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Catalyst-free 1:2 annulation of quinolines with trifluoroacetylacetylenes: an access to functionalized oxazinoquinolines

Kseniya V. Belyaeva,[a] Lina P. Nikitina,[a] Andrei V. Afonin,[a] Alexander V. Vashchenko,[a] Vasiliy M. Muzalevskiy,[b] Valentin G. Nenajdenko *[b] and Boris A. Trofimov*[a]

[a]*A. E. Favorsky Irkutsk Institute of Chemistry, Siberian Branch, Russian Academy of Sciences, 1 Favorsky Str., 664033, Irkutsk, Russia*
[b]*Moscow State University, Department of Chemistry, Leninskie Gory, Moscow 119992, Russia*
E-mail: boris_trofimov@irioch.irk.ru
E-mail: nenajdenko@org.chem.msu.ru

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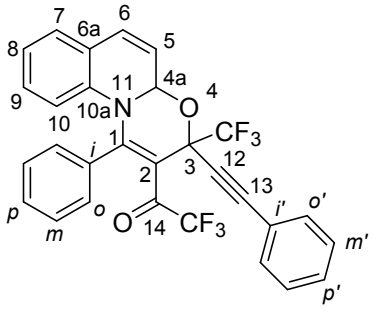
General methods. NMR spectra were recorded on a Bruker DPX-400 spectrometer (400.1 MHz for ^{1}H and 100.6 MHz for ^{13}C) and AV-400 spectrometers (40.5 MHz for ^{15}N and 379.5 MHz for ^{19}F) in $CDCl_3$. The internal standards were HMDS (for ^{1}H) or the residual solvent signals (for ^{13}C), CH_3NO_2 (for ^{15}N) and $CFCl_3$ (for ^{19}F). IR spectra were recorded on a two-beam Bruker Vertex 70 spectrometer. Elemental analysis was carried out on a FLASH EA 1112 Series analyzer. Mass spectra were recorded on Mass spectrometer Agilent 6210 HRMS-TOF-ESI. Electrostatic sputtering, registration of positive ions. Sample Solvent - MeCN with the addition of 0.1% heptafluorobutanoic acid and with the addition of calibration mixture for mass spectrometer. Melting points were determined on a Kofler hot stage apparatus. Commercial samples of quinolines **1a-g** and isoquinoline **4a** were used. Aryltrifluoroacetylacetylenes **2a-h**[1] and naphthyridines **4b**,**4c**[2] were obtained according to the literature procedures. Monitoring of the reaction course was carried out by IR spectroscopy following the disappearance of the absorption band of the C≡C bond in starting acetylene **2** at 2174-2202 cm^{-1}. The products **3a-o** and **5a-c** were purified by column chromatography. Column and thin-layer chromatography were carried out on silica gel (0.06-0.2 mm) with chloroform/benzene/ethanol (20:4:1, for **3a,d,f,g,i,l,m, 5a**) or hexane/dichloromethane (1:1 for **3b,c,e,h,j,k,n,o** and **5b,c**) mixtures as eluent.

General procedure and characterization data of compounds 3 and 5



2,2,2-Trifluoro-1-[1-phenyl-3-(phenylethynyl)-3-(trifluoromethyl)-3*H*,4a*H*-[1,3]oxazino[3,2-*a*]quinolin-2-yl]ethanone (3a). The mixture of acetylene **2a** (0.119 g, 0.6 mmol) and quinoline **1a** (0.039 g, 0.3 mmol) was stirred for 2 h at the room temperature in the argon atmosphere. The reaction mixture was passed through a column (eluent – chloroform/benzene/ethanol) to obtain 1,3-oxazinoquinoline **3a** (0.118 g, 91%) as light-yellow powder, mp 180-181 °C (ethanol). Initial acetylene **2a** was recovered (0.021 g, conversion was 82%). IR (microlayer): 2235 (C≡C), 1713 (C=O), 1654 (C=C), 1204, 1180, 1154, 1095 (C-F) cm^{-1}. (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 55:45 (^{1}H NMR).

(3*S**,4a*S**)-**3a**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.55-7.40 (m, 7H, $H_{o,o',m,p}$ from Ph), 7.33-7.28 (m, 4H, $H_{m,m'}$ from Ph), 7.21 (d, $^{3}J_{8,9}$ = 7.3 Hz, 1H, H-7), 6.95 (d, $^{3}J_{6,7}$ = 9.8 Hz, 1H, H-6), 6.92 (m, 1H, H-8), 6.82 (m, 1H, H-9), 6.33 (d, $^{3}J_{10,11}$ = 8.1 Hz, 1H, H-10), 6.16 (dd, $^{3}J_{5a,6}$ = 4.4 Hz, $^{3}J_{6,7}$ = 9.8 Hz, 1H, H-5), 5.71 (d, $^{3}J_{5a,6}$ = 4.4 Hz, 1H, H-4a) ppm.

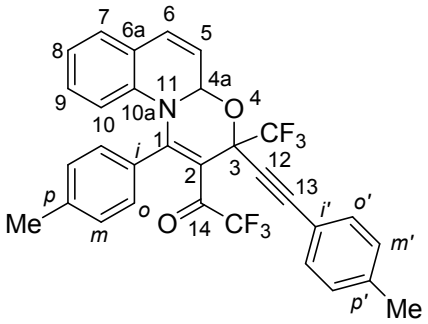
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 184.6 (q, $^{2}J_{CF}$ = 35.7 Hz, C-14), 158.2 (C-1), 135.1 (C-10a), 134.0 (C_i from Ph), 132.8 (C_p from Ph), 132.2 ($C_{o'}$ from Ph), 130.2 (C-2), 130.1 (C-6), 130.0 ($C_{o,m}$ from Ph), 129.7 ($C_{p'}$ from Ph), 129.0 (C-9), 128.5 (C-7), 128.4 ($C_{m'}$ from Ph), 122.7 (C-8), 122.2 (C-6a), 120.9 ($C_{i'}$ from Ph), 120.7 (q, $^{1}J_{CF}$ = 284.4 Hz, CF_3), 118.1 (C-10), 118.0 (C-5), 115.4 [C(O)$\underline{C}F_3$], 89.6 (C-13), 81.7 (C-12), 79.9 (q, $^{4}J_{CF}$ = 0.2 Hz, C-4a), 74.9 (q, $^{2}J_{CF}$ = 31.4 Hz, C-3) ppm.

^{15}N NMR (40.5 MHz, $CDCl_3$): δ -260.9 (N-11) ppm.

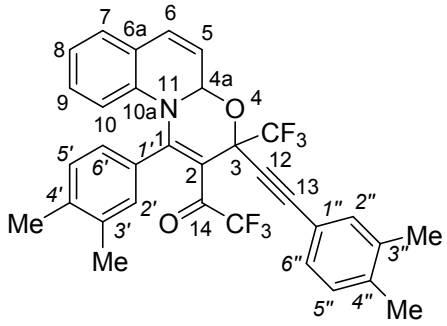
^{19}F NMR (376.5 MHz, $CDCl_3$): δ -72.4 [s, $C(O)CF_3$], -77.2 (s, CF_3) ppm.

(3*R**,4a*S**)-**3a** as an isomer in a mixture with the (3*S**,4a*S**)-**3a** isomer (ratio is 55:45): ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.55-7.40 (m, 7H, $H_{o,o',m,p}$ from Ph), 7.33-7.28 (m, 4H, $H_{m,m'}$ from Ph), 7.18 (d, $^{3}J_{8,9}$ = 7.3 Hz, 1H, H-7), 6.93 (d, $^{3}J_{6,7}$ = 9.8 Hz, 1H, H-6), 6.86 (m, 1H, H-8), 6.85 (m, 1H, H-9), 6.34 (d, $^{3}J_{10,11}$ = 8.3 Hz, 1H, H-10), 6.09 (dd, $^{3}J_{5a,6}$ = 4.6 Hz, $^{3}J_{6,7}$ = 9.8 Hz, 1H, H-5), 5.91 (d, $^{3}J_{5a,6}$ = 4.6 Hz, 1H, H-4a) ppm.

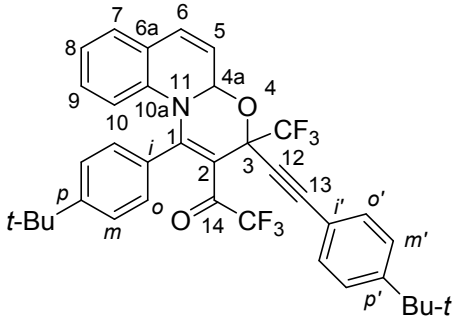
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 185.3 ($^2J_{CF}$ = 36.8 Hz, C-14), 152.6 (C-1), 135.4 (C-10a), 134.3 (C_i from Ph), 132.4 (C-2; $C_{o'}$ from Ph), 132.1 (C_p from Ph), 130.4 (C-6), 130.0 ($C_{o,m}$ from Ph), 129.4 ($C_{p'}$ from Ph), 129.0 (C-9), 128.6 (C-7), 128.5 ($C_{m'}$ from Ph), 122.4 (C-8), 122.3 (C-6a), 122.0 (q, $^1J_{CF}$ = 284.4 Hz, CF_3), 121.4 ($C_{i'}$ from Ph), 117.7 (C-10), 117.5 (C-5), 114.9 [q, $^1J_{CF}$ = 291.1 Hz, C(O)$\underline{C}F_3$], 89.2 (C-13), 81.7 (C-12), 80.6 (q, $^4J_{CF}$ = 2.4 Hz, C-4a), 73.4 (q, $^2J_{CF}$ = 31.4 Hz, C-3) ppm.
^{15}N NMR (40.5 MHz, $CDCl_3$): δ -269.0 (N-11) ppm.
^{19}F NMR (376.5 MHz, $CDCl_3$): δ -73.4 [q, $^6J_{F,F}$ = 2.2 Hz, C(O)CF_3], -75.5 (q, $^6J_{F,F}$ = 2.2 Hz, CF_3) ppm.
HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{29}H_{18}F_6NO_2^+$: 526.1236; found: 526.1215.
Found: C, 66.21; H, 3.25; F, 21.42; N, 2.58. Calc. for $C_{29}H_{17}F_6NO_2$ (525.45): C, 66.29; H, 3.26; F, 21.69; N, 2.67.



2,2,2-Trifluoro-1-[1-(4-methylphenyl)-3-[(4-methylphenyl)ethynyl]-3-(trifluoromethyl)-3*H*,4a*H*-[1,3]oxazino[3,2-*a*]quinolin-2-yl]ethanone (3b). Analogously, from quinoline **1a** (0.0325 g, 0.25 mmol) and acetylene **2b** (0.106 g, 0.5 mmol) in 0.2 ml MeCN (20-24 °C, 24 h) 1,3-oxazinoquinoline **3b** was obtained. Eluent was mixture of hexane/dichloromethane. First fraction, yellow crystals, 0.110 g, mp 85-87 °C (hexane), (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 40:60 (^{19}F NMR). Second fraction, yellow crystals, 0.017 g, mp 123-125 °C (hexane), (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 87:13. Total yield 0.127 g, 92%, (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 43:57 (^{19}F NMR).
(3*S**,4a*S**)-**3b**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.36 (m, 2H, H_o from Ph), 7.34 (m, 2H, $H_{o'}$ from Ph), 7.23 (d, 2H, H_m from Ph), 7.21 (d, $^3J_{7,8}$ = 7.4 Hz, 1H, H-7), 7.11 (m, 2H, $H_{m'}$ from Ph), 6.94 (d, $^3J_{5,6}$ = 9.8 Hz, 1H, H-6), 6.91 (m, 1H, H-8), 6.85 (m, 1H, H-9), 6.36 (d, $^3J_{9,10}$ = 8.1 Hz, 1H, H-10), 6.17 (dd, $^3J_{4a,5}$ = 4.7 Hz, $^3J_{5,6}$ = 9.9 Hz, 1H, H-5), 5.71 (d, $^3J_{4a,5}$ = 4.7 Hz, 1H, H-4a), 2.41 (s, 3H, Me), 2.34 (s, 3H, Me') ppm.
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 184.4 (q, $^2J_{CF}$ = 35.8 Hz, C-14), 158.3 (C-1), 143.6 (C_p from Ph), 139.8 ($C_{p'}$ from Ph), 135.0 (C-10a), 132.1 ($C_{o'}$ from Ph), 131.1 (C_i from Ph), 130.5 (C_m from Ph), 129.9 (C-6), 129.7 (C-2), 129.0 (C-9), 128.9 (C_o from Ph), 128.8 ($C_{m'}$ from Ph), 128.3 (C-7), 122.4 (C-8), 122.0 (C-6a), 121.9 (q, $^1J_{CF}$ = 286.4 Hz, CF_3), 117.9 (C-10), 117.8 (C-5), 117.7 ($C_{i'}$ from Ph), 115.3 [q, $^1J_{CF}$ = 293.4 Hz, C(O)$\underline{C}F_3$], 89.6 (C-13), 81.0 (C-12), 79.6 (C-4a), 74.8 (q, $^2J_{CF}$ = 34.7 Hz, C-3), 21.6 (Me), 21.5 (Me') ppm.
^{19}F NMR (376.3 MHz, $CDCl_3$): δ -73.7 [s, C(O)CF_3], -78.6 (s, CF_3) ppm.
(3*R**,4a*S**)-**3b**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.45 (m, 2H, H_o from Ph), 7.39 (m, 2H, $H_{o'}$ from Ph), 7.24 (m, 2H, H_m from Ph), 7.19 (d, $^3J_{7,8}$ = 7.1 Hz, 1H, H-7), 7.13 (m, 2H, $H_{m'}$ from Ph), 6.96 (d, $^3J_{5,6}$ = 9.8 Hz,1H, H-6), 6.89 (m, 1H, H-8), 6.85 (m, 1H, H-9), 6.39 (d, $^3J_{9,10}$ = 8.1 Hz, 1H, H-10), 6.11 (dd, $^3J_{4a,5}$ = 4.6 Hz, $^3J_{5,6}$ = 9.7 Hz, 1H, H-5), 5.93 (d, $^3J_{4a,5}$ = 4.6 Hz, 1H, H-4a), 2.42 (s, 3H, Me), 2.35 (s, 3H, Me') ppm.
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 185.2 (q, $^2J_{CF}$ = 36.9 Hz, C-14), 152.6 (C-1), 142.6 (C_p from Ph), 139.5 ($C_{p'}$ from Ph), 135.4 (C-10a), 132.0 ($C_{o'}$ from Ph), 131.4 (C_i from Ph), 130.5 (C_m from Ph), 130.2 (C-6), 130.0 (C-2), 129.0 (C-9), 128.9 (C_o from Ph), 128.8 ($C_{m'}$ from Ph), 128.4 (C-7), 123.1 (q, $^1J_{CF}$ = 289.3 Hz, CF_3), 122.1 (C-8), 122.0 (C-6a), 118.2 ($C_{i'}$ from Ph), 117.5 (C-10), 117.3 (C-5), 114.8 [q, $^1J_{CF}$ = 293.0 Hz, C(O)$\underline{C}F_3$], 86.2 (C-13), 80.4 (C-12), 80.2 (q, $^4J_{CF}$ = 2.2 Hz, C-4a), 73.2 (q, $^2J_{CF}$ = 31.7 Hz, C-3), 21.6 (Me), 21.5 (Me') ppm.
^{19}F NMR (376.3 MHz, $CDCl_3$): δ -74.7 [q, J = 2.0 Hz, 3F, C(O)CF_3], -76.9 (q, J = 2.0 Hz, 3F, CF_3) ppm.
HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{31}H_{22}F_6NO_2^+$: 554.1549; found: 554.1550.



1-[1-(3,4-Dimethylphenyl)-3-[(3,4-dimethylphenyl)ethynyl]-3-(trifluoromethyl)-3*H*,4a*H*-[1,3]oxazino[3,2-*a*]quinolin-2-yl]-2,2,2-trifluoroethanone (3c). Analogously, from quinoline **1a** (0.0325 g, 0.25 mmol) and acetylene **2c** (0.122 g, 0.5 mmol) in 0.2 ml MeCN (20-24 °C, 24 h) 1,3-oxazinoquinoline **3c** was obtained as yellow crystals, 0.130 g, 89%, mp 104-106 °C (hexane), (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 45:55 (^{19}F NMR). Eluent was mixture of hexane/dichloromethane.
(3*S**,4a*S**)-**3c**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.30-7.20 (m, 7H, H-7, H-2', H-5', H-6', H-2'', H-5'', H-6''), 6.94 (m, 1H, H-6), 6.91 (m, 1H, H-8), 6.86 (m, 1H, H-9), 6.44 (d, $^{3}J_{9,10}$ = 7.1 Hz, 1H, H-10), 6.19 (dd, $^{3}J_{4a,5}$ = 4.4 Hz, $^{3}J_{5,6}$ = 9.8 Hz, 1H, H-5), 5.74 (d, $^{3}J_{4a,5}$ = 4.4 Hz, 1H, H-4a), 2.32 (s, 3H, Me-4'), 2.26 (s, 3H, Me-3'), 2.25 (s, 3H, Me-3''), 2.23 (s, 3H, Me-4'') ppm.
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 185.2 (q, $^{2}J_{CF}$ = 35.8 Hz, C-14), 158.4 (C-1), 142.3 (C-4'), 138.5 (C-4''), 138.2 (C-3'), 136.7 (C-3''), 135.2 (C-10a), 133.1 (C-2'), 133.0 (C-2''), 131.5 (C-1'), 131.0 (C-5'), 130.8 (C-2), 129.9 (C-6), 129.6 (C-5''), 129.5 (C-6'), 129.4 (C-9), 128.8 (C-6''), 128.3 (C-7), 122.2 (C-8), 122.1 (C-6a), 121.9 (q, $^{1}J_{CF}$ = 286.0 Hz, CF_3), 118.0 (C-1''), 117.9 (C-10), 117.8 (C-5), 115.3 [q, $^{1}J_{CF}$ = 293.0 Hz, C(O)$\underline{C}F_3$], 89.7 (C-13), 80.8 (C-12), 79.6 (C-4a), 74.8 (q, $^{2}J_{CF}$ = 34.3 Hz, C-3), 19.9 (Me-4'), 19.7 (Me-3', Me-3''), 19.4 (Me-4'') ppm.
^{19}F NMR (376.3 MHz, $CDCl_3$): δ -73.6 [s, C(O)CF_3], -78.6 (s, CF_3) ppm.
(3*R**,4a*S**)-**3c**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.34 (m, 1H, H-2'), 7.30-7.20 (m, 6H, H-7, H-5', H-6', H-2'', H-5'', H-6''), 6.94 (m, 1H, H-6), 6.91 (m, 1H, H-8), 6.86 (m, 1H, H-9), 6.46 (d, $^{3}J_{9,10}$ = 7.4 Hz, 1H, H-10), 6.12 (dd, $^{3}J_{4a,5}$ = 4.6 Hz, $^{3}J_{5,6}$ = 9.8 Hz, 1H, H-5), 5.93 (d, $^{3}J_{4a,5}$ = 4.6 Hz, 1H, H-4a), 2.31 (s, 3H, Me-4'), 2.26 (s, 3H, Me-3'), 2.25 (s, 3H, Me-3''), 2.23 (s, 3H, Me-4'') ppm.
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 185.2 (q, $^{2}J_{CF}$ = 36.9 Hz, C-14), 152.7 (C-1), 141.3 (C-4'), 138.5 (C-4''), 138.2 (C-3'), 136.6 (C-3''), 135.9 (C-10a), 133.1 (C-2'), 133.0 (C-2''), 131.8 (C-1'), 131.0 (C-5'), 130.9 (C-2), 130.2 (C-6), 129.6 (C-5''), 129.5 (C-6'), 129.4 (C-9), 128.8 (C-6''), 128.3 (C-7), 123.1 (q, $^{1}J_{CF}$ = 289.3 Hz, CF_3), 122.1 (C-6a), 122.0 (C-8), 118.5 (C-1''), 117.6 (C-10), 117.3 (C-5), 114.8 [q, $^{1}J_{CF}$ = 293.4 Hz, C(O)$\underline{C}F_3$], 86.3 (C-13), 80.3 (C-12), 80.1 (q, $^{4}J_{CF}$ = 2.6 Hz, C-4a), 73.2 (q, $^{2}J_{CF}$ = 31.0 Hz, C-3), 19.9 (Me-4'), 19.7 (Me-3', Me-3''), 19.4 (Me-4'') ppm.
^{19}F NMR (376.3 MHz, $CDCl_3$): δ -74.6 [q, $^{6}J_{F,F}$ = 2.2 Hz, C(O)CF_3], -76.9 (q, $^{6}J_{F,F}$ = 2.2 Hz, CF_3) ppm.
HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{33}H_{26}F_6NO_2^+$: 582.1862; found: 582.1867.



1-[1-(4-*tert*-Butylphenyl)-3-[(4-*tert*-butylphenyl)ethynyl]-3-(trifluoromethyl)-3*H*,4a*H*-[1,3]oxazino[3,2-*a*]quinolin-2-yl]-2,2,2-trifluoroethanone (3d). Analogously, from quinoline **1a** (0.013 g, 0.1 mmol) and acetylene **2d** (0.051 g, 0.2 mmol) in 0.1 ml MeCN (20-24 °C, 24 h) 1,3-

oxazinoquinoline **3d** (0.048 g, 75%) was obtained as a yellow oil. Eluent was mixture of chloroform/benzene/ethanol. Initial acetylene **2d** was recovered (0.007 g, conversion was 86%). IR (microlayer): 2235 (C≡C), 1711 (C=O), 1655, 1607 (C=C), 1205, 1156, 1090 (C-F) cm^{-1}. (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 50:50 (^{1}H NMR).

(3*S**,4a*S**)-**3d**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.45-7.35 (m, 6H, $H_{o,o',m}$ from Ph), 7.30 (m, 2H, $H_{m'}$ from Ph), 7.18 (d, $^3J_{8,9}$ = 7.3 Hz, 1H, H-7), 6.92 (d, $^3J_{6,7}$ = 9.9 Hz, 1H, H-6), 6.89 (m, 1H, H-8), 6.81 (m, 1H, H-9), 6.33 (d, $^3J_{10,11}$ = 8.1 Hz, 1H, H-10), 6.14 (dd, $^3J_{5a,6}$ = 4.4 Hz, $^3J_{6,7}$ = 9.9 Hz, 1H, H-5), 5.70 (d, $^3J_{5a,6}$ = 4.4 Hz, 1H, H-4a), 1.29 (s, 9H, 3Me from *t*-Bu), 1.26 (s, 9H, 3Me' from *t*-Bu') ppm.

^{13}C NMR (100.6 MHz, $CDCl_3$): δ 185.0 (q, $^2J_{CF}$ = 35.4 Hz, C-14), 158.1 (C-1), 156.8 (C_p from Ph), 153.0 ($C_{p'}$ from Ph), 135.3 (C-10a), 132.0 ($C_{o'}$ from Ph), 131.2 (C_i from Ph), 130.4 (C-2), 130.1 (C-6), 129.0 (C-9), 128.5 (C_o from Ph; C-7), 126.9 (C_m from Ph), 125.4 ($C_{m'}$ from Ph), 122.5 (C-8), 122.2 (C-6a), 122.1 (q, $^1J_{CF}$ = 284.4 Hz, CF_3), 118.1 (C-5; C-10), 118.0 ($C_{i'}$ from Ph), 115.0 [q, $^1J_{CF}$ = 291.1 Hz, C(O)$\underline{C}F_3$], 89.7 (C-13), 80.7 (C-12), 80.4 (C-4a), 75.0 (q, $^2J_{CF}$ = 31.5 Hz, C-3), 35.3 (C from *t*-Bu), 35.0 (C' from *t*-Bu), 31.3 (3Me from *t*-Bu), 31.2 (3Me' from *t*-Bu') ppm.

^{19}F NMR (376.5 MHz, $CDCl_3$): δ -73.5 [s, C(O)CF_3], -75.5 (s, CF_3) ppm.

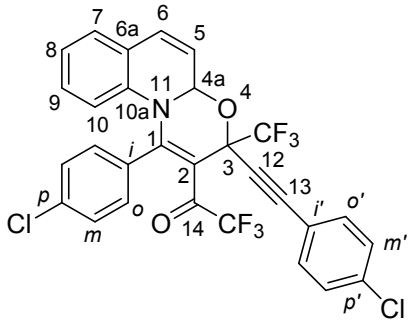
(3*R**,4a*S**)-**3d**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.45-7.35 (m, 6H, $H_{o,o',m}$ from Ph), 7.30 (m, 2H, $H_{m'}$ from Ph), 7.16 (d, $^3J_{8,9}$ = 7.3 Hz, 1H, H-7), 6.90 (d, $^3J_{6,7}$ = 9.7 Hz, 1H, H-6), 6.87 (m, 1H, H-8), 6.85 (m, 1H, H-9), 6.34 (d, $^3J_{10,11}$ = 8.0 Hz, 1H, H-10), 6.10 (dd, $^3J_{5a,6}$ = 4.6 Hz, $^3J_{6,7}$ = 9.7 Hz, 1H, H-5), 5.89 (d, $^3J_{5a,6}$ = 4.6 Hz, 1H, H-4a), 1.27 (s, 9H, 3Me from *t*-Bu), 1.26 (s, 9H, 3Me' from *t*-Bu') ppm.

^{13}C NMR (100.6 MHz, $CDCl_3$): δ 185.3 (q, $^2J_{CF}$ = 35.4 Hz, C-14), 155.9 (C_p from Ph), 152.8 ($C_{p'}$ from Ph), 152.6 (C-1), 135.7 (C-10a), 132.1 ($C_{o'}$ from Ph), 131.5 (C_i from Ph), 130.4 (C-2), 130.1 (C-6), 129.0 (C-9), 128.5 (C_o from Ph; C-7), 126.9 (C_m from Ph), 125.5 ($C_{m'}$ from Ph), 123.3 (q, $^1J_{CF}$ = 284.4 Hz, CF_3), 122.3 (C-6a), 122.2 (C-8), 118.5 ($C_{i'}$ from Ph), 117.7 (C-10), 117.6 (C-5), 114.6 [q, $^1J_{CF}$ = 291.1 Hz, C(O)CF_3], 86.4 (C-13), 81.4 (C-12), 79.8 (q, $^4J_{CF}$ = 2.6 Hz, C-4a), 73.4 (q, $^2J_{CF}$ = 31.4 Hz, C-3), 35.2 (C from *t*-Bu), 35.0 (C' from *t*-Bu), 31.3 (3Me from *t*-Bu), 31.2 (3Me' from *t*-Bu') ppm.

^{19}F NMR (376.5 MHz, $CDCl_3$): δ -72.4 [q, $^6J_{F,F}$ = 2.2 Hz, C(O)CF_3], -77.2 (q, $^6J_{F,F}$ = 2.2 Hz, CF_3) ppm.

HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{37}H_{34}F_6NO_2^+$: 638.2488; found: 638.2462.

Found: C, 69.40; H, 5.15; N, 2.08; F, 17.69. Calc. for $C_{37}H_{33}F_6NO_2$ (637.67): C, 69.69; H, 5.22; N, 2.20; F, 17.88.

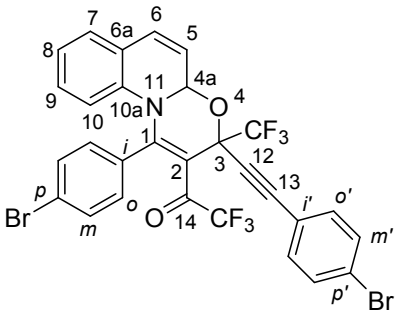


1-[1-(4-Chlorophenyl)-3-[(4-chlorophenyl)ethynyl]-3-(trifluoromethyl)-3*H*,4a*H*-[1,3]oxazino[3,2-*a*]quinolin-2-yl]-2,2,2-trifluoroethanone (3e). Analogously, from quinoline **1a** (0.0325 g, 0.25 mmol) and acetylene **2e** (0.117 g, 0.5 mmol) in 0.2 ml MeCN (20-24 °C, 24 h) 1,3-oxazinoquinoline **3e** was obtained. Eluent was mixture of hexane/dichloromethane. First fraction, yellow crystals, 0.124 g, mp 197-199 °C (hexane), (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 50:50 (^{19}F NMR). Second fraction, yellow crystals, 0.012 g, mp 190-191 °C (hexane), (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 100:0. Total yield 0.134 g, 90%, (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 55:45 (^{19}F NMR).

(3*S**,4a*S**)-**3e**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.42 (m, 4H, $H_{o,o'}$ from Ph), 7.37 (m, 2H, H_m from Ph), 7.29 (m, 2H, $H_{m'}$ from Ph), 7.23 (d, $^3J_{7,8}$ = 7.3 Hz, 1H, H-7), 6.97 (d, 1H, H-6), 6.92(m, 1H, H-8), 6.90 (m, 1H, H-9), 6.31 (d, $^3J_{9,10}$ = 8.0 Hz, 1H, H-10), 6.17 (dd, $^3J_{4a,5}$ = 4.4 Hz, $^3J_{5,6}$ = 9.8 Hz, 1H, H-5), 5.67 (d, $^3J_{4a,5}$ = 4.4 Hz, 1H, H-4a) ppm.

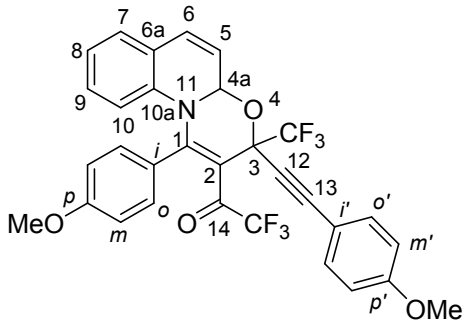
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 184.2 (q, $^2J_{CF}$ = 36.1 Hz, C-14), 156.9 (C-1), 139.2 (C_p from Ph), 135.5 (C-10a), 135.0 ($C_{p'}$ from Ph), 133.3 ($C_{o'}$ from Ph), 132.2 (C_i from Ph), 131.0 (C-2), 130.3 ($C_{o,m}$ from Ph),

130.1 (C-6), 129.1 (C-9), 128.6 ($C_{m'}$ from Ph), 128.5 (C-7), 122.9 (C-8), 122.1 (C-6a), 121.7 (q, $^1J_{CF}$ = 286.0 Hz, CF_3), 119.1 ($C_{i'}$ from Ph), 117.8 (C-10), 117.7 (C-5), 115.2 [q, $^1J_{CF}$ = 293.8 Hz, C(O)$\underline{C}F_3$], 88.4 (C-13), 81.8 (C-12), 79.8 (C-4a), 74.6 (q, $^2J_{CF}$ = 35.0 Hz, C-3) ppm.
^{19}F NMR (376.3 MHz, $CDCl_3$): δ -73.7 [s, C(O)CF_3], -78.6 (s, CF_3) ppm.
(3*R**,4a*S**)-**3e**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.45 (m, 2H, H_m from Ph), 7.43 (m, 4H, $H_{o,o'}$ from Ph), 7.30 (m, 2H, $H_{m'}$ from Ph), 7.21 (d, $^3J_{7,8}$ = 7.3 Hz, 1H, H-7), 6.97 (d, 1H, H-6), 6.92(m, 1H, H-8), 6.90 (m, 1H, H-9), 6.35 (d, $^3J_{9,10}$ = 7.2 Hz, 1H, H-10), 6.11 (dd, $^3J_{4a,5}$ = 4.5 Hz, $^3J_{5,6}$ = 9.7 Hz, 1H, H-5), 5.91 (d, $^3J_{4a,5}$ = 4.5 Hz, 1H, H-4a) ppm.
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 185.1 (q, $^2J_{CF}$ = 37.2 Hz, C-14), 151.1 (C-1), 138.4 (C_p from Ph), 135.8 (C-10a), 134.5 ($C_{p'}$ from Ph), 133.4 ($C_{o'}$ from Ph), 132.5 (C_i from Ph), 131.2 (C-6), 131.1 (C-2), 130.3 ($C_{o,m}$ from Ph), 129.0 (C-9), 128.7 ($C_{m'}$ from Ph), 128.6 (C-7), 123.0 (q, $^1J_{CF}$ = 289.3 Hz, CF_3), 122.5 (C-8), 122.2 (C-6a), 119.6 ($C_{i'}$ from Ph), 117.4 (C-10), 117.2 (C-5), 114.7 [q, $^1J_{CF}$ = 293.0 Hz, C(O)$\underline{C}F_3$], 85.1 (C-13), 82.1 (C-12), 80.3 (q, $^4J_{CF}$ = 2.6 Hz, C-4a), 73.1 (q, $^2J_{CF}$ = 31.7 Hz, C-3) ppm.
^{19}F NMR (376.3 MHz, $CDCl_3$): δ -74.7 [q, $^6J_{F,F}$ = 2.2 Hz, C(O)CF_3], -76.9 (q, $^6J_{F,F}$ = 2.2 Hz, CF_3) ppm.
HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{29}H_{16}Cl_2F_6NO_2^+$: 594.0457; found: 594.0461.



1-[1-(4-Bromophenyl)-3-[(4-bromophenyl)ethynyl]-3-(trifluoromethyl)-3*H*,4a*H*-[1,3]oxazino[3,2-*a*]quinolin-2-yl]-2,2,2-trifluoroethanone (3f). Analogously, from quinoline **1a** (0.039 g, 0.3 mmol) and acetylene **2f** (0.166 g, 0.6 mmol) in 0.3 ml MeCN (20-24 °C, 4 h) 1,3-oxazinoquinoline **3f** (0.114 g, 56%) was obtained as a yellow oil. Eluent was mixture of chloroform/benzene/ethanol. IR (microlayer): 2237 (C≡C), 1712 (C=O), 1655 (C=C), 1204, 1158, 1098 (C-F) cm^{-1}. (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 60:40 (^{1}H NMR).
(3*S**,4a*S**)-**3f**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.55 (m, 2H, H_m from Ph), 7.42 (m, 2H, $H_{m'}$ from Ph), 7.35-7.27 (m, 4H, $H_{o,o'}$ from Ph), 7.20 (m, 1H, H-7), 6.90 (m, 3H, H-6, H-8, H-9), 6.30 (m, 1H, H-10), 6.14 (dd, $^3J_{5a,6}$ = 4.4 Hz, $^3J_{6,7}$ = 9.6 Hz, 1H, H-5), 5.66 (d, $^3J_{5a,6}$ = 4.4 Hz, 1H, H-4a) ppm.
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 184.0 (q, $^2J_{CF}$ = 35.5 Hz, C-14), 157.0 (C-1), 135.1 (C-10a), 133.8 ($C_{o'}$ from Ph), 133.4 (C_m from Ph), 132.8 (C_i from Ph), 131.8 ($C_{o,m'}$ from Ph), 130.2 (C-6), 129.3 (C-9), 128.7 (C-7), 128.5 (C-2), 127.9 (C_p from Ph), 124.3 ($C_{p'}$ from Ph), 123.2 (C-8), 122.3 (C-6a), 121.8 (q, $^1J_{CF}$ = 284.6 Hz, CF_3), 119.7 ($C_{i'}$ from Ph), 118.0 (C-10), 117.8 (C-5), 115.5 [q, $^1J_{CF}$ = 291.3 Hz, C(O)$\underline{C}F_3$], 88.7 (C-13), 82.0 (C-12), 80.0 (C-4a), 75.0 (q, $^2J_{CF}$ = 31.0 Hz, C-3) ppm.
^{19}F NMR (376.5 MHz, $CDCl_3$): δ -72.2 [s, C(O)CF_3], -77.1 (s, CF_3) ppm.
(3*R**,4a*S**)-**3f**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.55 (m, 2H, H_m from Ph), 7.42 (m, 2H, $H_{m'}$ from Ph), 7.35-7.27 (m, 4H, $H_{o,o'}$ from Ph), 7.20 (m, 1H, H-7), 6.90 (m, 3H, H-6, H-8, H-9), 6.30 (m, 1H, H-10), 6.07 (dd, $^3J_{5a,6}$ = 4.4 Hz, $^3J_{6,7}$ = 9.6 Hz, 1H, H-5), 5.86 (d, $^3J_{5a,6}$ = 4.4 Hz, 1H, H-4a) ppm.
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 185.2 (q, $^2J_{CF}$ = 36.4 Hz, C-14), 151.3 (C-1), 135.2 (C-10a), 133.6 ($C_{o'}$ from Ph), 133.4 (C_m from Ph), 133.1 (C_i from Ph), 131.7 ($C_{m'}$ from Ph), 131.4 (C_o from Ph), 130.4 (C-6), 129.3 (C-9), 128.8 (C-7), 128.5 (C-2), 127.0 (C_p from Ph), 124.0 ($C_{p'}$ from Ph), 122.7 (C-8), 122.3 (C-6a), 122.2 (q, $^1J_{CF}$ = 284.2 Hz, CF_3), 120.2 ($C_{i'}$ from Ph), 117.4 (C-10), 117.0 (C-5), 115.0 [q, $^1J_{CF}$ = 290.8 Hz, C(O)$\underline{C}F_3$], 85.3 (C-13), 82.6 (C-12), 80.5 (q, $^4J_{CF}$ = 2.0 Hz, C-4a), 73.5 (q, $^2J_{CF}$ = 31.5 Hz, C-3) ppm.
^{19}F NMR (376.5 MHz, $CDCl_3$): δ -73.2 [q, $^6J_{F,F}$ = 2.2 Hz, C(O)CF_3], -75.4 (q, $^6J_{F,F}$ = 2.2 Hz, CF_3) ppm.
HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{29}H_{16}Br_2F_6NO_2^+$: 681.9446; found: 681.9415.

Found: C, 50.69; H, 2.14; N, 1.98; Br, 23.48; F, 16.94. Calc. for $C_{29}H_{15}Br_2F_6NO_2$ (683.24): C, 50.98; H, 2.21; N, 2.05; Br, 23.39; F, 16.68.



2,2,2-Trifluoro-1-[1-(4-methoxyphenyl)-3-[(4-methoxyphenyl)ethynyl]-3-(trifluoromethyl)-3*H*,4a*H*-[1,3]oxazino[3,2-*a*]quinolin-2-yl]ethanone (3g). Analogously, from quinoline **1a** (0.039 g, 0.3 mmol) and acetylene **2g** (0.137 g, 0.6 mmol) in 0.3 ml MeCN (20-24 °C, 3 h) 1,3-oxazinoquinoline **3g** (0.123 g, 74%) was obtained as a bright-yellow oil. Eluent was mixture of chloroform/benzene/ethanol. Initial acetylene **2g** was recovered (0.008 g, conversion was 94%). IR (microlayer): 2232 (C≡C), 1705 (C=O), 1655, 1604 (C=C), 1202, 1177, 1158, 1095 (C-F) cm^{-1}. (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 50:50 (^{1}H NMR).

(3*S**,4a*S**)-**3g**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.45-7.35 (m, 4H, $H_{o,o'}$ from Ph), 7.19 (d, $^3J_{8,9}$ = 7.0 Hz, 1H, H-7), 6.95-6.80 (m, 7H, H-6, H-8, H-9, $H_{m,m'}$ from Ph), 6.37 (d, $^3J_{10,11}$ = 8.0 Hz, 1H, H-10), 6.14 (dd, $^3J_{5a,6}$ = 4.4 Hz, $^3J_{6,7}$ = 9.6 Hz, 1H, H-5), 5.69 (d, $^3J_{5a,6}$ = 4.4 Hz, 1H, H-4a), 3.82 (s, 3H, OMe), 3.76 (s, 3H, OMe') ppm.

^{13}C NMR (100.6 MHz, $CDCl_3$): δ 184.5 (q, $^2J_{CF}$ = 35.5 Hz, C-14), 163.4 (C_p from Ph), 160.6 ($C_{p'}$ from Ph), 158.3 (C-1), 135.3 (C-10a), 133.8 ($C_{o'}$ from Ph), 132.1 (C_o from Ph), 130.1 (C-6), 129.0 (C-9), 128.5 (C-2; C-7), 126.4 (C_i from Ph), 122.6 (C-8), 122.2 (C-6a), 120.7 (q, $^1J_{CF}$ = 284.7 Hz, CF_3), 118.1 (C-10), 118.0 (C-5), 115.4 (C_m from Ph), 115.1 [q, $^1J_{CF}$ = 291.0 Hz, C(O)$\underline{C}F_3$], 114.0 ($C_{m'}$ from Ph), 113.1 ($C_{i'}$ from Ph), 89.6 (C-13), 80.7 (C-12), 79.7 (C-4a), 74.8 (q, $^2J_{CF}$ = 31.2 Hz, C-3), 55.6 (OMe), 55.4 (OMe') ppm.

^{19}F NMR (376.5 MHz, $CDCl_3$): δ -72.2 [s, C(O)CF_3], -77.4 (s, CF_3) ppm.

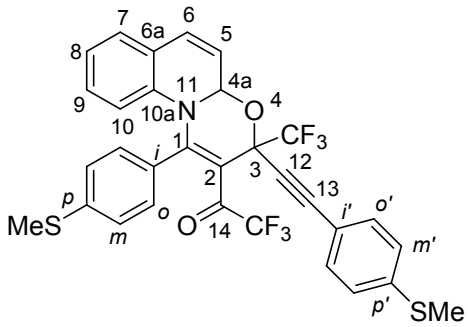
(3*R**,4a*S**)-**3g**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.45-7.35 (m, 4H, $H_{o,o'}$ from Ph), 7.15 (d, $^3J_{8,9}$ = 6.8 Hz, 1H, H-7), 6.95-6.80 (m, 7H, H-6, H-8, H-9, $H_{m,m'}$ from Ph), 6.37 (d, $^3J_{10,11}$ = 8.0 Hz, 1H, H-10), 6.06 (dd, $^3J_{5a,6}$ = 4.4 Hz, $^3J_{6,7}$ = 9.4 Hz, 1H, H-5), 5.88 (d, $^3J_{5a,6}$ = 4.4 Hz, 1H, H-4a), 3.82 (s, 3H, OMe), 3.76 (s, 3H, OMe') ppm.

^{13}C NMR (100.6 MHz, $CDCl_3$): δ 185.4 (q, $^2J_{CF}$ = 36.2 Hz, C-14), 162.7 (C_p from Ph), 160.5 ($C_{p'}$ from Ph), 152.5 (C-1), 135.7 (C-10a), 133.9 ($C_{o'}$ from Ph), 132.1 (C_o from Ph), 130.3 (C-6), 129.0 (C-9), 128.6 (C-7), 128.5 (C-2), 126.7 (C_i from Ph), 122.3 (C-6a; C-8), 122.1 (q, $^1J_{CF}$ = 284.7 Hz, CF_3), 117.7 (C-10), 117.6 (C-5), 115.4 (C_m from Ph), 114.9 [q, $^1J_{CF}$ = 290.8 Hz, C(O)$\underline{C}F_3$], 114.1 ($C_{m'}$ from Ph), 113.6 ($C_{i'}$ from Ph), 86.2 (C-13), 80.3 (q, $^4J_{CF}$ = 2.6 Hz, C-4a), 80.1 (C-12), 73.3 (q, $^2J_{CF}$ = 31.1 Hz, C-3), 55.6 (OMe'), 55.4 (OMe) ppm.

^{19}F NMR (376.5 MHz, $CDCl_3$): δ -73.4 [q, $^6J_{F,F}$ = 2.2 Hz, C(O)CF_3], -75.5 (q, $^6J_{F,F}$ = 2.2 Hz, CF_3) ppm.

HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{31}H_{22}F_6NO_4^+$: 586.1448; found: 586.1423.

Found: C, 63.30; H, 3.48; N, 2.68; F, 19.13. Calc. for $C_{31}H_{21}F_6NO_4$ (585.50): C, 63.59; H, 3.62; N, 2.39; F, 19.47.



2,2,2-Trifluoro-1-[1-[4-(methylthio)phenyl]-3-{[4-(methylthio)phenyl]ethynyl}-3-(trifluoromethyl)-3*H*,4a*H*-[1,3]oxazino[3,2-*a*]quinolin-2-yl]ethanone (3h). Analogously, from quinoline **1a** (0.0325 g, 0.25 mmol) and acetylene **2h** (0.122 g, 0.5 mmol) in 0.2 ml MeCN (20-24 °C, 24 h) 1,3-oxazinoquinoline **3h** was obtained. Eluent was mixture of hexane/dichloromethane. First fraction, yellow-brown crystals, 0.012 g, mp 88-90 °C (hexane), (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 13:87 (^{19}F NMR). Second fraction, yellow-brown crystals, 0.118 g, mp 131-133 °C (hexane), (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 50:50. Total yield 0.130 g, 84%, (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 45:55 (^{19}F NMR).

(3*S**,4a*S**)-**3h**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.44 (m, 2H, H_o from Ph), 7.38 (m, 2H, $H_{o'}$ from Ph), 7.25 (m, 2H, H_m from Ph), 7.21 (m, 1H, H-7), 7.16 (m, 2H, $H_{m'}$ from Ph), 6.96 (m, 1H, H-6), 6.93 (m, 1H, H-8), 6.89 (m, 1H, H-9), 6.42 (d, $^3J_{9,10}$ = 8.2 Hz, 1H, H-10), 6.19 (dd, $^3J_{4a,5}$ = 4.6 Hz, $^3J_{5,6}$ = 10.2 Hz, 1H, H-5), 5.73 (d, $^3J_{4a,5}$ = 4.6 Hz, 1H, H-4a), 2.51 (s, 3H, SMe), 2.46 (s, 3H, SMe') ppm.

^{13}C NMR (100.6 MHz, $CDCl_3$): δ 184.2 (q, $^2J_{CF}$ = 36.5 Hz, C-14), 157.9 (C-1), 145.9 (C_p from Ph), 141.1 ($C_{p'}$ from Ph), 134.9 (C-10a), 132.4 ($C_{o'}$ from Ph), 132.3 (C_m from Ph), 130.2 ($C_{m'}$ from Ph), 130.1 ($C_i$from Ph), 130.0 (C-2), 129.9 (C-6), 128.9 (C-9, C_o from Ph), 128.4 (C-7), 126.1 (C-8), 122.6 (C-6a), 121.8 (q, $^1J_{CF}$ = 286.8 Hz, CF_3), 117.8 (C-5, C-10), 116.7 ($C_{i'}$ from Ph), 114.8 [q, $^1J_{CF}$ = 293.4 Hz, C(O)$\underline{C}F_3$], 89.2 (C-13), 81.6 (C-12), 79.7 (C-4a), 74.8 (q, $^2J_{CF}$ = 34.6 Hz, C-3), 15.0 (SMe), 14.6 (SMe') ppm.

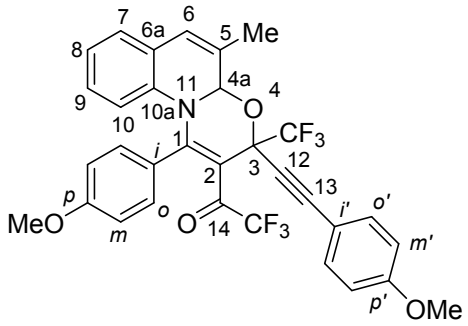
^{19}F NMR (376.3 MHz, $CDCl_3$): δ -73.6 [s, C(O)CF_3], -78.7 (s, CF_3) ppm.

(3*R**,4a*S**)-**3h**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.44 (m, 2H, H_o from Ph), 7.40 (m, 2H, $H_{o'}$ from Ph), 7.25 (m, 2H, H_m from Ph), 7.23 (m, 1H, H-7), 7.18 (m, 2H, $H_{m'}$ from Ph), 6.96 (m, 1H, H-6), 6.93 (m, 1H, H-8), 6.89 (m, 1H, H-9), 6.42 (d, $^3J_{9,10}$ = 8.4 Hz, 1H, H-10), 6.11 (dd, $^3J_{4a,5}$ = 4.7 Hz, $^3J_{5,6}$ = 10.1 Hz, 1H, H-5), 5.92 (d, $^3J_{4a,5}$ = 4.7 Hz, 1H, H-4a), 2.20 (s, 3H, SMe), 2.46 (s, 3H, SMe') ppm.

^{13}C NMR (100.6 MHz, $CDCl_3$): δ 185.1 (q, $^2J_{CF}$ = 37.6 Hz, C-14), 152.0 (C-1), 144.7 (C_p from Ph), 140.8 ($C_{i',p'}$ from Ph), 135.3 (C-10a), 132.4 ($C_{m,o'}$ from Ph), 130.2 ($C_{m'}$ from Ph), 129.9 (C-2, C-6), 129.7 (C_i from Ph), 128.9 (C-9, C_o from Ph), 128.5 (C-7), 125.4 (C-8), 123.0 (q, $^1J_{CF}$ = 289.3 Hz, CF_3), 122.2 (C-6a), 117.3 (C-5, C-10), 114.4 [q, $^1J_{CF}$ = 293.0 Hz, C(O)$\underline{C}F_3$], 85.8 (C-13), 81.0 (C-12), 80.2 (q, $^4J_{CF}$ = 2.6 Hz, C-4a), 74.8 (q, $^2J_{CF}$ = 31.3 Hz, C-3), 15.0 (SMe), 14.6 (SMe') ppm.

^{19}F NMR (376.3 MHz, $CDCl_3$): δ -74.7 [q, $^6J_{F,F}$ = 2.2 Hz, C(O)CF_3], -76.9 (q, $^6J_{F,F}$ = 2.2 Hz, CF_3) ppm.

HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{31}H_{22}F_6NO_2S_2^+$: 618.0991; found: 618.0990.



2,2,2-Trifluoro-1-[1-(4-methoxyphenyl)-3-[(4-methoxyphenyl)ethynyl]-5-methyl-3-(trifluoromethyl)-3*H*,4a*H*-[1,3]oxazino[3,2-*a*]quinolin-2-yl]ethanone (3i). Analogously, from quinoline **1b** (0.021 g, 0.15 mmol) and acetylene **2g** (0.068 g, 0.3 mmol) (20-24 °C, 6 h) 1,3-

oxazinoquinoline **3i** (0.072 g, 80%) was obtained as a yellow oil. Eluent was mixture of chloroform/benzene/ethanol. Initial acetylene **2g** was recovered (0.009 g, conversion was 87%). IR (microlayer): 2231 (C≡C), br 1694 (C=O), 1604 (C=C), 1177, 1074 (C-F) cm^{-1}. (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 75:25 (^{1}H NMR).

(3*S**,4a*S**)-**3i**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.39 (m, 4H, $H_{o,o'}$ from Ph), 7.12 (d, $^3J_{8,9}$ = 7.0 Hz, 1H, H-7), 6.95-6.75 (m, 6H, H-8, H-9, $H_{m,m'}$ from Ph), 6.63 (s, 1H, H-6), 6.32 (d, $^3J_{10,11}$ = 8.0 Hz, 1H, H-10), 5.46 (s, 1H, H-4a), 3.84 (s, 3H, OMe), 3.79 (s, 3H, OMe'), 2.17 (s, 3H, Me) ppm.

^{13}C NMR (100.6 MHz, $CDCl_3$): δ 184.4 (q, $^2J_{CF}$ = 35.3 Hz, C-14), 163.4 (C_p from Ph), 160.6 ($C_{p'}$ from Ph), 158.2 (C-1), 134.1 (C-10a), 133.8 ($C_{o'}$ from Ph), 132.2 (C_o from Ph), 128.5 (C-2; C-9), 127.8 (C-7), 127.6 (C-5), 127.5 (C_i from Ph), 125.7 (C-6), 123.2 (C-8), 122.7 (C-6a), 120.4 (q, $^1J_{CF}$ = 284.4 Hz, CF_3), 117.8 (C-10), 115.4 (C_m from Ph), 114.9 [q, $^1J_{CF}$ = 290.7 Hz, C(O)$\underline{C}F_3$], 114.1 ($C_{m'}$ from Ph), 113.3 ($C_{i'}$ from Ph), 89.3 (C-13), 83.5 (C-4a), 80.2 (C-12), 74.7 (q, $^2J_{CF}$ = 31.0 Hz, C-3), 55.7 (OMe), 55.5 (OMe'), 19.4 (Me) ppm.

^{19}F NMR (376.5 MHz, $CDCl_3$): δ -72.0 [s, C(O)CF_3], -77.2 (s, CF_3) ppm.

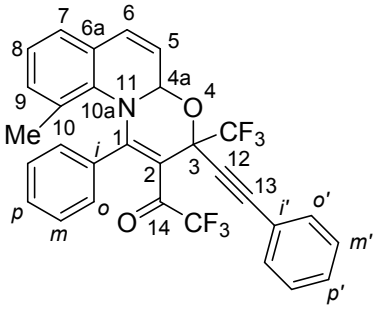
(3*R**,4a*S**)-**3i**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.39 (m, 4H, $H_{o,o'}$ from Ph), 7.09 (d, $^3J_{8,9}$ = 7.0 Hz, 1H, H-7), 6.95-6.75 (m, 6H, H-8, H-9, $H_{m,m'}$ from Ph), 6.61 (s, 1H, H-6), 6.32 (d, $^3J_{10,11}$ = 8.0 Hz, 1H, H-10), 5.70 (s, 1H, H-4a), 3.84 (s, 3H, OMe), 3.78 (s, 3H, OMe'), 2.13 (s, 3H, Me) ppm.

The signals of (3*R**,4a*S**)-**3n** in the ^{13}C NMR spectrum are overlapped with those of the major isomer.

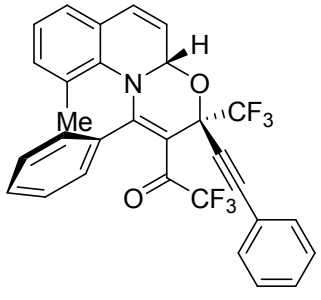
^{19}F NMR (376.5 MHz, $CDCl_3$): δ -73.4 [q, $^6J_{F,F}$ = 2.2 Hz, C(O)CF_3], -75.2 (q, $^6J_{F,F}$ = 2.2 Hz, CF_3) ppm.

HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{32}H_{24}F_6NO_4^+$: 600.1604; found: 600.1582.

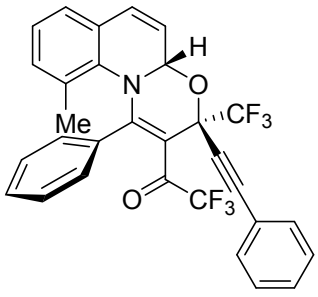
Found: C, 63.82; H, 3.85; N, 2.27; F, 18.74. Calc. for $C_{32}H_{23}F_6NO_4$ (599.53): C, 64.11; H, 3.87; N, 2.34; F, 19.01.



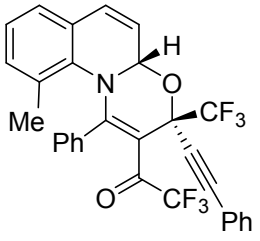
2,2,2-Trifluoro-1-[10-methyl-1-phenyl-3-(phenylethynyl)-3-(trifluoromethyl)-3*H*,4a*H*-[1,3]oxazino[3,2-*a*]quinolin-2-yl]ethanone (3j). Analogously, from quinoline **1e** (0.036 g, 0.25 mmol) and acetylene **2a** (0.099 g, 0.5 mmol) in 0.2 ml MeCN (20-24 °C, 204 h) 1,3-oxazinoquinoline **3j** was obtained as pale yellow crystals, 0.074 g, 87%, mp 177-179 °C (hexane). Eluent was mixture of hexane/dichloromethane. Mixture of three isomers, ratio is 26:53:21 (^{19}F NMR). Initial acetylene **2a** was recovered (0.037 g, conversion was 62%).



(3*S**,4a*S**)-diastereomer, atropomer **A**



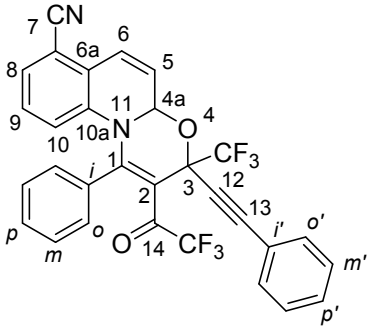
(3*S**,4a*S**)-diastereomer, atropomer **B**



(3*R**,4a*S**)-diastereomer

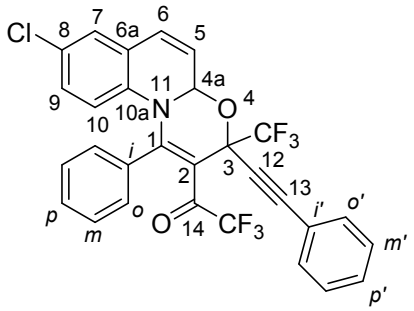
(3*S**,4a*S**)-**3j(A)**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.47 (m, 2H, H_o from Ph), 7.40-7.30 (m, 8H, $H_{o',m,m',p,p'}$ from Ph), 7.01 (m, 1H, H-7), 6.99 (m, 1H, H-8), 6.81 (dd, $^3J_{5,6}$ = 9.4 Hz, 1H, H-6), 6.72 (m, 1H, H-9), 6.18 (dd, $^3J_{4a,5}$ = 4.1 Hz, $^3J_{5,6}$ = 9.0 Hz, 1H, H-5), 5.73 (d, $^3J_{4a,5}$ = 4.1 Hz, 1H, H-4a), 1.87 (s, 3H, Me) ppm.

^{13}C NMR (100.6 MHz, $CDCl_3$): δ 183.2 (q, $^2J_{CF}$ = 35.8 Hz, C-14), 157.2 (C-1), 134.6 (C-10a), 133.1 (C_p from Ph), 133.0 (C_i from Ph), 132.1 ($C_{o'}$ from Ph), 132.0 (C-9), 130.9 ($C_{m'}$ from Ph), 130.1 (C-6), 129.7 (C-2), 129.5 ($C_{p'}$ from Ph), 128.2 (C_m from Ph), 126.7 (C_o from Ph), 125.3 (C-10), 124.4 (C-7), 123.3 (C-8), 122.5 (q, $^1J_{CF}$ = 291.2 Hz, CF_3), 122.4 (C-6a), 120.7 ($C_{i'}$ from Ph), 117.6 (C-5), 115.0 [q, $^1J_{CF}$ = 292.7 Hz, C(O)$\underline{C}F_3$], 88.9 (C-13), 81.1 (C-4a), 80.6 (C-12), 74.8 (q, $^2J_{CF}$ = 34.3 Hz, C-3), 21.2 (Me) ppm.
^{19}F NMR (376.3 MHz, $CDCl_3$): δ -73.4 [s, C(O)CF_3], -75.3 (s, CF_3) ppm.
(3*S**,4a*S**)-**3j(B)**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.30 (m, 2H, H_o from Ph), 7.40-7.30 (m, 6H, $H_{o',m',p,p'}$ from Ph), 7.10 (t, $^3J_{7,8}$ = 7.1 Hz, $^3J_{8,9}$ = 7.1 Hz, 1H, H-8), 7.01 (m, 1H, H-7), 6.92 (m, 2H, H_m from Ph), 6.71 (m, 1H, H-6), 6.61 (d, $^3J_{8,9}$ = 7.1 Hz, 1H, H-9), 6.14 (dd, $^3J_{4a,5}$ = 4.3 Hz, $^3J_{5,6}$ = 9.9 Hz, 1H, H-5), 5.73 (d, $^3J_{4a,5}$ = 4.3 Hz, 1H, H-4a), 1.67 (s, 3H, Me) ppm.
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 185.0 (q, $^2J_{CF}$ = 36.5 Hz, C-14), 161.2 (C-1), 134.8 (C-10a), 133.5 (C_p from Ph), 133.4 (C_i from Ph), 132.1 ($C_{o'}$ from Ph, C-9), 130.8 ($C_{m'}$ from Ph), 129.9 (C-6), 129.5 (C-2), 129.1 ($C_{p'}$ from Ph), 128.3 (C_m from Ph), 126.2 (C_o from Ph), 126.1 (C-10), 124.4 (C-7), 123.3 (C-8), 122.8 (q, $^1J_{CF}$ = 187.7 Hz, CF_3), 122.4 (C-6a), 120.7 ($C_{i'}$ from Ph), 117.6 (C-5), 114.7 [q, $^1J_{CF}$ = 291.9 Hz, C(O)$\underline{C}F_3$], 89.7 (C-13), 81.4 (C-4a), 81.1 (C-12), 74.3 (q, $^2J_{CF}$ = 32.8 Hz, C-3), 20.8 (Me) ppm.
^{19}F NMR (376.3 MHz, $CDCl_3$): δ -73.4 [s, C(O)CF_3], -76.8 (s, CF_3) ppm.
(3*R**,4a*S**)-**3j**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.47 (m, 2H, H_o from Ph), 7.40-7.30 (m, 8H, $H_{o',m,m',p,p'}$ from Ph), 7.10 (t, $^3J_{7,8}$ = 8.0 Hz, $^3J_{8,9}$ = 8.0 Hz, 1H, H-8), 7.01 (m, 1H, H-7), 6.71 (m, 1H, H-6), 6.60 (d, $^3J_{8,9}$ = 8.0 Hz, 1H, H-9), 6.38 (dd, $^3J_{4a,5}$ = 1.3 Hz, $^3J_{5,6}$ = 9.4 Hz, 1H, H-5), 5.81 (br s, 1H, H-4a), 1.72 (s, 3H, Me) ppm.
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 185.3 (q, $^2J_{CF}$ = 36.5 Hz, C-14), 151.9 (C-1), 134.3 (C-10a), 133.9 (C_i from Ph), 132.9 (C_p from Ph), 132.1 ($C_{o'}$ from Ph), 131.9 (C-9), 130.9 ($C_{m'}$ from Ph), 130.3 (C-6), 129.3 (C-2), 129.2 ($C_{p'}$ from Ph), 128.2 (C_m from Ph), 127.5 (C_o from Ph), 125.8 (C-10), 124.4 (C-7), 123.6 (C-6a), 123.4 (C-8), 122.9 (q, $^1J_{CF}$ = 285.6 Hz, CF_3), 120.7 ($C_{i'}$ from Ph), 117.7 (C-5), 115.3 [q, $^1J_{CF}$ = 285.6 Hz, C(O)$\underline{C}F_3$], 85.9 (C-13), 81.9 (C-12), 80.6 (C-4a), 73.3 (q, $^2J_{CF}$ = 35.0 Hz, C-3), 18.3 (Me) ppm.
^{19}F NMR (376.3 MHz, $CDCl_3$): δ -74.5 [q, $^6J_{F,F}$ = 2.0 Hz, C(O)CF_3], -76.4 (q, $^6J_{F,F}$ = 2.0 Hz, CF_3) ppm.
HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{30}H_{20}F_6NO_2^+$: 540.1393; found: 540.1393.

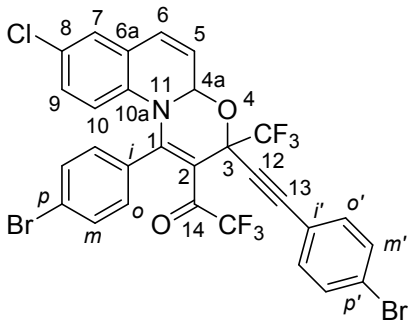


1-Phenyl-3-(phenylethynyl)-2-(trifluoroacetyl)-3-(trifluoromethyl)-3*H*,4a*H*-[1,3]oxazino[3,2-*a*]quinoline-7-carbonitrile (3k). Analogously, from quinoline **1d** (0.0385 g, 0.25 mmol) and acetylene **2a** (0.099 g, 0.5 mmol) in 0.2 ml MeCN (20-24 °C, 24 h) 1,3-oxazinoquinoline **3k** was obtained as pale yellow crystals, 0.124 g, 90%, mp 107-109 °C (hexane), (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 41:59 (^{19}F NMR). Eluent was mixture of hexane/dichloromethane.
(3*S**,4a*S**)-**3k**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.60-7.30 (m, 11H, $H_{o,o',m,m',p,p'}$ from Ph, H-8), 7.24 (d, $^3J_{5,6}$ = 7.6 Hz, 1H, H-6), 6.95 (t, $^3J_{8,9}$ = 8.1 Hz, $^3J_{9,10}$ = 8.1 Hz, 1H, H-9), 6.60 (d, $^3J_{9,10}$ = 8.1 Hz, 1H, H-10), 6.43 (dd, $^3J_{5,6}$ = 10.0 Hz, $^3J_{4a,5}$ = 4.4 Hz, 1H, H-5), 5.79 (d, $^3J_{4a,5}$ = 4.4 Hz, 1H, H-4a) ppm.
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 184.4 (q, $^2J_{CF}$ = 36.7 Hz, C-14), 156.0 (C-1), 135.6 (C-10a), 133.0 (C_p from Ph), 132.8 (C_i from Ph), 132.0 ($C_{o'}$ from Ph), 130.1 ($C_{o,m}$ from Ph), 129.8 (C-2), 129.5 (C-9), 128.9 ($C_{p'}$ from Ph), 128.2 ($C_{m'}$ from Ph), 126.4 (C-8), 126.1 (C-6), 123.8 (C-6a), 121.7 (q, $^1J_{CF}$ = 286.0 Hz, CF_3), 121.4 (C-5, C-10), 120.9 ($C_{i'}$ from Ph), 116.6 (CN), 115.0 [q, $^1J_{CF}$ = 293.4 Hz, C(O)$\underline{C}F_3$], 111.0 (C-7), 90.2 (C-13), 80.7 (C-12), 79.1 (C-4a), 74.8 (q, $^2J_{CF}$ = 34.8 Hz, C-3) ppm.
^{19}F NMR (376.3 MHz, $CDCl_3$): δ -74.1 [s, C(O)CF_3], -78.6 (s, CF_3) ppm.

(3*R**,4a*S**)-**3k**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.60-7.30 (m, 11H, $H_{o,o',m,m',p,p'}$ from Ph, H-8), 7.20 (d, $^3J_{5,6}$ = 8.6 Hz, 1H, H-6), 6.91 (t, $^3J_{8,9}$ = 8.1 Hz, $^3J_{9,10}$ = 8.1 Hz, 1H, H-9), 6.63 (dd, $^3J_{5,6}$ = 8.6 Hz, $^3J_{4a,5}$ = 4.6 Hz, 1H, H-5), 6.62 (q, $^3J_{9,10}$ = 8.1 Hz, 1H, H-10), 5.99 (d, $^3J_{4a,5}$ = 4.6 Hz, 1H, H-4a) ppm.
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 184.8 (q, $^2J_{CF}$ = 37.6 Hz, C-14), 150.9 (C-1), 135.9 (C-10a), 133.2 (C_i from Ph), 132.3 (C_p from Ph), 132.2 ($C_{o'}$ from Ph), 130.1 ($C_{o,m}$ from Ph), 129.8 (C-2), 129.5 (C-9), 128.9 ($C_{p'}$ from Ph), 128.3 ($C_{m'}$ from Ph), 126.4 (C-8), 126.2 (C-6), 124.0 (C-6a), 122.8 (q, $^1J_{CF}$ = 289.2 Hz, CF_3), 121.6 ($C_{i'}$ from Ph), 120.9 (C-5, C-10), 116.7 (CN), 114.6 [q, $^1J_{CF}$ = 293.0 Hz, C(O)$\underline{C}F_3$], 111.0 (C-7), 86.7 (C-13), 80.1 (C-12), 79.6 (q, $^4J_{CF}$ = 3.0 Hz, C-4a), 73.4 (q, $^2J_{CF}$ = 32.1 Hz, C-3) ppm.
^{19}F NMR (376.3 MHz, $CDCl_3$): δ -74.8 [q, $^6J_{F,F}$ = 2.2 Hz, C(O)CF_3], -76.9 (q, $^6J_{F,F}$ = 2.2 Hz, CF_3) ppm.
HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{30}H_{17}F_6N_2O_2^+$: 551.1189; found: 551.1189.



1-[8-Chloro-1-henyl-3-(phenylethynyl)-3-(trifluoromethyl)-3*H*,4a*H*-[1,3]oxazino[3,2-*a*]quinolin-2-yl]-2,2,2-trifluoroethanone (3l). Analogously, from quinoline **1e** (0.082 g, 0.5 mmol) and acetylene **2a** (0.198 g, 1 mmol) (20-24 °C, 24 h) 1,3-oxazinoquinoline **3l** (0.162 g, 75%) was obtained as a yellow powder, mp 188-189 °C (ethanol). Eluent was mixture of chloroform/benzene/ethanol. Initial quinoline **1e** (0.024 g, conversion was 71%) and acetylene **2a** (0.046 g, conversion was 77%) were recovered. IR (microlayer): 2235 (C≡C), 1707 (C=O), 1655 (C=C), 1199, 1160, 1098 (C-F) cm^{-1}. (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 40:60 (^{1}H NMR).
(3*S**,4a*S**)-**3l**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.54 (m, 1H, H_p from Ph), 7.44 (m, 6H, $H_{o,o',m}$ from Ph), 7.35-7.28 (m, 3H, $H_{m',p'}$ from Ph), 7.19 (d, $^4J_{8,10}$ = 2.3 Hz, 1H, H-7), 6.87 (d, $^3J_{6,7}$ = 9.9 Hz, 1H, H-6), 6.81 (dd, $^4J_{8,10}$ = 2.3 Hz, $^3J_{10,11}$ = 8.8 Hz, 1H, H-9), 6.25 (d, $^3J_{10,11}$ = 8.8 Hz, 1H, H-10), 6.22 (dd, $^3J_{5a,6}$ = 4.4 Hz, $^3J_{6,7}$ = 9.9 Hz, 1H, H-5), 5.70 (d, $^3J_{5a,6}$ = 4.4 Hz, 1H, H-4a) ppm.
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 184.5 (q, $^2J_{CF}$ = 35.7 Hz, C-14), 157.6 (C-1), 133.6 (C-10a; C_i from Ph), 133.0 (C_p from Ph), 132.3 ($C_{o'}$ from Ph), 130.1 (C-2; $C_{o,m}$ from Ph), 129.8 (C-6), 129.2 ($C_{p'}$ from Ph), 128.8 (C-9), 128.5 ($C_{m'}$ from Ph), 128.0 (C-7), 127.8 (C-8), 123.6 (C-6a), 121.9 (q, $^1J_{CF}$ = 284.3 Hz, CF_3), 120.7 ($C_{i'}$ from Ph), 119.4 (C-10), 119.1 (C-5), 115.3 [q, $^1J_{CF}$ = 291.1 Hz, C(O)$\underline{C}F_3$], 89.8 (C-13), 84.9 (C-12), 79.7 (C-4a), 74.9 (q, $^2J_{CF}$ = 31.2 Hz, C-3) ppm.
^{19}F NMR (376.5 MHz, $CDCl_3$): δ -72.5 [s, C(O)CF_3], -77.2 (s, CF_3) ppm.
(3*R**,4a*S**)-**3l**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.52-7.42 (m, 7H, $H_{o,o',m,p}$ from Ph), 7.33-7.28 (m, 3H, $H_{m',p'}$ from Ph), 7.13 (d, $^4J_{8,10}$ = 2.4 Hz, 1H, H-7), 6.83 (d, $^3J_{6,7}$ = 9.6 Hz, 1H, H-6), 6.75 (d, $^3J_{10,11}$ = 9.8 Hz, 1H, H-9), 6.26 (d, $^3J_{10,11}$ = 9.8 Hz, 1H, H-10), 6.13 (dd, $^3J_{5a,6}$ = 4.4 Hz, $^3J_{6,7}$ = 9.6 Hz, 1H, H-5), 5.90 (d, $^3J_{5a,6}$ = 4.4 Hz, 1H, H-4a) ppm.
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 185.2 (q, $^2J_{CF}$ = 36.9 Hz, C-14), 152.0 (C-1), 133.9 (C-10a; C_i from Ph), 132.3 ($C_{p,o'}$ from Ph), 132.2 (C-2), 130.1 ($C_{o,m}$ from Ph), 129.5 (C-6), 129.4 ($C_{p'}$ from Ph), 128.7 (C-9), 128.4 ($C_{m'}$ from Ph), 128.0 (C-7), 127.5 (C-8), 123.7 (C-6a), 123.1 (q, $^1J_{CF}$ = 287.4 Hz, CF_3), 121.2 ($C_{i'}$ from Ph), 118.9 (C-10), 118.8 (C-5), 114.9 [q, $^1J_{CF}$ = 291.1 Hz, C(O)$\underline{C}F_3$], 86.5 (C-13), 81.4 (C-12), 80.2 (q, $^4J_{CF}$ = 2.6 Hz, C-4a), 73.4 (q, $^2J_{CF}$ = 31.8 Hz, C-3) ppm.
^{19}F NMR (376.5 MHz, $CDCl_3$): δ -73.4 [q, $^6J_{F,F}$ = 2.2 Hz, C(O)CF_3], -75.5 (q, $^6J_{F,F}$ = 2.2 Hz, CF_3) ppm.
HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{29}H_{17}ClF_6NO_2^+$: 560.0847; found: 560.0828.
Found: C, 61.92; H, 3.03; N, 2.52; Cl, 6.10; F, 20.47. Calc. for $C_{29}H_{16}ClF_6NO_2$ (559.89): C, 62.21; H, 2.88; N, 2.50; Cl, 6.33; F, 20.36.



1-[1-(4-Bromophenyl)-3-[(4-bromophenyl)ethynyl]-8-chloro-3-(trifluoromethyl)-3*H*,4a*H*-[1,3]oxazino[3,2-*a*]quinolin-2-yl]-2,2,2-trifluoroethanone (3m). Analogously, from quinoline **1e** (0.049 g, 0.3 mmol) and acetylene **2g** (0.166 g, 0.6 mmol) in 0.3 ml MeCN (20-24 °C, 8 h) 1,3-oxazinoquinoline **3m** (0.156 g, 81%) was obtained as a yellow powder, mp 85-93 °C (ethanol). Eluent was mixture of chloroform/benzene/ethanol. Initial acetylene **2g** was recovered (0.017 g, conversion was 90%). IR (microlayer): 2237 (C≡C), 1716 (C=O), 1655 (C=C), 1205, 1158, 1106 (C-F) cm^{-1}. (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 40:60 (^{1}H NMR).

(3*S**,4a*S**)-**3m**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.58 (m, 2H, H_m from Ph), 7.44 (m, 2H, $H_{m'}$ from Ph), 7.35-7.25 (m, 4H, $H_{o,o'}$ from Ph), 7.16 (d, $^4J_{8,10}$ = 2.2 Hz, 1H, H-7), 6.87 (m, 1H, H-6), 6.81 (m, 1H, H-9), 6.23 (m, 1H, H-10), 6.20 (dd, $^3J_{5a,6}$ = 4.4 Hz, $^3J_{6,7}$ = 9.6 Hz, 1H, H-5), 5.65 (d, $^3J_{5a,6}$ = 4.4 Hz, 1H, H-4a) ppm.

^{13}C NMR (100.6 MHz, $CDCl_3$): δ 184.2 (q, $^2J_{CF}$ = 35.8 Hz, C-14), 156.3 (C-1), 133.6 ($C_{o',m}$ from Ph), 133.3 (C-10a), 132.4 (C_i from Ph), 131.9 ($C_{o,m'}$ from Ph), 130.3 (C-2), 129.3 (C-6), 129.0 (C-9), 128.2 (C-7), 128.1 (C-8), 127.2 (C_p from Ph), 124.4 ($C_{p'}$ from Ph), 123.6 (C-6a), 121.7 (q, $^1J_{CF}$ = 284.8 Hz, CF_3), 119.6 ($C_{i'}$ from Ph), 119.3 (C-10), 119.0 (C-5), 115.3 [q, $^1J_{CF}$ = 291.1 Hz, C(O)$\underline{C}F_3$], 89.0 (C-13), 81.7 (C-12), 79.9 (C-4a), 75.2 (q, $^2J_{CF}$ = 31.6 Hz, C-3) ppm.

^{19}F NMR (376.5 MHz, $CDCl_3$): δ -72.3 [s, C(O)CF_3], -77.2 (s, CF_3) ppm.

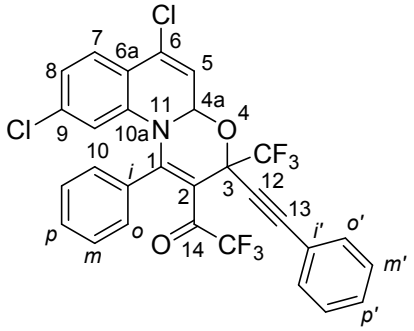
(3*R**,4a*S**)-**3m**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.58 (m, 2H, H_m from Ph), 7.44 (m, 2H, $H_{m'}$ from Ph), 7.35-7.25 (m, 4H, $H_{o,o'}$ from Ph), 7.15 (d, $^4J_{8,10}$ = 2.2 Hz, 1H, H-7), 6.87 (m, 1H, H-6), 6.81 (m, 1H, H-9), 6.23 (m, 1H, H-10), 6.13 (dd, $^3J_{5a,6}$ = 4.4 Hz, $^3J_{6,7}$ = 9.6 Hz, 1H, H-5), 5.86 (d, $^3J_{5a,6}$ = 4.4 Hz, 1H, H-4a) ppm.

^{13}C NMR (100.6 MHz, $CDCl_3$): δ 185.1 (q, $^2J_{CF}$ = 36.3 Hz, C-14), 150.7 (C-1), 133.8 ($C_{o'}$ from Ph), 133.7 (C-10a), 133.6 (C_m from Ph), 132.7 (C_i from Ph), 131.8 ($C_{o,m'}$ from Ph), 131.1 (C-2), 129.5 (C-6), 128.9 (C-9), 128.2 (C-7; C-8), 127.9 (C_p from Ph), 124.2 ($C_{p'}$ from Ph), 123.8 (C-6a), 122.9 (q, $^1J_{CF}$ = 285.0 Hz, CF_3), 120.1 ($C_{i'}$ from Ph), 118.8 (C-10), 118.7 (C-5), 114.8 [q, $^1J_{CF}$ = 291.0 Hz, C(O)$\underline{C}F_3$], 85.6 (C-13), 82.2 (C-12), 80.3 (q, $^4J_{CF}$ = 2.6 Hz, C-4a), 73.4 (q, $^2J_{CF}$ = 31.5 Hz, C-3) ppm.

^{19}F NMR (376.5 MHz, $CDCl_3$): δ -73.2 [q, $^6J_{F,F}$ = 2.2 Hz, C(O)CF_3], -75.5 (q, $^6J_{F,F}$ = 2.2 Hz, CF_3) ppm.

HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{29}H_{15}Br_2ClF_6NO_2^+$: 715.9057; found: 715.9036.

Found: C, 48.25; H, 1.95; N, 1.95; Br, 22.04; Cl, 4.67; F, 15.59. Calc. for $C_{29}H_{14}Br_2ClF_6NO_2$ (717.68): C, 48.53; H, 1.97; N, 1.95; Br, 22.27; Cl, 4.94; F, 15.88.



1-[6,9-Dichloro-1-phenyl-3-(phenylethynyl)-3-(trifluoromethyl)-2,3-dihydro-1*H*,4a*H*-[1,3]oxazino[3,2-*a*]quinolin-2-yl]-2,2,2-trifluoroethanone (3n). Analogously, from quinoline **1f** (0.050 g, 0.25 mmol) and acetylene **2a** (0.099 g, 0.5 mmol) in 0.2 ml MeCN (20-24 °C, 48 h) 1,3-

oxazinoquinoline **3n** was obtained. Eluent was mixture of hexane/dichloromethane. First fraction, yellow crystals, 0.058 g, mp 149-151 °C (hexane), (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 49:51 (^{19}F NMR). Second fraction, yellow oil, 0.019 g, (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 75:25. Total yield 0.077 g, 52%, (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 55:45 (^{19}F NMR).

(3*S**,4a*S**)-**3n**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.66 (m, 2H, H_o from Ph), 7.50-7.43 (m, 5H, $H_{o',m,p}$ from Ph), 7.45 (d, $^{3}J_{7,8}$ = 7.8 Hz, 1H, H-7), 7.40-7.30 (m, 3H, $H_{m',p'}$ from Ph), 6.98 (dd, $^{3}J_{7,8}$ = 7.8 Hz, $^{4}J_{8,10}$ = 1.5 Hz, 1H, H-8), 6.36 (d, $^{3}J_{4a,5}$ = 4.4 Hz, 1H, H-5), 6.35 (d, $^{4}J_{8,10}$ = 1.5 Hz, 1H, H-10), 5.76 (d, $^{3}J_{4a,5}$ = 4.4 Hz, 1H, H-4a) ppm.

^{13}C NMR (100.6 Hz, $CDCl_3$): δ 184.4 (q, $^{2}J_{CF}$ = 36.3 Hz, C-14), 155.9 (C-1), 136.5 (C-10a), 135.8 (C-6), 133.8 (C_i from Ph), 133.1 (C_p from Ph), 132.8 (C-9), 132.3($C_{o'}$ from Ph), 130.1 ($C_{o,m}$ from Ph), 130.0 ($C_{p'}$ from Ph), 129.8 (C-2), 128.4 ($C_{m'}$ from Ph), 127.3 (C-7), 122.7 (C-8), 121.7 (q, $^{1}J_{CF}$ = 284.0 Hz, CF_3), 120.3 ($C_{i'}$ from Ph), 118.7 (C-6a), 117.7 (C-5), 115.8 (C-10), 115.0 [q, $^{1}J_{CF}$ = 291.2 Hz, C(O)$\underline{C}F_3$], 94.7 (q, $^{2}J_{CF}$ = 35.3 Hz, C-3), 87.1 (C-13), 80.1 (C-4a; C-12) ppm.

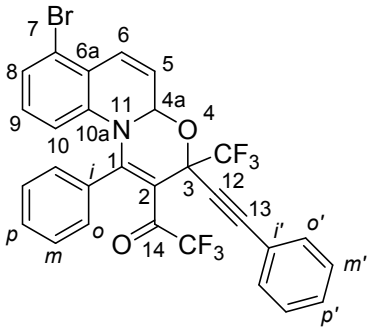
^{19}F NMR (376.3 Hz, $CDCl_3$): δ -74.1 [s, C(O)CF_3], -78.5 (s, CF_3) ppm.

(3*R**,4a*S**)-**3n**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.64 (m, 2H, H_o from Ph), 7.50-7.43 (m, 5H, $H_{o',m,p}$ from Ph), 7.45 (d, $^{3}J_{7,8}$ = 8.5 Hz, 1H, H-7), 7.40-7.30 (m, 3H, $H_{m',p'}$ from Ph), 6.94 (dd, $^{3}J_{7,8}$ = 7.8 Hz, $^{4}J_{8,10}$ = 1.5 Hz, 1H, H-8), 6.39 (d, $^{4}J_{8,10}$ = 1.5 Hz, 1H, H-10), 6.30 (d, $^{3}J_{4a,5}$ = 4.4 Hz, 1H, H-5), 5.95 (d, $^{3}J_{4a,5}$ = 4.4 Hz, 1H, H-4a) ppm.

^{13}C NMR (100.6 Hz, $CDCl_3$): δ 185.7 ($^{2}J_{CF}$ = 36.1 Hz, C-14), 151.0 (C-1), 136.8 (C-10a), 135.8 (C-6), 134.2 (C_i from Ph), 133.2 (C-9), 132.4 (C_p from Ph), 132.1 ($C_{o'}$ from Ph), 130.1 ($C_{o,m}$ from Ph), 129.8 (C-2), 129.6 ($C_{p'}$ from Ph), 128.3 ($C_{m'}$ from Ph), 127.3 (C-7), 122.8 (q, $^{1}J_{CF}$ = 284.7 Hz, CF_3), 122.4 (C-8), 120.9 ($C_{i'}$ from Ph), 118.8 (C-6a), 117.6 (C-5), 115.4 (C-10), 114.6 [q, $^{1}J_{CF}$ = 291.7 Hz, C(O)$\underline{C}F_3$], 90.2 (C-13), 80.6 (q, $^{4}J_{CF}$ = 2.6 Hz, C-4a), 80.5 (C-12), 73.7 (q, $^{2}J_{CF}$ = 33.5 Hz, C-3) ppm.

^{19}F NMR (376.3 Hz, $CDCl_3$): δ -74.8 [q, $^{6}J_{F,F}$ = 2.0 Hz, C(O)CF_3], -77.0 (q, $^{6}J_{F,F}$ = 2.0 Hz, CF_3) ppm.

HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{29}H_{16}{}^{[35]}Cl_2F_6NO_2^+$: 594.0457; found: 594.0459; m/z $[M+H]^+$ Calcd for $C_{29}H_{16}{}^{[37]}Cl_2F_6NO_2^+$: 596.0429; found: 596.0433.

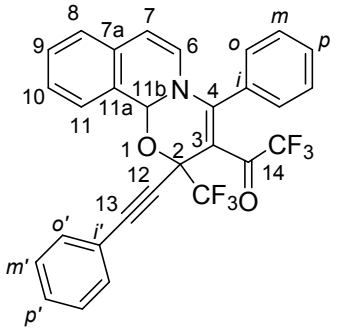


1-[7-Bromo-1-phenyl-3-(phenylethynyl)-3-(trifluoromethyl)-3*H*,4a*H*-[1,3]oxazino[3,2-*a*]quinolin-2-yl]-2,2,2-trifluoroethanone (3o). Analogously, from quinoline **1g** (0.052 g, 0.25 mmol) and acetylene **2a** (0.099 g, 0.5 mmol) in 0.2 ml MeCN (20-24 °C, 48 h) 1,3-oxazinoquinoline **3o** was obtained. Eluent was mixture of hexane/dichloromethane. First fraction, yellow crystals, 0.114 g, mp 83-85 °C (hexane), (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 42:58 (^{19}F NMR). Second fraction, yellow crystals, 0.010 g, mp 87-89 °C (hexane), (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 86:14. Total yield 0.124 g, 82%, (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 45:55 (^{19}F NMR).

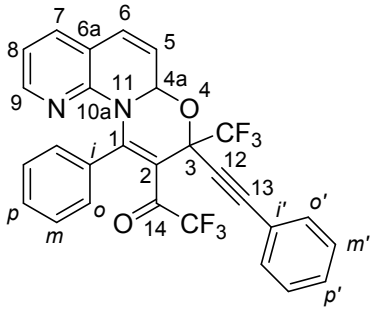
(3*S**,4a*S**)-**3o**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.57-7.40 (m, 7H, $H_{o,o',m,p}$ from Ph), 7.37-7.28 (m, 4H, $H_{m',p'}$ from Ph, H-8), 7.16 (d, $^{3}J_{5,6}$ = 7.9 Hz, 1H, H-6), 6.71 (t, $^{3}J_{8,9}$ = 8.2 Hz, $^{3}J_{9,10}$ = 8.2 Hz, 1H, H-9), 6.33 (d, $^{3}J_{9,10}$ = 8.3 Hz, 1H, H-10), 6.28 (dd, $^{3}J_{5,6}$ = 10.2 Hz, $^{3}J_{4a,5}$ = 4.6 Hz, 1H, H-5), 5.72 (d, $^{3}J_{4a,5}$ = 4.6 Hz, 1H, H-4a) ppm.

^{13}C NMR (100.6 MHz, $CDCl_3$): δ 184.5 (q, $^{2}J_{CF}$ = 36.5 Hz, C-14), 157.0 (C-1), 136.4 (C-10a), 133.5 ($C_{i'}$ from Ph), 132.8 ($C_{p'}$ from Ph), 132.1 ($C_{o'}$ from Ph), 129.9 ($C_{o,m}$ from Ph), 129.8 (C-2), 129.7 (C_p from Ph), 129.4 (C-6), 129.3 (C-9), 128.3 ($C_{m'}$ from Ph), 126.7 (C-8), 121.7 (q, $^{1}J_{CF}$ = 286.8 Hz, CF_3), 121.1

(C_i from Ph), 120.5 (C-6a), 119.3 (C-10), 118.9 (C-5), 117.8 (C-7), 115.1 [q, $^1J_{CF}$ = 293.4 Hz, C(O)$\underline{C}F_3$], 89.8 (C-13), 81.1 (C-12), 79.4 (C-4a), 74.8 (q, $^2J_{CF}$ = 34.6 Hz, C-3) ppm.
^{19}F NMR (376.3 MHz, $CDCl_3$): δ -74.0 [s, C(O)CF_3], -78.6 (s, CF_3) ppm.
(3*R**,4a*S**)-**3o**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.57-7.40 (m, 7H, $H_{o,o',m,p}$ from Ph), 7.37-7.28 (m, 4H, $H_{m',p'}$ from Ph, H-6), 7.14 (d, $^3J_{5,6}$ = 8.0 Hz, 1H, H-6), 6.88 (t, $^3J_{8,9}$ = 8.1 Hz, $^3J_{9,10}$ = 8.1 Hz,1H, H-9), 6.39 (d, $^3J_{9,10}$ = 8.1 Hz, 1H, H-10), 6.23 (dd, $^3J_{5,6}$ = 10.1 Hz, $^3J_{4a,5}$ = 4.7 Hz, 1H, H-5), 5.93 (d, $^3J_{4a,5}$ = 4.7 Hz, 1H, H-4a) ppm.
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 185.2 ($^2J_{CF}$ = 37.6 Hz, C-14), 151.7 (C-1), 136.8 (C-10a), 133.9 ($C_{i'}$ from Ph), 132.8 ($C_{p'}$ from Ph), 132.2 ($C_{o'}$ from Ph), 129.9 ($C_{o,m}$ from Ph), 129.8 (C-2), 129.4 (C-6), 129.3 (C_p from Ph; C-7), 128.2 ($C_{m'}$ from Ph), 126.4 (C-8), 122.9 (q, $^1J_{CF}$ = 289.3 Hz, CF_3), 121.3 (C_i from Ph), 121.2 (C-6a), 117.8 (C-7), 117.4 (C-10), 117.0 (C-5), 114.7 [q, $^1J_{CF}$ = 293.0 Hz, C(O)$\underline{C}F_3$], 86.4 (C-13), 80.5 (C-12), 79.9 (q, $^4J_{CF}$ = 2.6 Hz,C-4a), 73.3 (q, $^2J_{CF}$ = 31.3 Hz, C-3) ppm.
^{19}F NMR (376.3 MHz, $CDCl_3$): δ -74.8 [q, $^6J_{F,F}$ = 2.2 Hz, C(O)CF_3], -77.0 (q, $^6J_{F,F}$ = 2.2 Hz, CF_3) ppm.
HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{29}H_{17}{}^{[79]}BrF_6NO_2^+$: 604.0341; found: 604.0341; m/z $[M+H]^+$ Calcd for $C_{29}H_{17}{}^{[81]}BrF_6NO_2^+$: 606.0323; found: 606.0322.



2,2,2-Trifluoro-1-[4-phenyl-2-(phenylethynyl)-2-(trifluoromethyl)-2*H*,11b*H*-[1,3]oxazino[2,3-*a*]isoquinolin-3-yl]ethanone (5a). Analogously, from isoquinoline **4a** (0.012 g, 0.15 mmol) and acetylene **2a** (0.076 g, 0.3 mmol) (20-24 °C, 3 h) 1,3-oxazinoisoquinoline **5a** (0.190 g, 72%) was obtained as a yellow powder, mp 163-165 °C (hexane). Eluent was mixture of chloroform/benzene/ethanol. Initial acetylene **2a** was recovered (0.004 g, conversion was 98%). IR (microlayer): 2233 (C≡C), 1678 (C=O), 1646 (C=C), 1190, 1162 (C-F) cm^{-1}. (2*R**,11b*R**):(2*S**,11b*R**)-isomers ratio is 85:15 (^{1}H NMR).
(2*R**,11b*R**)-**5a**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.65-7.30 (m, 13H, H-9, H-10, H-11, $H_{o,m,p,o',m',p'}$ from Ph), 7.23 (d, $^3J_{8,9}$ = 7.6 Hz, 1H, H-8), 6.43 (d, $^3J_{6,7}$ = 7.8 Hz, 1H, H-6), 6.23 (s, 1H, H-11b), 5.96 (d, $^3J_{6,7}$ = 7.8 Hz, 1H, H-7) ppm.
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 180.8 (q, $^2J_{CF}$ = 34.5 Hz, C-14), 161.0 (C-4), 133.4 ($C_{i,p}$ from Ph), 132.3 ($C_{o'}$ from Ph), 131.8 (C-3), 130.3 (C-6), 129.9 (C-7a), 129.5 ($C_{o,m}$ from Ph), 129.0 (C-9), 128.5 ($C_{m'}$ from Ph), 128.4 ($C_{p'}$ from Ph), 127.8 (C-11), 125.9 (C-10), 125.6 (C-11a), 124.4 (C-8), 122.8 (q, $^1J_{CF}$ = 284.7 Hz, CF_3), 121.2 ($C_{i'}$ from Ph), 115.9 [q, $^1J_{CF}$ = 291.0 Hz, C(O)$\underline{C}F_3$], 107.7 (C-7), 88.5 (C-13), 81.7 (C-12), 80.8 (C-11b), 75.5 (q, $^2J_{CF}$ = 34.1 Hz, C-2) ppm.
^{19}F NMR (376.5 MHz, $CDCl_3$): δ -70.7 [C(O)CF_3], -75.8 (CF_3) ppm.
(2*S**,11b*R**)-**5a**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 7.65-7.30 (m, 13H, H-9, H-10, H-11, $H_{o,m,p,o',m',p'}$ from Ph), 7.17 (d, $^3J_{8,9}$ = 7.4 Hz, 1H, H-8), 6.54 (s, 1H, H-11b), 6.28 (d, $^3J_{6,7}$ = 7.8 Hz, 1H, H-6), 5.81 (d, $^3J_{6,7}$ = 7.8 Hz, 1H, H-7) ppm.
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 183.2 (q, $^2J_{CF}$ = 35.7 Hz, C-14), 154.2 (C-5), 134.0 ($C_{o'}$ from Ph), 132.9 (C_p from Ph), 132.6 (C_i from Ph), 131.5 (C-3), 130.3 (C-6), 130.1 (C-7a), 129.6 ($C_{o,m}$ from Ph), 129.0 ($C_{m'}$ from Ph), 128.8 (C-9), 128.4 ($C_{p'}$ from Ph), 127.7 (C-11), 125.0 (C-11a), 124.8 (C-10), 124.2 (C-8), 121.7 (q, $^1J_{CF}$ = 284.6 Hz, CF_3), 121.5 ($C_{i'}$ from Ph), 115.2 [q, $^1J_{CF}$ = 290.2 Hz, C(O)$\underline{C}F_3$], 105.8 (C-7), 85.8 (C-13), 83.5 (C-12), 81.2 (C-11b), 72.8 (q, $^2J_{CF}$ = 31.8 Hz, C-2) ppm.
^{19}F NMR (376.5 MHz, $CDCl_3$): δ -72.9 [C(O)CF_3], -74.1 (CF_3) ppm.
HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{29}H_{18}F_6NO_2^+$: 526.1236; found: 526.1225.
Found: C, 66.02; H, 3.21; N, 2.47; F, 21.98. Calc. for $C_{29}H_{17}F_6NO_2$ (525.45): C, 66.29; H, 3.26; N, 2.67; F, 21.69.



2,2,2-Trifluoro-1-[10-phenyl-8-(phenylethynyl)-8-(trifluoromethyl)-6a*H*,8*H*-[1,3]oxazino[3,2-*a*]-1,8-naphthyridin-9-yl]ethanone (5b). Analogously, from naphthyridine **4b** (0.0325 g, 0.25 mmol) and acetylene **2a** (0.099 g, 0.5 mmol) in 0.2 ml MeCN (20-24 °C, 24 h) 1,3-oxazinoquinoline **5b** was obtained. Eluent was mixture of hexane/dichloromethane. First fraction, pale brown crystals, 0.020 g, mp 75-77 °C (hexane), (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 6:94 (^{19}F NMR). Second fraction, pale brown crystals, 0.062 g, mp 80-82 °C (hexane), (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 45:55. Total yield 0.082 g, 62%, (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 40:60 (^{19}F NMR).

(3*S**,4a*S**)-**5b**: (400.1 MHz, $CDCl_3$): δ 7.77 (dd, $^3J_{8,9}$ = 4.9 Hz, $^4J_{7,9}$ = 1.8 Hz, 1H, H-9), 7.55 (m, 2H, H_o from Ph), 7.50-7.30 (m, 9H, H-7, $H_{m,p,o',m',p'}$ from Ph), 6.92 (d, $^3J_{5,6}$ = 9.8 Hz, 1H, H-6), 6.83 (dd, $^3J_{8,9}$ = 4.9 Hz, $^3J_{7,8}$ = 7.4 Hz, 1H, H-8), 6.22 (dd, $^3J_{4a,5}$ = 4.4 Hz, $^3J_{5,6}$ = 9.8 Hz, 1H, H-5), 5.91 (d, $^3J_{4a,5}$ = 4.4 Hz, 1H, H-4a) ppm.

^{13}C NMR (100.6 MHz, $CDCl_3$): δ 184.7 (q, $^2J_{CF}$ = 36.5 Hz, C-14), 156.8 (C-1), 147.7 (C-10a), 147.5 (C-9), 135.4 (C_i from Ph), 135.2 (C-7), 132.1 ($C_{o'}$ from Ph), 131.4 (C_p from Ph), 130.5 (C-6), 129.6 ($C_{p'}$ from Ph), 129.4 (C-2), 128.9 (C_o from Ph), 128.8 (C_m from Ph), 128.2 ($C_{m'}$ from Ph), 122.0 (q, $^1J_{CF}$ = 286.4 Hz, CF_3), 120.6 ($C_{i'}$ from Ph), 118.9 (C-8), 118.3 (C-5), 116.1 (C-6a), 115.0 [q, $^1J_{CF}$ = 272.0 Hz, C(O)$\underline{C}F_3$], 89.7 (C-13), 81.1 (C-12), 79.9 (C-4a), 74.5 (q, $^2J_{CF}$ = 32.4 Hz, C-3) ppm.

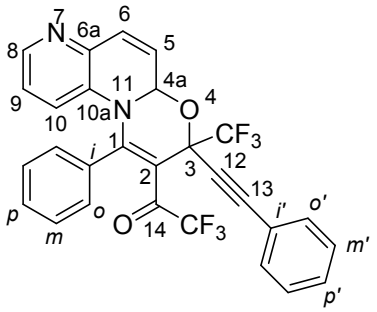
^{19}F NMR (376.3 MHz, $CDCl_3$): δ -74.0 [s, C(O)CF_3], -78.3 (s, CF_3) ppm.

(3*R**,4a*S**)-**5b**: ^{1}H NMR (400.13 MHz, $CDCl_3$): δ 7.71 (dd, $^3J_{8,9}$ = 4.9 Hz, $^4J_{7,9}$ = 1.8 Hz, 1H, H-9), 7.50-7.30 (m, 11H, H-7, $H_{o,m,p,o',m',p'}$ from Ph), 6.89 (d, $^3J_{5,6}$ = 9.5 Hz, 1H, H-6), 6.79 (dd, $^3J_{8,9}$ = 4.9 Hz, $^3J_{7,8}$ = 7.4 Hz, 1H, H-8), 6.15 (dd, $^3J_{5,6}$ = 9.5 Hz, $^3J_{4a,5}$ = 4.4 Hz, 1H, H-5), 6.12 (d, $^3J_{4a,5}$ = 4.4 Hz, 1H, H-4a) ppm.

^{13}C NMR (100.6 MHz, $CDCl_3$): δ 185.1 ($^2J_{CF}$ = 36.7 Hz, C-14), 151.9 (C-1), 147.9 (C-10a), 147.5 (C-9), 135.8 (C_i from Ph), 135.2 (C-7), 132.2 ($C_{o'}$ from Ph), 131.4 (C_p from Ph), 130.5 (C-6), 129.4 (C-2), 129.3 ($C_{p'}$ from Ph), 128.9 (C_o from Ph), 128.8 (C_m from Ph), 128.3 ($C_{m'}$ from Ph), 123.0 (q, $^1J_{CF}$ = 289.3 Hz, CF_3), 121.2 ($C_{i'}$ from Ph), 118.5 (C-8), 118.1 (C-5), 116.3 (C-6a), 114.6 [q, $^1J_{CF}$ = 276.8 Hz, C(O)$\underline{C}F_3$], 86.5 (C-13), 80.8 (C-12), 80.3 (q, $^4J_{CF}$ = 2.6 Hz, C-4a), 73.1 (q, $^2J_{CF}$ = 31.7 Hz, C-3) ppm.

^{19}F NMR (376.3 MHz, $CDCl_3$): δ -74.8 [q, $^6J_{F,F}$ = 2.2 Hz, C(O)CF_3], -77.0 (q, $^6J_{F,F}$ = 2.2 Hz, CF_3) ppm.

HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{28}H_{17}F_6N_2O_2^+$: 527.1189; found: 527.1185.



2,2,2-Trifluoro-1-[1-phenyl-3-(phenylethynyl)-3-(trifluoromethyl)-3*H*,4a*H*-[1,3]oxazino[3,2-*a*]-1,5-naphthyridin-2-yl]ethanone (5c). Analogously, from naphthyridine **4c** (0.0325 g, 0.25 mmol) and acetylene **2a** (0.099 g, 0.5 mmol) in 0.2 ml MeCN (20-24 °C, 24 h) 1,3-oxazinoquinoline **5c** was obtained

as brown powder, 0.096 g, 73%, mp 125-127 °C (hexane), (3*S**,4a*S**):(3*R**,4a*S**)-isomers ratio is 55:45 (^{19}F NMR). Eluent was mixture of hexane/dichloromethane.

(3*S**,4a*S**)-**5c**: (400.1 MHz, $CDCl_3$): δ 8.18 (dd, $^3J_{8,9}$ = 4.7 Hz, $^4J_{8,10}$ = 1.2 Hz, 1H, H-8), 7.60-7.25 (m, 10H, $H_{o,m,p,o',m',p'}$ from Ph), 7.19 (d, $^3J_{5,6}$ = 10.6 Hz, 1H, H-6), 6.79 (dd, $^3J_{8,9}$ = 4.7 Hz, $^3J_{9,10}$ = 10.1 Hz, 1H, H-9), 6.60 (d, $^3J_{9,10}$ = 10.1 Hz, 1H, H-10), 6.44 (dd, $^3J_{4a,5}$ = 4.4 Hz, $^3J_{5,6}$ = 10.1 Hz, 1H, H-5), 5.76 (d, $^3J_{4a,5}$ = 4.4 Hz, 1H, H-4a) ppm.

^{13}C NMR (100.6 MHz, $CDCl_3$): δ 184.3 (q, $^2J_{CF}$ = 36.5 Hz, C-14), 156.7 (C-1), 143.5 (C-8), 141.0 (C-6a), 133.0 (C_p from Ph), 132.8 (C_i from Ph), 132.1 (C-10a, $C_{o'}$ from Ph), 131.6 (C-6), 130.1 ($C_{o,m}$ from Ph), 130.0 (C-2), 129.7 ($C_{p'}$ from Ph), 128.3 ($C_{m'}$ from Ph), 124.2 (C-5), 122.8 (C-10), 122.1 (C-9), 121.8 (q, $^1J_{CF}$ = 286.2 Hz, CF_3), 120.4 ($C_{i'}$ from Ph), 115.5 [q, $^1J_{CF}$ = 282.3 Hz, C(O)$\underline{C}F_3$], 89.9 (C-13), 80.9 (C-12), 79.1 (C-4a), 74.4 (q, $^2J_{CF}$ = 35.2 Hz, C-3) ppm.

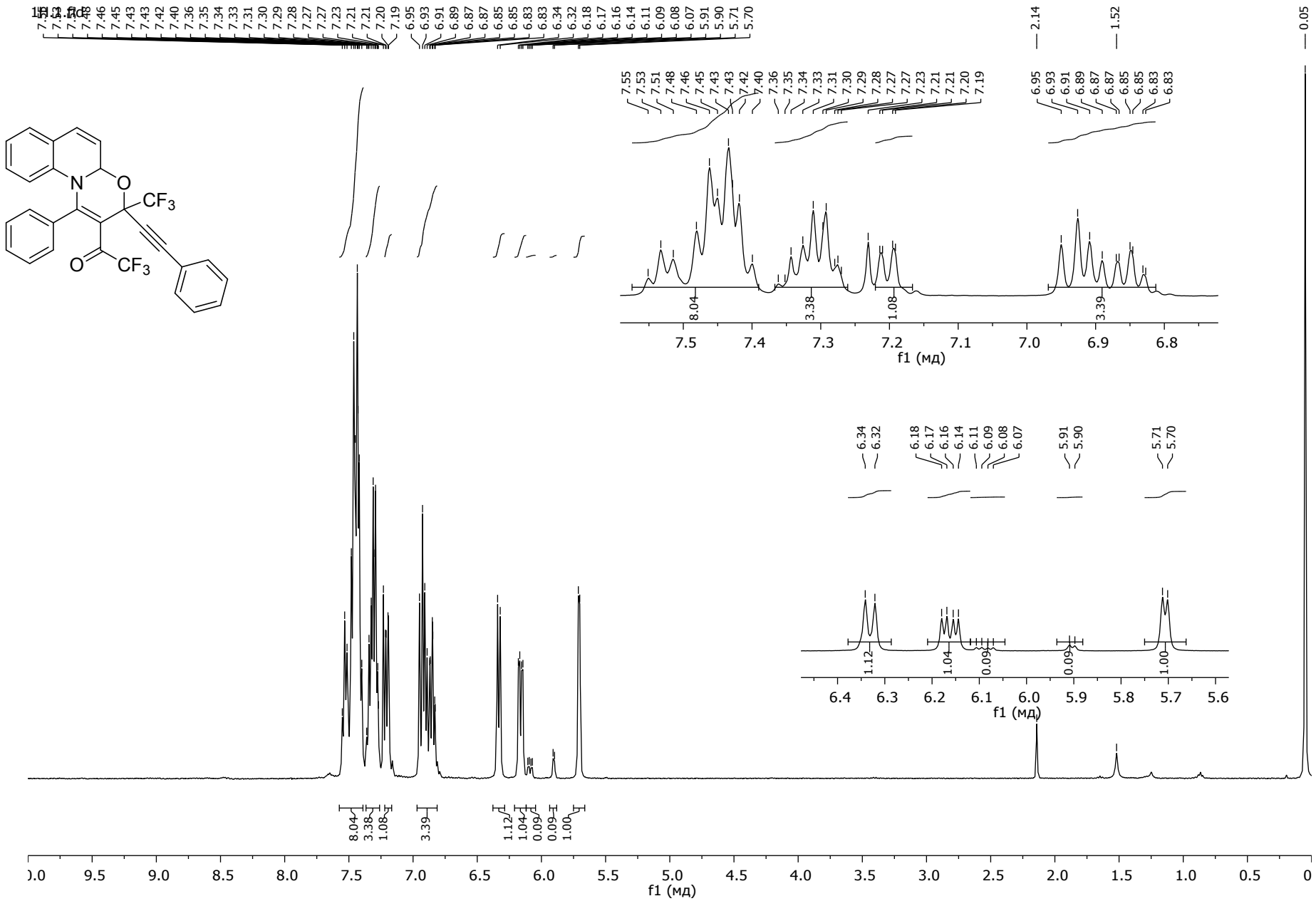
^{19}F NMR (376.3 MHz, $CDCl_3$): δ -73.9 [s, C(O)CF_3], -78.6 (s, CF_3) ppm.

(3*R**,4a*S**)-**5c**: ^{1}H NMR (400.1 MHz, $CDCl_3$): δ 8.13 (dd, $^3J_{8,9}$ = 4.6 Hz, $^4J_{8,10}$ = 1.1 Hz, 1H, H-8), 7.60-7.25 (m, 10H, $H_{o,m,p,o',m',p'}$ from Ph), 7.16 (d, $^3J_{5,6}$ = 10.6 Hz, 1H, H-6), 6.74 (dd, $^3J_{8,9}$ = 4.6 Hz, $^3J_{9,10}$ = 8.5 Hz, 1H, H-9), 6.60 (d, $^3J_{9,10}$ = 8.5 Hz, 1H, H-10), 6.37 (dd, $^3J_{4a,5}$ = 4.5 Hz, $^3J_{5,6}$ = 10.1 Hz, 1H, H-5), 5.97 (d, $^3J_{4a,5}$ = 4.5 Hz, 1H, H-4a) ppm.

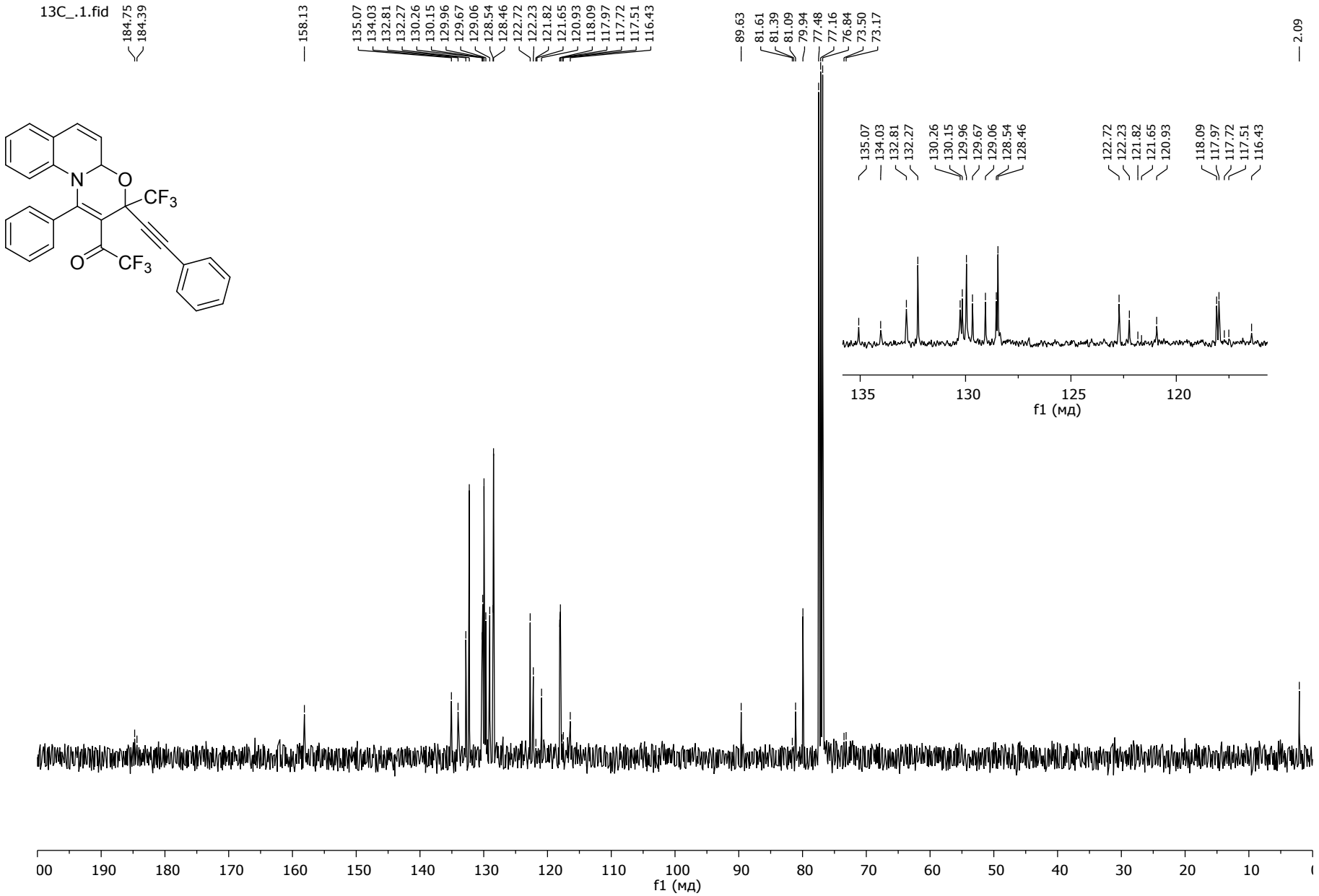
^{13}C NMR (100.6 MHz, $CDCl_3$): δ 185.3 (q, $^2J_{CF}$ = 37.4 Hz, C-14), 151.2 (C-1), 143.1 (C-8), 141.0 (C-6a), 133.1 (C_i from Ph), 132.8 (C_p from Ph), 132.4 (C-10a), 132.2 ($C_{o'}$ from Ph), 131.8 (C-6), 130.1 ($C_{o,m}$ from Ph), 130.0 (C-2), 129.4 ($C_{p'}$ from Ph), 128.2 ($C_{m'}$ from Ph), 123.9 (C-5), 122.9 (q, $^1J_{CF}$ = 289.5 Hz, CF_3), 122.7 (C-10), 121.6 (C-9), 121.0 ($C_{i'}$ from Ph), 115.1 [q, $^1J_{CF}$ = 293.2 Hz, C(O)$\underline{C}F_3$], 89.9 (C-13), 80.9 (C-12), 79.6 (q, $^4J_{CF}$ = 3.1 Hz, C-4a), 73.6 (q, $^2J_{CF}$ = 30.6 Hz, C-3) ppm.

^{19}F NMR (376.3 MHz, $CDCl_3$): δ -74.8 [q, *J* = 2.0 Hz, C(O)CF_3], -76.9 (q, $^6J_{F,F}$ = 2.0 Hz, CF_3) ppm.

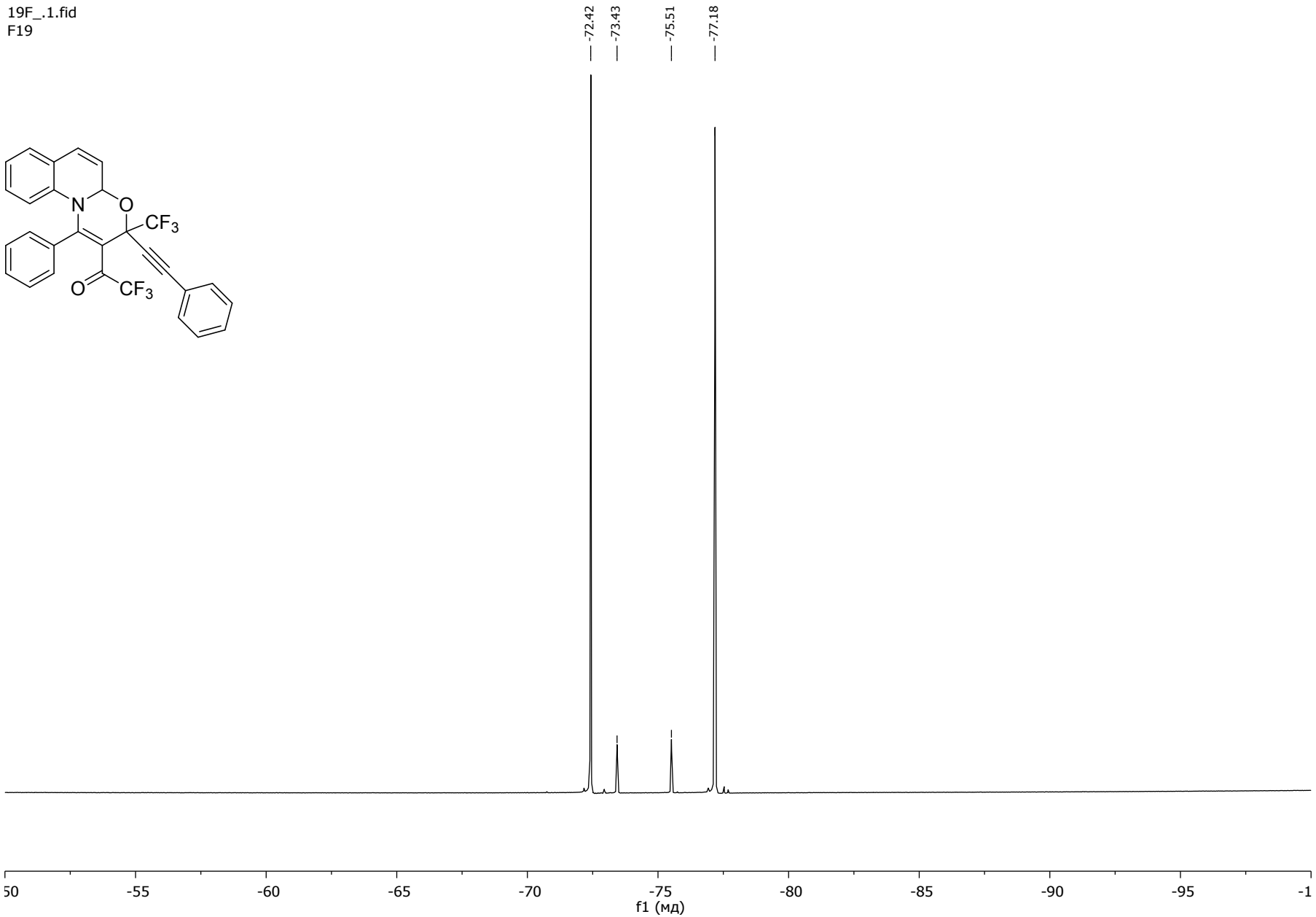
HRMS (ESI-TOF): m/z $[M+H]^+$ Calcd for $C_{28}H_{17}F_6N_2O_2^+$: 527.1189; found: 527.1183.



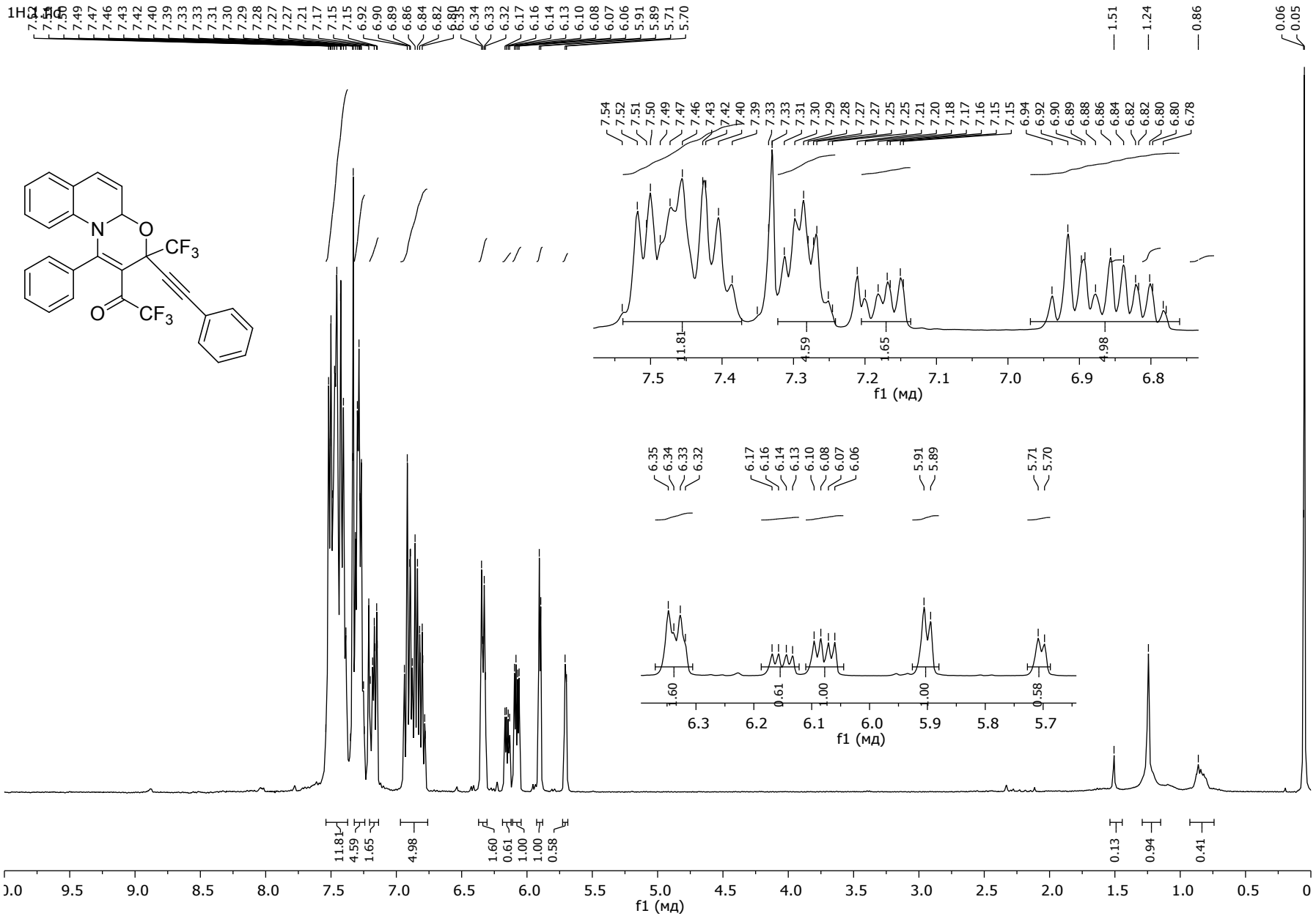
^{1}H NMR spectrum of (3*S**,4a*S**)-**3a** (400.1 MHz, $CDCl_3$)



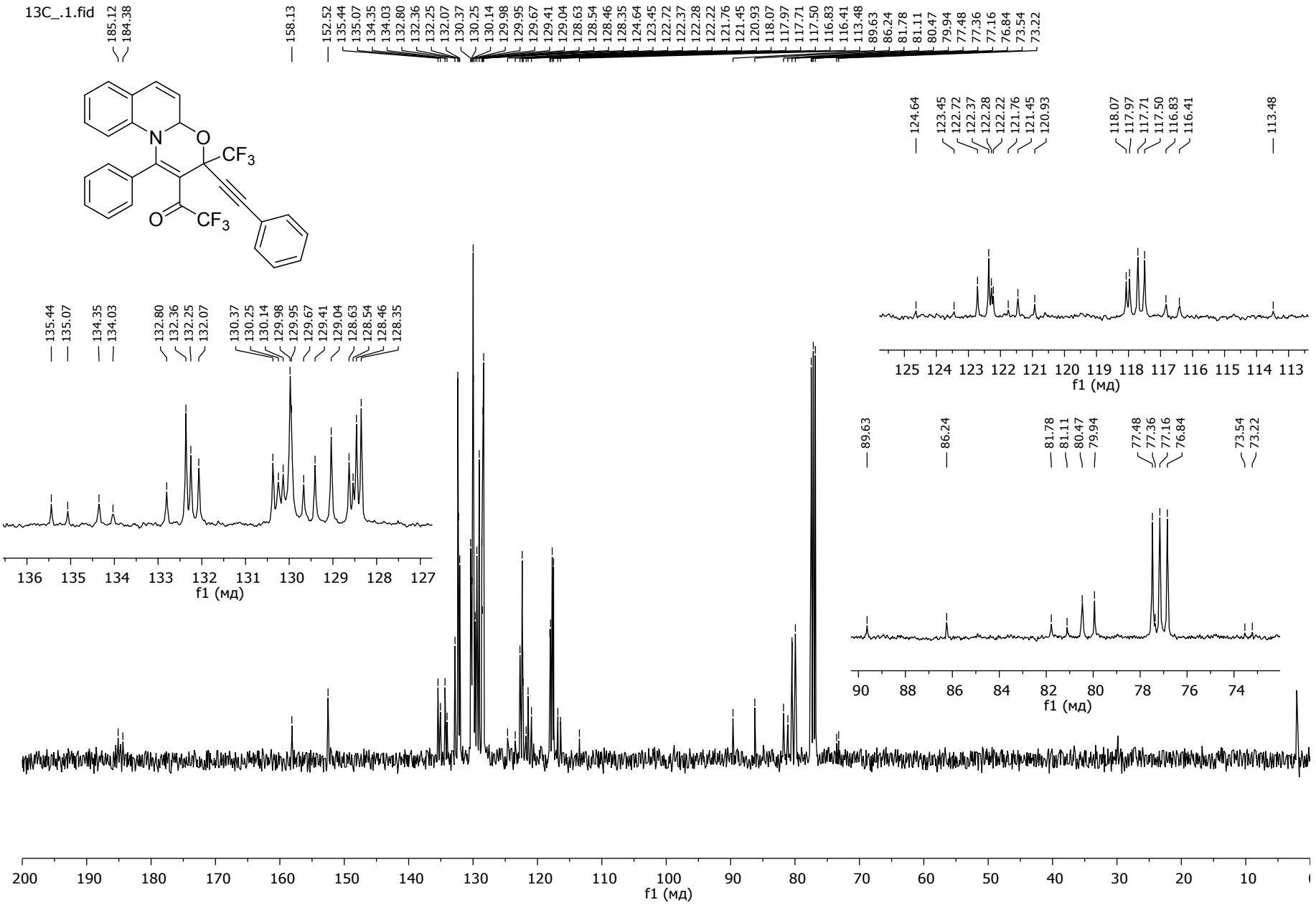
^{13}C NMR spectrum of (3*S**,4a*S**)-**3a** (100.6 MHz, $CDCl_3$)



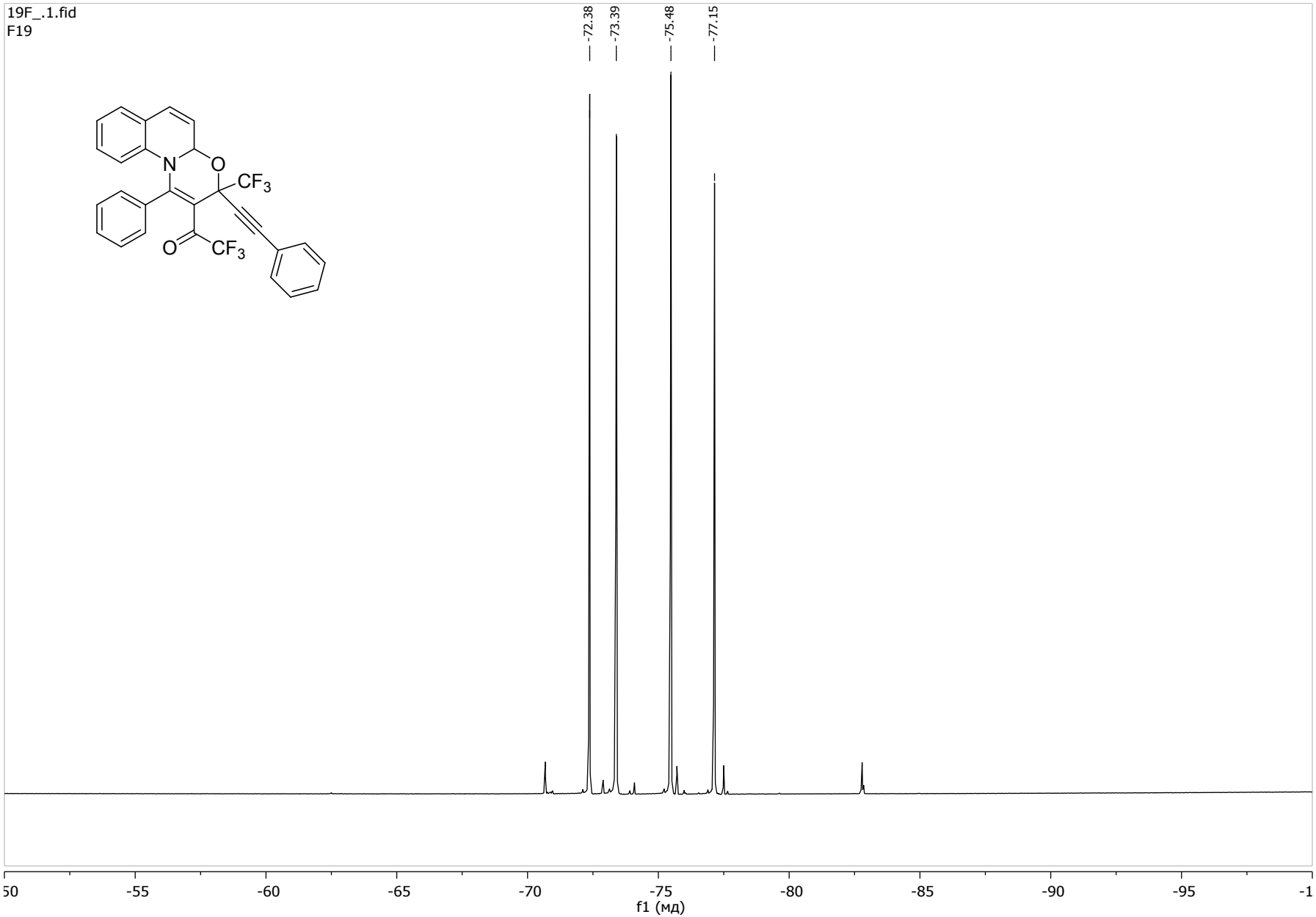
^{19}F NMR spectrum of (3*S**,4a*S**)-**3a** (376.5 MHz, $CDCl_3$)



^{1}H NMR spectrum of **3a** (signals at 0.86, 1.24 ppm are from hexane and 1.51 ppm – is from water) (400.1 MHz, $CDCl_3$)

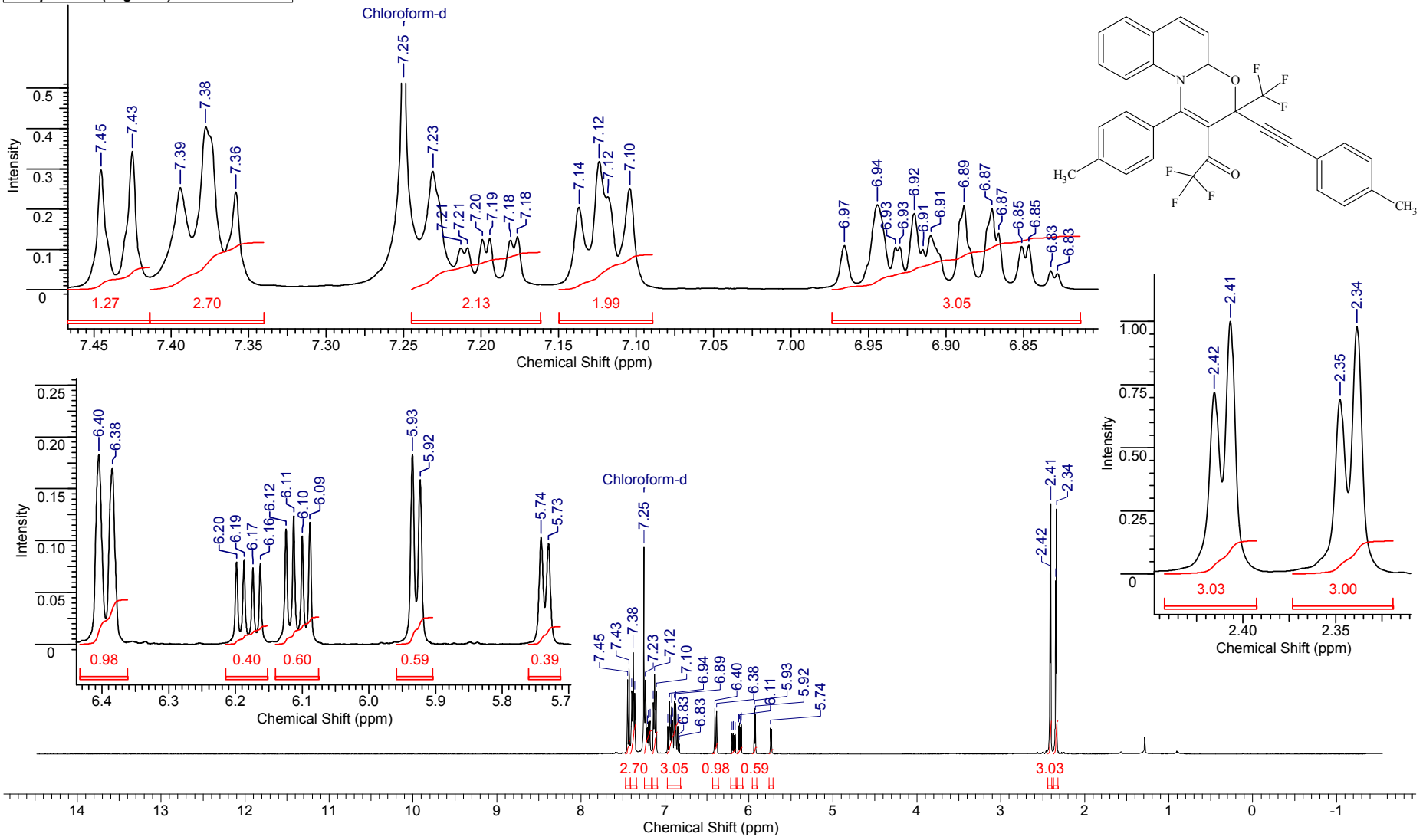


^{13}C NMR spectrum of **3a** (100.6 MHz, $CDCl_3$)



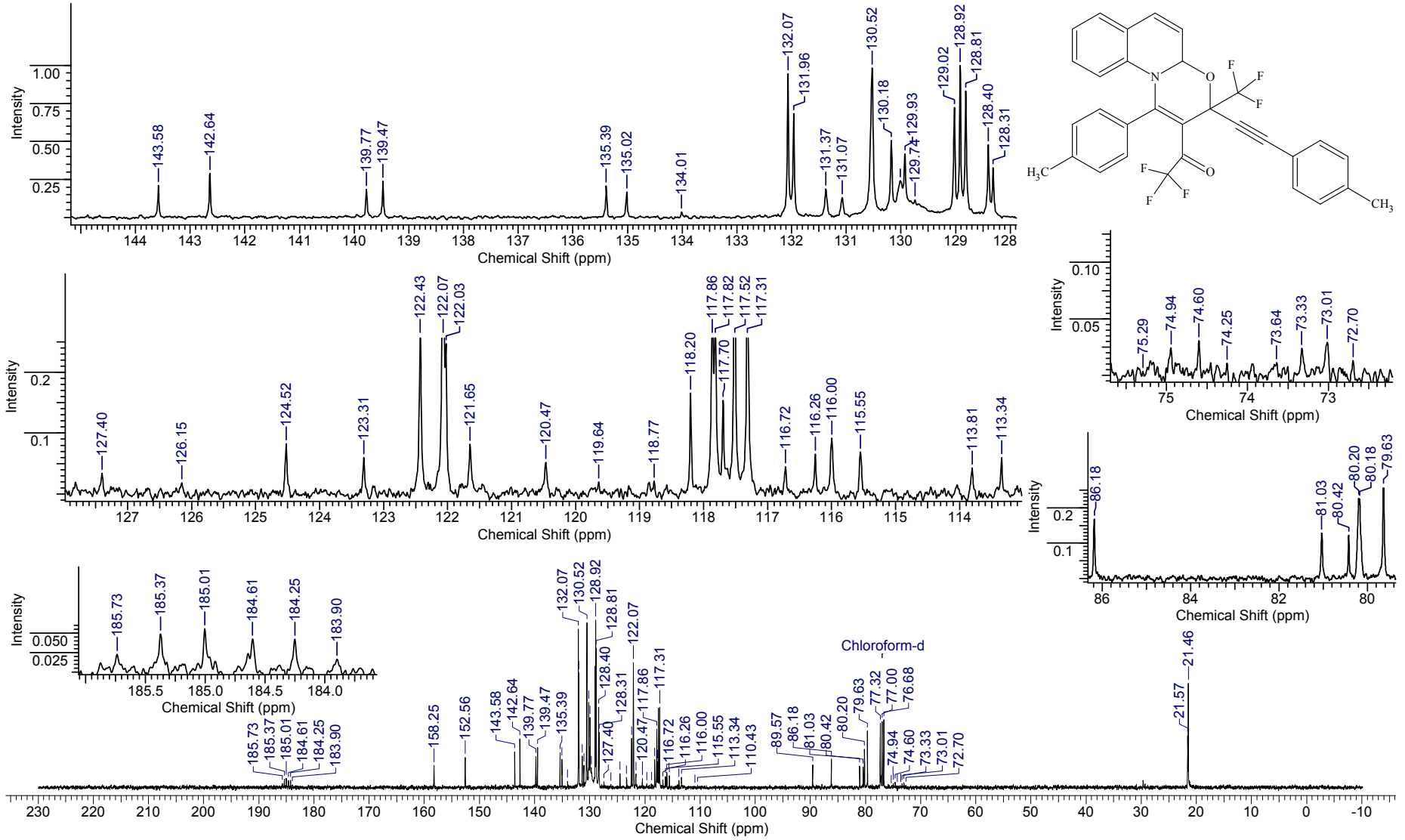
^{19}F NMR spectrum of **3a** (376.5 MHz, $CDCl_3$)

Acquisition Time (sec)	2.5559	***Comment***	Imported from UXNMR.			***Date***	14 Apr 2018 14:01:24
File Name	D:\Comp_316\BN\output\2018\04.äï ðåëü\BM-1347-1.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	16384	***Points Count***	65536
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	6410.26
Temperature (degree C)	27.000						



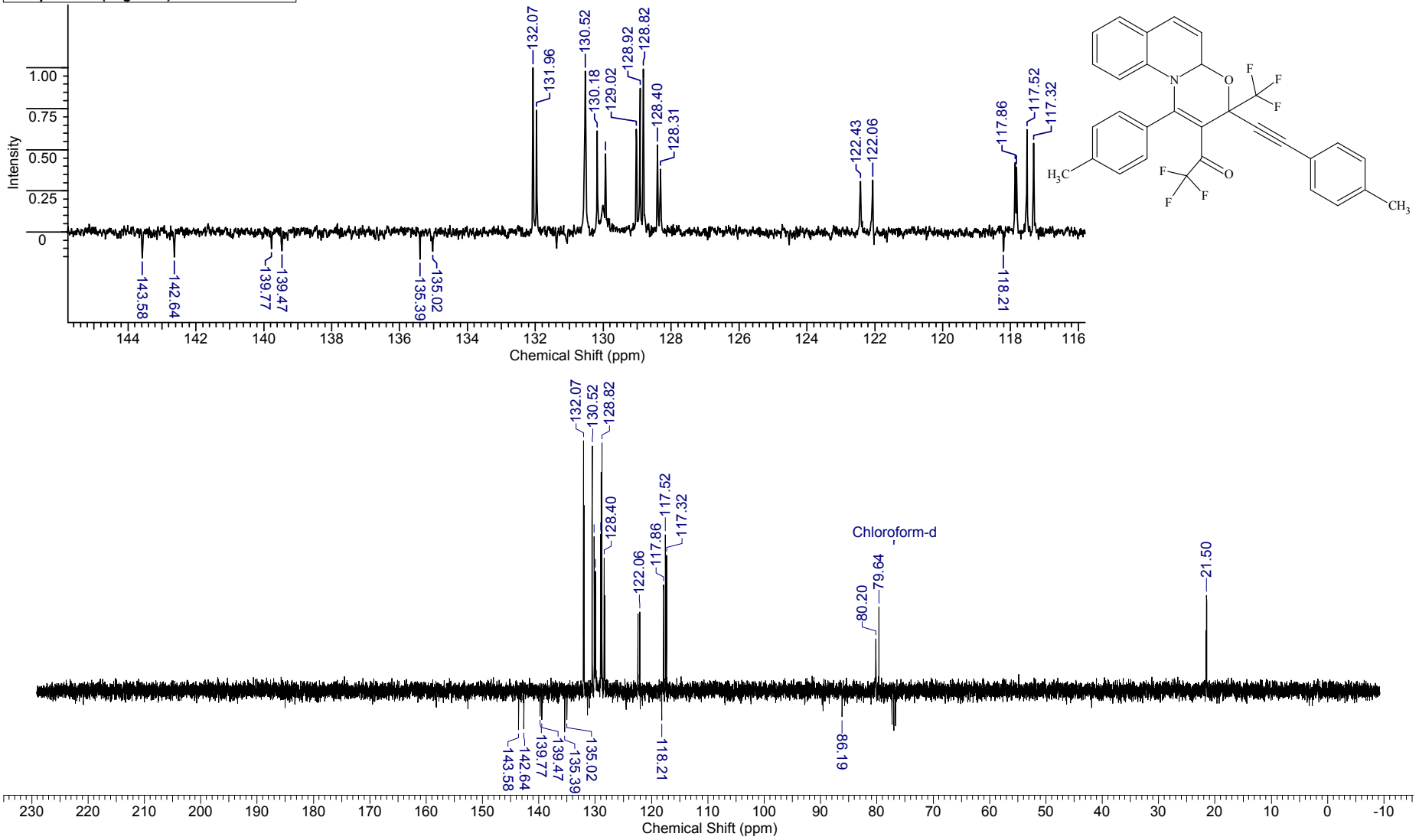
^{1}H NMR spectrum of **3b** (400.1 MHz, $CDCl_3$)

Acquisition Time (sec)	0.4999	***Comment***	Imported from UXNMR.			***Date***	15 May 2018 15:04:26
File Name	D:\Comp_316\BN\output\2018\05.ì àé\BM-1347-1B.C_002001r			***Frequency (MHz)***	100.61	***Nucleus***	13C
Number of Transients	300	***Original Points Count***	12076	***Points Count***	65536	***Pulse Sequence***	zgpg30
Solvent	DEUTERIUM OXIDE			***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000



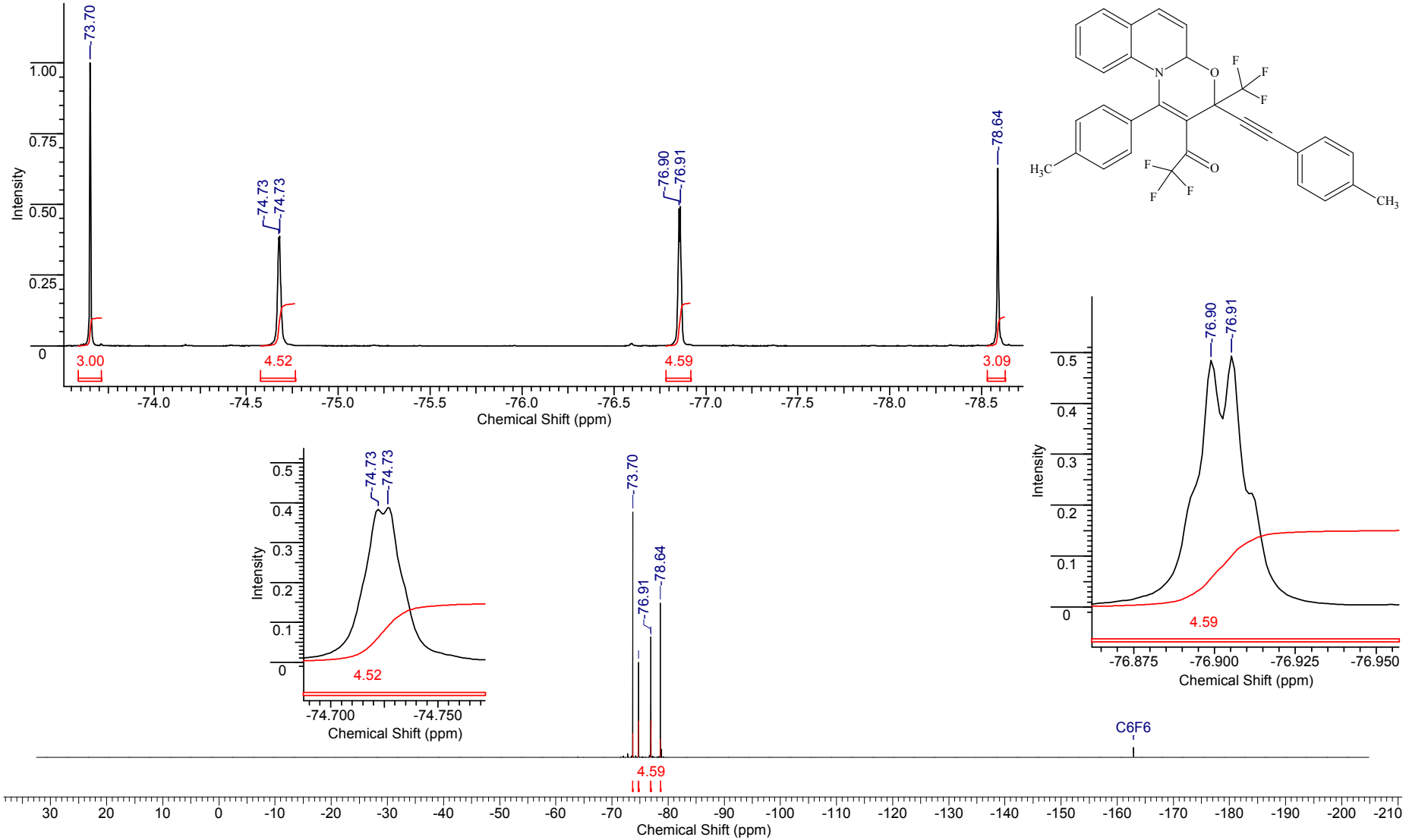
^{13}C NMR spectrum of **3b** (100.6 MHz, $CDCl_3$)

Acquisition Time (sec)	1.3664	***Comment***	Imported from UXNMR.			***Date***	25 May 2018 15:43:00
File Name	D:\Comp_316\BN\output\2018\05.ì àé\BM-1347-1B.Capt_004001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	41	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	jmod	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	23980.81
Temperature (degree C)	27.000						



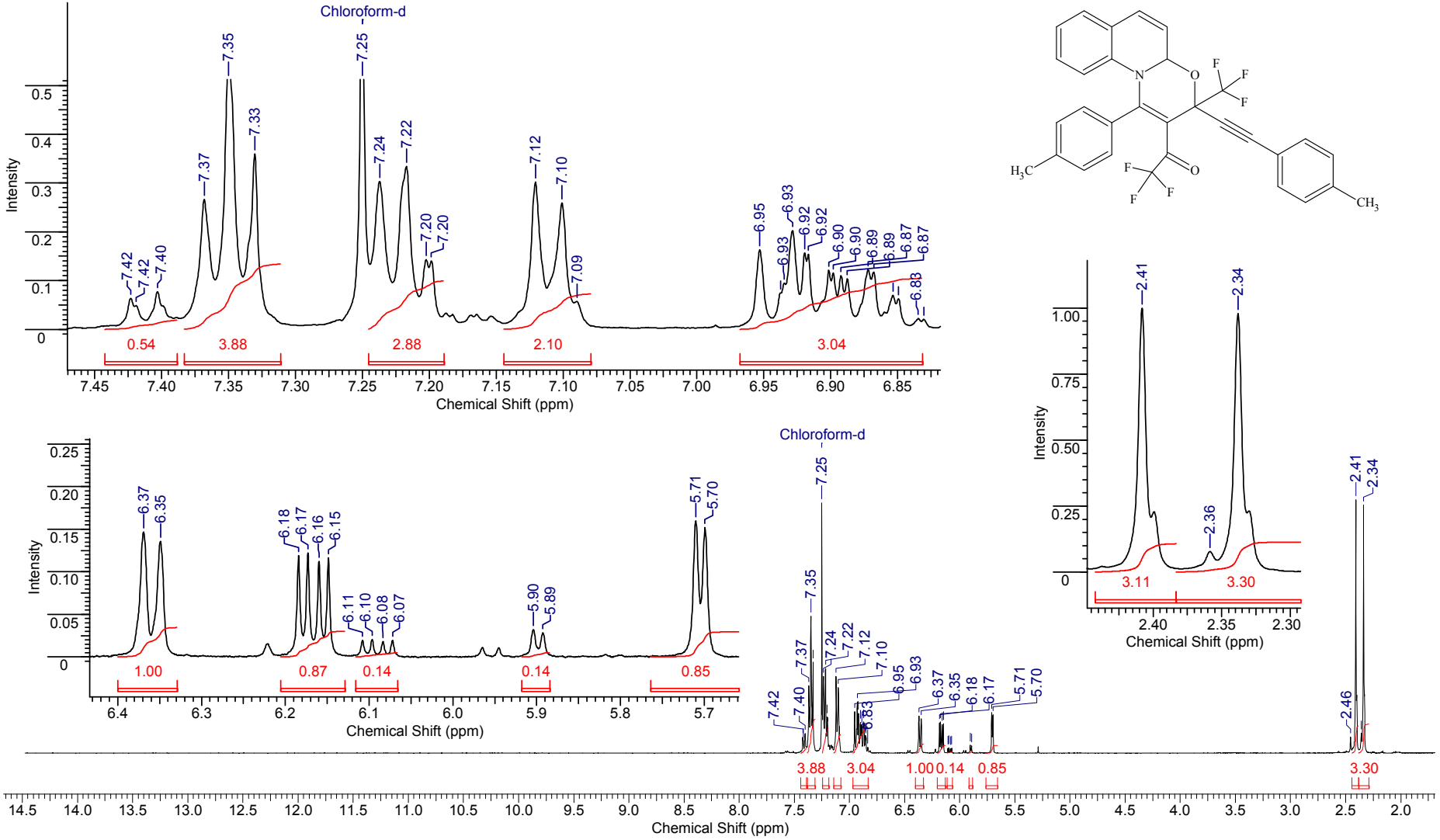
^{13}C NMR (APT) spectrum of **3b** (100.6 MHz, $CDCl_3$)

Acquisition Time (sec)	1.5000	***Date***	Apr 16 2018				
File Name	D:\Comp_316\BN\DOC (BN)\vasiliy\SPEC_BM_F_2018.04.27\BM-1347-1_20180416_01\FLUORINE_01					***Frequency (MHz)***	376.31
Nucleus	19F	***Number of Transients***	16	***Original Points Count***	133929	***Points Count***	262144
Pulse Sequence	s2pul	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	89285.71	***Temperature (degree C)***	22.000



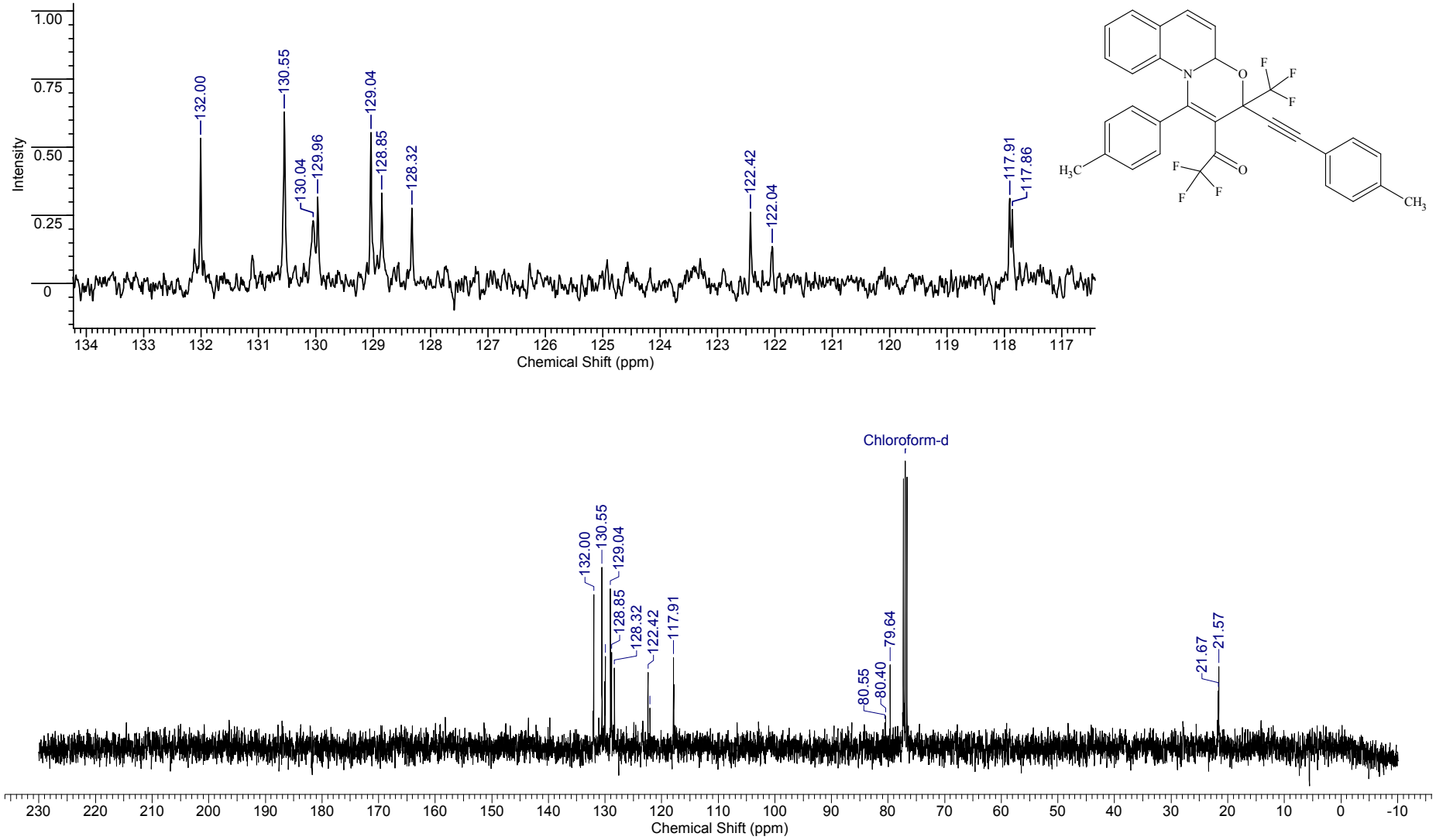
^{19}F NMR spectrum of **3b** (376.3 MHz, $CDCl_3$)

Acquisition Time (sec)	2.5559	***Comment***	Imported from UXNMR.			***Date***	14 Apr 2018 14:07:34
File Name	D:\Comp_316\BN\output\2018\04.äï ðåëü\BM-1347-2.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	16384	***Points Count***	65536
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	6410.26
Temperature (degree C)	27.000						



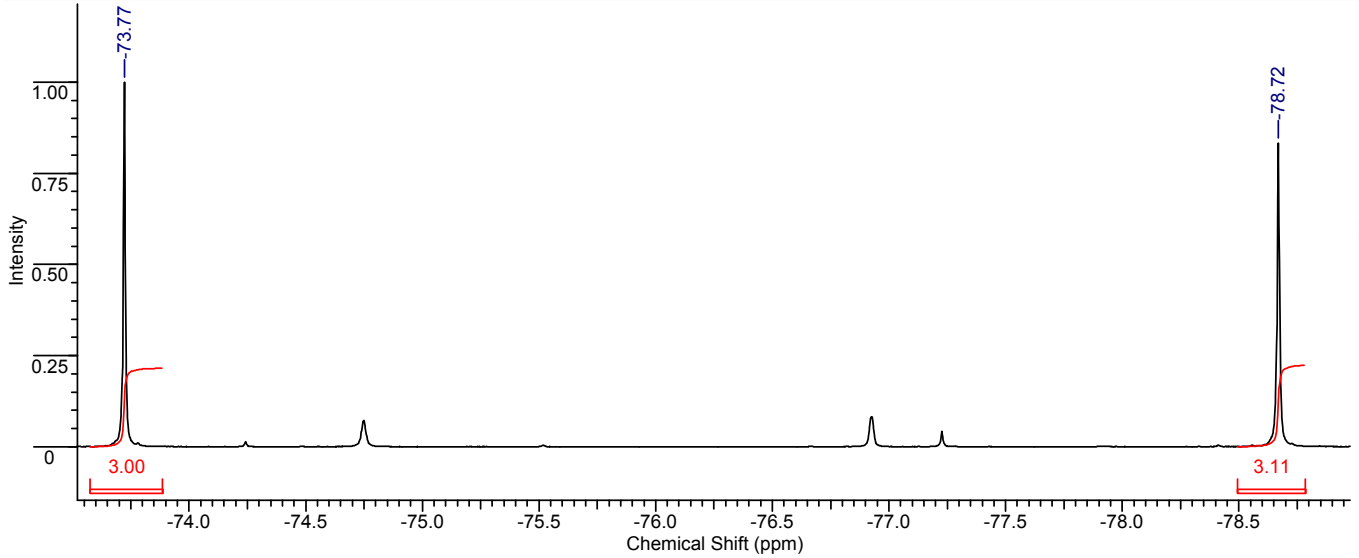
^{1}H NMR spectrum of (3*S**,4a*S**)-**3b** (400.1 MHz, $CDCl_3$)

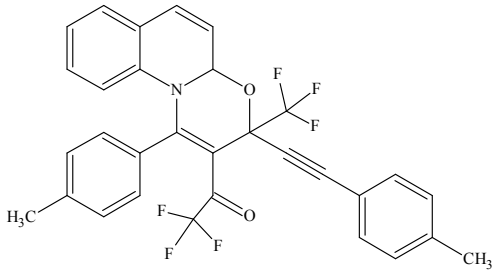
Acquisition Time (sec)	0.4999	***Comment***	Imported from UXNMR.			***Date***	14 Apr 2018 14:10:30
File Name	D:\Comp_316\BN\output\2018\04.àï ðåëü\BM-1347-2.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	72	***Original Points Count***	12076	***Points Count***	65536
Pulse Sequence	zgpg30	***Solvent***	DEUTERIUM OXIDE			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						

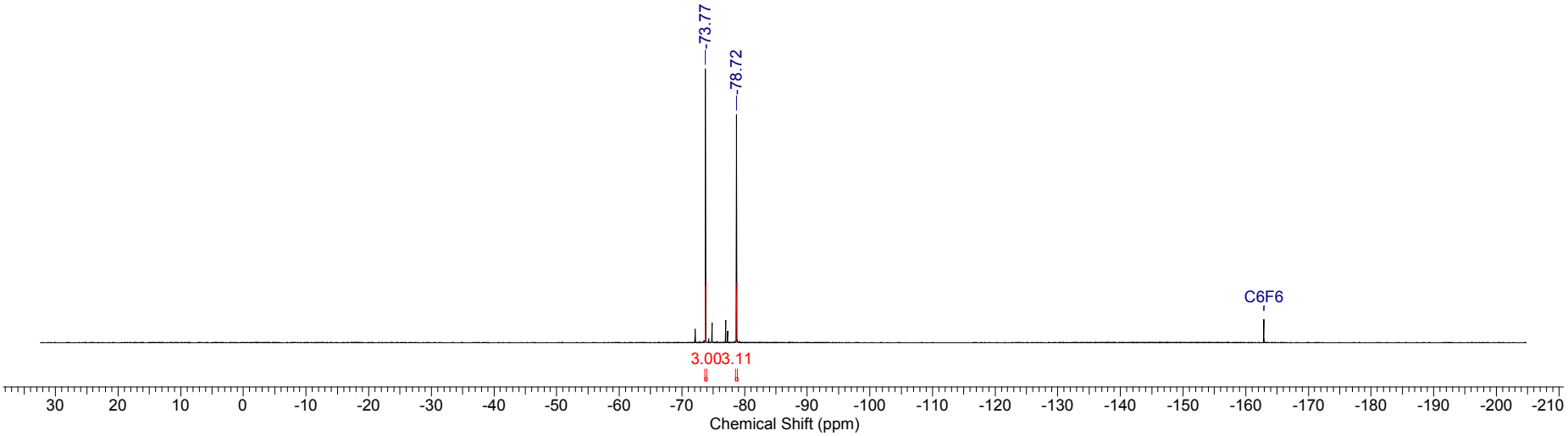


^{13}C NMR spectrum of (3*S**,4a*S**)-**3b** (100.6 MHz, $CDCl_3$)

Acquisition Time (sec)	1.5000	***Date***	Apr 16 2018				
File Name	D:\Comp_316\BN\DOC (BN)\vasiliy\SPEC_BM_F_2018.04.27\BM-1347-2_20180416_01\FLUORINE_01					***Frequency (MHz)***	376.31
Nucleus	19F	***Number of Transients***	16	***Original Points Count***	133929	***Points Count***	262144
Pulse Sequence	s2pul	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	89285.71	***Temperature (degree C)***	22.000

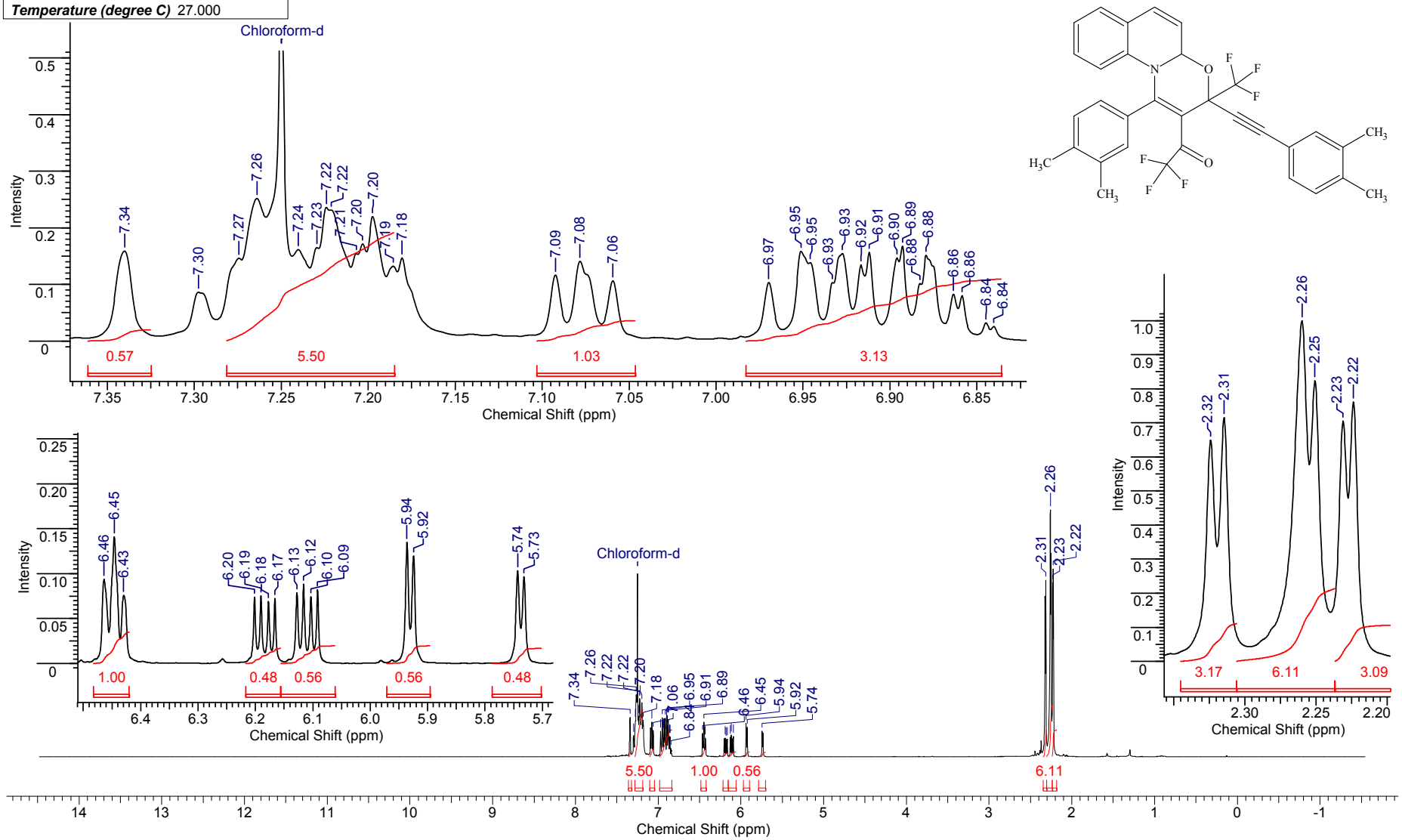






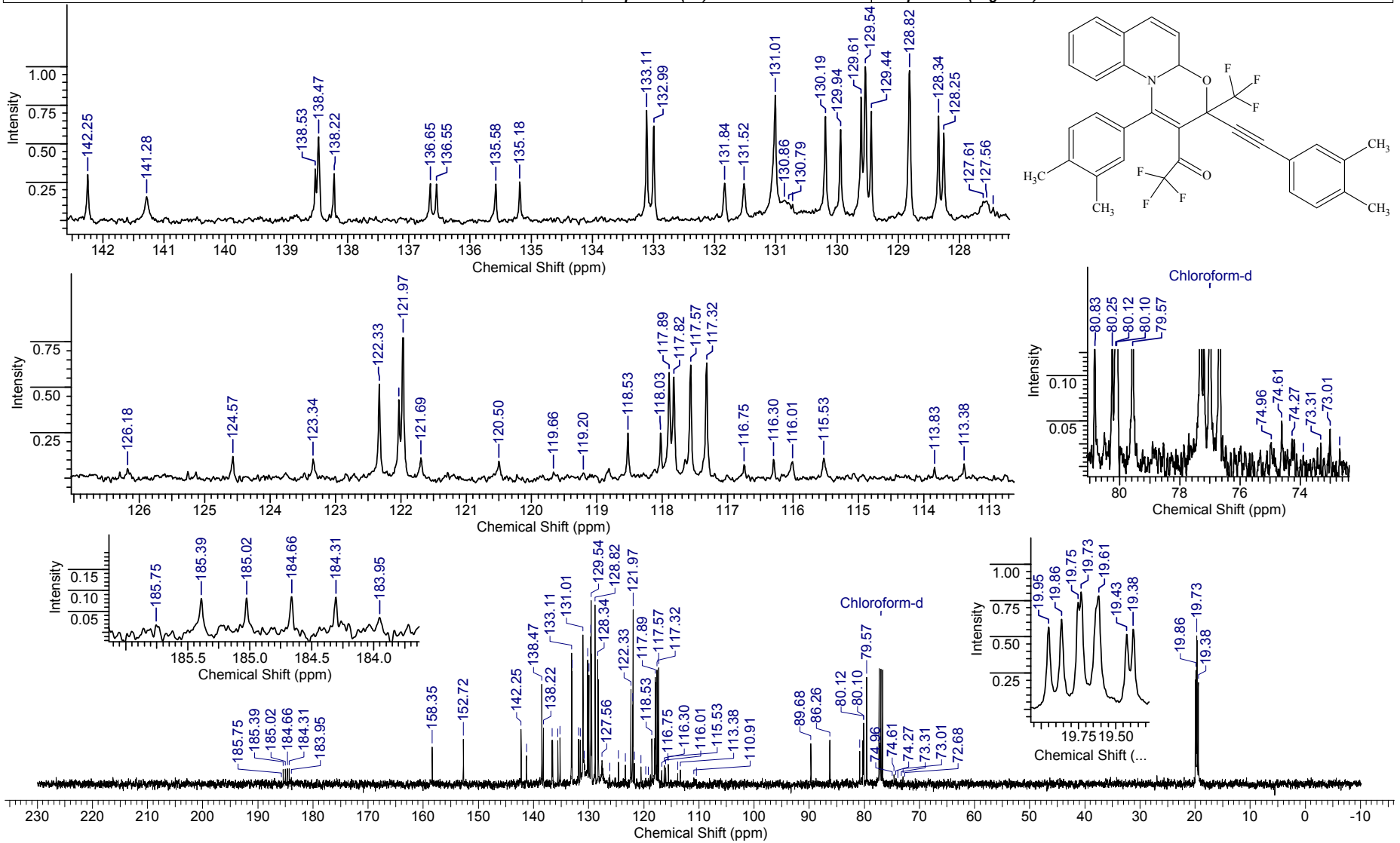
^{19}F NMR spectrum of (3*S**,4a*S**)-**3b** (376.3 MHz, $CDCl_3$)

Acquisition Time (sec)	2.5559	***Comment***	Imported from UXNMR.			***Date***	23 Apr 2018 15:47:18
File Name	D:\Comp_316\BN\output\2018\04.äï ðåëü\BM-1359.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	32	***Original Points Count***	16384	***Points Count***	65536
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	6410.26
Temperature (degree C)	27.000						



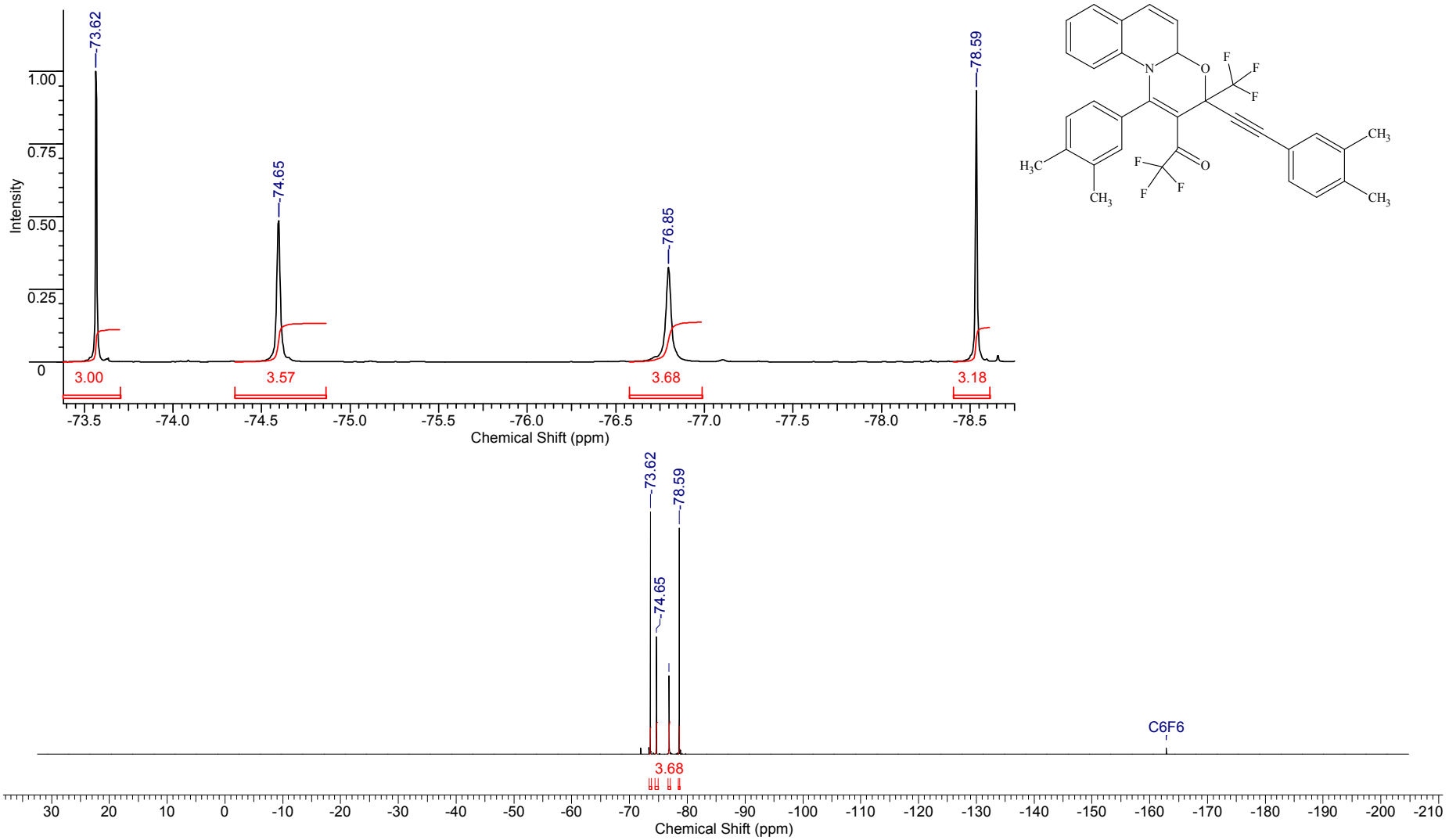
^{1}H NMR spectrum of **3c** (400.1 MHz, $CDCl_3$)

Acquisition Time (sec)	0.4999	***Comment***	Imported from UXNMR.			***Date***	23 Apr 2018 15:52:04
File Name	D:\Comp_316\BN\output\2018\04.äï ðåëü\BM-1359.C_002001r			***Frequency (MHz)***	100.61	***Nucleus***	13C
Number of Transients	129	***Original Points Count***	12076	***Points Count***	65536	***Pulse Sequence***	zgpg30
Solvent	DEUTERIUM OXIDE			***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000

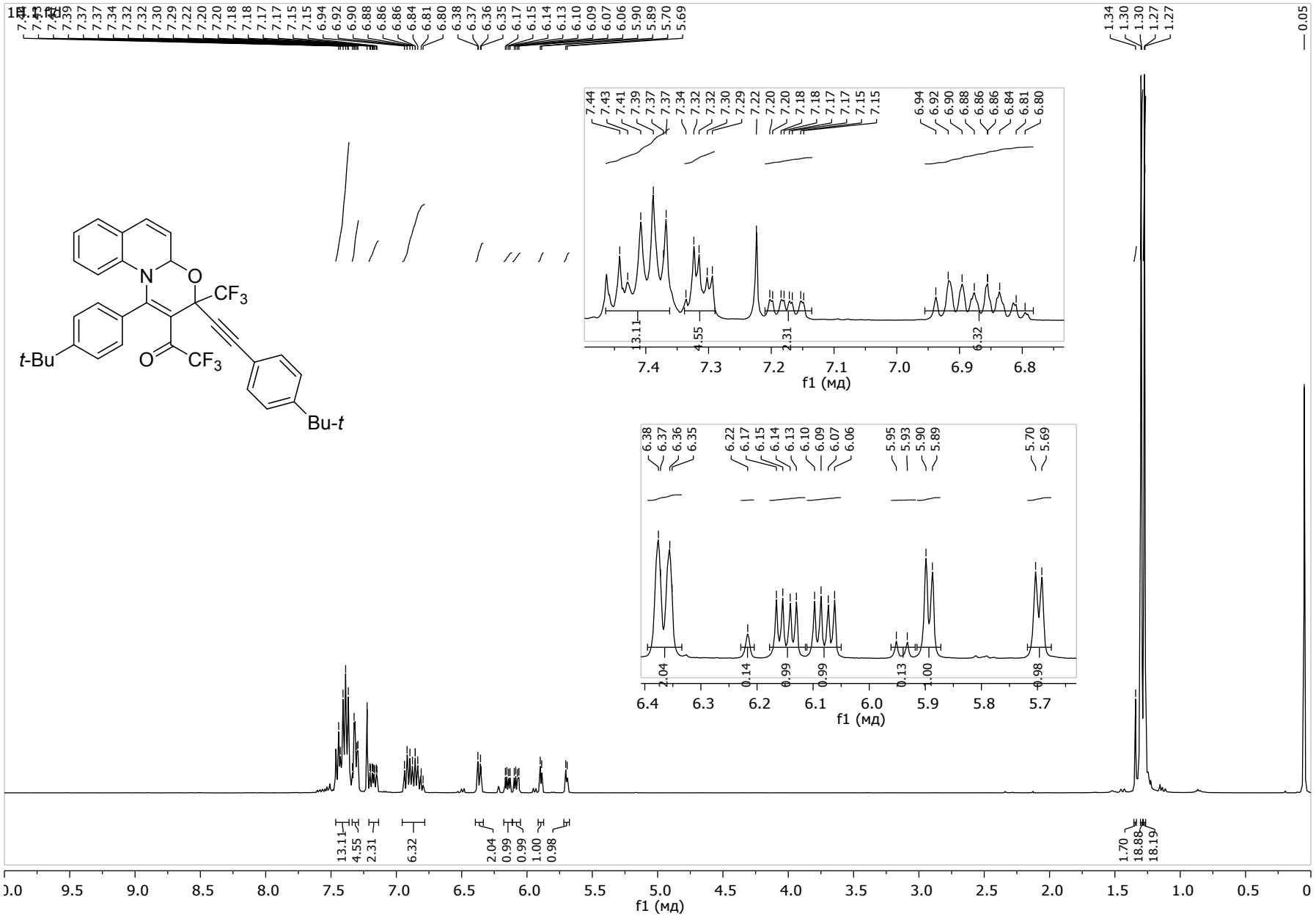


^{13}C NMR spectrum of **3c** (100.6 MHz, $CDCl_3$)

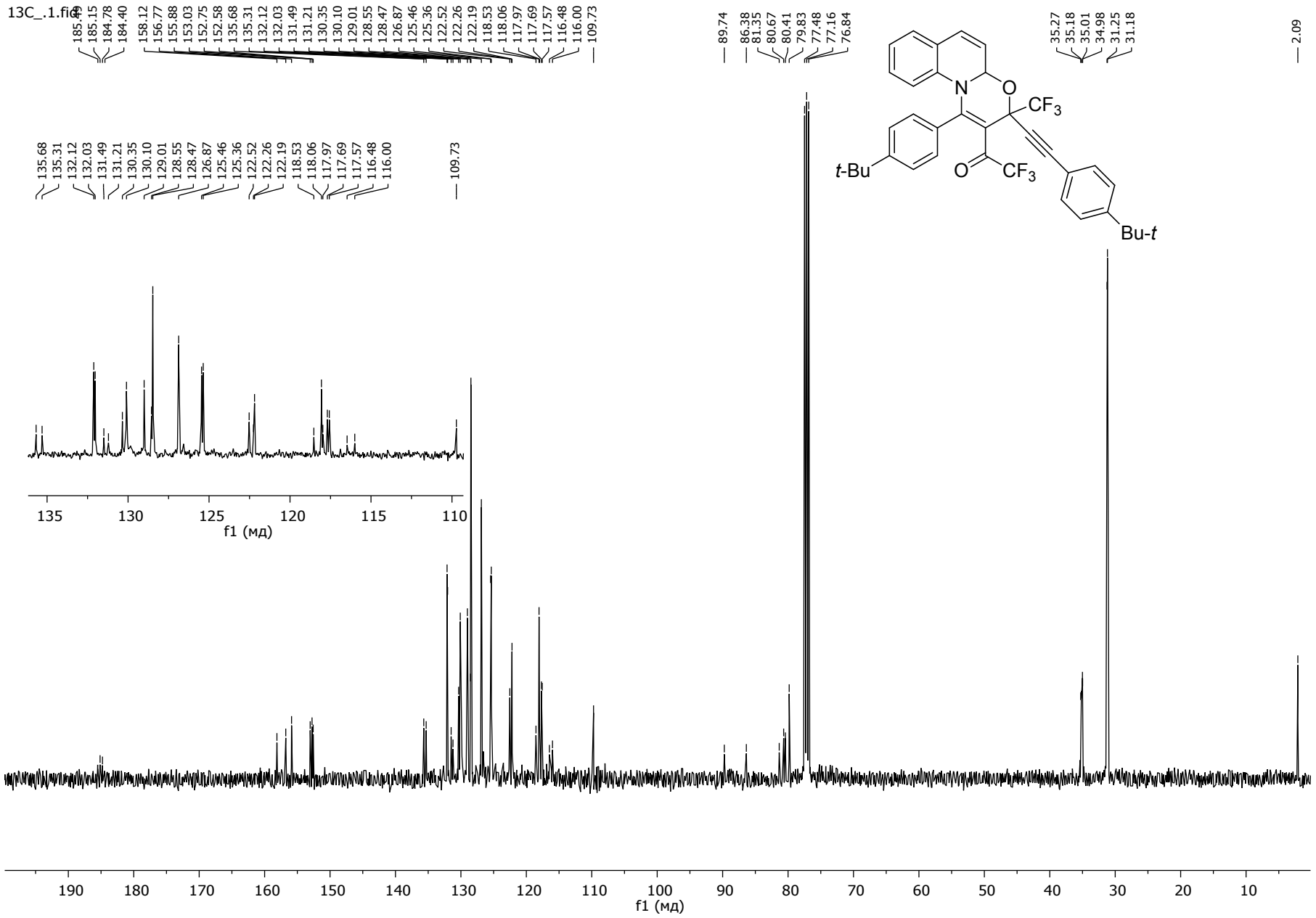
Acquisition Time (sec)	0.7340	***Date***	Apr 24 2018				
File Name	D:\Comp_316\BN\DOC (BN)\vasiliy\SPEC_BM_F_2018.04.27\bm1359-f_20180424_01\FLUORINE_01					***Frequency (MHz)***	376.31
Nucleus	19F	***Number of Transients***	100	***Original Points Count***	65536	***Points Count***	65536
Pulse Sequence	s2pul	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	89285.71
Temperature (degree C)	22.000						



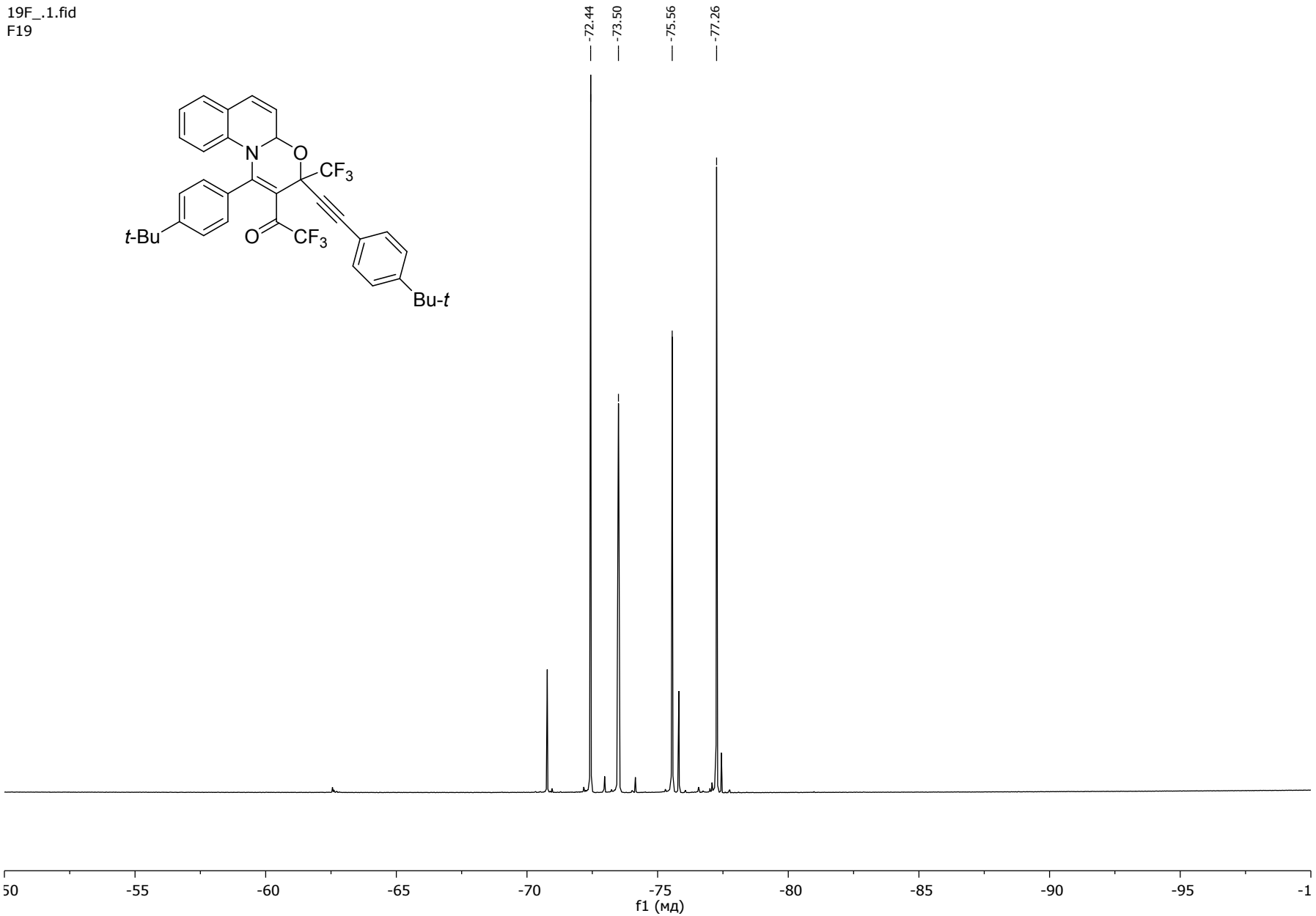
^{19}F NMR spectrum of **3c** (376.3 MHz, $CDCl_3$)



^{1}H NMR spectrum of **3d** (400.1 MHz, $CDCl_3$)

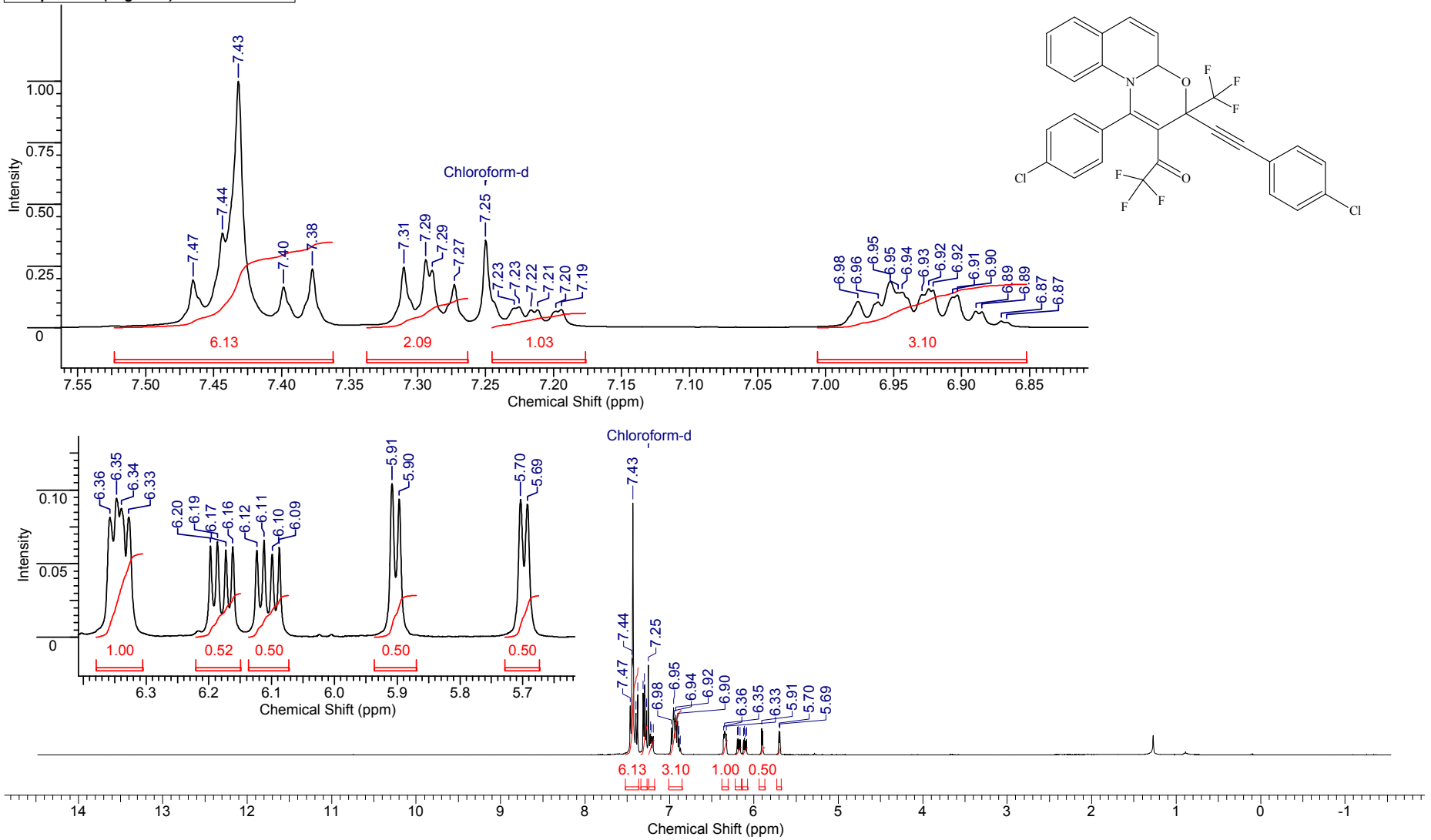


^{13}C NMR spectrum of **3d** (100.6 MHz, $CDCl_3$)



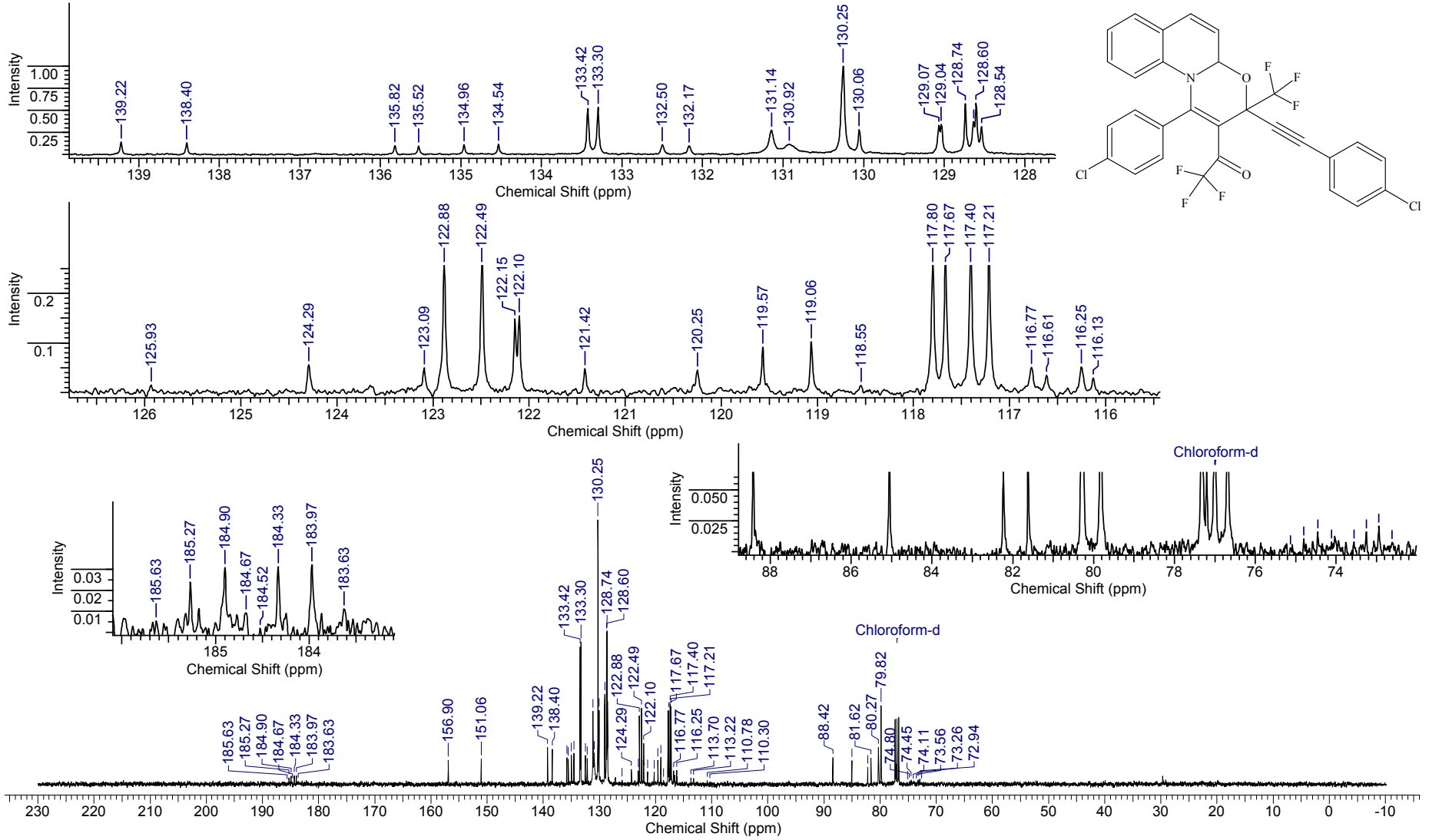
^{19}F NMR spectrum of **3d** (376.5 MHz, $CDCl_3$)

Acquisition Time (sec)	2.5559	***Comment***	Imported from UXNMR.			***Date***	14 Apr 2018 14:18:48
File Name	D:\Comp_316\BN\output\2018\04.äï ðåëü\BM-1339-2.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	16384	***Points Count***	65536
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	6410.26
Temperature (degree C)	27.000						



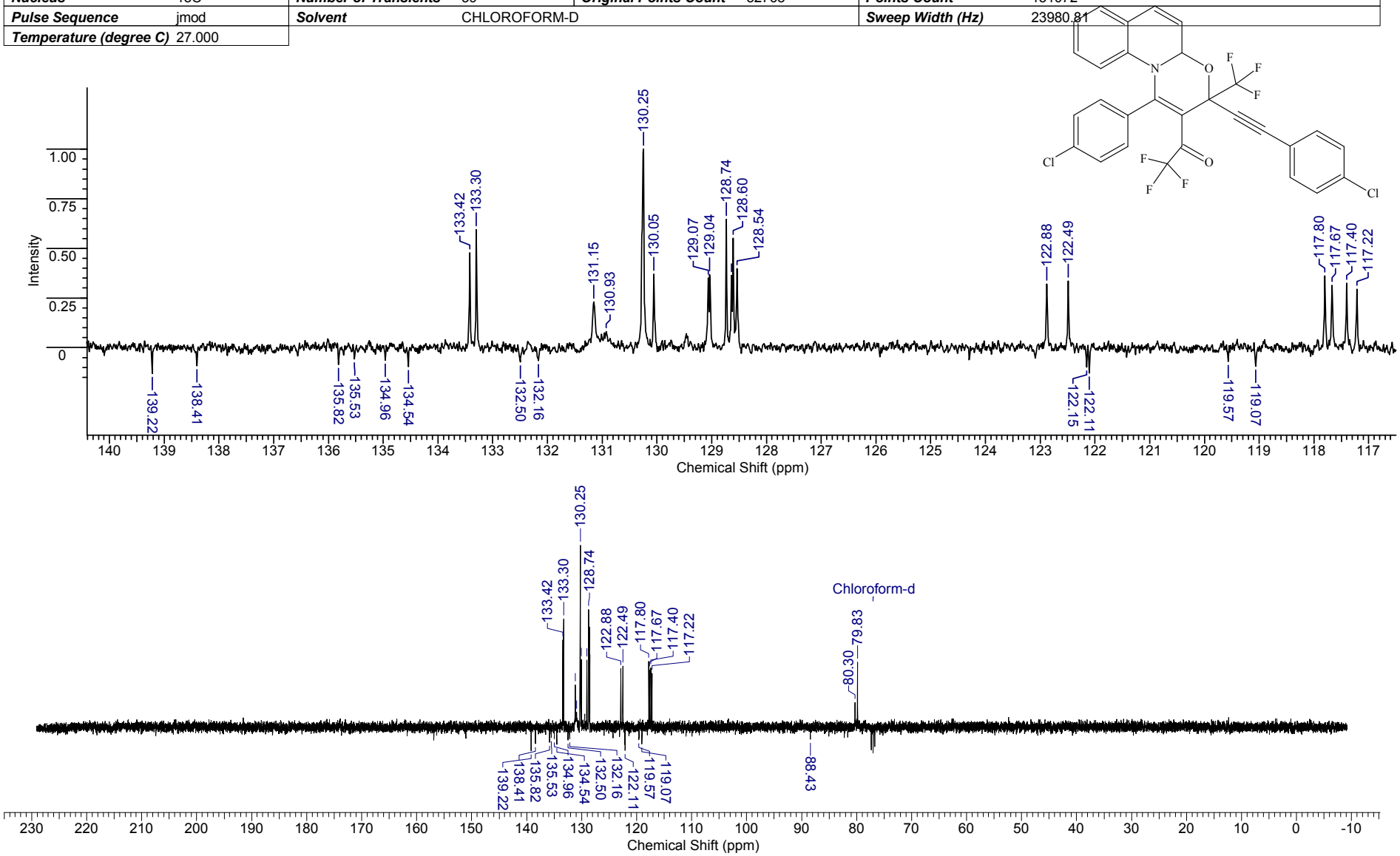
^{1}H NMR spectrum of **3e** (400.1 MHz, $CDCl_3$)

Acquisition Time (sec)	0.4999	***Comment***	Imported from UXNMR.			***Date***	14 Apr 2018 14:26:14
File Name	D:\Comp_316\BN\output\2018\04.äï ðåëü\BM-1339-2.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	262	***Original Points Count***	12076	***Points Count***	65536
Pulse Sequence	zgpg30	***Solvent***	DEUTERIUM OXIDE			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



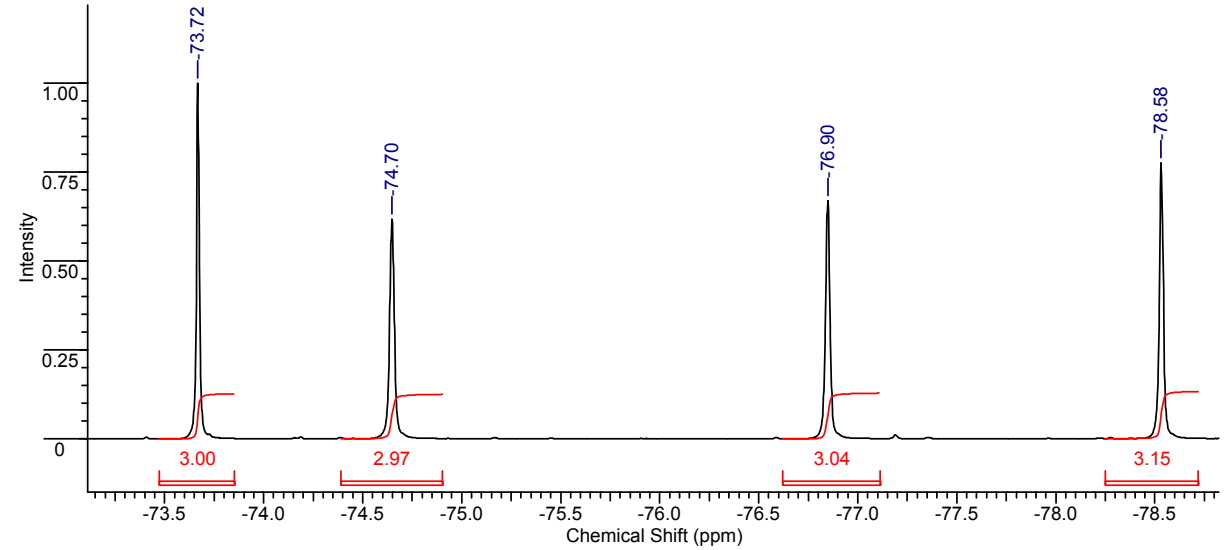
^{13}C NMR spectrum of **3e** (100.6 MHz, $CDCl_3$)

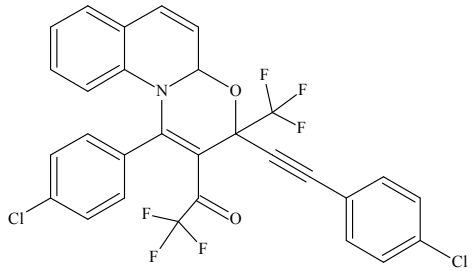
Acquisition Time (sec)	1.3664	***Comment***	Imported from UXNMR.			***Date***	25 May 2018 15:46:34
File Name	D:\Comp_316\BN\output\2018\05.ì àé\BM-1339-2.Capt_004001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	39	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	jmod	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	23980.81
Temperature (degree C)	27.000						

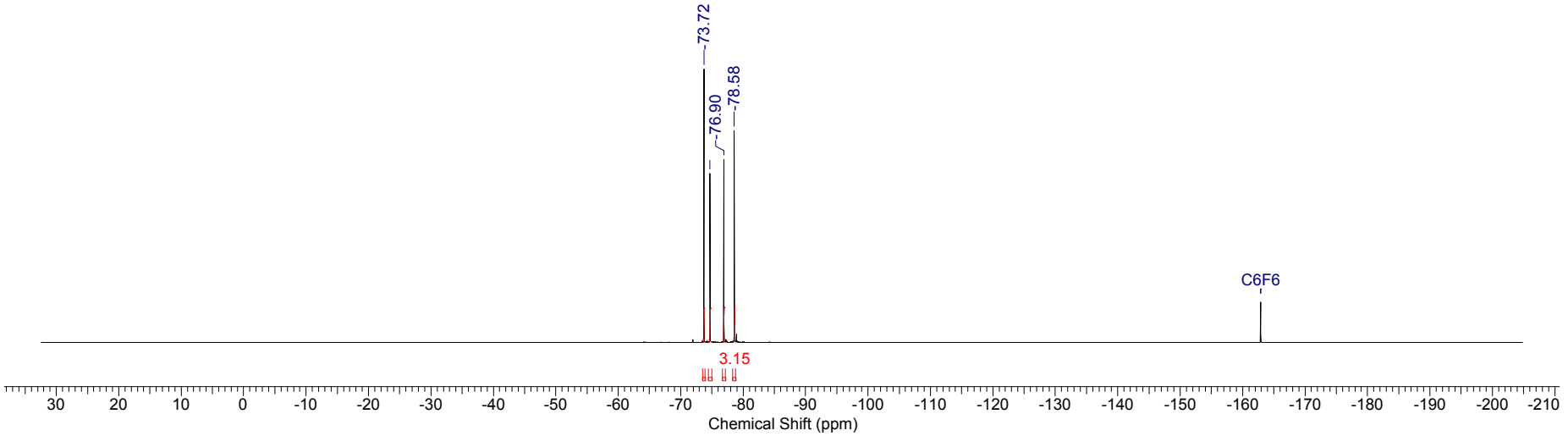


^{13}C NMR (APT) spectrum of **3e** (100.6 MHz, $CDCl_3$)

Acquisition Time (sec)	1.5000	***Date***	Apr 16 2018				
File Name	D:\Comp_316\BN\DOC (BN)\vasiliy\SPEC_BM_F_2018.04.27\BM-1339-2_20180416_01\FLUORINE_01					***Frequency (MHz)***	376.31
Nucleus	19F	***Number of Transients***	16	***Original Points Count***	133929	***Points Count***	262144
Pulse Sequence	s2pul	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	89285.71	***Temperature (degree C)***	22.000

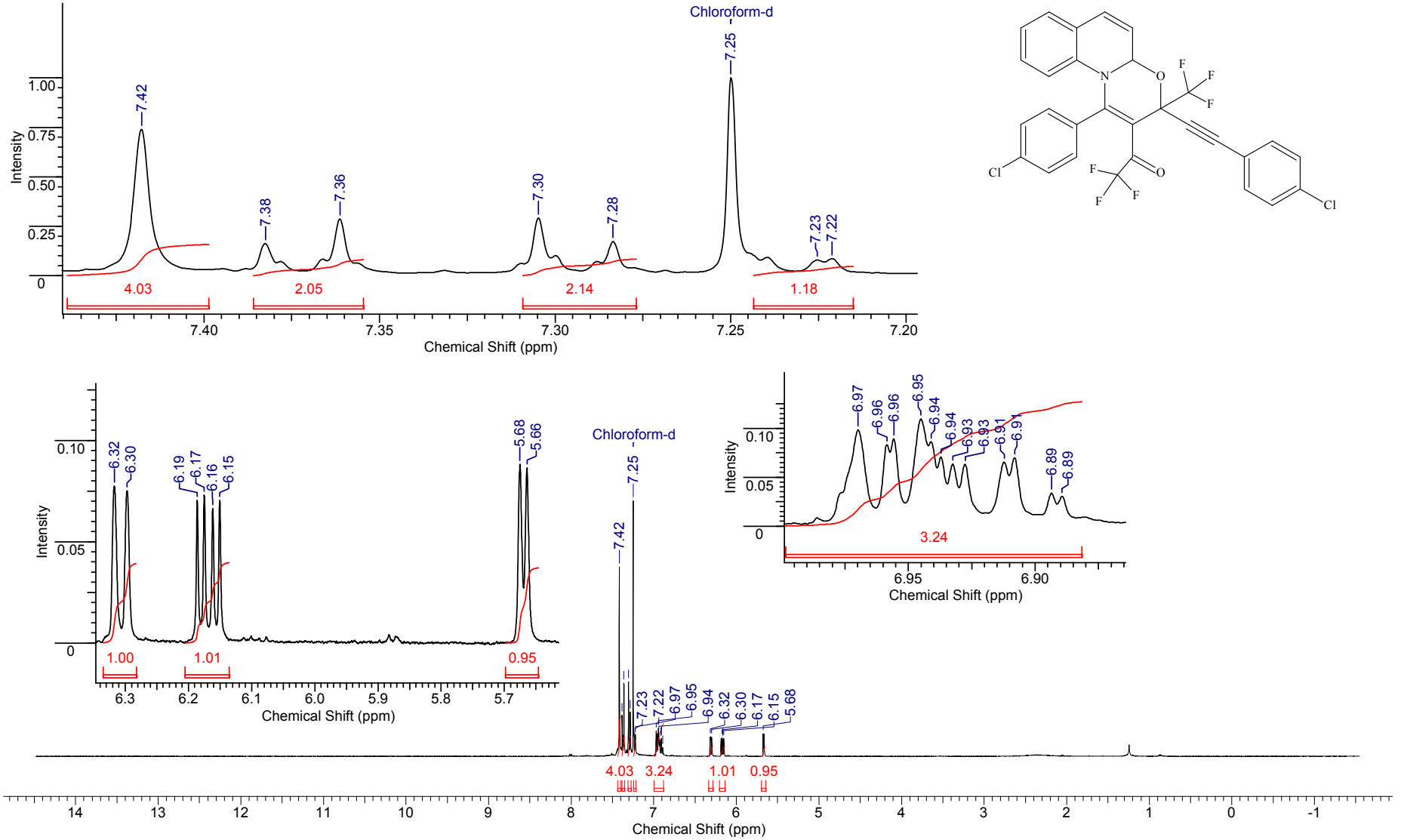






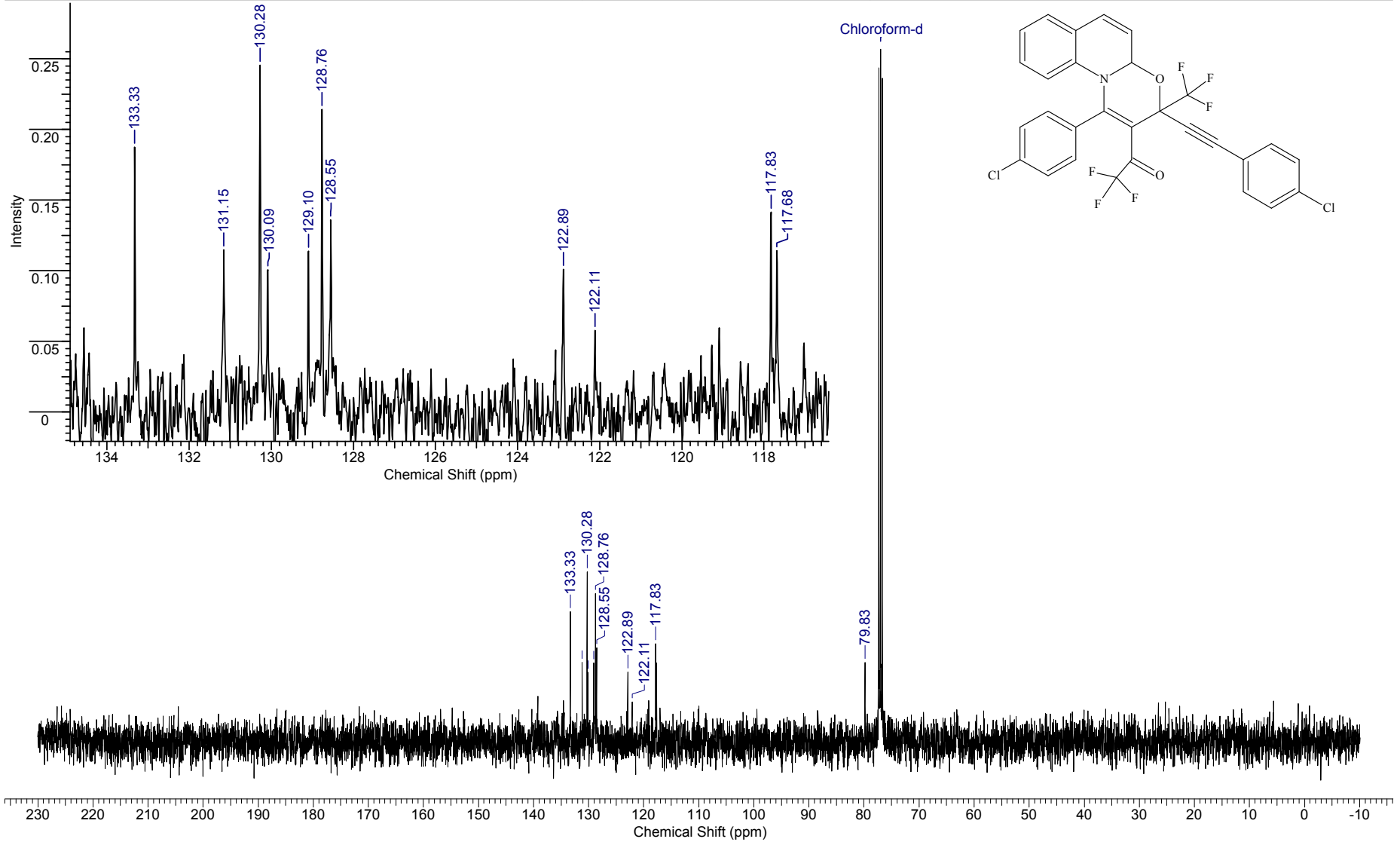
^{19}F NMR spectrum of **3e** (376.3 MHz, $CDCl_3$)

Acquisition Time (sec)	2.5559	***Comment***	Imported from UXNMR.	***Date***	21 May 2018 15:46:10
File Name	D:\Comp_316\BN\output\2018\05.ì àé\BM-1339-3.H_001001r	***Frequency (MHz)***	400.13	***Nucleus***	1H
Number of Transients	4	***Original Points Count***	16384	***Points Count***	65536	***Pulse Sequence***	zg30
Solvent	CHLOROFORM-D	***Sweep Width (Hz)***	6410.26	***Temperature (degree C)***	27.000



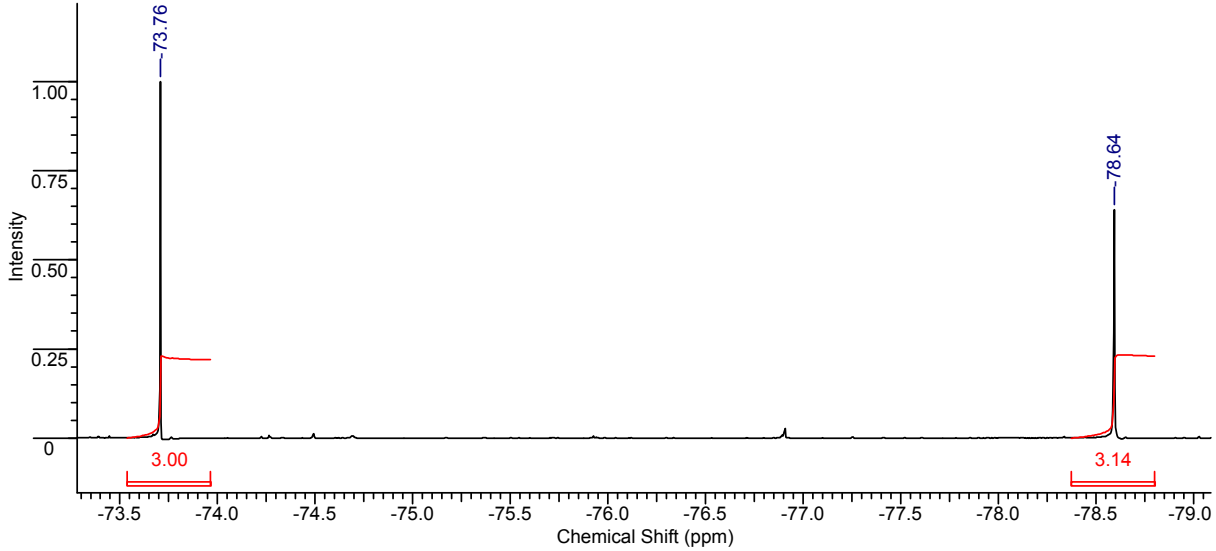
^{1}H NMR spectrum of (3*S**,4a*S**)-**3e** (400.1 MHz, $CDCl_3$)

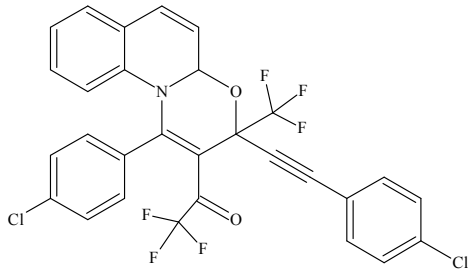
Acquisition Time (sec)	0.4999	***Comment***	Imported from UXNMR.			***Date***	21 May 2018 15:51:26
File Name	D:\Comp_316\BN\output\2018\05.ì àé\BM-1339-3.C_002001r			***Frequency (MHz)***	100.61	***Nucleus***	13C
Number of Transients	133	***Original Points Count***	12076	***Points Count***	65536	***Pulse Sequence***	zgpg30
Solvent	DEUTERIUM OXIDE			***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000

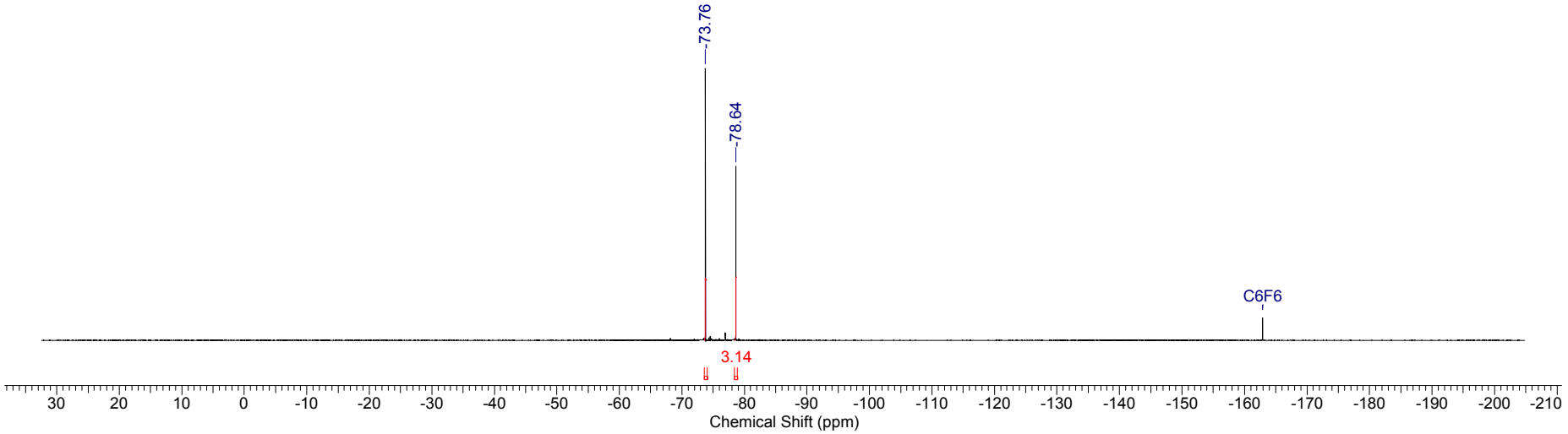


^{13}C NMR spectrum of (3*S**,4a*S**)-**3e** (100.6 MHz, $CDCl_3$)

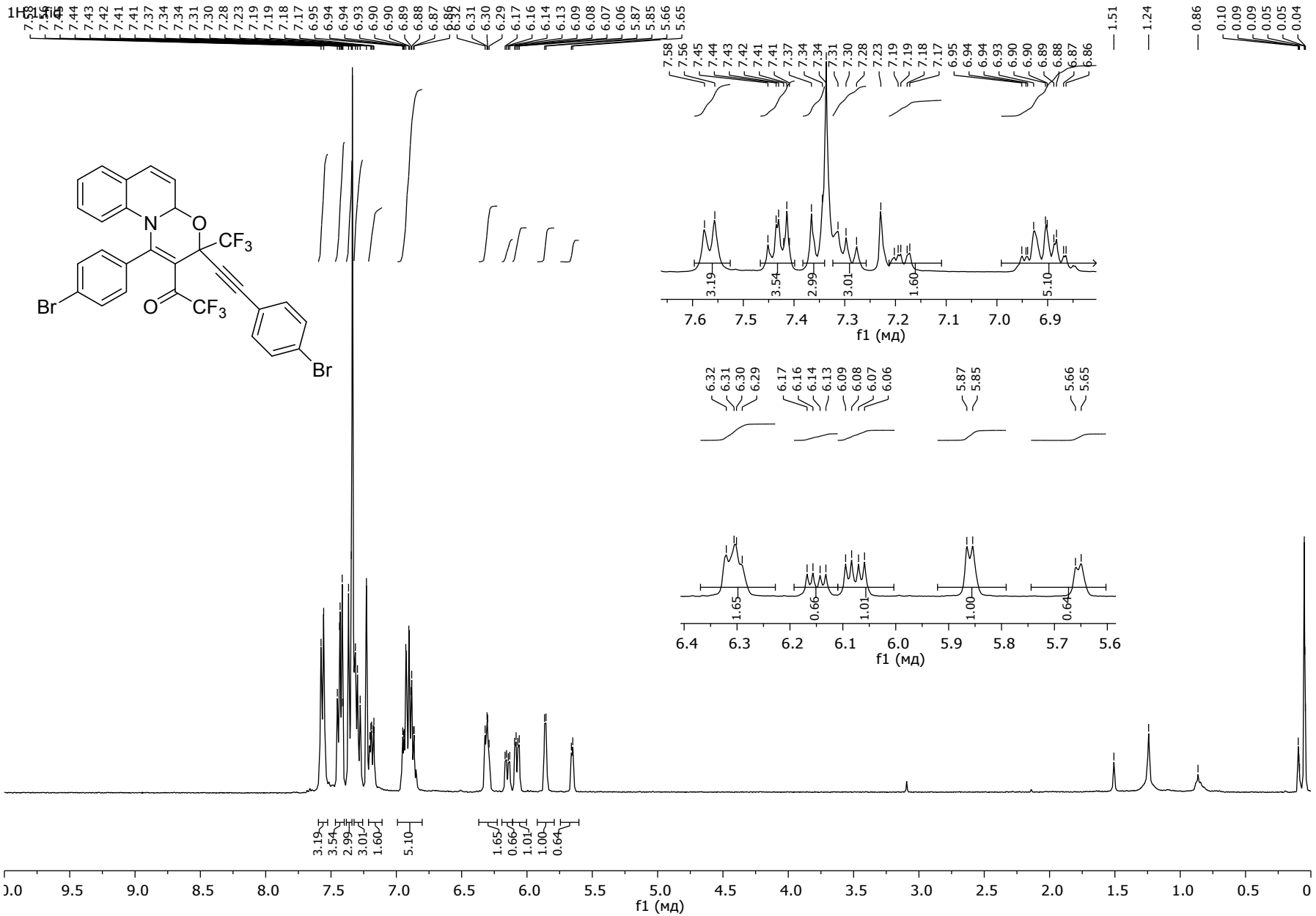
Acquisition Time (sec)	0.7340	***Date***	May 22 2018	***File Name***	D:\Comp_316\BN\output\F19\F_2018\2018.05.22\bm1339-3-f_20180522_01\FLUORINE_01		
Frequency (MHz)	376.31	***Nucleus***	19F	***Number of Transients***	1000	***Original Points Count***	65536
Points Count	65536	***Pulse Sequence***	s2pul	***Solvent***	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	***Temperature (degree C)***	22.000				



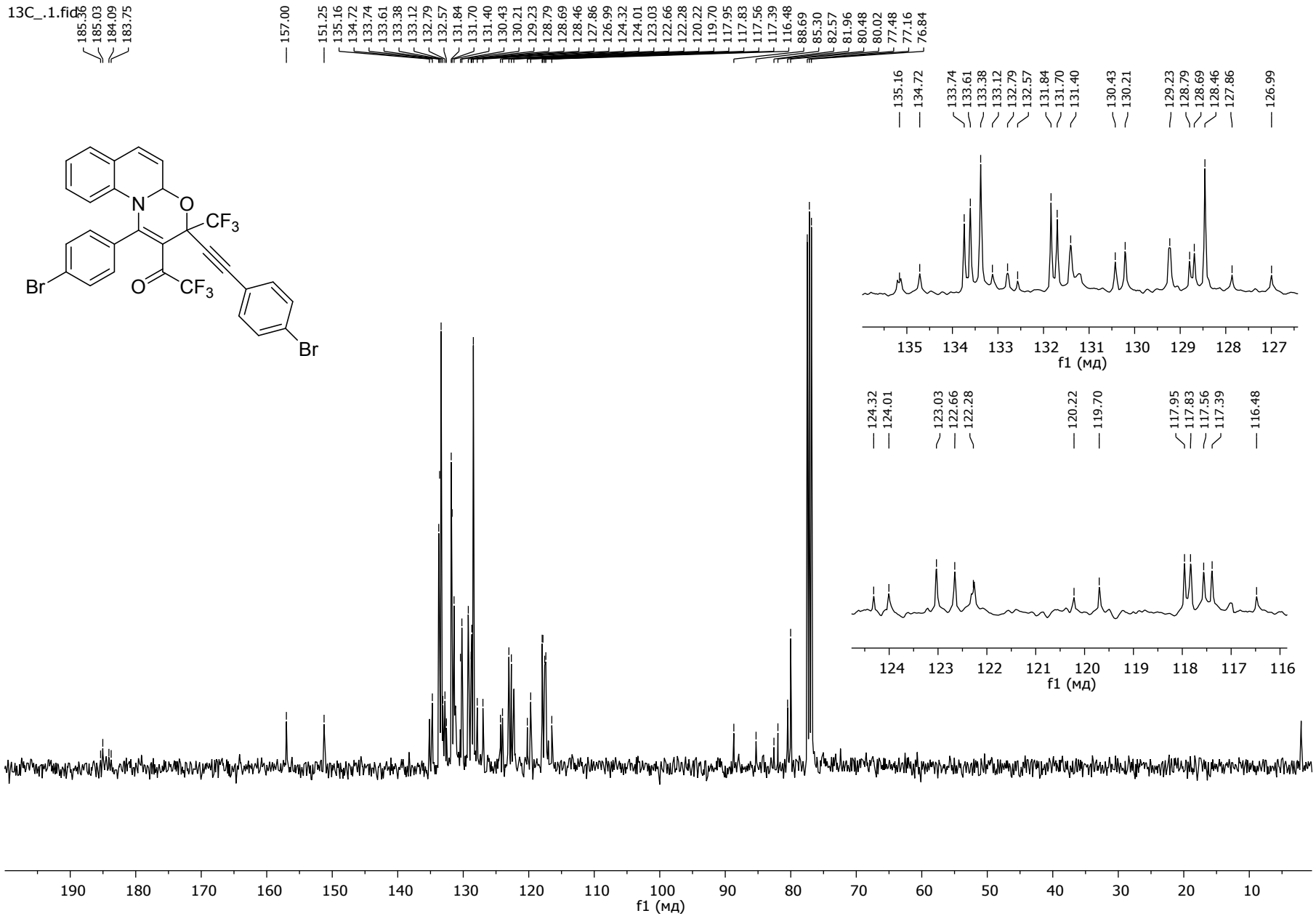




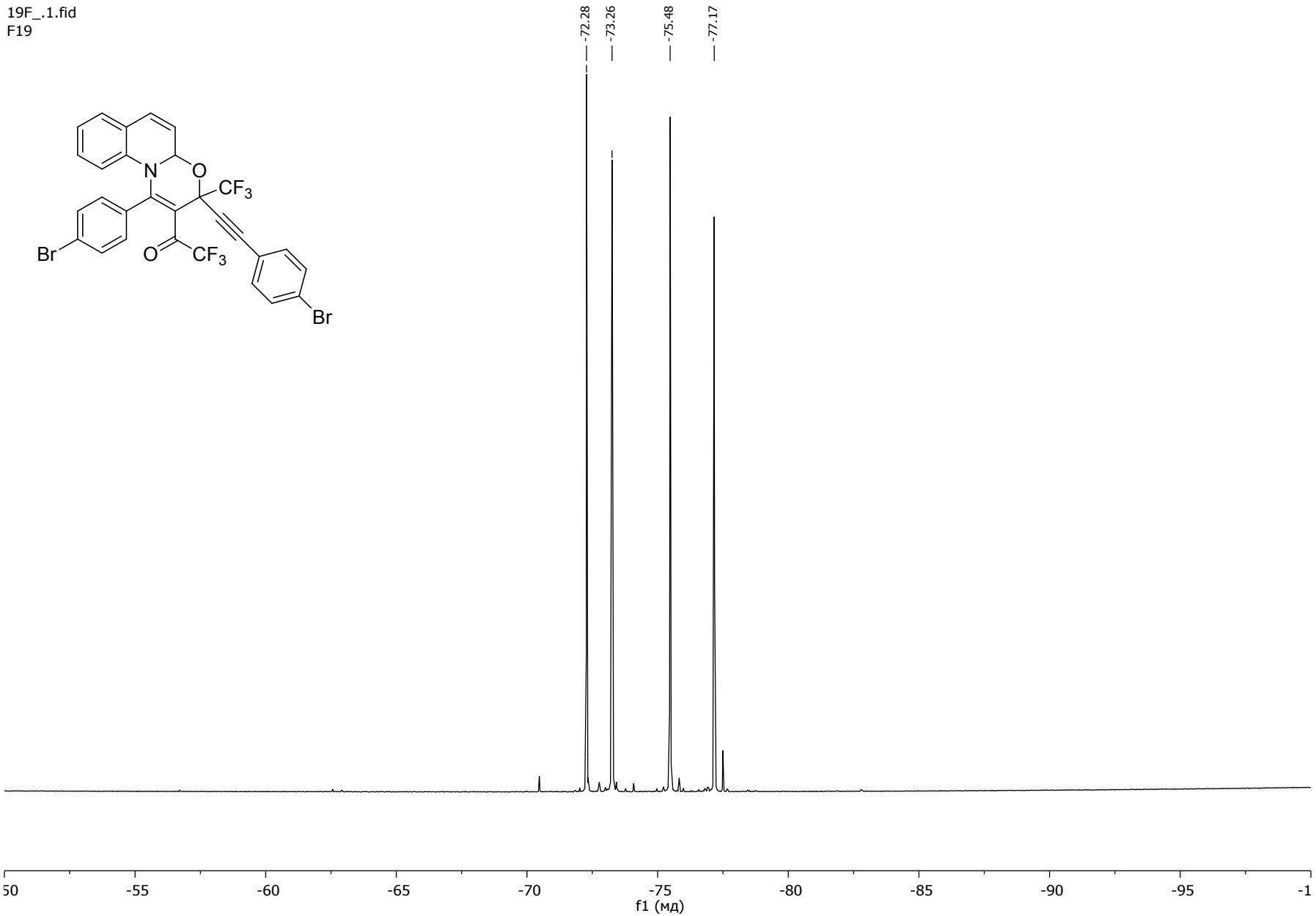
^{19}F NMR spectrum of (3*S**,4a*S**)-**3e** (376.3 MHz, $CDCl_3$)



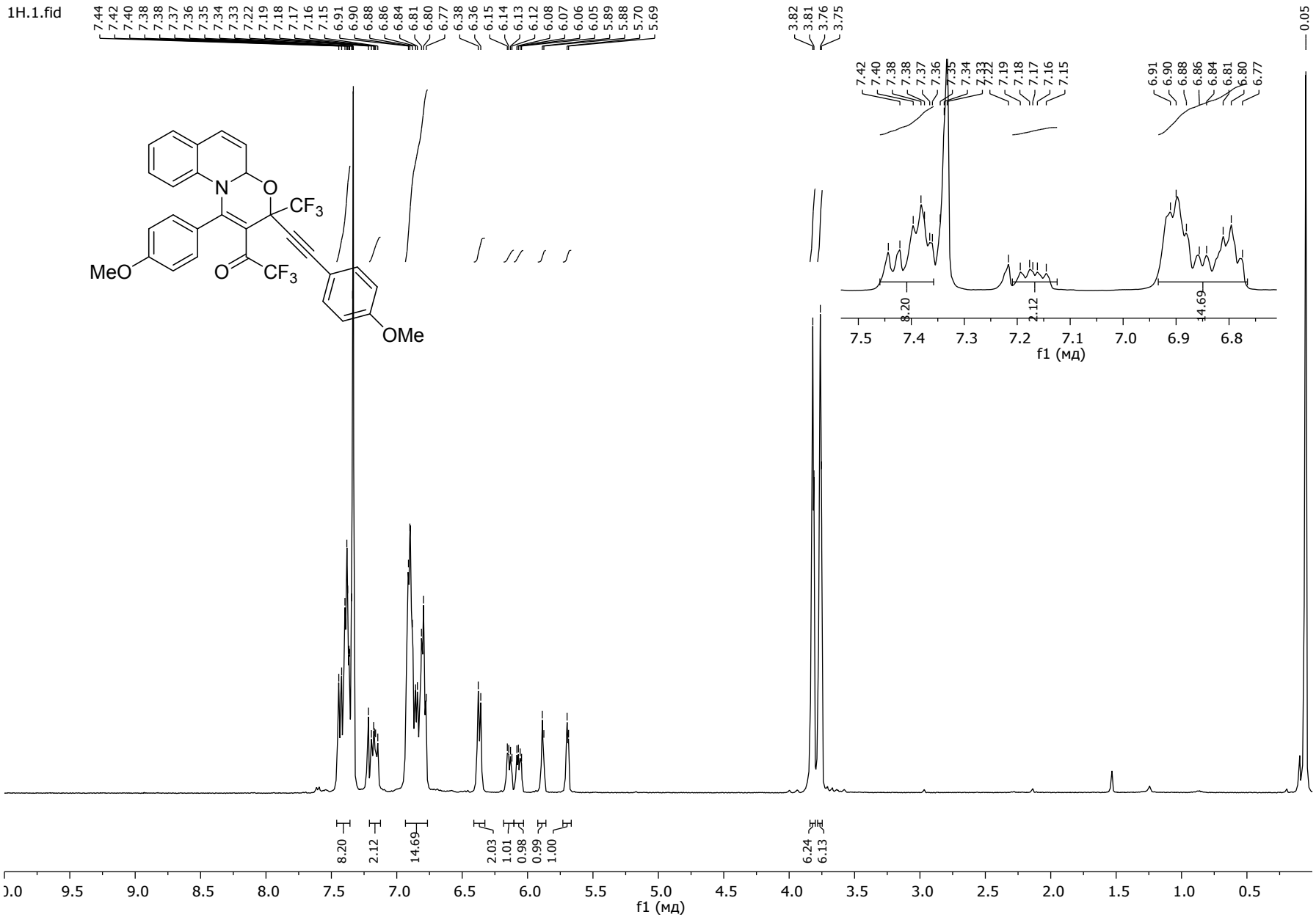
^{1}H NMR spectrum of **3f** (400.1 MHz, $CDCl_3$)



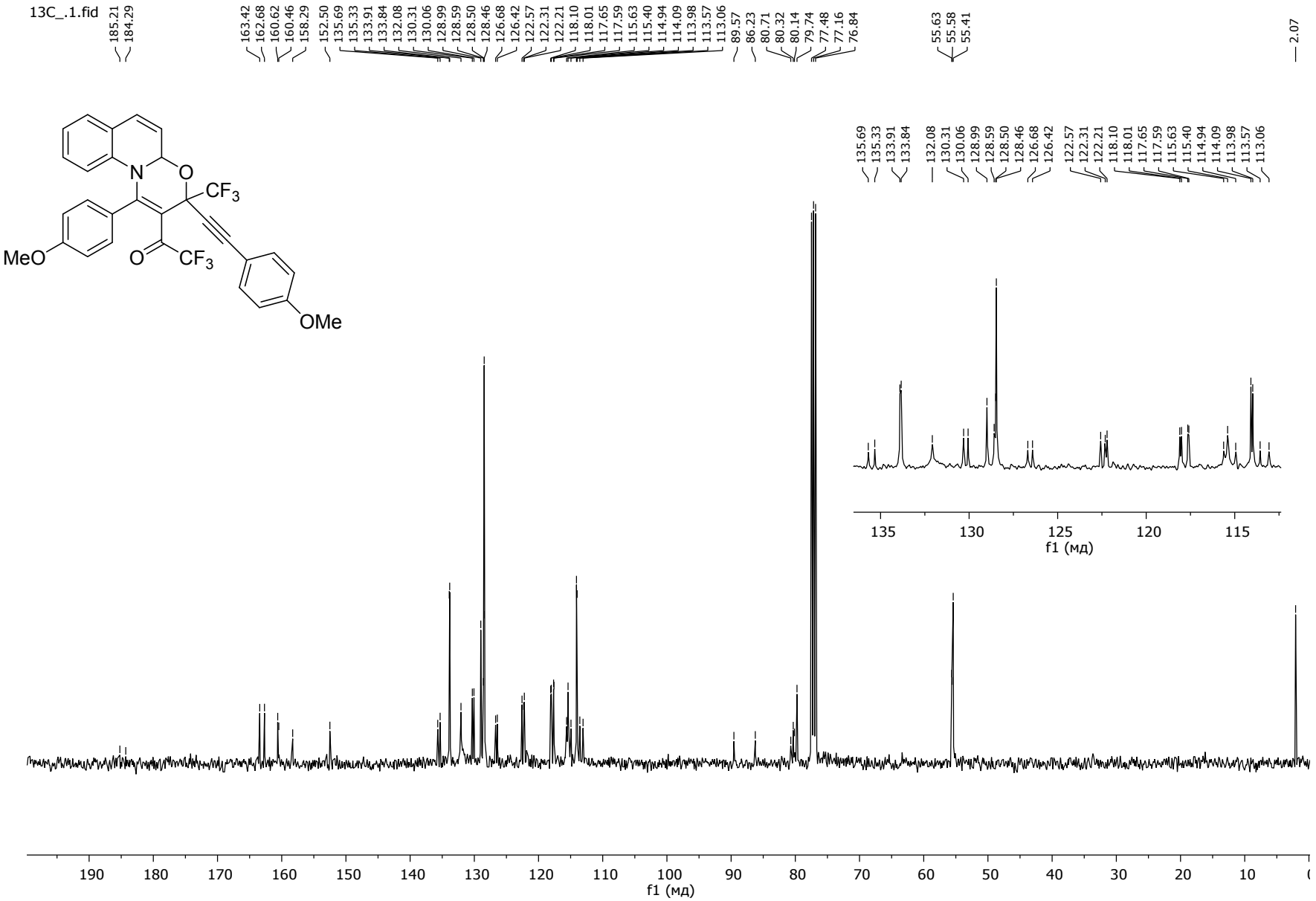
^{13}C NMR spectrum of **3f** (100.6 MHz, $CDCl_3$)



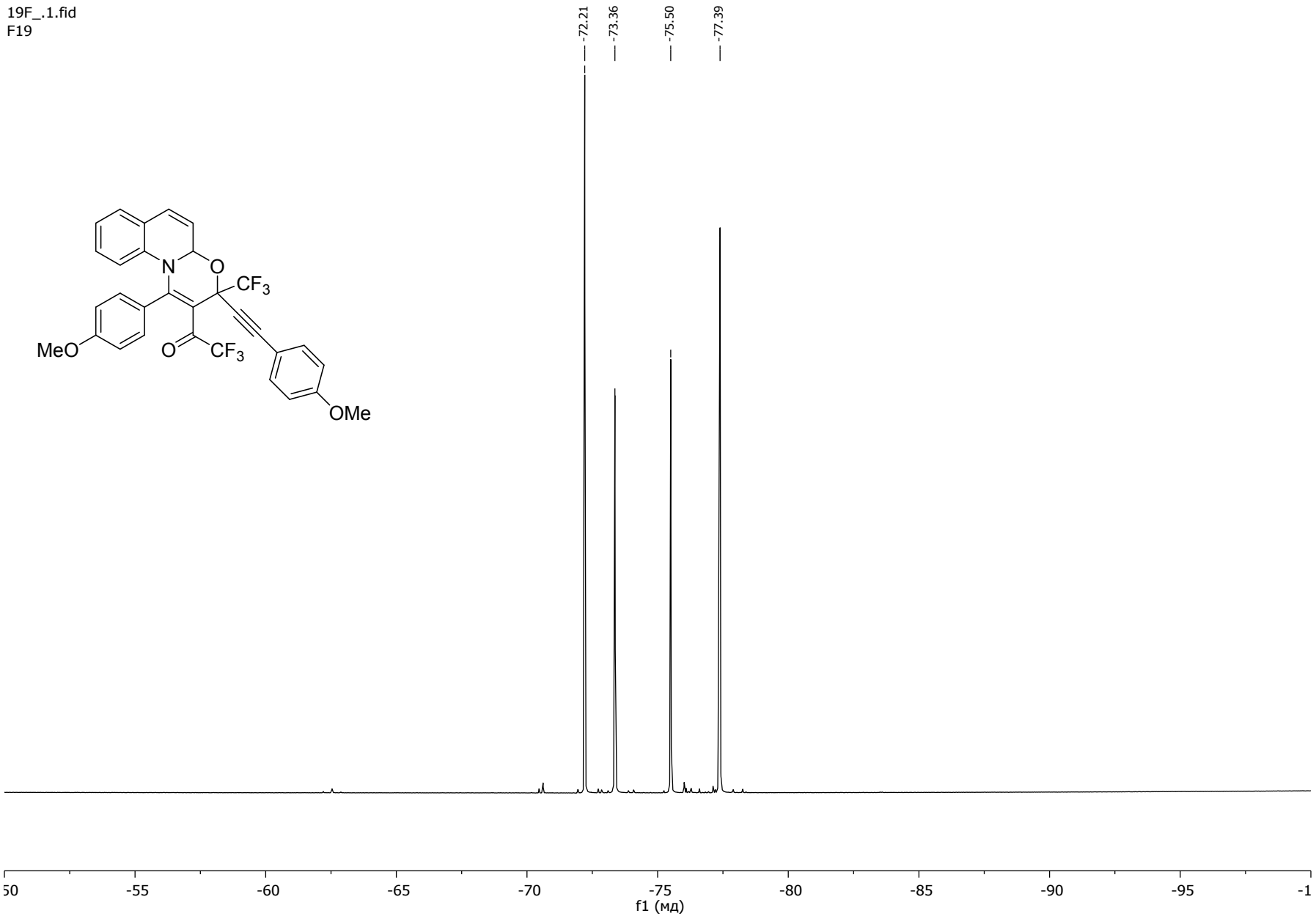
^{19}F NMR spectrum of **3f** (376.5 MHz, $CDCl_3$)



^{1}H NMR spectrum of **3g** (400.1 MHz, $CDCl_3$)

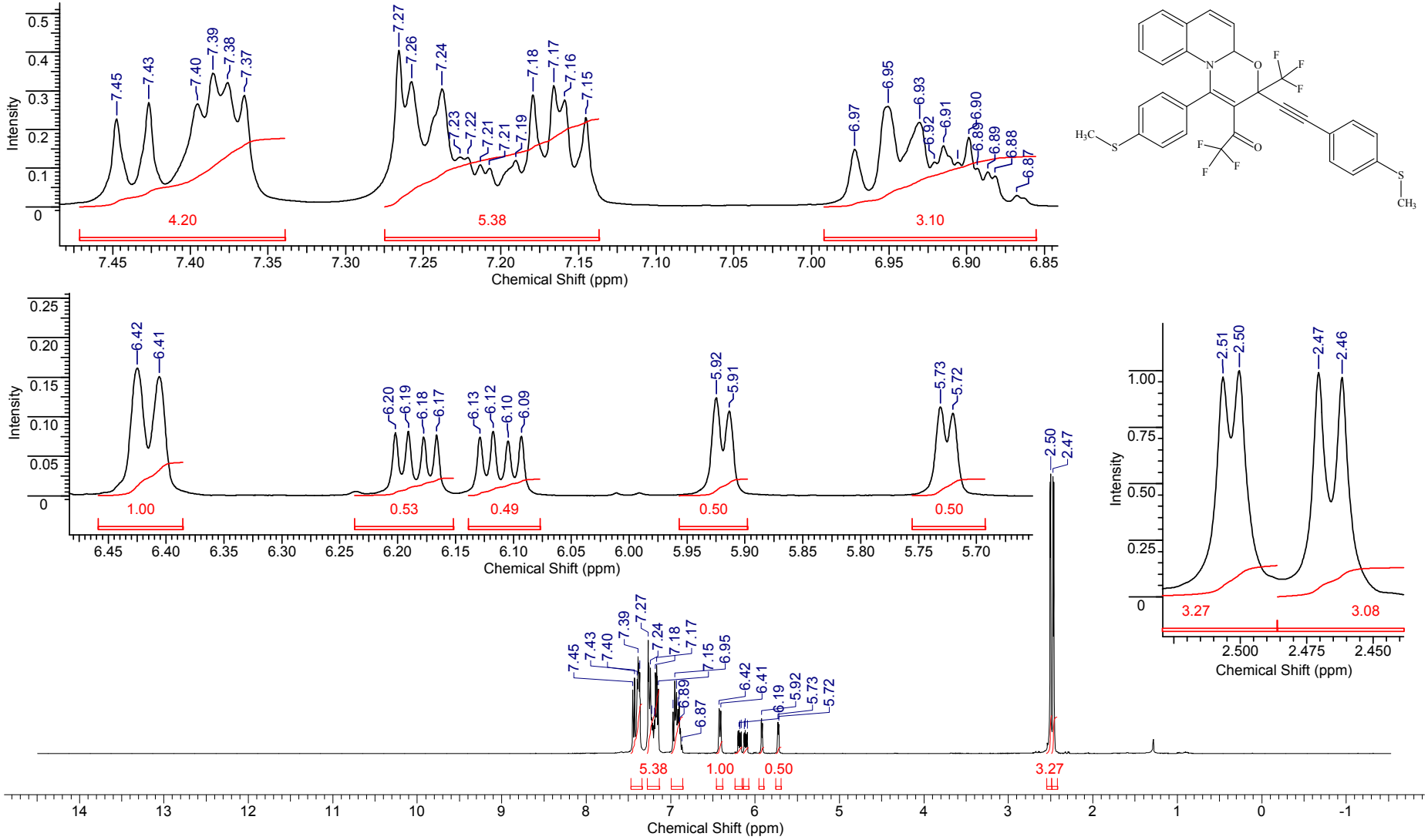


^{13}C NMR spectrum of **3g** (100.6 MHz, $CDCl_3$)



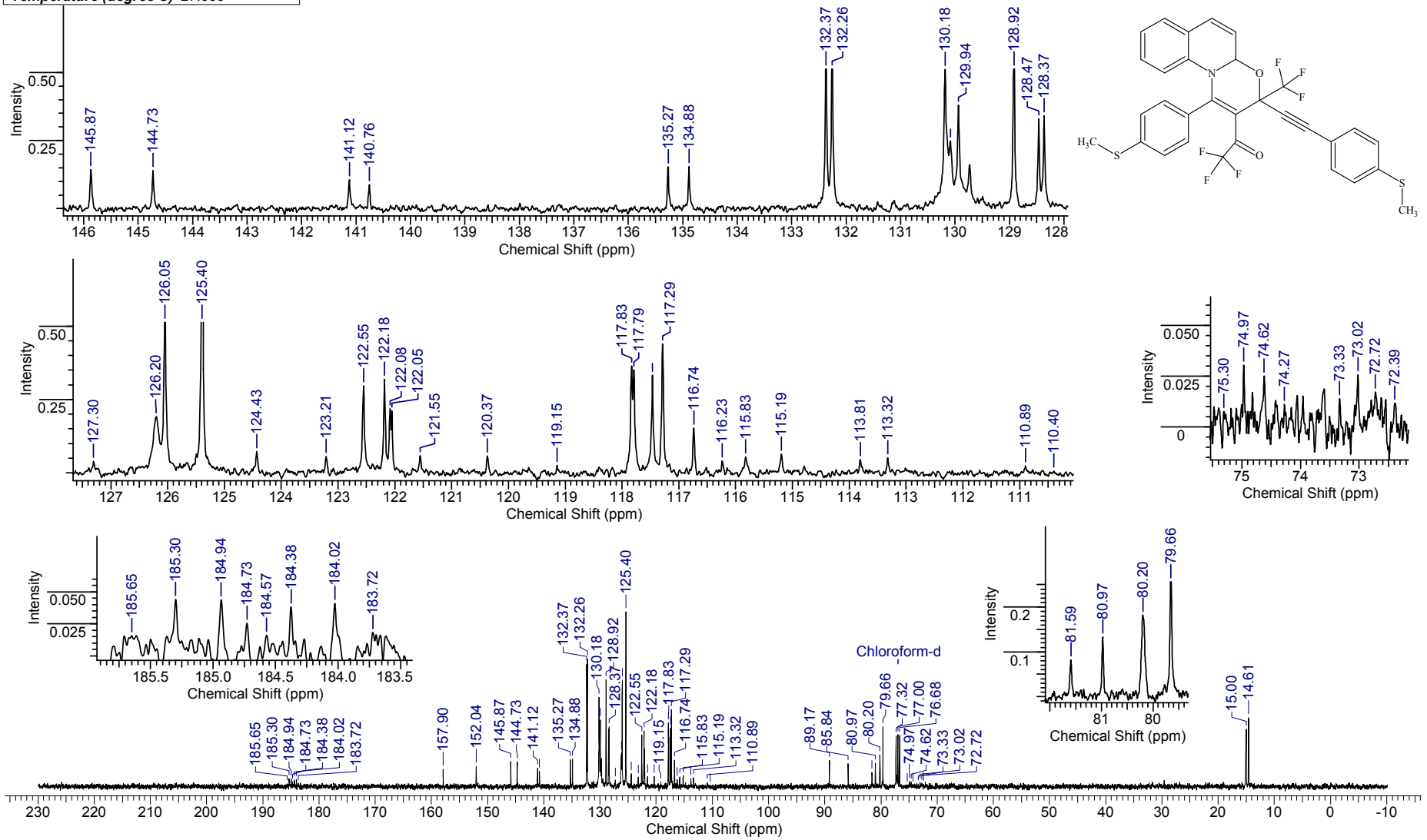
^{19}F NMR spectrum of **3g** (376.5 MHz, $CDCl_3$)

Acquisition Time (sec)	2.5559	***Comment***	Imported from UXNMR.			***Date***	14 Apr 2018 14:11:54
File Name	D:\Comp_316\BN\output\2018\04.äï ðåëü\BM-1341-2.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	16384	***Points Count***	65536
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	6410.26
Temperature (degree C)	27.000						



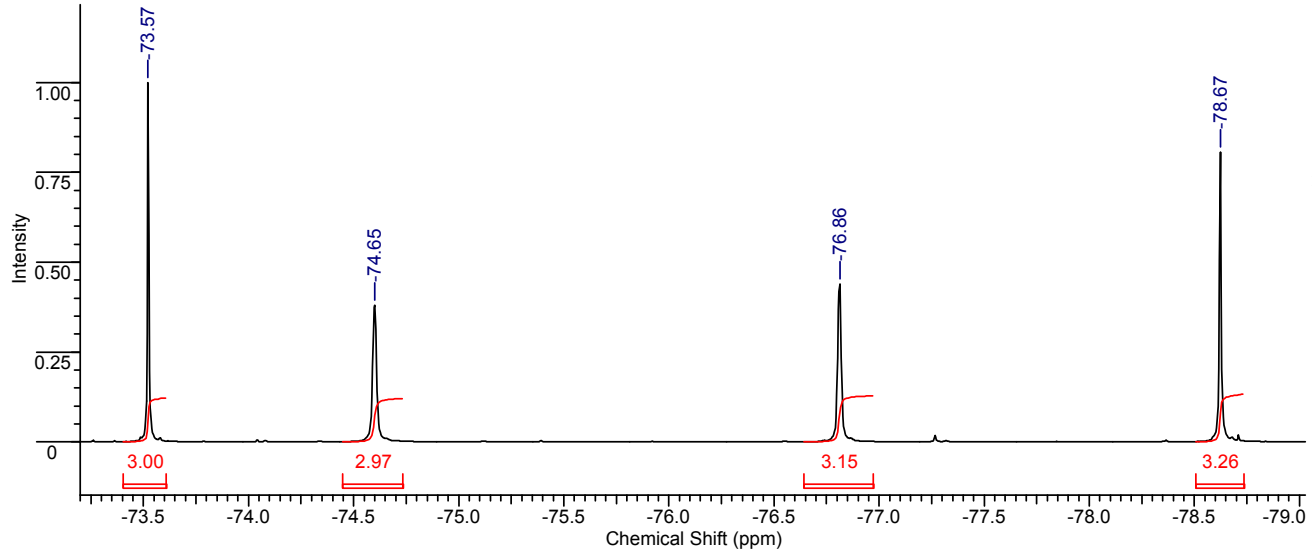
^{1}H NMR spectrum of **3h** (400.1 MHz, $CDCl_3$)

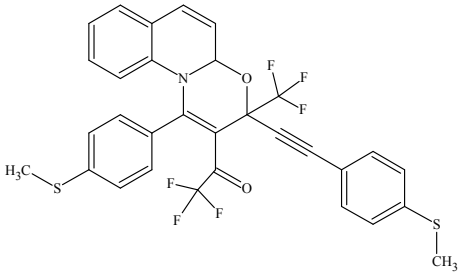
Acquisition Time (sec)	0.4999	***Comment***	Imported from UXNMR.			***Date***	14 Apr 2018 14:17:12
File Name	D:\Comp_316\BN\output\2018\04.äï ðåëü\BM-1341-2.H_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	170	***Original Points Count***	12076	***Points Count***	65536
Pulse Sequence	zgpg30	***Solvent***	DEUTERIUM OXIDE			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						

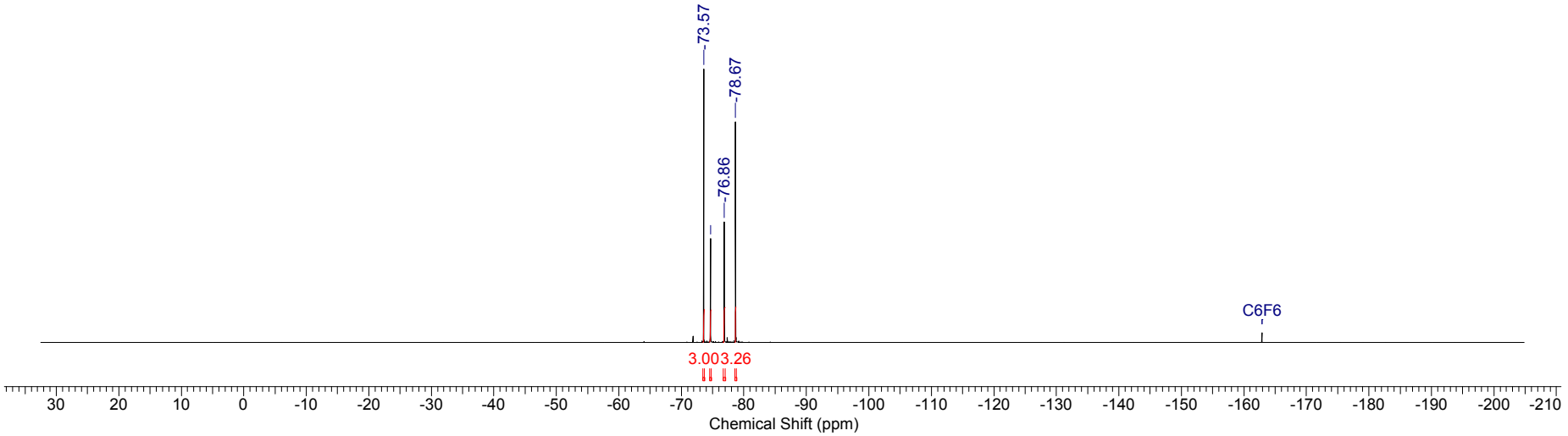


^{13}C NMR spectrum of **3h** (100.6 MHz, $CDCl_3$)

Acquisition Time (sec)	0.7340	***Date***	Apr 17 2018				
File Name	D:\Comp_316\BN\DOC (BN)\vasiliy\SPEC_BM_F_2018.04.27\bm1341-2-f_20180417_01\FLUORINE_01					***Frequency (MHz)***	376.31
Nucleus	19F	***Number of Transients***	100	***Original Points Count***	65536	***Points Count***	65536
Pulse Sequence	s2pul	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	89285.71	***Temperature (degree C)***	22.000

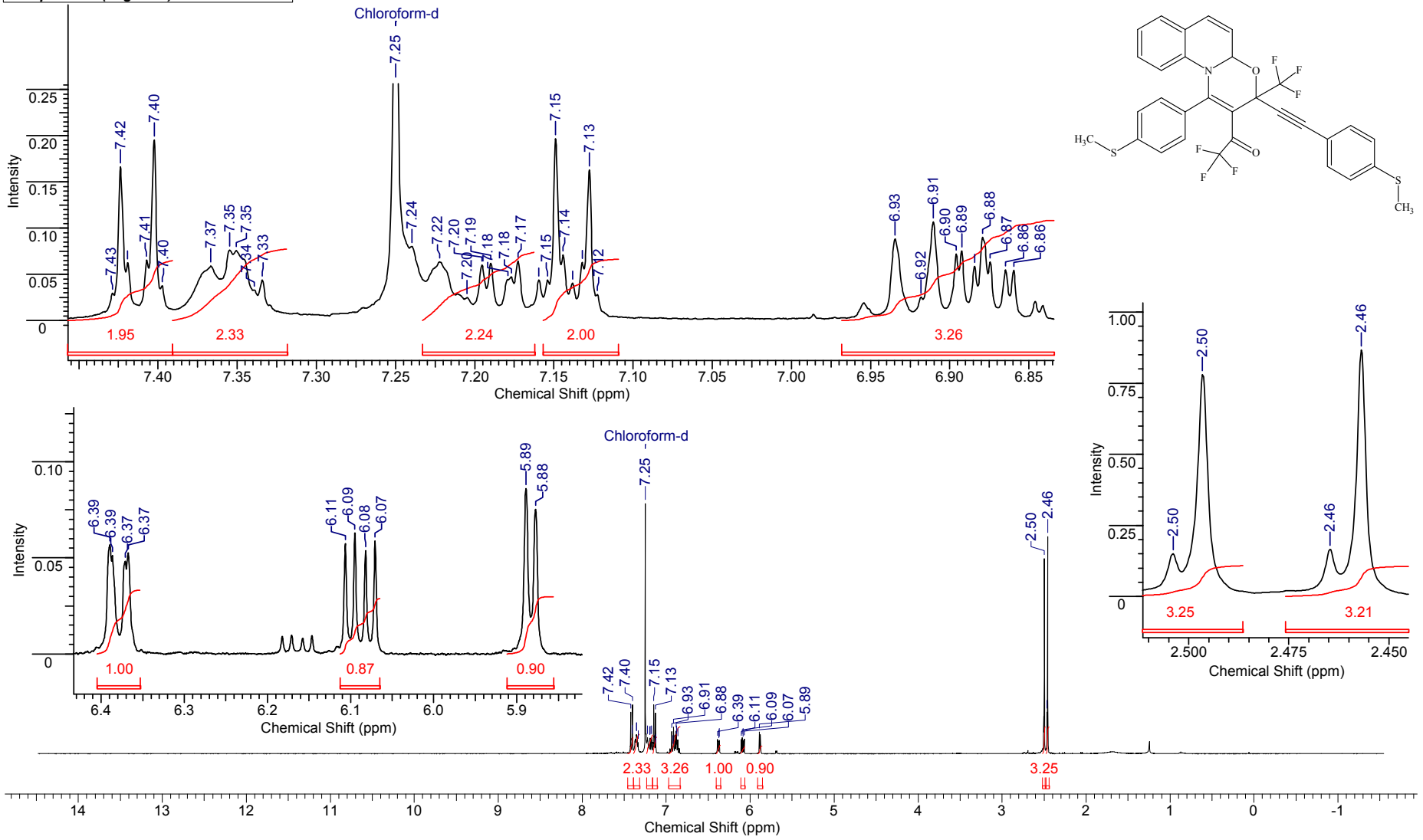






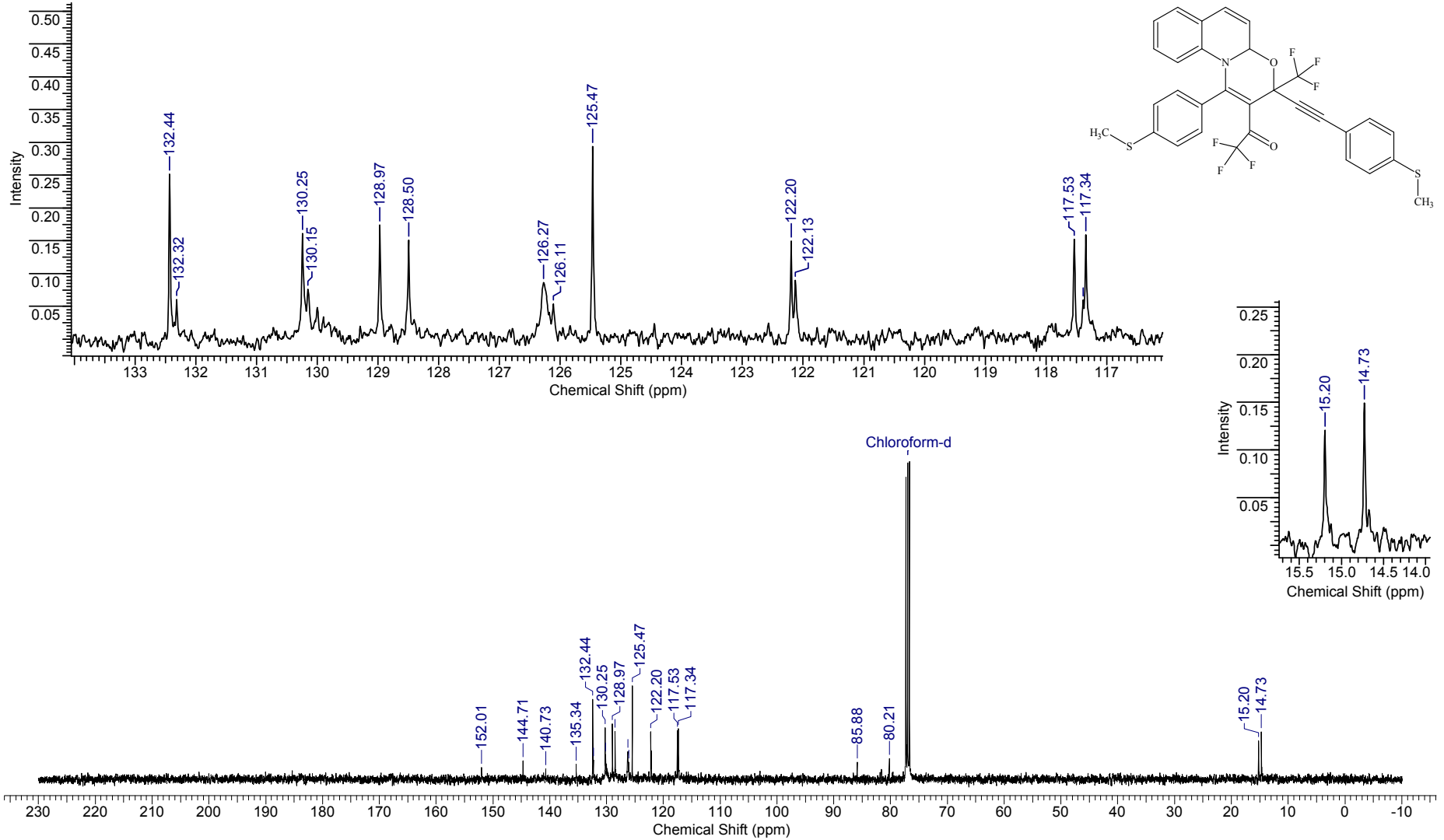
^{19}F NMR spectrum of **3h** (376.3 MHz, $CDCl_3$)

Acquisition Time (sec)	2.5559	***Comment***	Imported from UXNMR.			***Date***	17 Apr 2018 15:18:38
File Name	D:\Comp_316\BN\output\2018\04.äï ðåëü\BM-1341-1.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	16384	***Points Count***	65536
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	6410.26
Temperature (degree C)	27.000						



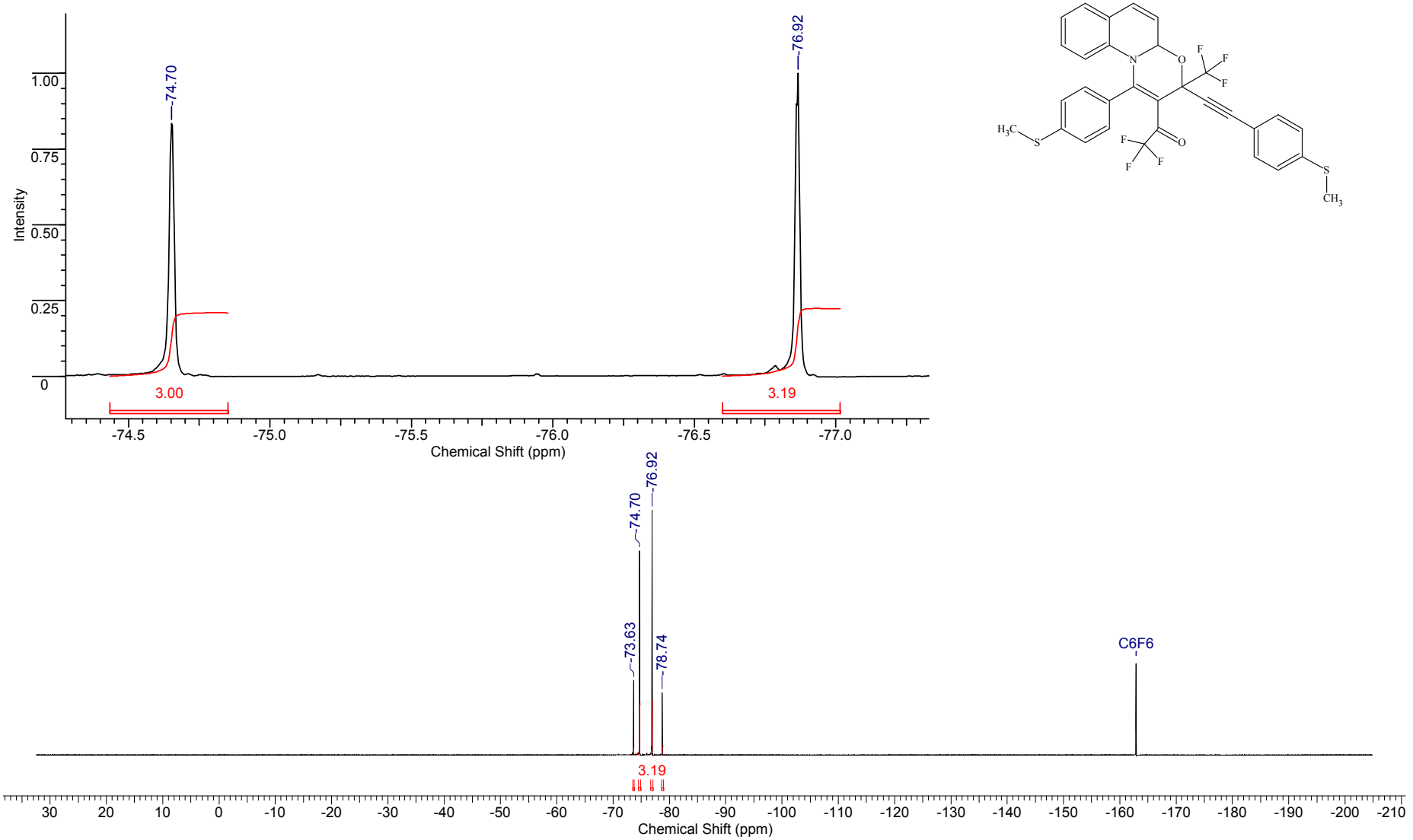
^{1}H NMR spectrum of (3*R**,4a*S**)-**3h** (400.1 MHz, $CDCl_3$)

Acquisition Time (sec)	0.4999	***Comment***	Imported from UXNMR.			***Date***	17 Apr 2018 15:46:46
File Name	D:\Comp_316\BN\output\2018\04.àï ðåëü\BM-1341-1.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	1024	***Original Points Count***	12076	***Points Count***	65536
Pulse Sequence	zgpg30	***Solvent***	DEUTERIUM OXIDE			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						

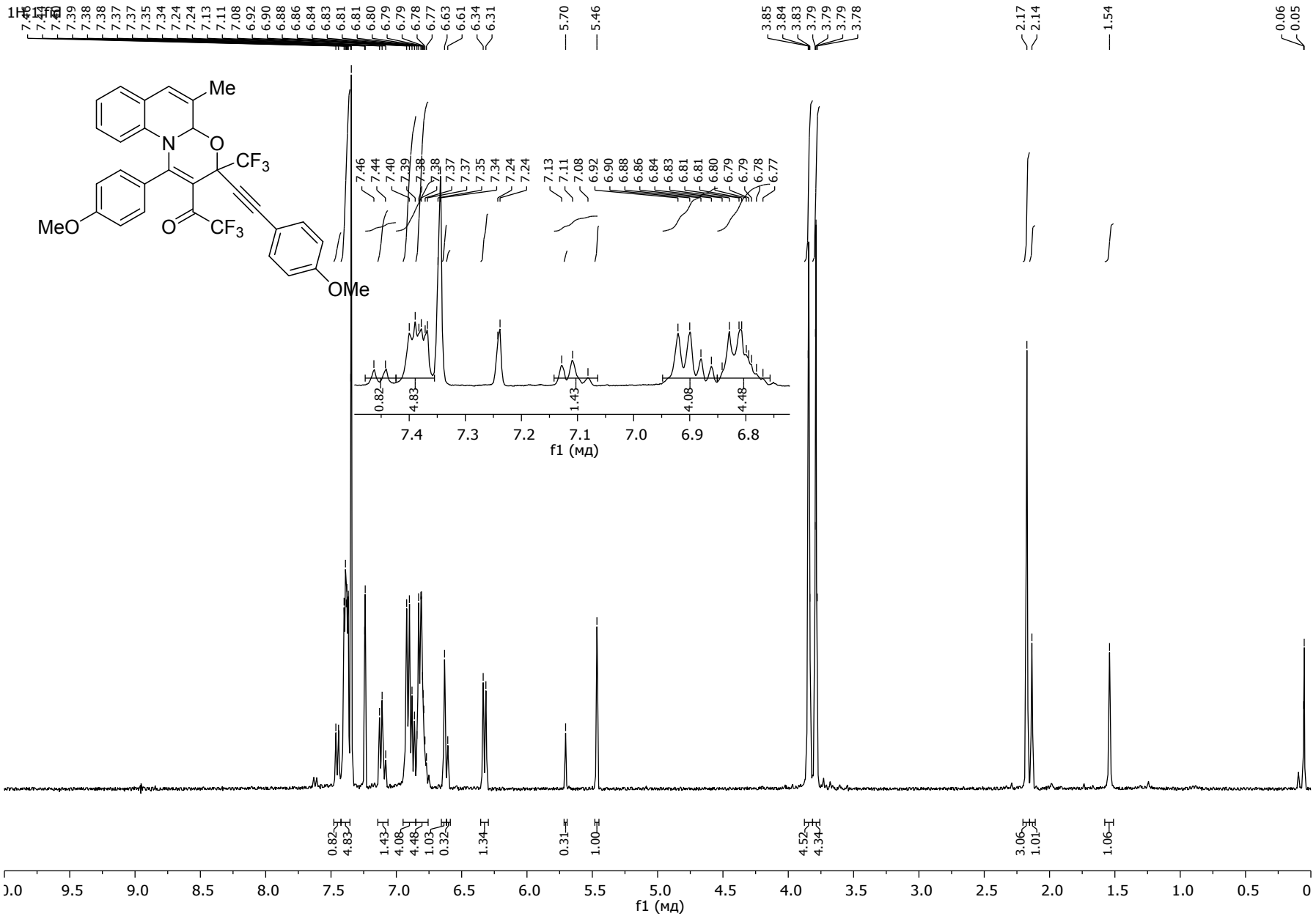


^{13}C NMR spectrum of (3*R**,4a*S**)-**3h** (100.6 MHz, $CDCl_3$)

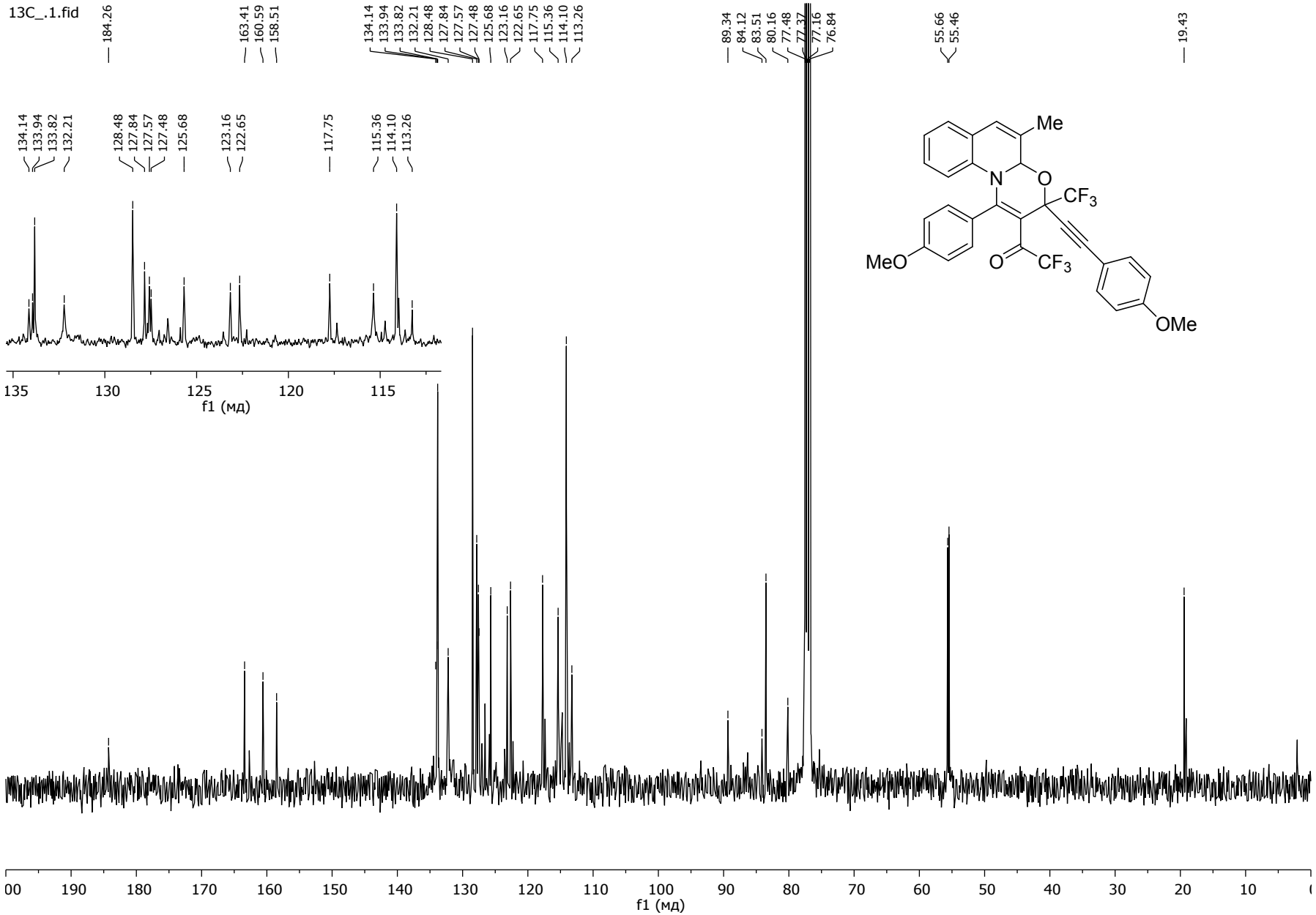
Acquisition Time (sec)	0.7340	***Date***	Apr 17 2018				
File Name	D:\Comp_316\BN\DOC (BN)\vasiliy\SPEC_BM_F_2018.04.27\bm1341-1-f_20180417_01\FLUORINE_01					***Frequency (MHz)***	376.31
Nucleus	19F	***Number of Transients***	100	***Original Points Count***	65536	***Points Count***	65536
Pulse Sequence	s2pul	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	89285.71	***Temperature (degree C)***	22.000



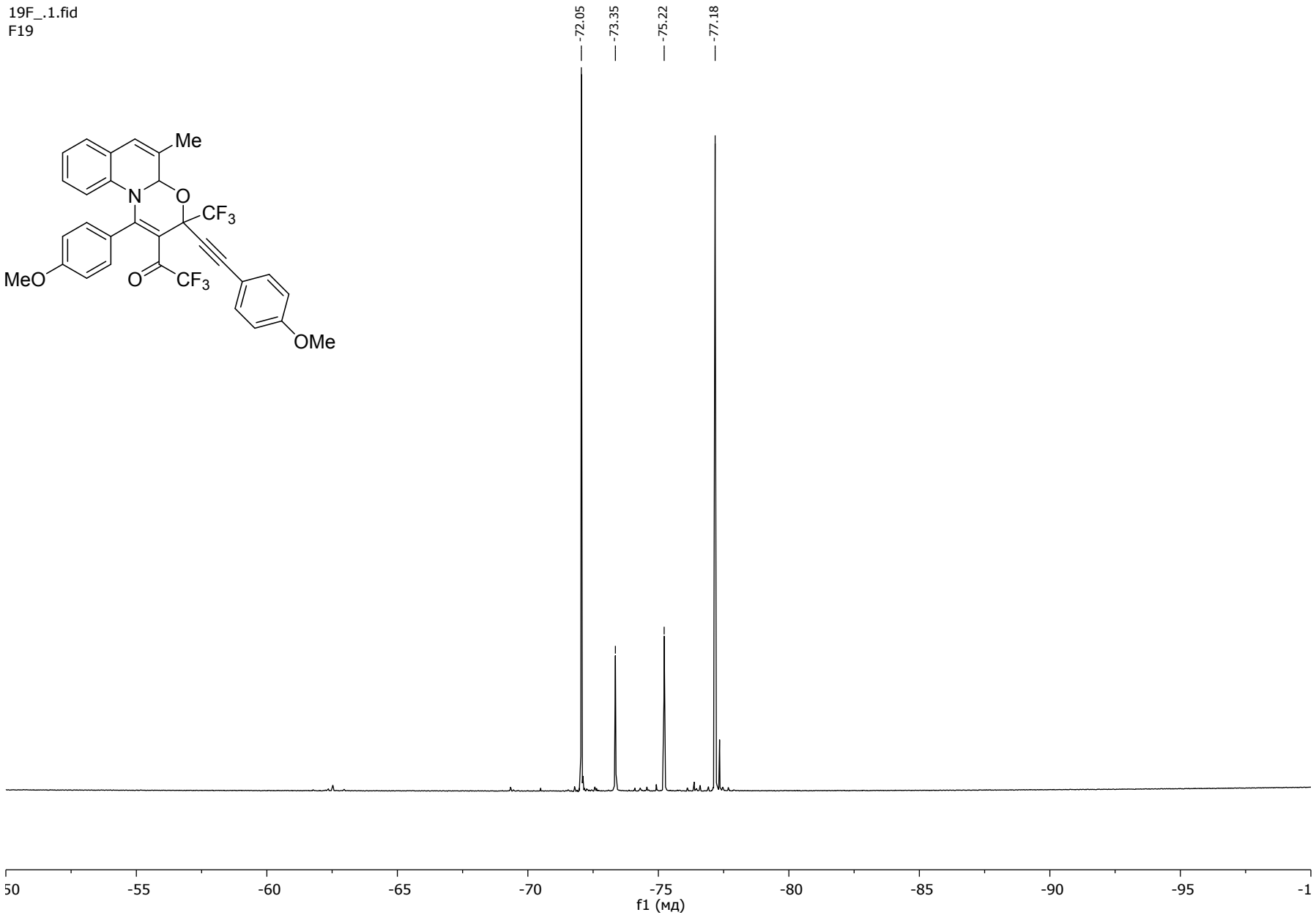
^{19}F NMR spectrum of (3*R**,4a*S**)-**3h** (376.3 MHz, $CDCl_3$)



^{1}H NMR spectrum of **3i** (400.1 MHz, $CDCl_3$)

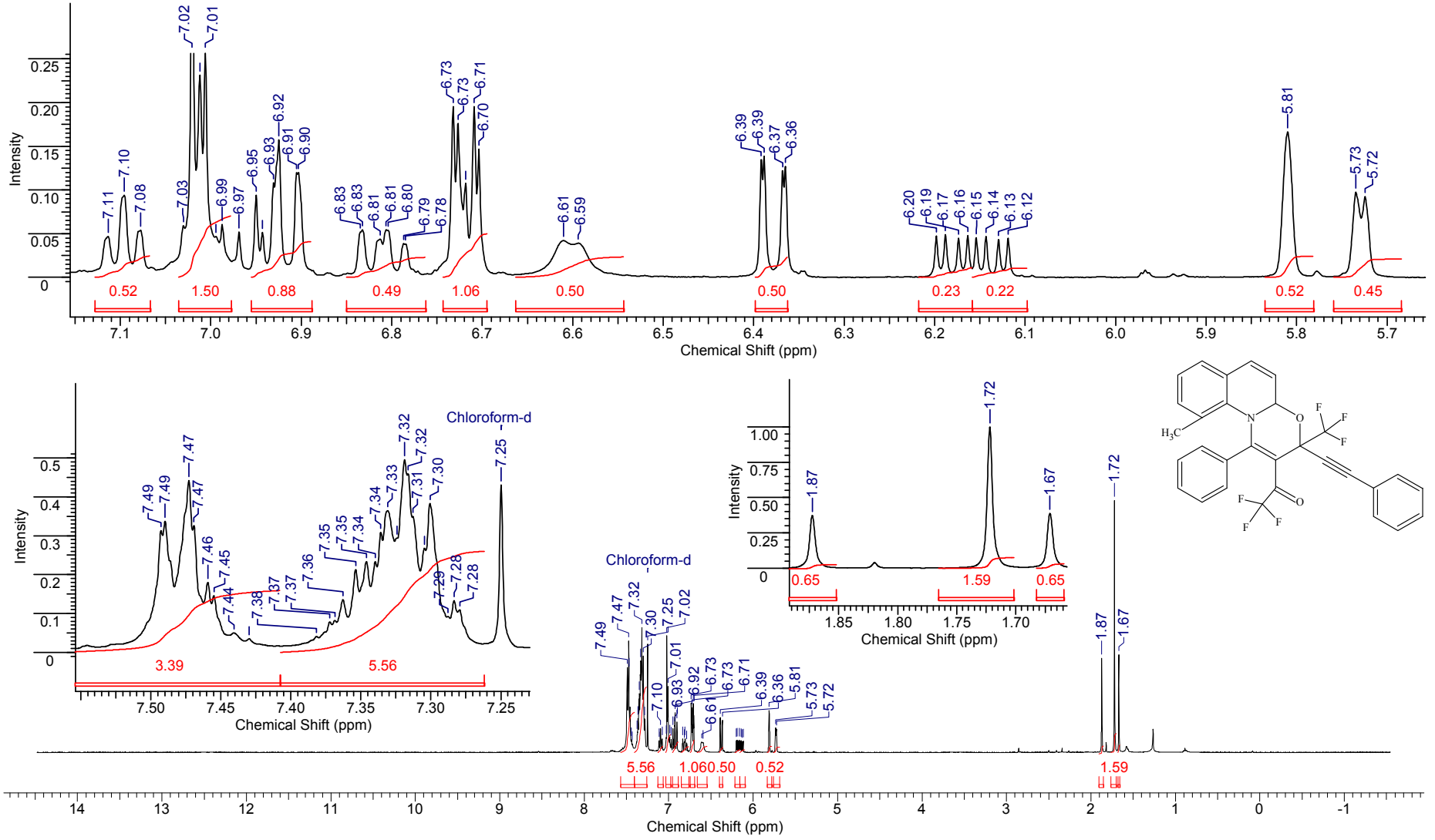


^{13}C NMR spectrum of **3i** (100.6 MHz, $CDCl_3$)



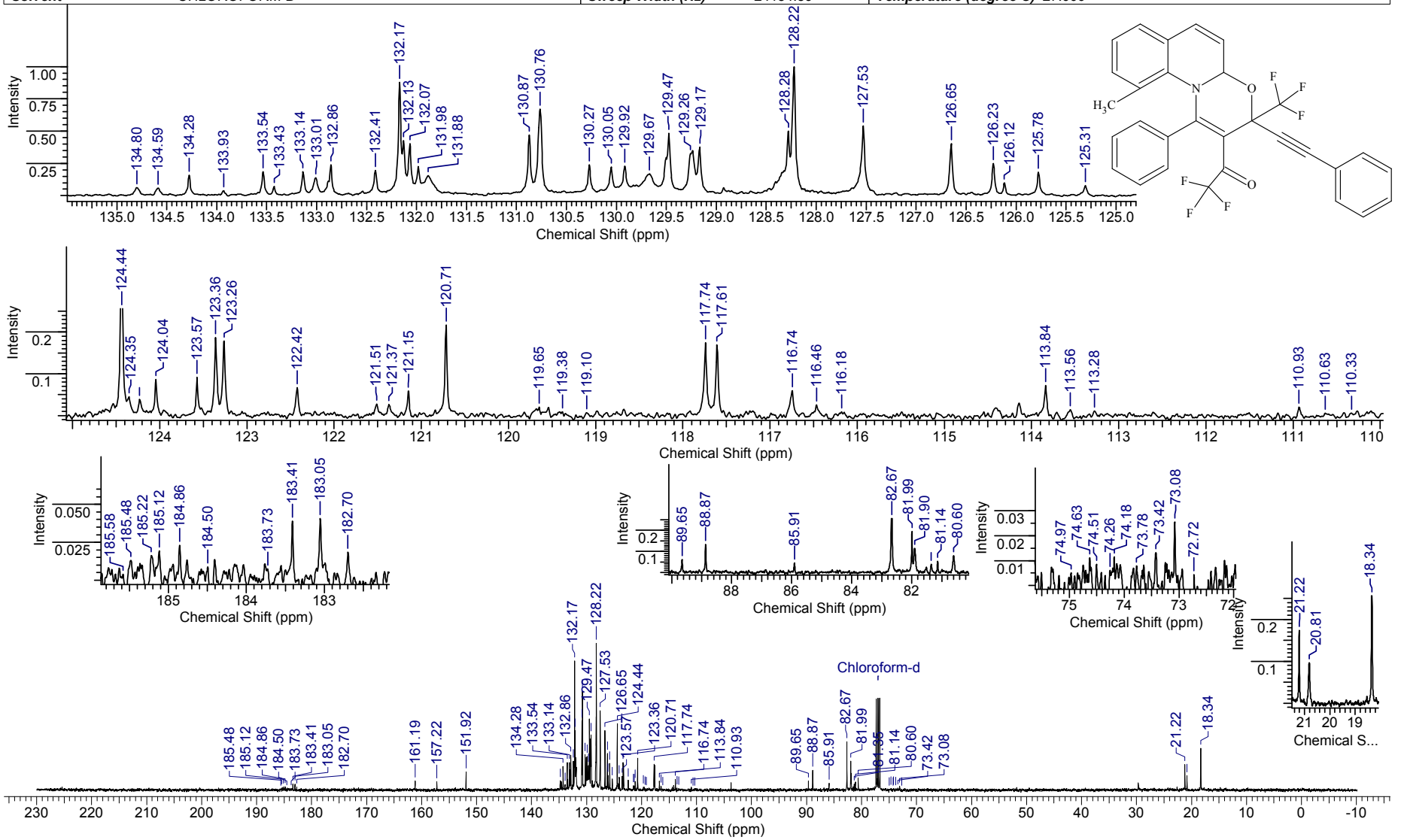
^{19}F NMR spectrum of **3i** (376.5 MHz, $CDCl_3$)

Acquisition Time (sec)	2.5559	***Comment***	Imported from UXNMR.			***Date***	27 Apr 2018 15:19:56
File Name	D:\Comp_316\BN\output\2018\04.àï ðåëü\BM-1352.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	16384	***Points Count***	65536
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	6410.26
Temperature (degree C)	27.000						



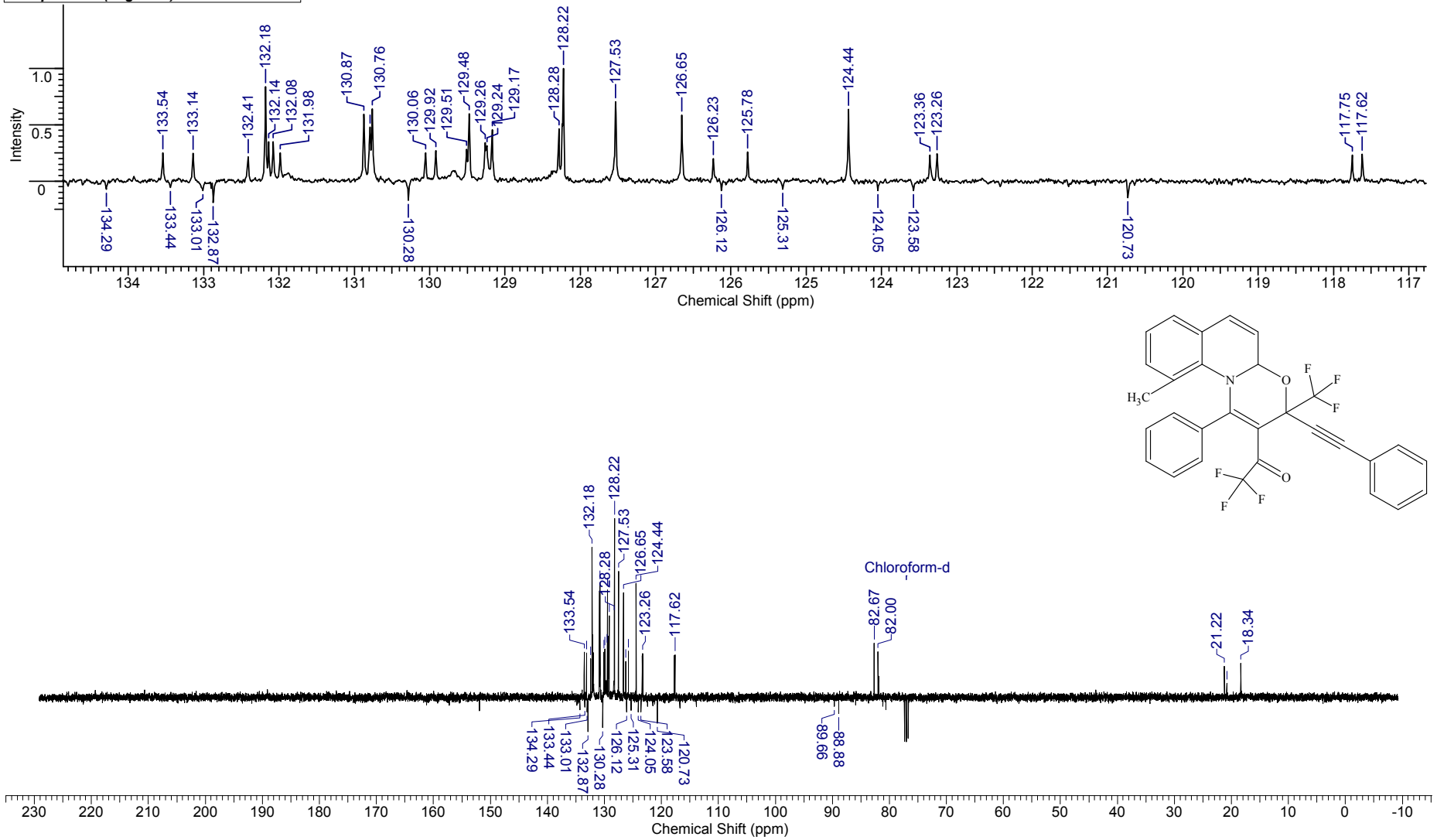
^{1}H NMR spectrum of **3j** (400.1 MHz, $CDCl_3$)

Acquisition Time (sec)	0.4999	***Comment***	Imported from UXNMR.			***Date***	28 May 2018 16:04:12
File Name	D:\Comp_316\BN\output\2018\05.ì àé\BM-1352-B2.C_002001r			***Frequency (MHz)***	100.61	***Nucleus***	13C
Number of Transients	1024	***Original Points Count***	12076	***Points Count***	65536	***Pulse Sequence***	zgpg30
Solvent	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000



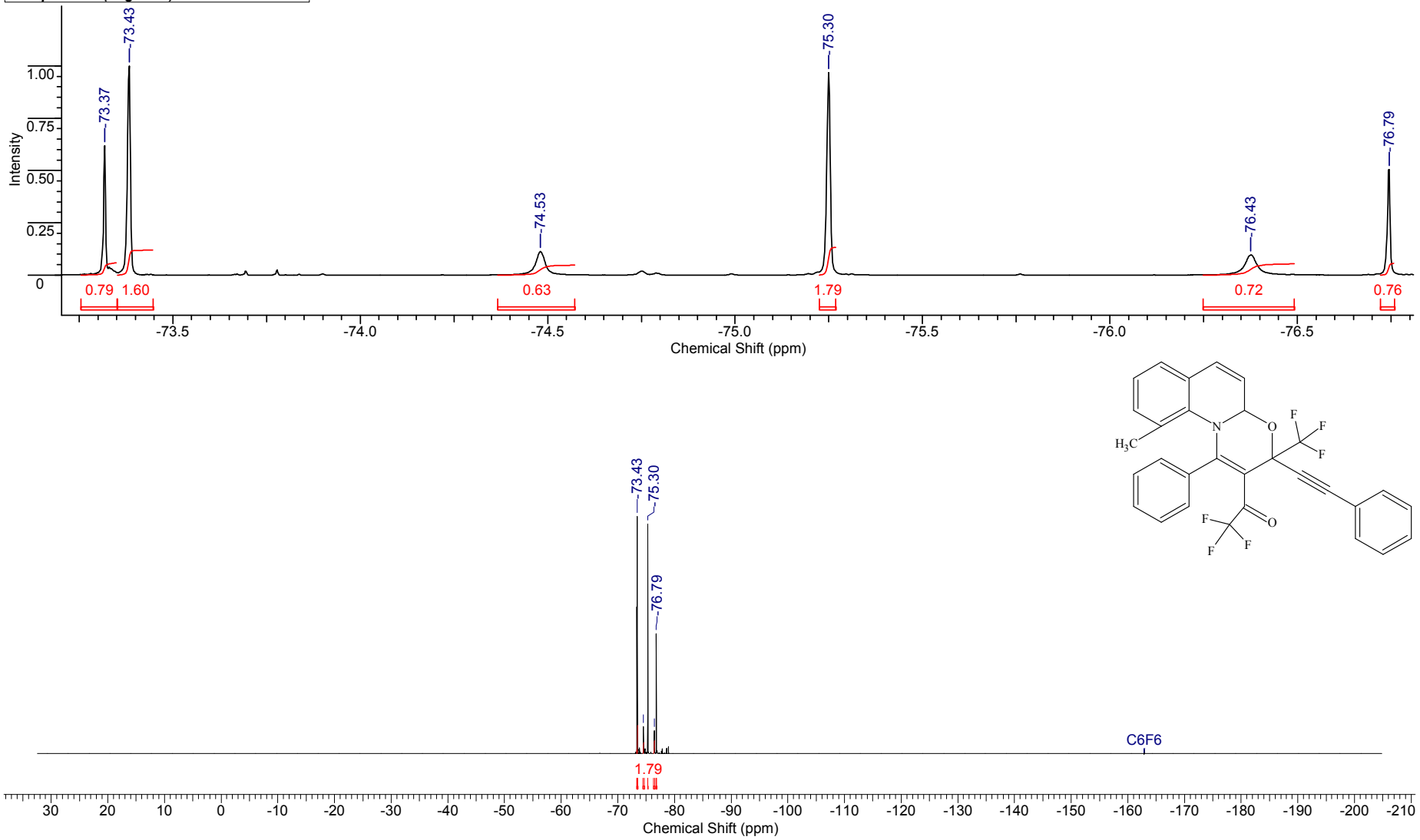
^{13}C NMR spectrum of **3j** (100.6 MHz, $CDCl_3$)

Acquisition Time (sec)	1.3664	***Comment***	Imported from UXNMR.			***Date***	27 Apr 2018 15:36:56
File Name	D:\Comp_316\BN\output\2018\04.àï ðåëü\BM-1352.Capt_004001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	132	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	jmod	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	23980.81
Temperature (degree C)	27.000						



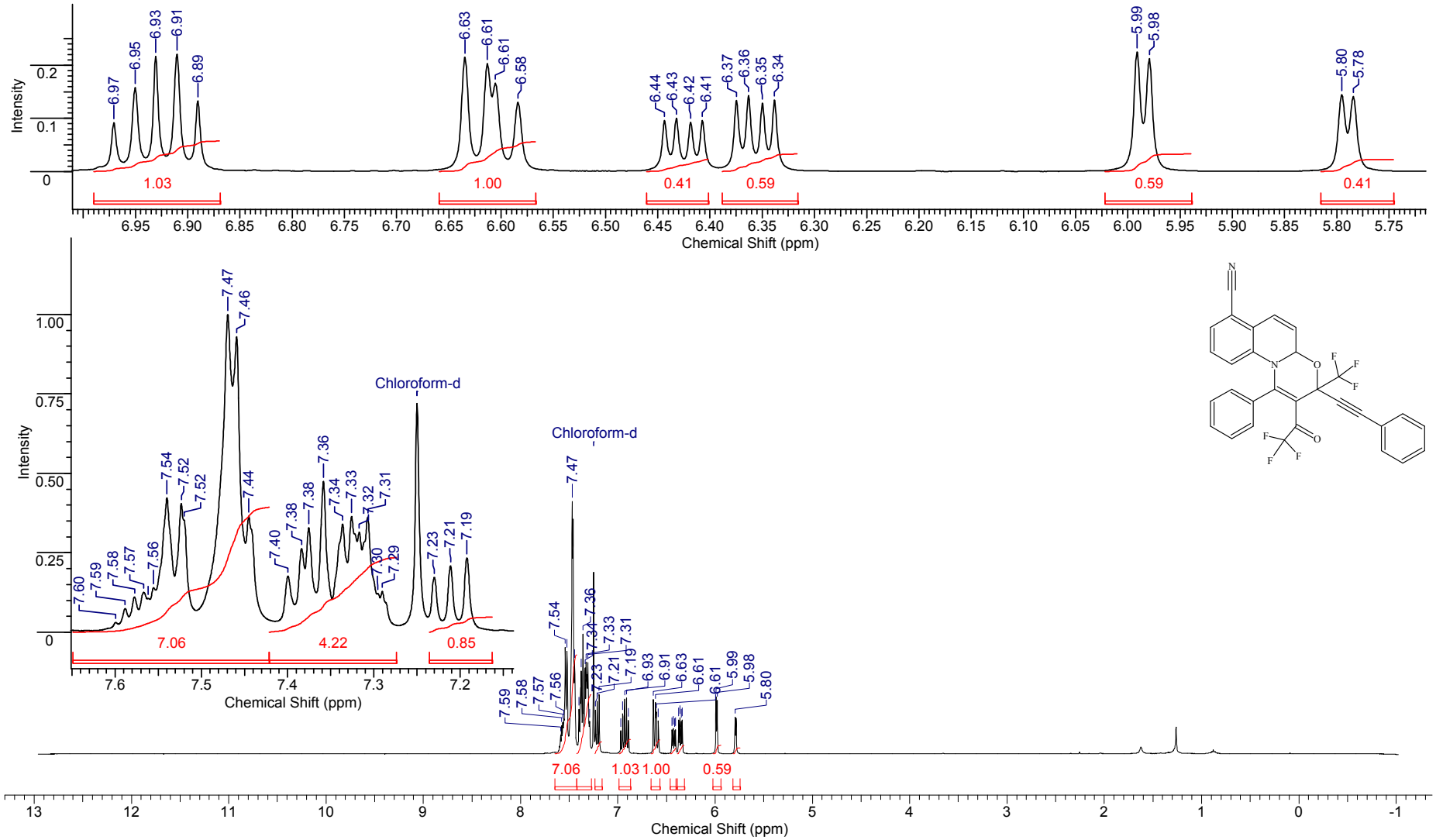
^{13}C NMR (APT) spectrum of **3j** (100.6 MHz, $CDCl_3$)

Acquisition Time (sec)	1.0000	***Date***	Apr 27 2018		
File Name	D:\Comp_316\BN\DOC (BN)\vasiliy\SPEC_BM_F_2018.04.27\BM-1352_20180427_01\FLUORINE_01			***Frequency (MHz)***	376.31
Nucleus	19F	***Number of Transients***	16	***Original Points Count*** 89286	***Points Count*** 131072
Pulse Sequence	s2pul	***Solvent***	CHLOROFORM-D		***Sweep Width (Hz)*** 89285.71
Temperature (degree C)	22.000				



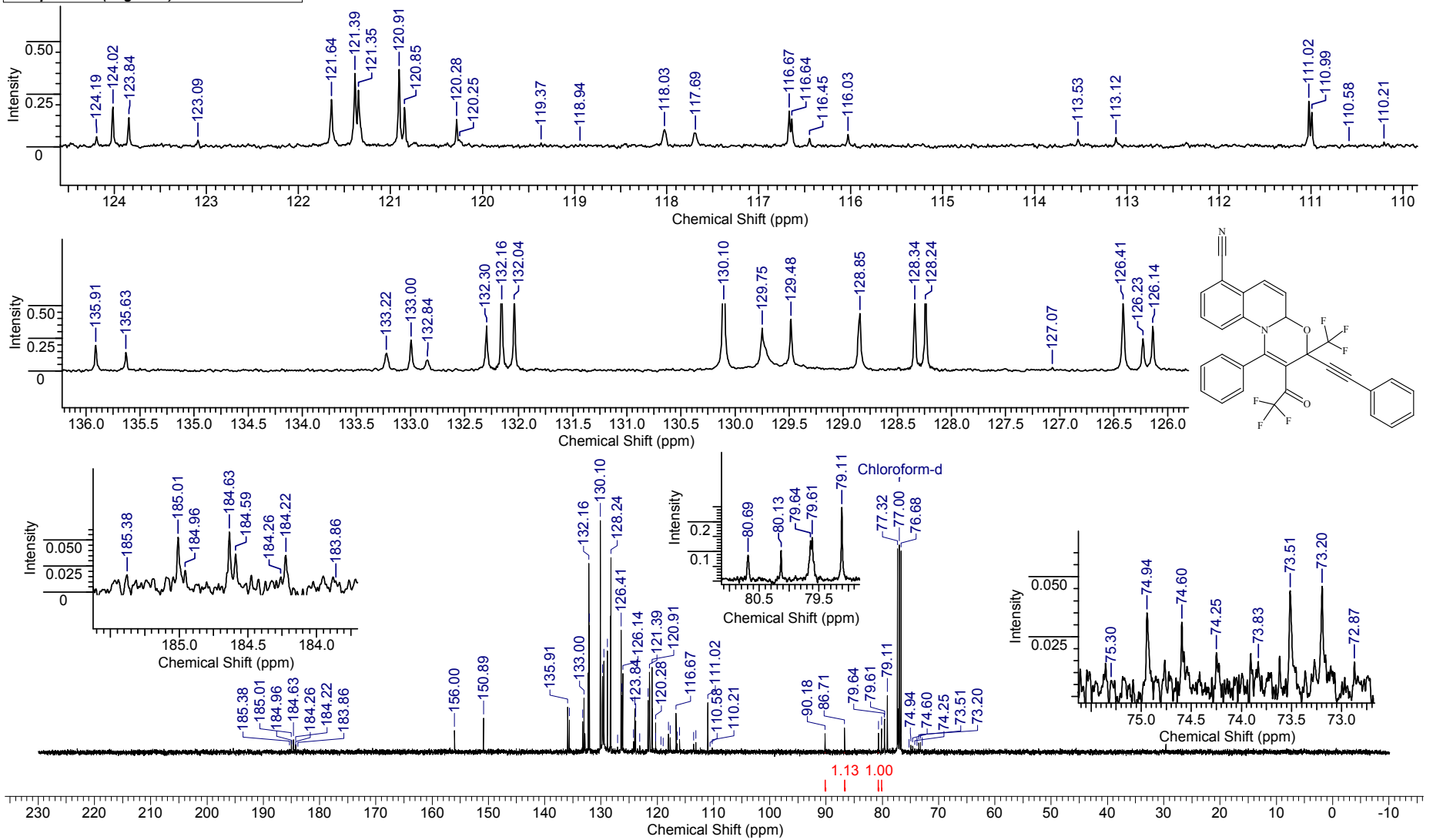
^{19}F NMR spectrum of **3j** (376.3 MHz, $CDCl_3$)

Acquisition Time (sec)	2.9295	***Comment***	Imported from UXNMR.			***Date***	25 Apr 2018 21:35:16
File Name	D:\Comp_316\BN\output\2018\04.àï ðåëü\BM-1356\BM-1356_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	8	***Original Points Count***	16384	***Points Count***	65536
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	5592.84
Temperature (degree C)	27.000						



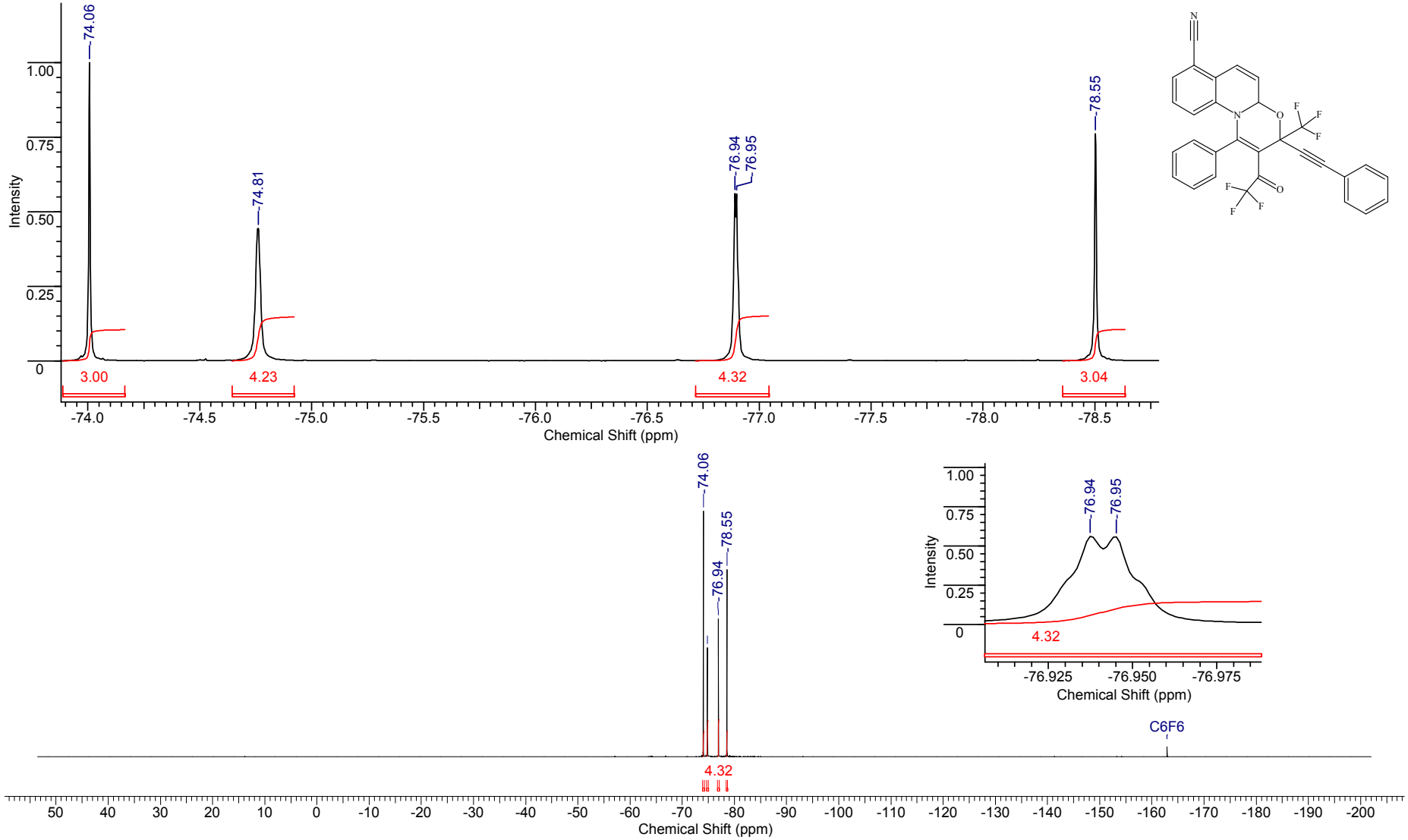
^{1}H NMR spectrum of **3k** (400.1 MHz, $CDCl_3$)

Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	25 Apr 2018 21:51:34
File Name	D:\Comp_316\BN\output\2018\04.äï ðåëü\BM-1356\BM-1356_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	368	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						

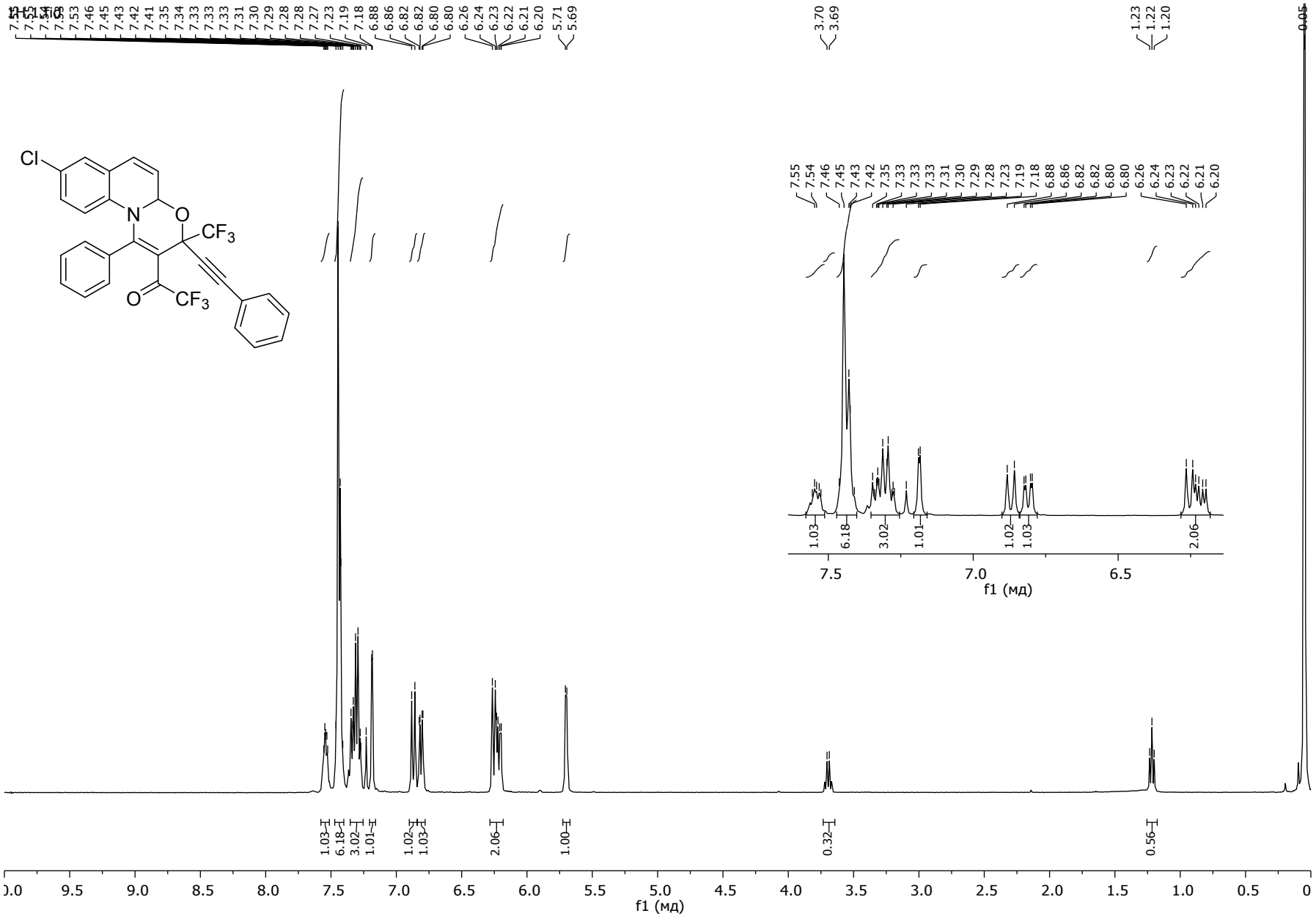


^{13}C NMR spectrum of **3k** (100.6 MHz, $CDCl_3$)

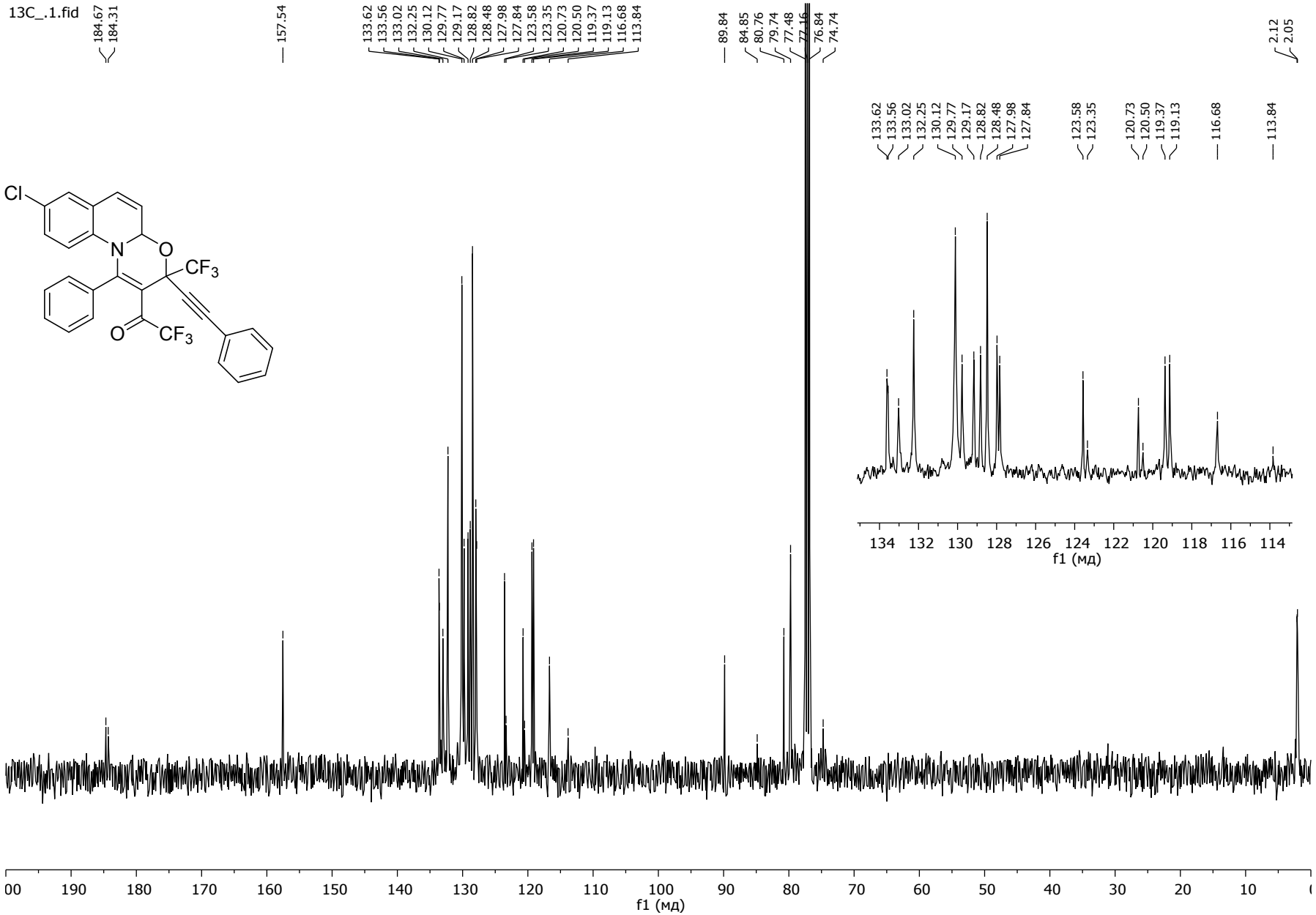
Acquisition Time (sec)	2.7263	***Date***	Apr 26 2018				
File Name	D:\Comp_316\BN\DOC (BN)\vasiliy\SPEC_BM_F_2018.04.27\BM-1356-F_20180426_01\FLUORINE_01					***Frequency (MHz)***	376.31
Nucleus	19F	***Number of Transients***	8	***Original Points Count***	262144	***Points Count***	262144
Pulse Sequence	s2pul	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	96153.84	***Temperature (degree C)***	22.000



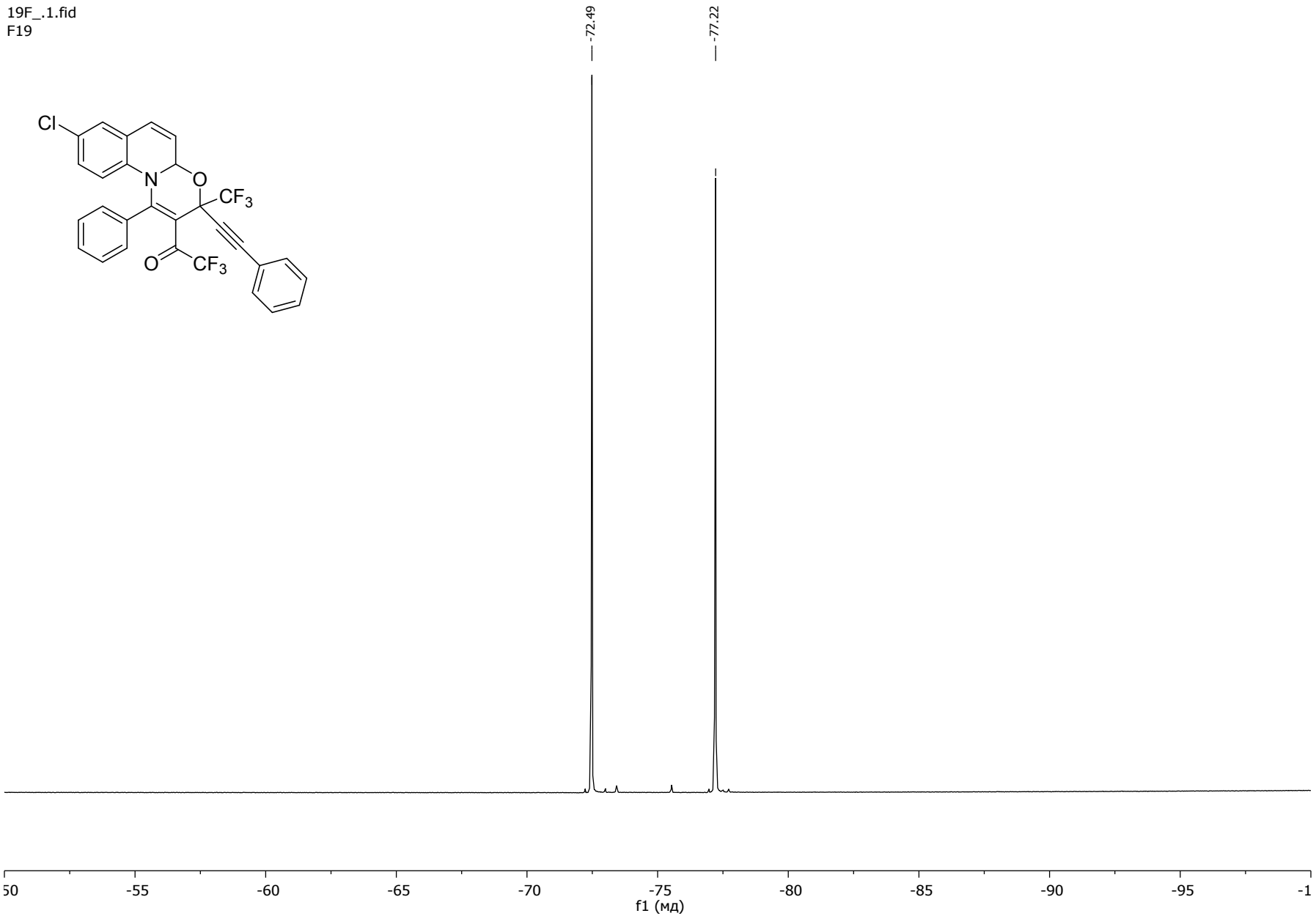
^{19}F NMR spectrum of **3k** (376.3 MHz, $CDCl_3$)



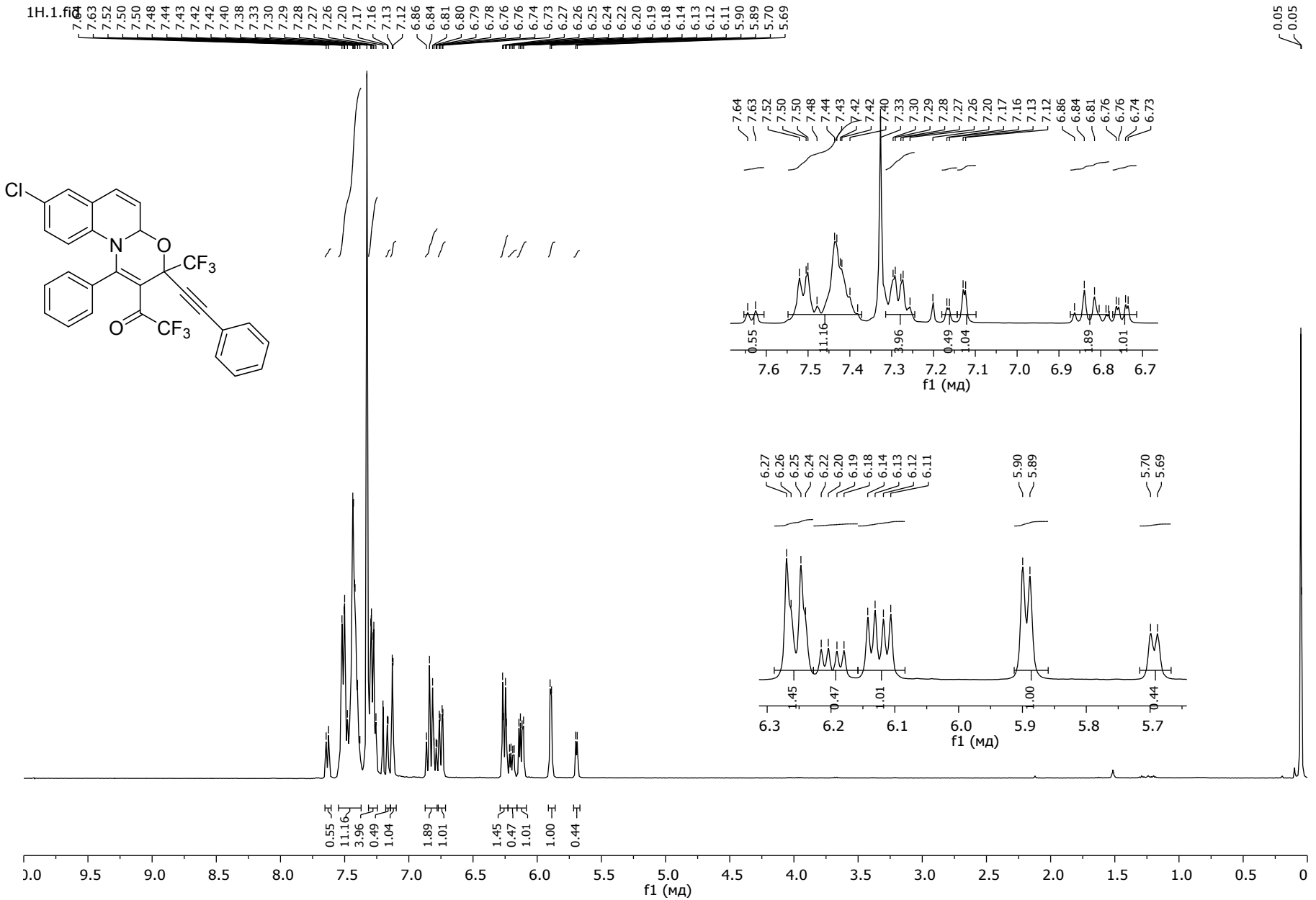
^{1}H NMR spectrum of (3*S**,4a*S**)-**3l** (400.1 MHz, $CDCl_3$)



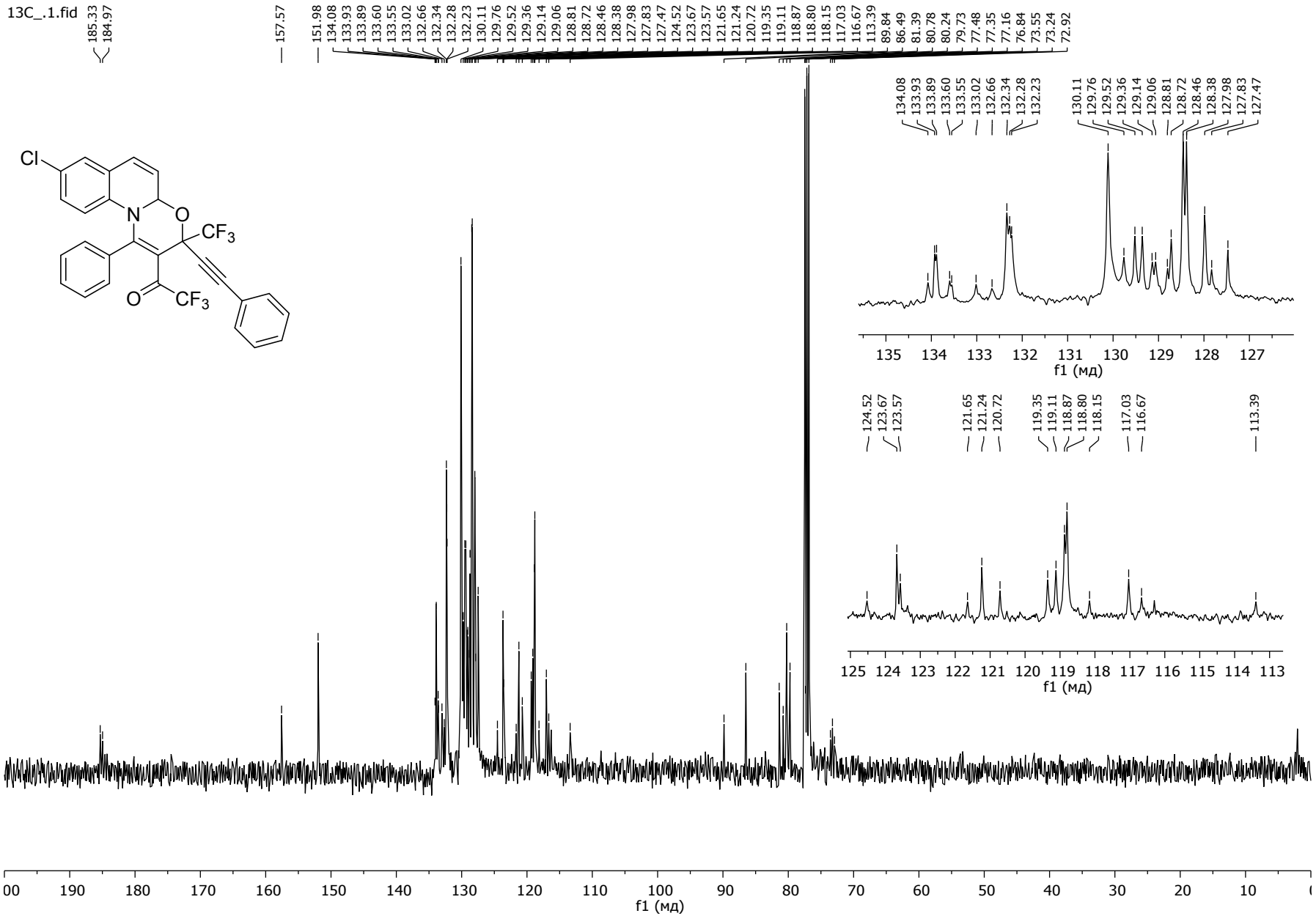
^{13}C NMR spectrum of (3*S**,4a*S**)-**3l** (100.6 MHz, $CDCl_3$)



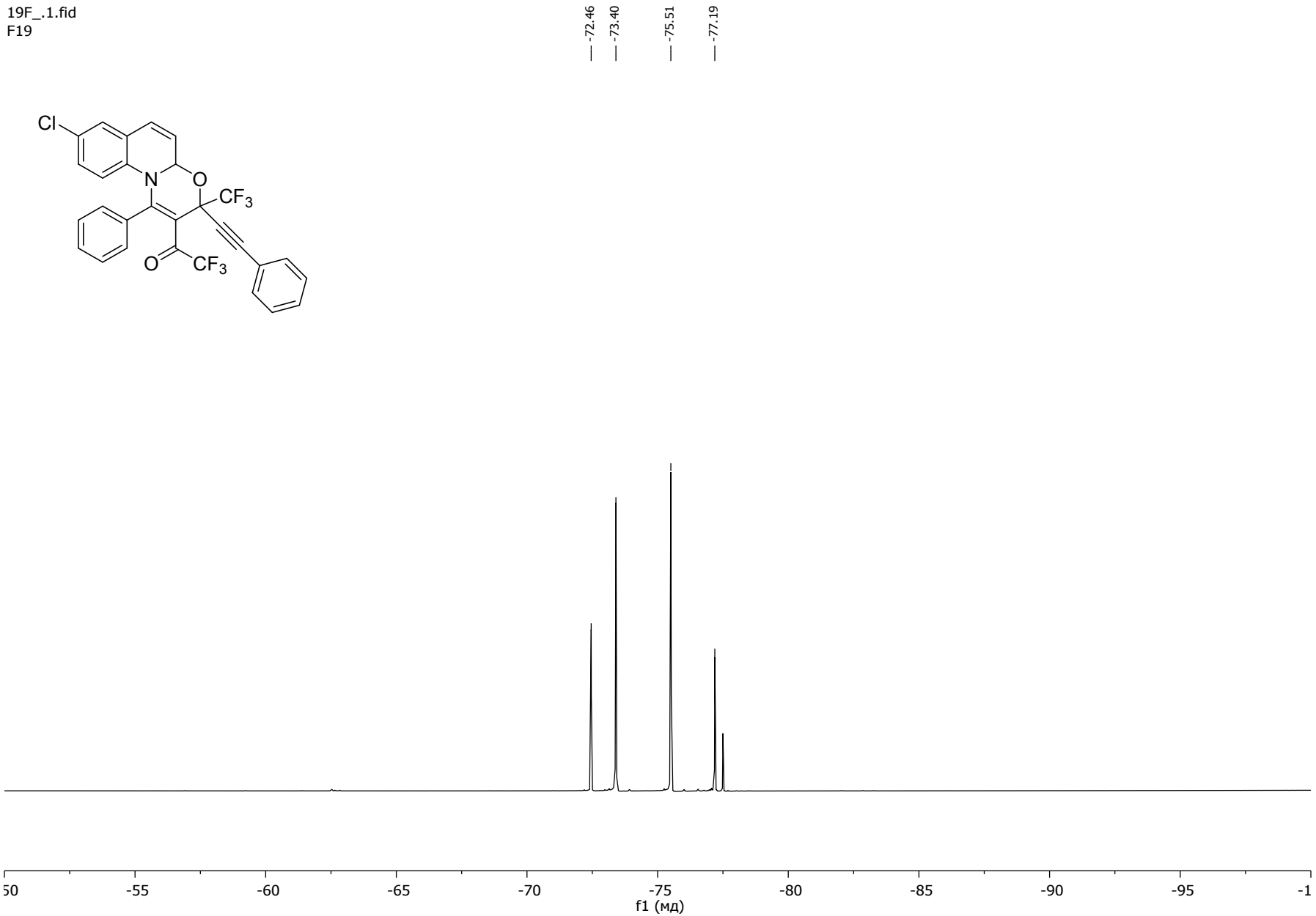
^{19}F NMR spectrum of (3*S**,4a*S**)-**3l** (376.5 MHz, $CDCl_3$)



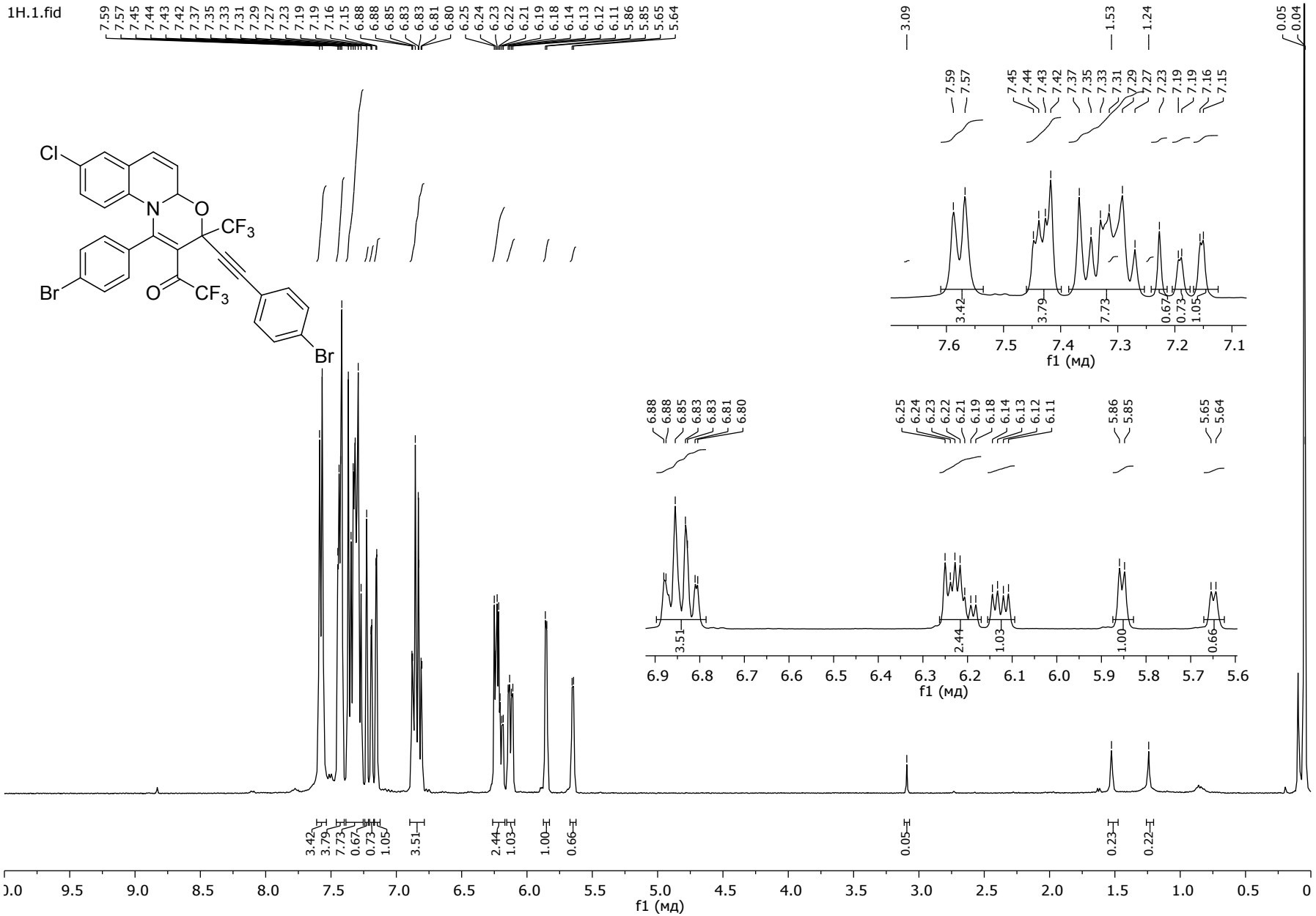
^{1}H NMR spectrum of **3l** (400.1 MHz, $CDCl_3$)



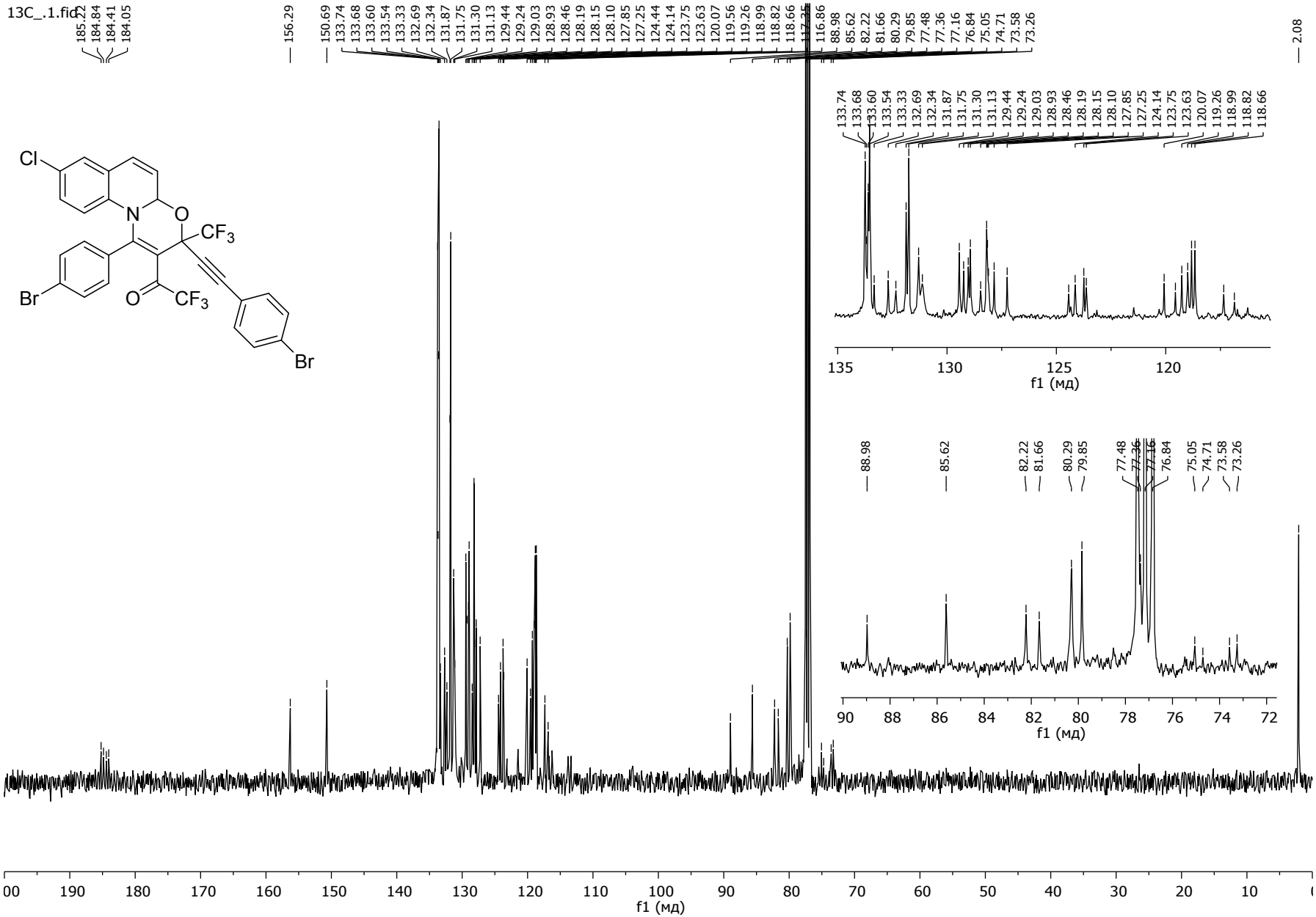
^{13}C NMR spectrum of **3l** (100.6 MHz, $CDCl_3$)



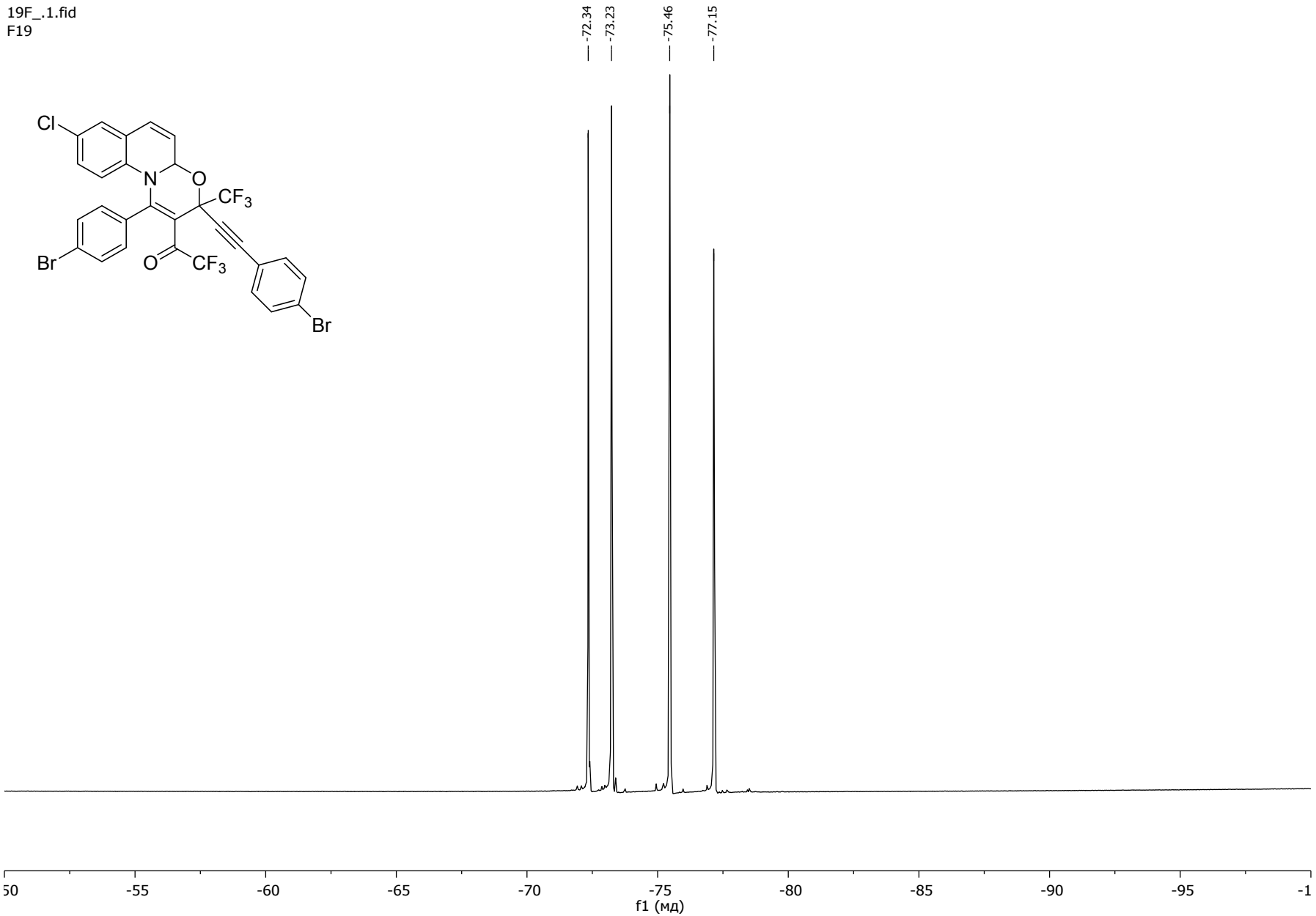
^{19}F NMR spectrum of **3l** (376.5 MHz, $CDCl_3$)



^{1}H NMR spectrum of **3m** (400.1 MHz, $CDCl_3$)



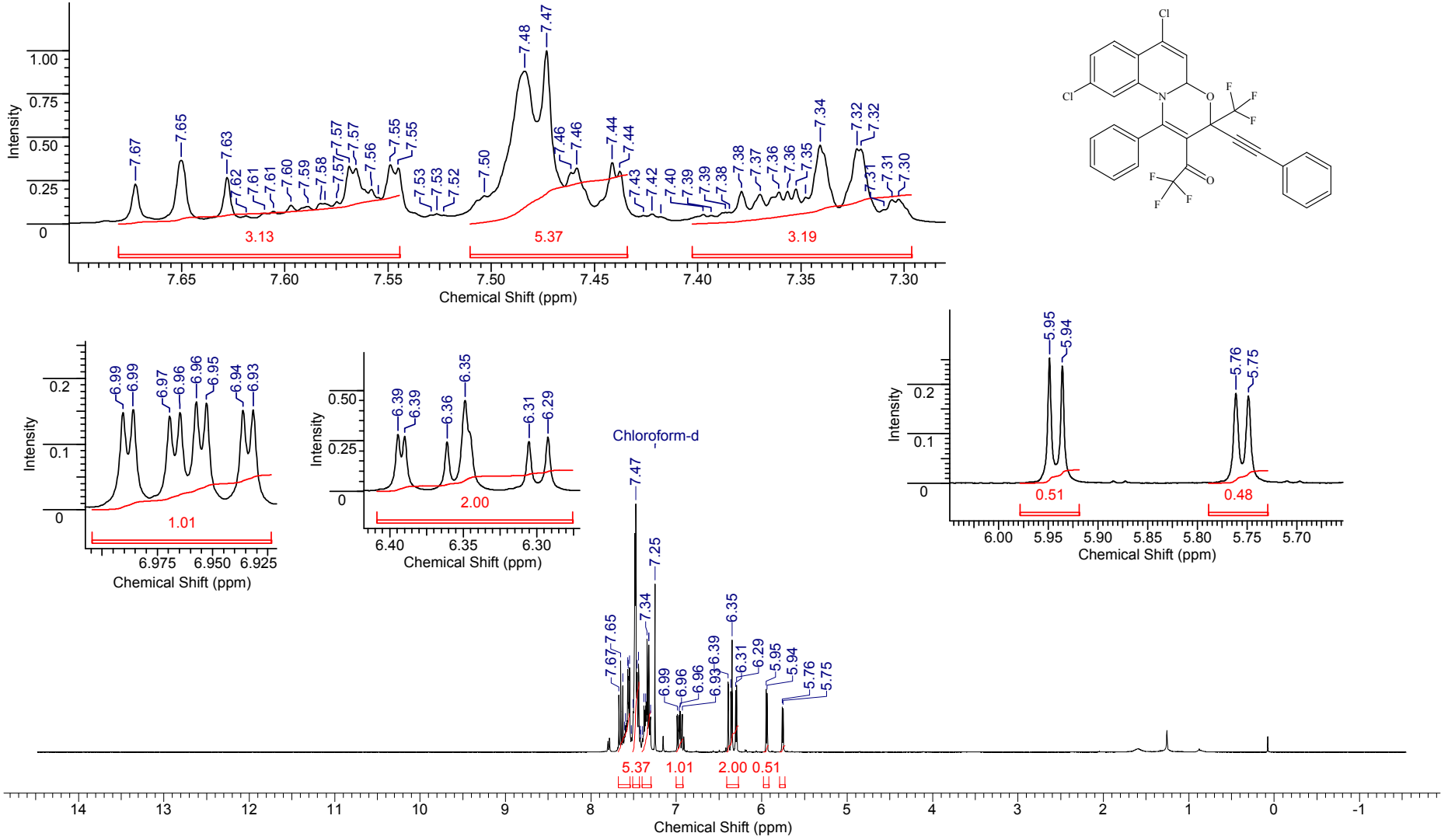
^{13}C NMR spectrum of **3m** (100.6 MHz, $CDCl_3$)



^{19}F NMR spectrum of **3m** (376.5 MHz, $CDCl_3$)

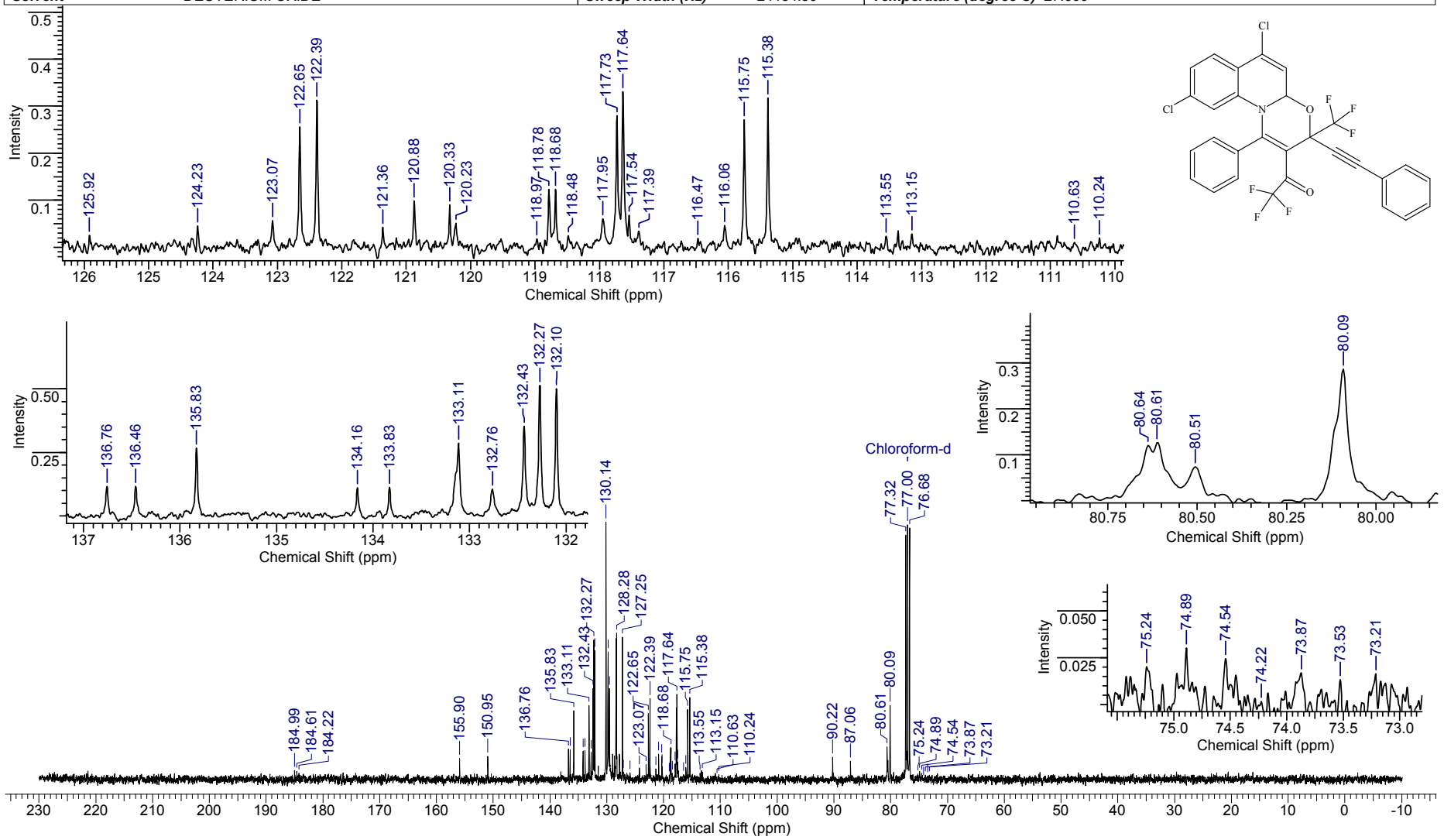
FW	594.3308	**Formula**	$C_{29}H_{15}Cl_2F_6NO_2$

Acquisition Time (sec)	2.5559	**Comment**	Imported from UXNMR.			**Date**	06 Jun 2018 17:14:16
File Name	F:\2018\06. èþ í ü\BM-1363-2B2.H_001001r			**Frequency (MHz)**	400.13	**Nucleus**	1H **Number of Transients** 4
Original Points Count	16384	**Points Count**	65536	**Pulse Sequence**	zg30	**Solvent**	CHLOROFORM-D
Sweep Width (Hz)	6410.26	**Temperature (degree C)**	27.000				



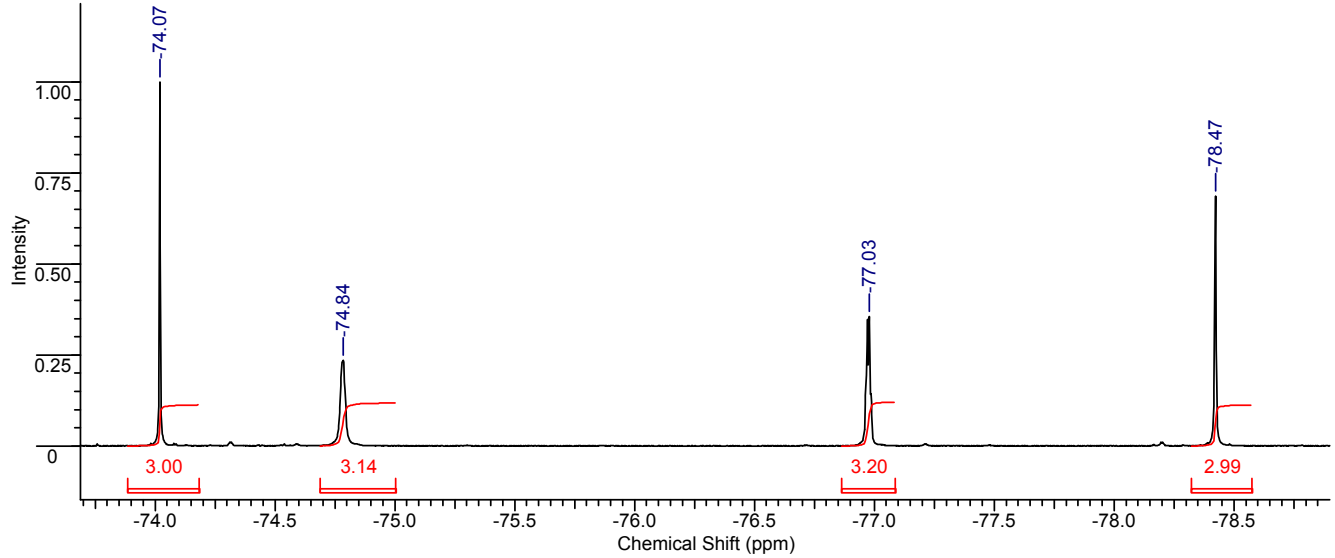
^{1}H NMR spectrum of **3n** (400.1 MHz, $CDCl_3$)

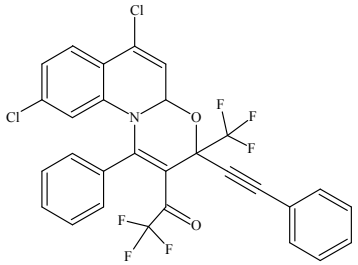
FW	594.3308	***Formula***	$C_{29}H_{15}Cl_2F_6NO_2$				
Acquisition Time (sec)	0.4999	***Comment***	Imported from UXNMR.			***Date***	06 Jun 2018 17:41:28
File Name	F:\2018\06. èþ í ü\BM-1363-2B2.C_002001r			***Frequency (MHz)***	100.61	***Nucleus***	13C
Number of Transients	951	***Original Points Count***	12076	***Points Count***	65536	***Pulse Sequence***	zgpg30
Solvent	DEUTERIUM OXIDE			***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000

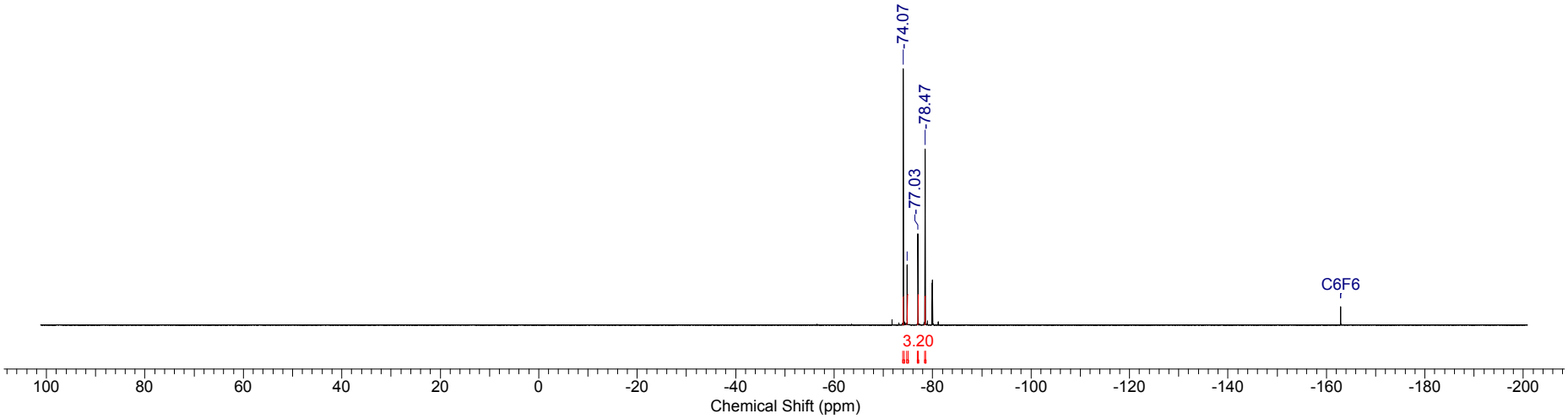


^{13}C NMR spectrum of **3n** (100.6 MHz, $CDCl_3$)

FW	594.3308	***Formula***	$C_{29}H_{15}Cl_2F_6NO_2$				
Acquisition Time (sec)	2.3069	***Date***	Jun 7 2018	***File Name***	I:\SPEC_BM_F_2018.04.27\BM-1363-2B2-F_20180607_01\FLUORINE_01		
Frequency (MHz)	376.32	***Nucleus***	19F	***Number of Transients***	8	***Original Points Count***	262144
Points Count	262144	***Pulse Sequence***	s2pul	***Solvent***	CHLOROFORM-D		
Sweep Width (Hz)	113636.37	***Temperature (degree C)***	22.000				



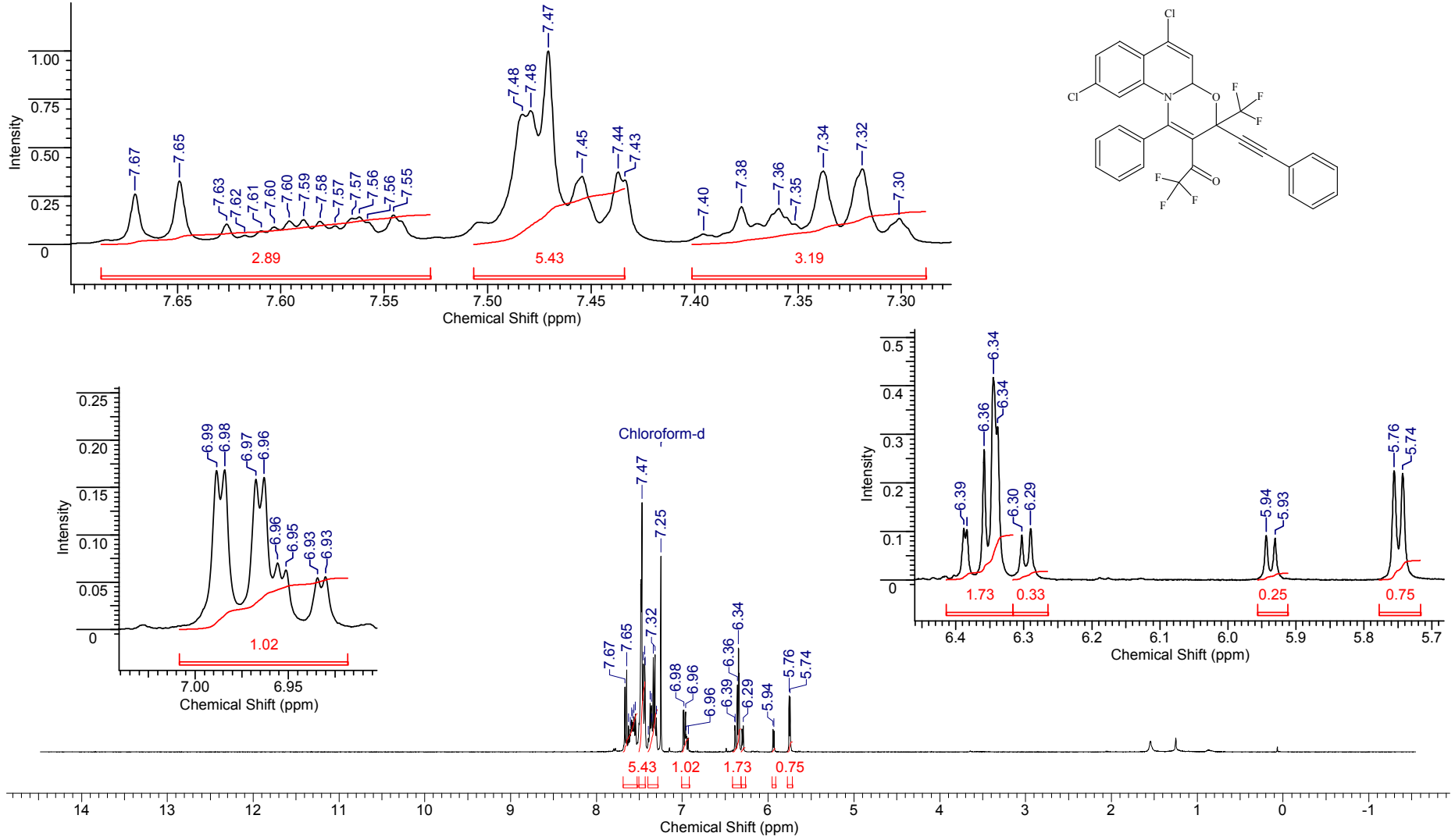




^{19}F NMR spectrum of **3n** (376.3 MHz, $CDCl_3$)

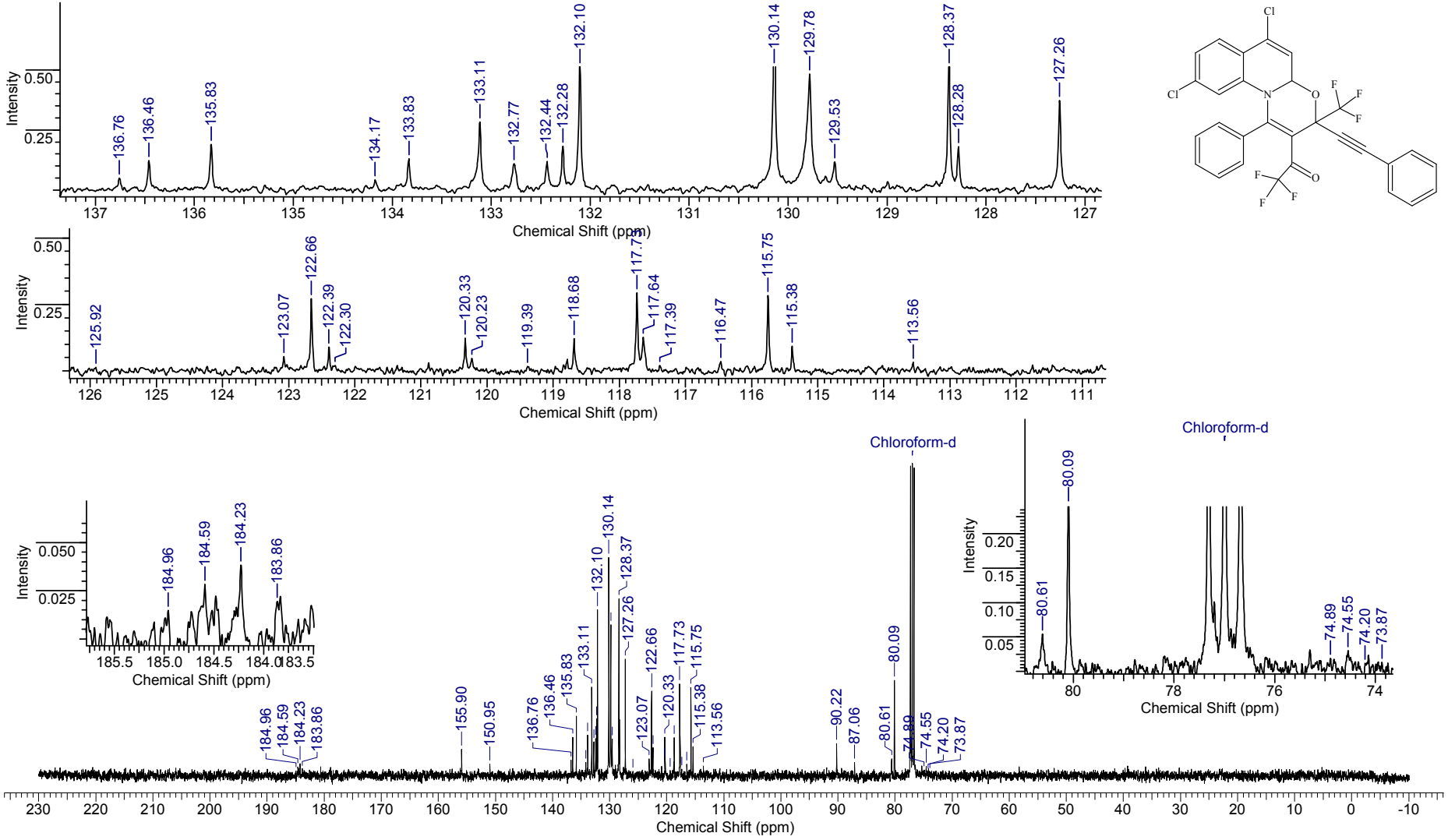
FW	594.3308	***Formula***	$C_{29}H_{15}Cl_2F_6NO_2$

Acquisition Time (sec)	2.5559	***Comment***	Imported from UXNMR.			***Date***	02 Jun 2018 13:27:08
File Name	F:\2018\06. èþ í ü\BM-1363-3.H_001001r			***Frequency (MHz)***	400.13	***Nucleus***	1H ***Number of Transients*** 4
Original Points Count	16384	***Points Count***	65536	***Pulse Sequence***	zg30	***Solvent***	CHLOROFORM-D
Sweep Width (Hz)	6410.26	***Temperature (degree C)***	27.000				



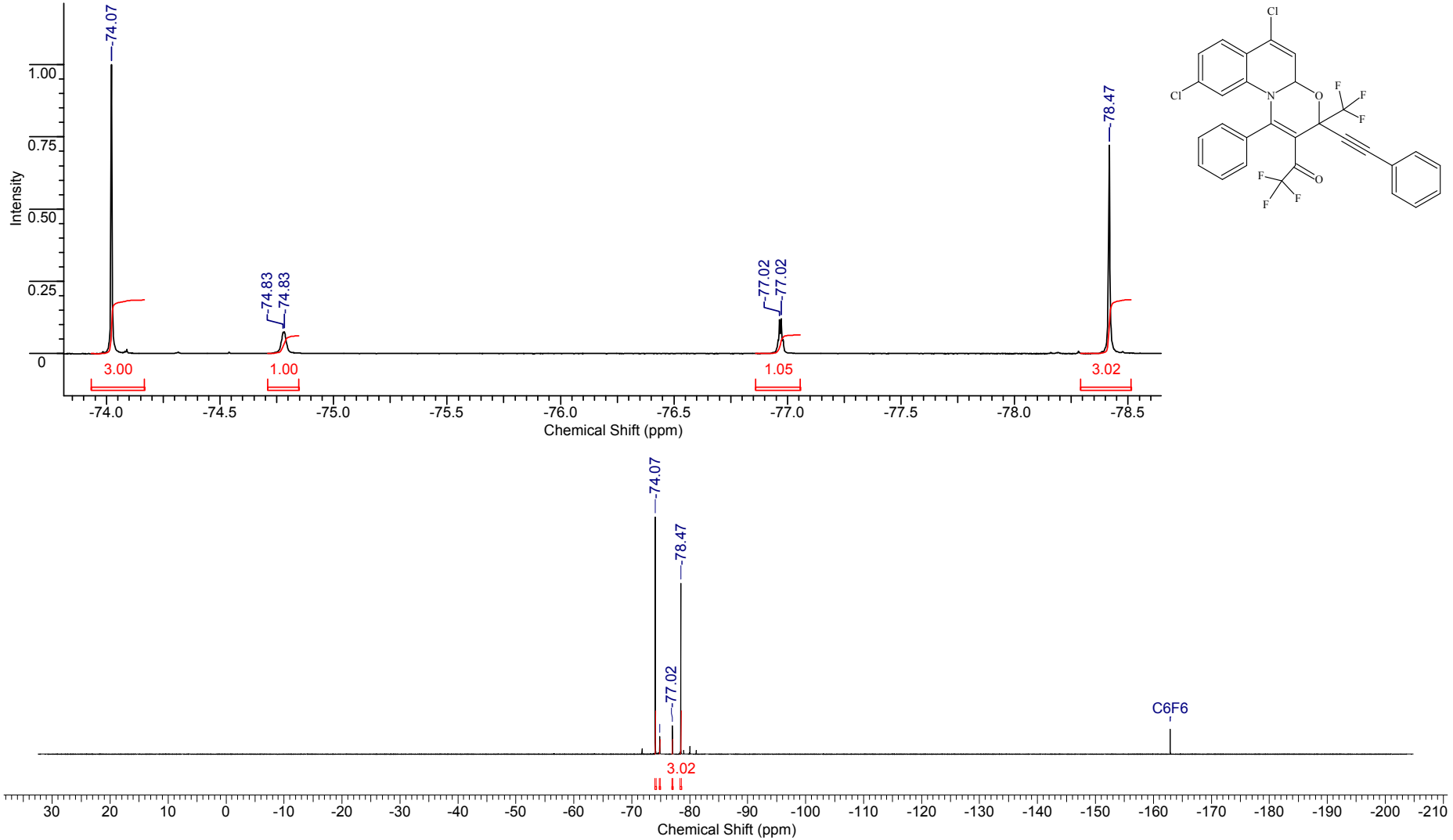
^{1}H NMR spectrum of (3*S**,4a*S**)-**3n** (400.1 MHz, $CDCl_3$)

FW	594.3308	***Formula***	$C_{29}H_{15}Cl_2F_6NO_2$				
Acquisition Time (sec)	0.4999	***Comment***	Imported from UXNMR.			***Date***	05 Jun 2018 15:01:20
File Name	F:\2018\06. èþ í ü\BM-1363-3.C_002001r			***Frequency (MHz)***	100.61	***Nucleus***	13C
Original Points Count	12076	***Points Count***	65536	***Pulse Sequence***	zgpg30	***Solvent***	DEUTERIUM OXIDE
Sweep Width (Hz)	24154.59	***Temperature (degree C)***	27.000				



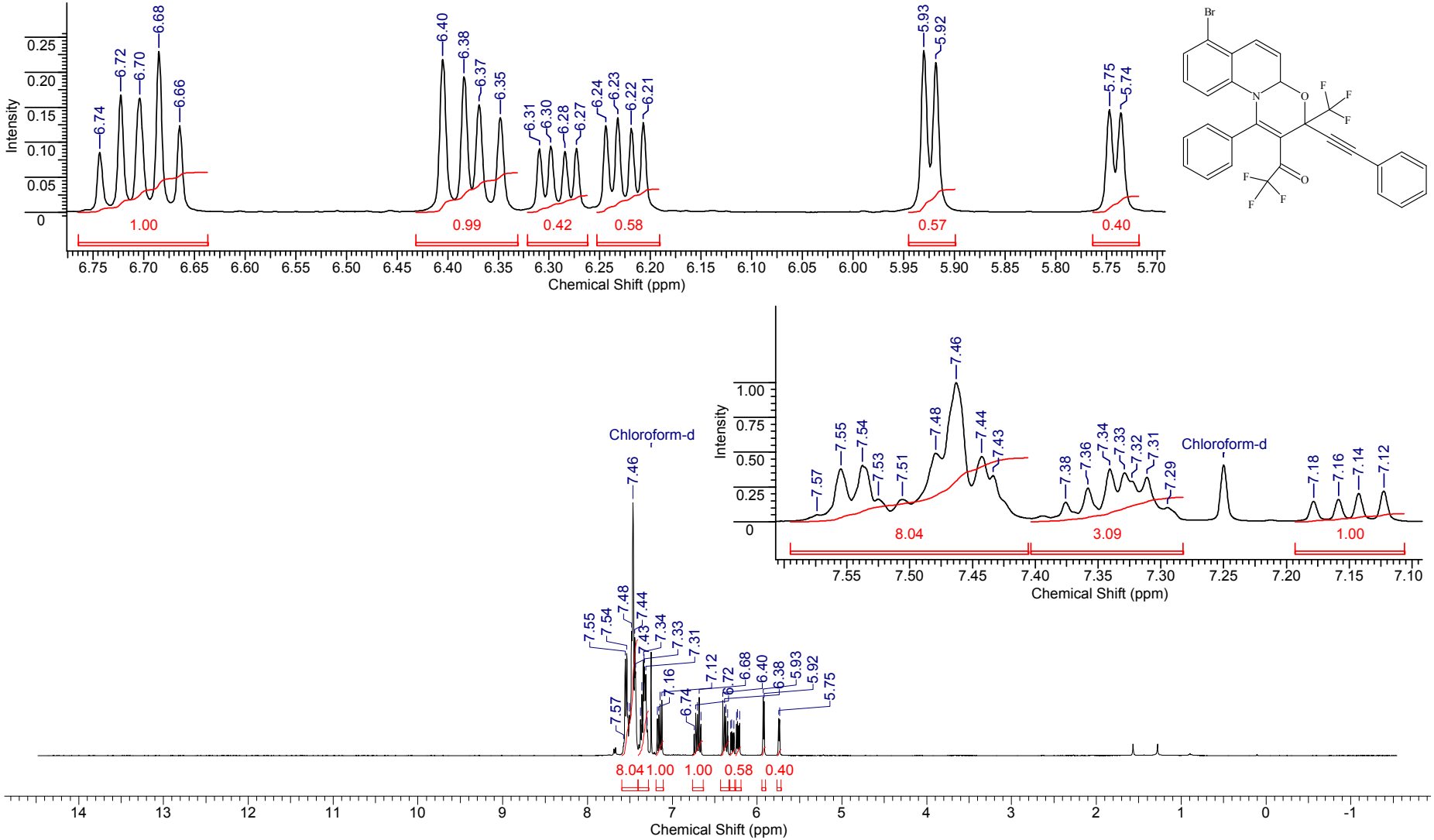
^{13}C NMR spectrum of (3*S**,4a*S**)-**3n** (100.6 MHz, $CDCl_3$)

FW	594.3308	***Formula***	$C_{29}H_{15}Cl_2F_6NO_2$				
Acquisition Time (sec)	2.0000	***Date***	Jun 4 2018	***File Name***	I:\SPEC_BM_F_2018.04.27\BM-1363-3_20180604_01\FLUORINE_01		
Frequency (MHz)	376.31	***Nucleus***	19F	***Number of Transients***	16	***Original Points Count***	178571
Points Count	262144	***Pulse Sequence***	s2pul	***Solvent***	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	***Temperature (degree C)***	23.000				



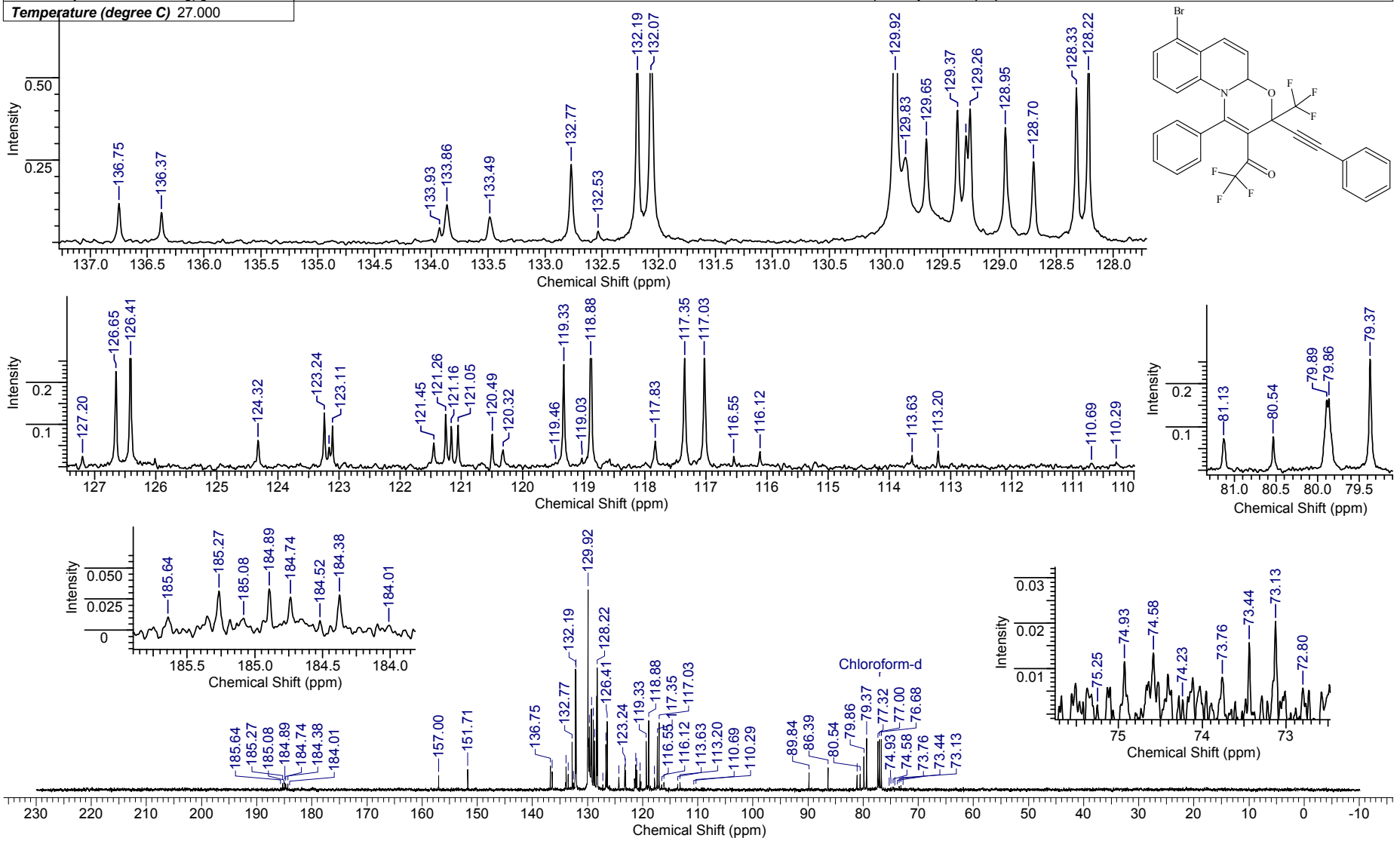
^{19}F NMR spectrum of (3*S**,4a*S**)-**3n** (376.3 MHz, $CDCl_3$)

Acquisition Time (sec)	2.5559	***Comment***	Imported from UXNMR.			***Date***	25 Apr 2018 17:17:32
File Name	D:\Comp_316\BN\output\2018\04.àï ðåëü\BM-1355-1.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	8	***Original Points Count***	16384	***Points Count***	65536
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	6410.26
Temperature (degree C)	27.000						



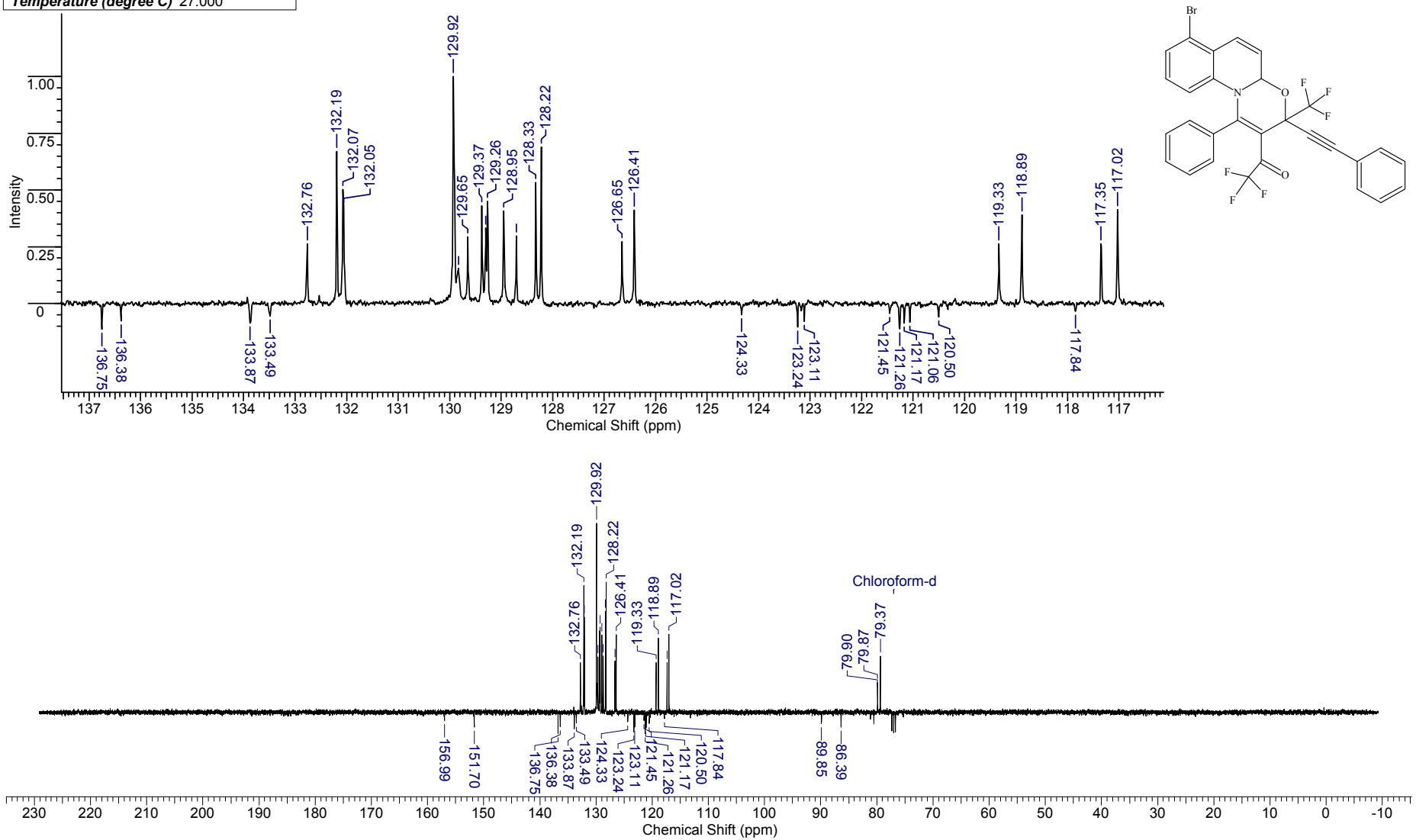
^{1}H NMR spectrum of **3o** (400.1 MHz, $CDCl_3$)

Acquisition Time (sec)	0.4999	***Comment***	Imported from UXNMR.			***Date***	25 Apr 2018 17:26:58
File Name	D:\Comp_316\BN\output\2018\04.àï ðåëü\BM-1355-1.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	329	***Original Points Count***	12076	***Points Count***	65536
Pulse Sequence	zgpg30	***Solvent***	DEUTERIUM OXIDE			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



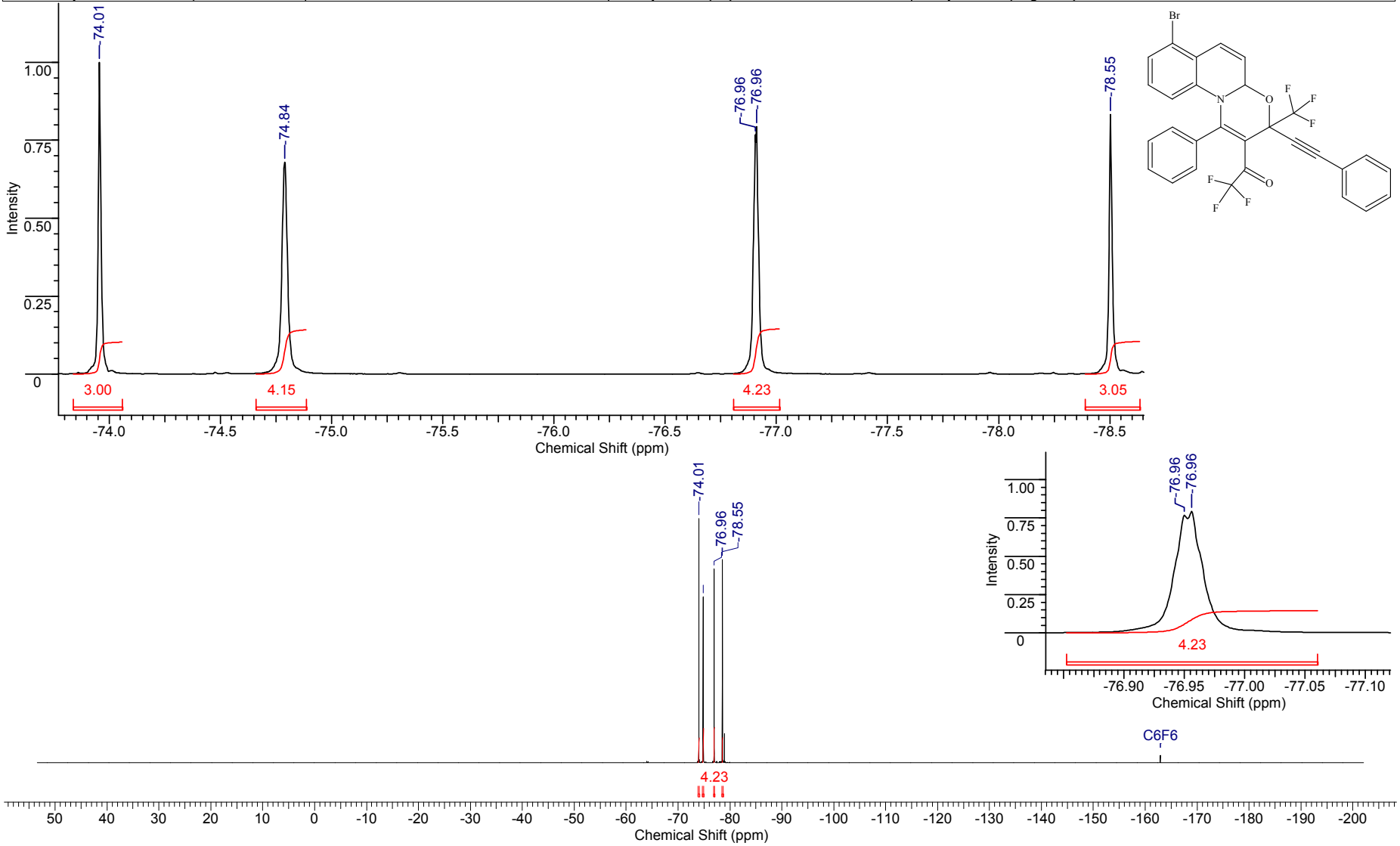
^{13}C NMR spectrum of **3o** (100.6 MHz, $CDCl_3$)

Acquisition Time (sec)	1.3664	***Comment***	Imported from UXNMR.			***Date***	27 Apr 2018 15:44:22
File Name	D:\Comp_316\BN\output\2018\04.àï ðåëü\BM-1355-1.Capt_004001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	78	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	jmod	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	23980.81
Temperature (degree C)	27.000						



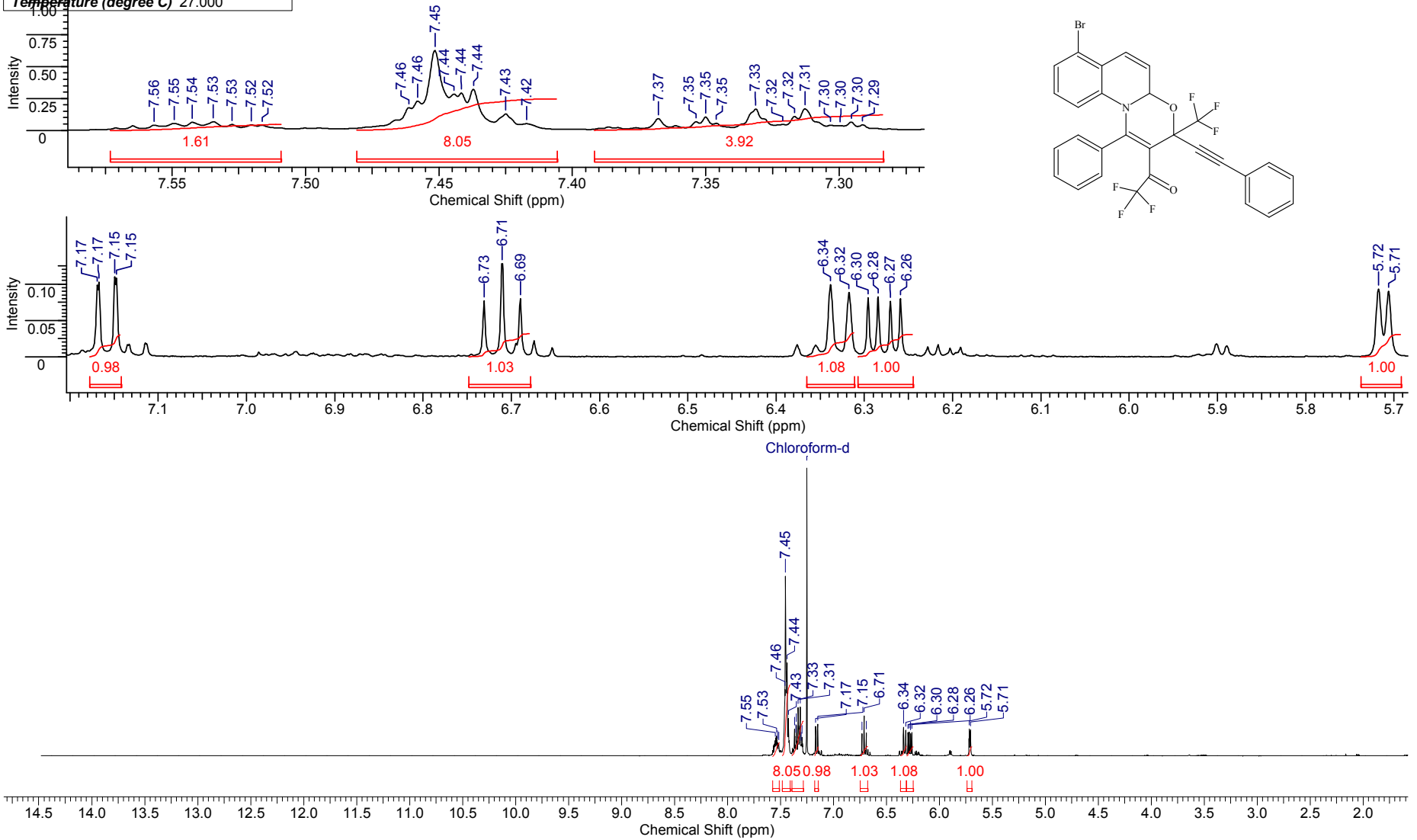
^{13}C NMR (APT) spectrum of **3o** (100.6 MHz, $CDCl_3$)

Acquisition Time (sec)	2.7263	***Date***	Apr 26 2018				
File Name	D:\Comp_316\BN\DOC (BN)\vasiliy\SPEC_BM_F_2018.04.27\BM-1355-1-F_20180426_01\FLUORINE_01					***Frequency (MHz)***	376.31
Nucleus	19F	***Number of Transients***	8	***Original Points Count***	262144	***Points Count***	262144
Pulse Sequence	s2pul	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	96153.84	***Temperature (degree C)***	22.000



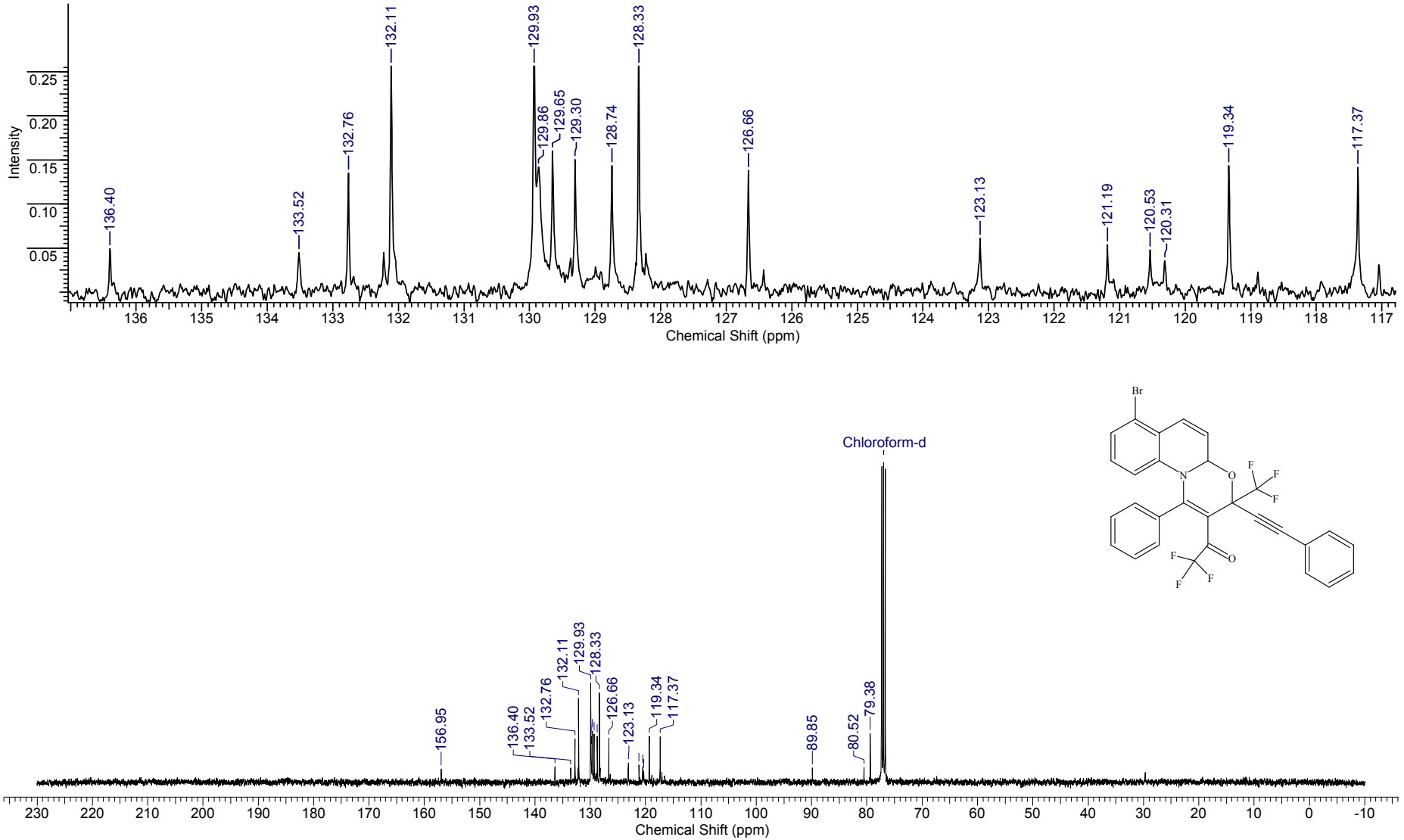
^{19}F NMR spectrum of **3o** (376.3 MHz, $CDCl_3$)

Acquisition Time (sec)	2.5559	***Comment***	Imported from UXNMR.	***Date***	25 Apr 2018 16:58:56
File Name	D:\Comp_316\BN\output\2018\04.äï ðåëü\BM-1355-2.H_001001r			***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	13	***Original Points Count*** 16384	***Points Count*** 65536
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D		***Sweep Width (Hz)*** 6410.26
Temperature (degree C)	27.000				



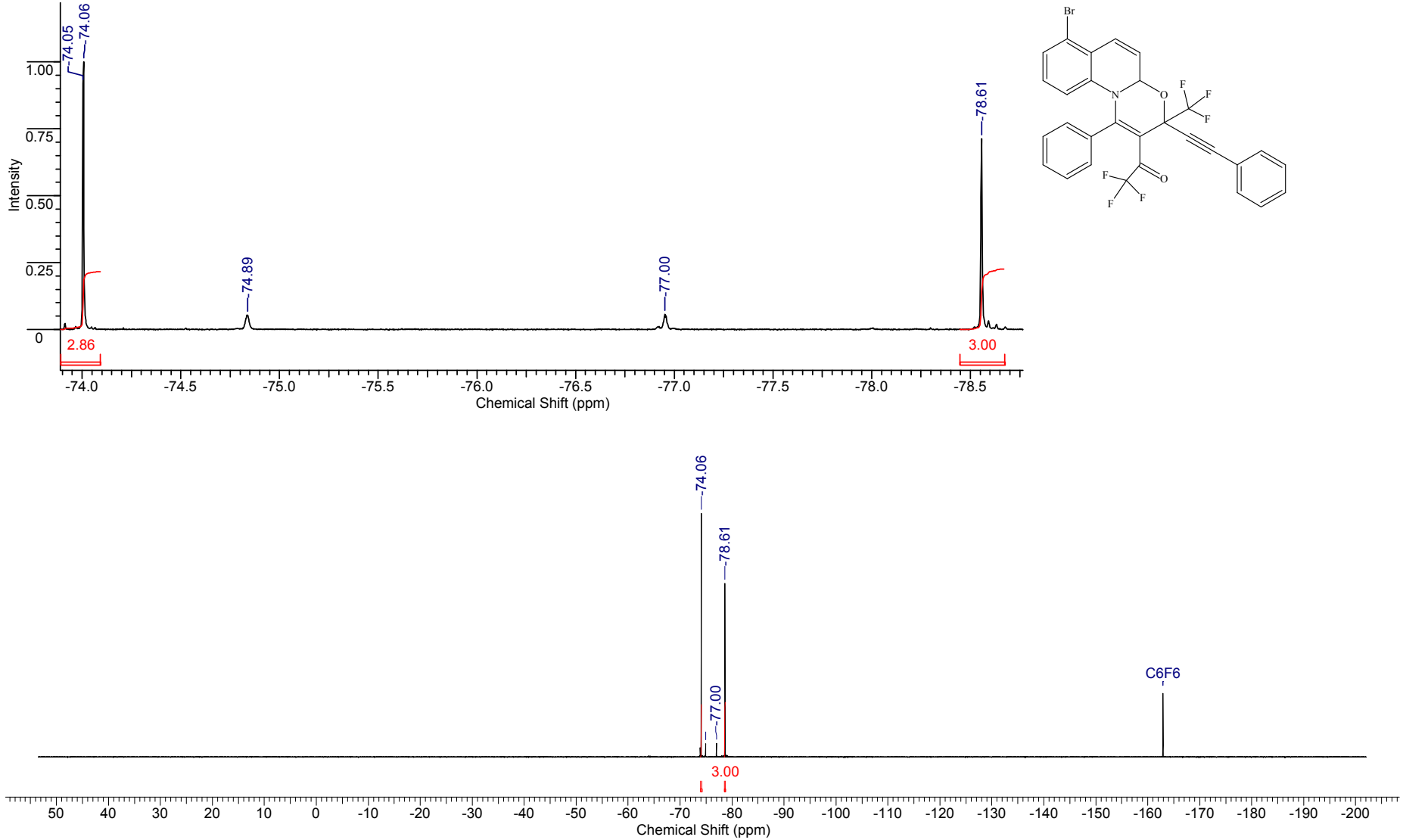
^{1}H NMR spectrum of (3*S**,4a*S**)-**3o** (400.1 MHz, $CDCl_3$)

Acquisition Time (sec)	0.4999	***Comment***	Imported from UXNMR.			***Date***	24 May 2018 12:59:56
File Name	D:\Comp_316\BN\output\2018\05.ì àé\BM-1355-2B.C_002001r			***Frequency (MHz)***	100.61	***Nucleus***	13C
Number of Transients	1809	***Original Points Count***	12076	***Points Count***	65536	***Pulse Sequence***	zgpg30
Solvent	DEUTERIUM OXIDE			***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000

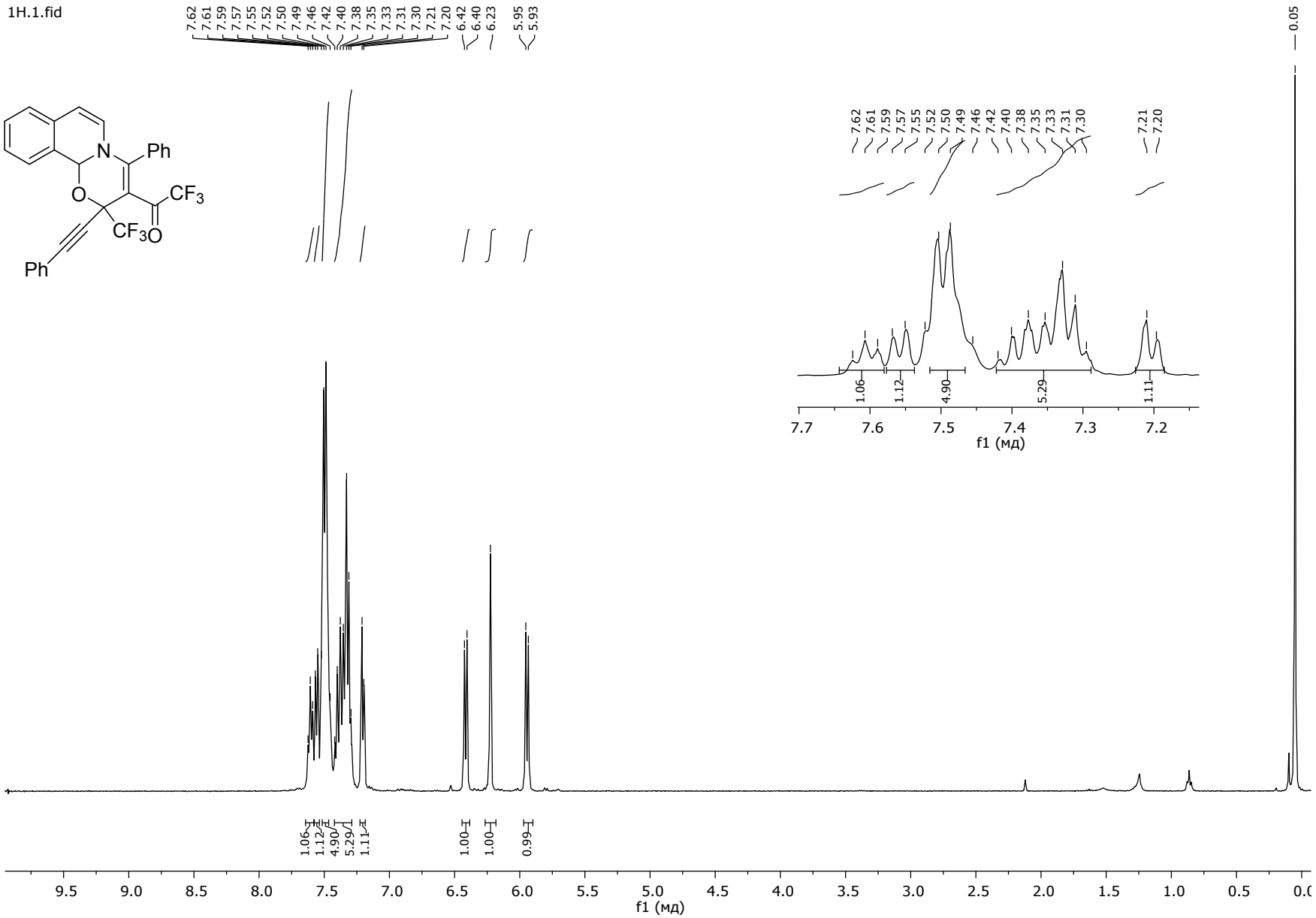


^{13}C NMR spectrum of (3*S**,4a*S**)-**3o** (100.6 MHz, $CDCl_3$)

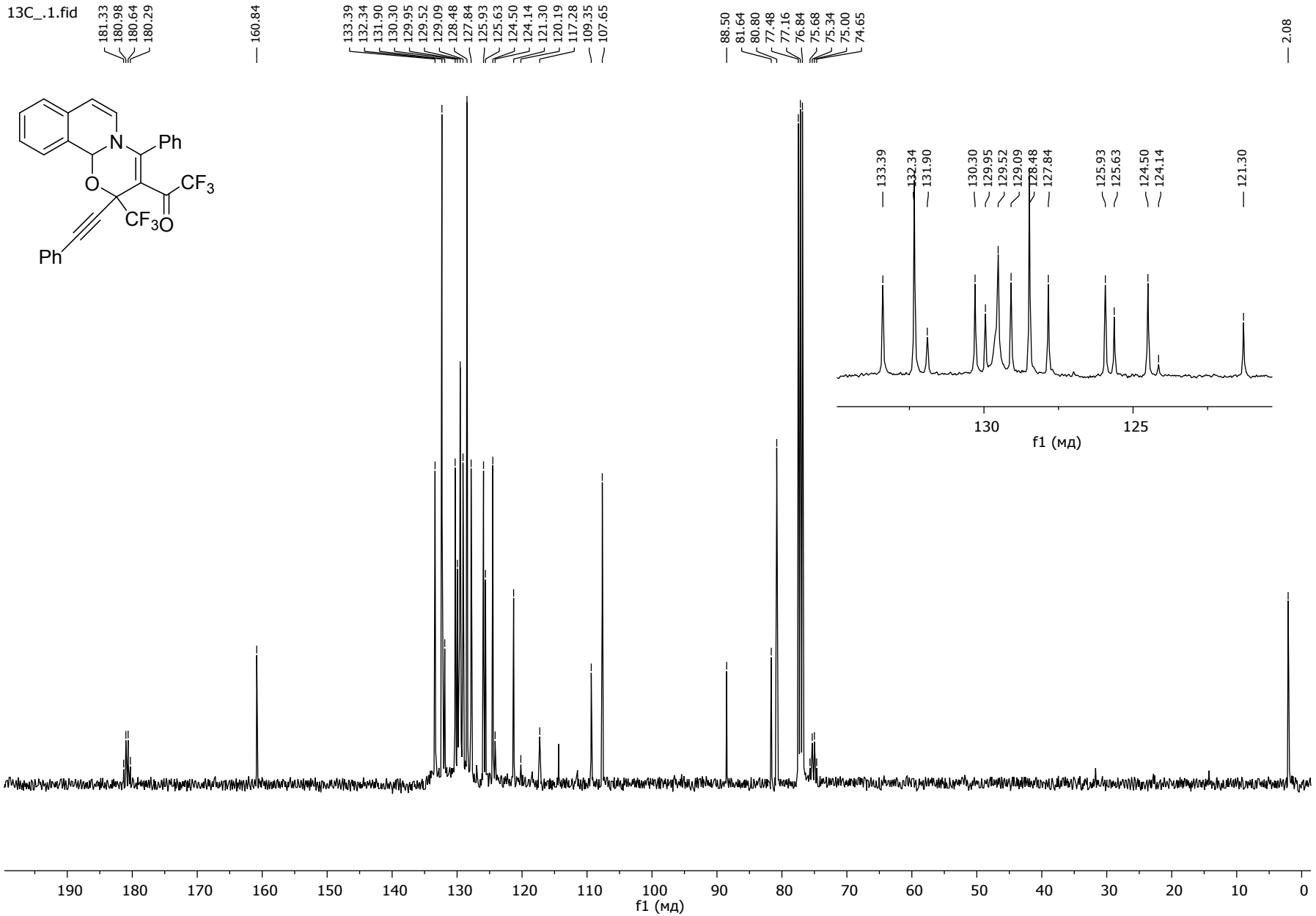
Acquisition Time (sec)	2.7263	***Date***	Apr 26 2018				
File Name	D:\Comp_316\BN\DOC (BN)\vasiliy\SPEC_BM_F_2018.04.27\BM1355-2-F_20180426_01\FLUORINE_01					***Frequency (MHz)***	376.31
Nucleus	19F	***Number of Transients***	8	***Original Points Count***	262144	***Points Count***	262144
Pulse Sequence	s2pul	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	96153.84	***Temperature (degree C)***	22.000



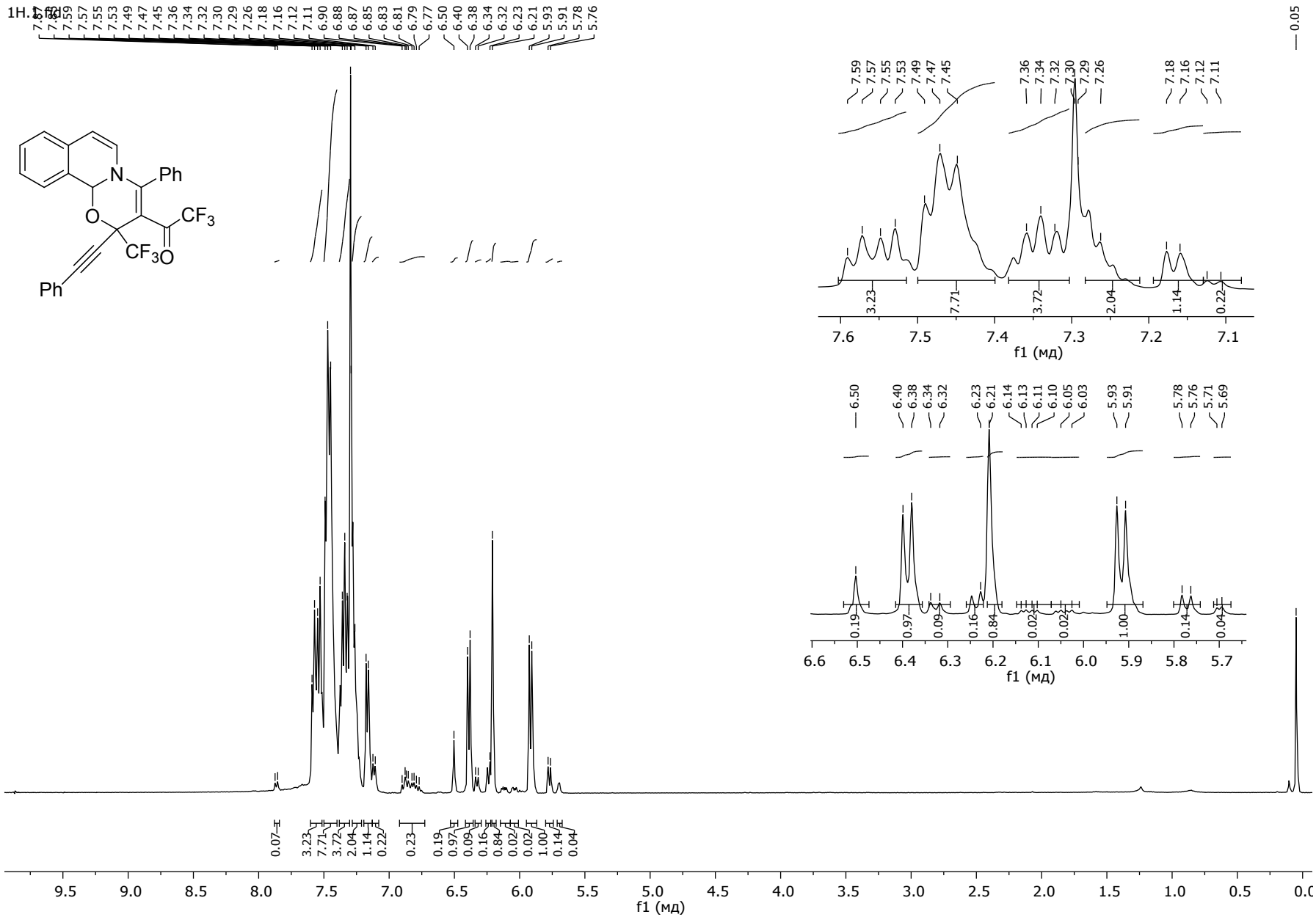
^{19}F NMR spectrum of (3*S**,4a*S**)-**3o** (376.3 MHz, $CDCl_3$)



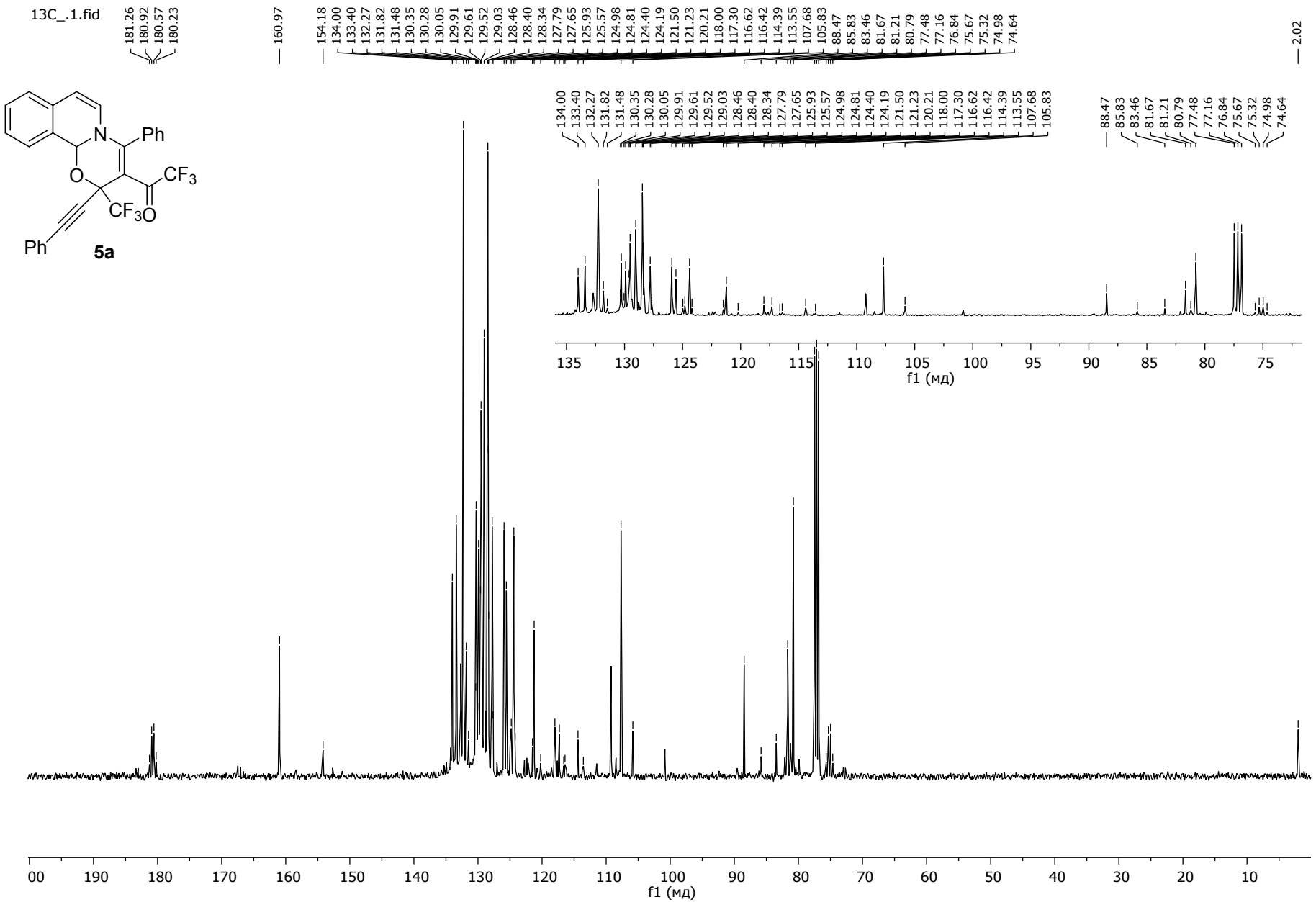
^{1}H NMR spectrum of (2*R**,11b*R**)-**5a** (400.1 MHz, $CDCl_3$)



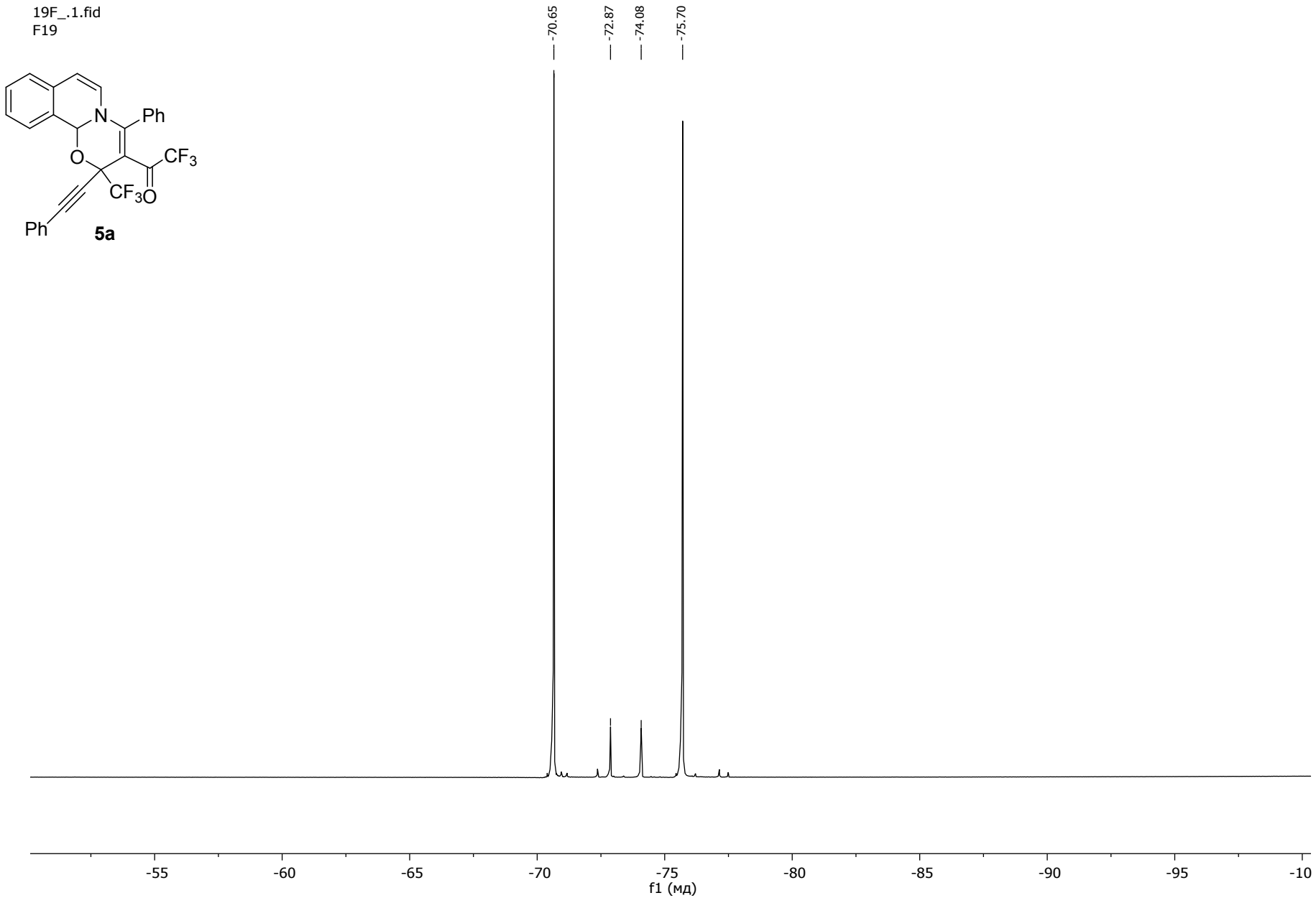
^{13}C NMR spectrum of (2*R**,11b*R**)-**5a** (100.6 MHz, $CDCl_3$)



^{1}H NMR spectrum of **5a** (400.1 MHz, $CDCl_3$)

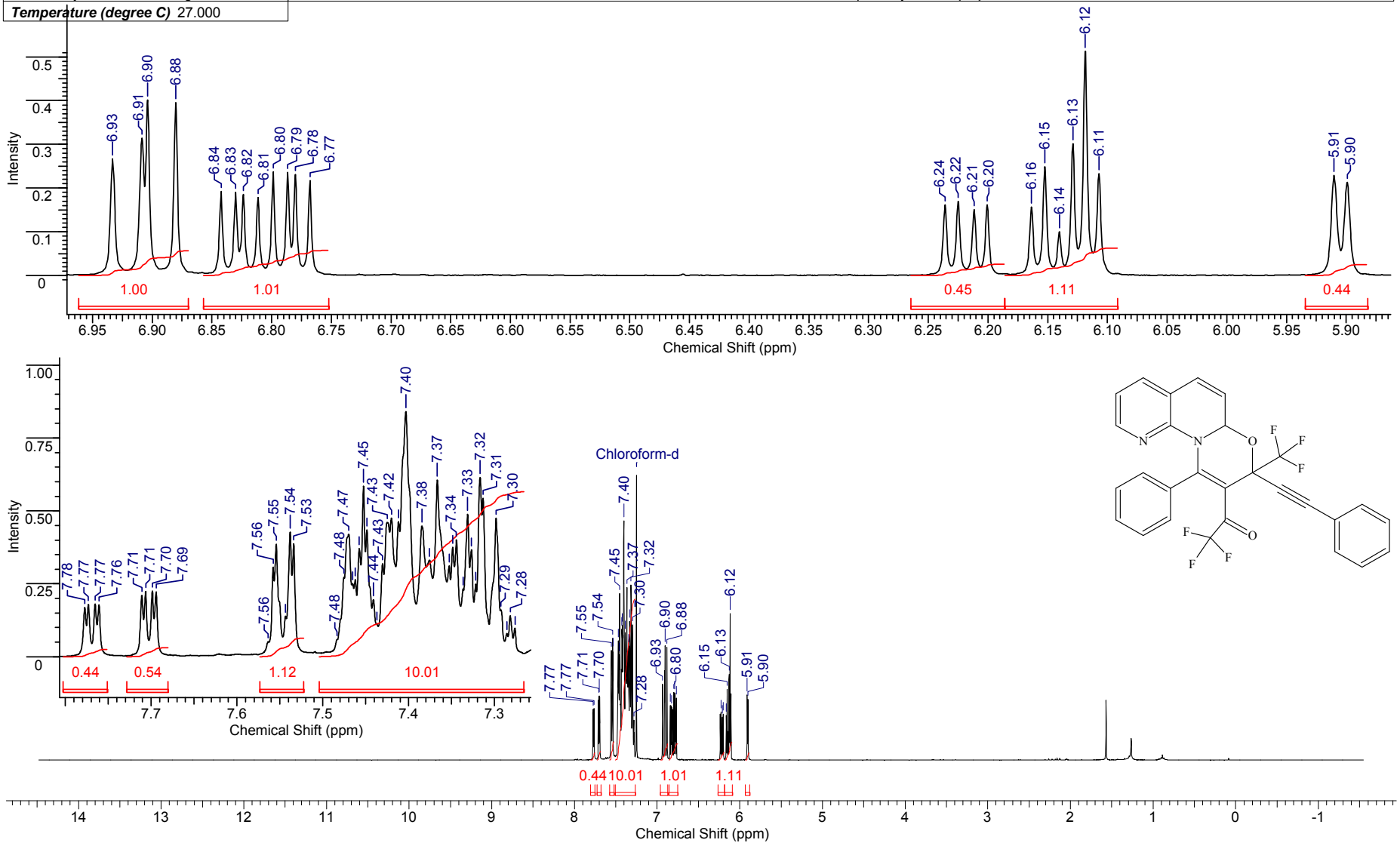


^{13}C NMR spectrum of **5a** (100.6 MHz, $CDCl_3$)



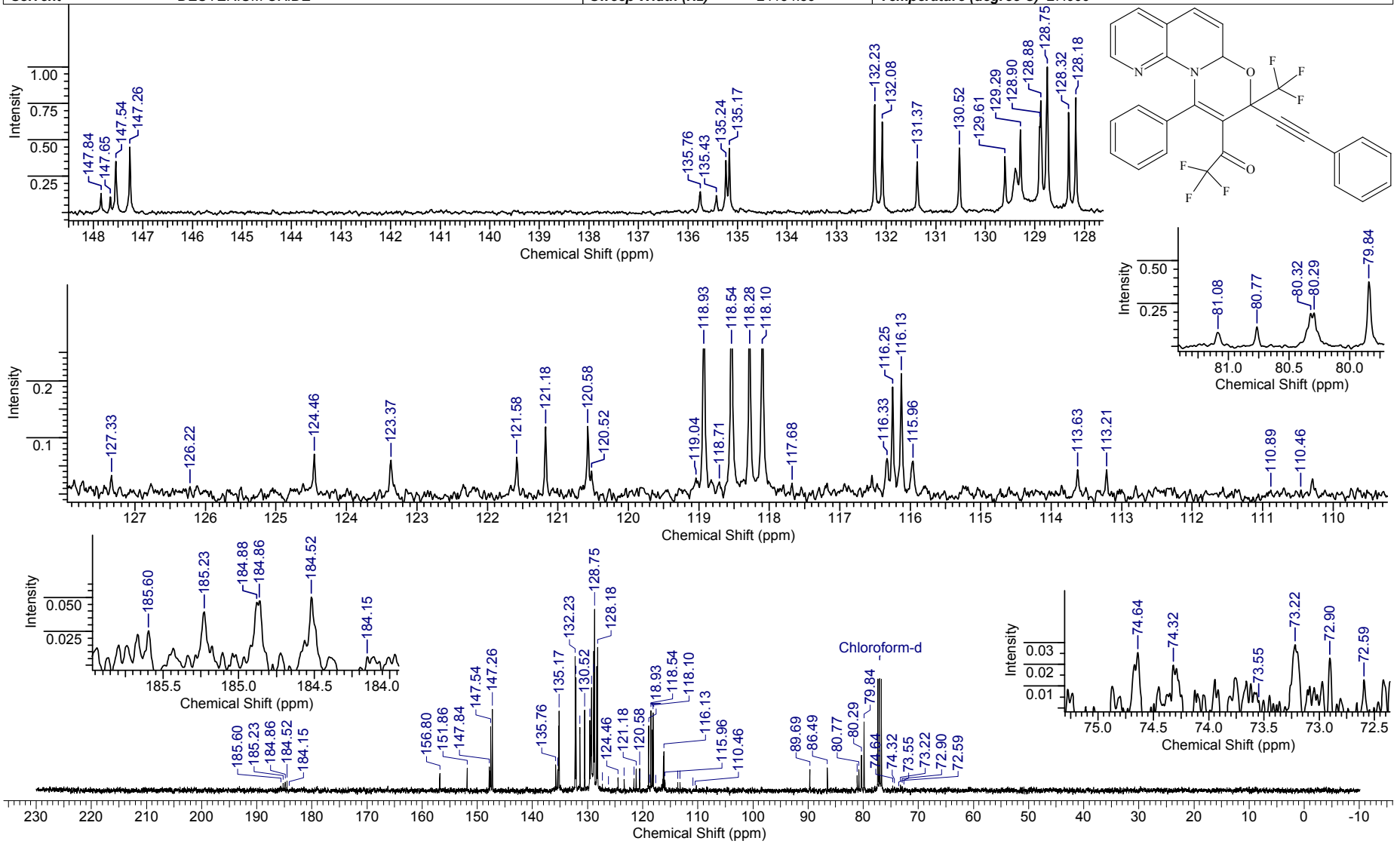
^{19}F NMR spectrum of **5a** (376.5 MHz, $CDCl_3$)

Acquisition Time (sec)	2.5559	***Comment***	Imported from UXNMR.			***Date***	21 Apr 2018 13:38:54
File Name	D:\Comp_316\BN\output\2018\04.äï ðåëü\BM-1357-2.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	16384	***Points Count***	65536
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	6410.26
Temperature (degree C)	27.000						



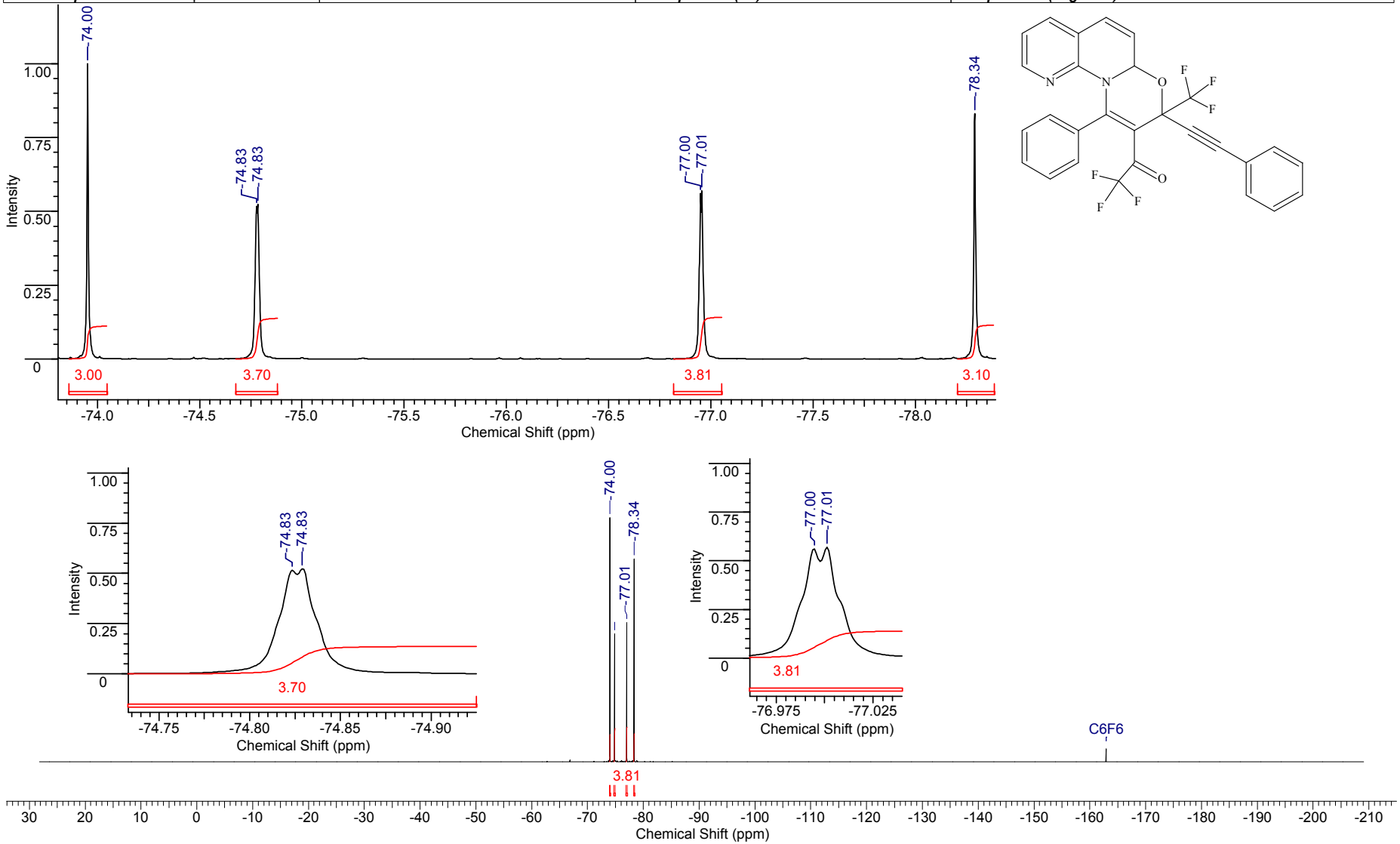
^{1}H NMR spectrum of **5b** (400.1 MHz, $CDCl_3$)

Acquisition Time (sec)	0.4999	***Comment***	Imported from UXNMR.			***Date***	15 May 2018 14:54:30
File Name	D:\Comp_316\BN\output\2018\05.ì àé\BM-1357-2B.C_002001r			***Frequency (MHz)***	100.61	***Nucleus***	13C
Number of Transients	400	***Original Points Count***	12076	***Points Count***	65536	***Pulse Sequence***	zgpg30
Solvent	DEUTERIUM OXIDE			***Sweep Width (Hz)***	24154.59	***Temperature (degree C)***	27.000



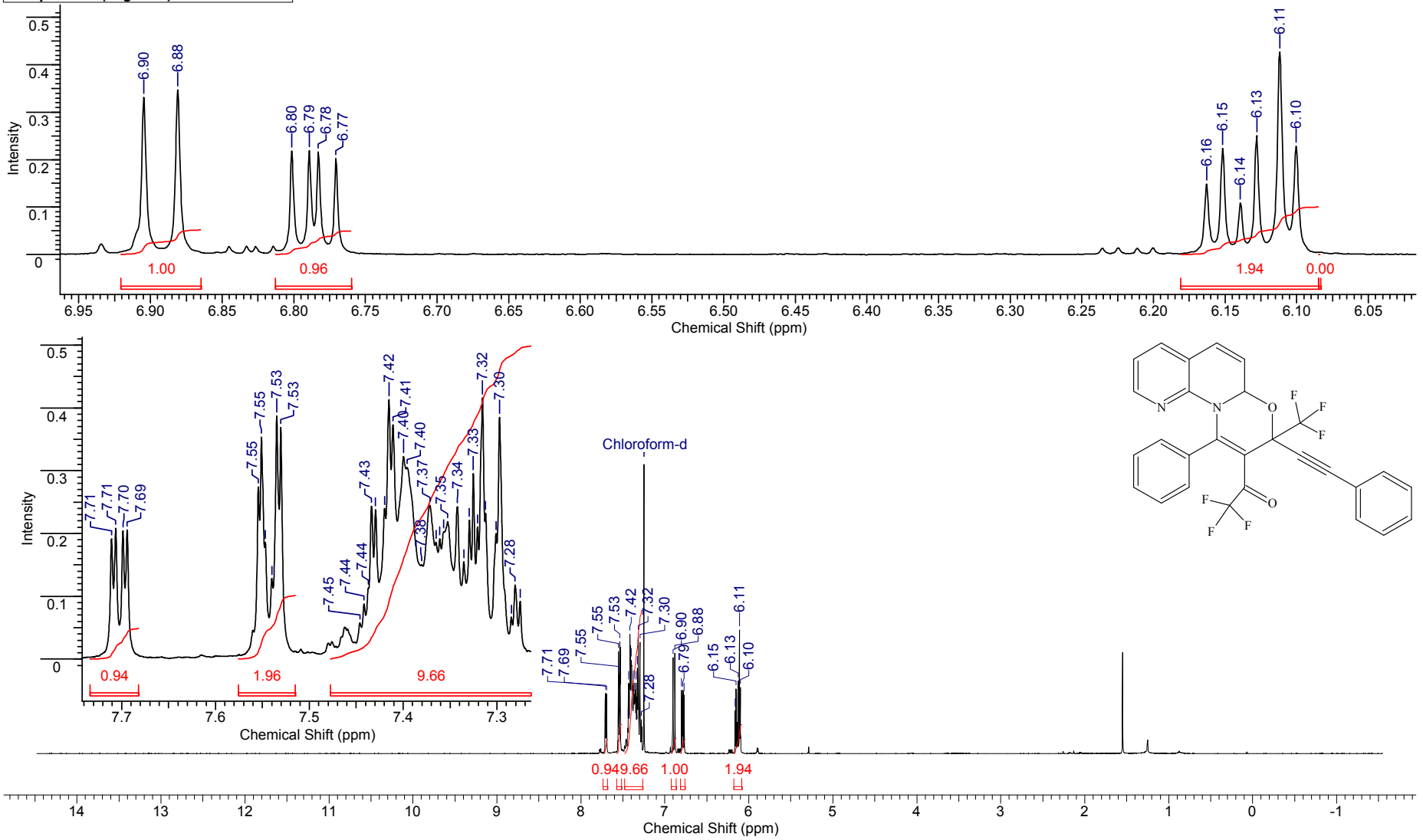
^{13}C NMR spectrum of **5b** (100.6 MHz, $CDCl_3$)

Acquisition Time (sec)	1.5000	***Comment***	STANDARD FLUORINE PARAMETERS			***Date***	Apr 23 2018
File Name	D:\Comp_316\BN\DOC (BN)\vasiliy\SPEC_BM_F_2018.04.27\BM-1357-2_20180423_01\FLUORINE_01					***Frequency (MHz)***	376.31
Nucleus	19F	***Number of Transients***	8	***Original Points Count***	133929	***Points Count***	262144
Pulse Sequence	s2pul	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	89285.71	***Temperature (degree C)***	22.000



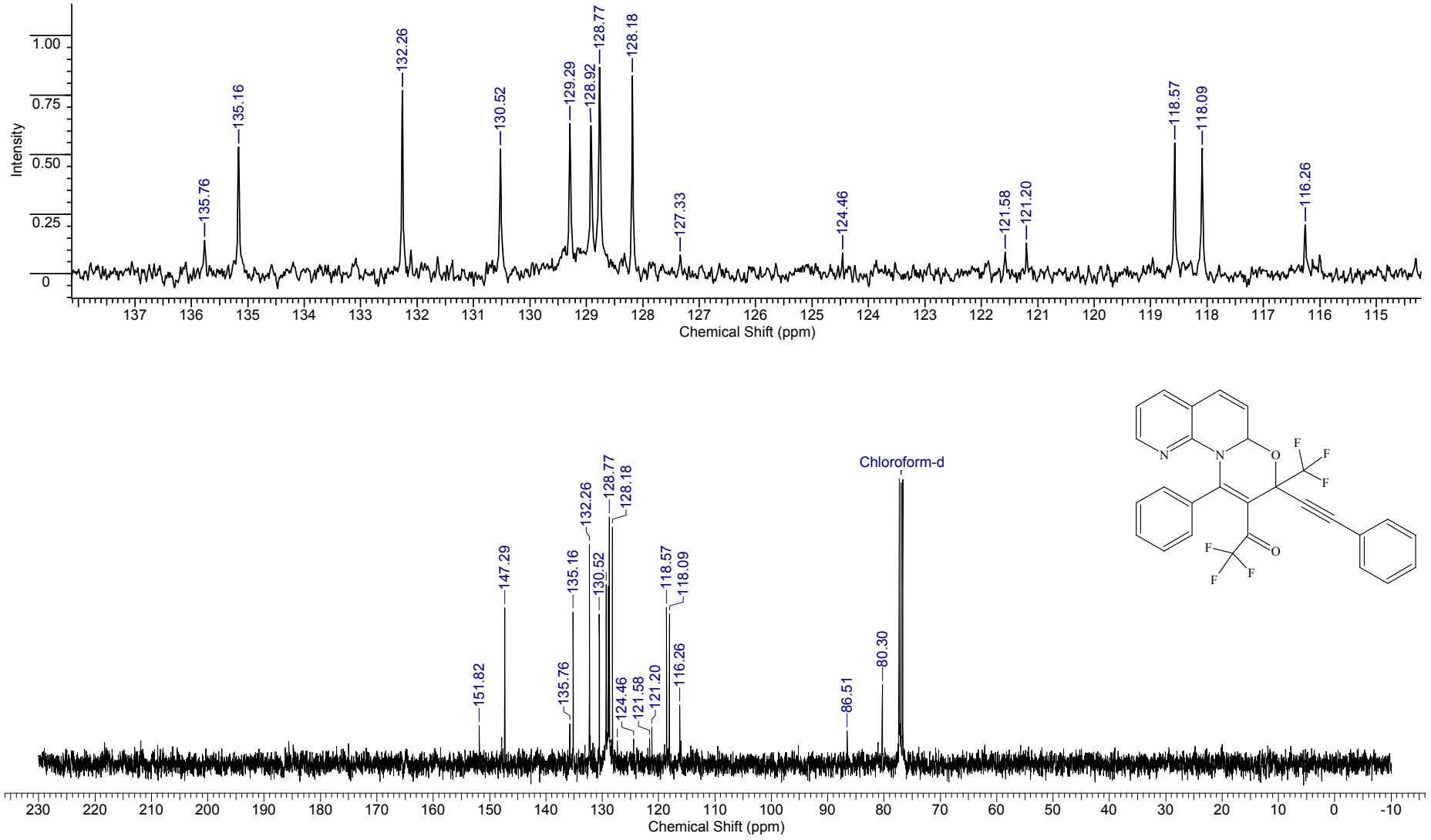
^{19}F NMR spectrum of **5b** (376.3 MHz, $CDCl_3$)

Acquisition Time (sec)	2.5559	***Comment***	Imported from UXNMR.			***Date***	21 Apr 2018 13:32:04
File Name	D:\Comp_316\BN\output\2018\04.äï ðåëü\BM-1357-1.H_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	4	***Original Points Count***	16384	***Points Count***	65536
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	6410.26
Temperature (degree C)	27.000						



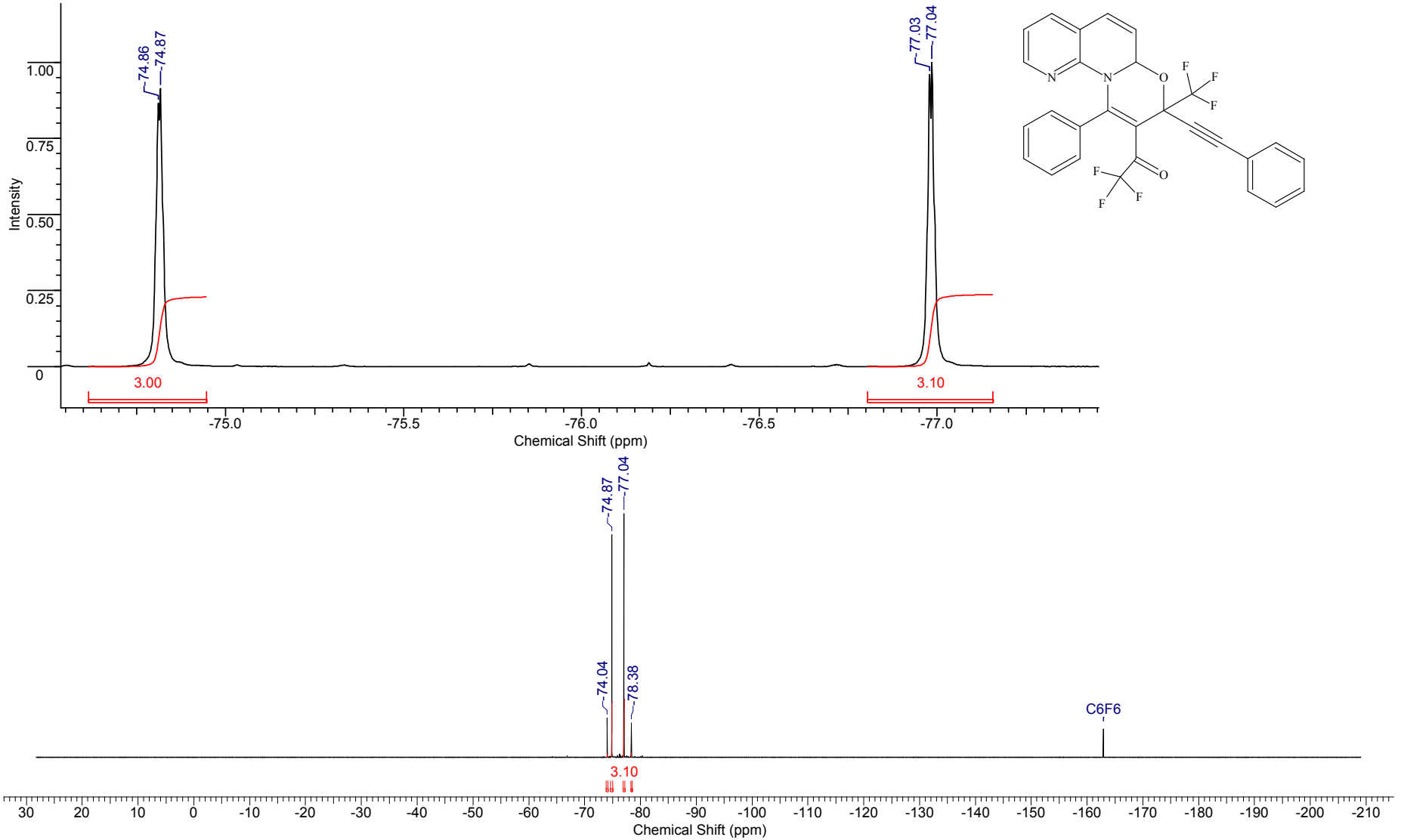
^{1}H NMR spectrum of (3*R**,4a*S**)-**5b** (400.1 MHz, $CDCl_3$)

Acquisition Time (sec)	0.4999	***Comment***	Imported from UXNMR.			***Date***	21 Apr 2018 13:37:10
File Name	D:\Comp_316\BN\output\2018\04.äï ðåëü\BM-1357-1.C_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	140	***Original Points Count***	12076	***Points Count***	65536
Pulse Sequence	zgpg30	***Solvent***	DEUTERIUM OXIDE			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



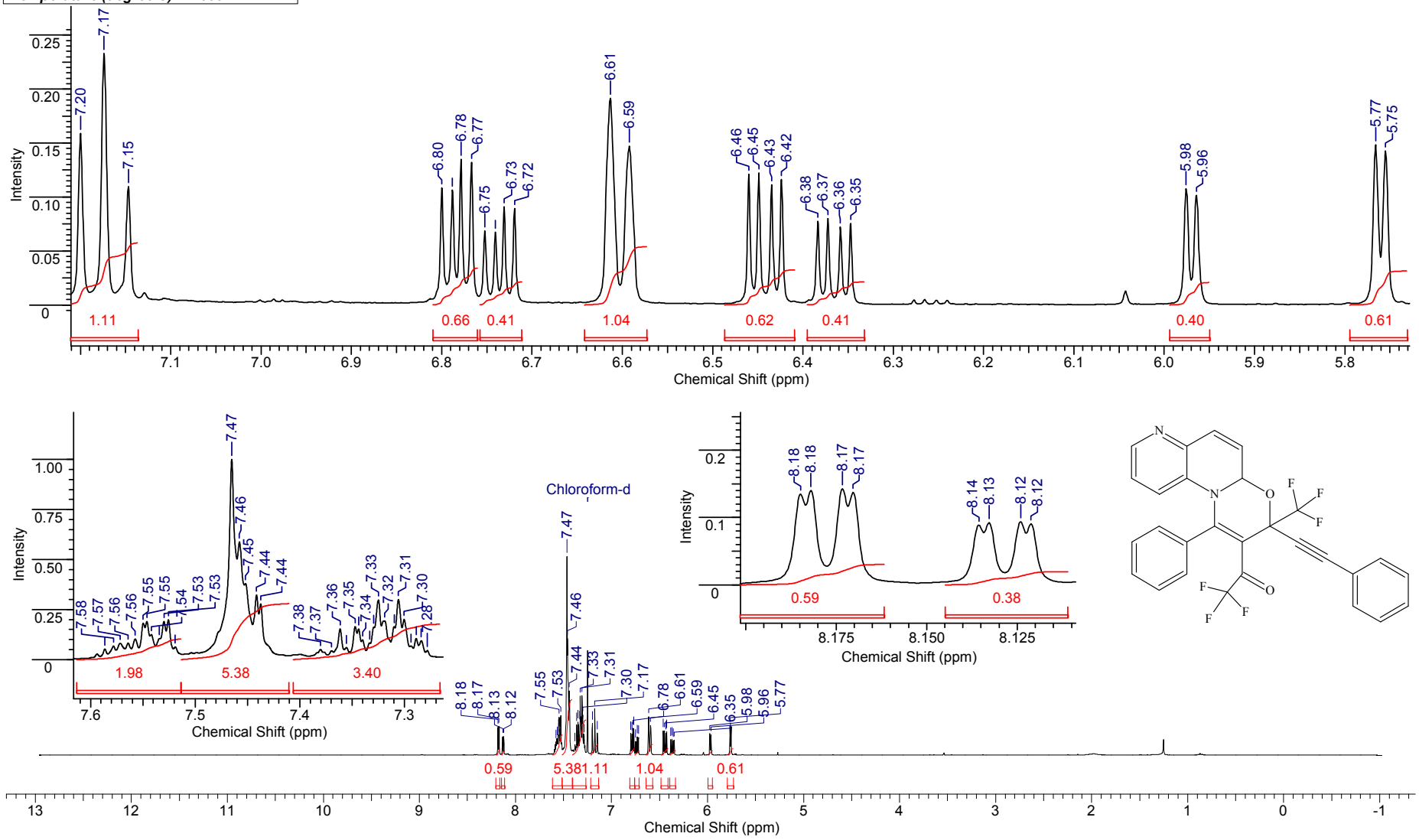
^{13}C NMR spectrum of (3*R**,4a*S**)-**5b** (100.6 MHz, $CDCl_3$)

Acquisition Time (sec)	1.5000	***Date***	Apr 23 2018				
File Name	D:\Comp_316\BN\DOC (BN)\vasiliy\SPEC_BM_F_2018.04.27\BM-1357-1_20180423_01\FLUORINE_01					***Frequency (MHz)***	376.31
Nucleus	19F	***Number of Transients***	8	***Original Points Count***	133929	***Points Count***	262144
Pulse Sequence	s2pul	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	89285.71	***Temperature (degree C)***	22.000



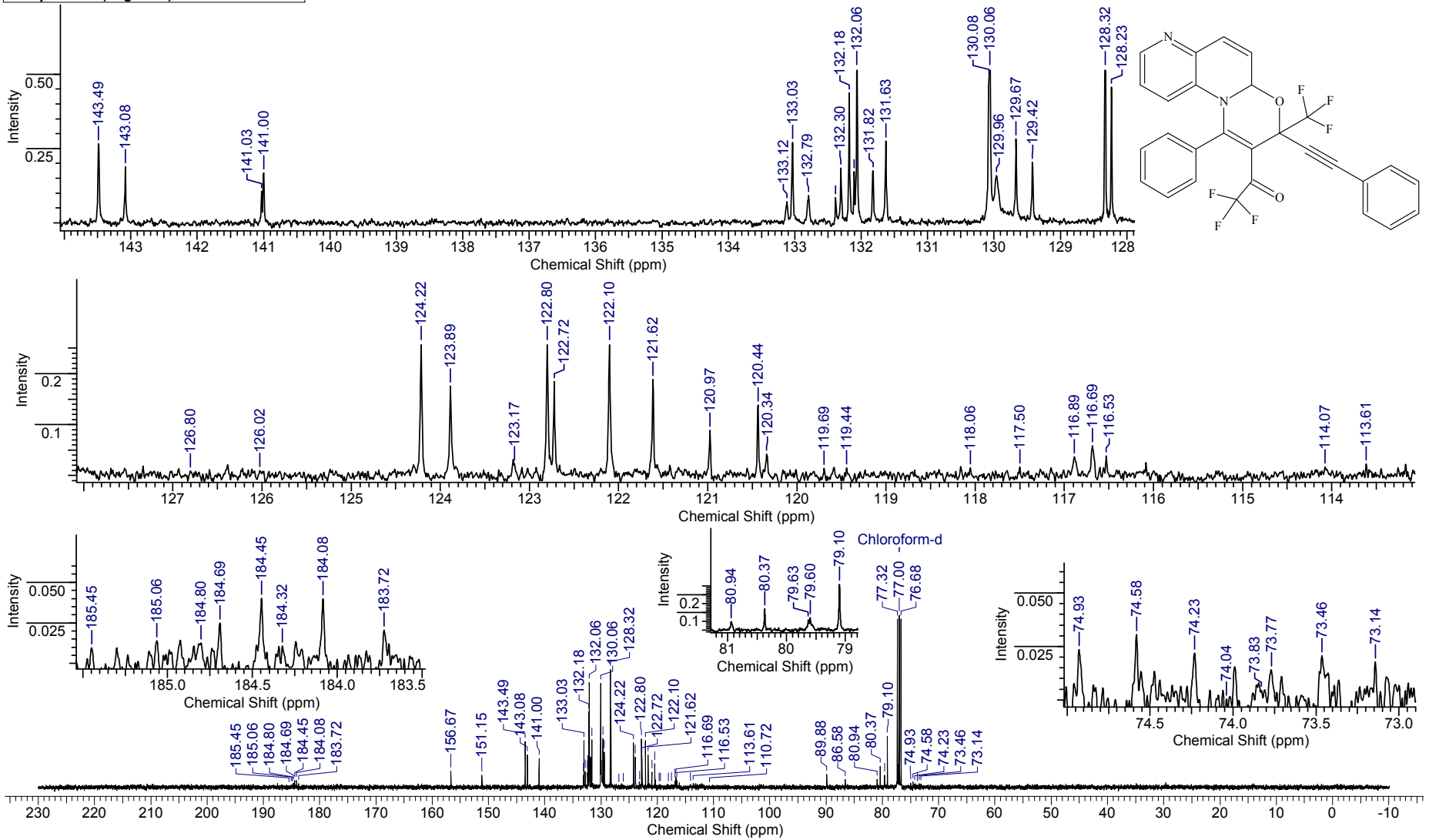
^{19}F NMR spectrum of (3*R**,4a*S**)-**5b** (376.3 MHz, $CDCl_3$)

Acquisition Time (sec)	2.9295	***Comment***	Imported from UXNMR.			***Date***	21 Apr 2018 22:17:06
File Name	D:\Comp_316\BN\output\2018\04.àï ðåëü\BM-1358-3\BM-1358-3_001001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	8	***Original Points Count***	16384	***Points Count***	65536
Pulse Sequence	zg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	5592.84
Temperature (degree C)	27.000						



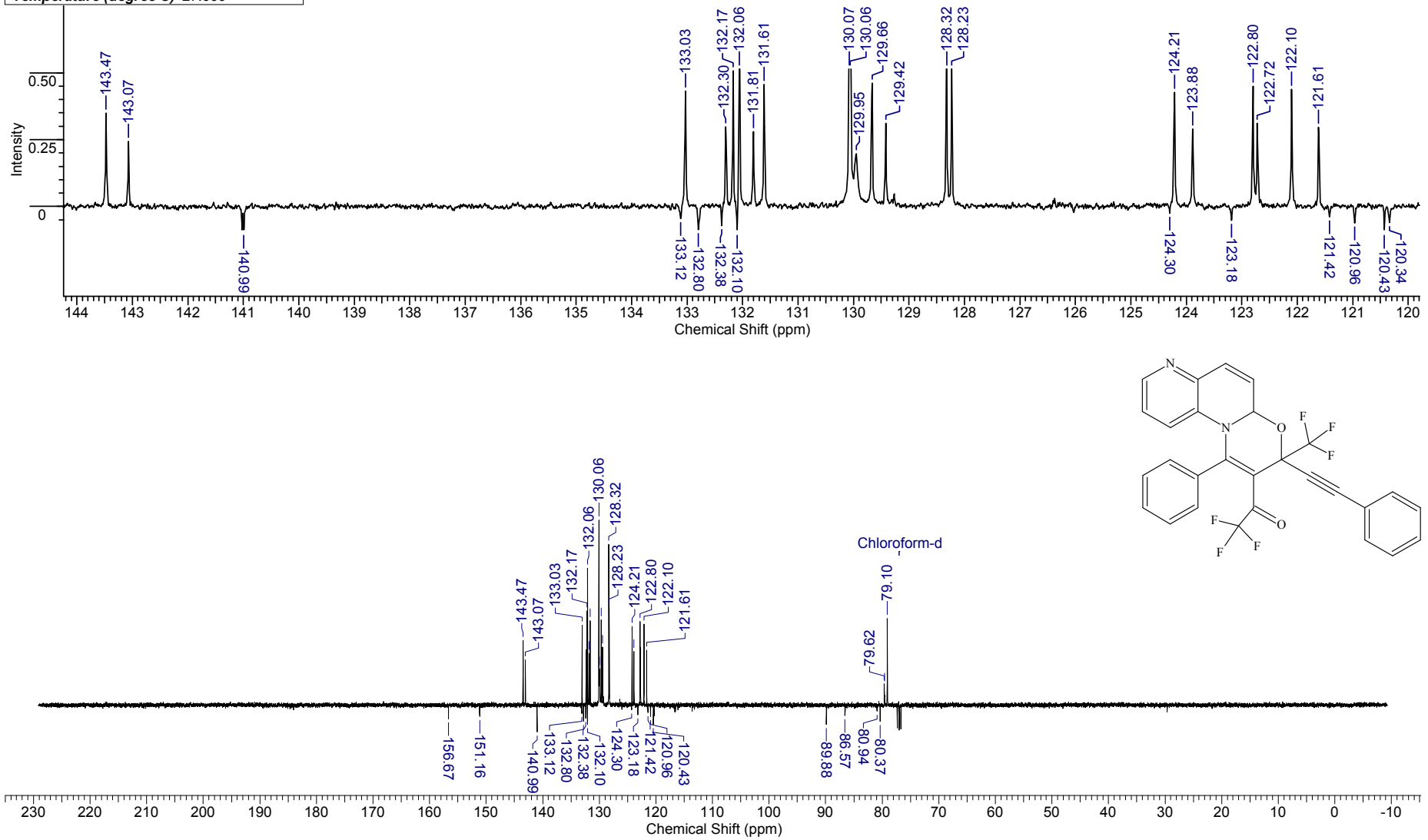
^{1}H NMR spectrum of **5c** (400.1 MHz, $CDCl_3$)

Acquisition Time (sec)	0.6783	***Comment***	Imported from UXNMR.			***Date***	21 Apr 2018 22:27:22
File Name	D:\Comp_316\BN\output\2018\04.äï ðåëü\BM-1358-3\BM-1358-3_002001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	192	***Original Points Count***	16384	***Points Count***	131072
Pulse Sequence	zgpg30	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	24154.59
Temperature (degree C)	27.000						



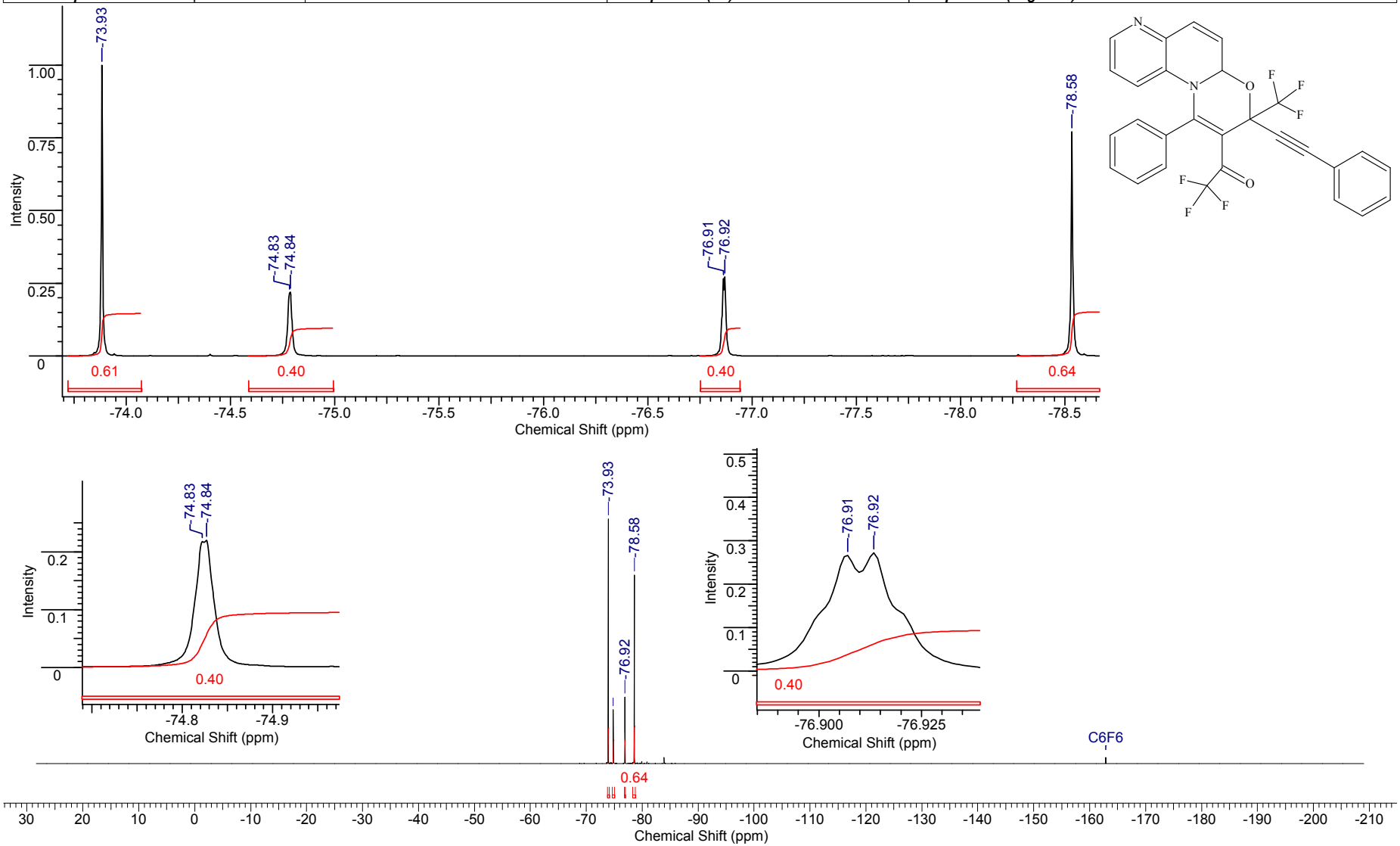
^{13}C NMR spectrum of **5c** (100.6 MHz, $CDCl_3$)

Acquisition Time (sec)	1.3664	***Comment***	Imported from UXNMR.			***Date***	26 Apr 2018 11:55:34
File Name	D:\Comp_316\BN\output\2018\04.àï ðåëü\BM-1358-3APT.CApt_004001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	173	***Original Points Count***	32768	***Points Count***	131072
Pulse Sequence	jmod	***Solvent***	CHLOROFORM-D			***Sweep Width (Hz)***	23980.81
Temperature (degree C)	27.000						



^{13}C NMR (APT) spectrum of **5c** (100.6 MHz, $CDCl_3$)

Acquisition Time (sec)	1.5000	***Date***	Apr 23 2018				
File Name	D:\Comp_316\BN\DOC (BN)\vasiliy\SPEC_BM_F_2018.04.27\BM-1358-3_20180423_01\FLUORINE_01					***Frequency (MHz)***	376.31
Nucleus	19F	***Number of Transients***	8	***Original Points Count***	133929	***Points Count***	262144
Pulse Sequence	s2pul	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	89285.71	***Temperature (degree C)***	22.000



^{19}F NMR spectrum of **5c** (376.3 MHz, $CDCl_3$)

X-ray diffraction structural analysis data

The determination of the unit cell and the data collection for 2,2,2-trifluoro-1-[1-phenyl-3-(2-phenylethynyl)-3-(trifluoromethyl)-3*H*,4a*H*-[1,3]oxazino[3,2-*a*]quinolin-2-yl]-1-ethanone (**3a**) was performed on a Bruker D8 VENTURE PHOTON 100 CMOS diffractometer with MoK_α radiation (λ = 0.71073) at 100.0(2) K using the ω–φ scan technique. A specimen of $C_{29}H_{17}F_6N_1O_2$, approximate dimensions 0.5 mm x 0.5 mm x 0.5 mm, pale yellow cylinder-like crystal was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The integration of the data using an monoclinic unit cell with *P2₁* space group yielded a total of 38293 reflections to a maximum θ angle of 30.91° (0.69 Å resolution), of which 6736 were independent (average redundancy 5.685, completeness = 92.6%, Rint = 3.58%, Rsig = 3.68%) and 5807 (86.21%) were greater than 2σ(F2). The final cell constants of **a** = 9.2784(4) Å, **b** = 14.1722(6) Å, **c** = 9.8379(4) Å, β=114.0770(10)°, Z= 2, volume = 1181.09(9) Å^3, are based upon the refinement of the XYZ-centroids of 9178 reflections above 20 σ(I) with 4.808° < 2θ < 60.79°. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.716. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9400 and 0.9400. The structure was solved and refined using the Bruker SHELXTL Software Package.[3] The H atoms were determined from a difference Fourier synthesis.

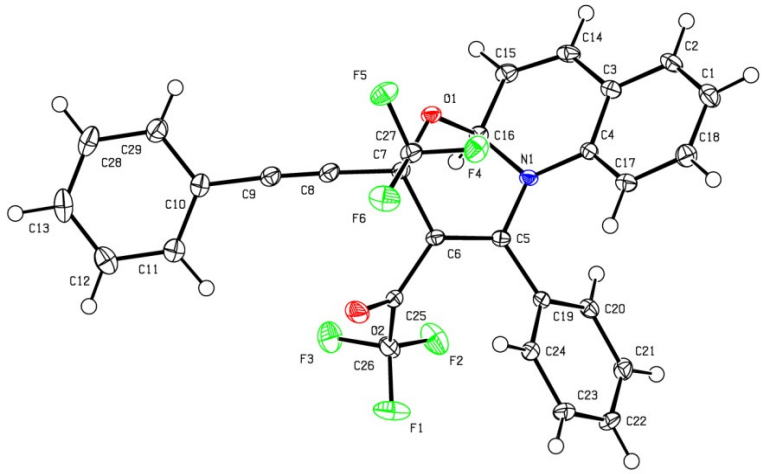


Figure 1. X-ray structure of 2,2,2-trifluoro-1-[1-phenyl-3-(phenylethynyl)-3-(trifluoromethyl)-3*H*,4a*H*-dihydro-[1,3]oxazino[3,2-*a*]quinolin-2-yl]ethanone (**3a**). Thermal ellipsoids set at 50% probability.

The final anisotropic full-matrix least-squares refinement on F2 with 343 variables converged at R1 = 3.66%, for the observed data and wR2 = 7.46% for all data. The goodness-of-fit was 1.023. The largest peak in the final difference electron density synthesis was 0.27 e$^-$/Å^3 and the largest hole was -0.23 e$^-$/Å^3 with an RMS deviation of 0.054 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.477 g/cm^3 and F(000), 536 e$^-$. CCDC **1545029**.

Bond precision:	C-C = 0.0031 Å	Wavelength = 0.71073
Cell: a=9.2784(4)	b=14.1722(6)	c=9.8379(4)
alpha=90	beta=114.077(1)	gamma=90
Temperature: 100 K		
	Calculated	**Reported**
Volume	1181.09(9)	1181.09(9)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C29 H17 F6 N O2	C29 H17 F6 N O2

Sum formula	C29 H17 F6 N O2	C29 H17 F6 N O2
Mr	525.44	525.44
Dx,g cm-3	1.477	1.477
Z	2	2
Mu (mm-1)	0.125	0.125
F000	536.0	536.0
F000’	536.38	
h,k,lmax	13,20,14	12,20,14
Nref	7456[3864]	6736
Tmin,Tmax	0.939,0.939	0.534,0.746
Tmin’	0.939	

Correction method= # Reported T Limits: Tmin=0.534 Tmax=0.746 AbsCorr = MULTI-SCAN

Data completeness= 1.74/0.90 Theta(max)= 30.907

R(reflections)= 0.0366(5807) wR2(reflections)= 0.0746(6736)

S = 1.023 Npar= 412

References

1 V. M. Muzalevskiy, A. Yu. Rulev, A. R. Romanov, E. V. Kondrashov, I. A. Ushakov, V. A. Chertkov, V. G. Nenajdenko. *J. Org. Chem.* **2017**, *82*, 7200–7214

2 B. A. Trofimov, K. V. Belyaeva, L. P. Nikitina, A. V. Afonin, A. V. Vashchenko, V. M. Muzalevskiy, V. G. Nenajdenko, *Chem. Commun.* **2018**, *54*, 2268-2271.

3 G.M. Sheldrick. *Acta Crystallogr*. **2008**, *D64*, 112-122.