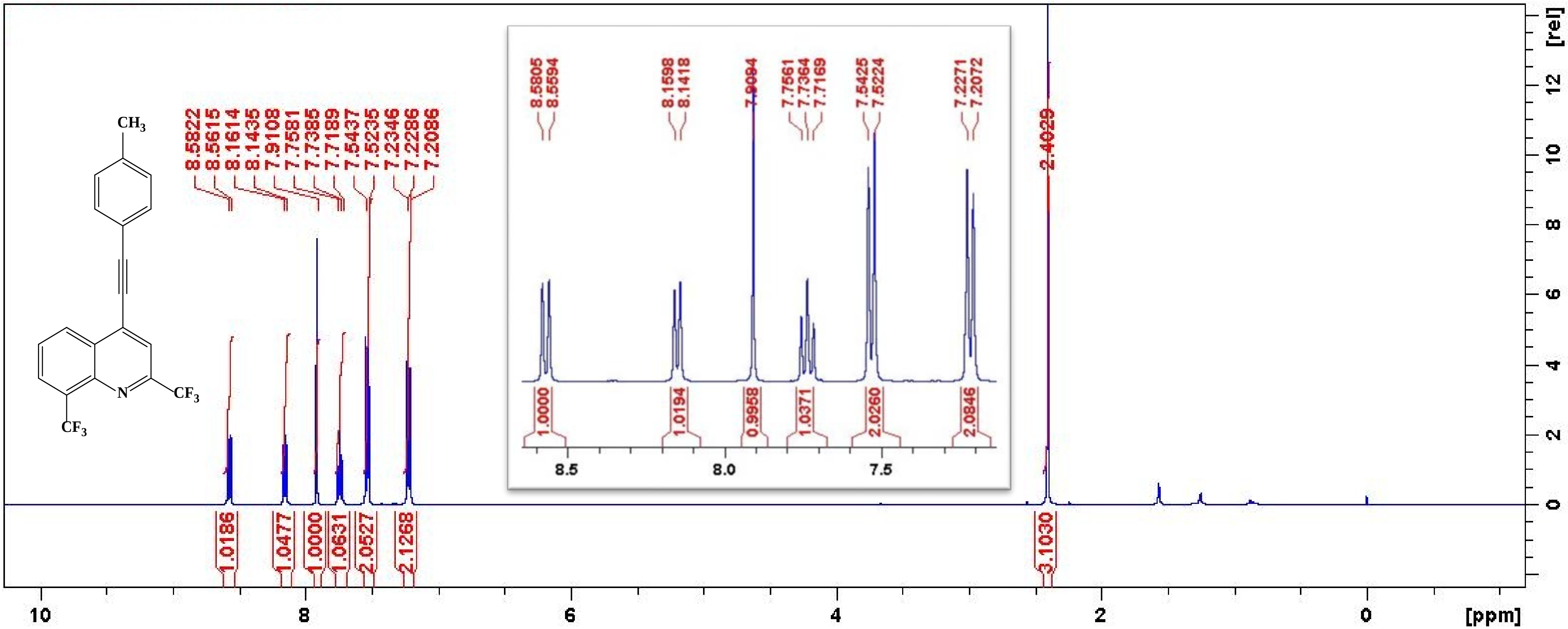
HMBC spectrum of **4A**



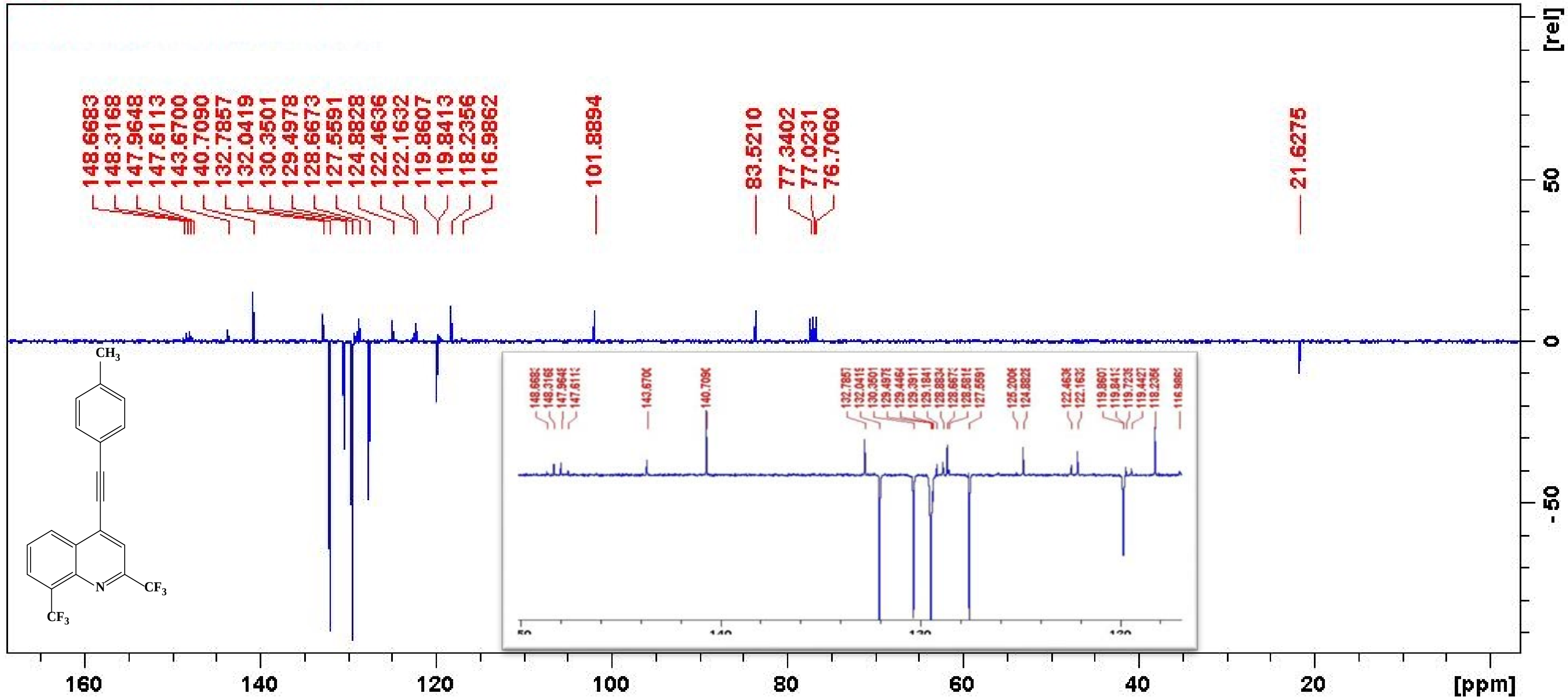
HRMS of **4A**


SA3
MS_Direct_151211_33 36 (0.169) Cm (34:37)
1: TOF MS ES+
2.39e4
100
%
0
366.0722
367.0749
298.0829
397.0505
247.1592
240.9858
234.2068
290.2688
262.2400
279.1619
312.0948
319.2836
336.3146
341.2693
363.3119
357.2442
368.0814
396.0490
401.0513
424.3630
429.3230
452.3978
468.3908
473.3449
496.4138
512.4174
540.4480
556.4449
N
CF3
CF3
220 230 240 250 260 270 280 290 300 310 320 330 340 350 360 370 380 390 400 410 420 430 440 450 460 470 480 490 500 510 520 530 540 550 560 570 580 590
m/z

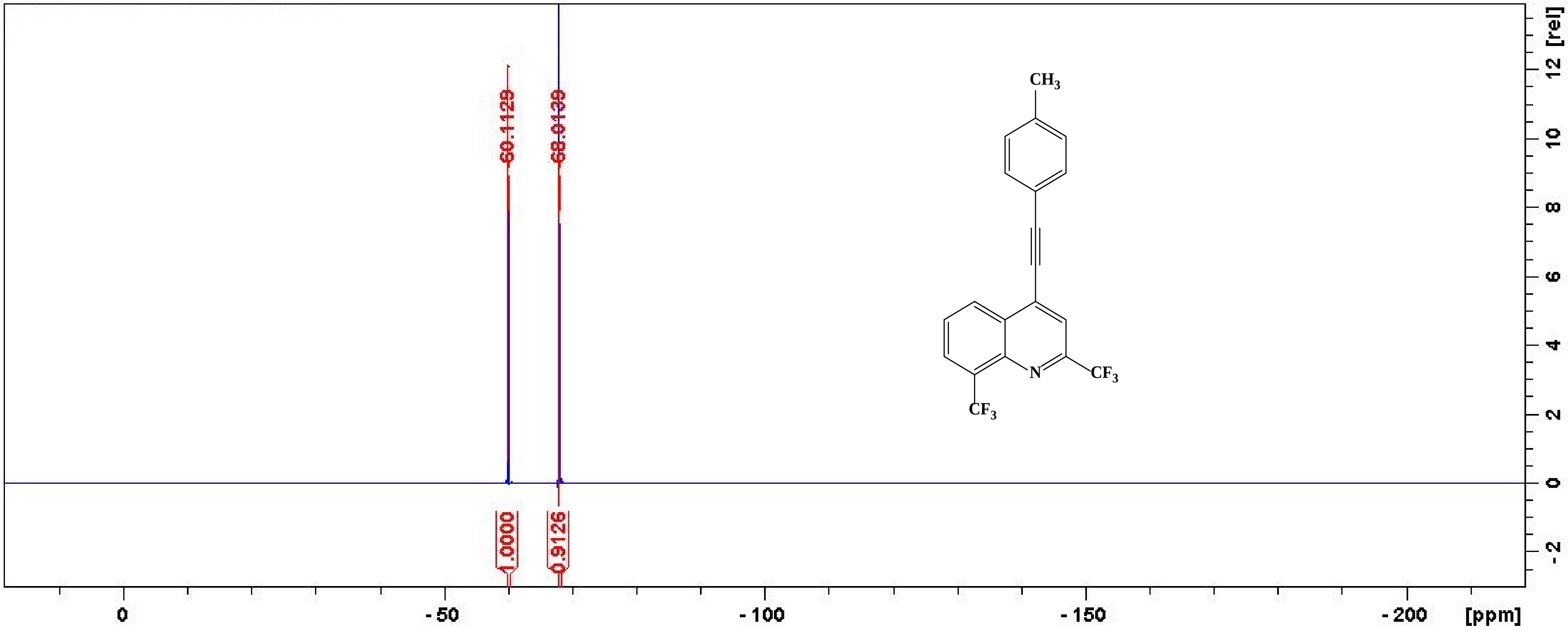
[1]H NMR spectrum of **4B (CDCl₃, 400 MHz)**



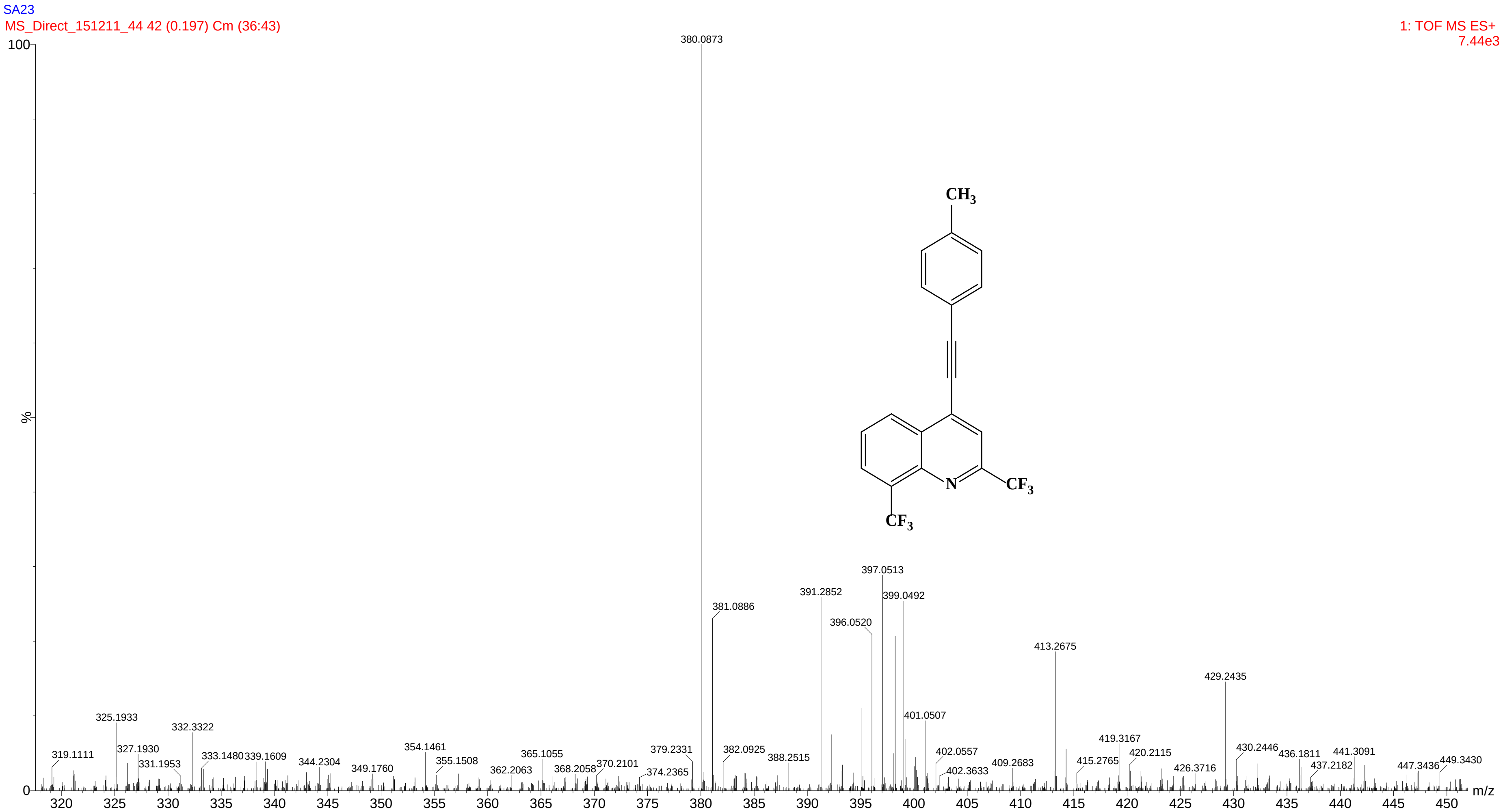
^{13}C NMR spectrum of **4B (CDCl$_3$, 100 MHz)**



^{19}F NMR spectrum of **4B ($CDCl_3$, 376 MHz)**

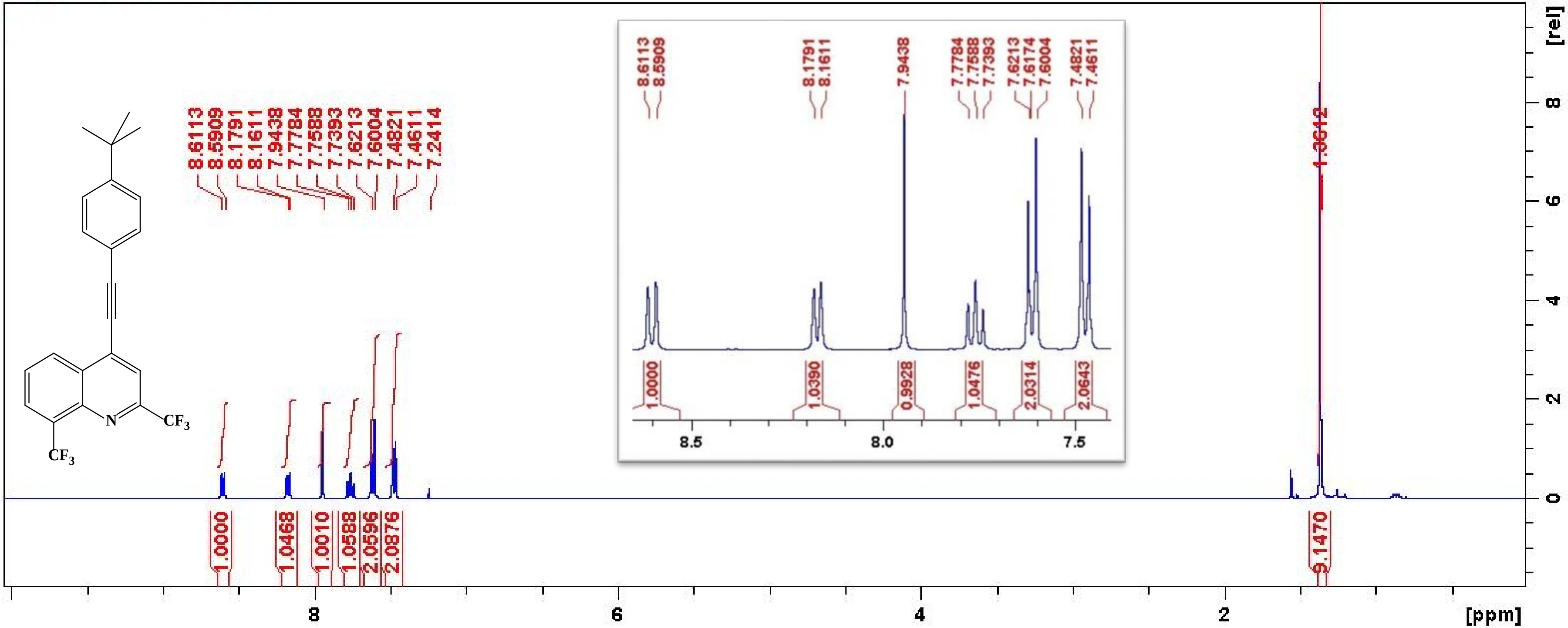


HRMS of **4B**

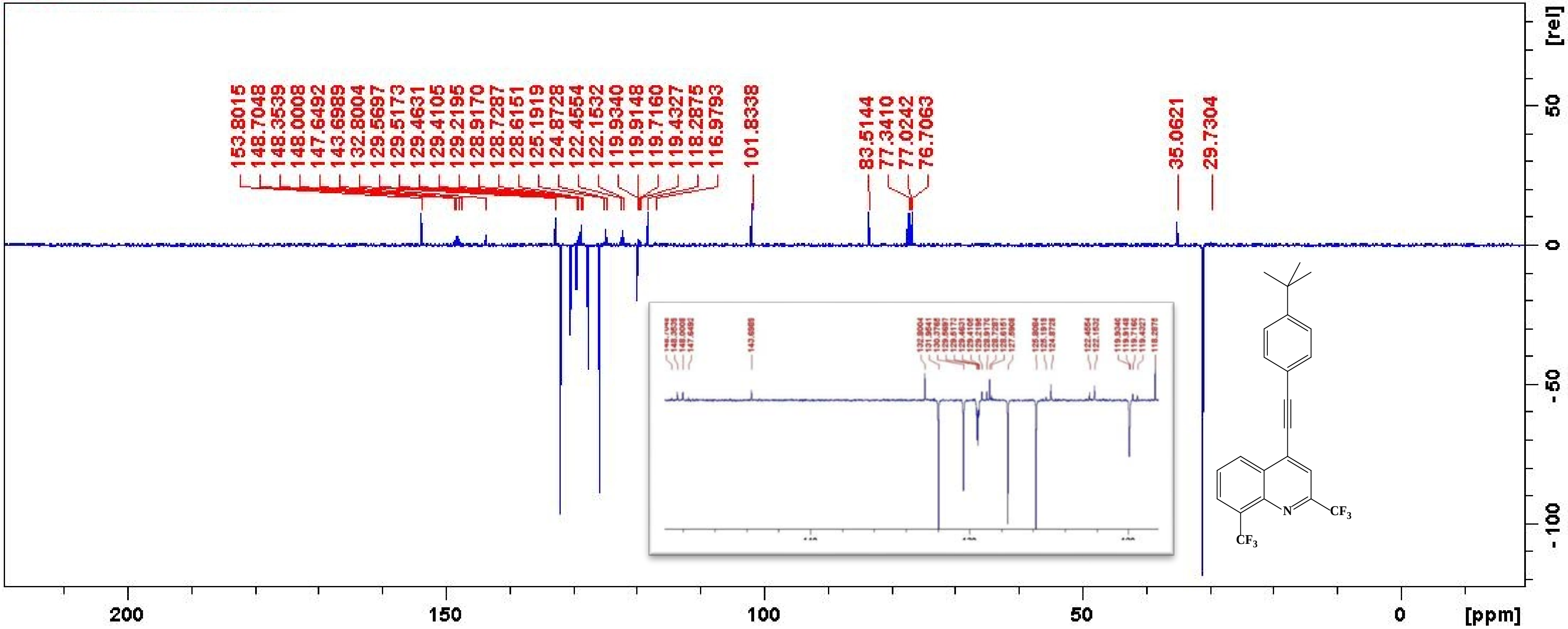


SA23
MS_Direct_151211_44 42 (0.197) Cm (36:43)
1: TOF MS ES+
7.44e3
100
%
0
m/z
380.0873
381.0886
391.2852
397.0513
399.0492
396.0520
413.2675
429.2435
401.0507
325.1933
332.3322
CH3
N
CF3
CF3

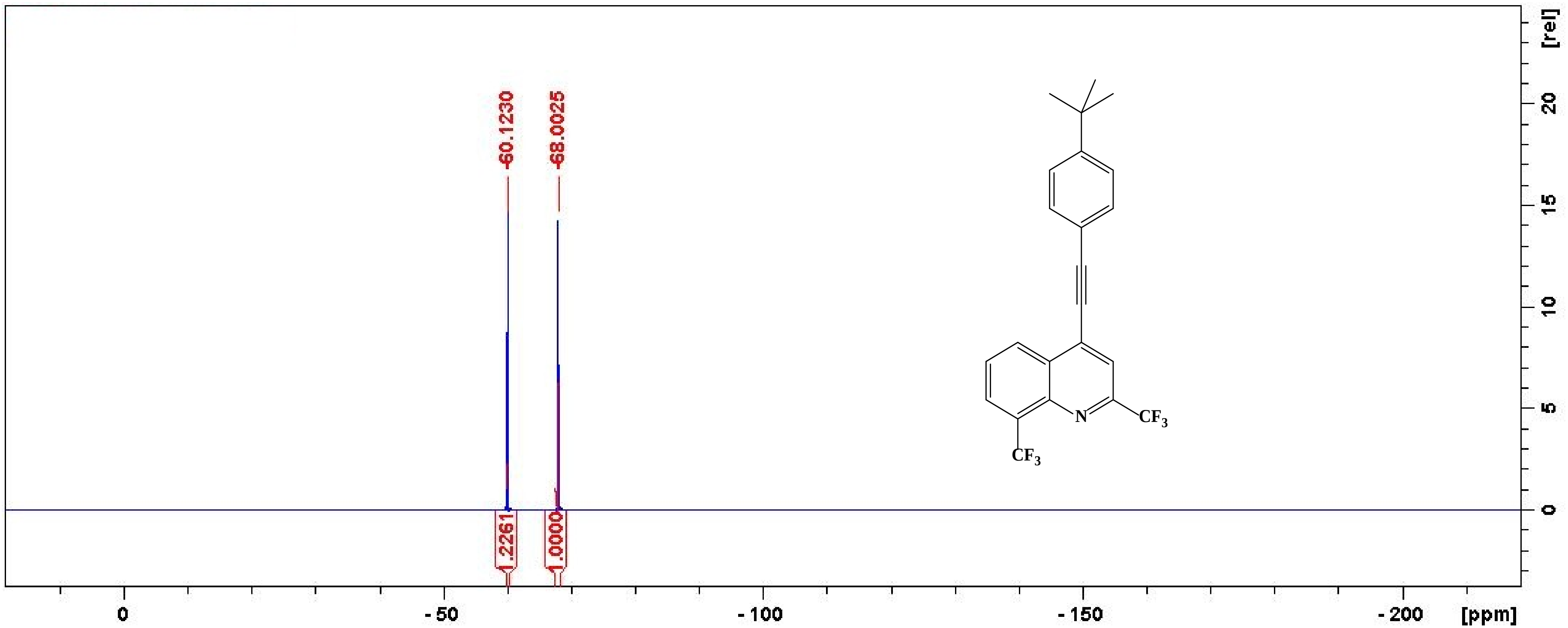
[1]H NMR spectrum of **4C ($CDCl_3$, 400 MHz)**



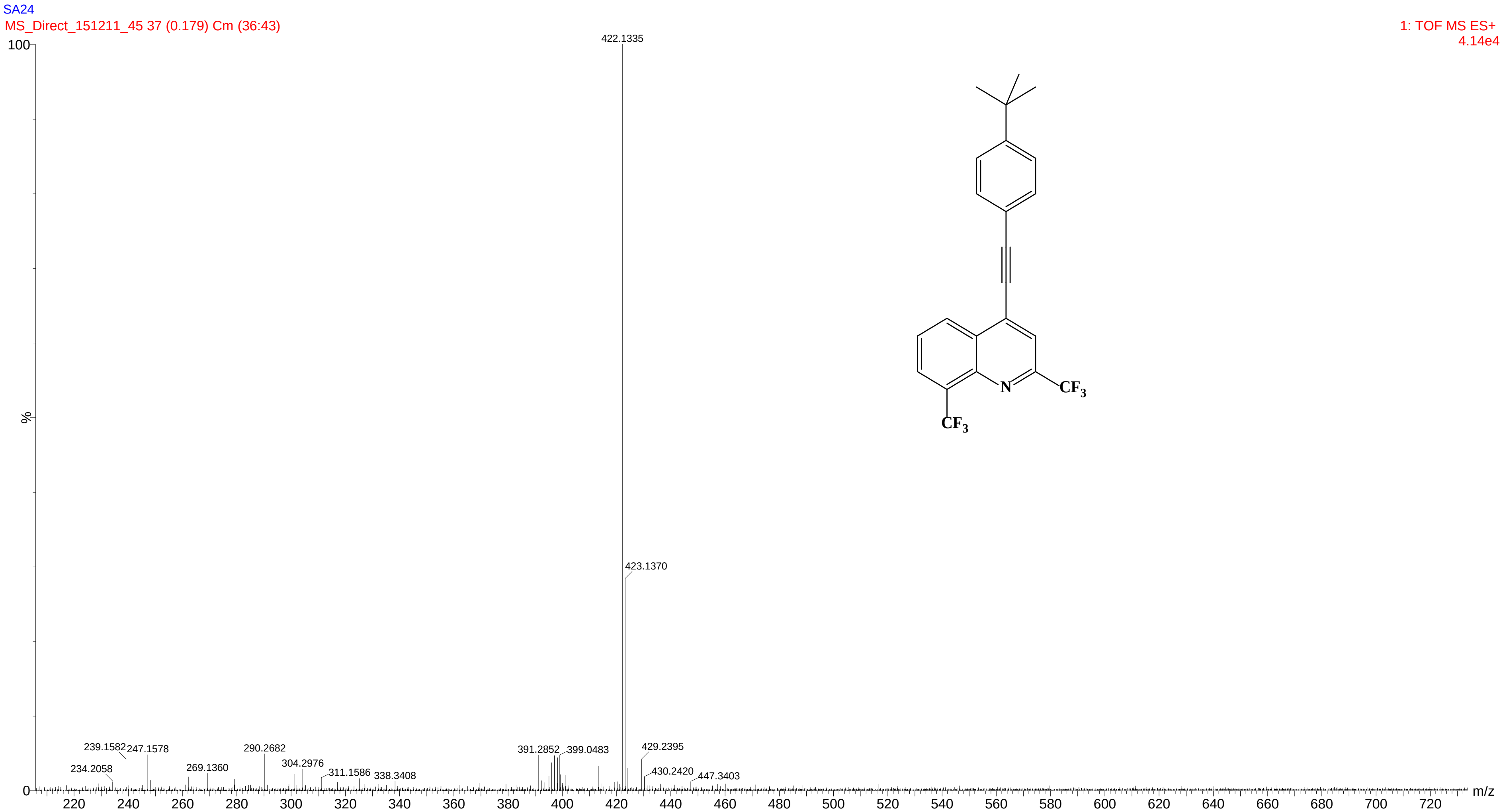
^{13}C NMR spectrum of **4C (CDCl$_3$, 100 MHz)**



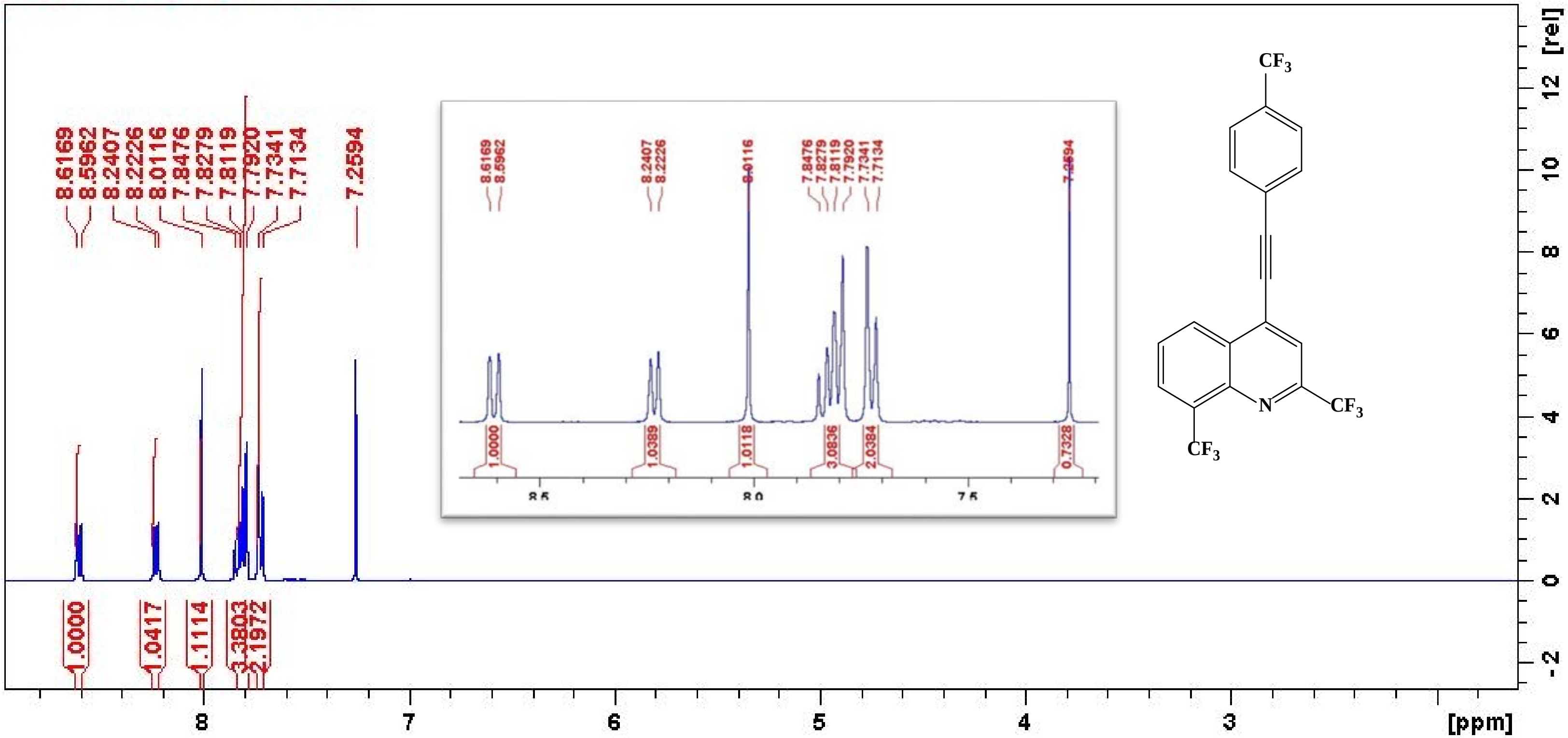
^{19}F NMR spectrum of **4C ($CDCl_3$, 376 MHz)**



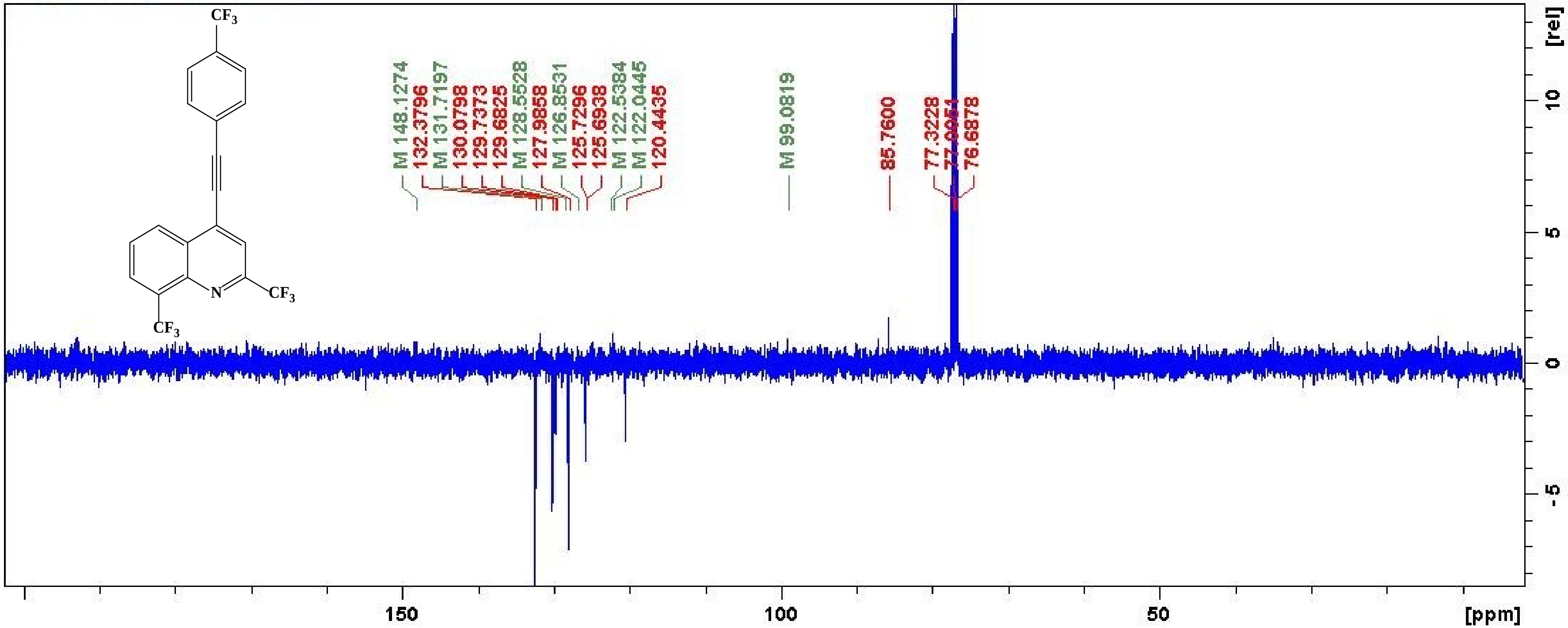
HRMS of **4C**


SA24
MS_Direct_151211_45 37 (0.179) Cm (36:43)
1: TOF MS ES+
4.14e4
100
%
0
422.1335
423.1370
239.1582
247.1578
234.2058
269.1360
290.2682
304.2976
311.1586
338.3408
391.2852
399.0483
429.2395
430.2420
447.3403
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
520
540
560
580
600
620
640
660
680
700
720
m/z
N
CF_3
CF_3

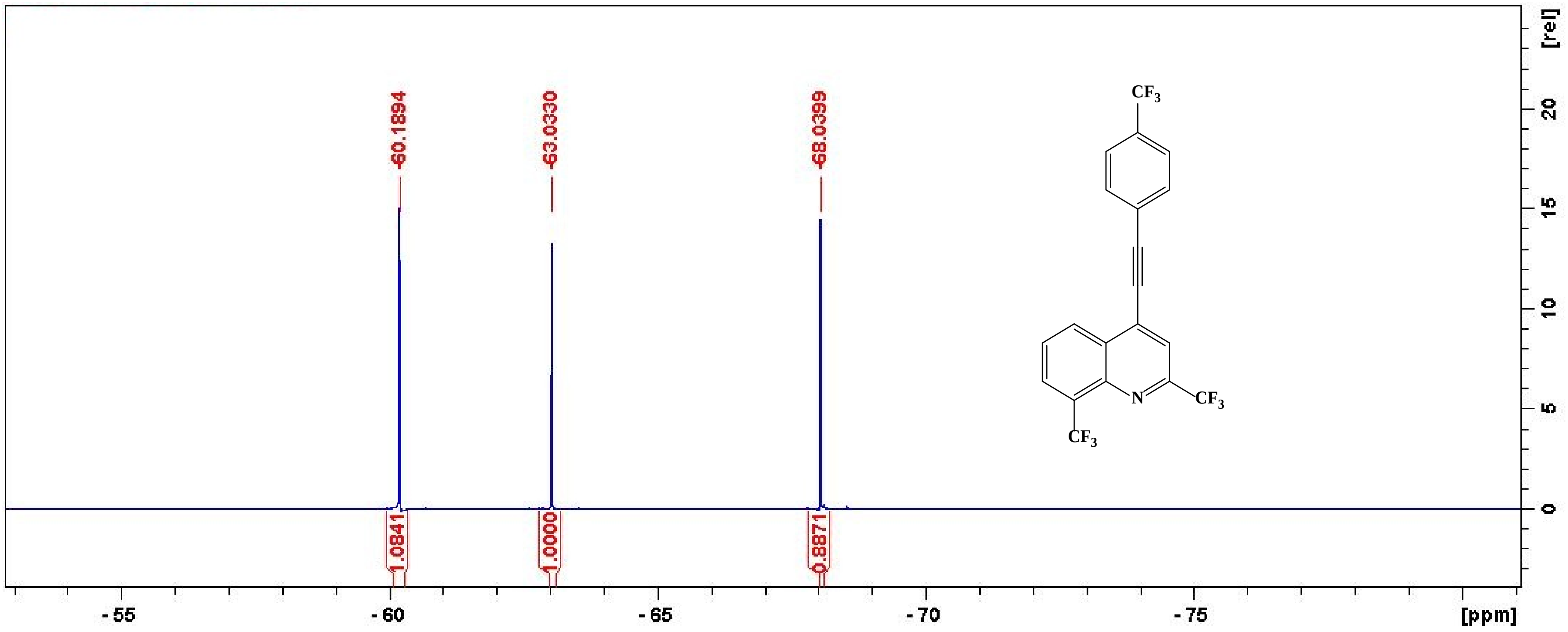
[1]H NMR spectrum of **4D ($CDCl_3$, 400 MHz)**



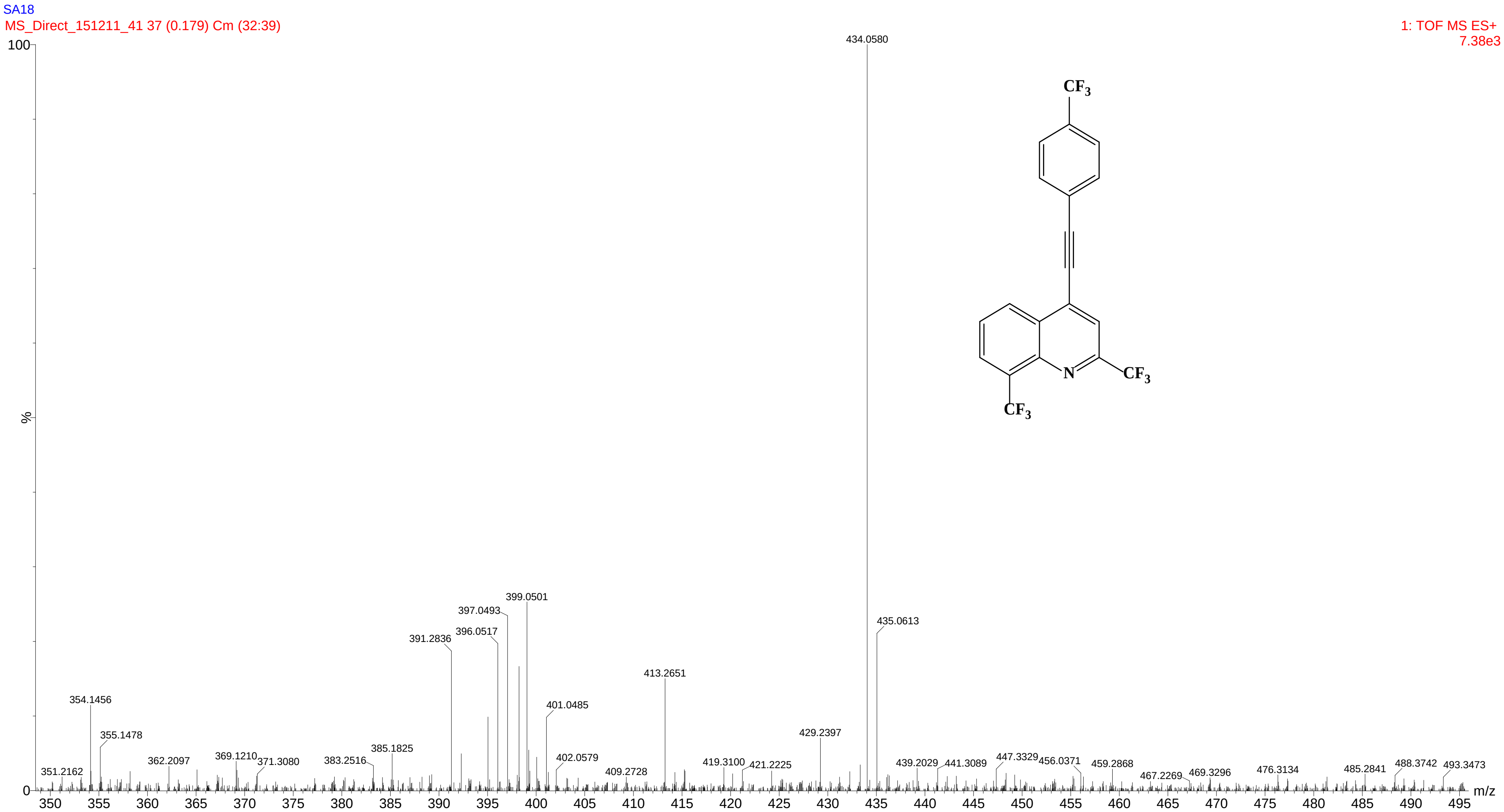
^{13}C NMR spectrum of **4D ($CDCl_3$, 100 MHz)**



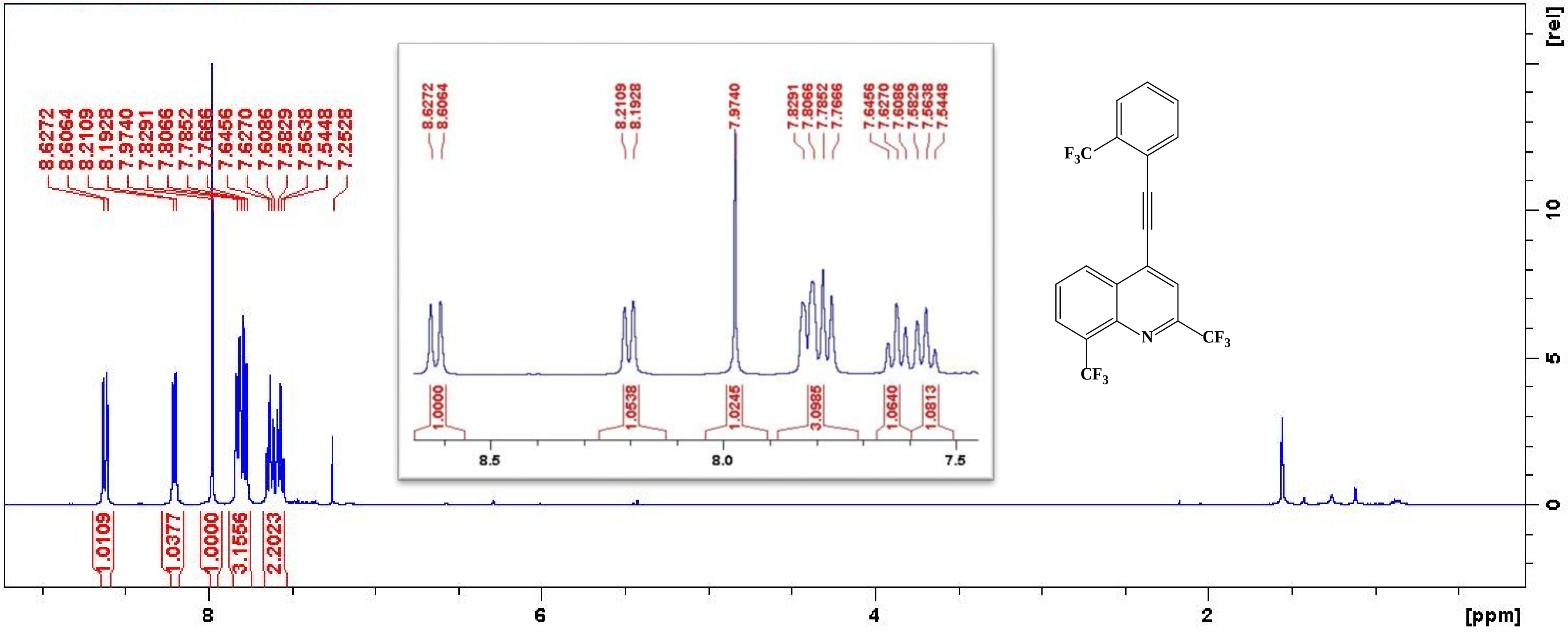
^{19}F NMR spectrum of **4D (CDCl$_3$, 376 MHz)**



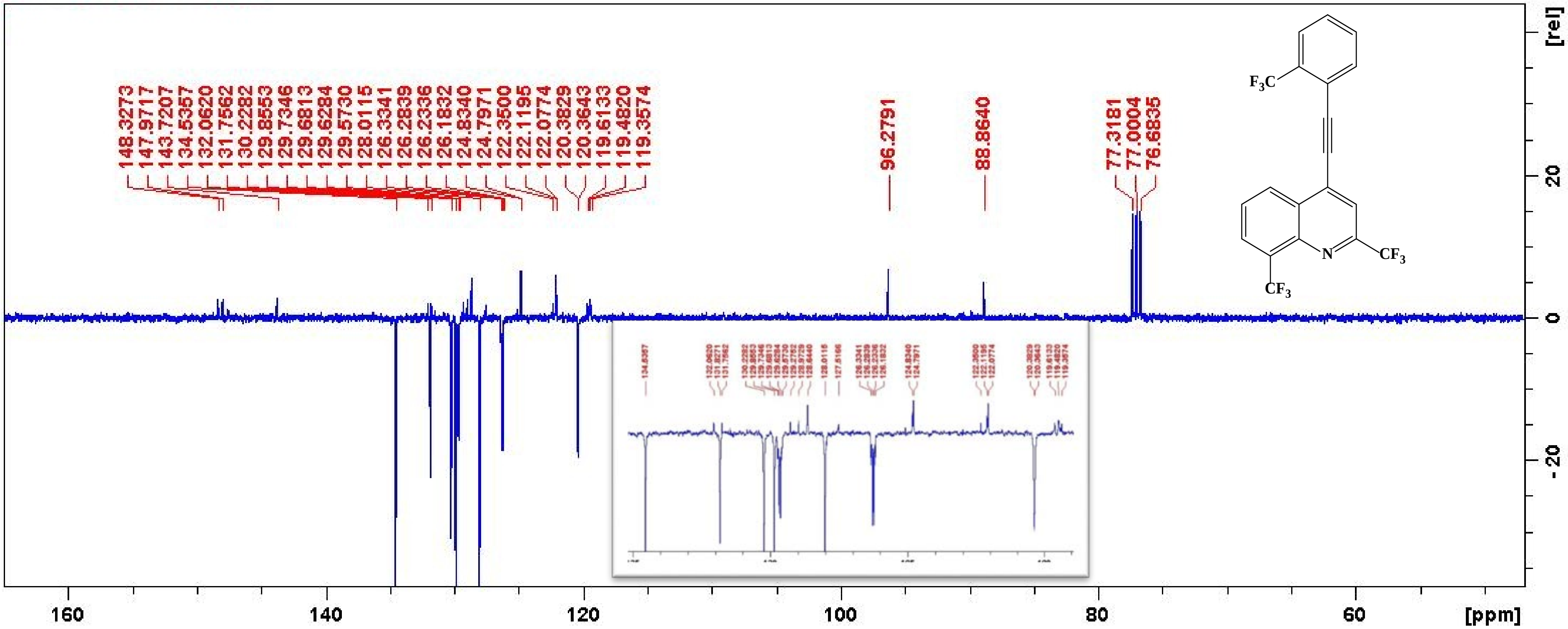
HRMS of **4D**


SA18
MS_Direct_151211_41 37 (0.179) Cm (32:39)
1: TOF MS ES+
7.38e3
434.0580
435.0613
399.0501
397.0493
396.0517
391.2836
413.2651
401.0485
354.1456
355.1478
429.2397
m/z
%
CF3
N

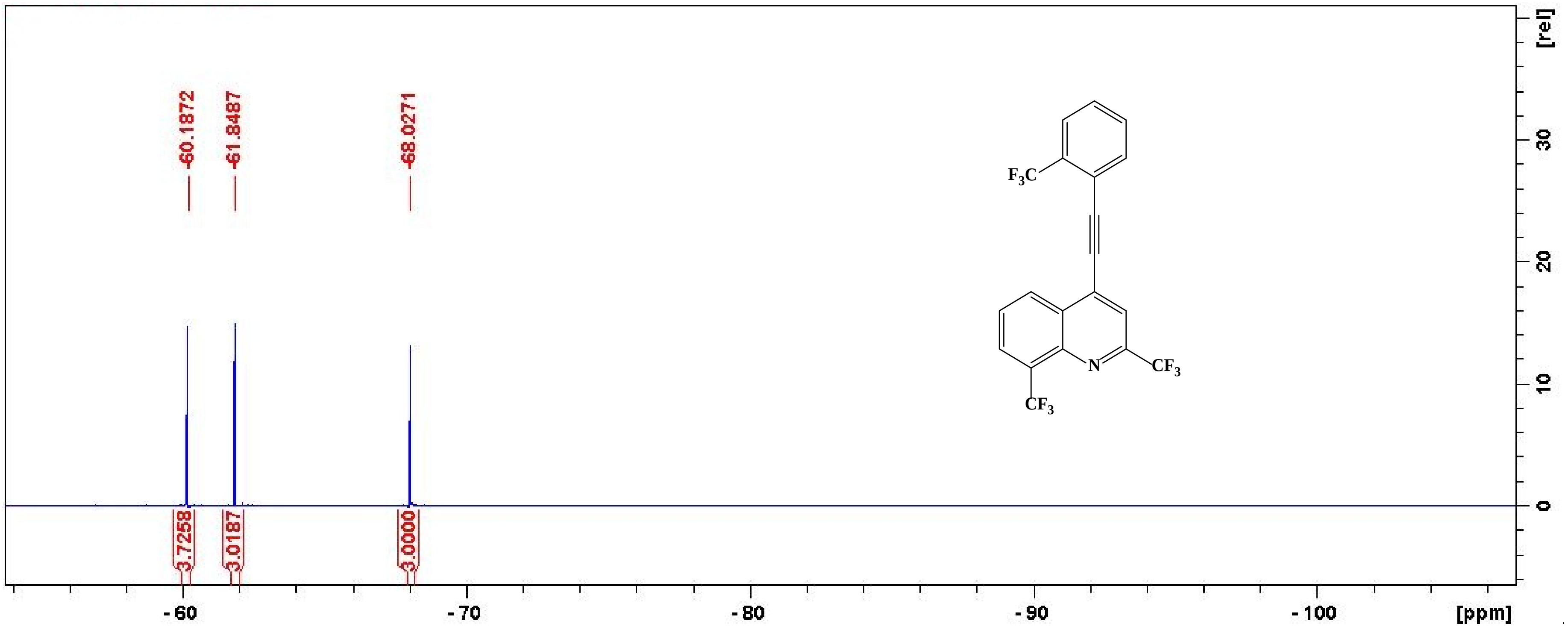
[1]H NMR spectrum of **4E (CDCl3, 400 MHz)**



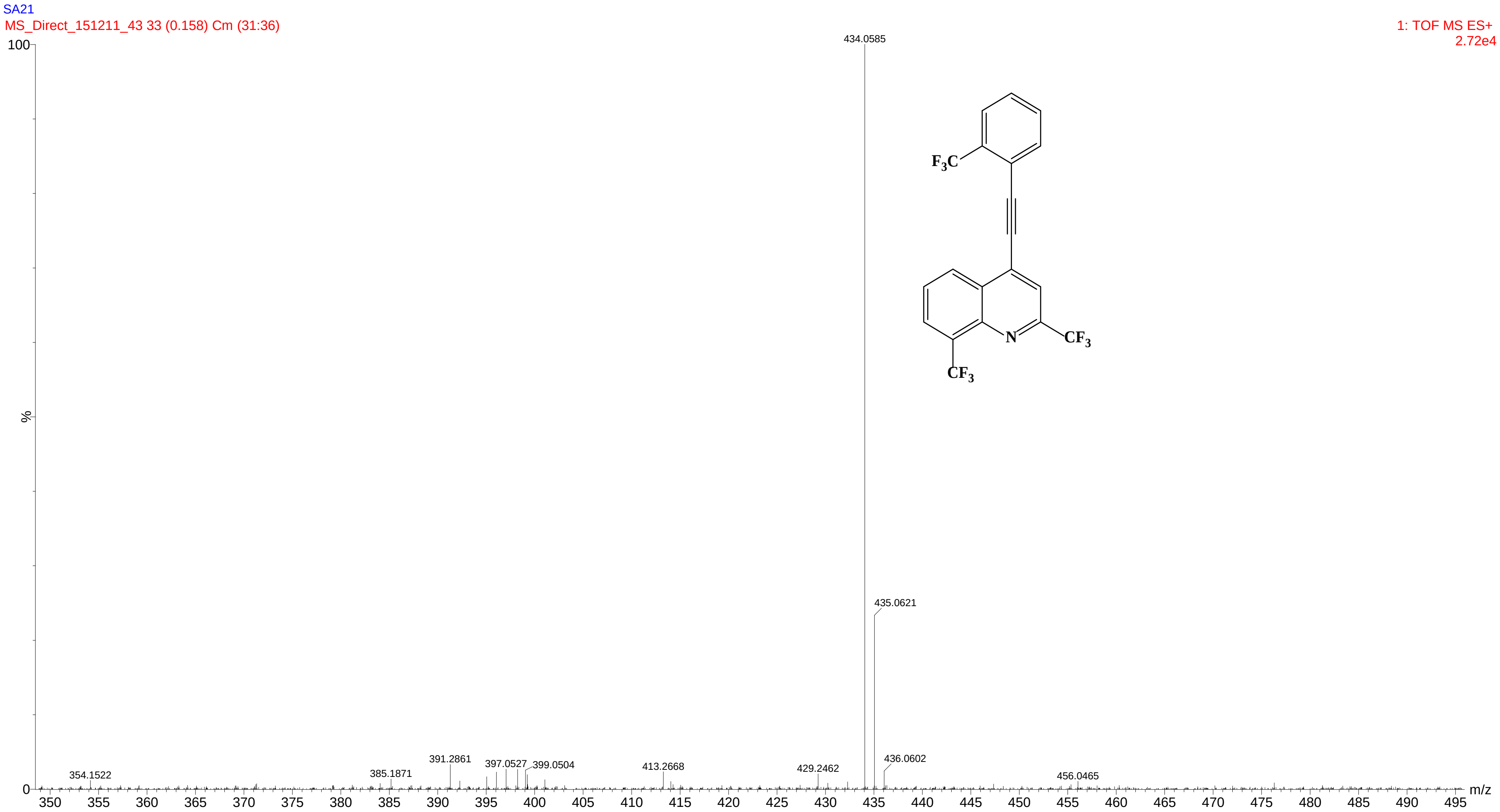
^{13}C NMR spectrum of **4E** **(CDCl$_3$, 100 MHz)**



[19]F NMR spectrum of **4E (CDCl3, 376 MHz)**

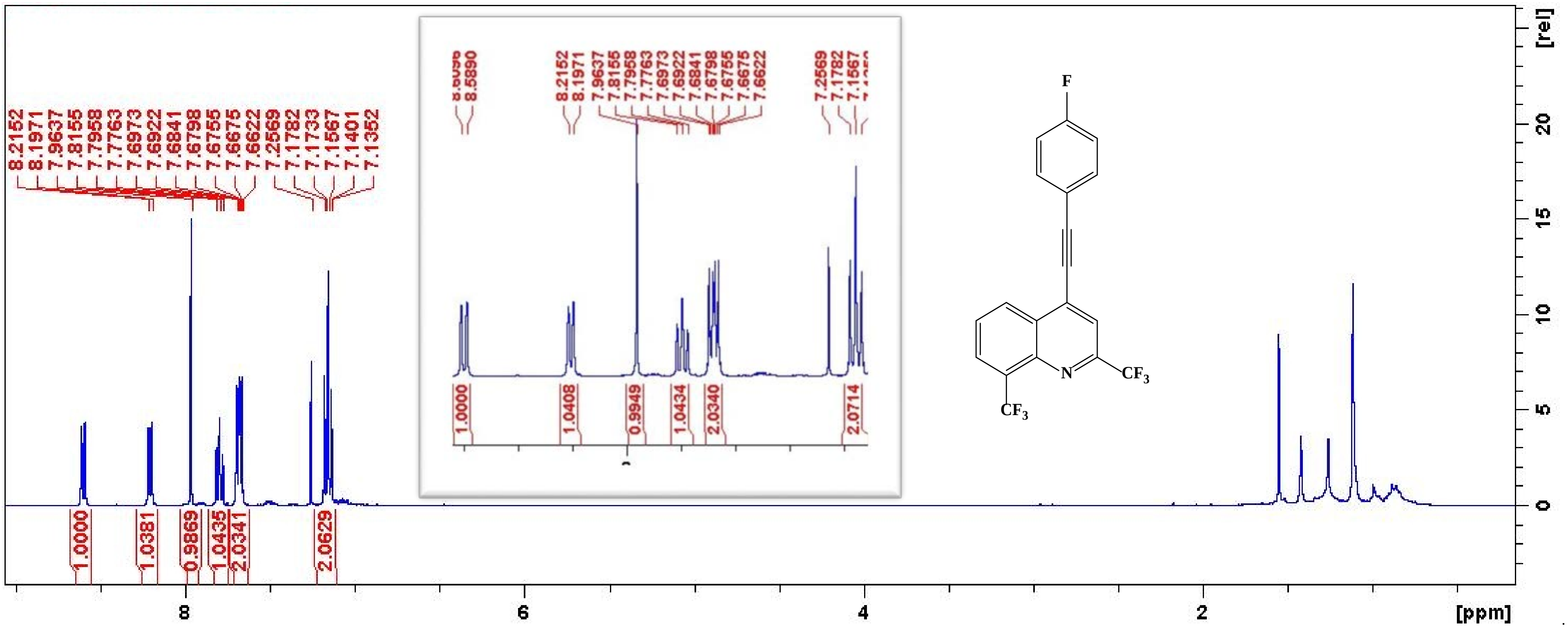


HRMS of **4E**

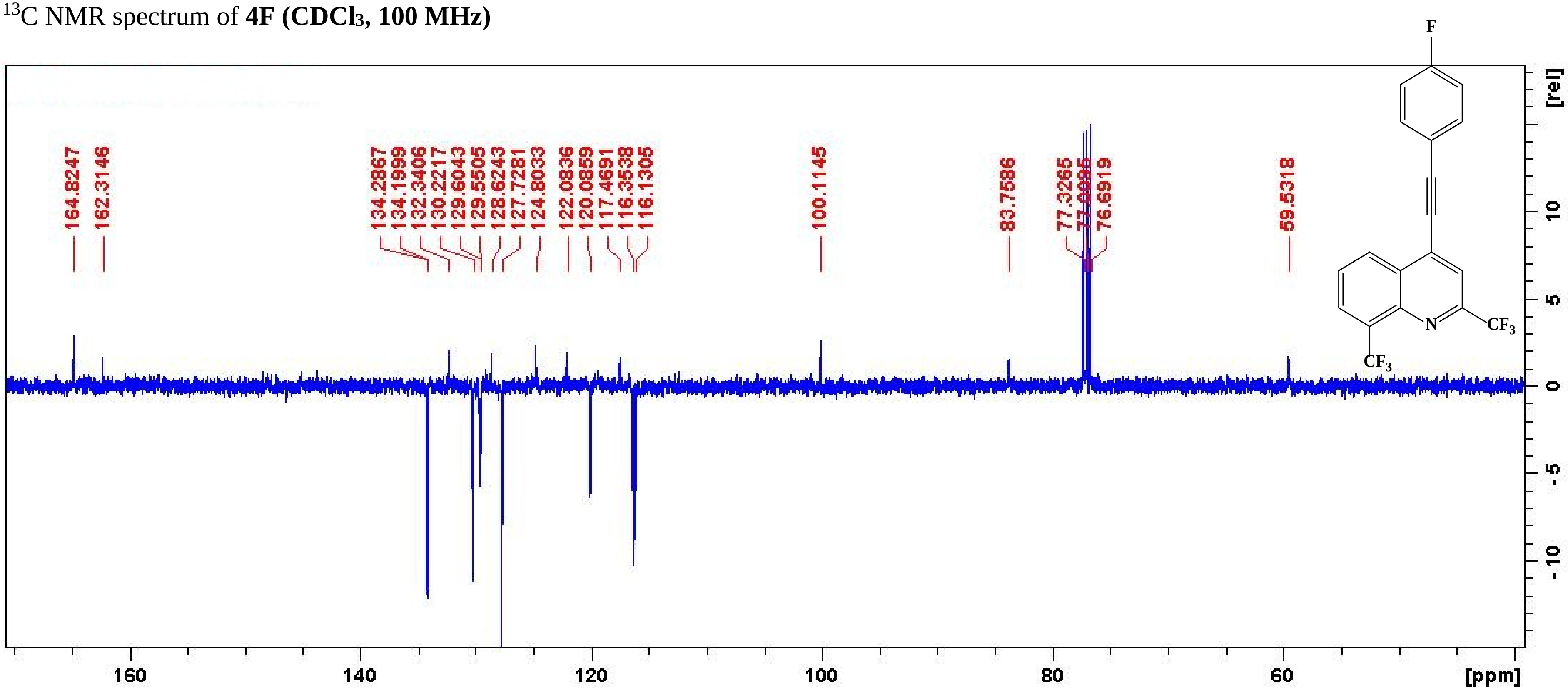


SA21
MS_Direct_151211_43 33 (0.158) Cm (31:36)
1: TOF MS ES+
2.72e4
434.0585
435.0621
436.0602
354.1522
385.1871
391.2861
397.0527
399.0504
413.2668
429.2462
456.0465
100
%
0
m/z
F3C
N
CF3
CF3

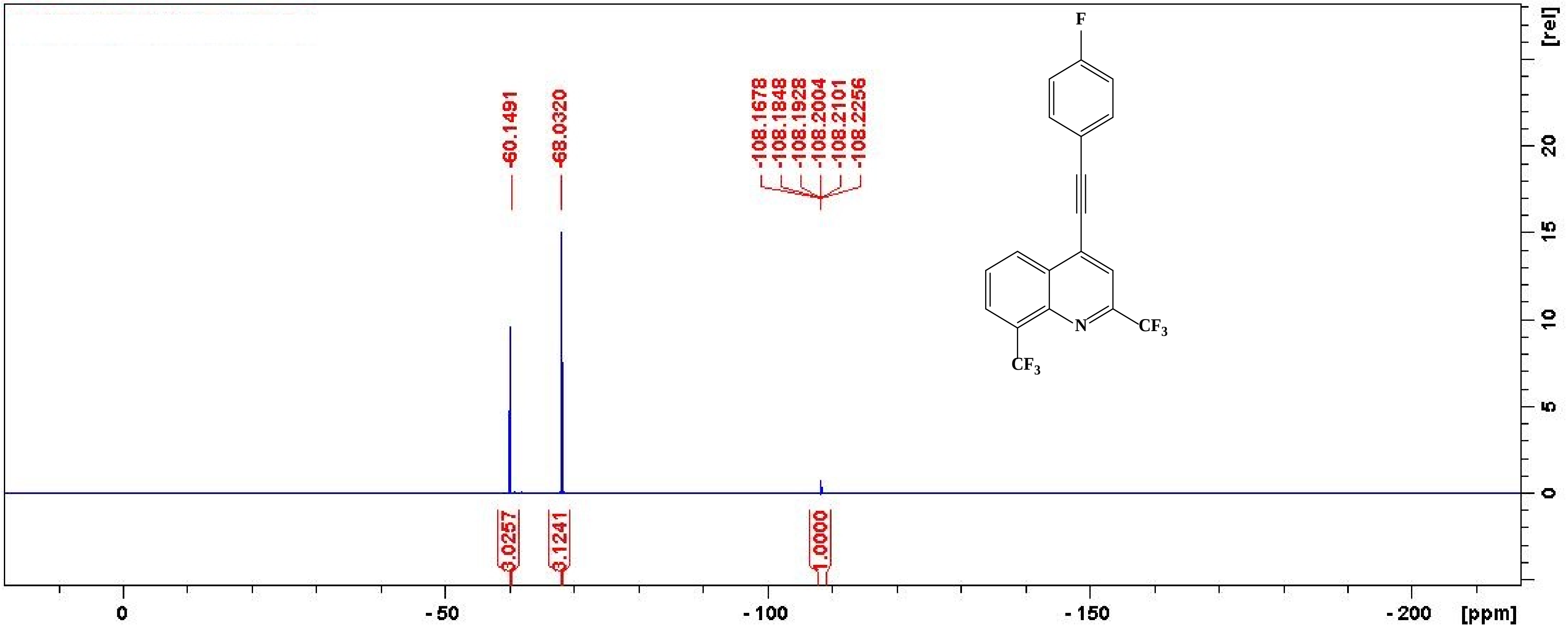
[1]H NMR spectrum of **4F (CDCl₃, 400 MHz)**



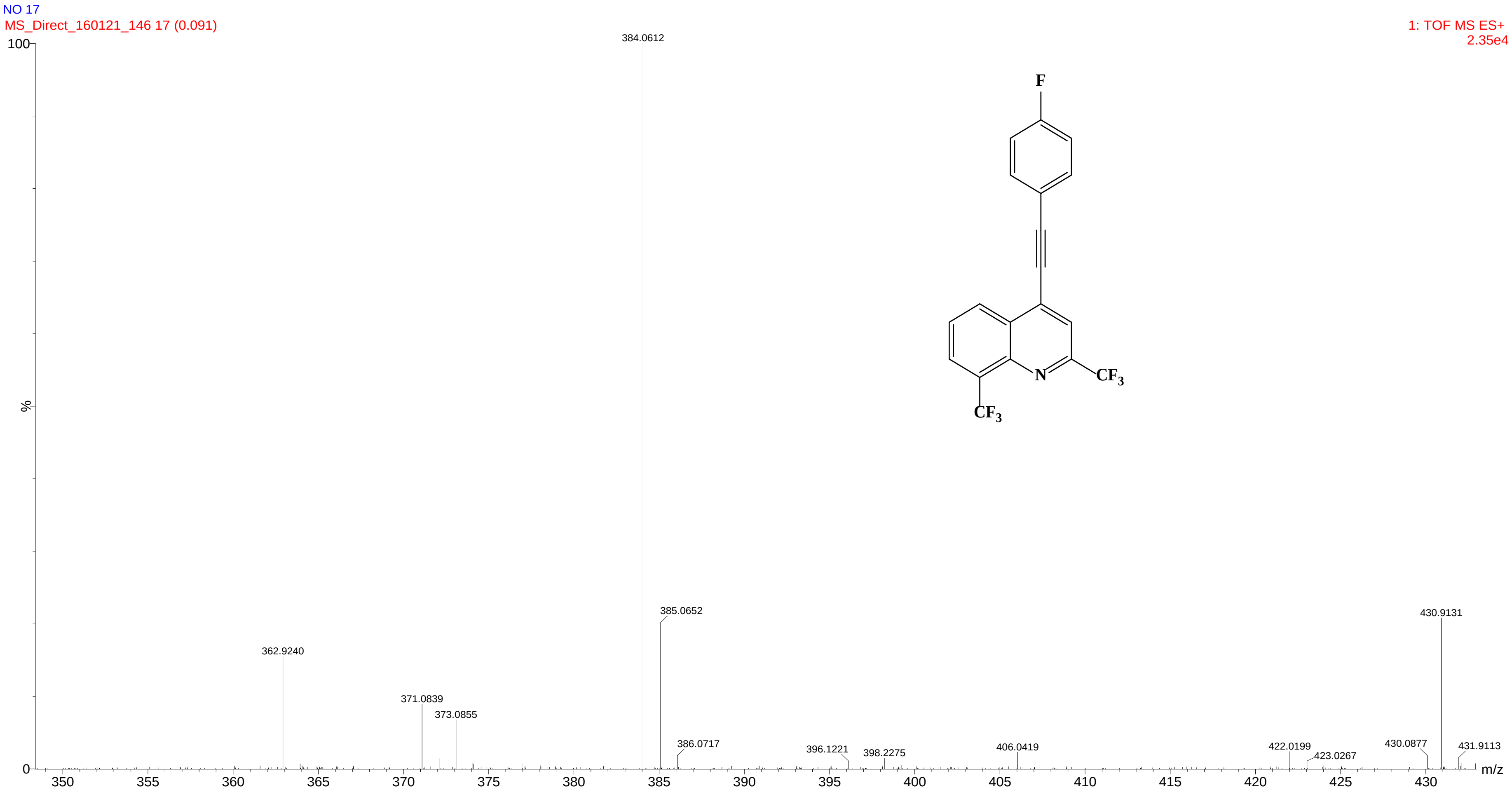
^{13}C NMR spectrum of **4F (CDCl$_3$, 100 MHz)**



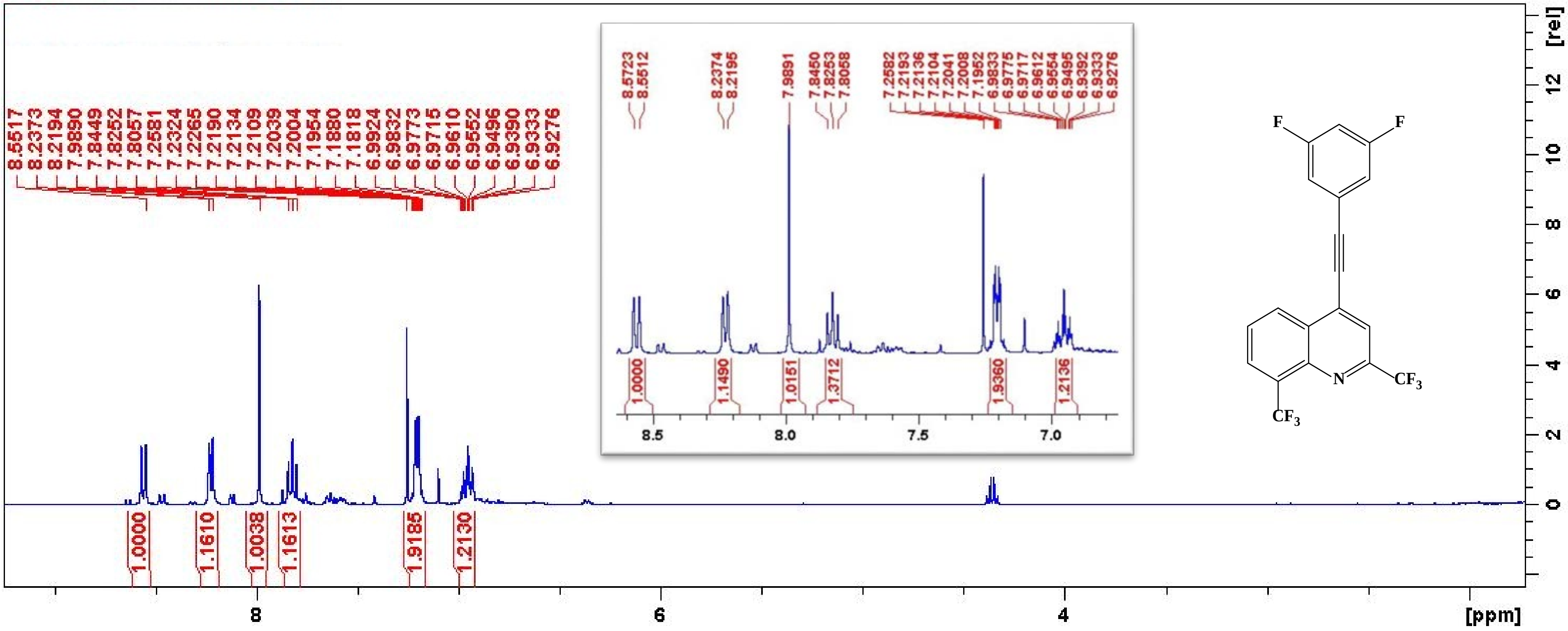
[19]F NMR spectrum of **4F (CDCl₃, 376 MHz)**



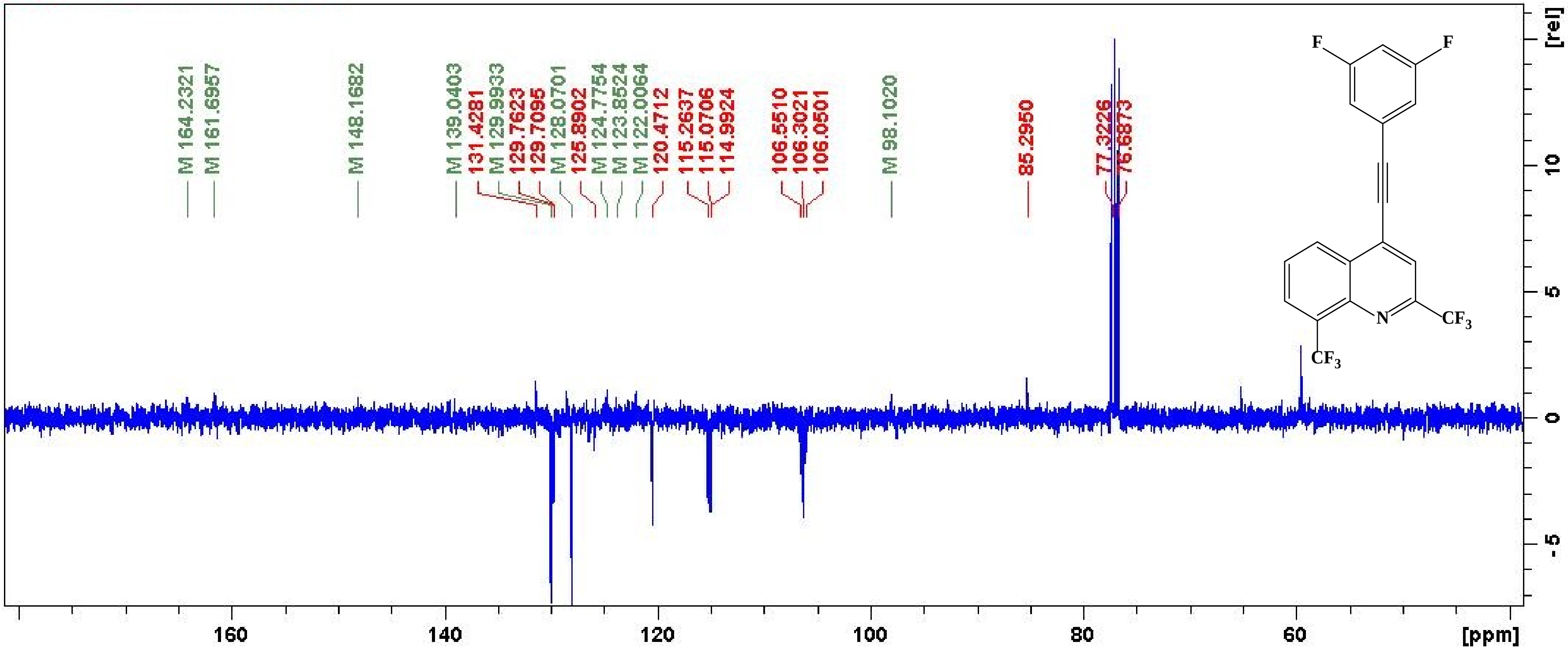
HRMS of **4F**


NO 17
MS_Direct_160121_146 17 (0.091)
1: TOF MS ES+
2.35e4
100
%
0
384.0612
385.0652
430.9131
362.9240
371.0839
373.0855
386.0717
396.1221
398.2275
406.0419
422.0199
423.0267
430.0877
431.9113
350
355
360
365
370
375
380
385
390
395
400
405
410
415
420
425
430
m/z
F
N
CF3
CF3

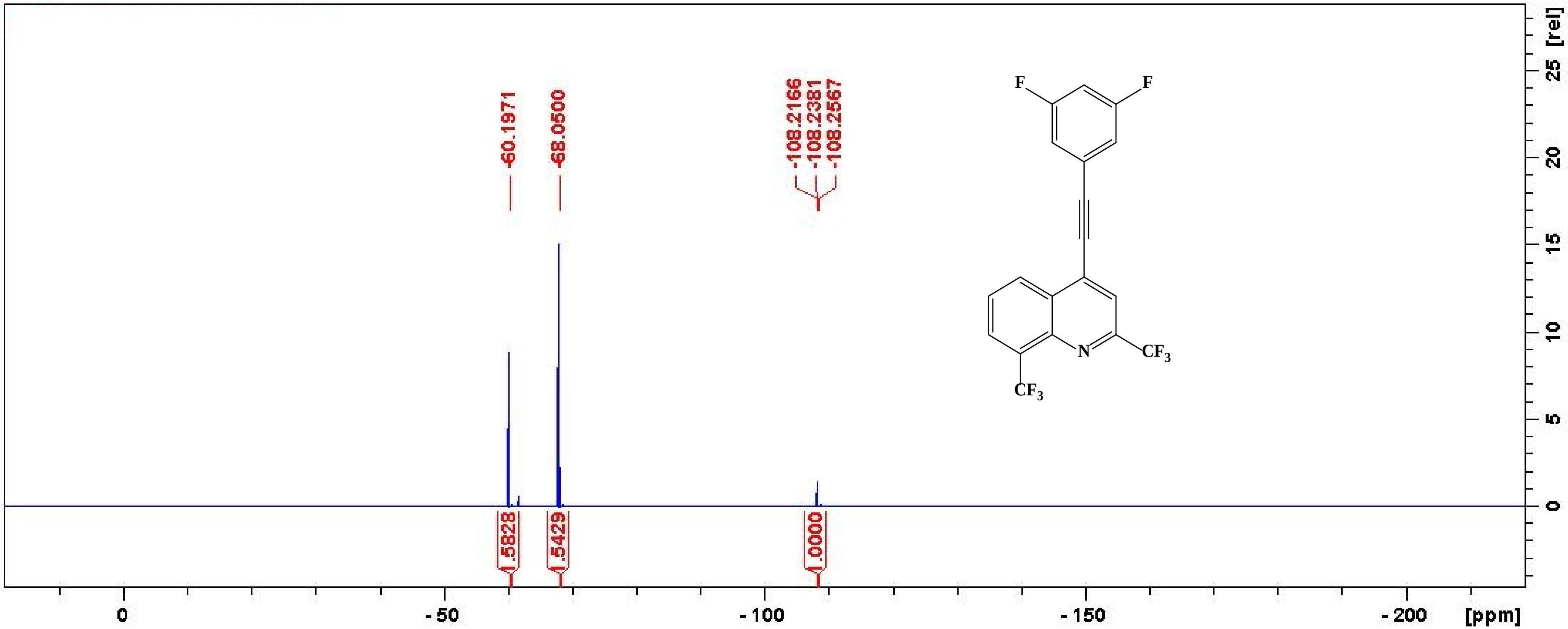
[1]H NMR spectrum of **4G (CDCl₃, 400 MHz)**



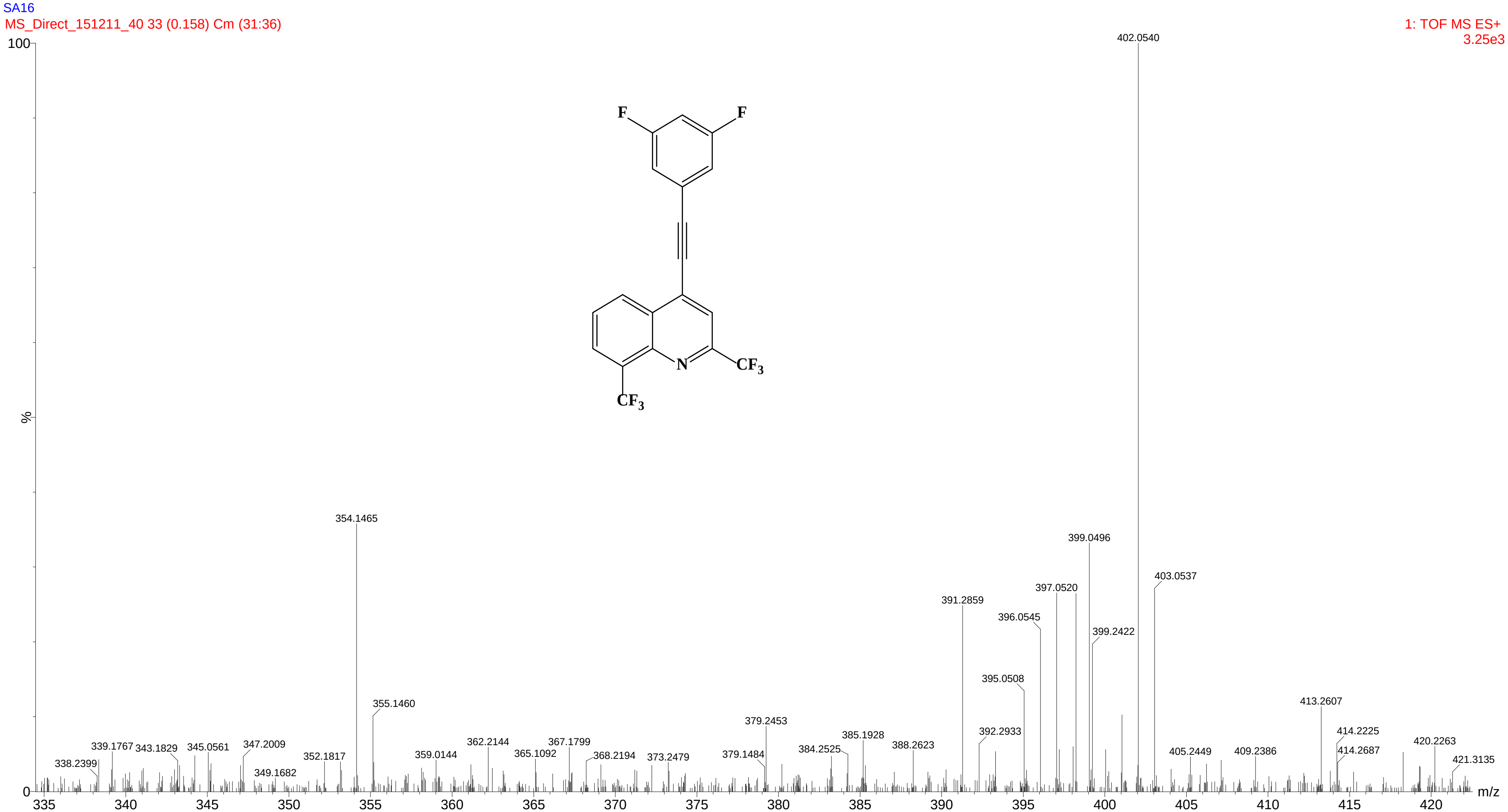
^{13}C NMR spectrum of **4G ($CDCl_3$, 100 MHz)**



^{19}F NMR spectrum of **4G (CDCl$_3$, 376 MHz)**

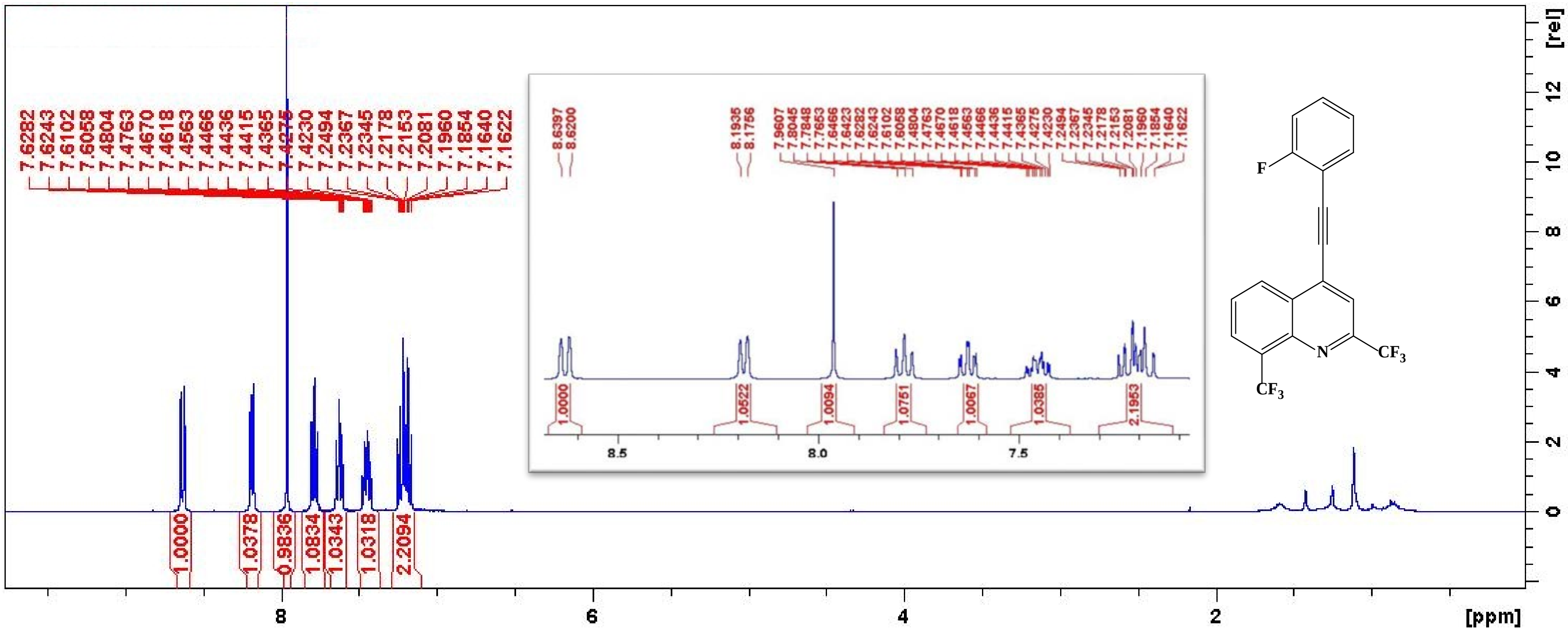


HRMS of **4G**

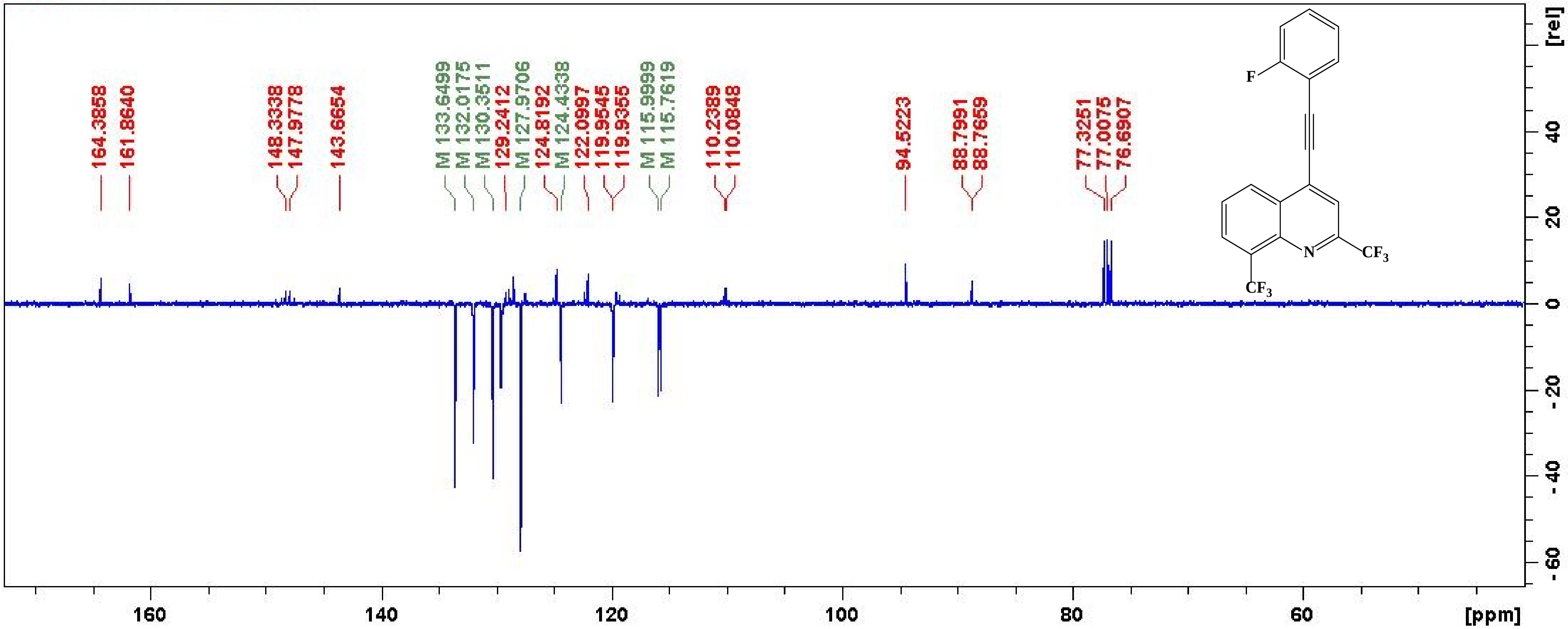


SA16
MS_Direct_151211_40 33 (0.158) Cm (31:36)
1: TOF MS ES+
3.25e3
100
%
0
F
F
N
CF3
CF3
402.0540
354.1465
399.0496
403.0537
397.0520
391.2859
396.0545
399.2422
395.0508
355.1460
413.2607
379.2453
392.2933
414.2225
385.1928
347.2009
420.2263
339.1767
343.1829
345.0561
362.2144
367.1799
388.2623
384.2525
414.2687
352.1817
359.0144
365.1092
368.2194
373.2479
379.1484
405.2449
409.2386
421.3135
338.2399
349.1682
335
340
345
350
355
360
365
370
375
380
385
390
395
400
405
410
415
420
m/z

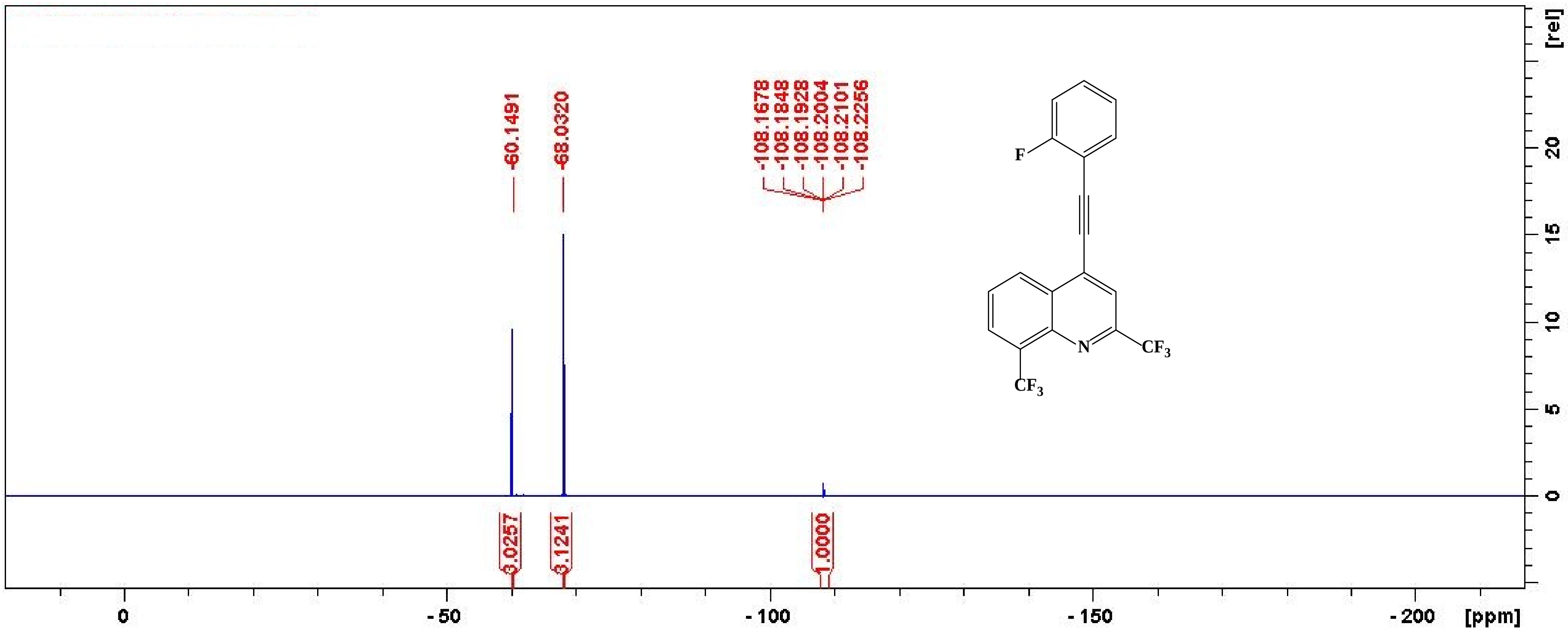
[1]H NMR spectrum of **4H ($CDCl_3$, 400 MHz)**



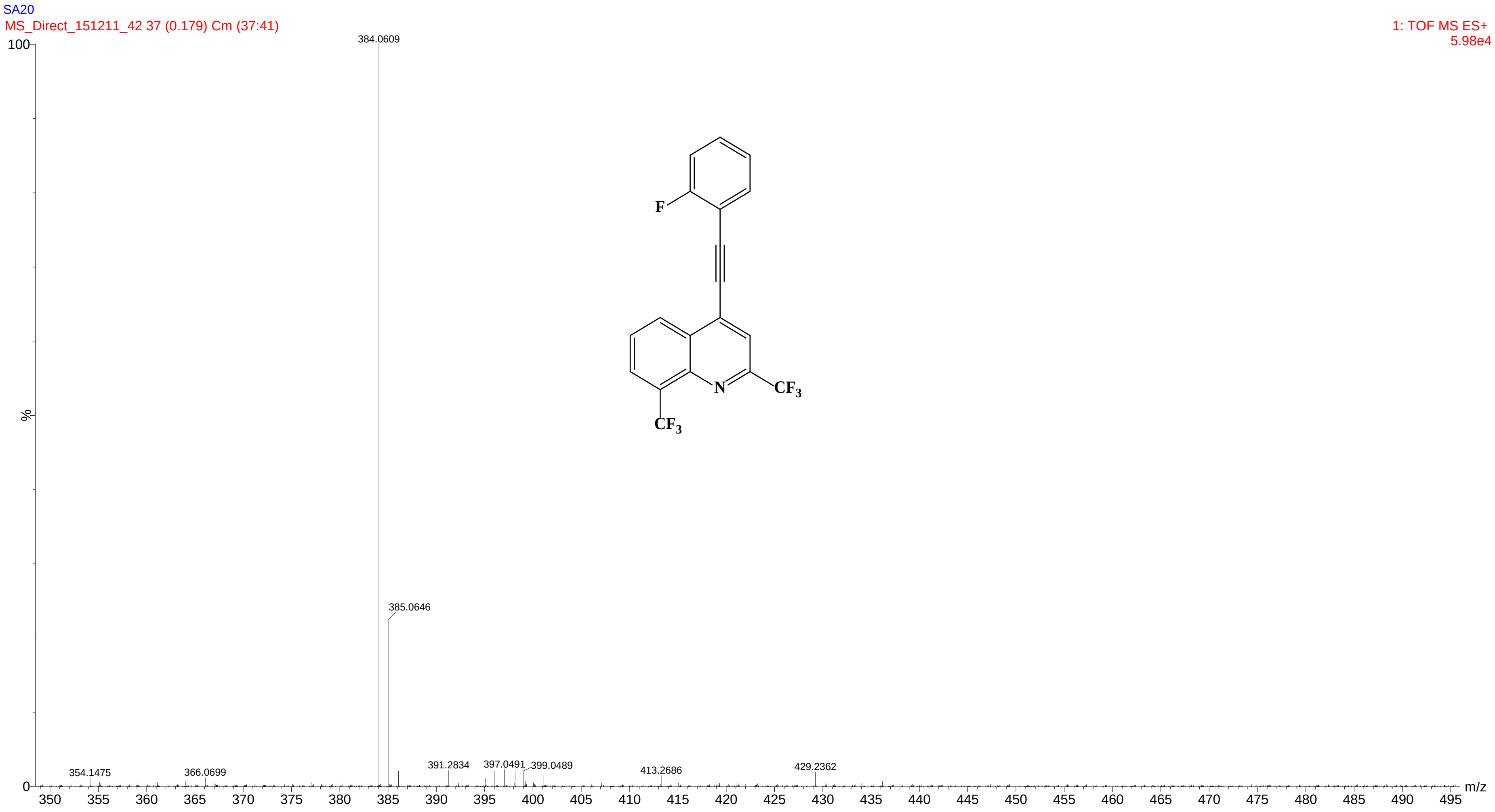
^{13}C NMR spectrum of **4H ($CDCl_3$, 100 MHz)**



^{19}F NMR spectrum of **4H (CDCl$_3$, 376 MHz)**

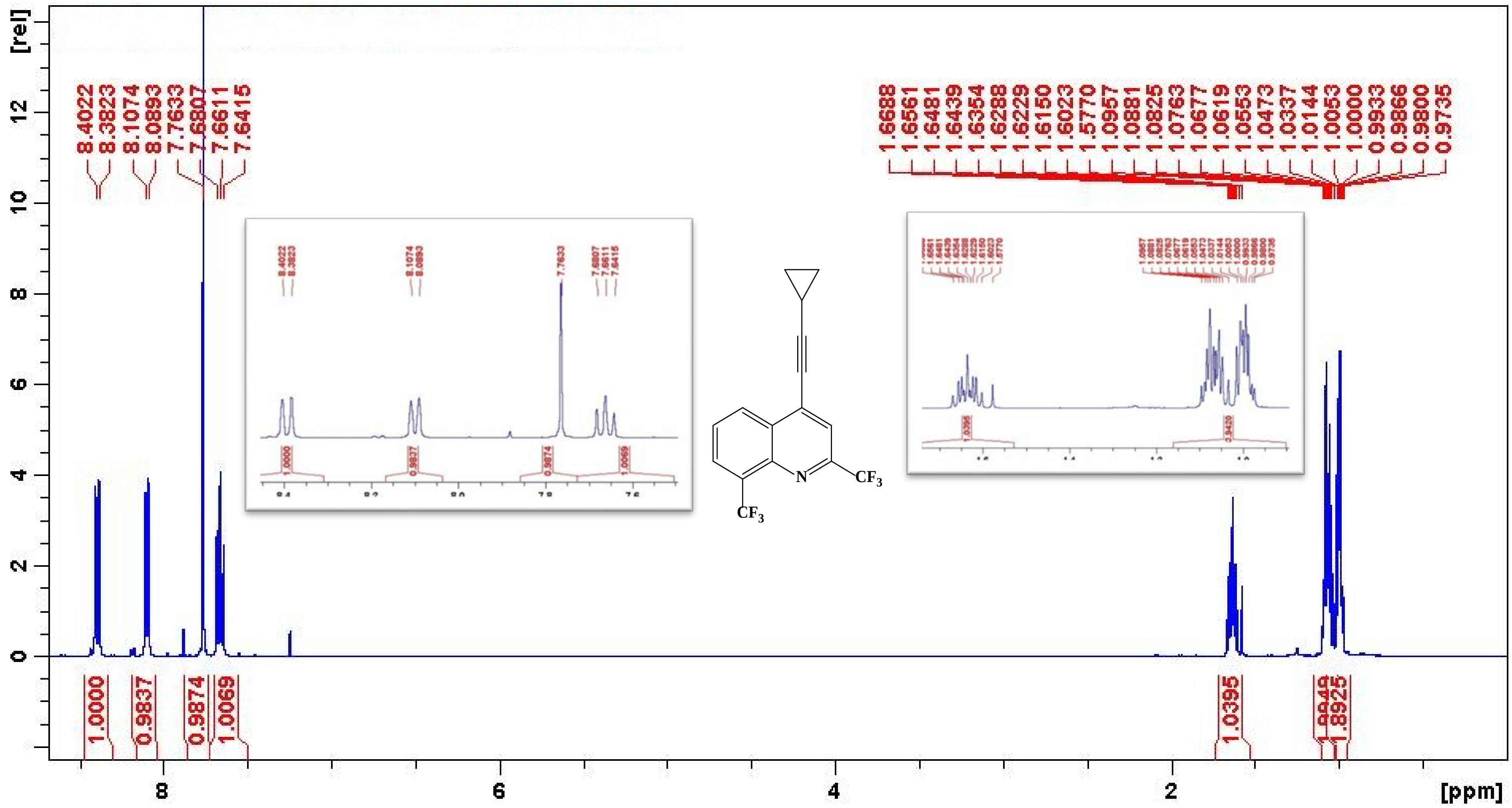


HRMS of **4H**

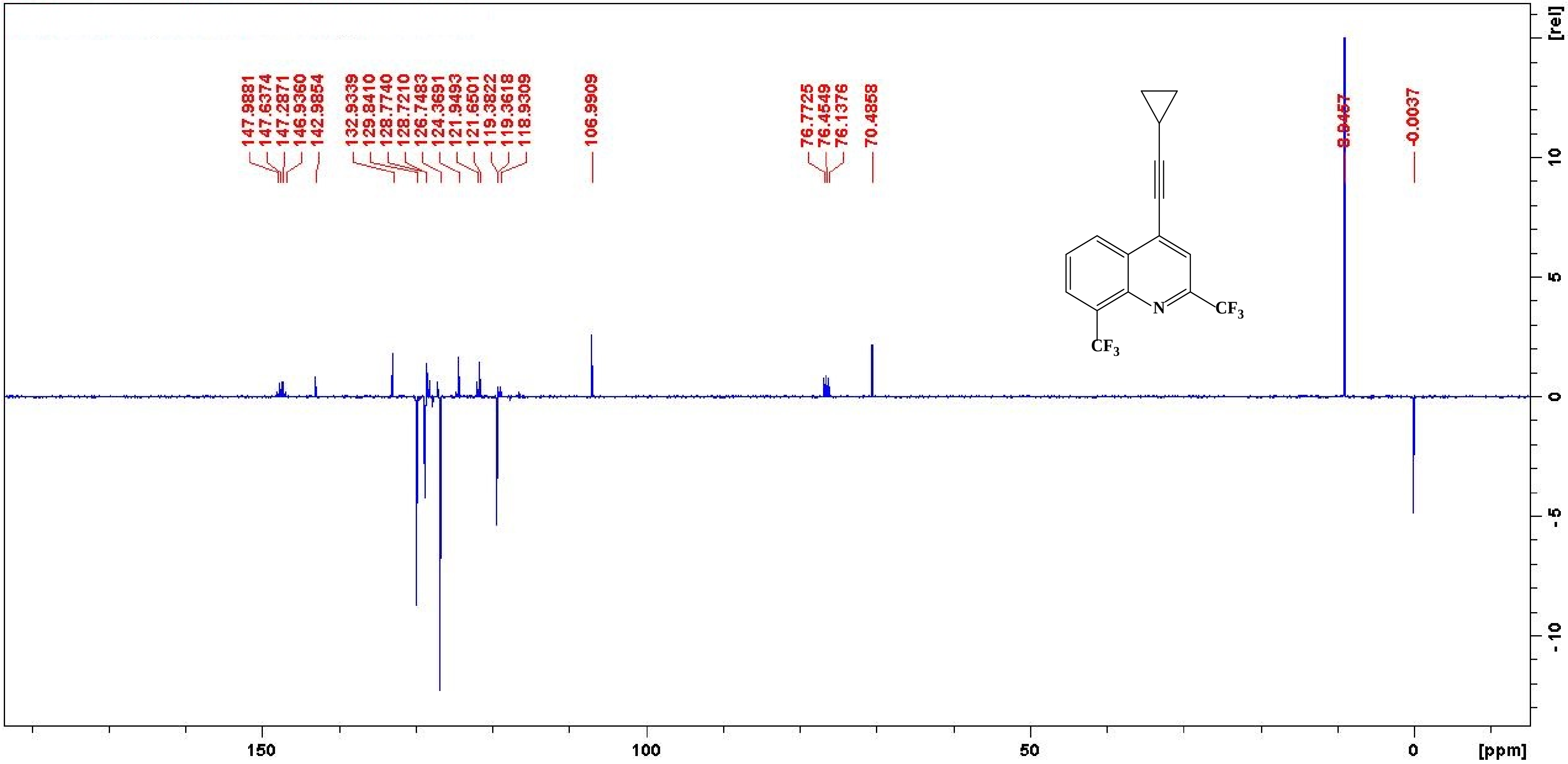


SA20
MS_Direct_151211_42 37 (0.179) Cm (37:41)
1: TOF MS ES+
5.98e4
100
%
0
384.0609
385.0646
354.1475
366.0699
391.2834
397.0491
399.0489
413.2686
429.2362
350
355
360
365
370
375
380
385
390
395
400
405
410
415
420
425
430
435
440
445
450
455
460
465
470
475
480
485
490
495
m/z
F
N
CF3
CF3

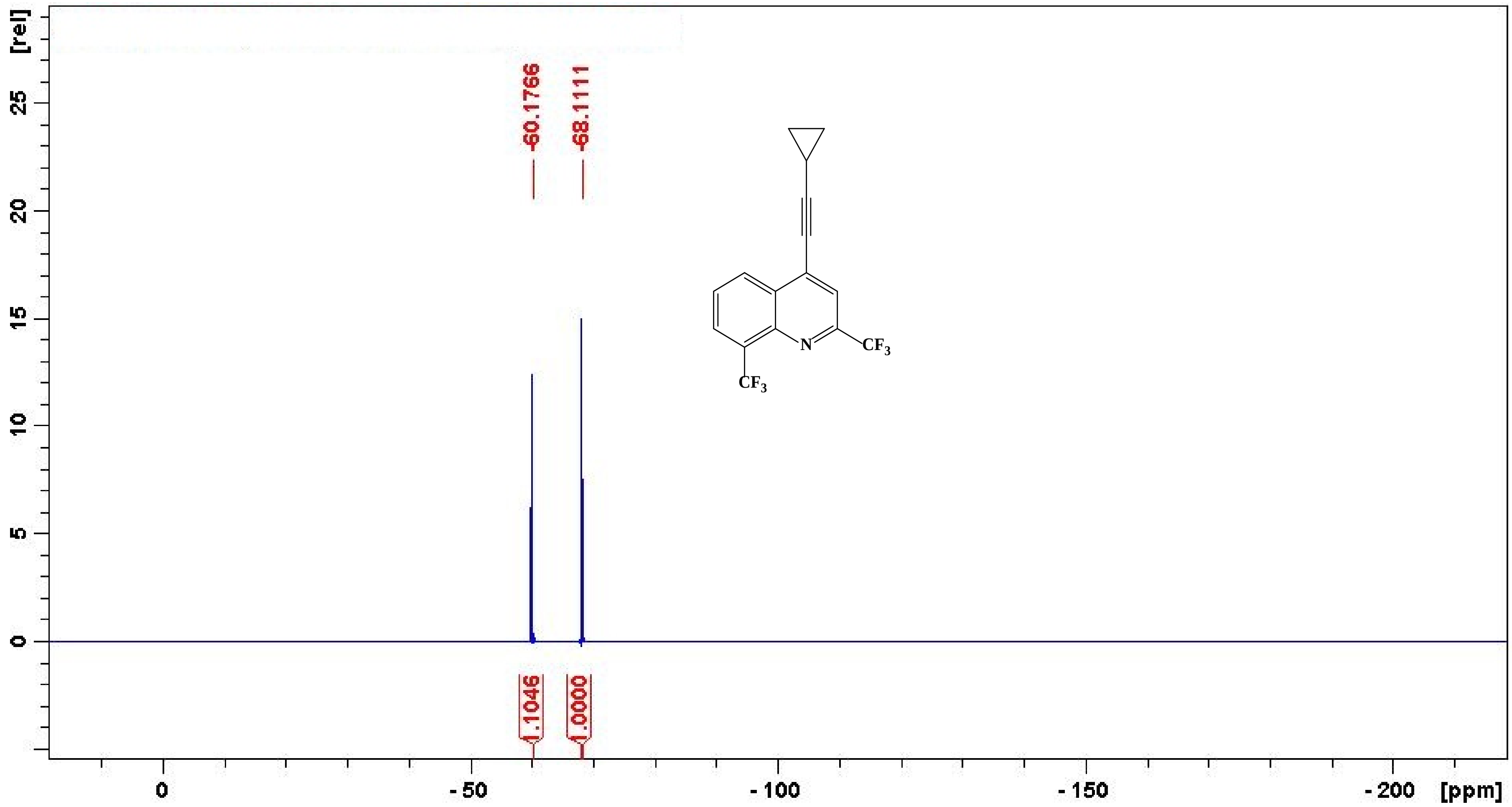
[1]H NMR spectrum of **4I (CDCl₃, 400 MHz)**



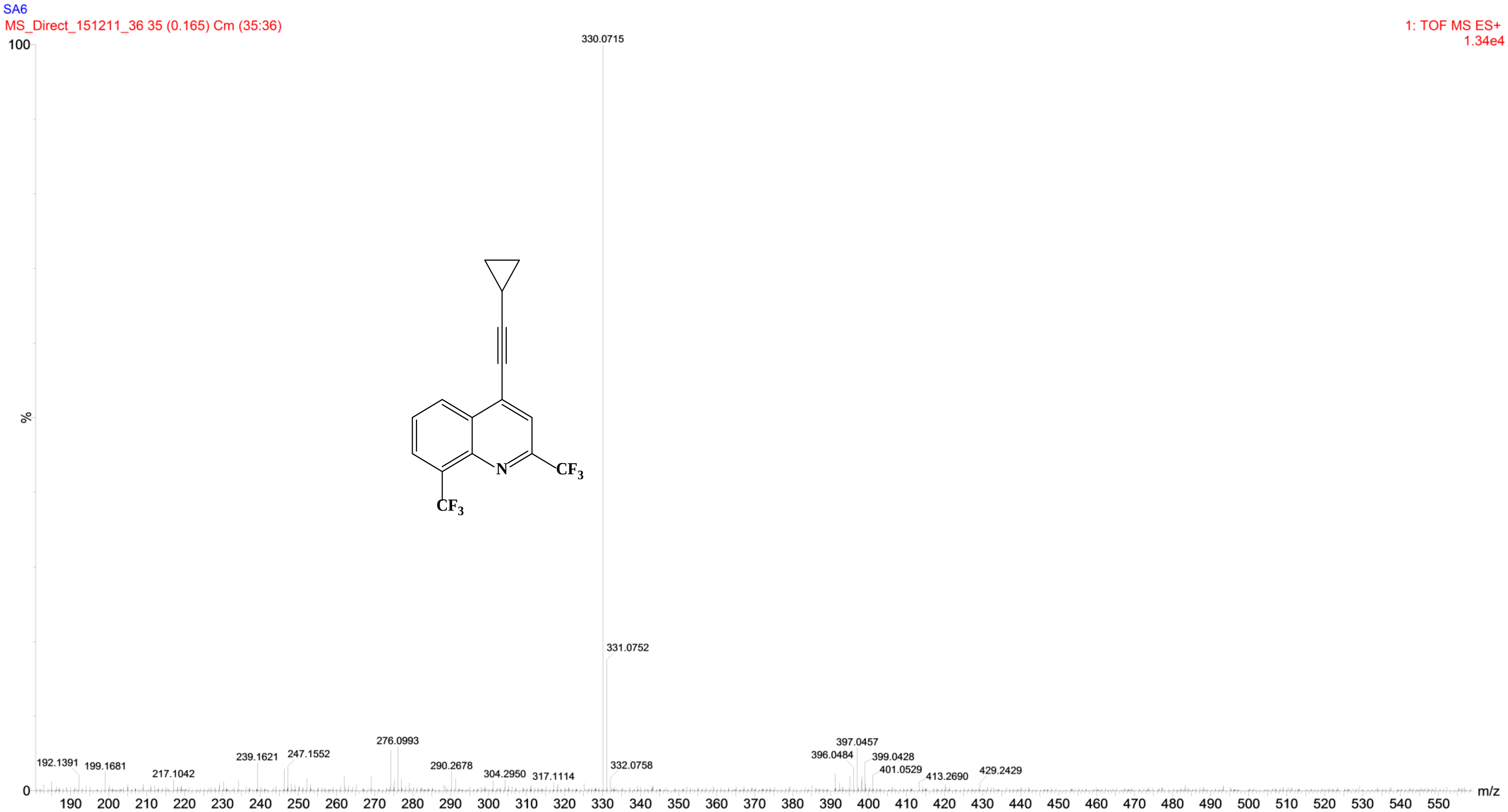
[13]C NMR spectrum of **4l (CDCl$_3$, 100 MHz)**



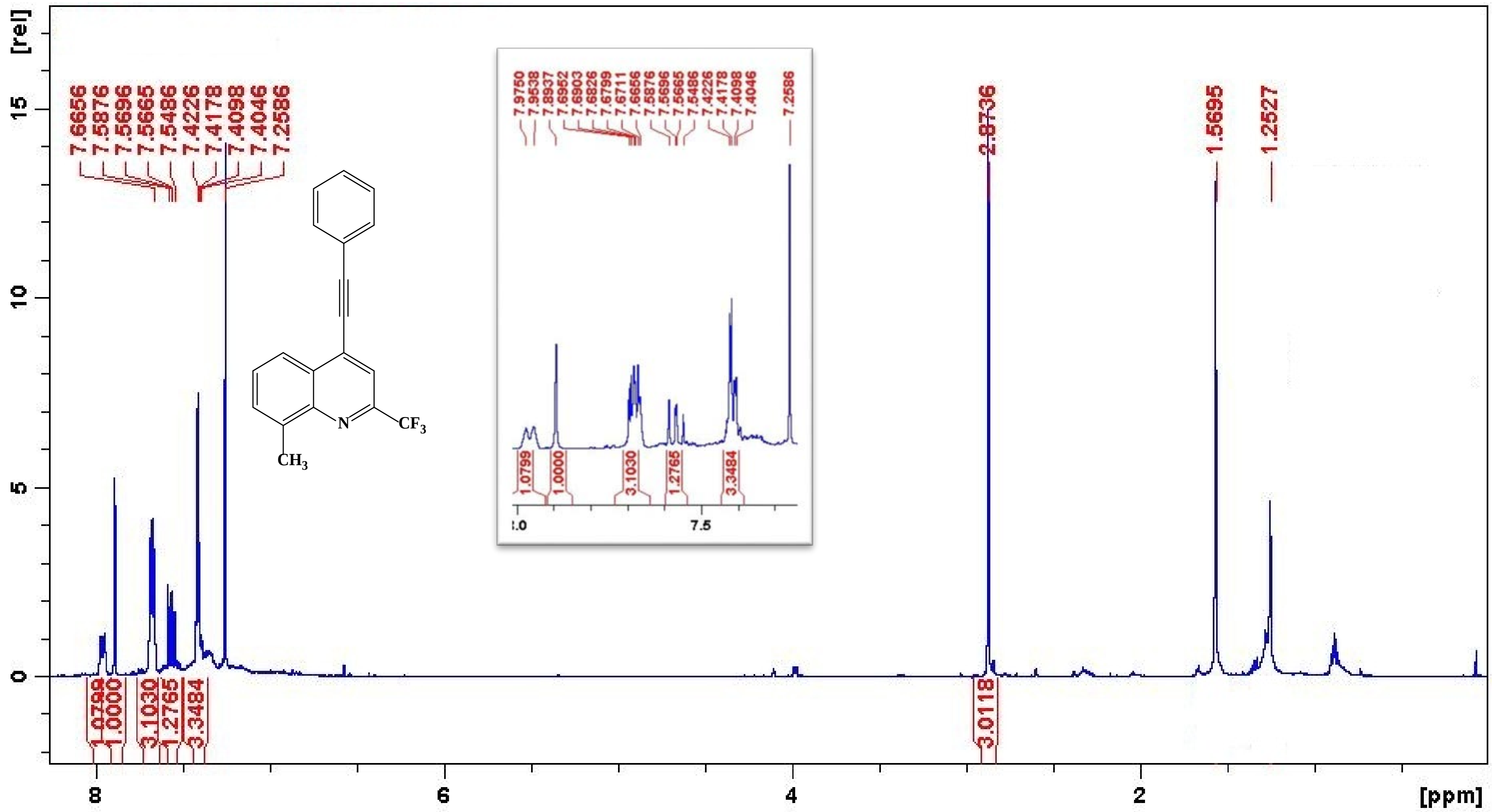
^{19}F NMR spectrum of **4l (CDCl$_3$, 376 MHz)**



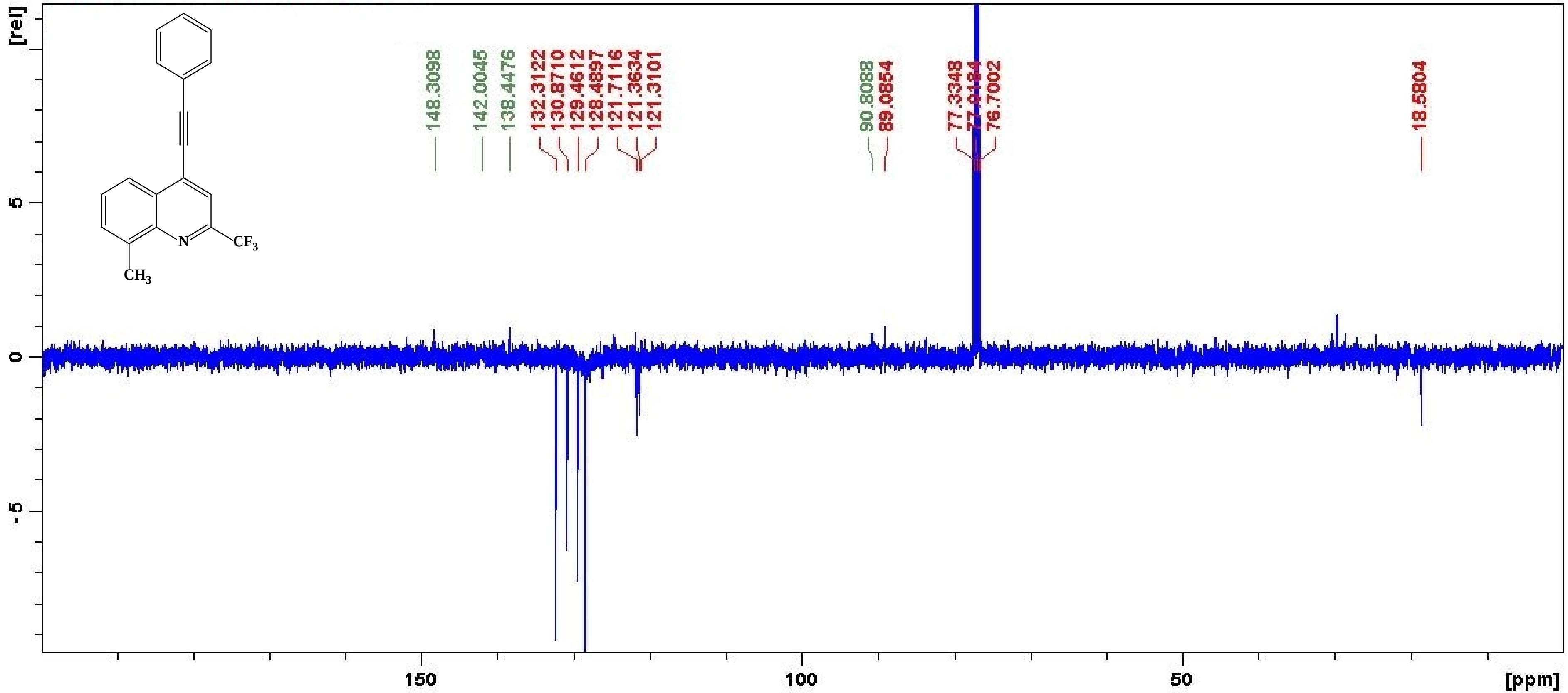
HRMS of **4I**


SA6
MS_Direct_151211_36 35 (0.165) Cm (35:36)
1: TOF MS ES+
1.34e4
100
%
0
330.0715
331.0752
192.1391
199.1681
217.1042
239.1621
247.1552
276.0993
290.2678
304.2950
317.1114
332.0758
396.0484
397.0457
399.0428
401.0529
413.2690
429.2429
m/z
N
CF3
CF3

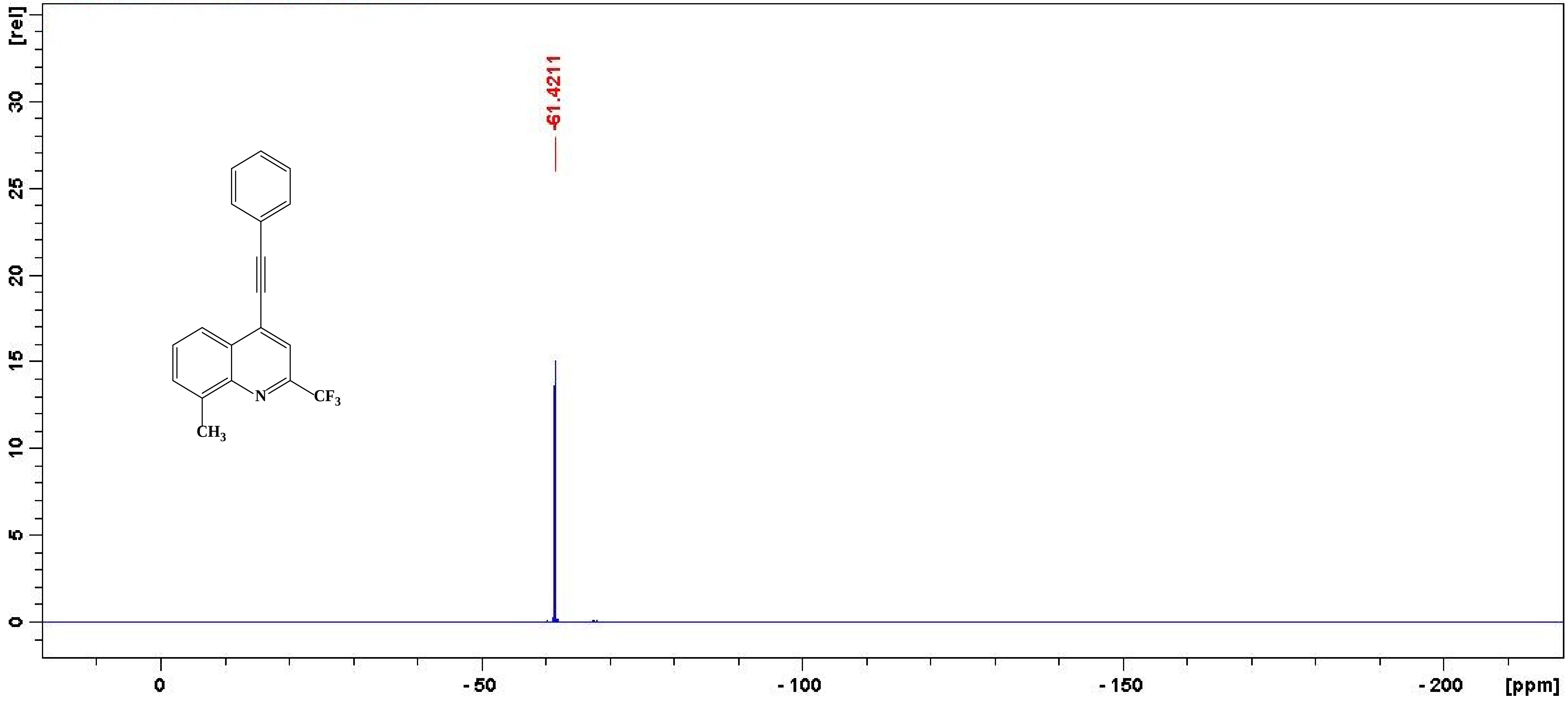
^{1}H NMR spectrum of **4J ($CDCl_3$, 400 MHz)**



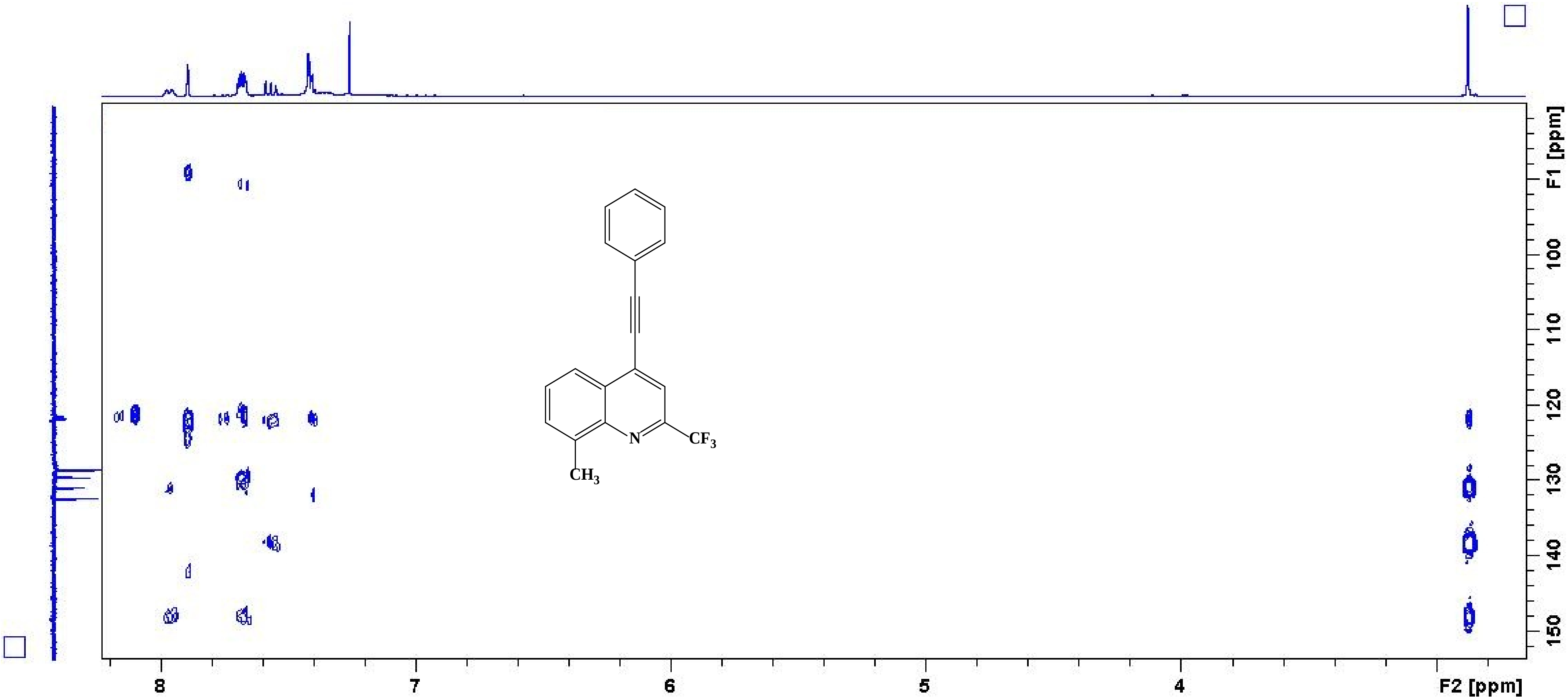
^{13}C NMR spectrum of **4J ($CDCl_3$, 100 MHz)**



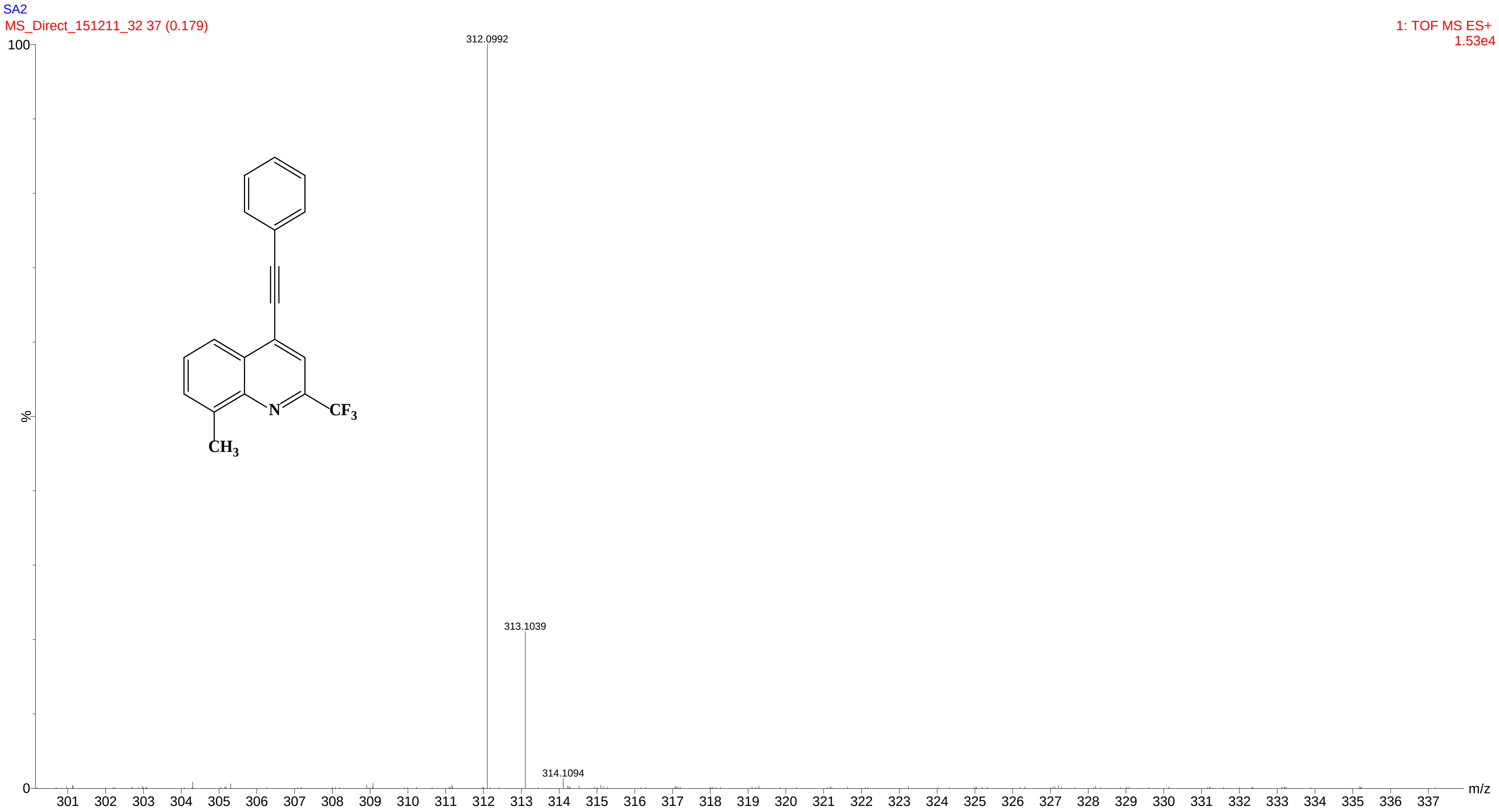
^{19}F NMR spectrum of **4J ($CDCl_3$, 376 MHz)**



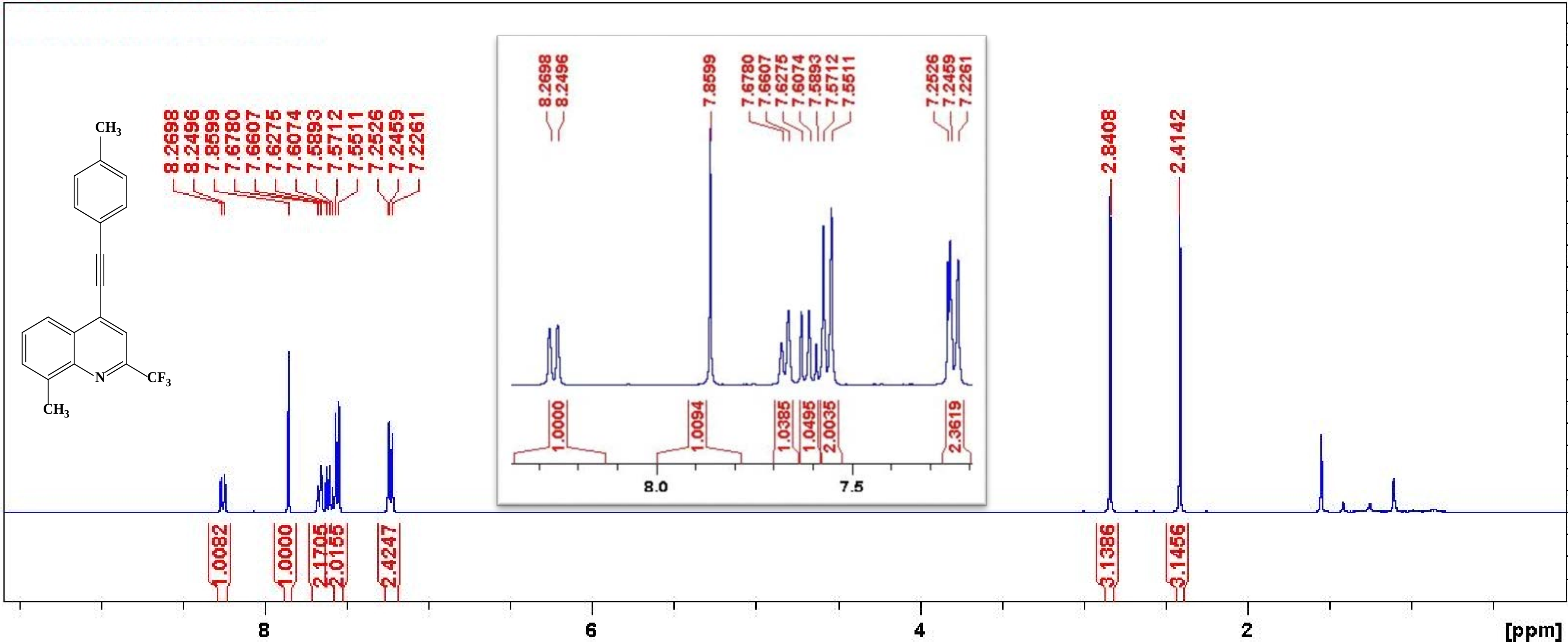
HMBC spectrum of **4J**



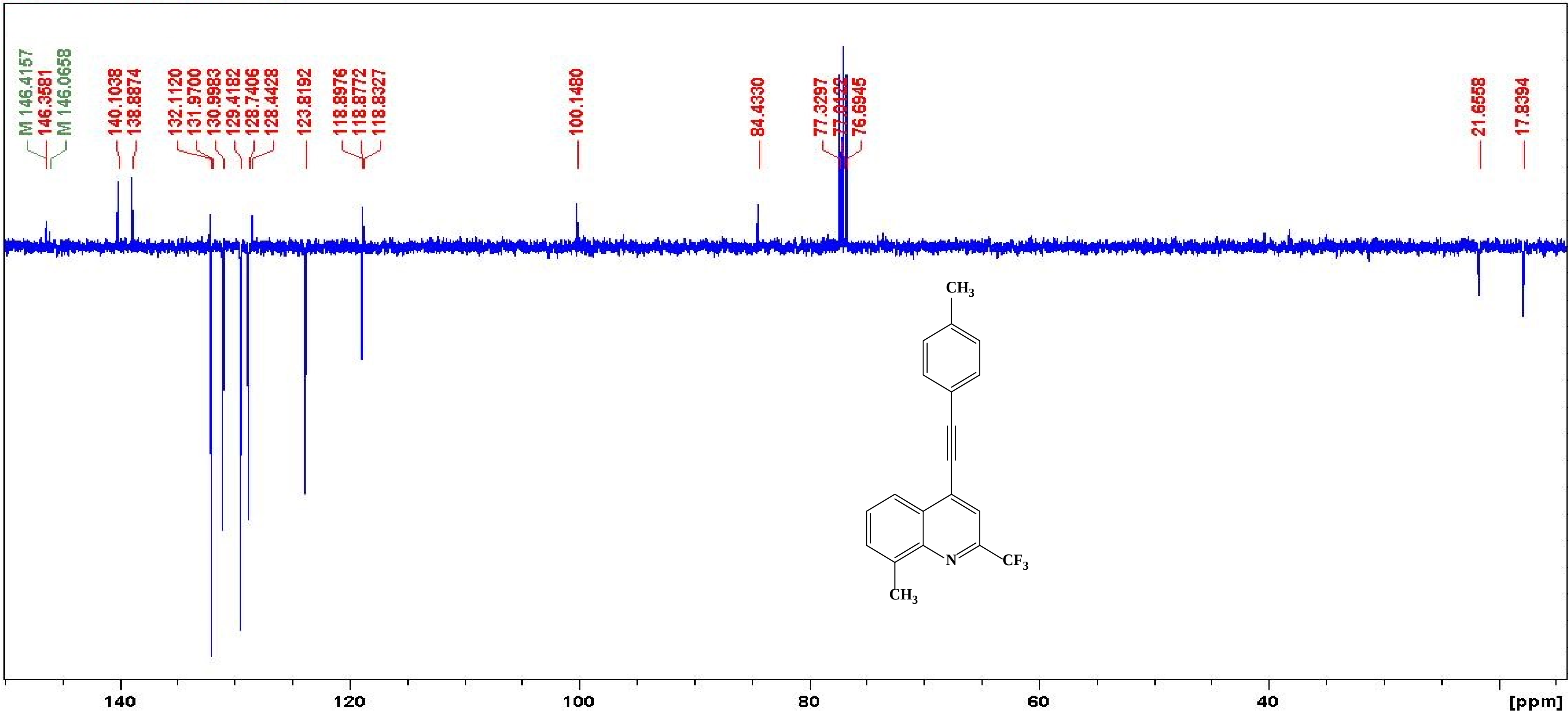
HRMS of **4J**


SA2
MS_Direct_151211_32 37 (0.179)
1: TOF MS ES+
1.53e4
100
%
0
312.0992
313.1039
314.1094
301
302
303
304
305
306
307
308
309
310
311
312
313
314
315
316
317
318
319
320
321
322
323
324
325
326
327
328
329
330
331
332
333
334
335
336
337
m/z
N
CF_3
CH_3

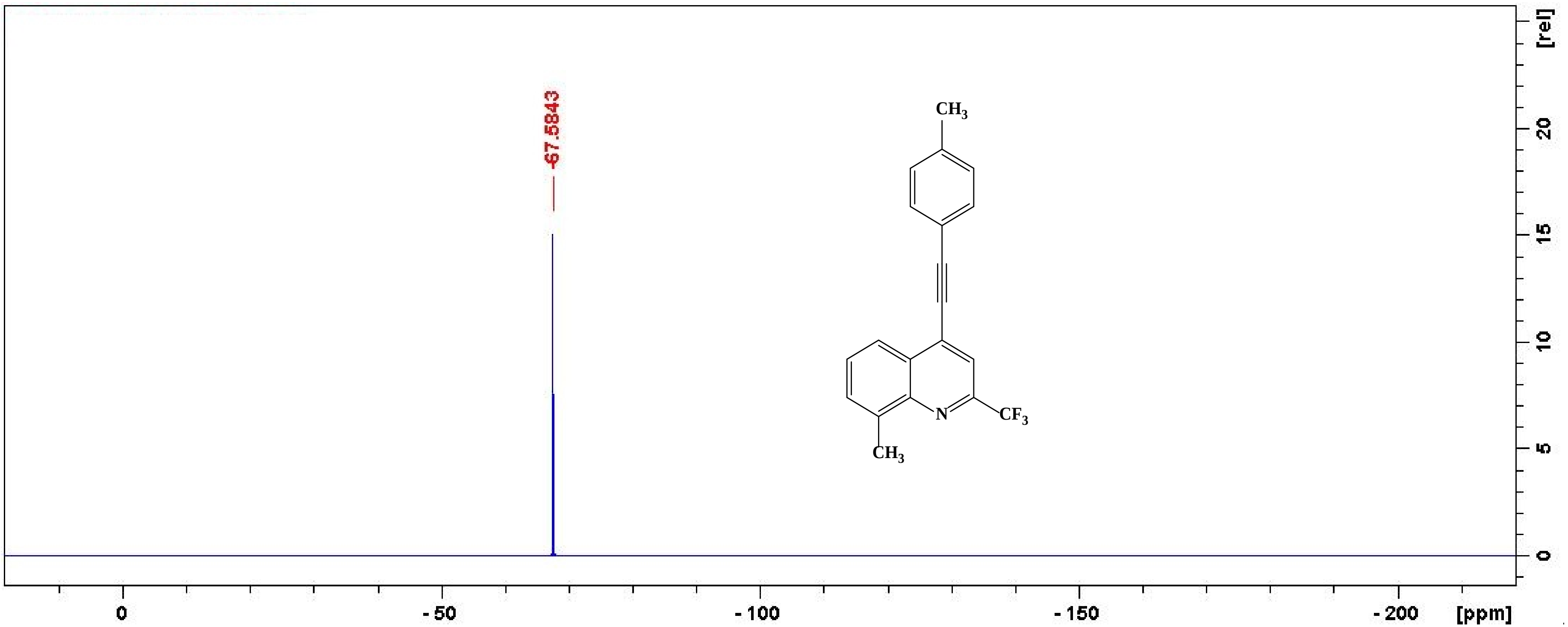
[1]H NMR spectrum of **4K (CDCl3, 400 MHz)**



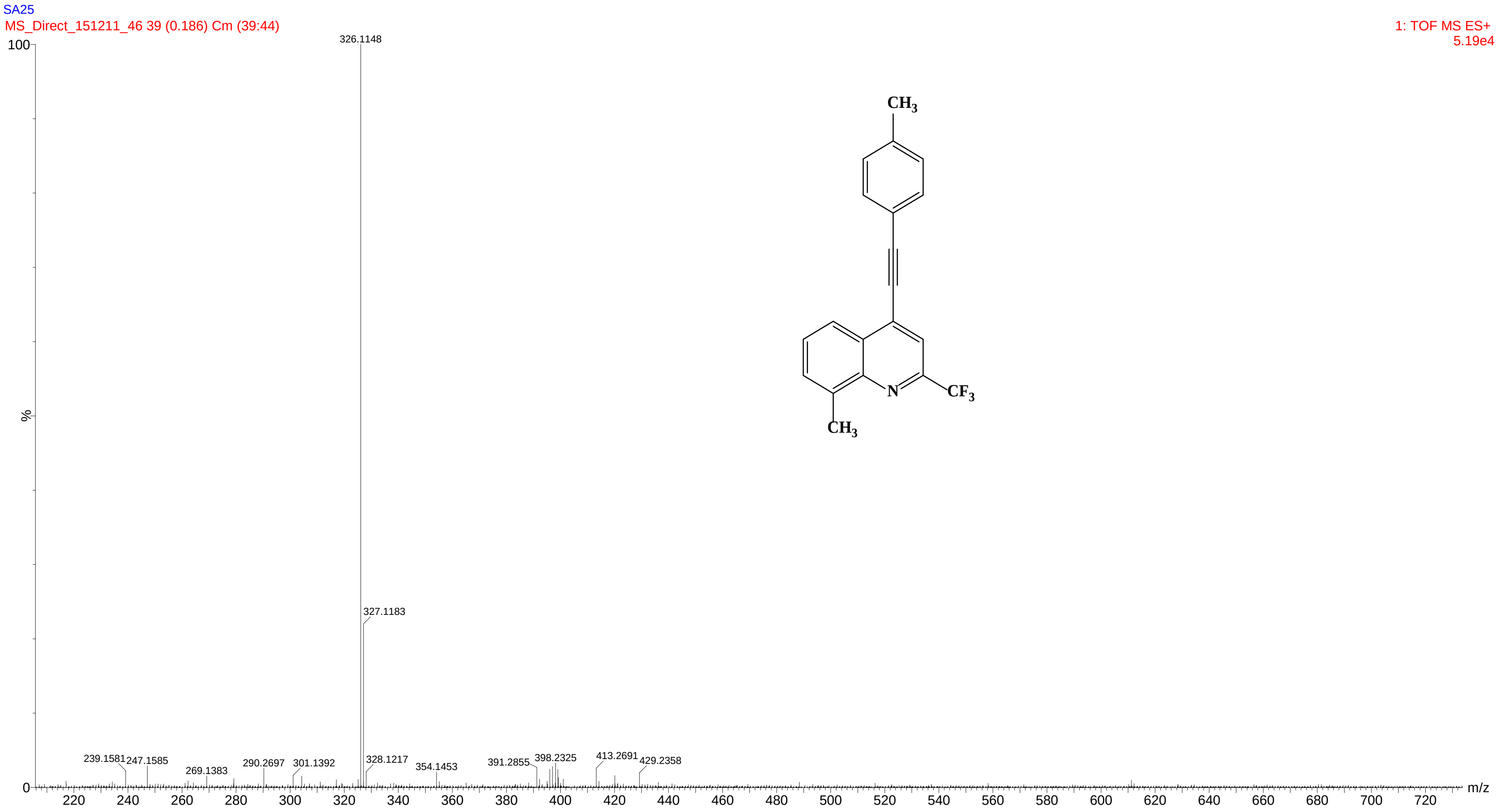
^{13}C NMR spectrum of **4K (CDCl$_3$, 100 MHz)**



[19]F NMR spectrum of **4K (CDCl$_3$, 376 MHz)**

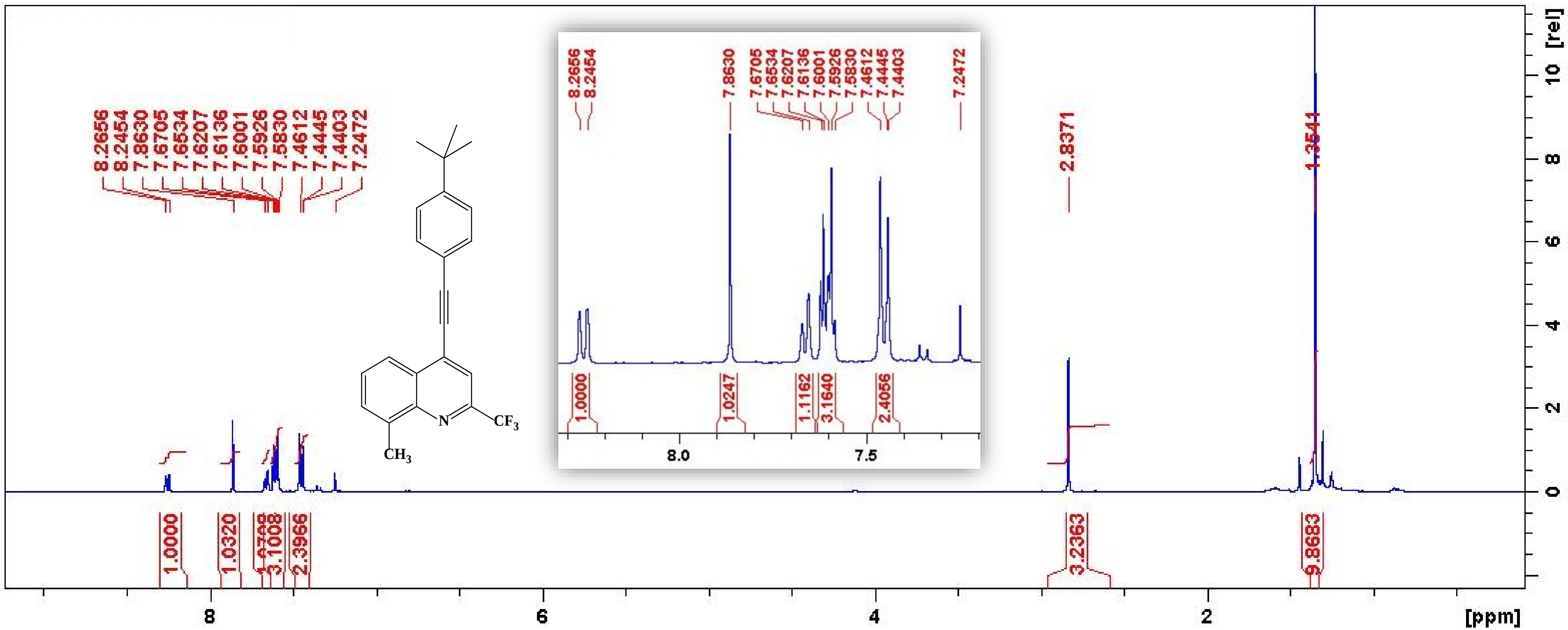


HRMS of **4K**

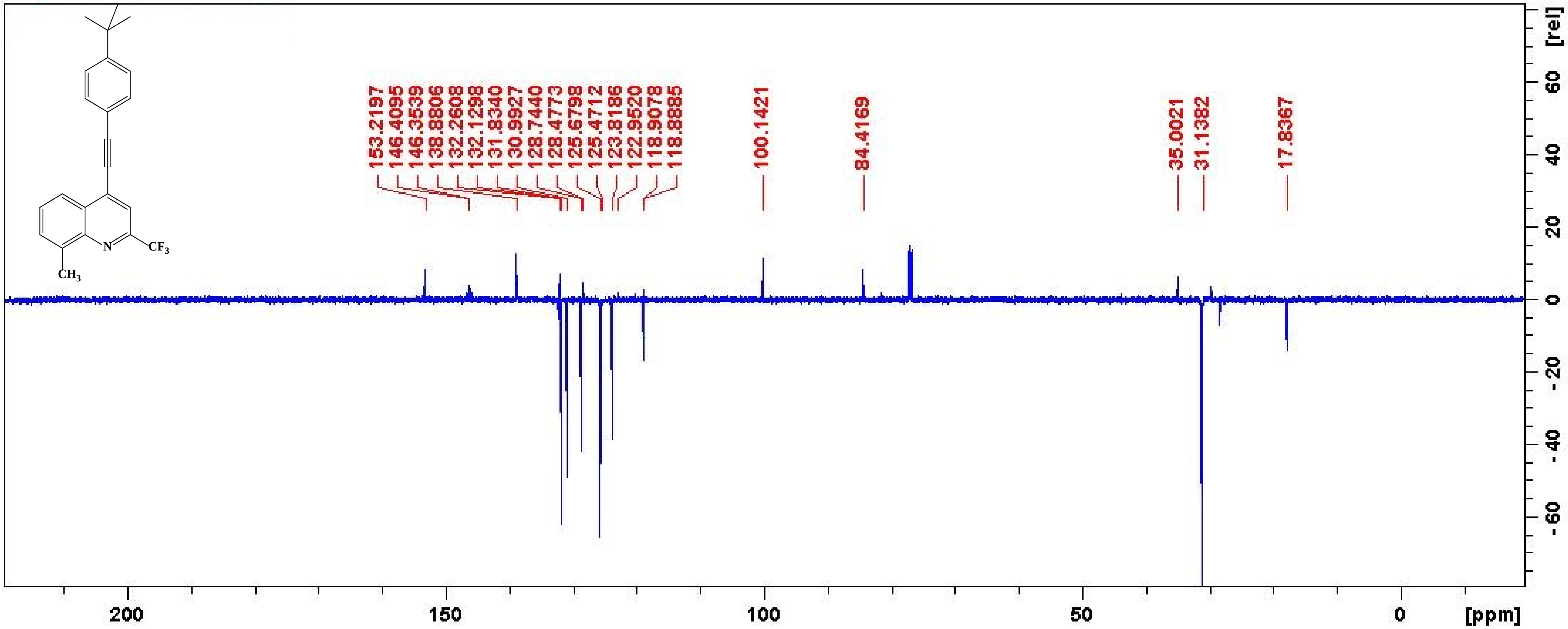


SA25
MS_Direct_151211_46 39 (0.186) Cm (39:44)
1: TOF MS ES+
5.19e4
100
%
0
326.1148
327.1183
239.1581
247.1585
269.1383
290.2697
301.1392
328.1217
354.1453
391.2855
398.2325
413.2691
429.2358
m/z
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
520
540
560
580
600
620
640
660
680
700
720
CH3
N
CF3
CH3

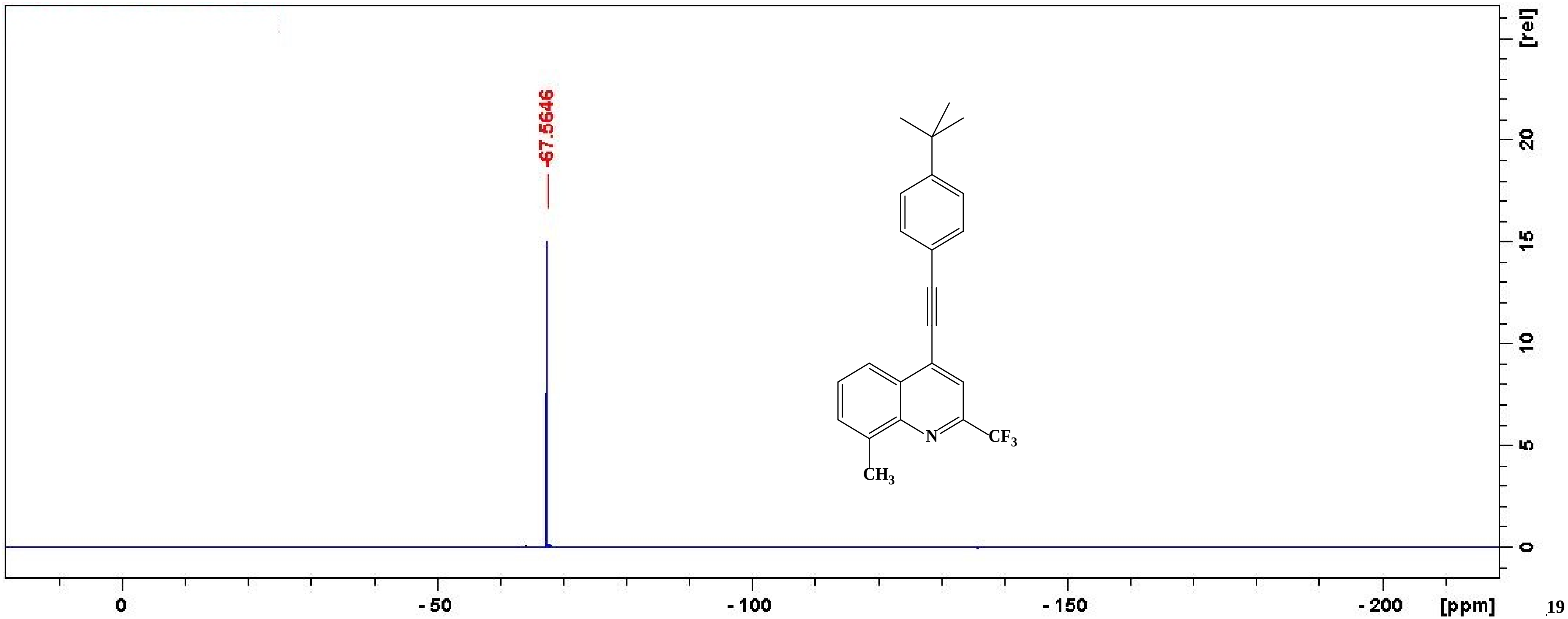
[1]H NMR spectrum of **4L ($CDCl_3$, 400 MHz)**



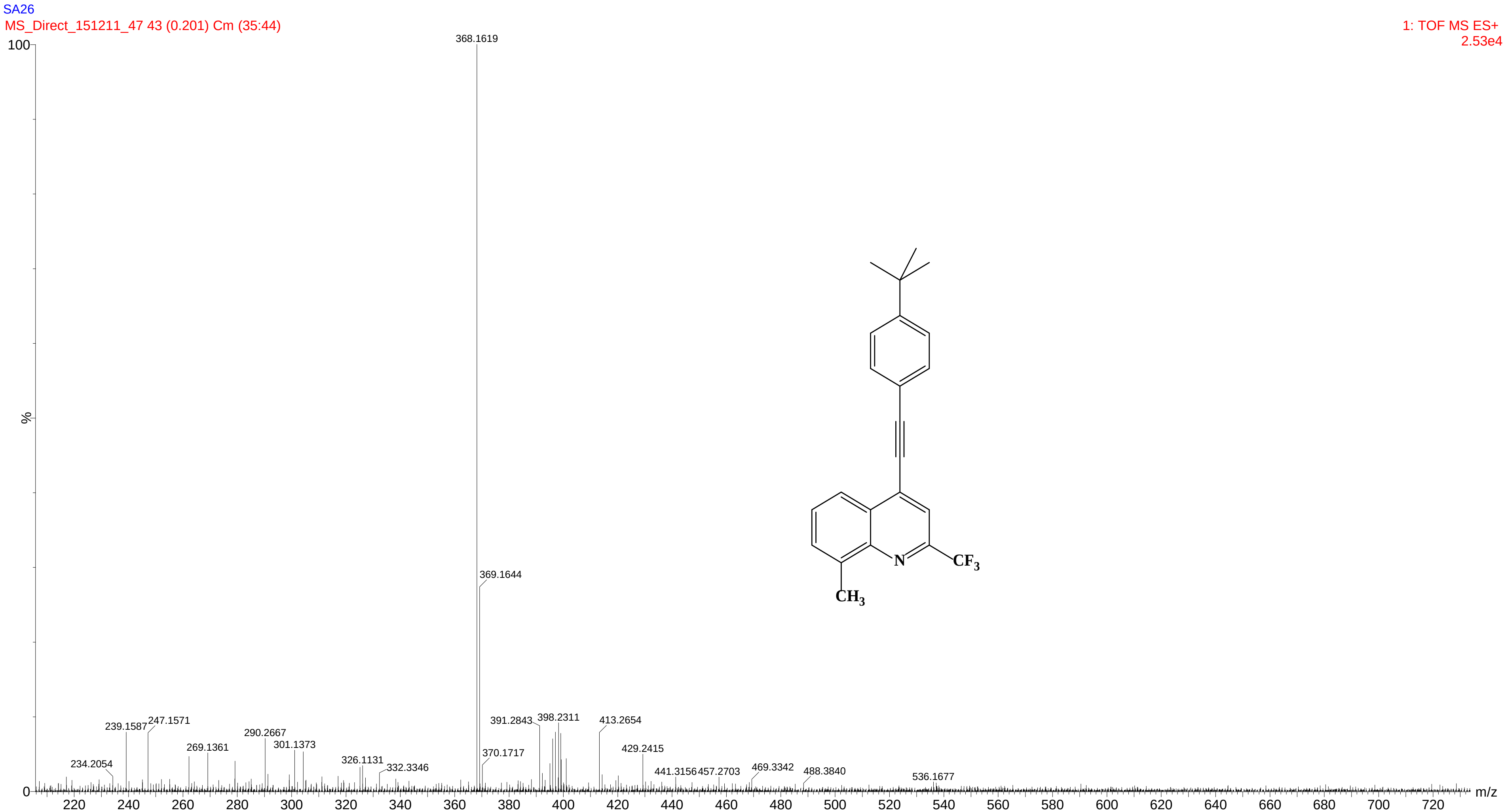
^{13}C NMR spectrum of **4L ($CDCl_3$, 100 MHz)**



[19]F NMR spectrum of **4L (CDCl₃, 376 MHz)**

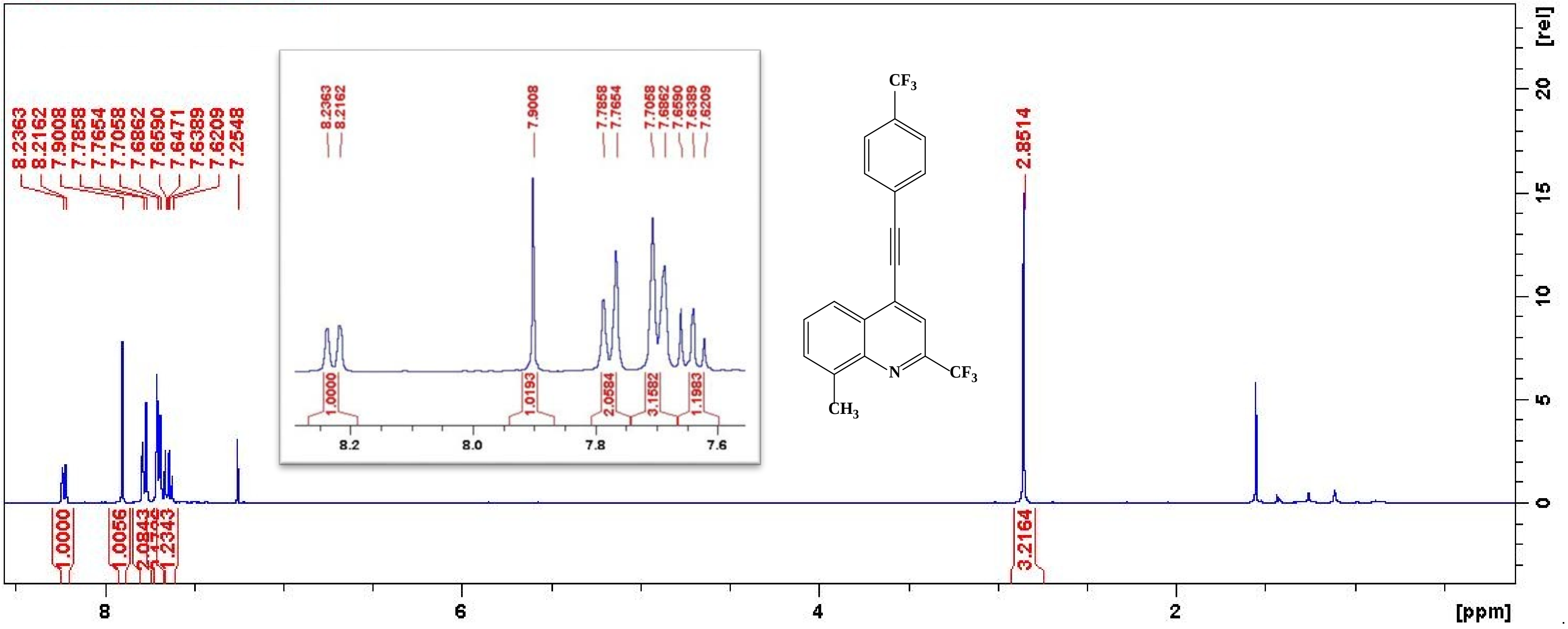


HRMS of **4L**

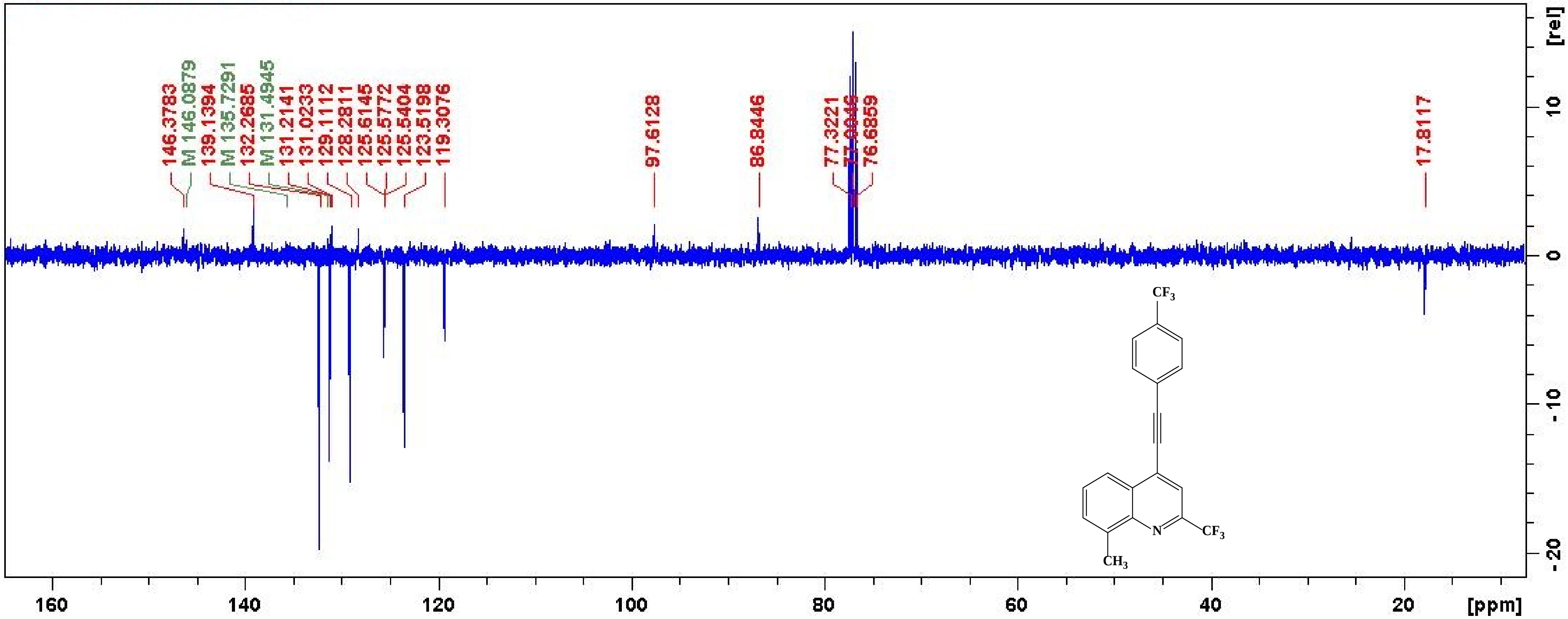


SA26
MS_Direct_151211_47 43 (0.201) Cm (35:44)
1: TOF MS ES+
2.53e4
100
%
0
368.1619
369.1644
239.1587
247.1571
234.2054
269.1361
290.2667
301.1373
326.1131
332.3346
370.1717
391.2843
398.2311
413.2654
429.2415
441.3156
457.2703
469.3342
488.3840
536.1677
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
520
540
560
580
600
620
640
660
680
700
720
m/z
N
CF3
CH3

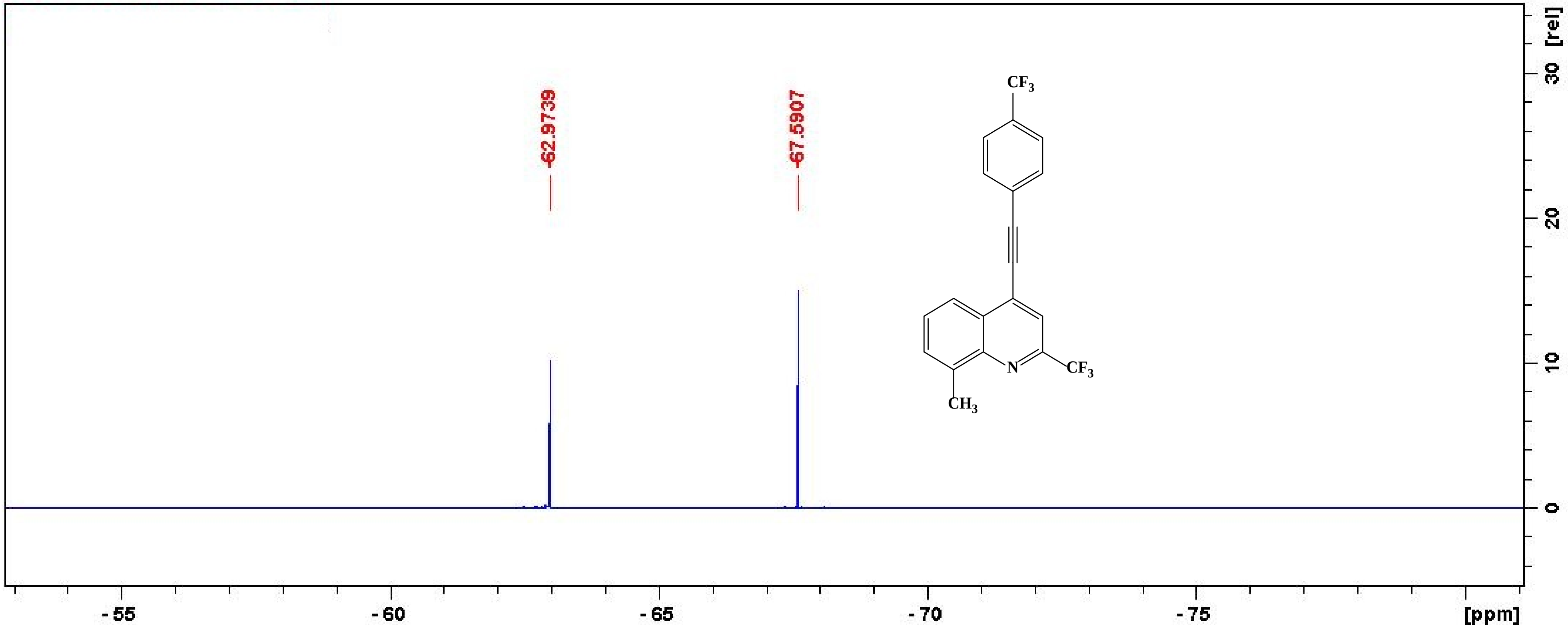
[1]H NMR spectrum of **4M (CDCl3, 400 MHz)**



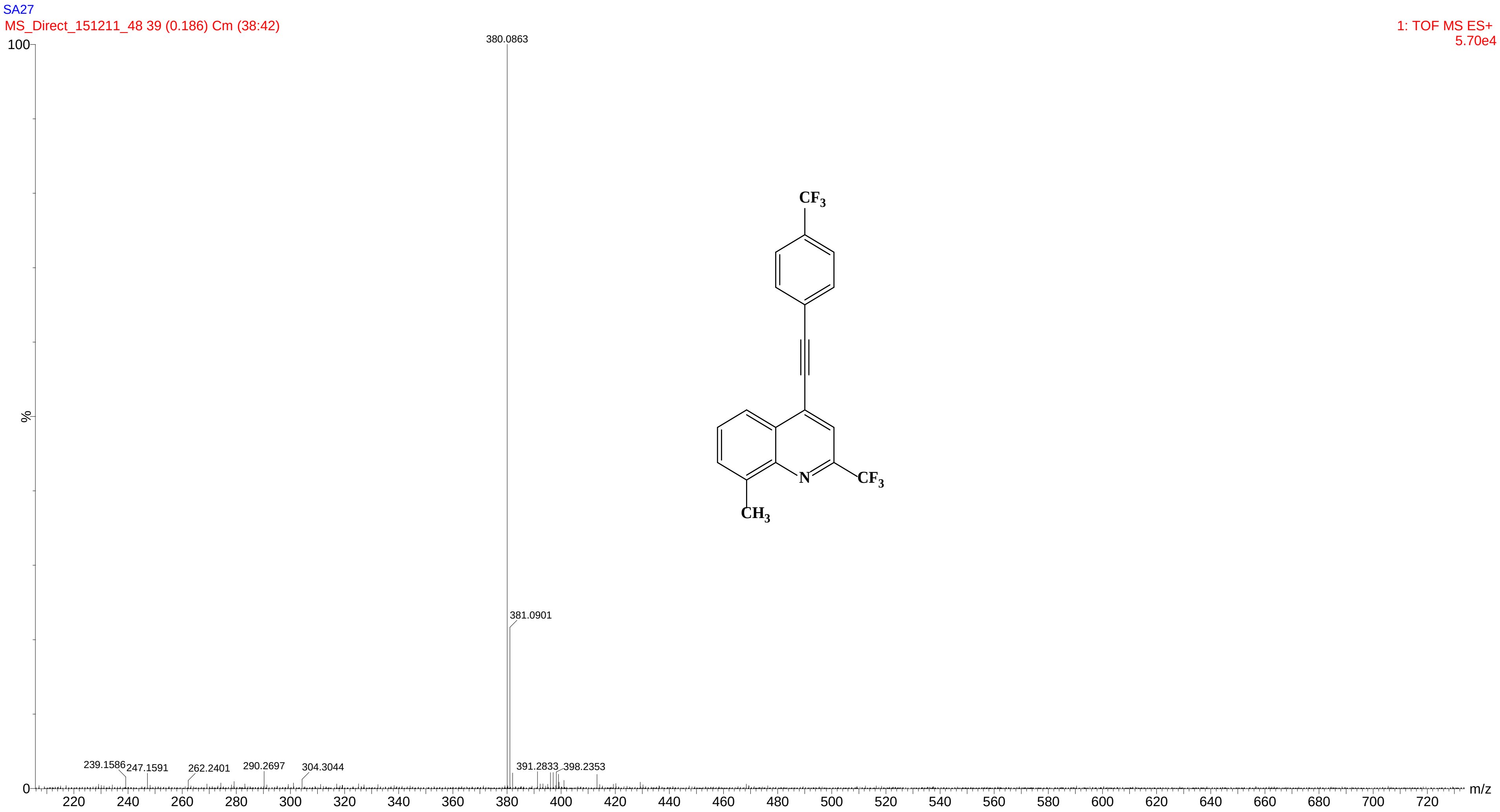
[13]C NMR spectrum of **4M (CDCl₃, 100 MHz)**



^{19}F NMR spectrum of **4M ($CDCl_3$, 376 MHz)**

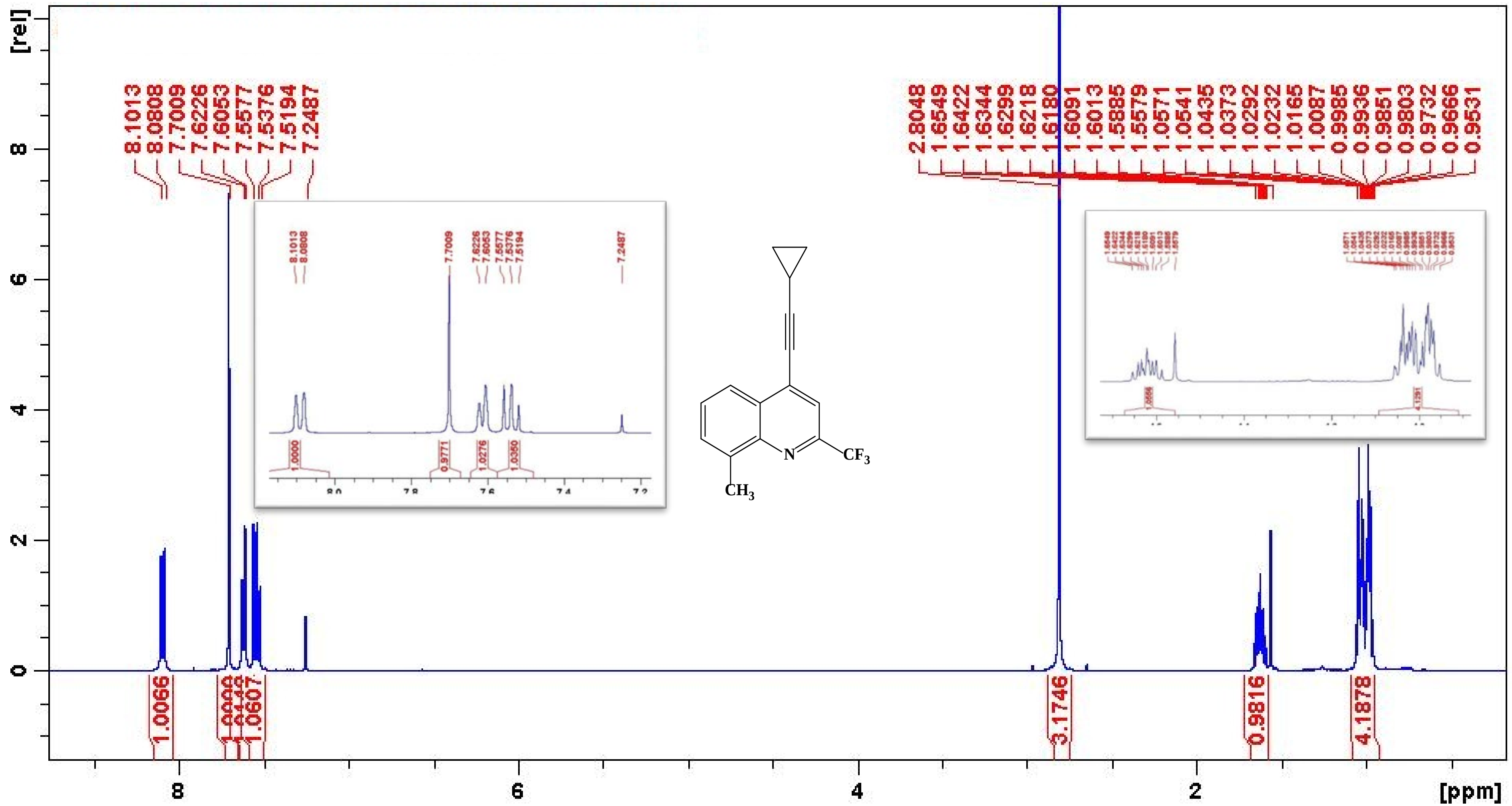


HRMS of **4M**

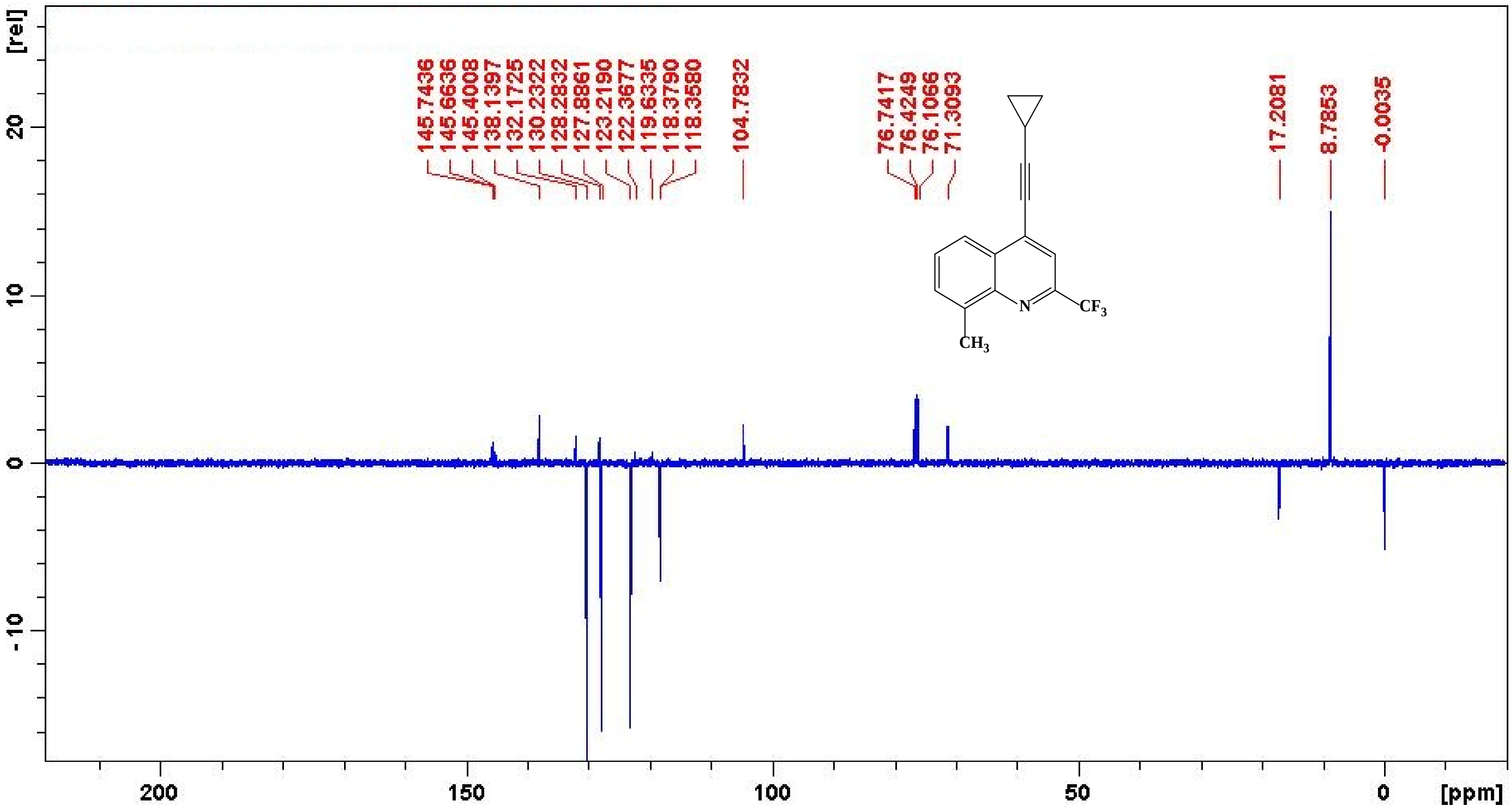


SA27
MS_Direct_151211_48 39 (0.186) Cm (38:42)
1: TOF MS ES+
5.70e4
380.0863
381.0901
239.1586
247.1591
262.2401
290.2697
304.3044
391.2833
398.2353
100
%
0
m/z
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
520
540
560
580
600
620
640
660
680
700
720
CF3
N
CF3
CH3

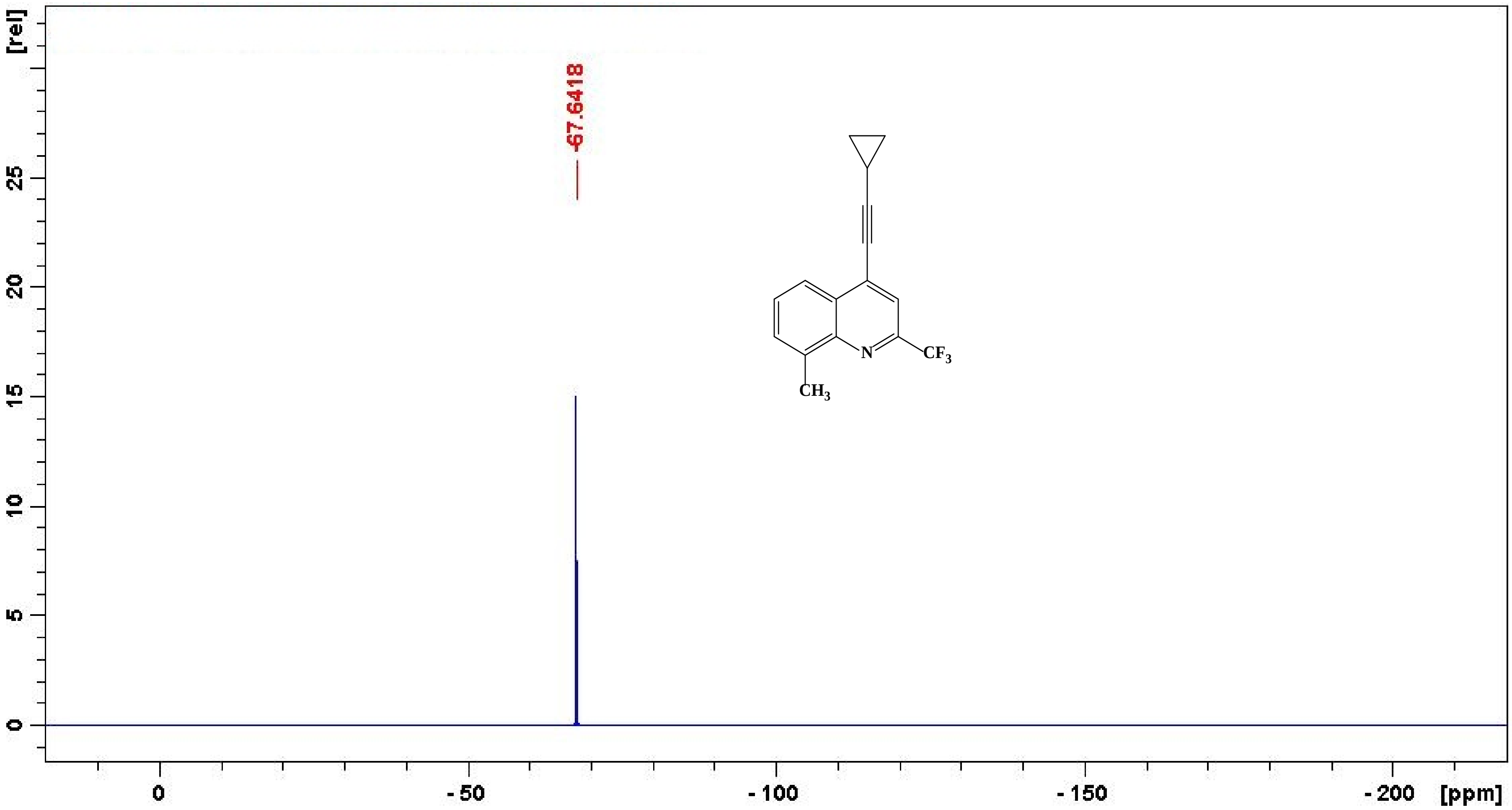
[1]H NMR spectrum of **4N ($CDCl_3$, 400 MHz)**



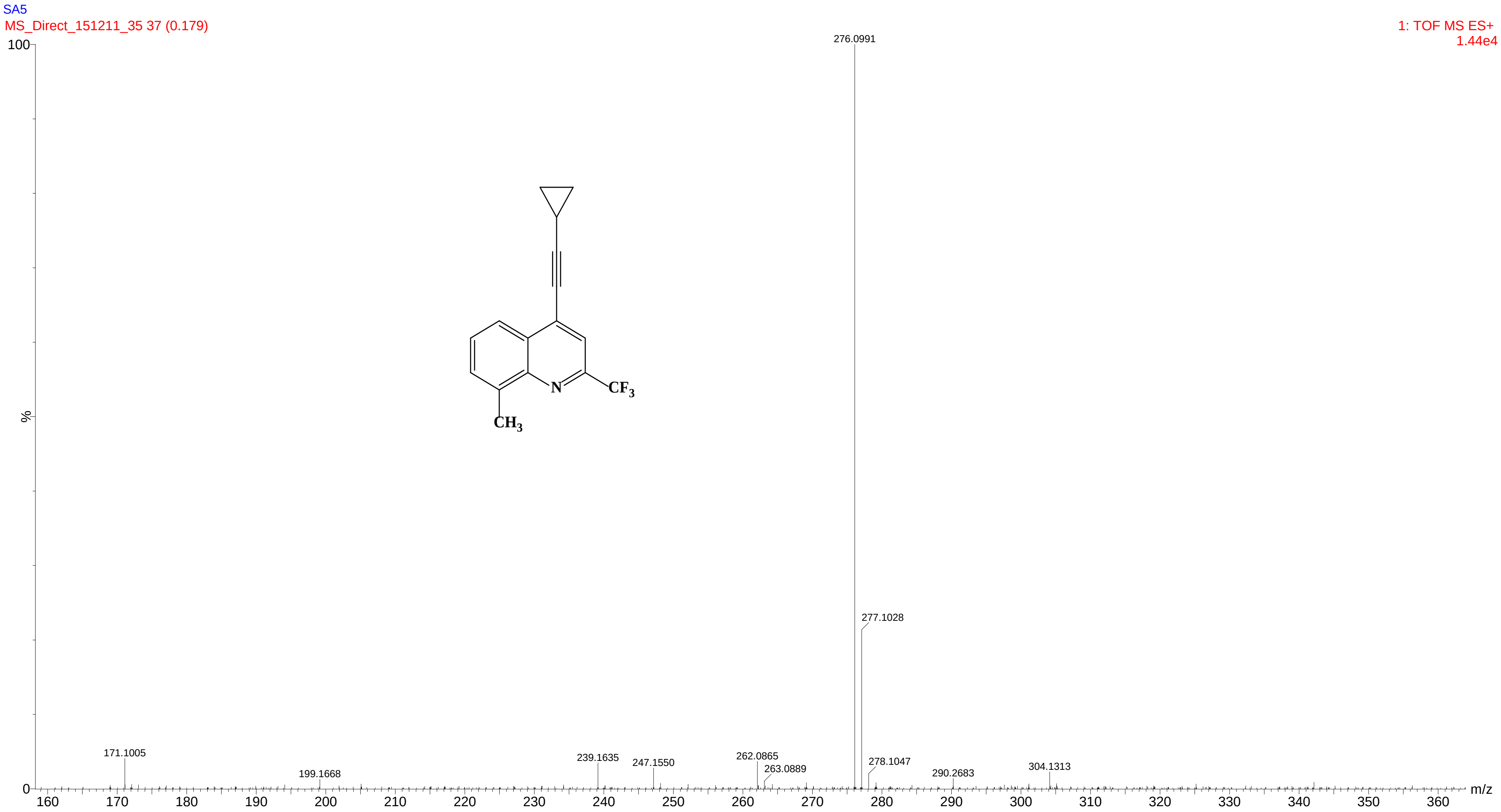
[13]C NMR spectrum of **4N (CDCl3, 100 MHz)**



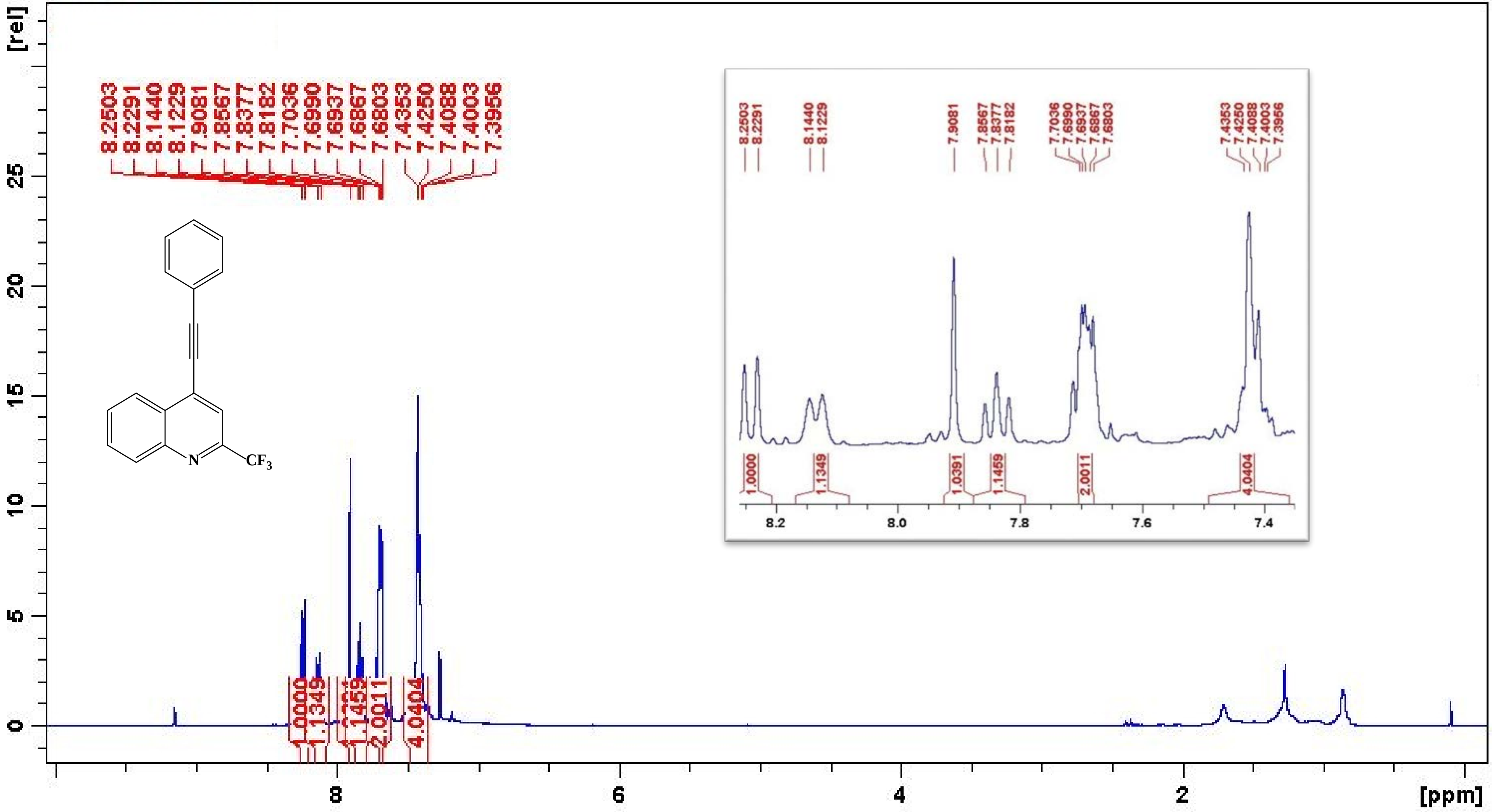
[19]F NMR spectrum of **4N (CDCl$_3$, 376 MHz)**



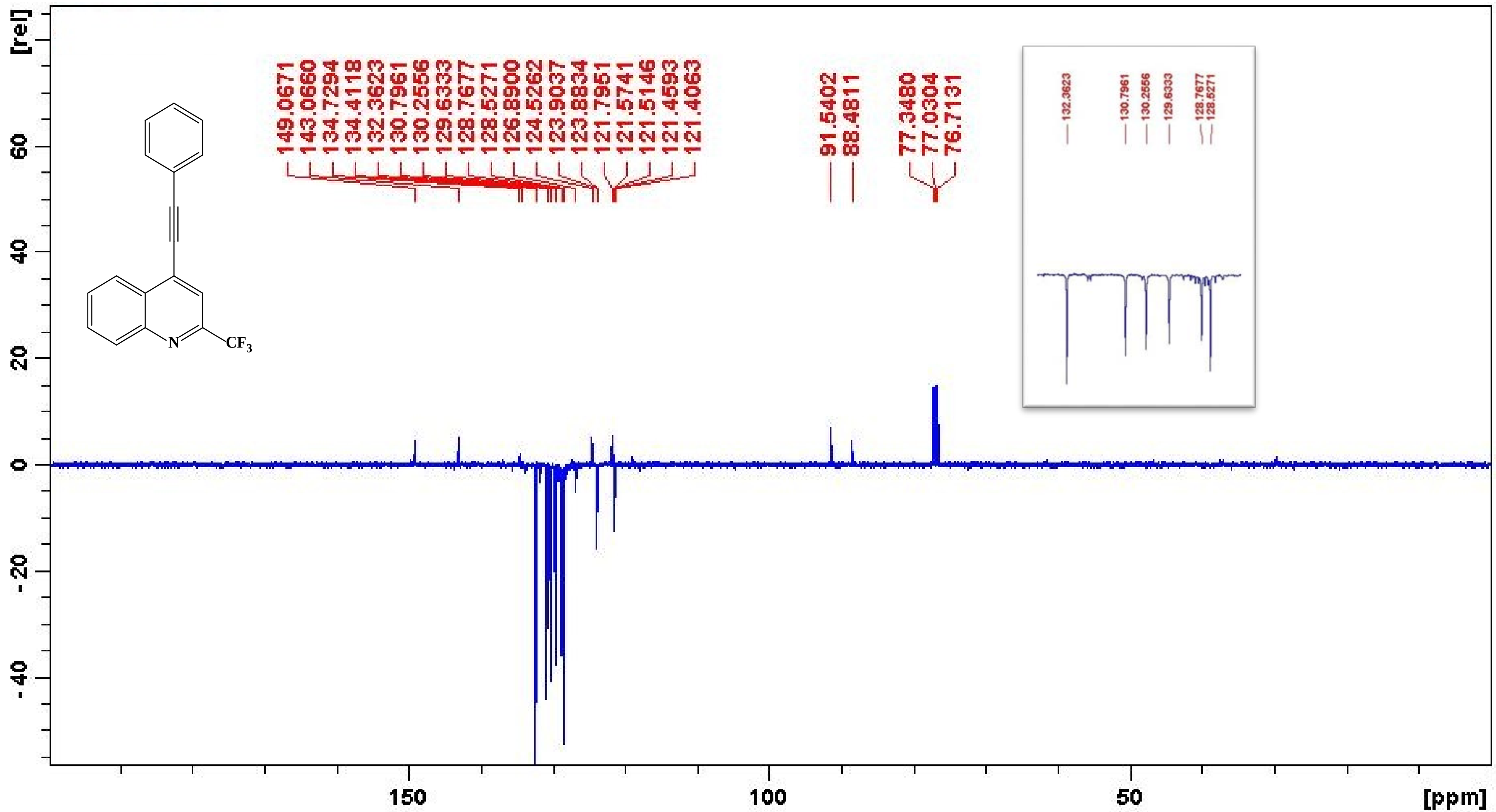
HRMS of **4N**


SA5
MS_Direct_151211_35 37 (0.179)
1: TOF MS ES+
1.44e4
276.0991
277.1028
171.1005
199.1668
239.1635
247.1550
262.0865
263.0889
278.1047
290.2683
304.1313
N
CF3
CH3
100
%
0
160
170
180
190
200
210
220
230
240
250
260
270
280
290
300
310
320
330
340
350
360
m/z

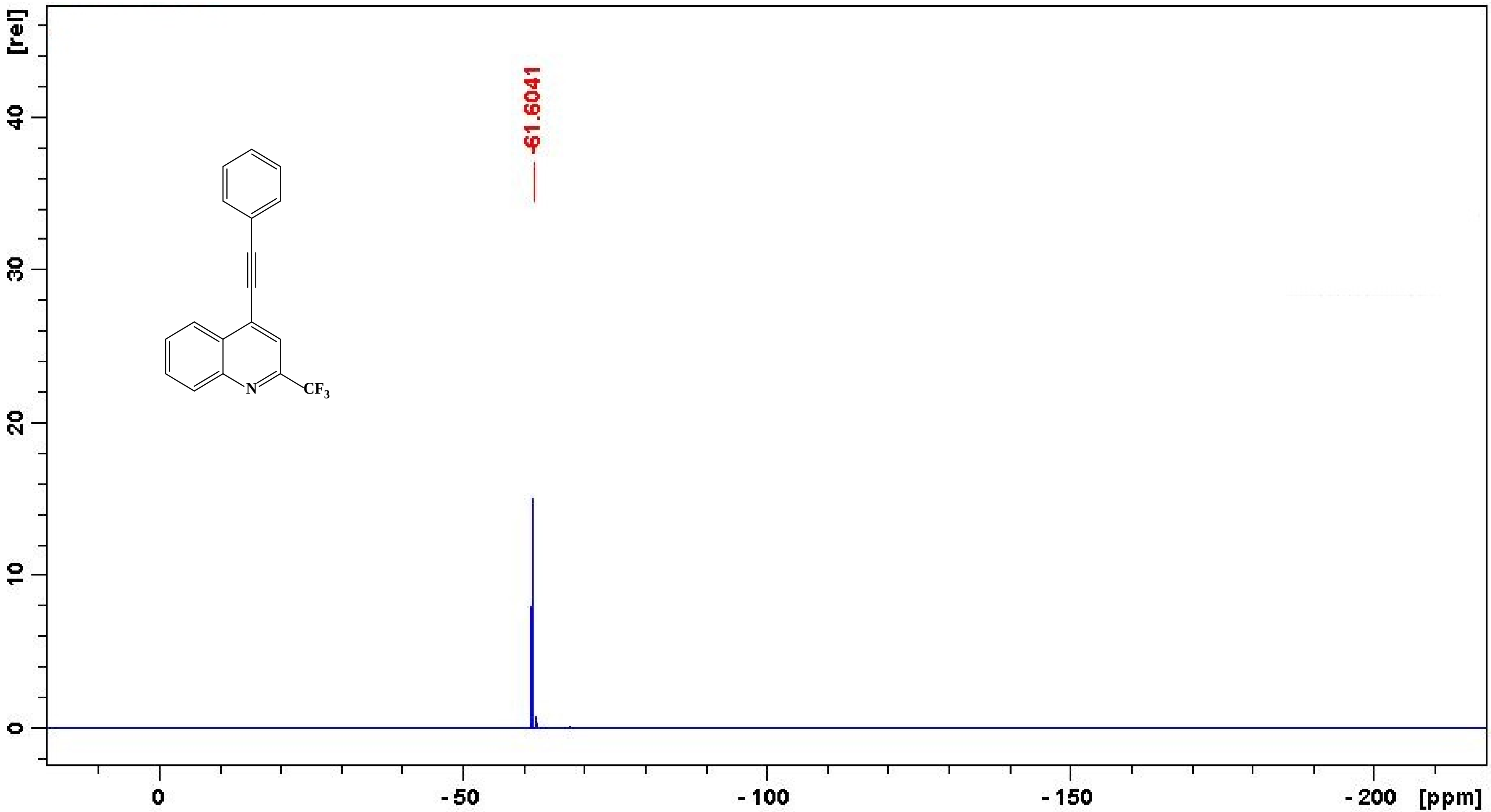
[1]H NMR spectrum of **4O ($CDCl_3$, 400 MHz)**



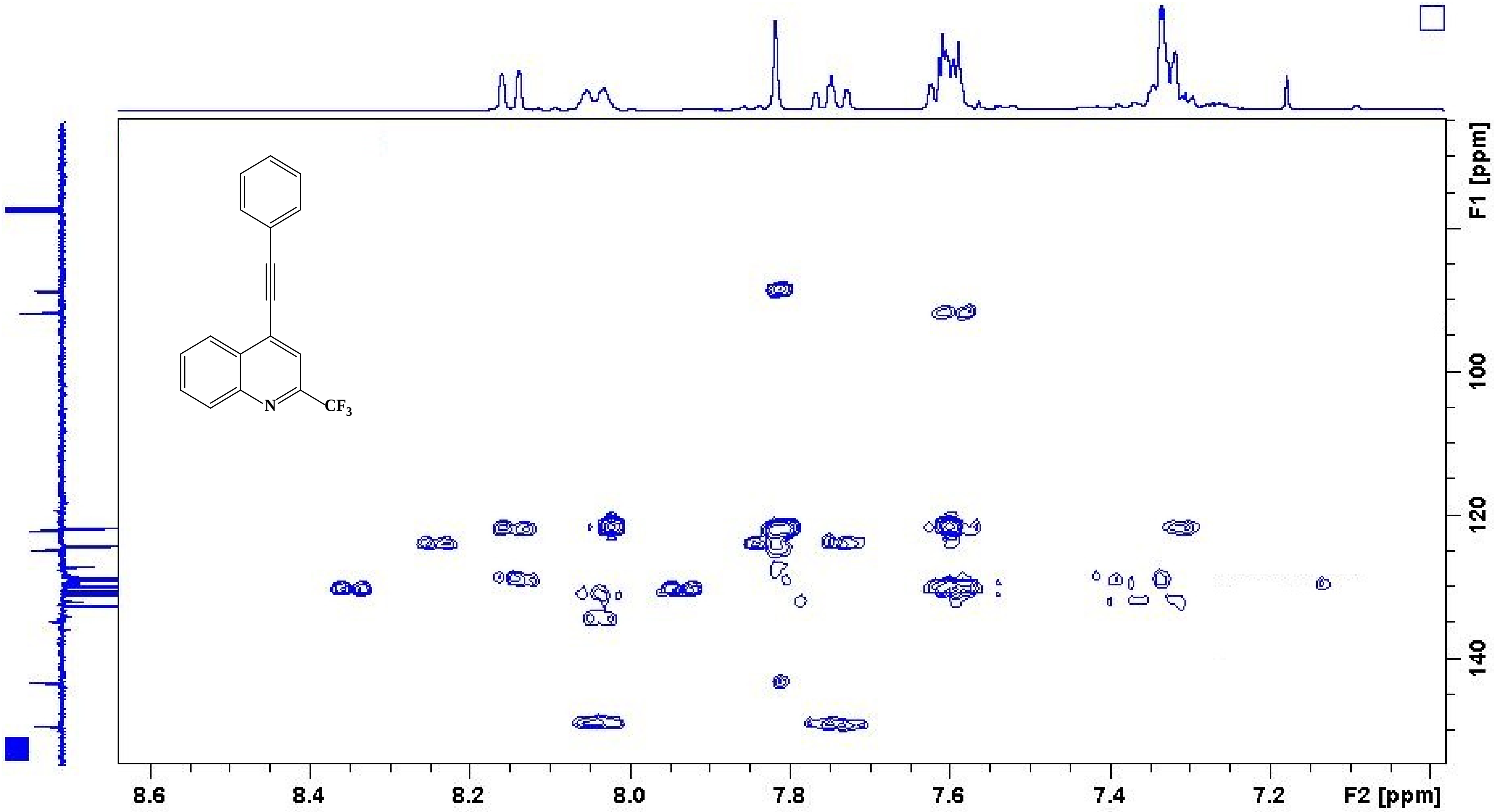
^{13}C NMR spectrum of **4O (CDCl$_3$, 100 MHz)**



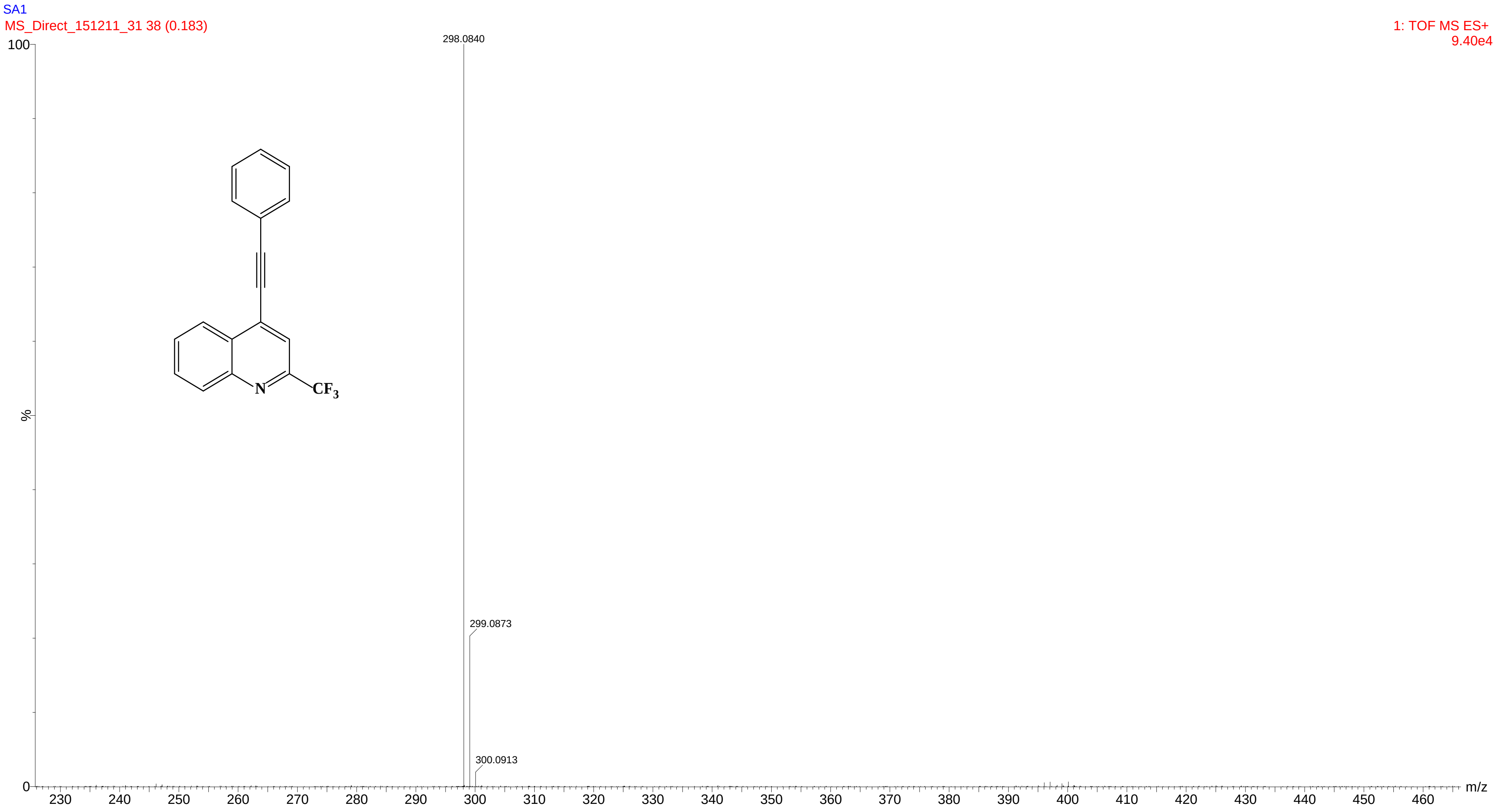
^{19}F NMR spectrum of **4O ($CDCl_3$, 376 MHz)**



HMBC spectrum of **4O**

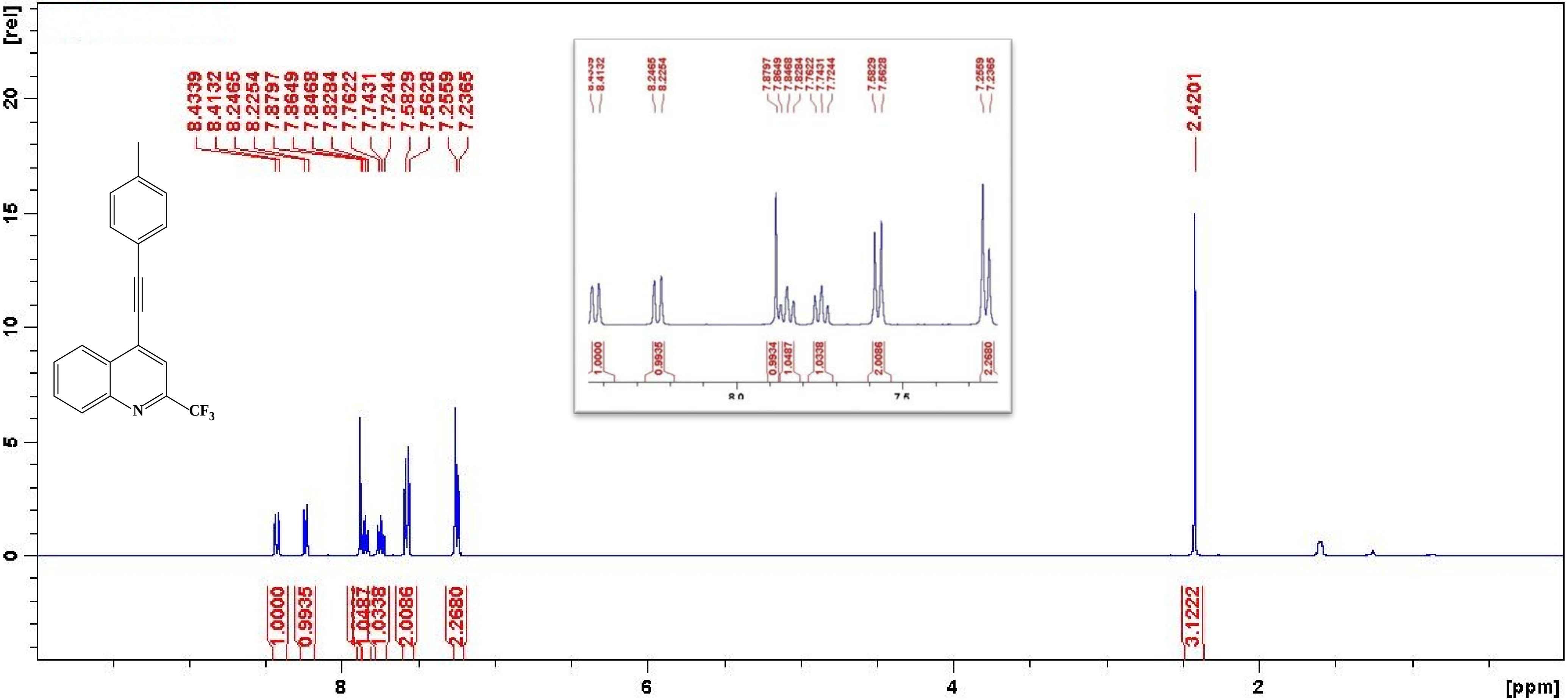


HRMS of **4O**

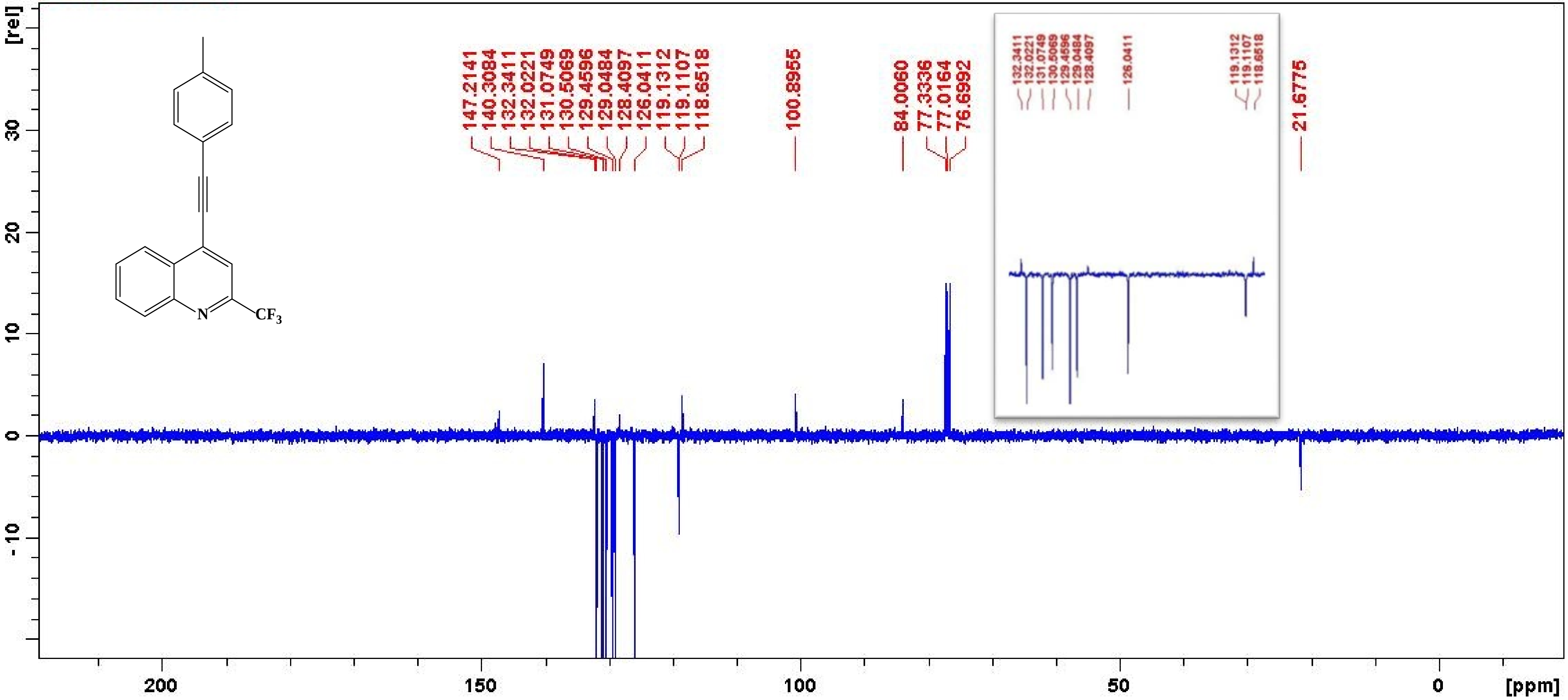


SA1
MS_Direct_151211_31 38 (0.183)
1: TOF MS ES+
9.40e4
298.0840
299.0873
300.0913
100
%
0
m/z
N
CF3

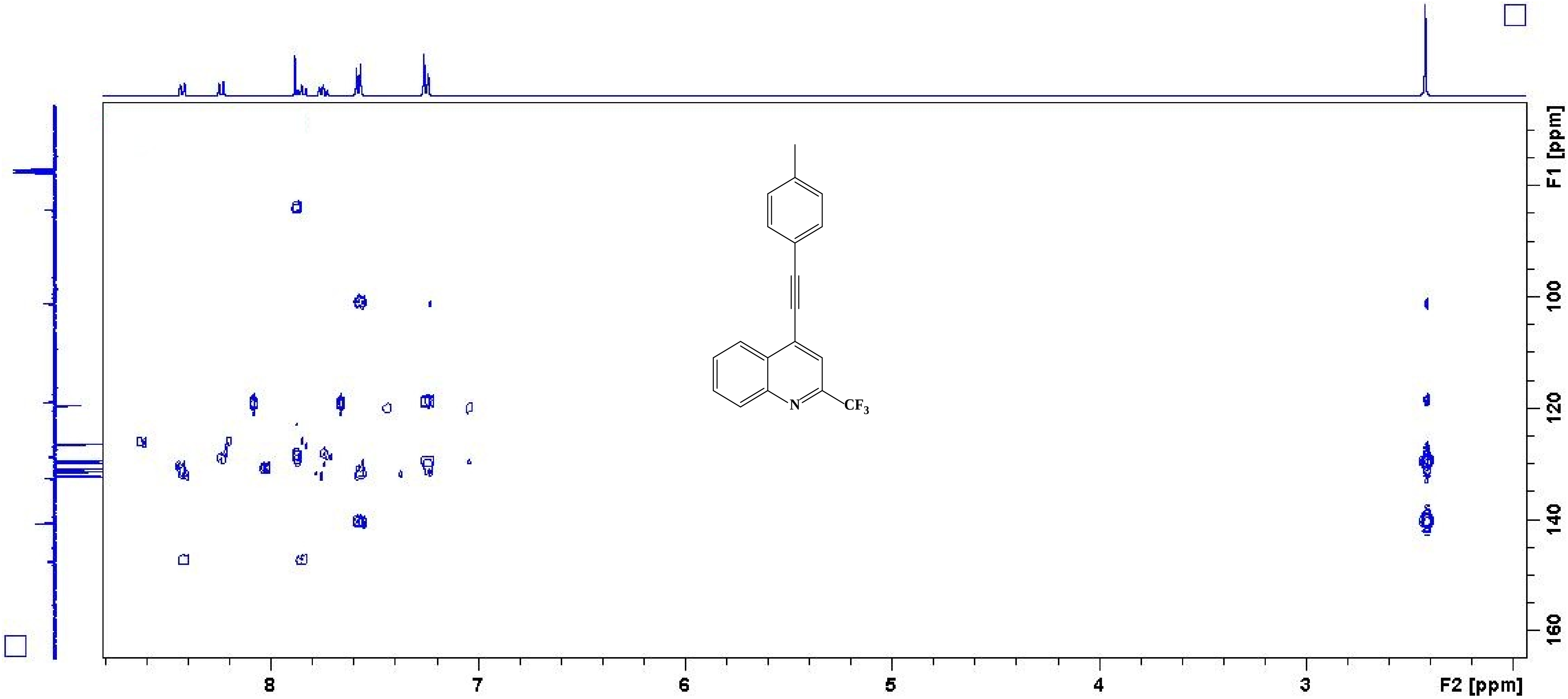
[1]H NMR spectrum of **4P (CDCl₃, 400 MHz)**



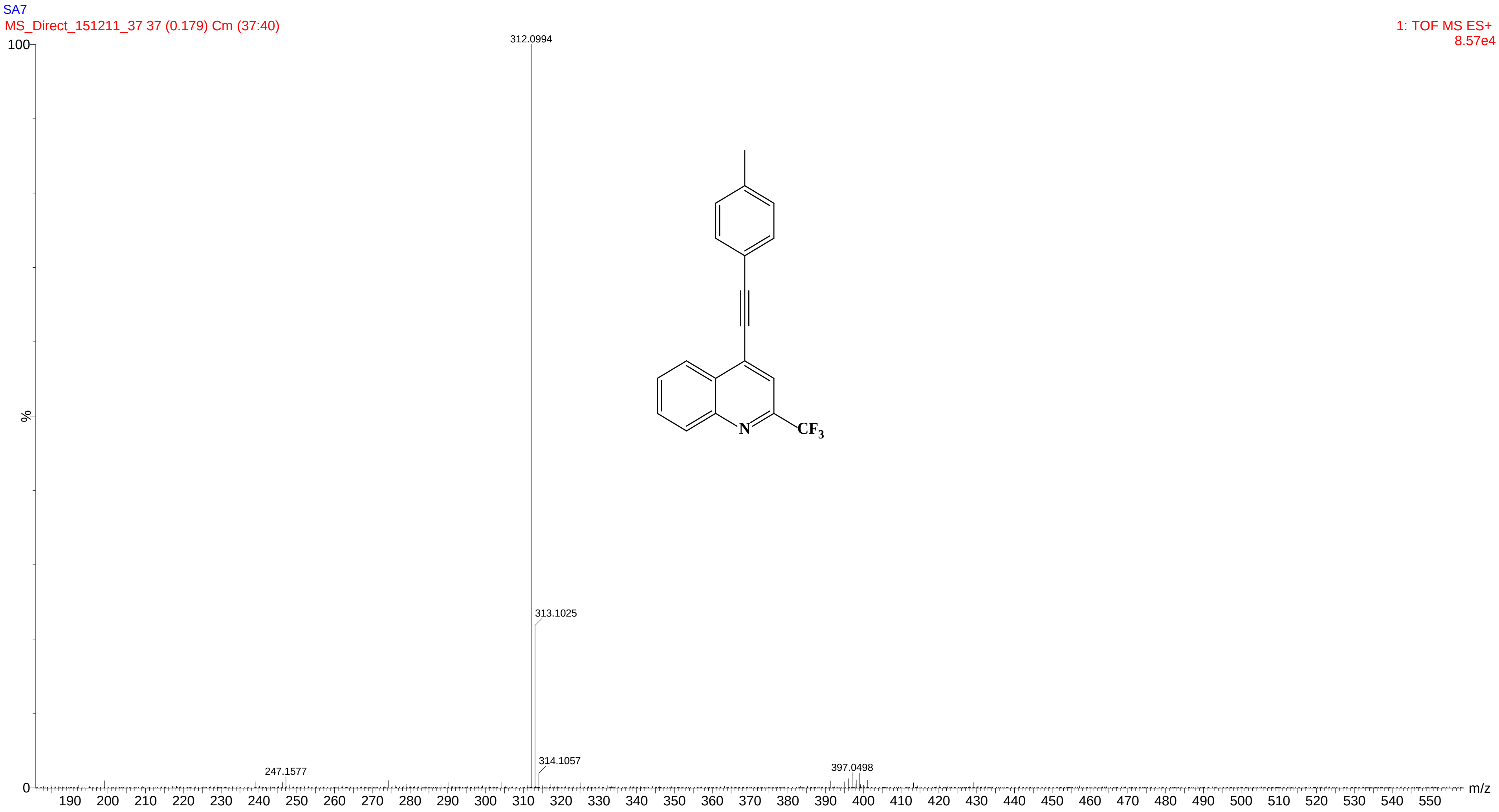
^{13}C NMR spectrum of **4P ($CDCl_3$, 100 MHz)**



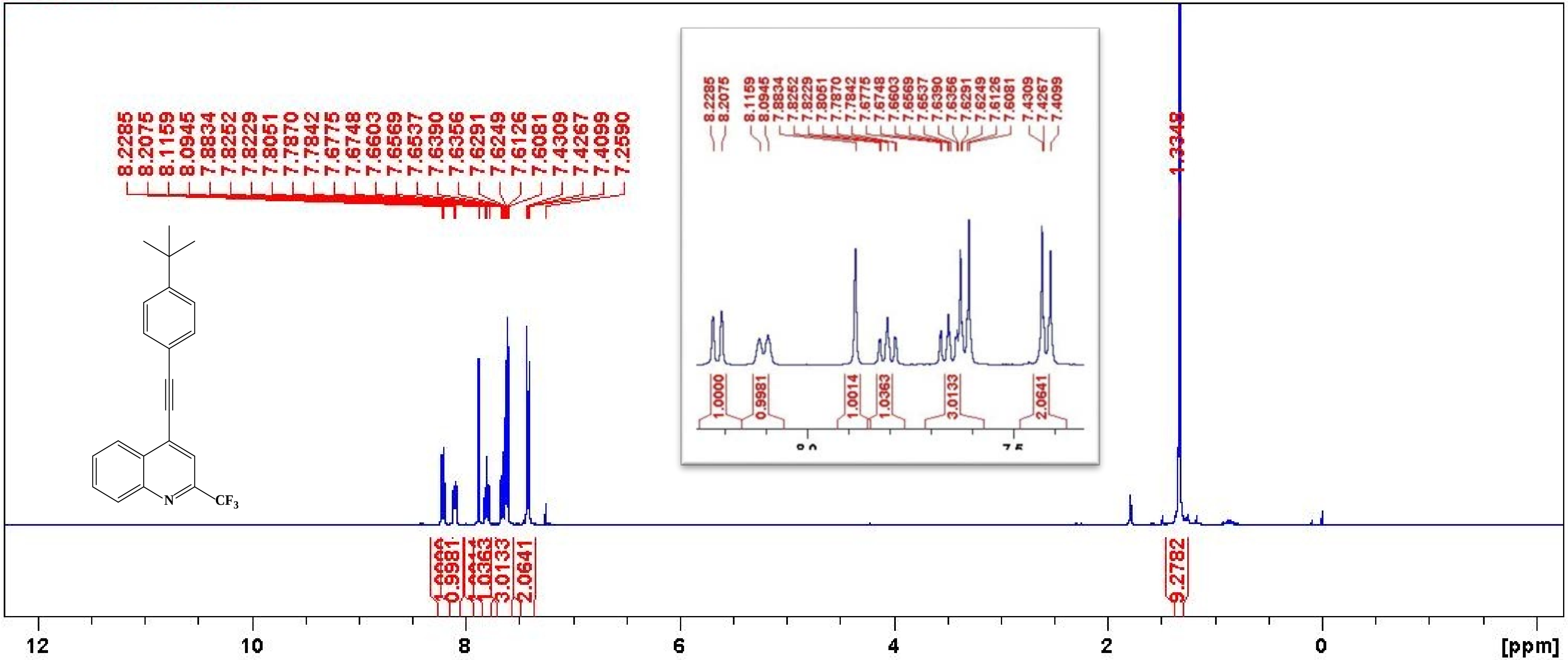
HMBC spectrum of **4P**



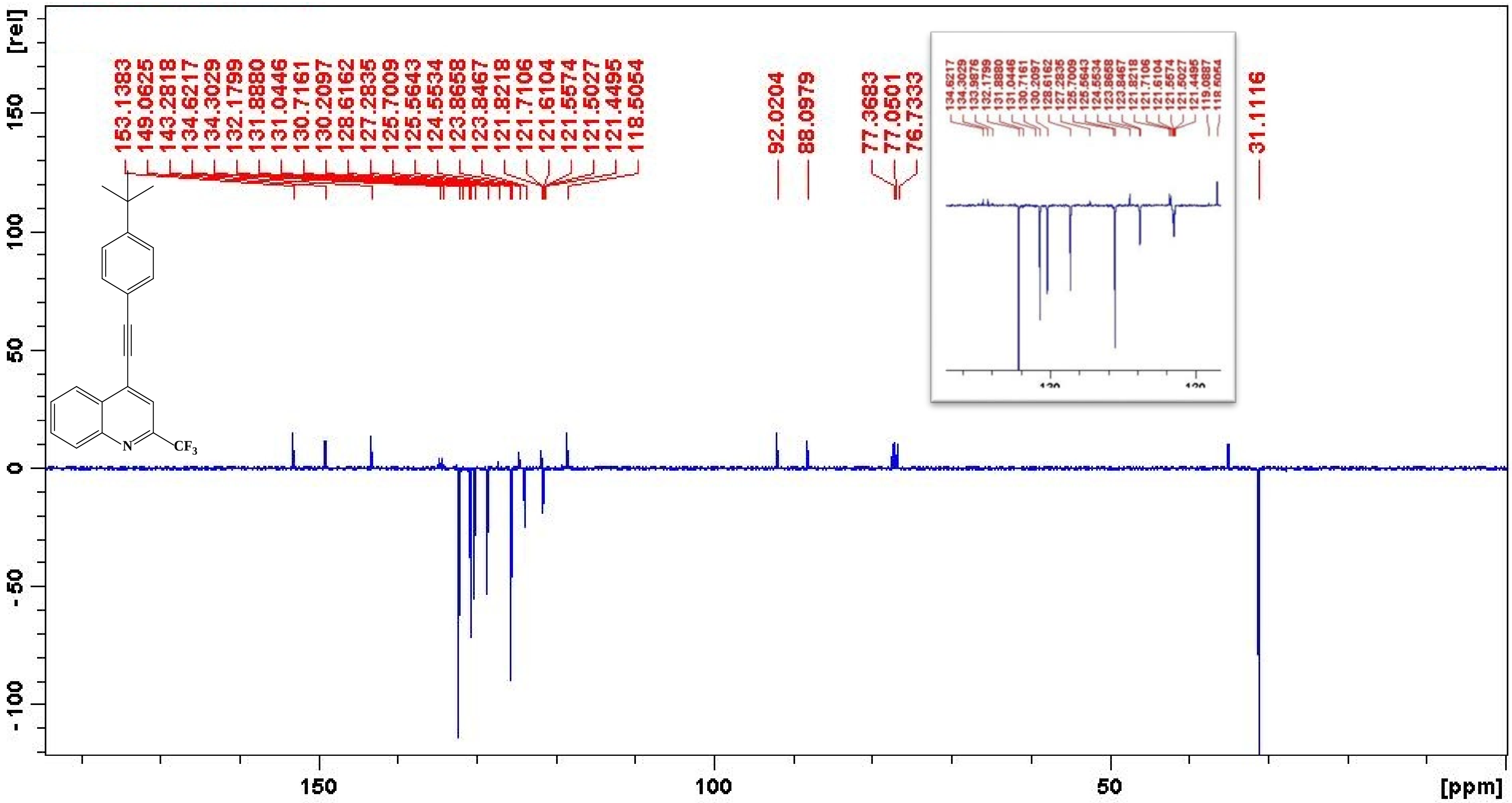
HRMS of **4P**


SA7
MS_Direct_151211_37 37 (0.179) Cm (37:40)
1: TOF MS ES+
8.57e4
100
%
0
312.0994
313.1025
314.1057
247.1577
397.0498
m/z
190 200 210 220 230 240 250 260 270 280 290 300 310 320 330 340 350 360 370 380 390 400 410 420 430 440 450 460 470 480 490 500 510 520 530 540 550
N
CF3

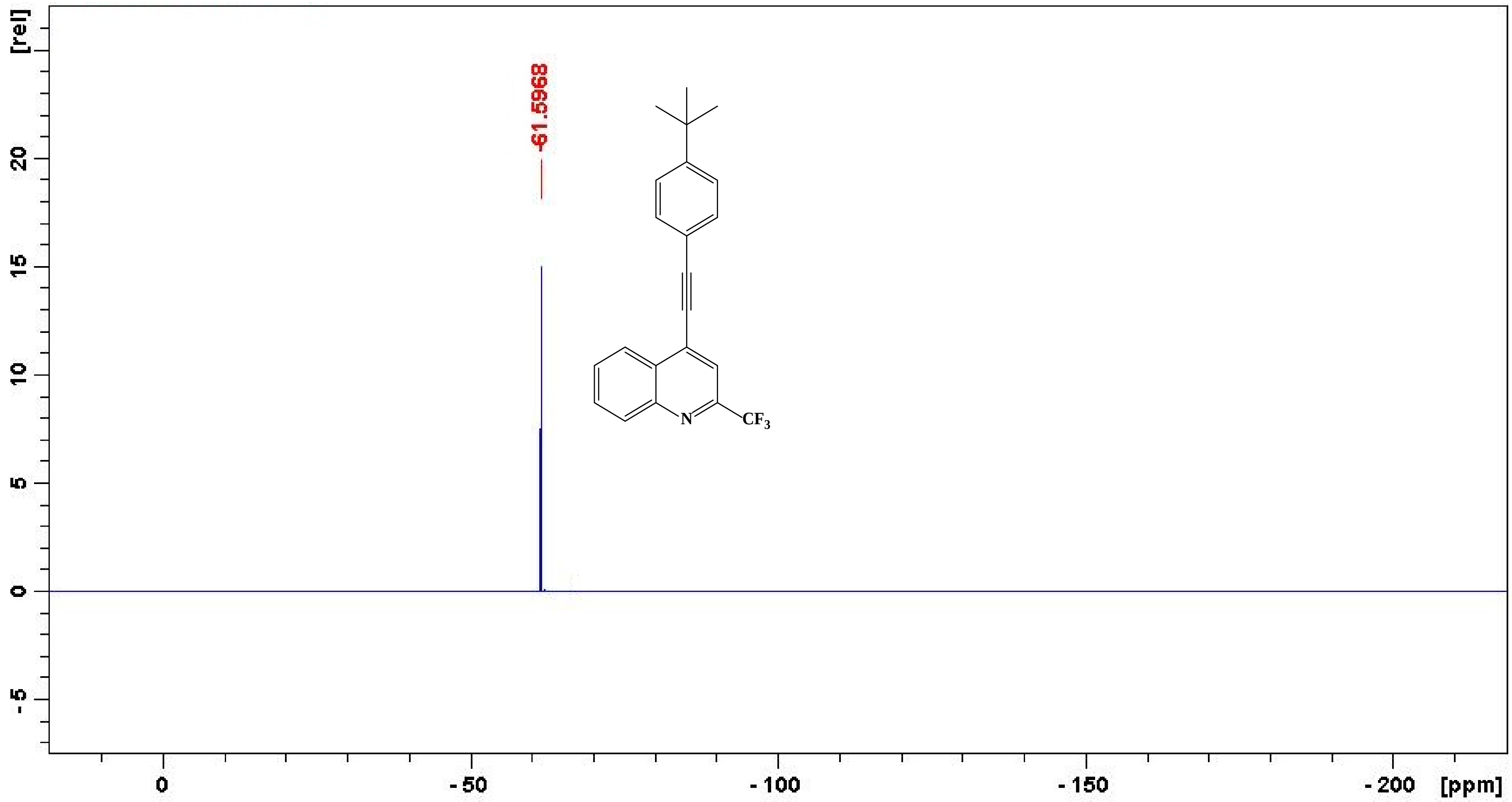
[1]H NMR spectrum of **4Q (CDCl3, 400 MHz)**



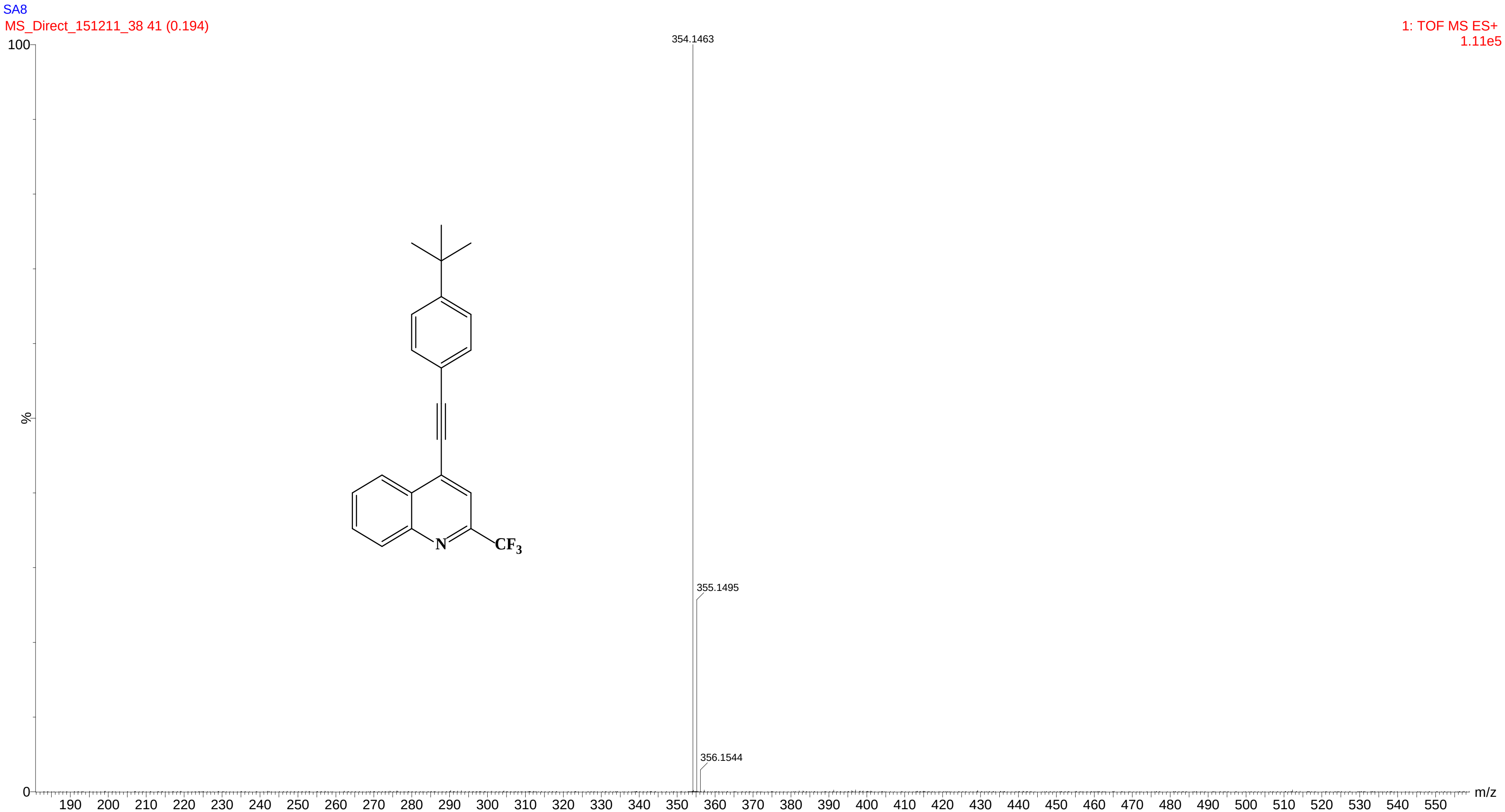
[13]C NMR spectrum of **4Q (CDCl₃, 100 MHz)**



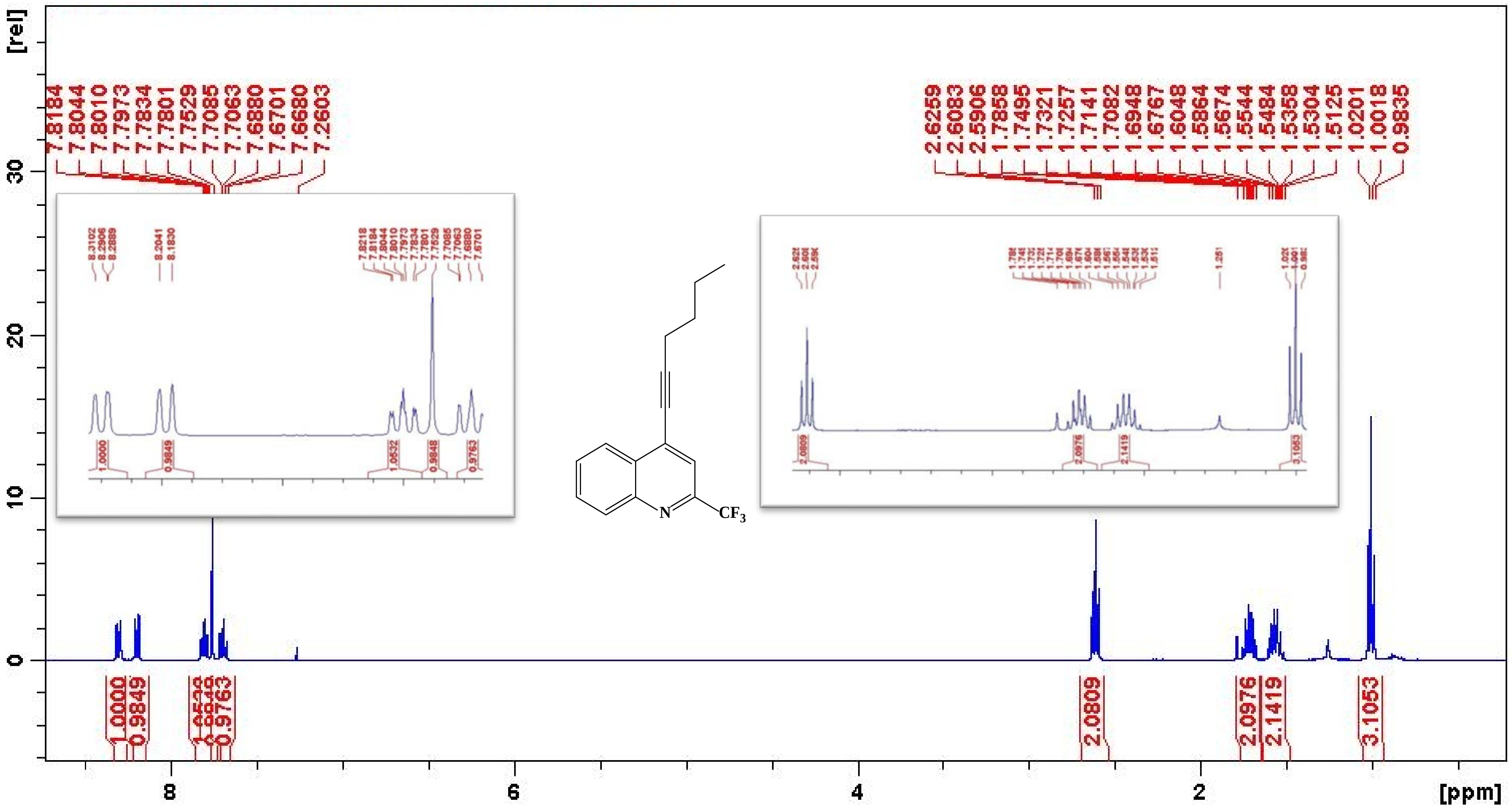
[19]F NMR spectrum of **4Q (CDCl3, 376 MHz)**



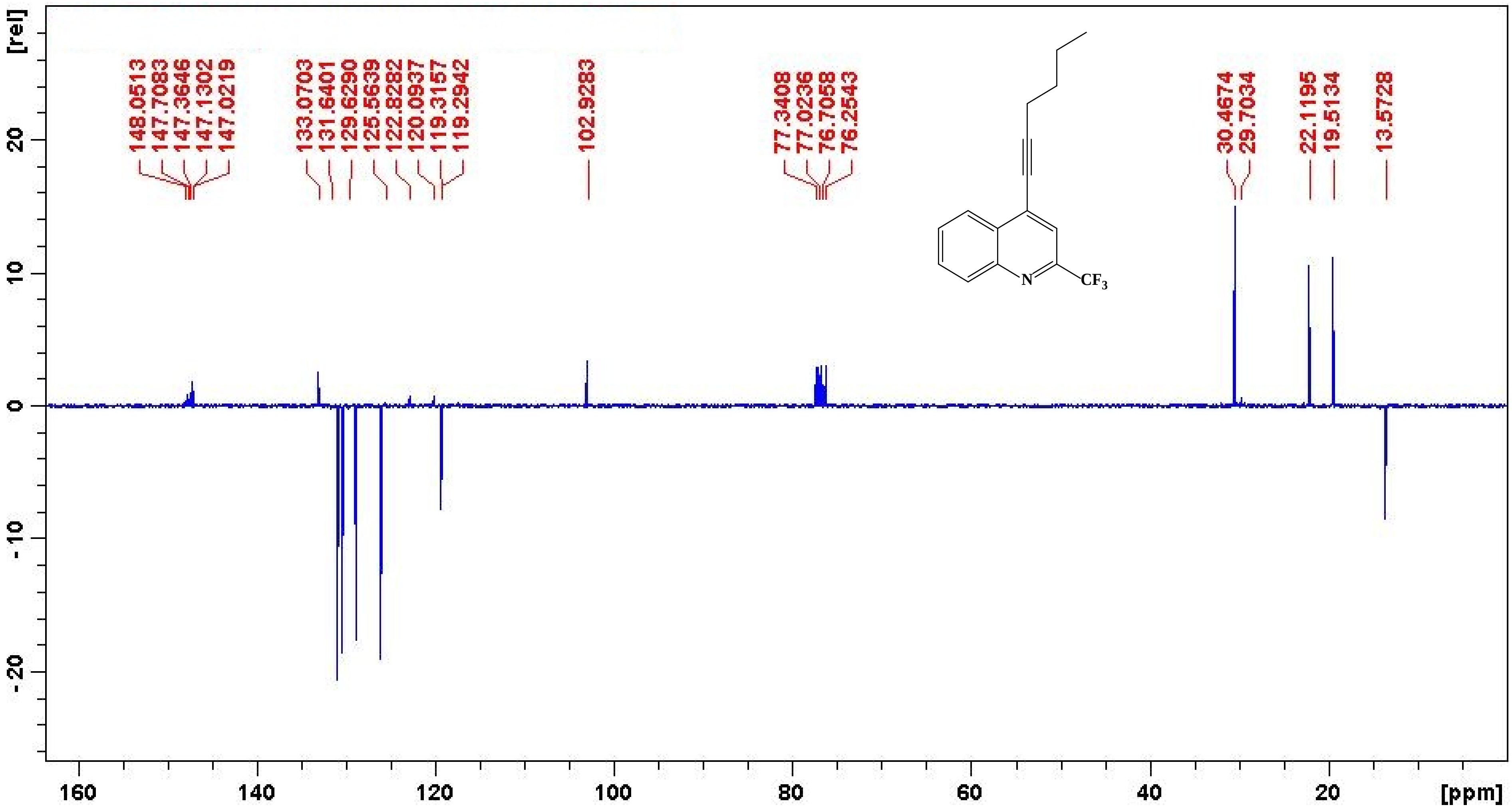
HRMS of **4Q**


SA8
MS_Direct_151211_38 41 (0.194)
1: TOF MS ES+
1.11e5
100
%
0
354.1463
355.1495
356.1544
N
CF3
190 200 210 220 230 240 250 260 270 280 290 300 310 320 330 340 350 360 370 380 390 400 410 420 430 440 450 460 470 480 490 500 510 520 530 540 550
m/z

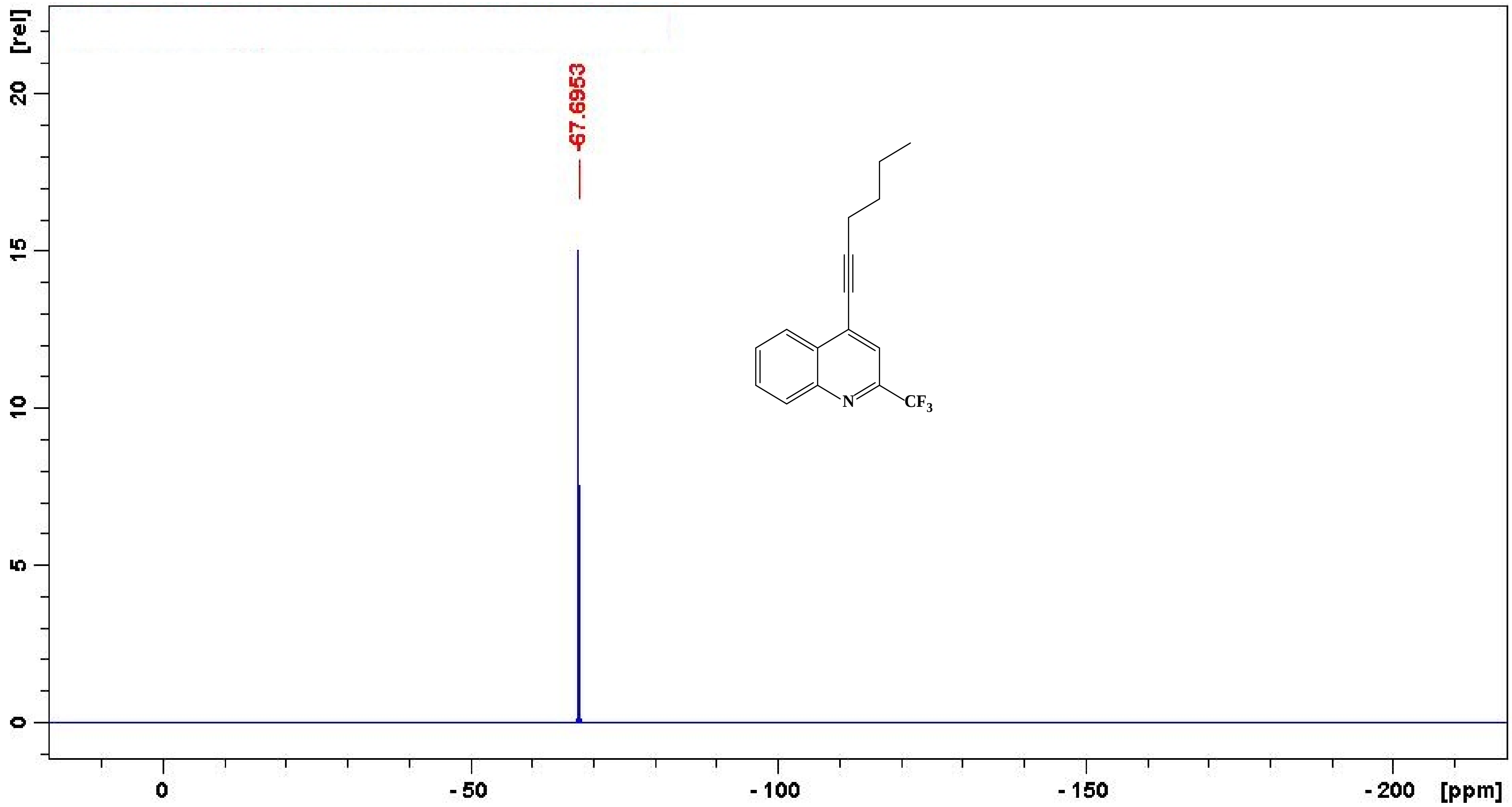
^{1}H NMR spectrum of **4R (CDCl$_3$, 400 MHz)**



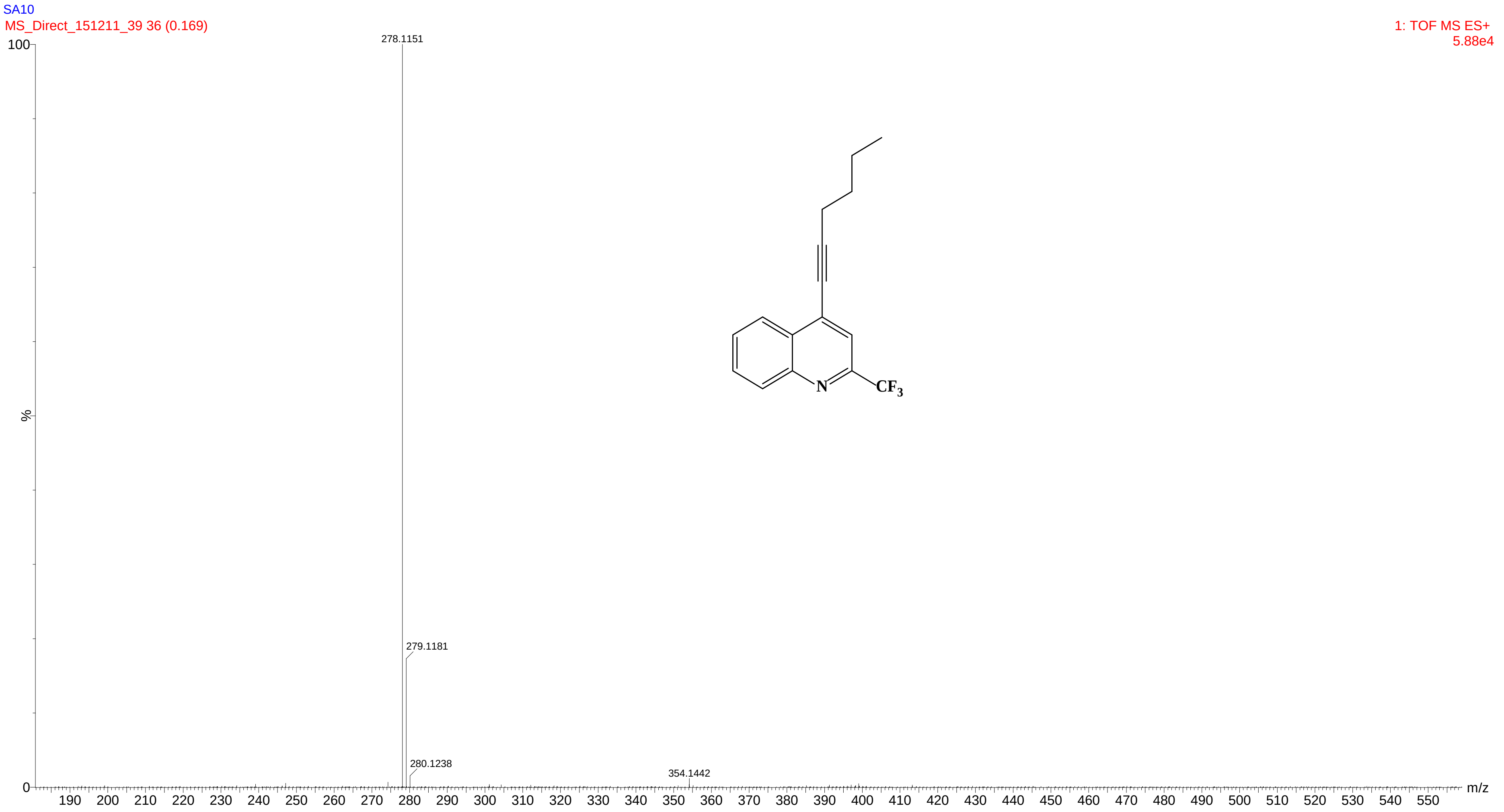
^{13}C NMR spectrum of **4R ($CDCl_3$, 100 MHz)**



^{19}F NMR spectrum of **4R ($CDCl_3$, 376 MHz)**

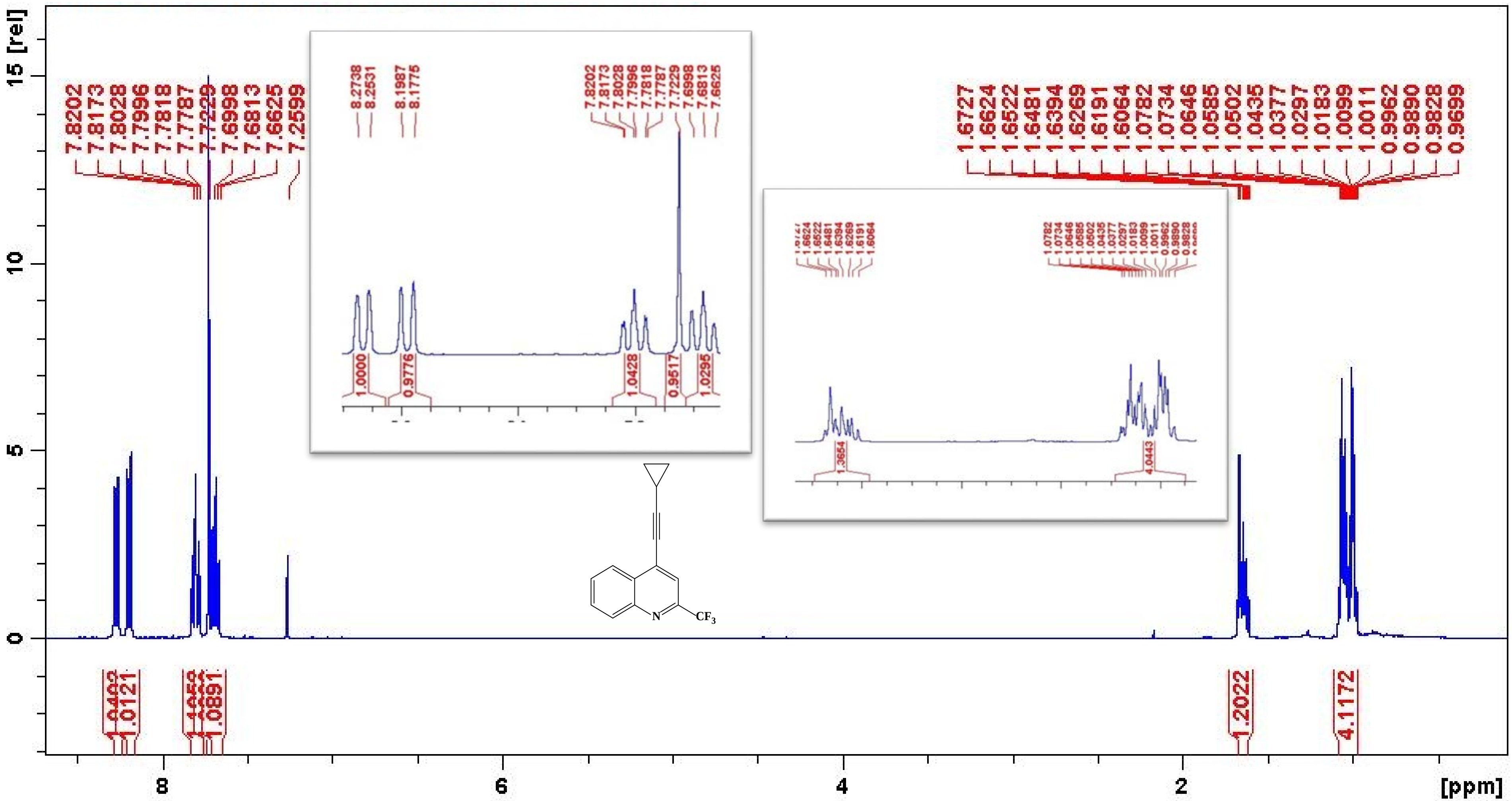


HRMS of **4R**

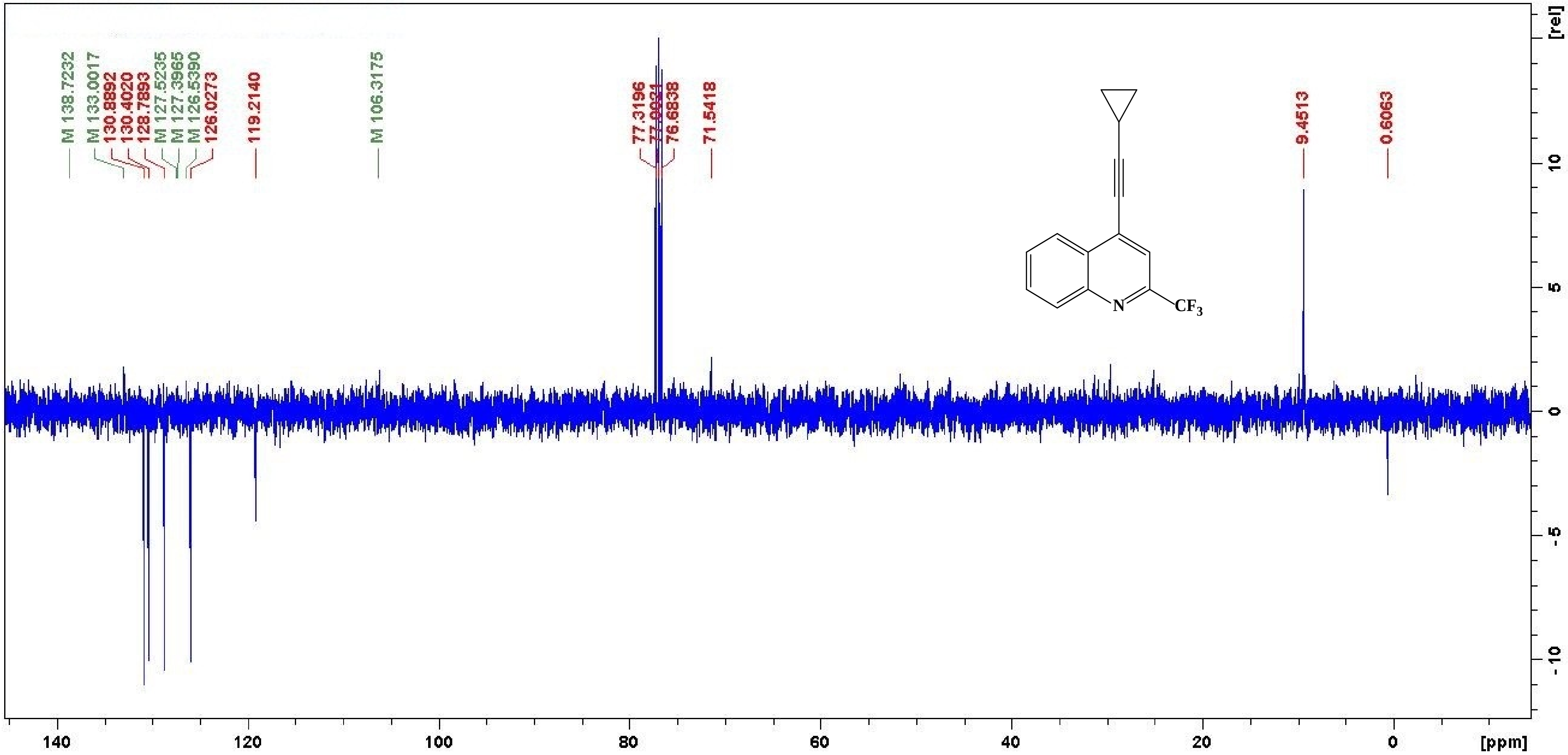


SA10
MS_Direct_151211_39 36 (0.169)
1: TOF MS ES+
5.88e4
100
%
0
278.1151
279.1181
280.1238
354.1442
190
200
210
220
230
240
250
260
270
280
290
300
310
320
330
340
350
360
370
380
390
400
410
420
430
440
450
460
470
480
490
500
510
520
530
540
550
m/z
N
CF3

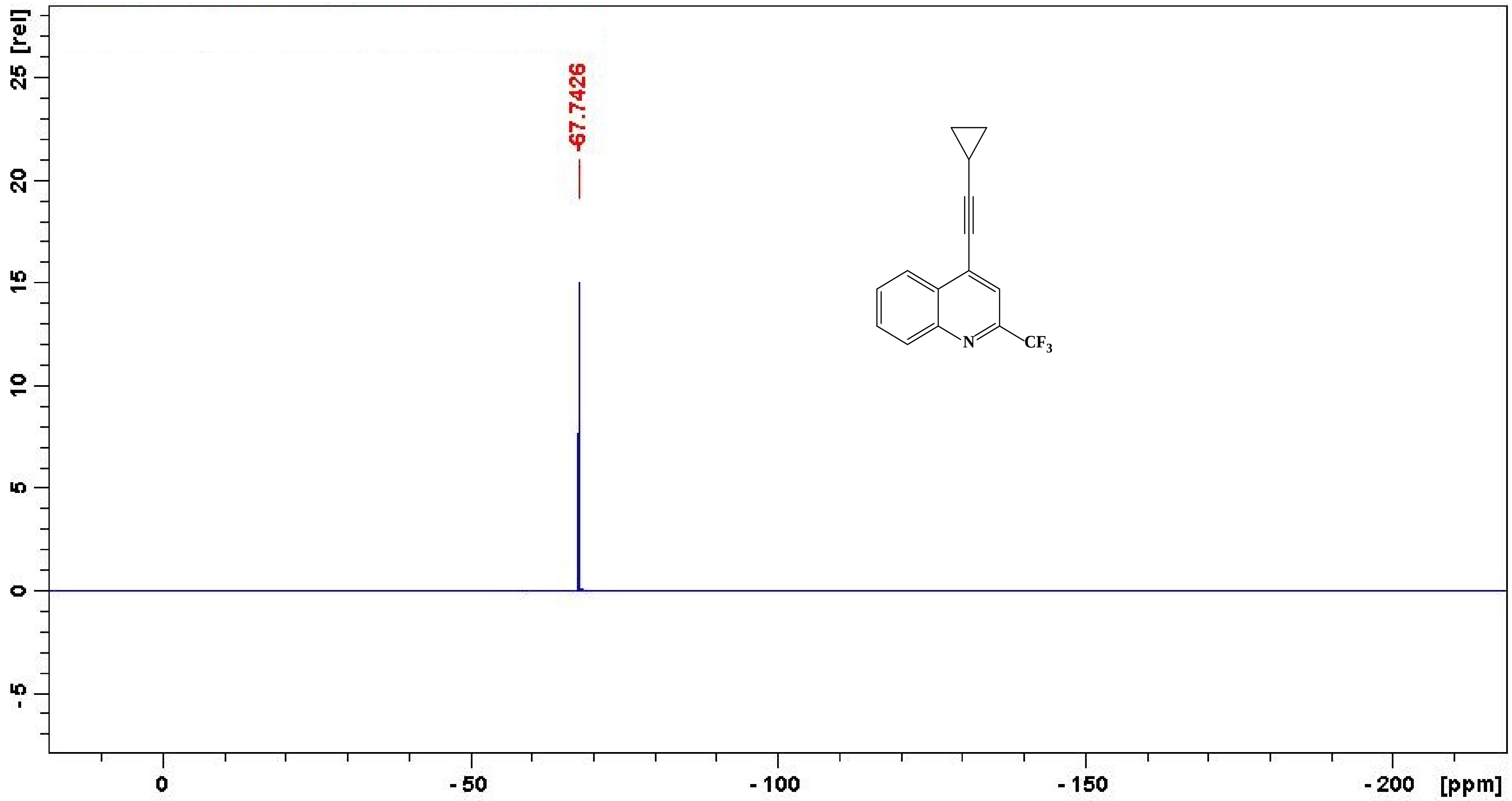
[1]H NMR spectrum of **4S (CDCl$_3$, 400 MHz)**



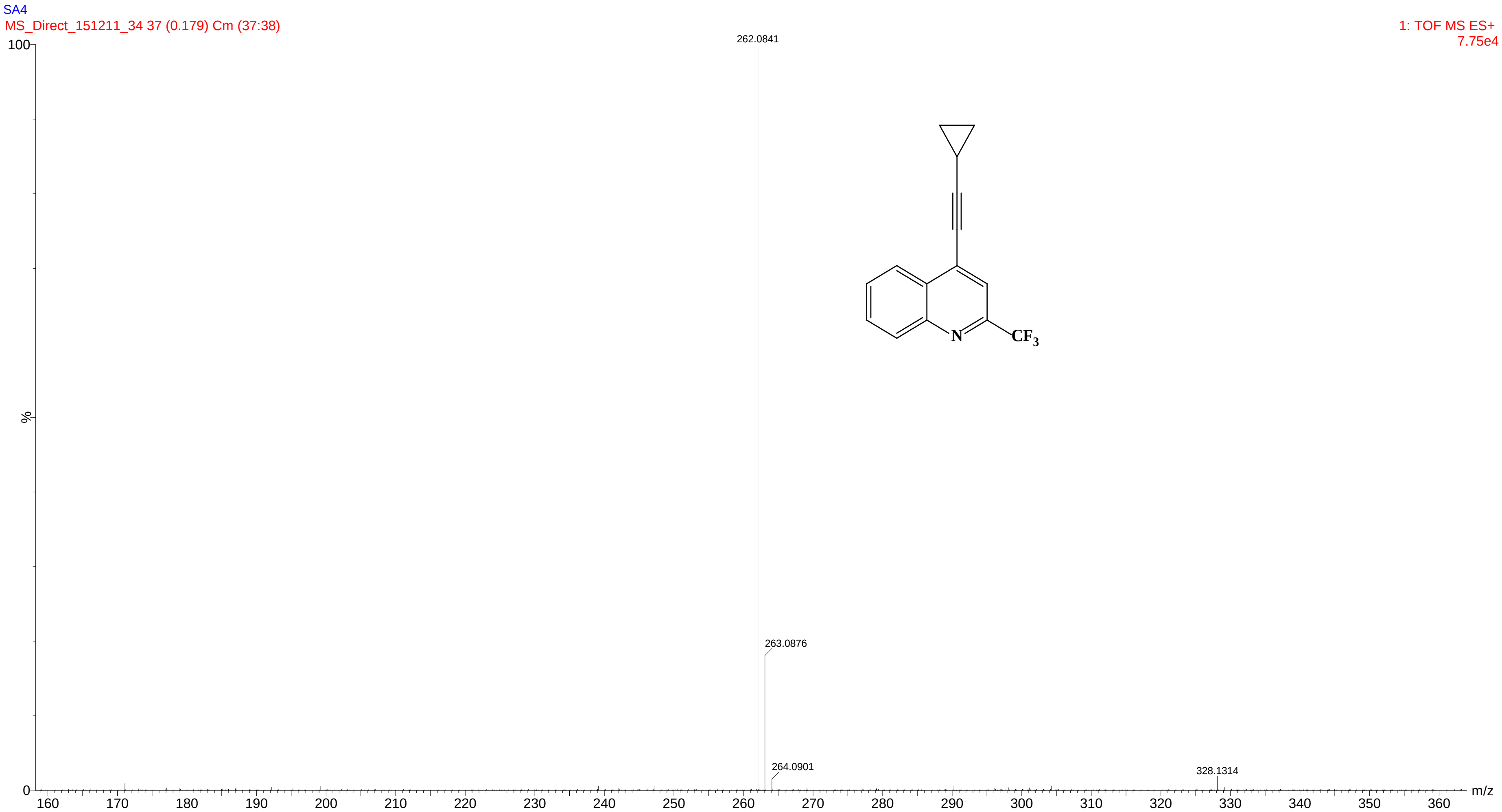
^{13}C NMR spectrum of **4S (CDCl$_3$, 100 MHz)**



^{19}F NMR spectrum of **4S (CDCl$_3$, 376 MHz)**



HRMS of **4S**


SA4
MS_Direct_151211_34 37 (0.179) Cm (37:38)
1: TOF MS ES+
7.75e4
262.0841
263.0876
264.0901
328.1314
100
%
0
m/z
160
170
180
190
200
210
220
230
240
250
260
270
280
290
300
310
320
330
340
350
360
N
CF_3