

Supporting Information

Visible Light Promotes Cascade Trifluoromethylation/Cyclization, Leading to Trifluoromethylated Polycyclic Quinazolinones, Benzimidazoles and Indoles

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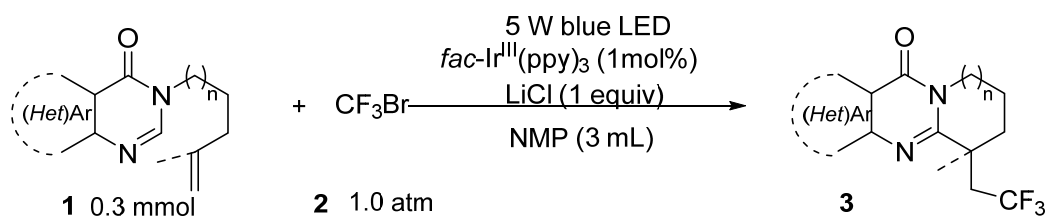
1. General information

The solvents were distilled by standard methods. Reagents were obtained from commercial suppliers and used without further purification unless otherwise noted. Silica gel column chromatography was carried out using silica gel 60 (230–400 mesh). Analytical thin-layer chromatography (TLC) was done using silica gel (silica gel 60 F254). TLC plates were analyzed by exposure to ultraviolet (UV) light and/or submersion in phosphomolybdic acid solution or submersion in KMnO₄ solution or iodine vapor. NMR experiments were carried out in deuterated chloroform (CDCl₃). ¹H NMR, ¹³C{¹H} NMR, and ¹⁹F NMR spectra were recorded at 400 or 600 MHz, 100 or 150 MHz, and 376 MHz spectrometers, respectively. Chemical shifts are reported as δ values relative to internal TMS (δ 0.00 ppm for ¹H NMR), chloroform (δ 7.26 ppm for ¹H NMR), chloroform (δ 77.00 ppm for ¹³C{¹H} NMR) in parts per million (ppm). The following abbreviations are used for the multiplicities: s, singlet; d, doublet; dd, doublet of doublet; t, triplet; q, quartet; and m, multiplet. Coupling constants (*J*) are reported in hertz (Hz). High-resolution mass spectra (HRMS) were recorded on a Micro TOF-QII mass instrument (ESI).

2. Synthesis of alkenyl-substituted substrates 1, 4 and 6

N-alkenyl quinazolinones, *N*-alkenyl pyrroles, *N*-alkenyl indoles, and *N*-alkenyl benzimidazoles were prepared according to the published procedure.^[1-3]

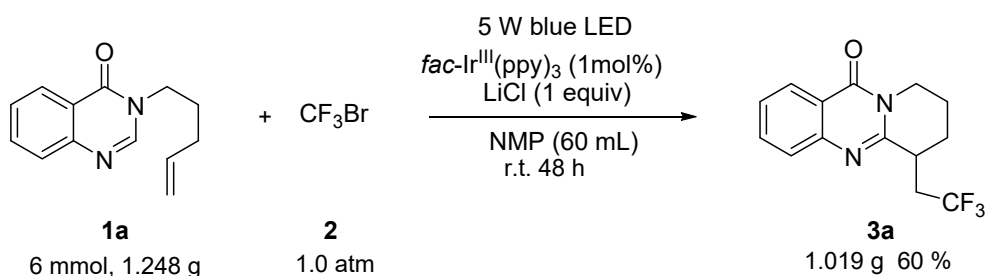
3. General procedure for the synthesis of products 3, 5 and 7



N-alkenyl quinazolinones **1** (0.3 mmol), *fac*-Ir^{III}(ppy)₃ (1.0 mol %), LiCl (0.3 mmol) and NMP (3 mL) were added into a 50 mL Schlenk flask, which was degassed with CF₃Br gas 3 times and refilled with CF₃Br (1 atm). Afterward, the reaction mixture was

stirred at room temperature under 5 W blue LED lamp ($h\nu = 460$ nm) for 16–48 h. The solvent was removed by vacuum distillation and the residue was purified by flash column chromatography on silica gel with petroleum ether and ethyl acetate as eluent. The preparation procedure of compounds **5** and **7** is as same as that of compounds **3**.

4. Procedure for the gram-scale synthesis of **3a**



3-(pent-4-en-1-yl) quinazolin-4(3H)-one **1a** (6 mmol), *fac*-Ir^(III)(ppy)₃ (1.0 mol %), LiCl (6 mmol) and NMP (60 mL) were added into a 100 mL Schlenk flask, which was degassed with CF₃Br gas 3 times and refilled with CF₃Br (1 atm). Afterward, the reaction mixture was stirred at room temperature under 4 × 5 W blue LED lamp ($h\nu = 460$ nm) for 48h. The solvent was removed by vacuum distillation and the residue was purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate as eluent (6/1) to obtain **3a** in yield of 60% (1.019 g)

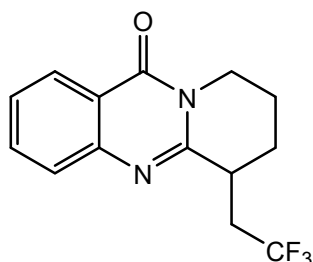
5. Radical trapping experiment

N-Alkenyl quinazolinones **1** (0.3 mmol), *fac*-Ir^(III)(ppy)₃ (1.0 mol %), LiCl (0.3 mmol), TEMPO or 1,1-diphenylethylene (0.6 mmol, 2 equiv.) and NMP (3 mL) were added into a 50 mL Schlenk flask, which was degassed with CF₃Br gas 3 times and refilled with CF₃Br (1 atm). Afterward, the reaction mixture was stirred at room temperature under 5 W blue LED lamp ($h\nu = 460$ nm) for 16 h. The solvent was removed by vacuum distillation and the residue was purified by flash column chromatography on silica gel with petroleum ether to obtain (3,3,3-trifluoroprop-1-ene-1,1-diyl)dibenzene **8**.

It is unfortunate that adduct CF₃-TEMPO could not be detected by ¹⁹F NMR.

6. Characterization data of products

6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-*b*]quinazolin-11-one (**3a**)^[4]



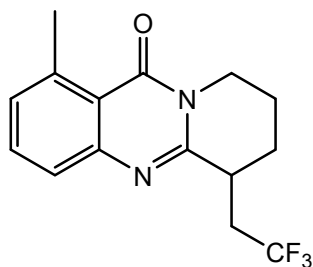
The desired pure product (70 mg, 83% yield) as a white crystal (mp 143–144 °C) was purified by flash column chromatography (PE/EA = 6/1).

¹H NMR (400 MHz, CDCl₃): (ppm) δ 8.26 (d, J = 8.0, 1H), 7.73 (t, J = 8.4 Hz, 1H), 7.63 (d, J = 8.0 Hz, 1H), 7.45 (t, J = 7.6 Hz, 1H), 4.36 – 4.29 (m, 1H), 3.99 – 3.91 (m, 1H), 3.61 – 3.47 (m, 1H), 3.22 – 3.15 (m, 1H), 2.46 – 2.30 (m, 2H), 2.07 – 2.00 (m, 2H), 1.72 – 1.62 (m, 1H).

¹³C NMR (150 MHz, CDCl₃): (ppm) δ 161.89 (s), 154.70 (s), 146.85 (s), 134.18 (s), 127.05 (q, J_{C-F} = 275.3 Hz), 126.96 (s), 126.64 (s), 126.57 (s), 120.22 (s), 41.13 (s), 36.09 (q, J_{C-F} = 28.2 Hz), 35.33 (q, J_{C-F} = 2.7 Hz), 25.10 (s), 20.60 (s).

¹⁹F NMR (376 MHz, CDCl₃): (ppm) δ -63.25 (t, J = 11.7 Hz).

1-methyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-*b*]quinazolin-11-one (**3b**)^[4]



The desired pure product (62 mg, 70% yield) as a white crystal (mp 135–136 °C) was purified by flash column chromatography (PE/EA = 5/1).

¹H NMR (400 MHz, CDCl₃): (ppm) δ 7.53 (t, J = 8.0, 1H), 7.44 (d, J = 8.0 Hz, 1H), 7.17 (d, J = 7.6 Hz, 1H), 4.22 – 4.16 (m, 1H), 3.94 – 3.88 (m, 1H), 3.59 – 3.45 (m, 1H),

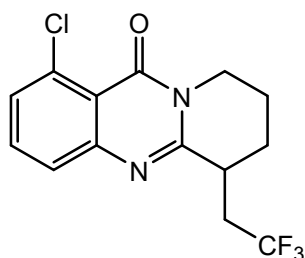
3.17 – 3.09 (m, 1H), 2.86 (s, 3H), 2.41 – 2.30 (m, 2H), 2.09 – 1.93 (m, 2H), 1.69 – 1.59 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 162.39 (s), 154.23 (s), 148.31 (s), 140.80 (s), 133.20 (s), 129.05 (s), 127.04 (q, $J_{\text{C-F}} = 275.4$ Hz), 125.09 (s), 118.69 (s), 41.00 (s), 36.07 (q, $J_{\text{C-F}} = 28.1$ Hz), 35.24 (s), 25.07 (s), 23.00 (s), 20.71 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.64 (t, $J = 11.3$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{15}\text{H}_{16}\text{F}_3\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ 297.1209, found 297.1204.

1-chloro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3c**)



The desired pure product (67 mg, 71% yield) as a white crystal (mp 129–130 °C) was purified by flash column chromatography (PE/EA = 5/1).

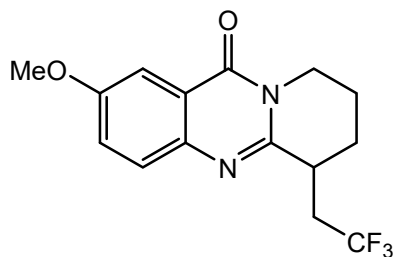
^1H NMR (400 MHz, CDCl_3): (ppm) δ 7.59 – 7.52 (m, 2H), 7.44 (d, $J = 7.6$ Hz, 1H), 4.26 – 4.19 (m, 1H), 3.98 – 3.92 (m, 1H), 3.56 – 3.42 (m, 1H), 3.19 – 3.12 (m, 1H), 2.42 – 2.32 (m, 2H), 2.10 – 1.95 (m, 2H), 1.71 – 1.63 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 159.89 (s), 155.43 (s), 149.15 (s), 133.81 (s), 133.46 (s), 129.16 (s), 126.96 (q, $J_{\text{C-F}} = 275.4$ Hz), 126.28 (s), 117.29 (s), 41.43 (s), 35.96 (q, $J_{\text{C-F}} = 28.4$ Hz), 35.39 (q, $J_{\text{C-F}} = 2.7$ Hz), 24.94 (s), 20.62 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.66 (t, $J_{\text{F-H}} = 11.3$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{14}\text{H}_{12}\text{ClF}_3\text{N}_2\text{NaO}$ $[\text{M} + \text{Na}]^+$ 339.0482, found 339.0472.

2-methoxy-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3d**)^[4]



The desired pure product (68 mg, 62% yield) as a white crystal (mp 98–100 °C) was purified by flash column chromatography (PE/EA = 6/1).

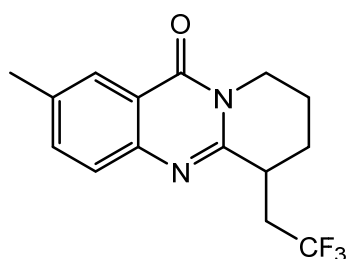
^1H NMR (400 MHz, CDCl_3): (ppm) δ 7.60 (d, J = 2.8 Hz, 1H), 7.54 (d, J = 9.2 Hz, 1H), 7.31 (dd, J = 9.2, 2.8 Hz, 1H), 4.34 – 4.28 (m, 1H), 4.00 – 3.88 (m, 4H), 3.58 – 3.44 (m, 1H), 3.20 – 3.13 (m, 1H), 2.42 – 2.30 (m, 2H), 2.05 – 1.99 (m, 2H), 1.70 – 1.60 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 161.74 (s), 158.19 (s), 152.33 (s), 141.54 (s), 128.55 (s), 127.07 (q, $J_{\text{C-F}}$ = 275.4 Hz), 124.58 (s), 120.88 (s), 105.78 (s), 55.77 (s), 41.25 (s), 36.10 (q, $J_{\text{C-F}}$ = 28.2 Hz), 35.13 (q, $J_{\text{C-F}}$ = 2.7 Hz), 25.16 (s), 20.64 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.66 (t, $J_{\text{F-H}}$ = 11.7 Hz).

HRMS (ESI): m/z calcd for $\text{C}_{15}\text{H}_{16}\text{F}_3\text{N}_2\text{O}_2$ [$\text{M} + \text{H}$] $^+$ 313.1158, found 313.1160.

2-methyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3e**)^[4]



The desired pure product (56 mg, 63% yield) as a white crystal (mp 109–110 °C) was purified by flash column chromatography (PE/EA = 5/1).

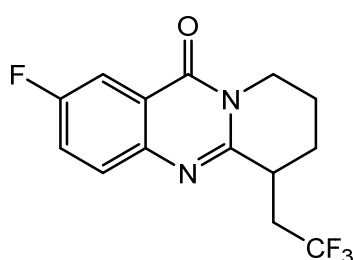
^1H NMR (400 MHz, CDCl_3): (ppm) δ 8.03 (s, 1H), 7.55 – 7.50 (m, 2H), 4.34 – 4.28 (m, 1H), 3.97 – 3.90 (m, 1H), 3.59 – 3.45 (m, 1H), 3.20 – 3.12 (m, 1H), 2.47 (s, 3H), 2.44 – 2.28 (m, 2H), 2.05 – 1.98 (m, 2H), 1.70 – 1.60 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 161.84 (s), 153.77 (s), 144.84 (s), 136.65 (s), 135.62 (s), 127.06 (q, $J_{\text{C-F}} = 275.6$ Hz), 126.73 (s), 125.94 (s), 119.89 (s), 41.06 (s), 36.06 (q, $J_{\text{C-F}} = 28.2$ Hz), 35.20 (q, $J_{\text{C-F}} = 2.7$ Hz), 25.10 (s), 21.25 (s), 20.59 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.66 (t, $J_{\text{F-H}} = 11.3$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{15}\text{H}_{16}\text{F}_3\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ 297.1209, found 297.1212.

2-fluoro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3f**)^[4]



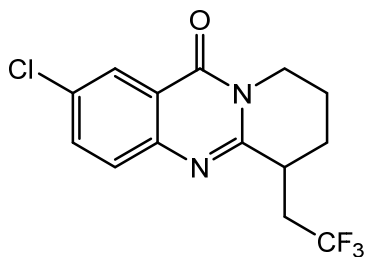
The desired pure product (47 mg, 52% yield) as a white crystal (mp 117–119 °C) was purified by flash column chromatography (PE/EA = 7/1).

^1H NMR (400 MHz, CDCl_3): (ppm) δ 7.85 (dd, $J = 8.4, 2.8$ Hz, 1H), 7.62 (dd, $J = 9.2, 5.2$ Hz, 1H), 7.45 – 7.40 (m, 1H), 4.33 – 4.27 (m, 1H), 3.98 – 3.91 (m, 1H), 3.57 – 3.43 (m, 1H), 3.20 – 3.12 (m, 1H), 2.45 – 2.31 (m, 2H), 2.06 – 1.99 (m, 2H), 1.73 – 1.61 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 161.19 (d, $J_{\text{C-F}} = 3.6$ Hz), 160.65 (d, $J_{\text{C-F}} = 246.5$ Hz), 154.02 (d, $J_{\text{C-F}} = 2.1$ Hz), 143.52 (d, $J_{\text{C-F}} = 2.0$ Hz), 129.39 (d, $J_{\text{C-F}} = 8.1$ Hz), 126.98 (q, $J_{\text{C-F}} = 275.4$ Hz), 122.79 (d, $J_{\text{C-F}} = 24.2$ Hz), 121.34 (d, $J_{\text{C-F}} = 8.7$ Hz), 111.32 (d, $J_{\text{C-F}} = 23.4$ Hz), 41.27 (s), 36.01 (q, $J_{\text{C-F}} = 28.2$ Hz), 35.24 (q, $J_{\text{C-F}} = 2.7$ Hz), 25.06 (s), 20.55 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.70 (t, $J_{\text{F-H}} = 11.7$ Hz), -113.43 – -113.49 (m).
HRMS (ESI): m/z calcd for $\text{C}_{14}\text{H}_{12}\text{F}_4\text{N}_2\text{NaO}$ $[\text{M} + \text{Na}]^+$ 323.0778, found 323.0774.

2-chloro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3g**)^[4]



The desired pure product (65 mg, 69% yield) as a white crystal (mp 100–102 °C) was purified by flash column chromatography (PE/EA = 4/1).

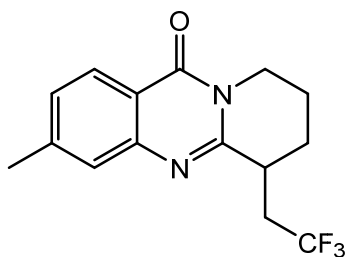
^1H NMR (400 MHz, CDCl_3): (ppm) δ 8.21 (d, $J = 2.4$ Hz, 1H), 7.65 (dd, $J = 8.4$ Hz, 2.4 Hz, 1H), 7.57 (d, $J = 8.8$ Hz, 1H), 4.34 – 4.28 (m, 1H), 3.99 – 3.92 (m, 1H), 3.57 – 3.44 (m, 1H), 3.21 – 3.14 (m, 1H), 2.46 – 2.30 (m, 2H), 2.07 – 2.01 (m, 2H), 1.72 – 1.63 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 160.82 (s), 155.05 (s), 145.31 (s), 134.57 (s), 132.20 (s), 128.66 (s), 126.95 (q, $J_{\text{C-F}} = 275.6$ Hz), 125.90 (s), 121.17 (s), 41.31 (s), 35.99 (q, $J_{\text{C-F}} = 28.2$ Hz), 35.34 (q, $J_{\text{C-F}} = 2.7$ Hz), 25.00 (s), 20.52 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.68 (t, $J_{\text{F-H}} = 11.3$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{14}\text{H}_{12}\text{ClF}_3\text{N}_2\text{NaO}$ $[\text{M} + \text{Na}]^+$ 339.0482, found 339.0486.

3-methyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3h**)^[4]



The desired pure product (63 mg, 71% yield) as a white crystal (mp 139–140 °C) was purified by flash column chromatography (PE/EA = 5/1).

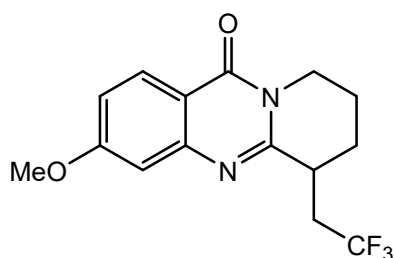
^1H NMR (400 MHz, CDCl_3): (ppm) δ 8.13 (d, $J = 8.0$ Hz, 1H), 7.42 (s, 1H), 7.26 (d, $J = 7.2$ Hz, 1H), 4.34 – 4.27 (m, 1H), 3.97 – 3.90 (m, 1H), 3.59 – 3.45 (m, 1H), 3.20 – 3.12 (m, 1H), 2.49 (s, 3H), 2.42 – 2.31 (m, 2H), 2.05 – 1.98 (m, 2H), 1.71 – 1.61 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 161.78 (s), 154.72 (s), 146.93 (s), 145.11 (s), 128.15 (s), 127.05 (q, $J_{\text{C-F}} = 275.3$ Hz), 126.62 (s), 126.43 (s), 117.81 (s), 40.99 (s), 36.07 (q, $J_{\text{C-F}} = 28.2$ Hz), 35.28 (q, $J_{\text{C-F}} = 2.6$ Hz), 25.11 (s), 21.81 (s), 20.59 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.67 (t, $J_{\text{F-H}} = 11.7$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{15}\text{H}_{16}\text{F}_3\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ 297.1209, found 297.1200.

3-methoxy-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3i**)^[4]



The desired pure product (46 mg, 49% yield) as a white crystal (mp 129–130 °C) was purified by flash column chromatography (PE/EA = 5/1).

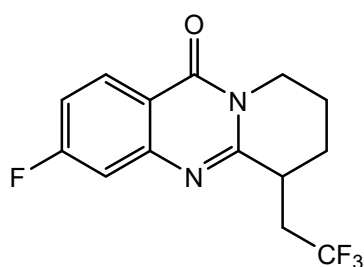
^1H NMR (400 MHz, CDCl_3): (ppm) δ 8.15 (d, $J = 8.8$ Hz, 1H), 7.04 – 7.00 (m, 2H), 4.32 – 4.26 (m, 1H), 3.98 – 3.91 (m, 4H), 3.59 – 3.45 (m, 1H), 3.20 – 3.13 (m, 1H), 2.44 – 2.32 (m, 2H), 2.06 – 1.99 (m, 2H), 1.72 – 1.62 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 164.49 (s), 161.44 (s), 155.42 (s), 149.10 (s), 128.20 (s), 127.04 (q, $J_{\text{C-F}} = 275.4$ Hz), 116.85 (s), 113.81 (s), 107.37 (s), 55.62 (s), 41.00 (s), 36.17 (q, $J_{\text{C-F}} = 28.2$ Hz), 35.36 (q, $J_{\text{C-F}} = 2.6$ Hz), 25.11 (s), 20.58 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.66 (t, $J_{\text{F-H}} = 11.3$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{15}\text{H}_{16}\text{F}_3\text{N}_2\text{O}_2$ $[\text{M} + \text{H}]^+$ 313.1158, found 313.1159.

3-fluoro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*] quinazolin-11-one (**3j**)^[4]



The desired pure product (64 mg, 71% yield) as a white crystal (mp 118–119 °C) was purified by flash column chromatography (PE/EA = 5/1).

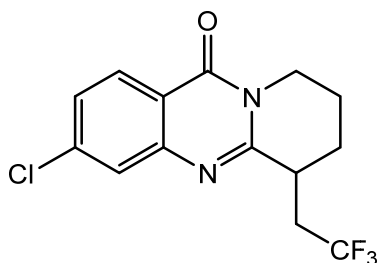
^1H NMR (400 MHz, CDCl_3): (ppm) δ 8.26 (dd, $J = 8.8, 6.4$ Hz, 1H), 7.26 (dd, $J = 10.0, 2.8$ Hz, 1H), 7.16 (td, $J = 8.4, 2.4$ Hz, 1H), 4.34 – 4.27 (m, 1H), 3.98 – 3.91 (m, 1H), 3.57 – 3.32 (m, 1H), 3.21 – 3.13 (m, 1H), 2.44 – 2.33 (m, 2H), 2.07 – 2.02 (m, 2H), 1.72 – 1.62 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 166.39 (d, $J_{\text{C-F}} = 252.5$ Hz), 161.14 (s), 156.13 (s), 148.94 (d, $J_{\text{C-F}} = 13.1$ Hz), 129.38 (d, $J_{\text{C-F}} = 10.5$ Hz), 126.96 (q, $J_{\text{C-F}} = 275.4$ Hz), 116.95 (d, $J_{\text{C-F}} = 1.8$ Hz), 115.42 (d, $J_{\text{C-F}} = 23.6$ Hz), 112.14 (d, $J_{\text{C-F}} = 21.6$ Hz), 41.14 (s), 36.01 (q, $J_{\text{C-F}} = 28.4$ Hz), 35.41 (q, $J_{\text{C-F}} = 2.7$ Hz), 25.00 (s), 20.54 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.67 (t, $J_{\text{F-H}} = 11.7$ Hz), -104.04 – -104.10 (m).

HRMS (ESI): m/z calcd for $\text{C}_{14}\text{H}_{12}\text{F}_4\text{N}_2\text{NaO}$ [$\text{M} + \text{Na}$] $^+$ 323.0778, found 323.0762.

3-chloro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3k**)^[4]



The desired pure product (56 mg, 59% yield) as a white crystal (mp 147–148 °C) was purified by flash column chromatography (PE/EA = 5/1).

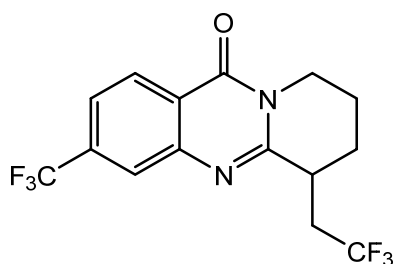
^1H NMR (400 MHz, CDCl_3): (ppm) δ 8.18 (d, $J = 8.4$ Hz, 1H), 7.63 (d, $J = 2.0$ Hz, 1H), 7.39 (dd, $J = 8.8, 2.0$ Hz, 1H), 4.33 – 4.27 (m, 1H), 3.98 – 3.91 (m, 1H), 3.56 – 3.43 (m, 1H), 3.21 – 3.13 (s, 1H), 2.44 – 2.32 (m, 2H), 2.07 – 2.02 (m, 2H), 1.72 – 1.62 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 161.26 (s), 156.13 (s), 147.76 (s), 140.35 (s), 128.14 (s), 127.21 (s), 126.94 (q, $J_{\text{C-F}} = 275.6$ Hz), 126.52 (s), 118.66 (s), 41.22 (s), 35.99 (q, $J_{\text{C-F}} = 28.2$ Hz), 35.43 (q, $J_{\text{C-F}} = 2.7$ Hz), 25.01 (s), 20.54 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.68 (t, $J_{\text{F-H}} = 11.7$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{14}\text{H}_{13}\text{ClF}_3\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ 317.0663, found 317.0670.

6-(2,2,2-trifluoroethyl)-3-(trifluoromethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3l**)^[4]



The desired pure product (62 mg, 59% yield) as a white crystal (mp 115–117 °C) was purified by flash column chromatography (PE/EA = 5/1).

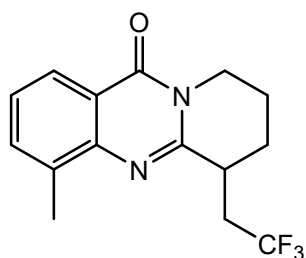
^1H NMR (400 MHz, CDCl_3): (ppm) δ 8.36 (d, $J = 8.4$ Hz, 1H), 7.93 (s, 1H), 7.65 (d, $J = 8.4$ Hz, 1H), 4.37 – 4.30 (m, 1H), 4.02 – 3.95 (m, 1H), 3.59 – 3.45 (m, 1H), 3.24 – 3.16 (m, 1H), 2.48 – 2.33 (m, 2H), 2.10 – 2.03 (m, 2H), 1.74 – 1.64 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 161.08 (s), 156.34 (s), 146.76 (s), 135.77 (q, $J_{\text{C-F}} = 32.7$ Hz), 127.84 (s), 126.91 (q, $J_{\text{C-F}} = 275.7$ Hz), 124.63 (q, $J_{\text{C-F}} = 4.0$ Hz), 123.38 (q, $J_{\text{C-F}} = 271.4$ Hz), 122.50 (q, $J_{\text{C-F}} = 3.5$ Hz), 122.44 (s), 41.40 (s), 35.97 (q, $J_{\text{C-F}} = 28.4$ Hz), 35.47 (q, $J_{\text{C-F}} = 2.6$ Hz), 24.99 (s), 20.52 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.62 (s), -63.72 (t, $J_{\text{F-H}} = 10.9$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{15}\text{H}_{13}\text{F}_6\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ 351.0927, found 351.0934.

4-methyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3m**)^[4]



The desired pure product (57 mg, 64% yield) as a white crystal (mp 116–117 °C) was purified by flash column chromatography (PE/EA = 6/1).

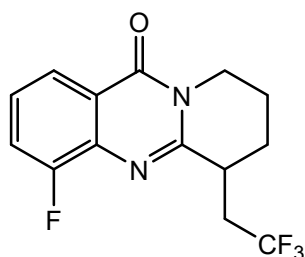
¹H NMR (400 MHz, CDCl₃): (ppm) δ 8.10 (d, J = 8.0 Hz, 1H), 7.56 (d, J = 7.2 Hz, 1H), 7.33 (t, J = 7.6 Hz, 1H), 4.35 – 4.28 (m, 1H), 3.98 – 3.91 (m, 1H), 3.63 – 3.49 (m, 1H), 3.21 – 3.13 (m, 1H), 2.57 (s, 3H), 2.46 – 2.33 (m, 2H), 2.06 – 2.00 (m, 2H), 1.70 – 1.60 (m, 1H).

¹³C NMR (150 MHz, CDCl₃): (ppm) δ 162.17 (s), 153.37 (s), 145.23 (s), 135.49 (s), 134.61 (s), 127.11 (q, J_{C-F} = 275.4 Hz), 126.11 (s), 124.24 (s), 120.08 (s), 40.94 (s), 36.01 (q, J_{C-F} = 28.4 Hz), 35.46 (q, J_{C-F} = 2.6 Hz), 25.26 (s), 20.75 (s), 17.10 (s).

¹⁹F NMR (376 MHz, CDCl₃): (ppm) δ -63.64 (t, J_{F-H} = 11.7 Hz).

HRMS (ESI): m/z calcd for C₁₅H₁₅F₃N₂NaO [M + H]⁺ 319.1029, found 319.1013.

4-fluoro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3n**)



The desired pure product (42 mg, 47% yield) as a white crystal (mp 128–129 °C) was purified by flash column chromatography (PE/EA = 6/1).

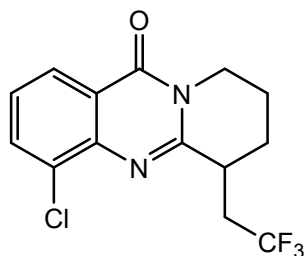
¹H NMR (400 MHz, CDCl₃): (ppm) δ 8.03 (dd, J = 7.6, 0.8 Hz, 1H), 7.47 – 7.35 (m, 2H), 4.35 – 4.28 (m, 1H), 4.01 – 3.94 (m, 1H), 3.63 – 3.49 (m, 1H), 3.26 – 3.18 (m, 1H), 2.49 – 2.34 (m, 2H), 2.09 – 2.00 (m, 2H), 1.74 – 1.64 (m, 1H).

¹³C NMR (150 MHz, CDCl₃): (ppm) δ 160.98 (d, J = 3.3 Hz), 156.74 (d, J = 254.6 Hz), 155.43 (s), 136.39 (d, J_{C-F} = 11.7 Hz), 126.96 (q, J_{C-F} = 275.7 Hz), 126.55 (d, J_{C-F} = 7.5 Hz), 122.13 (s), 122.10 (s), 119.52 (d, J_{C-F} = 18.8 Hz), 41.36 (s), 35.99 (q, J_{C-F} = 28.4 Hz), 35.63 (q, J_{C-F} = 2.7 Hz), 24.91 (s), 20.55 (s).

¹⁹F NMR (376 MHz, CDCl₃): (ppm) δ -63.52 (t, J_{F-H} = 11.3 Hz), -126.45 – -126.49 (m).

HRMS (ESI): m/z calcd for C₁₄H₁₂F₄N₂NaO [M + Na]⁺ 323.0778, found 323.0774.

4-chloro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3o**)



The desired pure product (28 mg, 30% yield) as a white crystal (mp 141–142 °C) was purified by flash column chromatography (PE/EA = 6/1).

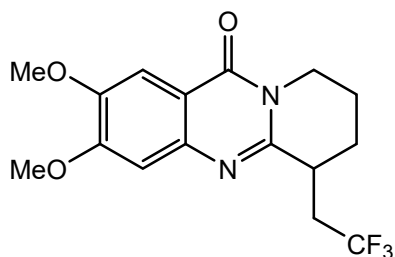
¹H NMR (400 MHz, CDCl₃): (ppm) δ 8.17 (dd, J = 8.0, 1.6 Hz, 1H), 7.81 (dd, J = 7.6, 1.2 Hz, 1H), 7.36 (t, J = 8.0 Hz, 1H), 4.33 – 4.26 (m, 1H), 4.04 – 3.95 (m, 1H), 3.71 – 3.57 (m, 1H), 3.26 – 3.18 (m, 1H), 2.50 – 2.36 (m, 2H), 2.09 – 2.02 (m, 2H), 1.73 – 1.63 (m, 1H).

¹³C NMR (150 MHz, CDCl₃): (ppm) δ 161.23 (s), 155.50 (s), 143.34 (s), 134.30 (s), 131.56 (s), 127.01 (q, J_{C-F} = 275.4 Hz), 126.49 (s), 125.34 (s), 121.61 (s), 41.33 (s), 35.86 (q, J_{C-F} = 28.2 Hz), 35.70 (q, J_{C-F} = 2.6 Hz), 24.93 (s), 20.62 (s).

¹⁹F NMR (376 MHz, CDCl₃): (ppm) δ -63.54 (t, J_{F-H} = 11.3 Hz).

HRMS (ESI): m/z calcd for C₁₄H₁₂ClF₃N₂NaO [M + Na]⁺ 339.0482, found 339.0479.

2,3-dimethoxy-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3p**)



The desired pure product (62 mg, 58% yield) as a white crystal (mp 182–183 °C) was purified by flash column chromatography (PE/EA = 5/2).

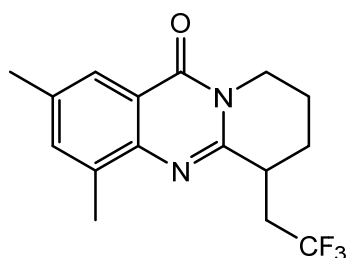
^1H NMR (400 MHz, CDCl_3): (ppm) δ 7.57 (s), 7.03 (s), 4.33 – 4.26 (m, 1H), 4.03 – 3.96 (m, 7H), 3.58 – 3.44 (m, 1H), 3.21 – 3.14 (m, 1H), 2.42 – 2.29 (m, 2H), 2.07 – 1.99 (m, 2H), 1.73 – 1.62 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 161.21 (s), 154.90 (s), 153.37 (s), 148.91 (s), 143.17 (s), 127.03 (q, $J_{\text{C-F}} = 275.4$ Hz), 113.51 (s), 107.25 (s), 105.46 (s), 56.25 (s), 56.22 (s), 41.20 (s), 36.22 (q, $J_{\text{C-F}} = 28.1$ Hz), 35.20 (q, $J_{\text{C-F}} = 2.7$ Hz), 25.16 (s), 20.60 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.67 (t, $J_{\text{F-H}} = 12.0$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{16}\text{H}_{18}\text{F}_3\text{N}_2\text{O}_3$ $[\text{M} + \text{H}]^+$ 343.1264, found 343.1274.

2,4-dimethyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3q**)



The desired pure product (29 mg, 31% yield) as a white crystal (mp 106–108 °C) was purified by flash column chromatography (PE/EA = 6/1).

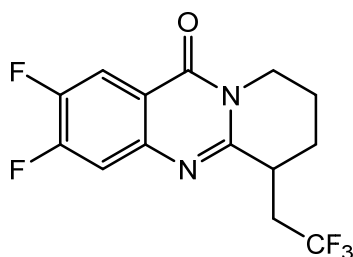
^1H NMR (400 MHz, CDCl_3): (ppm) δ 7.88 (s), 7.39 (s), 4.34 – 4.27 (m, 1H), 3.97 – 3.90 (m, 1H), 3.62 – 3.48 (m, 1H), 3.17 – 3.12 (m, 1H), 2.53 (s, 3H), 2.43 (s, 3H), 2.40 – 2.31 (m, 2H), 2.05 – 1.99 (m, 2H), 1.69 – 1.58 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 162.17 (s), 152.46 (s), 143.29 (s), 136.19 (s), 136.10 (s), 135.21 (s), 127.15 (q, $J_{\text{C-F}} = 275.3$ Hz), 123.59 (s), 119.85 (s), 40.92 (s), 36.02 (q, $J_{\text{C-F}} = 28.1$ Hz), 35.37 (q, $J_{\text{C-F}} = 2.7$ Hz), 25.30 (s), 21.25 (s), 20.79 (s), 16.97 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.65 (t, $J_{\text{F-H}} = 11.3$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{16}\text{H}_{18}\text{F}_3\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ 311.1366, found 311.1366.

2,3-difluoro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-*b*]quinazolin-11-one (**3r**)



The desired pure product (77 mg, 81% yield) as a white crystal (mp 123–124 °C) was purified by flash column chromatography (PE/EA = 6/1).

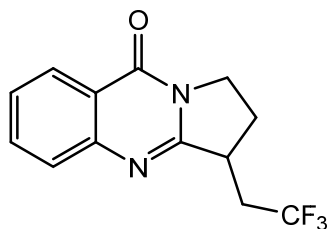
¹H NMR (400 MHz, CDCl₃): (ppm) δ 8.01 – 7.98 (m, 1H), 7.42 – 7.39 (m, 1H), 4.32 – 4.27 (m, 1H), 3.98 – 3.93 (m, 1H), 3.51 – 3.42 (m, 1H), 3.19 – 3.14 (m, 1H), 2.44 – 2.32 (m, 2H), 2.08 – 2.00 (m, 2H), 1.71 – 1.64 (m, 1H).

¹³C NMR (150 MHz, CDCl₃): (ppm) δ 160.43 (d, J_{C-F} = 3.0 Hz), 155.62 (d, J_{C-F} = 2.1 Hz), 154.78 (dd, J_{C-F} = 255.9, 14.7 Hz), 149.46 (dd, J_{C-F} = 249.9, 14.3 Hz), 144.57 (dd, J_{C-F} = 11.3, 2.4 Hz), 126.90 (q, J_{C-F} = 275.4 Hz), 117.05 (dd, J_{C-F} = 6.6, 2.1 Hz), 114.63 (d, J_{C-F} = 17.6 Hz), 113.83 (dd, J_{C-F} = 19.1, 2.3 Hz), 41.32 (s), 35.92 (q, J_{C-F} = 28.5 Hz), 35.32 (q, J_{C-F} = 2.7 Hz), 24.93 (s), 20.46 (s).

¹⁹F NMR (376 MHz, CDCl₃): (ppm) δ -63.77 (t, J_{F-H} = 10.9 Hz), -127.27 – -127.38 (m), -136.99 – -137.10 (m).

HRMS (ESI): m/z calcd for C₁₄H₁₁F₅N₂NaO [M + Na]⁺ 341.0684, found 341.0691.

3-(2,2,2-trifluoroethyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1H)-one (**3s**)^[4]



The desired pure product (43 mg, 56% yield) as a white crystal (mp 91–92 °C) was purified by flash column chromatography (PE/EA = 6/1).

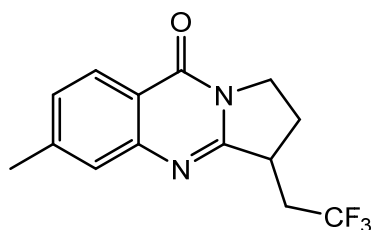
^1H NMR (600 MHz, CDCl_3): (ppm) δ 8.28 (dd, $J = 7.8, 1.2$ Hz, 1H), 7.75 – 7.72 (m, 1H), 7.66 (d, $J = 7.8$ Hz, 1H), 7.47 (t, $J = 7.8$ Hz, 1H), 4.41 – 4.37 (m, 1H), 3.97 – 3.92 (m, 1H), 3.55 – 3.50 (m, 1H), 3.31 – 3.23 (m, 1H), 2.70 – 2.66 (m, 1H), 2.34 – 2.24 (m, 1H), 2.07 – 2.00 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 160.69 (s), 158.49 (s), 148.85 (s), 134.25 (s), 127.04 (s), 126.64 (s), 126.55 (q, $J_{\text{C-F}} = 275.1$ Hz), 126.44 (s), 120.82 (s), 44.68 (s), 38.32 (q, $J_{\text{C-F}} = 2.9$ Hz), 35.95 (q, $J_{\text{C-F}} = 28.8$ Hz), 27.46 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -65.10 (t, $J_{\text{F-H}} = 10.5$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{13}\text{H}_{11}\text{F}_3\text{N}_2\text{NaO}$ $[\text{M} + \text{Na}]^+$ 291.0716, found 291.0710.

6-methyl-3-(2,2,2-trifluoroethyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1H)-one
(**3t**)^[5]



The desired pure product (46 mg, 54% yield) as a white crystal (mp 93–94 °C) was purified by flash column chromatography (PE/EA = 6/1).

^1H NMR (600 MHz, CDCl_3): (ppm) δ 8.17 (d, $J = 8.4$ Hz, 1H), 7.46 (s, 1H), 7.29 (d, $J = 7.8$ Hz, 1H), 4.39 – 4.36 (m, 1H), 3.96 – 3.90 (m, 1H), 3.53 – 3.48 (m, 1H), 3.29 – 3.21 (m, 1H), 2.69 – 2.65 (m, 1H), 2.50 (s, 3H), 2.32 – 2.23 (m, 1H), 2.06 – 1.99 (m, 1H).

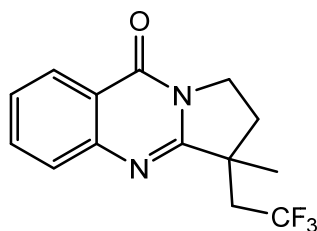
^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 160.61 (s), 158.53 (s), 148.96 (s), 145.24 (s), 128.16 (s), 126.78 (s), 126.55 (q, $J_{\text{C-F}} = 275.1$ Hz), 126.18 (s), 118.35 (s), 44.56 (s), 38.26 (q, $J_{\text{C-F}} = 2.7$ Hz), 35.92 (q, $J_{\text{C-F}} = 28.8$ Hz), 27.43 (s), 21.78 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -65.12 (t, $J_{\text{F-H}} = 10.5$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{14}\text{H}_{13}\text{F}_3\text{N}_2\text{NaO}$ $[\text{M} + \text{Na}]^+$ 305.0872, found 305.0881.

3-methyl-3-(2,2,2-trifluoroethyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1H)-one (**3u**)

[4]



The desired pure product (64 mg, 76% yield) as a white crystal (mp 95–96 °C) was purified by flash column chromatography (PE/EA = 4/1).

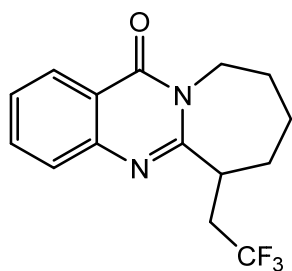
^1H NMR (600 MHz, CDCl_3): (ppm) δ 8.29 (d, $J = 8.0$ Hz, 1H), 7.74 (t, $J = 7.6$ Hz, 1H), 7.67 (d, $J = 8.4$ Hz, 1H), 7.48 – 7.44 (m, 1H), 4.33 – 4.27 (m, 1H), 4.07 – 4.00 (m, 1H), 2.99 – 2.87 (m, 1H), 2.62 – 2.49 (m, 1H), 2.43 – 2.35 (m, 1H), 2.30 – 2.24 (m, 1H), 1.49 (s, 3H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 162.38 (s), 160.81 (s), 149.15 (s), 134.13 (s), 127.16 (s), 126.46 (s), 126.42 (q, $J_{\text{C-F}} = 276.3$ Hz), 126.36 (s), 120.82 (s), 43.86 (q, $J_{\text{C-F}} = 2.0$ Hz), 44.30 (s), 41.38 (q, $J_{\text{C-F}} = 27.6$ Hz), 32.76 (s), 23.86 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -65.47 (t, $J_{\text{F-H}} = 11.3$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{14}\text{H}_{13}\text{F}_3\text{N}_2\text{NaO}$ [$\text{M} + \text{Na}$] $^+$ 305.0872, found 305.0871.

6-(2,2,2-trifluoroethyl)-7,8,9,10-tetrahydroazepino[2,1-*b*]quinazolin-12(6H)-one (**3v**)



The desired pure product (27 mg, 30% yield) as a white crystal (mp 96–97 °C) was purified by flash column chromatography (PE/EA = 4/1).

^1H NMR (600 MHz, CDCl_3): (ppm) δ 8.26 (d, $J = 7.8$ Hz, 1H), 7.72 (t, $J = 7.8$ Hz, 1H), 7.62 (d, $J = 7.8$ Hz, 1H), 7.45 (t, $J = 7.8$ Hz, 1H), 5.35 (d, $J = 13.8$ Hz, 1H), 3.55 (t, $J =$

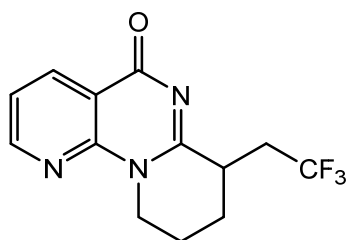
13.2 Hz, 1H), 3.41 – 3.32 (m, 2H), 2.49 – 2.39 (m, 1H), 2.21 (d, $J=13.8$ Hz, 1H), 2.10 – 2.07 (m, 1H), 1.94 – 1.89 (m, 1H), 1.85 – 1.78 (m, 1H), 1.63 – 1.50 (m, 2H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 161.87 (s), 158.27 (s), 146.75 (s), 134.12 (s), 127.18 (s), 127.16 (q, $J_{\text{C-F}} = 276.3$ Hz), 126.97 (s), 126.67 (s), 120.36 (s), 41.56 (s), 38.29 (s), 37.02 (q, $J_{\text{C-F}} = 27.6$ Hz), 32.32 (s), 27.93 (s), 27.10 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -64.14 (t, $J_{\text{F-H}} = 11.3$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{15}\text{H}_{15}\text{F}_3\text{N}_2\text{NaO}$ $[\text{M} + \text{Na}]^+$ 319.1029, found 319.1028.

7-(2,2,2-trifluoroethyl)-7,8,9,10-tetrahydro-5H-dipyrido[1,2-*a*:3',2'-*e*]pyrimidin-5-one
(**3w**)



The desired pure product (35 mg, 41% yield) as a colorless liquid was purified by flash column chromatography (PE/EA = 1/1).

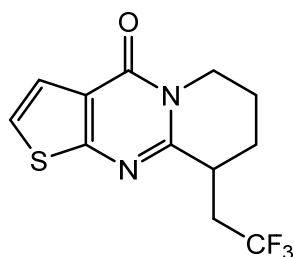
^1H NMR (400 MHz, CDCl_3): (ppm) δ 8.97 (dd, $J = 4.4, 2.0$ Hz, 1H), 8.60 (dd, $J = 7.6, 2.0$ Hz, 1H), 7.43 (dd, $J = 7.6, 4.4$ Hz, 1H), 4.37 – 4.30 (m, 1H), 4.00 – 3.94 (m, 1H), 3.72 – 3.58 (m, 1H), 3.29 – 3.22 (m, 1H), 2.53 – 2.39 (m, 2H), 2.10 – 2.04 (m, 2H), 1.77 – 1.67 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 162.05 (s), 158.93 (s), 156.73 (s), 156.07 (s), 136.45 (s), 126.88 (q, $J_{\text{C-F}} = 275.4$ Hz), 122.21 (s), 115.32 (s), 41.45 (s), 35.94 (q, $J_{\text{C-F}} = 28.5$ Hz), 35.64 (q, $J_{\text{C-F}} = 2.6$ Hz), 24.79 (s), 20.41 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.62 (t, $J_{\text{F-H}} = 11.3$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{13}\text{H}_{12}\text{F}_3\text{N}_3\text{NaO}$ $[\text{M} + \text{Na}]^+$ 306.0825, found 306.0812.

9-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-4H-pyrido[1,2-*a*]thieno[2,3-*d*]pyrimidin-4-one
(**3x**)



The desired pure product (60 mg, 69% yield) as a white crystal (mp 103–104 °C) was purified by flash column chromatography (PE/EA = 6/1).

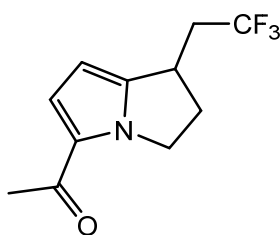
^1H NMR (400 MHz, CDCl_3): (ppm) δ 7.76 (d, $J = 5.2$ Hz, 1H), 7.26 (d, $J = 5.2$ Hz, 1H), 4.44 – 3.37 (m, 1H), 3.97 – 3.90 (m, 1H), 3.53 – 3.39 (m, 1H), 3.24 – 3.16 (m, 1H), 2.46 – 2.30 (m, 2H), 2.09 – 1.98 (m, 2H), 1.72 – 1.62 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 158.00 (s), 156.44 (s), 155.60 (s), 134.11 (s), 126.89 (q, $J_{\text{C-F}} = 275.6$ Hz), 124.79 (s), 121.15 (s), 40.92 (s), 36.18 (q, $J_{\text{C-F}} = 28.4$ Hz), 35.64 (q, $J_{\text{C-F}} = 2.7$ Hz), 25.01 (s), 20.45 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.69 (t, $J_{\text{F-H}} = 11.3$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{12}\text{H}_{11}\text{F}_3\text{N}_2\text{NaOS}$ $[\text{M} + \text{Na}]^+$ 311.0436, found 311.0430.

1-(1-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-pyrrolizin-5-yl)ethan-1-one (**5a**)



The desired pure product (44 mg, 63% yield) as a white crystal (mp 101–102°C) was purified by flash column chromatography (PE/EA = 4/1).

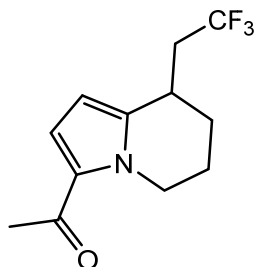
^1H NMR (400 MHz, CDCl_3): (ppm) δ 6.92 (d, $J = 4.0$ Hz, 1H), δ 5.94 (d, $J = 4.0$ Hz, 1H), 4.52 – 4.46 (m, 1H), 4.19 – 4.12 (m, 1H), 3.47 – 3.40 (m, 1H), 2.85 – 2.77 (m, 1H), 2.69 – 2.55 (m, 1H), 2.37 (s, 3H), 2.32 – 2.23 (m, 2H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 187.56 (s), 145.54 (s), 127.87 (s), 126.24 (q, $J_{\text{C-F}} = 275.6$ Hz), 121.68 (s), 101.44 (s), 47.36 (s), 38.05 (q, $J_{\text{C-F}} = 27.9$ Hz), 34.78 (s), 31.63 (q, $J_{\text{C-F}} = 2.9$ Hz), 25.86 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -65.27 (t, $J_{\text{F-H}} = 10.5$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{11}\text{H}_{13}\text{F}_3\text{NO}$ $[\text{M} + \text{H}]^+$ 232.0944, found 232.0945.

1-(8-(2,2,2-trifluoroethyl)-5,6,7,8-tetrahydroindolizin-3-yl)ethan-1-one (**5b**)



The desired pure product (44 mg, 53% yield) as a white crystal (mp 81–83°C) was purified by flash column chromatography (PE/EA = 4/1).

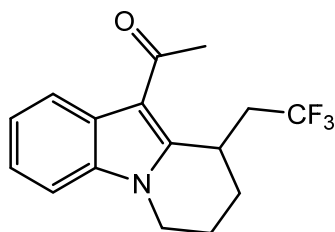
^1H NMR (400 MHz, CDCl_3): (ppm) δ 6.95 (d, $J = 4.4$ Hz, 1H), 6.00 (dd, $J = 4.0, 0.8$ Hz, 1H), 4.62 – 4.56 (m, 1H), 4.19 – 4.11 (m, 1H), 3.24 – 3.20 (m, 1H), 2.74 – 2.60 (m, 1H), 2.40 (s, 3H), 2.32 – 2.23 (m, 1H), 2.21 – 2.15 (m, 1H), 2.12 – 2.04 (m, 1H), 1.93 – 1.83 (m, 1H), 1.61 – 1.52 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 187.91 (s), 139.24 (s), 130.15 (s), 126.45 (q, $J_{\text{C-F}} = 276.0$ Hz), 119.61 (s), 105.81 (s), 46.03 (s), 39.18 (q, $J_{\text{C-F}} = 27.5$ Hz), 29.58 (q, $J_{\text{C-F}} = 2.9$ Hz), 27.06 (s), 25.78 (s), 21.80 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.93 (t, $J_{\text{F-H}} = 10.5$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{12}\text{H}_{14}\text{F}_3\text{NNaO}$ $[\text{M} + \text{Na}]^+$ 268.0920, found 268.0912.

1-(9-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydropyrido[1,2-*a*]indol-10-yl)ethan-1-one (**5e**)



The desired pure product (42 mg, 47% yield) as a white crystal (mp 107–108°C) was purified by flash column chromatography (PE/EA = 4/1).

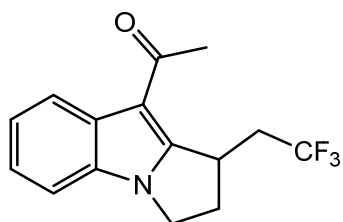
^1H NMR (600 MHz, CDCl_3): (ppm) δ 7.91 (d, $J = 7.8$ Hz, 1H), 7.37 – 7.28 (m, 3H), 4.34 – 4.31 (m, 1H), 4.25 – 4.23 (m, 1H), 3.94 – 3.89 (m, 1H), 2.89 – 2.80 (m, 1H), 2.71 (s, 3H), 2.36 – 2.27 (m, 2H), 2.23 – 2.12 (m, 2H), 1.91 – 1.85 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 193.74 (s), 147.00 (s), 136.11 (s), 126.53 (q, $J_{\text{C-F}} = 276.6$ Hz), 125.99 (s), 122.60 (s), 122.19 (s), 120.45 (s), 112.34 (s), 109.78 (s), 42.57 (s), 35.45 (q, $J_{\text{C-F}} = 27.2$ Hz), 31.58 (s), 28.54 (s), 22.49 (s), 17.30 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.31 (t, $J_{\text{F-H}} = 10.9$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{16}\text{H}_{16}\text{F}_3\text{NNaO}$ $[\text{M} + \text{Na}]^+$ 318.1076, found 318.1076.

1-(1-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-pyrrolo[1,2-*a*]indol-9-yl)ethan-1-one (**5f**)



The desired pure product (56 mg, 66% yield) as a white crystal (mp 112–113°C) was purified by flash column chromatography (PE/EA = 6/1).

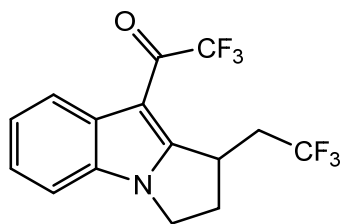
^1H NMR (400 MHz, CDCl_3): (ppm) δ 7.95 – 7.93 (m, 1H), 7.32 – 7.24 (m, 3H), 4.22 – 4.11 (m, 2H), 3.99 – 3.93 (m, 1H), 3.26 – 3.13 (m, 1H), 2.95 – 2.85 (m, 1H), 2.70 – 2.62 (m, 4H), 2.29 – 2.15 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 193.23 (s), 152.91 (s), 132.46 (s), 129.99 (s), 126.66 (q, $J_{\text{C-F}} = 276.0$ Hz), 122.30 (s), 122.28 (s), 121.03 (s), 110.53 (s), 110.30 (s), 43.27 (s), 35.64 (q, $J_{\text{C-F}} = 27.5$ Hz), 33.85 (q, $J_{\text{C-F}} = 3.0$ Hz), 32.11 (s), 30.42 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -64.59 (t, $J_{\text{F-H}} = 10.9$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{15}\text{H}_{14}\text{F}_3\text{NNaO}$ $[\text{M} + \text{Na}]^+$ 304.0920, found 304.0922.

2,2,2-trifluoro-1-(1-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-pyrrolo[1,2-*a*]indol-9-yl)ethan-1-one (**5g**)



The desired pure product (81 mg, 81% yield) as a white crystal (mp 126–128°C) was purified by flash column chromatography (PE/EA = 4/1).

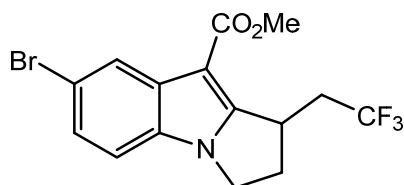
^1H NMR (400 MHz, CDCl_3): (ppm) δ 8.08 – 8.05 (m, 1H), 7.36 – 7.32 (m, 3H), 4.25 – 4.22 (m, 2H), 4.05 – 4.00 (m, 1H), 3.01 – 2.89 (m, 2H), 2.75 – 2.72 (m, 1H), 2.36 – 2.22 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 174.37 (q, $J_{\text{C-F}} = 36.5$ Hz), 157.35 (s), 132.75 (s), 128.97 (s), 126.29 (q, $J_{\text{C-F}} = 276.3$ Hz), 123.77 (s), 123.68 (s), 121.82 (q, $J_{\text{C-F}} = 3.9$ Hz), 117.10 (q, $J_{\text{C-F}} = 287.3$ Hz), 110.70 (s), 103.90 (s), 43.78 (s), 35.31 (q, $J_{\text{C-F}} = 27.8$ Hz), 34.50 (q, $J_{\text{C-F}} = 2.9$ Hz), 31.76 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -64.59 (t, $J_{\text{F-H}} = 10.5$ Hz), -75.40 (s).

HRMS (ESI): m/z calcd for $\text{C}_{15}\text{H}_{11}\text{F}_6\text{NNaO}$ $[\text{M} + \text{Na}]^+$ 358.0637, found 358.0641.

Methyl 1-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-pyrrolo[1,2-*a*]indole-9-carboxylate (**5h**)



The desired pure product (52 mg, 46% yield) as a white crystal (mp 92–93°C) was purified by flash column chromatography (PE/EA = 4/1).

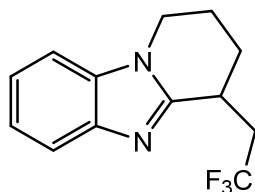
^1H NMR (400 MHz, CDCl_3): (ppm) δ 8.24 (d, $J = 1.6$ Hz, 1H), 7.32 (d, $J = 8.4$ Hz, 1H), 7.12 (d, $J = 8.4$ Hz, 1H), 4.22 – 4.08 (m, 2H), 3.92 – 3.88 (m, 4H), 3.36 – 3.24 (m, 1H), 2.99 – 2.90 (m, 1H), 2.65 – 2.60 (m, 1H), 2.33 – 2.19 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 164.90 (s), 153.22 (s), 132.13 (s), 130.97 (s), 126.54 (q, $J_{\text{C-F}} = 276.0$ Hz), 125.33 (s), 124.44 (s), 115.66 (s), 111.39 (s), 99.51 (s), 51.05 (s), 43.70 (s), 36.28 (q, $J_{\text{C-F}} = 27.6$ Hz), 33.43 (q, $J_{\text{C-F}} = 1.5$ Hz), 32.60 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -64.87 (t, $J_{F-H} = 10.5$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{15}\text{H}_{13}\text{BrF}_3\text{NNaO}$ $[\text{M} + \text{Na}]^+$ 397.9974, found 397.9972.

4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyridine (**7a**)^[6]



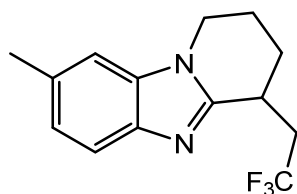
The desired pure product (53 mg, 70% yield) as a white crystal (mp 93 – 94 °C) was purified by flash column chromatography (PE/EA = 2/1).

^1H NMR (400 MHz, CDCl_3): (ppm) δ 7.72 – 7.70 (m, 1H), 7.29 – 7.22 (m, 3H), 4.21 – 4.16 (m, 1H), 3.96 – 3.89 (m, 1H), 3.55 – 3.45 (m, 1H), 3.42 – 3.34 (m, 1H), 2.46 – 2.43 (m, 1H), 2.37 – 2.23 (m, 2H), 2.11 – 2.00 (m, 1H), 1.75 – 1.65 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 152.13 (s), 142.42 (s), 134.75 (s), 126.76 (q, $J_{C-F} = 275.7$ Hz), 122.37 (s), 122.24 (s), 119.08 (s), 109.00 (s), 42.29 (s), 37.09 (q, $J_{C-F} = 28.2$ Hz), 31.41 (q, $J_{C-F} = 2.8$ Hz), 26.64 (s), 21.58 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.89 (t, $J_{F-H} = 11.3$ Hz).

8-methyl-4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyridine (**7b**)



The desired pure product (58 mg, 72% yield) as a white crystal (mp 94 – 95 °C) was purified by flash column chromatography (PE/EA = 10/1).

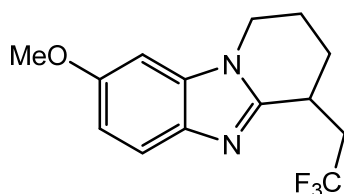
^1H NMR (400 MHz, CDCl_3): (ppm) δ 7.18 – 7.12 (m, 2H), 7.06 (d, $J = 6.0$ Hz, 1H), 4.22 – 4.17 (m, 1H), 3.99 – 3.92 (m, 1H), 3.60 – 3.41 (m, 2H), 2.65 (s, 3H), 2.47 – 2.43 (m, 1H), 2.38 – 2.22 (m, 2H), 2.13 – 2.02 (m, 1H), 1.79 – 1.69 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 151.27 (s), 141.85 (s), 134.43 (s), 129.22 (s), 126.82 (q, $J_{\text{C-F}} = 275.9$ Hz), 122.72 (s), 122.10 (s), 106.43 (s), 42.41 (s), 37.25 (q, $J_{\text{C-F}} = 27.9$ Hz), 31.41 (q, $J_{\text{C-F}} = 2.9$ Hz), 26.58 (s), 21.46 (s), 16.58 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.58 (t, $J_{\text{F-H}} = 11.3$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{14}\text{H}_{16}\text{F}_3\text{N}_2$ $[\text{M} + \text{H}]^+$ 269.1260, found 269.1255.

8-methoxy-4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyridine (**7c**)



The desired pure product (58 mg, 68% yield) as a white crystal (mp 130 – 131 °C) was purified by flash column chromatography (PE/EA = 5/1).

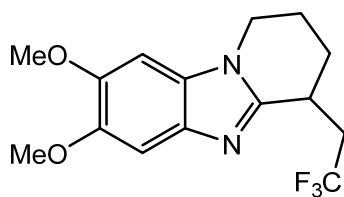
^1H NMR (400 MHz, CDCl_3): (ppm) δ 7.59 (d, $J = 8.8$ Hz, 1H), 6.90 (dd, $J = 8.8, 2.0$ Hz, 1H), 6.76 (d, $J = 2.4$ Hz, 1H), 4.19 – 4.15 (m, 1H), 3.95 – 3.89 (m, 1H), 3.86 (s, 3H), 3.54 – 3.35 (m, 2H), 2.48 – 2.40 (m, 1H), 2.37 – 2.26 (m, 2H), 2.14 – 2.02 (m, 1H), 1.76 – 1.66 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 156.29 (s), 151.30 (s), 136.85 (s), 135.33 (s), 126.78 (q, $J_{\text{C-F}} = 275.7$ Hz), 119.50 (s), 111.27 (s), 92.92 (s), 55.82 (s), 42.30 (s), 37.07 (q, $J_{\text{C-F}} = 27.9$ Hz), 31.44 (q, $J_{\text{C-F}} = 2.7$ Hz), 26.70 (s), 21.63 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.90 (t, $J_{\text{F-H}} = 11.3$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{14}\text{H}_{16}\text{F}_3\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ 285.1209, found 285.1205.

7,8-dimethoxy-4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyridine (**7d**)



The desired pure product (56 mg, 59% yield) as a white crystal (mp 148 – 149 °C) was purified by flash column chromatography (PE/EA = 3/1).

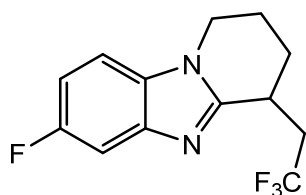
^1H NMR (400 MHz, CDCl_3): (ppm) δ 7.23 (s, 1H), 6.77 (s, 1H), 4.19 – 4.15 (m, 1H), 3.94 – 3.92 (m, 7H), 3.51 – 3.35 (m, 2H), 2.47 – 2.44 (m, 1H), 2.36 – 2.27 (m, 2H), 2.14 – 2.03 (m, 1H), 1.75 – 1.66 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 150.41 (s), 146.86 (s), 146.75 (s), 135.78 (s), 128.24 (s), 126.76 (q, $J_{\text{C-F}} = 275.6$ Hz), 101.39 (s), 92.21 (s), 56.37 (s), 56.20 (s), 42.34 (s), 37.12 (q, $J_{\text{C-F}} = 27.9$ Hz), 31.35 (q, $J_{\text{C-F}} = 2.6$ Hz), 26.66 (s), 21.65 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.93 (t, $J_{\text{F-H}} = 10.9$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{15}\text{H}_{18}\text{F}_3\text{N}_2\text{O}_2$ $[\text{M} + \text{H}]^+$ 315.1315, found 315.1309.

7-fluoro-4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-a]pyridine (7e)



The desired pure product (56 mg, 69% yield) as a white crystal (mp 106 – 107 °C) was purified by flash column chromatography (PE/EA = 5/1).

^1H NMR (400 MHz, CDCl_3): (ppm) δ 7.62 (dd, $J = 8.4, 4.8$ Hz, 1H), 7.03 – 6.97 (m, 2H), 4.20 – 4.15 (m, 1H), 3.97 – 3.90 (m, 1H), 3.53 – 3.36 (m, 2H), 2.49 – 2.28 (m, 3H), 2.15 – 2.04 (m, 1H), 1.78 – 1.69 (m, 1H).

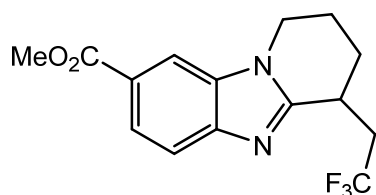
^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 159.39 (d, $J_{\text{C-F}} = 238.2$ Hz), 152.88 (d, $J_{\text{C-F}} = 2.7$ Hz), 138.81 (s), 134.88 (d, $J_{\text{C-F}} = 12.9$ Hz), 126.72 (q, $J_{\text{C-F}} = 275.6$ Hz), 119.79 (d,

$J_{C-F} = 10.1$ Hz), 110.57 (d, $J_{C-F} = 24.9$ Hz), 95.85 (d, $J_{C-F} = 27.2$ Hz), 42.51 (s), 37.05 (q, $J_{C-F} = 8.2$ Hz), 31.52 (q, $J_{C-F} = 2.9$ Hz), 26.63 (s), 21.59 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.93 (t, $J_{F-H} = 10.5$ Hz), -119.73 – -119.79(m).

HRMS (ESI): m/z calcd for $\text{C}_{13}\text{H}_{12}\text{F}_4\text{N}_2\text{Na}$ $[\text{M} + \text{Na}]^+$ 295.0829, found 295.0819.

Methyl 4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyridine-8-carboxylate (**7f**)



The desired pure product (63 mg, 67% yield) as a white crystal (mp 148 – 152 °C) was purified by flash column chromatography (PE/EA = 3/1).

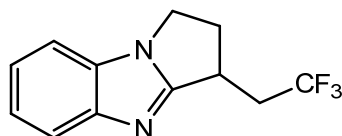
^1H NMR (400 MHz, CDCl_3): (ppm) δ 8.43 (s, 1H), 7.99 (dd, $J = 8.4, 1.6$ Hz, 1H), 7.31 (d, $J = 8.4$ Hz, 1H), 4.29 – 4.24 (m, 1H), 4.04 – 3.97 (m, 1H), 3.94 (s, 3H), 3.55 – 3.39 (m, 2H), 2.51 – 2.48 (m, 1H), 2.42 – 2.29 (m, 2H), 2.17 – 2.05 (m, 1H), 1.81 – 1.71 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 167.59 (s), 154.03 (s), 142.09 (s), 138.00 (s), 126.68 (q, $J_{C-F} = 275.6$ Hz), 124.65 (s), 123.98 (s), 121.50 (s), 108.72 (s), 52.06 (s), 42.63 (s), 37.03 (q, $J_{C-F} = 28.4$ Hz), 31.60 (q, $J_{C-F} = 2.9$ Hz), 26.51 (s), 21.56 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -68.63 (t, $J_{F-H} = 10.5$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{15}\text{H}_{15}\text{F}_3\text{N}_2\text{NaO}_2$ $[\text{M} + \text{Na}]^+$ 335.0978, found 335.0976.

3-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-benzo[*d*]pyrrolo[1,2-*a*]imidazole (**7g**)



The desired pure product (19 mg, 26% yield) as a white crystal (mp 94 – 98 °C) was purified by flash column chromatography (PE/EA = 4/1).

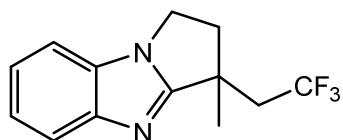
^1H NMR (400 MHz, CDCl_3): (ppm) δ 7.72 (t, $J = 7.2$ Hz, 1H), 7.33 – 7.30 (m, 1H), 7.26 – 7.23 (m, 2H), 4.21 – 4.16 (m, 1H), 4.06 – 3.99 (m, 1H), 3.61 – 3.55 (m, 1H), 3.22 – 3.10 (m, 1H), 3.05 – 2.98 (m, 1H), 2.55 – 2.46 (m, 1H), 2.37 – 2.23 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 160.54 (s), 148.33 (s), 132.31 (s), 126.39 (q, $J_{\text{C-F}} = 275.6$ Hz), 122.36 (s), 122.05 (s), 119.81 (s), 109.65 (s), 41.98 (s), 36.80 (q, $J_{\text{C-F}} = 28.5$ Hz), 33.65 (s), 30.78 (q, $J_{\text{C-F}} = 3.0$ Hz).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -65.38 (t, $J_{\text{F-H}} = 11.3$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{12}\text{H}_{12}\text{F}_3\text{N}_2$ $[\text{M} + \text{H}]^+$ 241.0947, found 241.0945.

3-methyl-3-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-benzo[*d*]pyrrolo[1,2-*a*]imidazole (7h)



The desired pure product (41 mg, 54% yield) as a white crystal (mp 76 – 77 °C) was purified by flash column chromatography (PE/EA = 4/1).

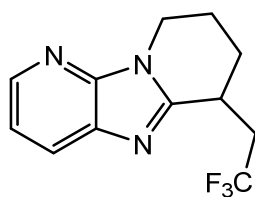
^1H NMR (400 MHz, CDCl_3): (ppm) δ 7.74 – 7.70 (m, 1H), 7.34 – 7.31 (m, 1H), 7.27 – 7.23 (m, 2H), 4.18 – 4.07 (m, 2H), 2.94 – 2.82 (m, 2H), 2.65 – 2.54 (m, 2H), 1.55 (s, 3H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 164.28 (s), 148.26 (s), 131.98 (s), 126.28 (q, $J_{\text{C-F}} = 276.5$ Hz), 122.31 (s), 122.00 (s), 119.89 (s), 109.71 (s), 41.93 (q, $J_{\text{C-F}} = 27.5$ Hz), 41.05 (s), 39.87 (s), 37.29 (q, $J_{\text{C-F}} = 2.0$ Hz), 24.63 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -61.23 (t, $J_{\text{F-H}} = 11.3$ Hz).

HRMS (ESI): m/z calcd for $\text{C}_{13}\text{H}_{14}\text{F}_3\text{N}_2$ $[\text{M} + \text{H}]^+$ 255.1104, found 255.1100.

6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydroimidazo[1,2-*a*:5,4-*b'*]dipyridine (7i)



The desired pure product (48 mg, 63% yield) as a white crystal (mp 115 – 116 °C) was purified by flash column chromatography (PE/EA = 2/1).

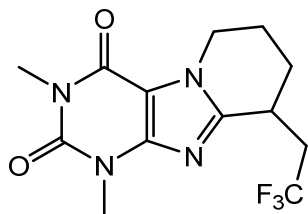
^1H NMR (400 MHz, CDCl_3): (ppm) δ 8.35 (d, J = 4.8 Hz, 1H), 7.97 (dd, J = 8.0, 1.2 Hz, 1H), 7.23 (dd, J = 8.0, 4.8 Hz, 1H), 4.51 – 4.46 (m, 1H), 4.08 – 4.01 (m, 1H), 3.53 – 3.40 (m, 2H), 2.52 – 2.30 (m, 3H), 2.14 – 2.03 (m, 1H), 1.82 – 1.72 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 153.62 (s), 147.77 (s), 143.44 (s), 134.76 (s), 126.70 (q, $J_{\text{C-F}}$ = 275.7 Hz), 126.57 (s), 118.49 (s), 41.45 (s), 36.91 (q, $J_{\text{C-F}}$ = 28.4 Hz), 31.73 (q, $J_{\text{C-F}}$ = 2.9 Hz), 26.65 (s), 21.48 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.93 (t, $J_{\text{F-H}}$ = 10.5 Hz).

HRMS (ESI): m/z calcd for $\text{C}_{12}\text{H}_{13}\text{F}_3\text{N}_3$ $[\text{M} + \text{H}]^+$ 256.1056, found 256.1063.

1,3-dimethyl-9-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydropyrido[2,1-*f*]purine-2,4(1H,3H)-dione (**7j**)



The desired pure product (66 mg, 70% yield) as a white crystal (mp 147 – 151 °C) was purified by flash column chromatography (PE/EA = 3/1).

^1H NMR (400 MHz, CDCl_3): (ppm) δ 4.58 – 4.54 (m, 1H), 4.16 – 4.11 (m, 1H), 3.55 (s, 3H), 3.38 (s, 3H), 3.31 – 3.22 (m, 2H), 2.41 – 2.39 (m, 1H), 2.33 – 2.19 (m, 2H), 2.05 – 1.97 (m, 1H), 1.74 – 1.67 (m, 1H).

^{13}C NMR (150 MHz, CDCl_3): (ppm) δ 155.07 (s), 151.66 (s), 150.58 (s), 148.08 (s), 126.44 (q, $J_{\text{C-F}}$ = 275.9 Hz), 106.99 (s), 44.70 (s), 36.93 (q, $J_{\text{C-F}}$ = 28.2 Hz), 30.94 (q, $J_{\text{C-F}}$ = 2.9 Hz), 29.68 (s), 27.79 (s), 25.83 (s), 21.24 (s).

^{19}F NMR (376 MHz, CDCl_3): (ppm) δ -63.86 (t, $J_{\text{F-H}}$ = 11.3 Hz).

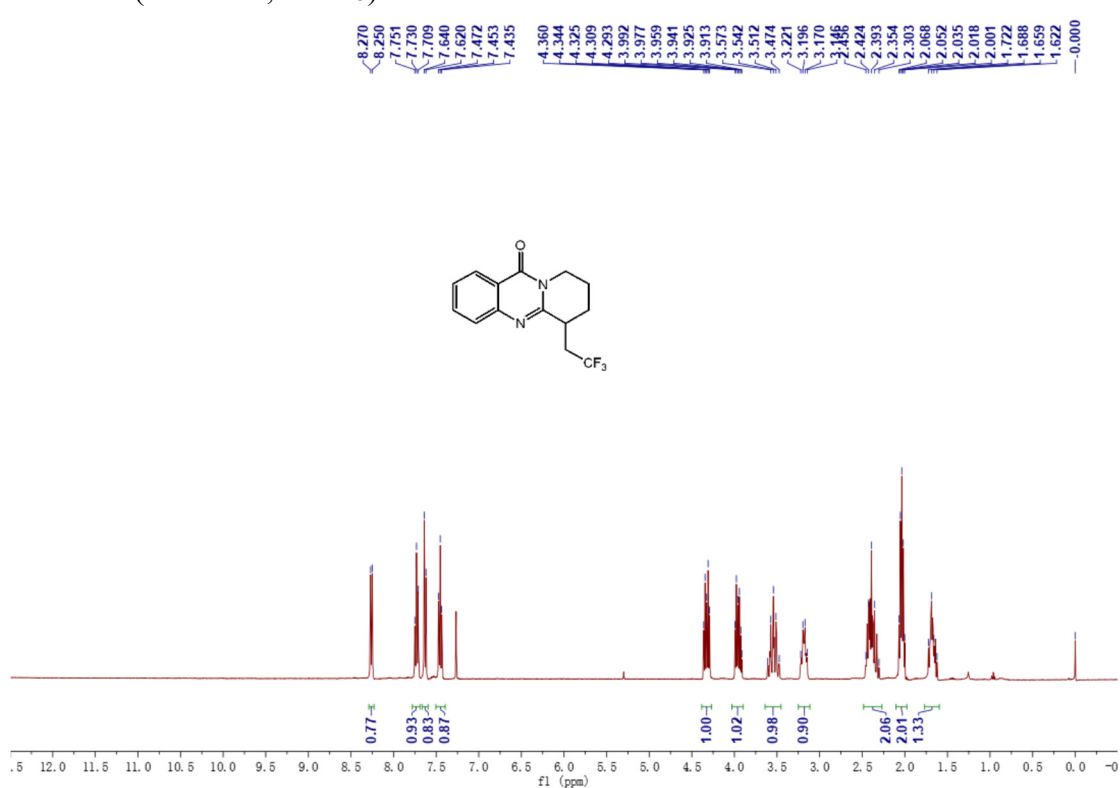
HRMS (ESI): m/z calcd for $\text{C}_{13}\text{H}_{15}\text{F}_3\text{N}_4\text{NaO}_2$ $[\text{M} + \text{Na}]^+$ 339.1039, found 339.1048.

7. Reference

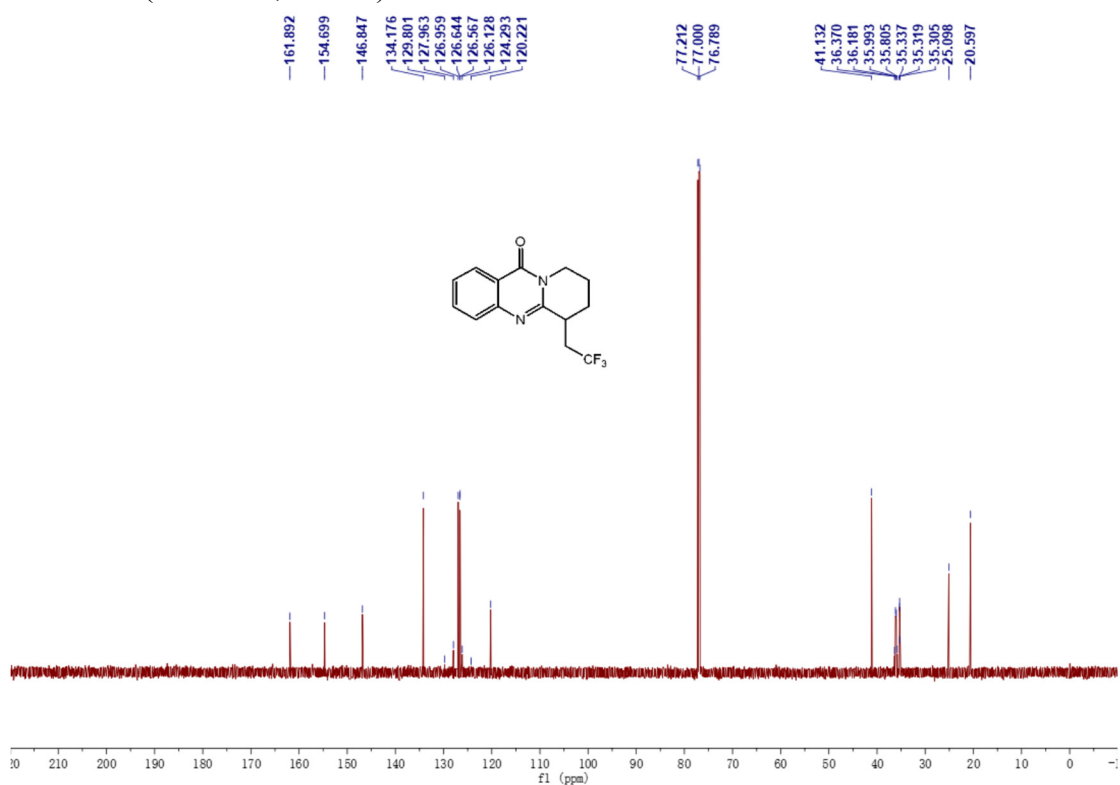
- [1] Yang J.; Sun B.; Ding H.; Huang P.-Y.; Tang X.-L.; Shi R.-C.; Yan Z.-Y.; Yu C.-M.; Jin C. *Green Chem.* **2021**, *23*, 575-581.
- [2] Yang R.; Yi D.; Shen K.; Fu Q.; Wei J.; Lu J.; Yang L.; Wang L.; Wei S.; Zhang Z. *Org. Lett.* **2022**, *24*, 2014-2019.
- [3] Wang Y.-X.; Qi S.-L.; Luan Y.-X.; Han X.-W.; Wang S.; Chen H.; Ye M. *J. Am. Chem. Soc.* **2018**, *140*, 5360-5364.
- [4] Sun B.; Huang P.; Yan Z.; Shi X.; Tang X.; Yang J.; Jin C. *Org. Lett.* **2021**, *23*, 1026-1031.
- [5] Zheng J.; Deng Z.; Zhang Y.; Cui S. *Adv. Syn. & Catal.* **2016**, *358*, 746-751.
- [6] Lin S.; Cui J.; Chen Y.; Li Y. *J. Org. Chem.* **2021**, *86*, 15768-15776.

8. The ^1H , ^{13}C and ^{19}F NMR spectra copy of compounds

6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-b]quinazolin-11-one (**3a**) :

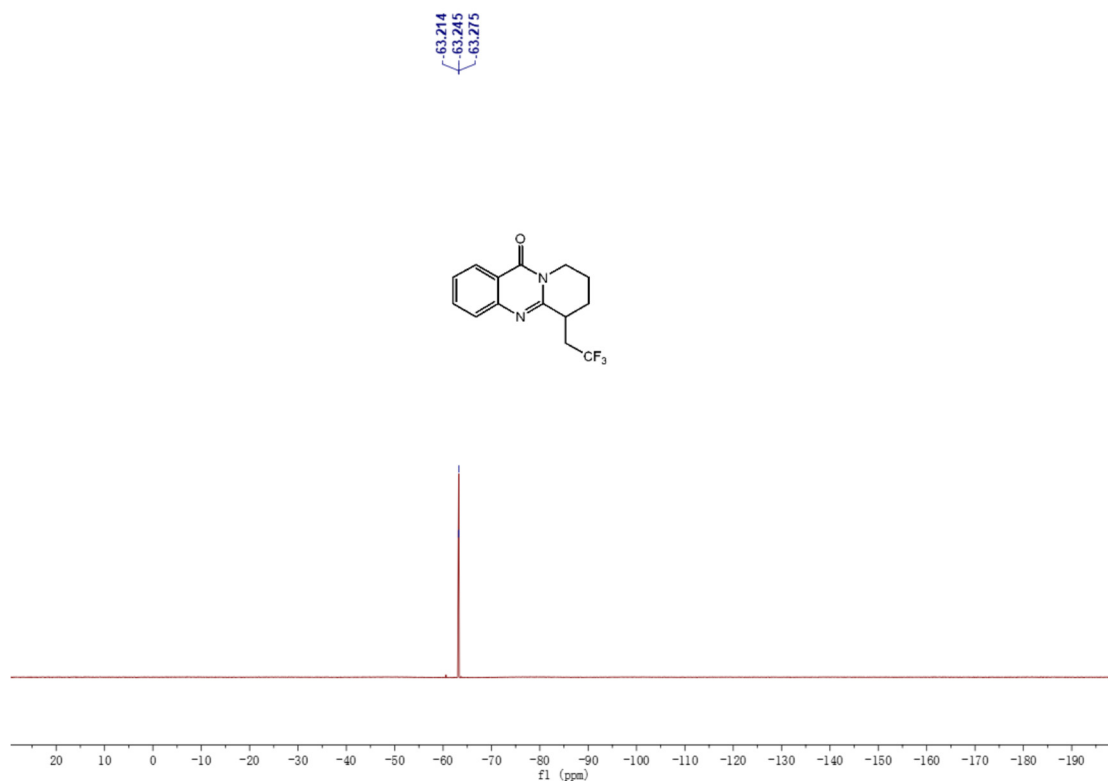


6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-b]quinazolin-11-one (**3a**) :

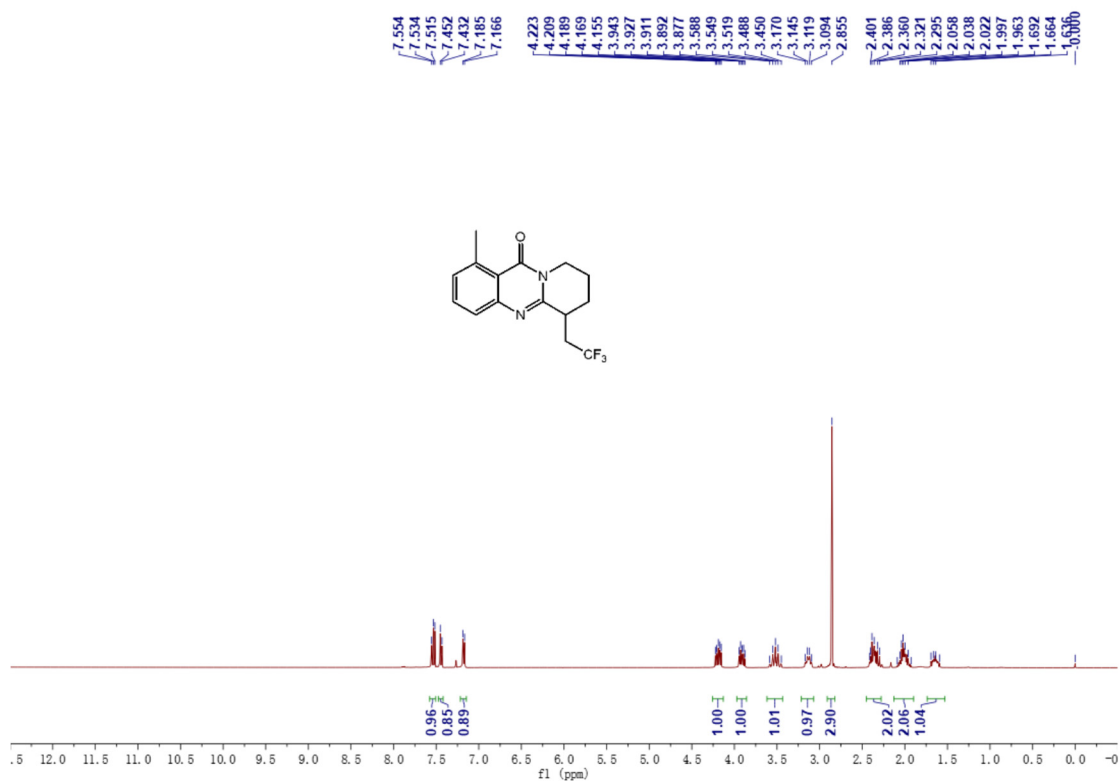


6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-b]quinazolin-11-one (**3a**) :

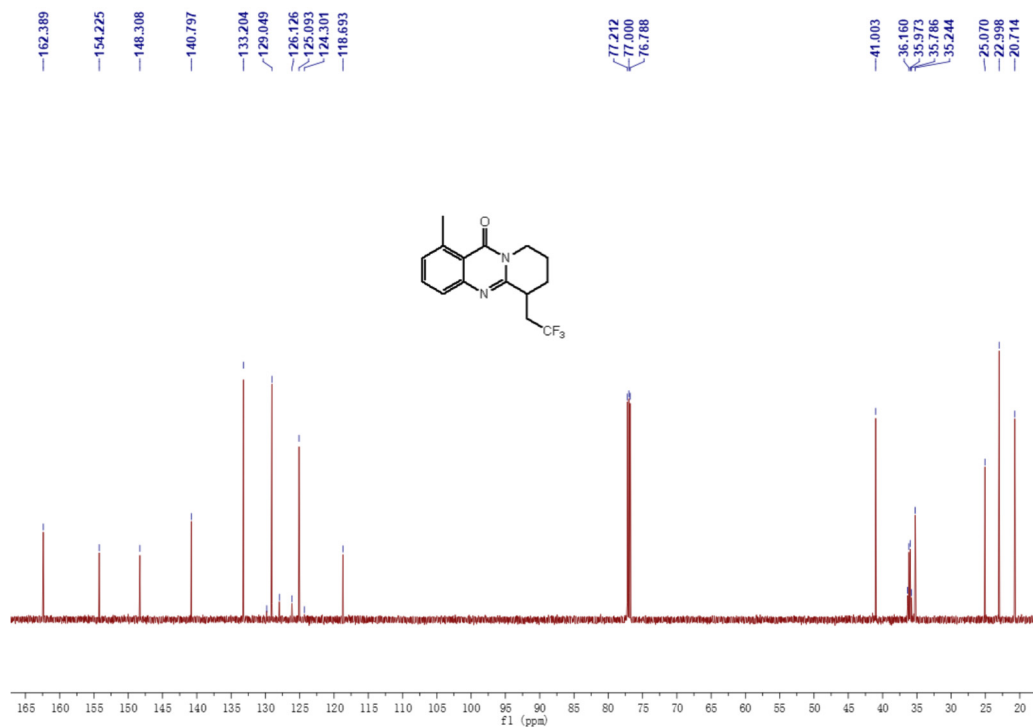
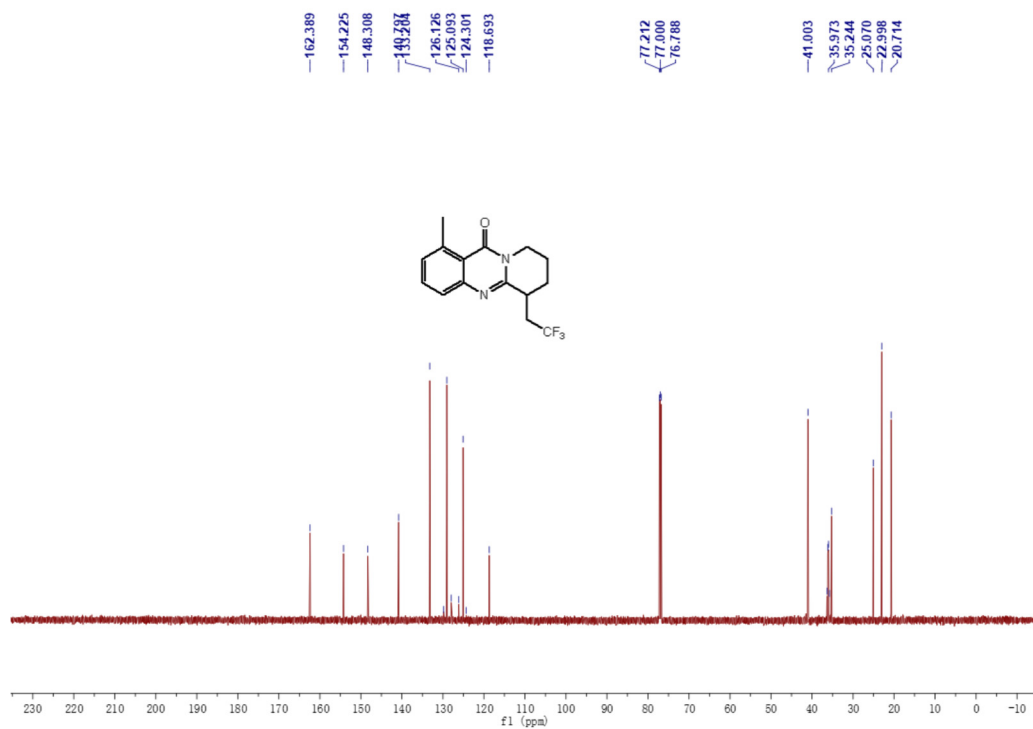
^{19}F NMR (376 MHz, CDCl_3)



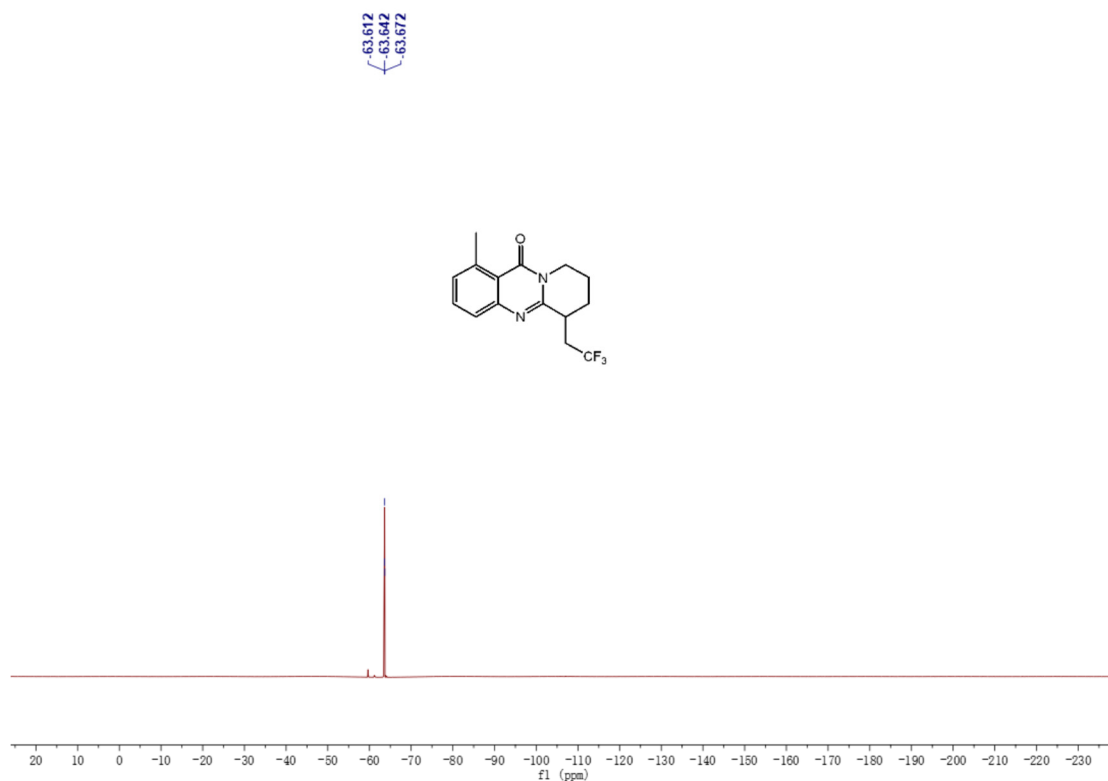
1-methyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-b]quinazolin-11-one (**3b**): ^1H NMR (400 MHz, CDCl_3)



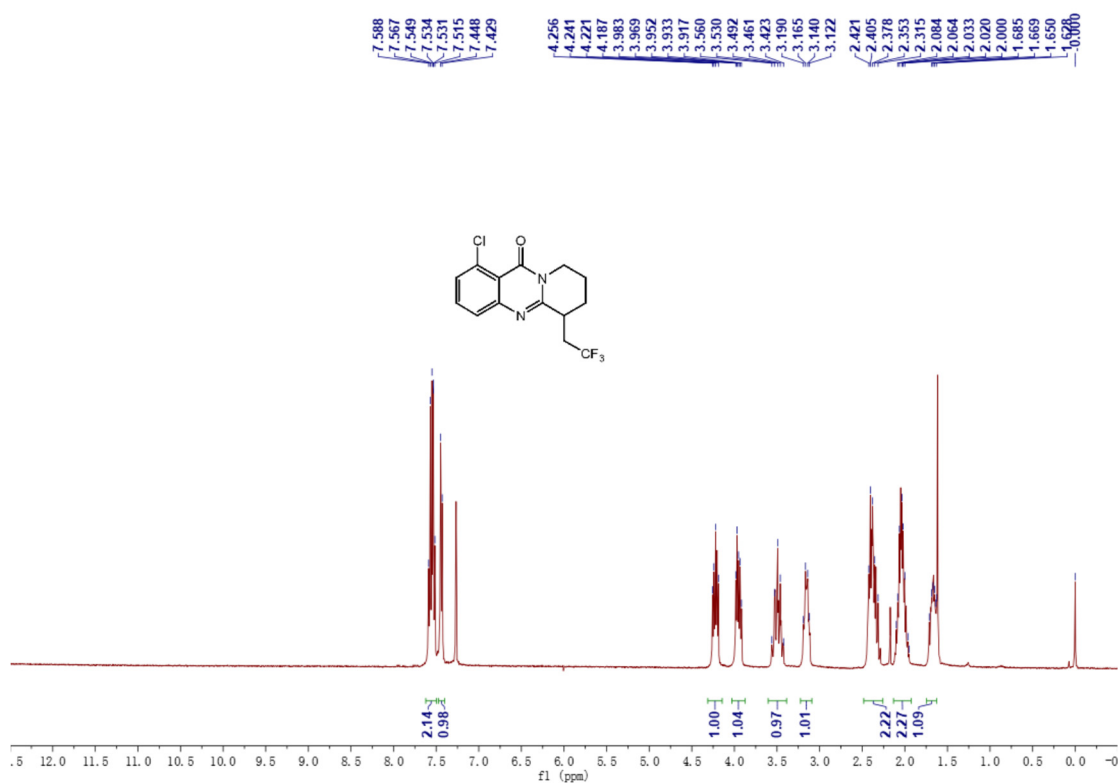
1-methyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3b**): ^{13}C NMR (150 MHz, CDCl_3)



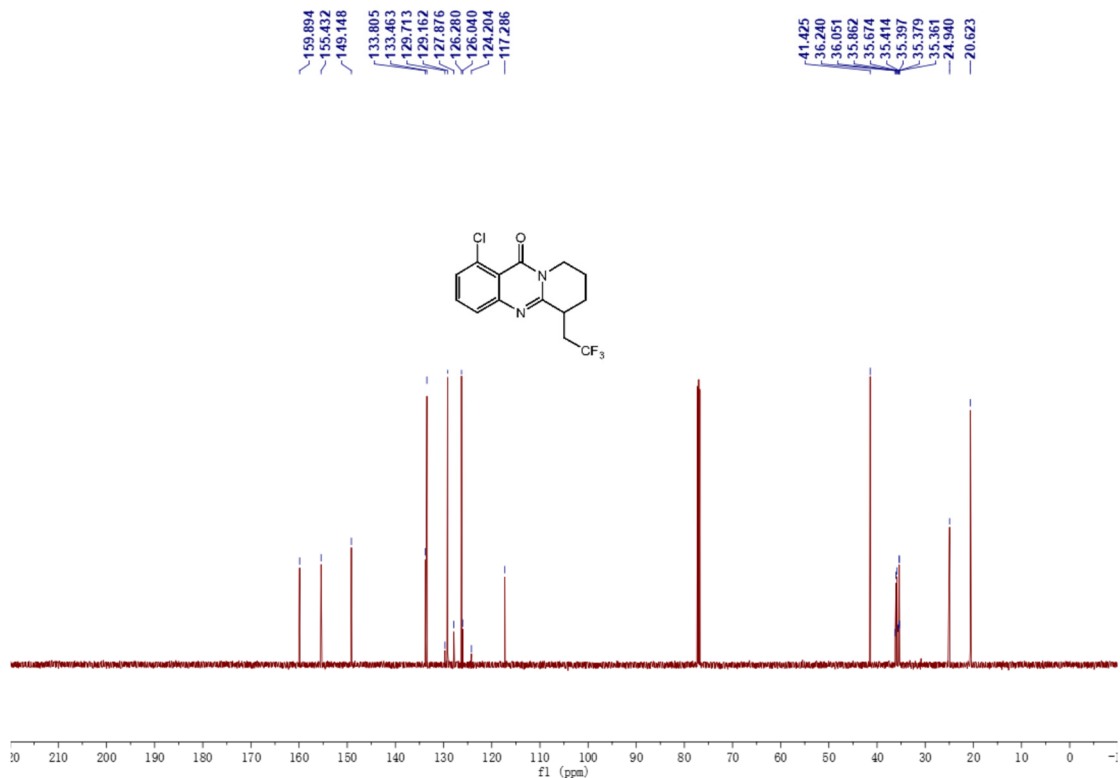
1-methyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3b**): ^{19}F NMR (376 MHz, CDCl_3)



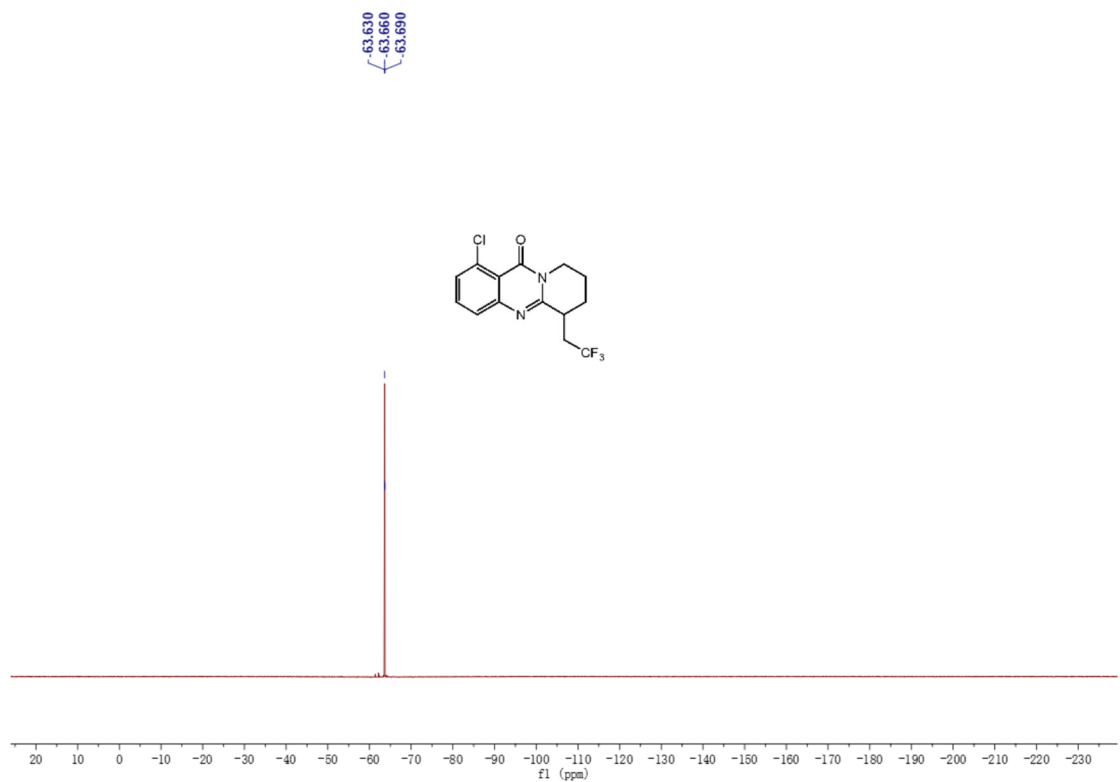
1-chloro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3c**): ^1H NMR (400 MHz, CDCl_3)



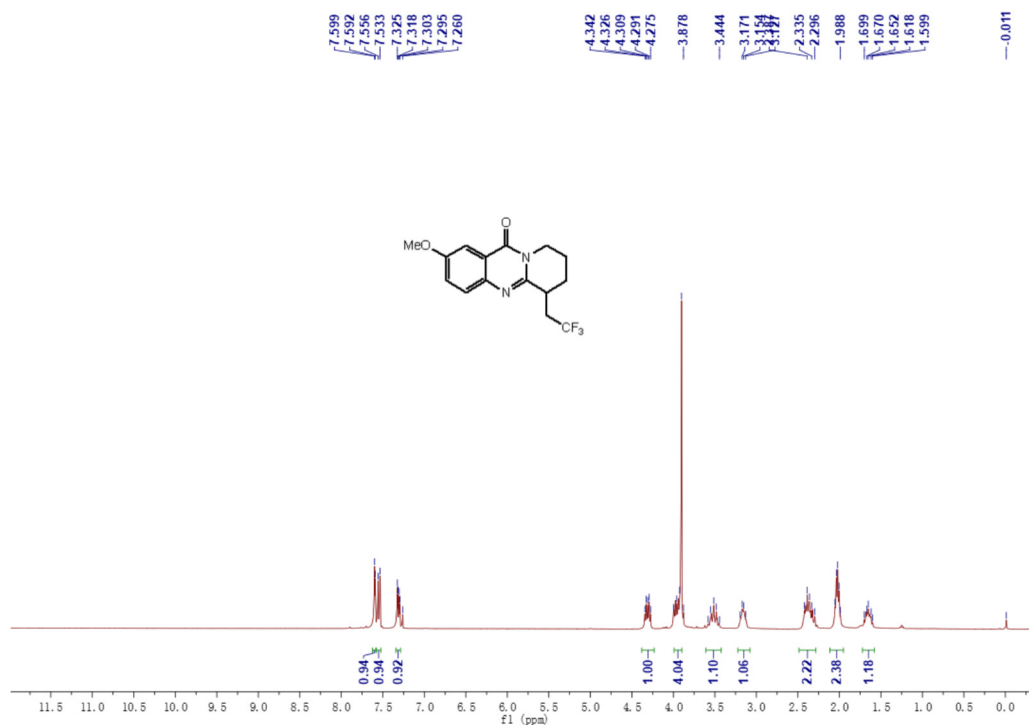
1-chloro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3c**): ^{13}C NMR (150 MHz, CDCl_3)



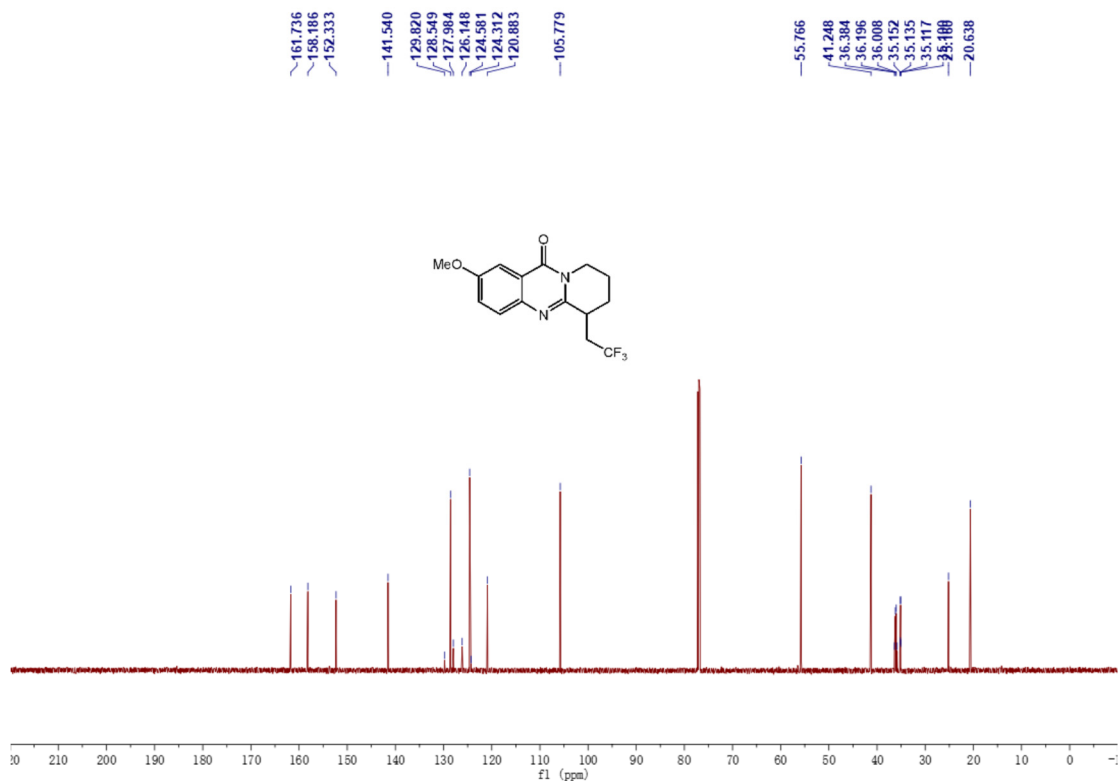
1-chloro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3c**): ^{19}F NMR (376 MHz, CDCl_3)



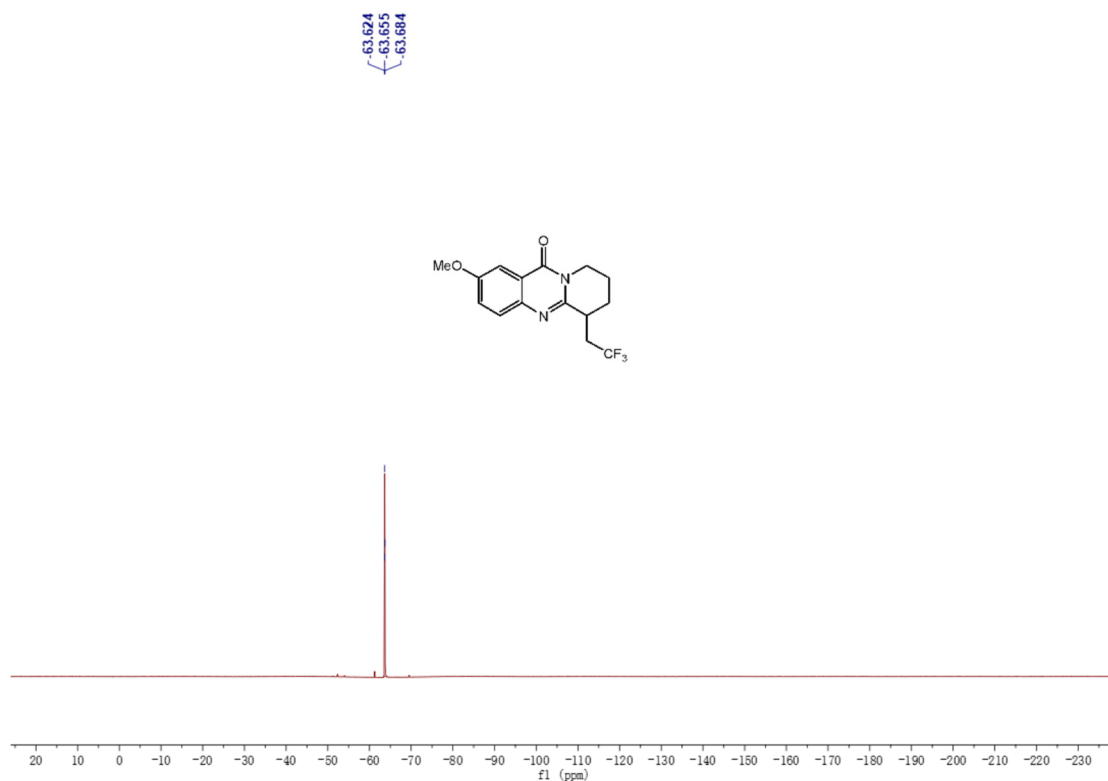
2-methoxy-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3d**) : ^1H NMR (400 MHz, CDCl_3)



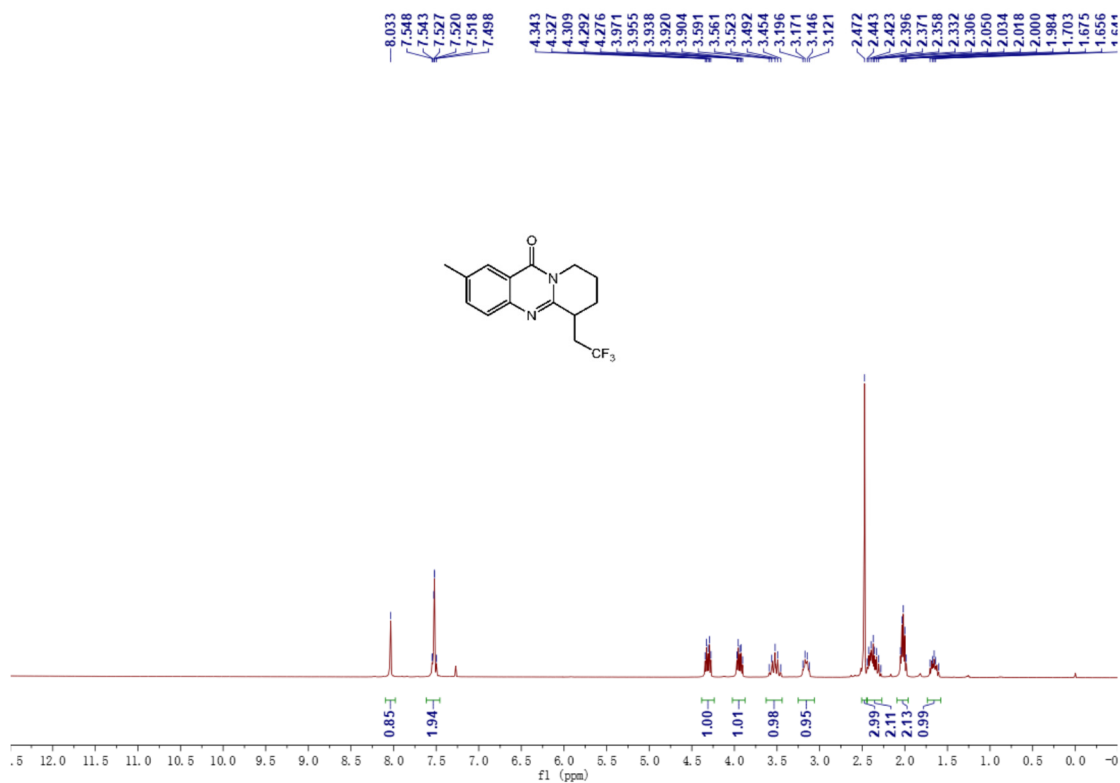
2-methoxy-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3d**) : ^{13}C NMR (150 MHz, CDCl_3)



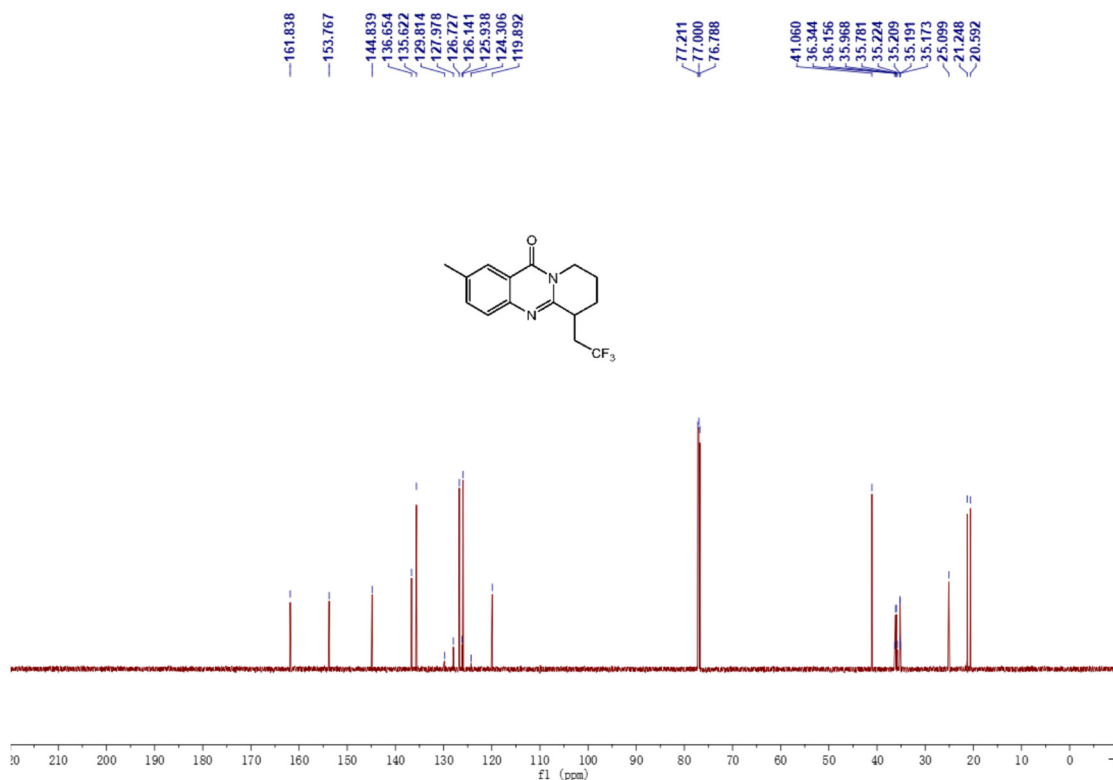
2-methoxy-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-*b*]quinazolin-11-one (**3d**) : ^{19}F NMR (376 MHz, CDCl_3)



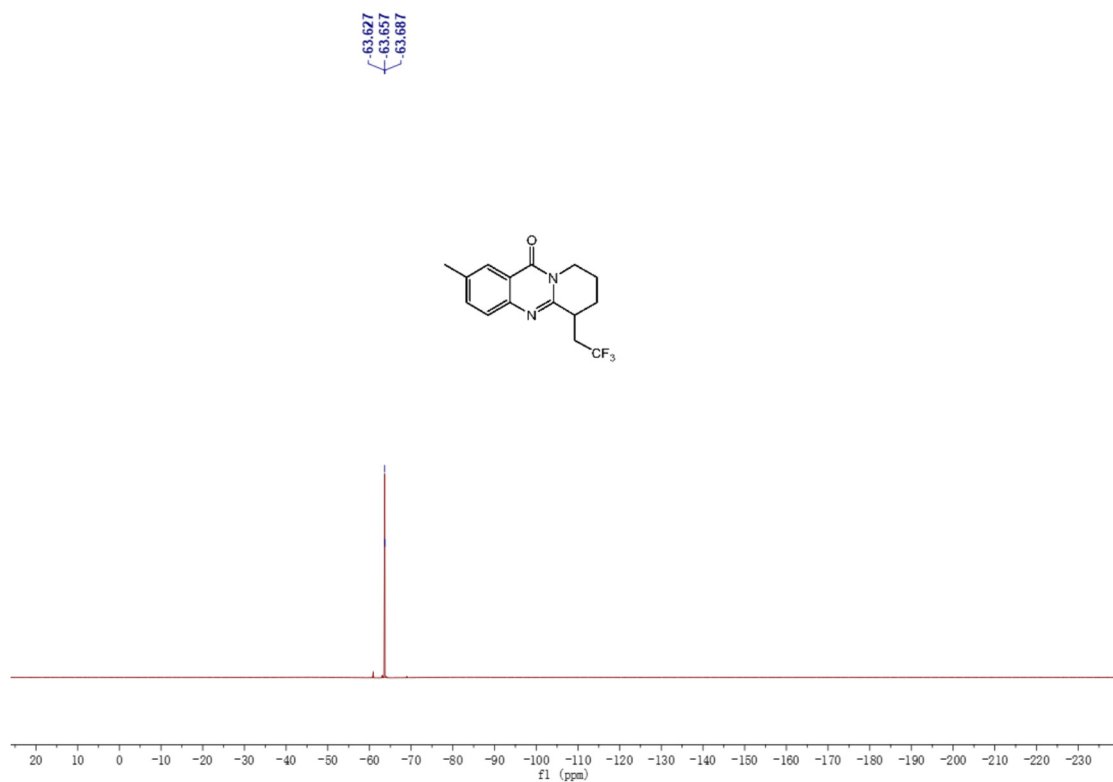
2-methyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-*b*]quinazolin-11-one (**3e**) : ^1H NMR (400 MHz, CDCl_3)



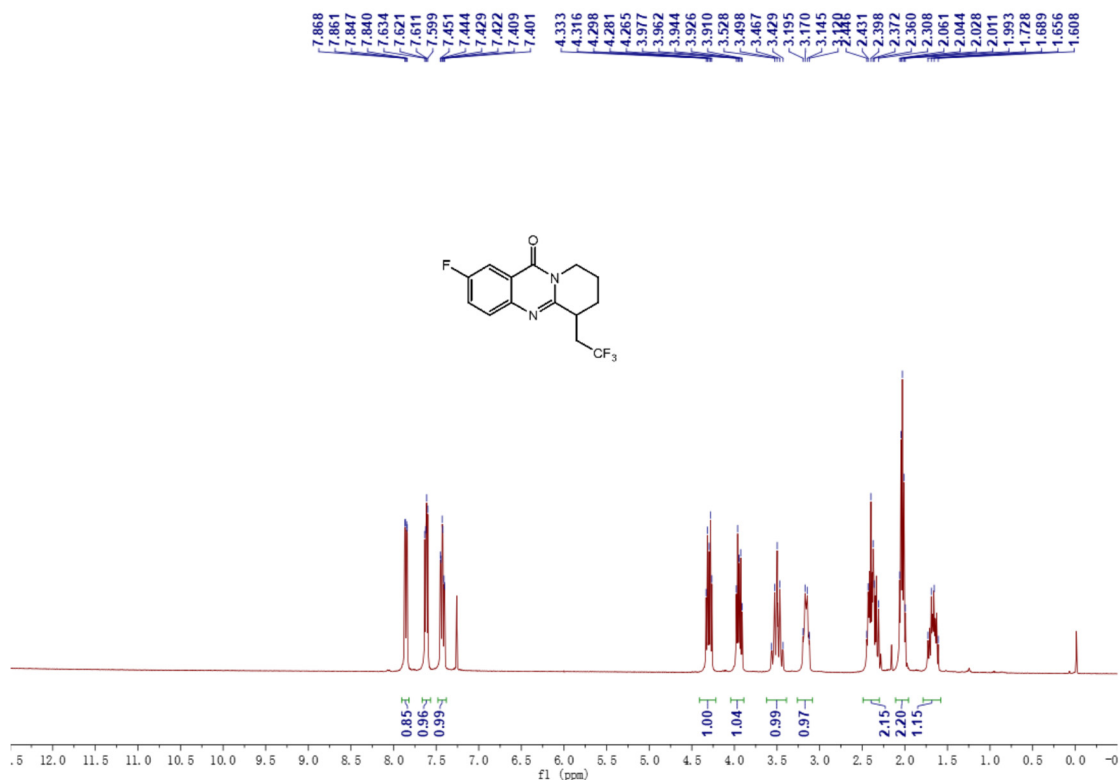
2-methyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-*b*]quinazolin-11-one (**3e**) : ^{13}C NMR (150 MHz, CDCl_3)



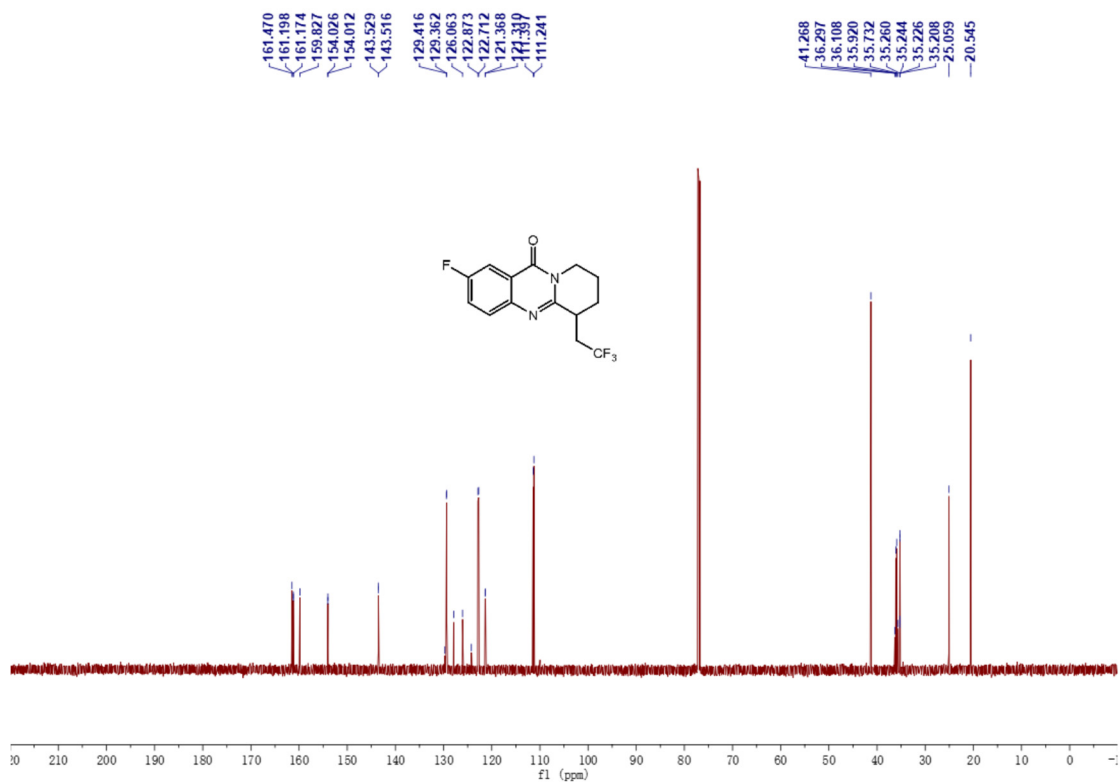
2-methyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-*b*]quinazolin-11-one (**3e**) : ^{19}F NMR (376 MHz, CDCl_3)

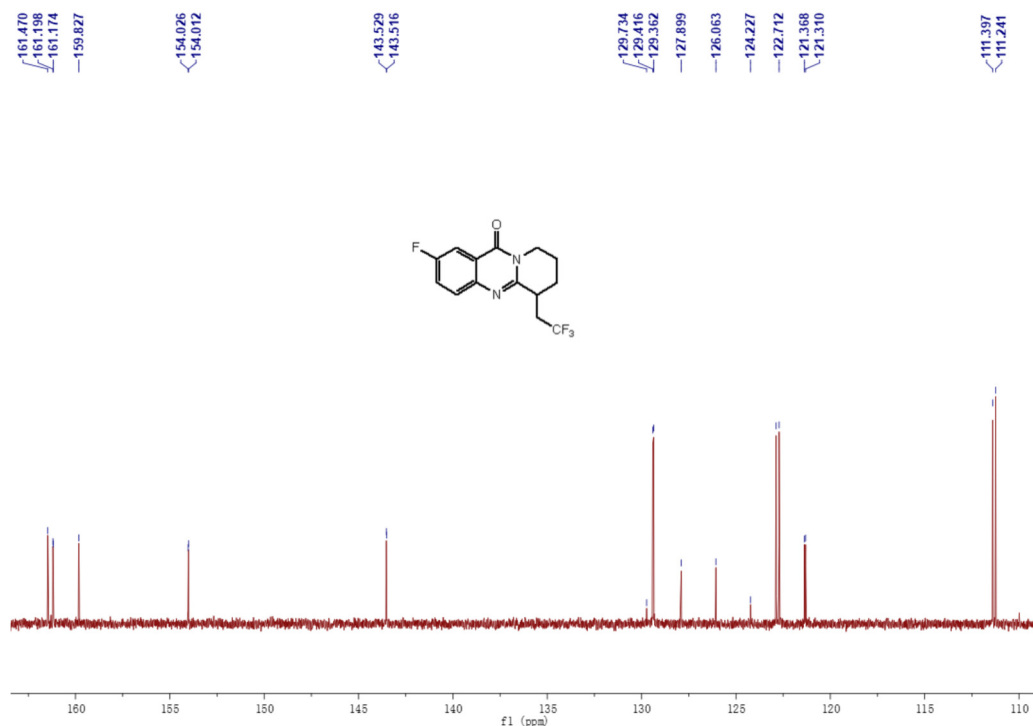


2-fluoro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-*b*]quinazolin-11-one (**3f**) : ^1H NMR (400 MHz, CDCl_3)



2-fluoro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-*b*]quinazolin-11-one (**3f**) : ^{13}C NMR (150 MHz, CDCl_3)

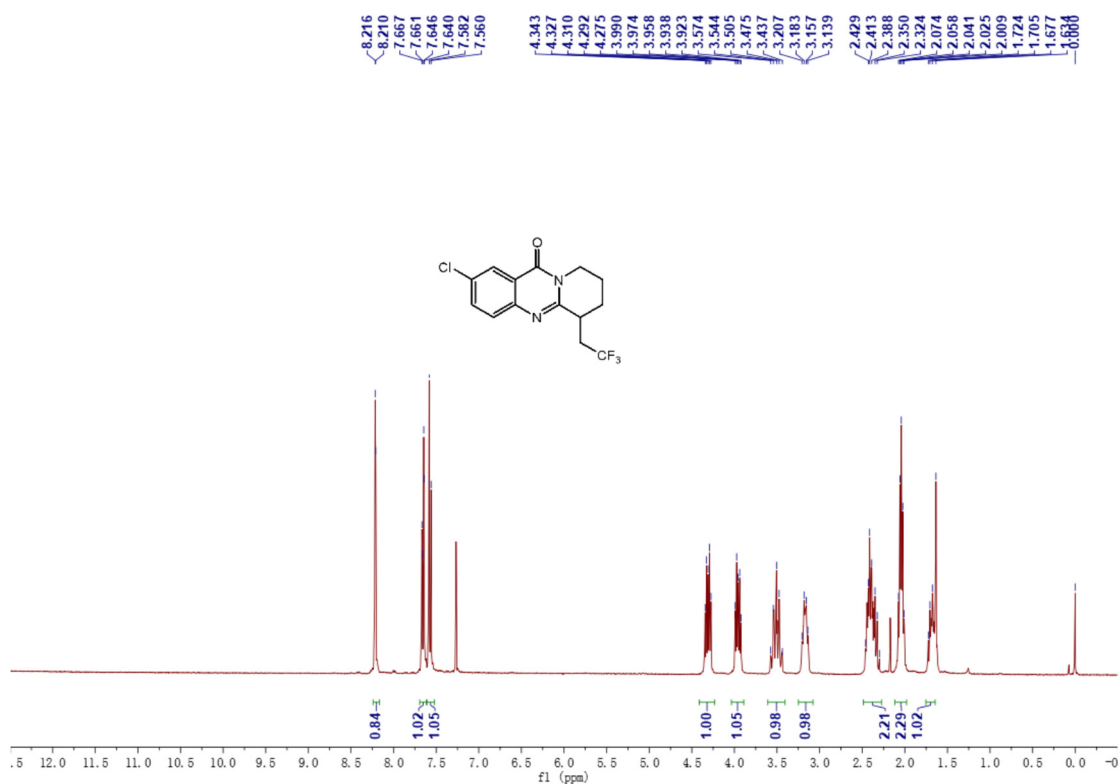




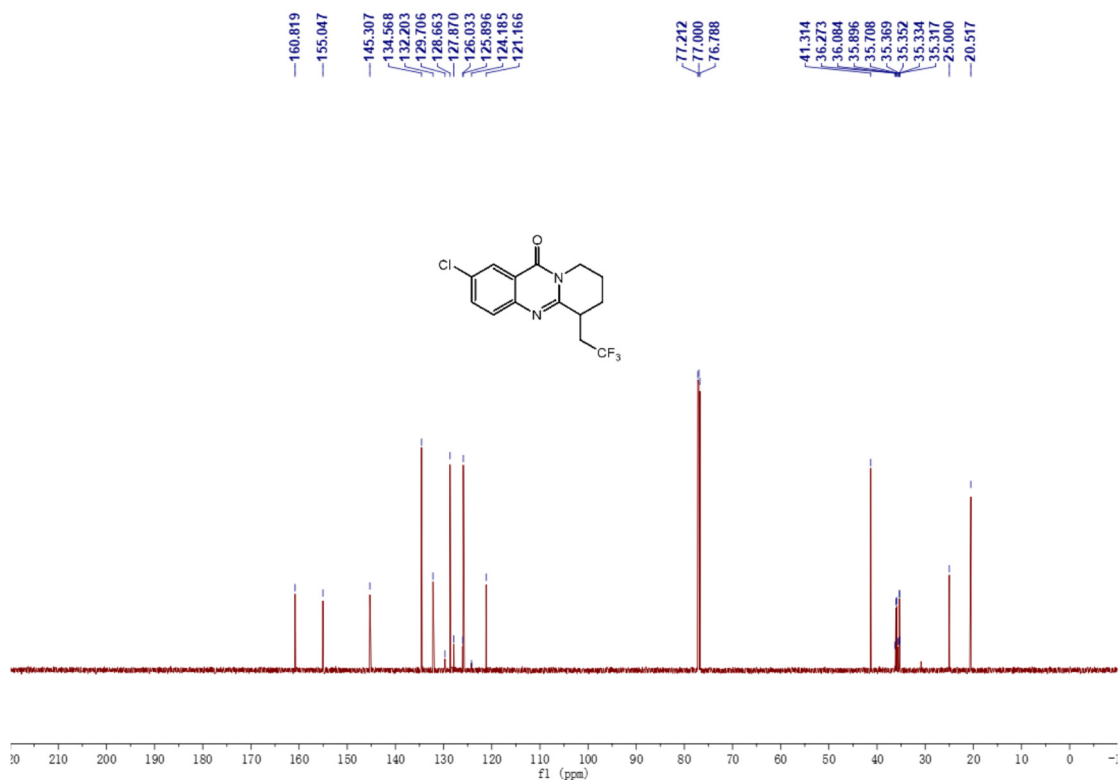
2-fluoro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3f**) : ^{19}F NMR (376 MHz, CDCl_3)



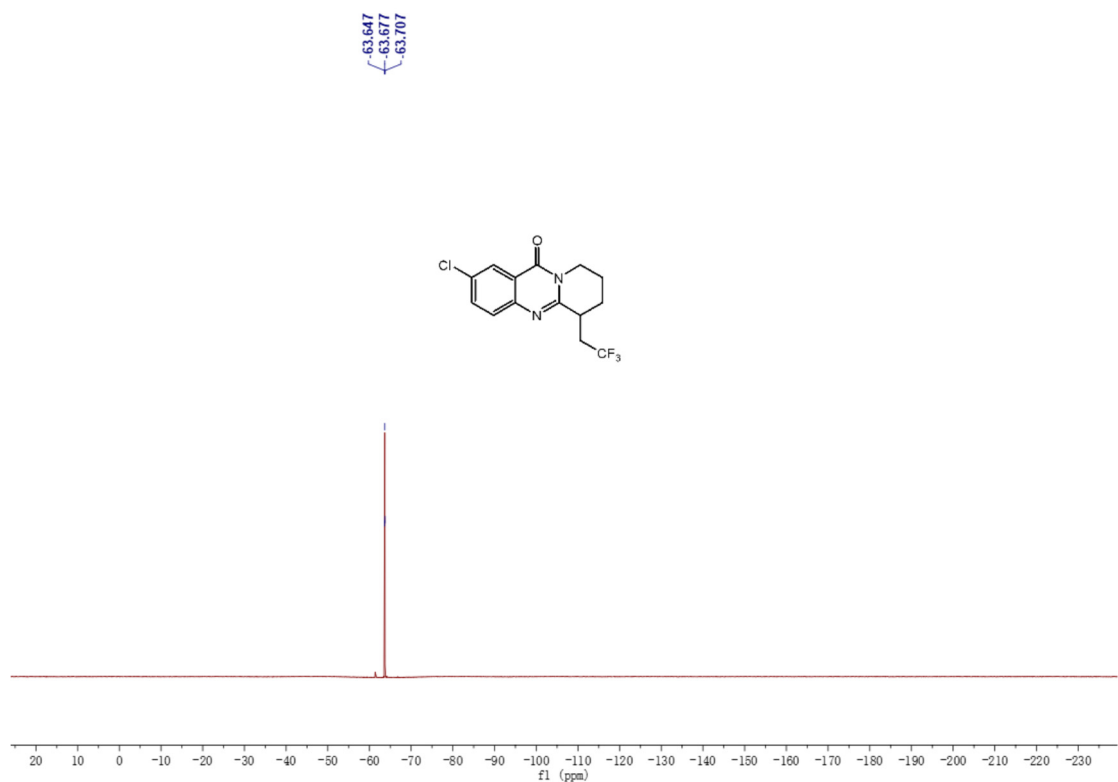
2-chloro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3g**) : ^1H NMR (400 MHz, CDCl_3)



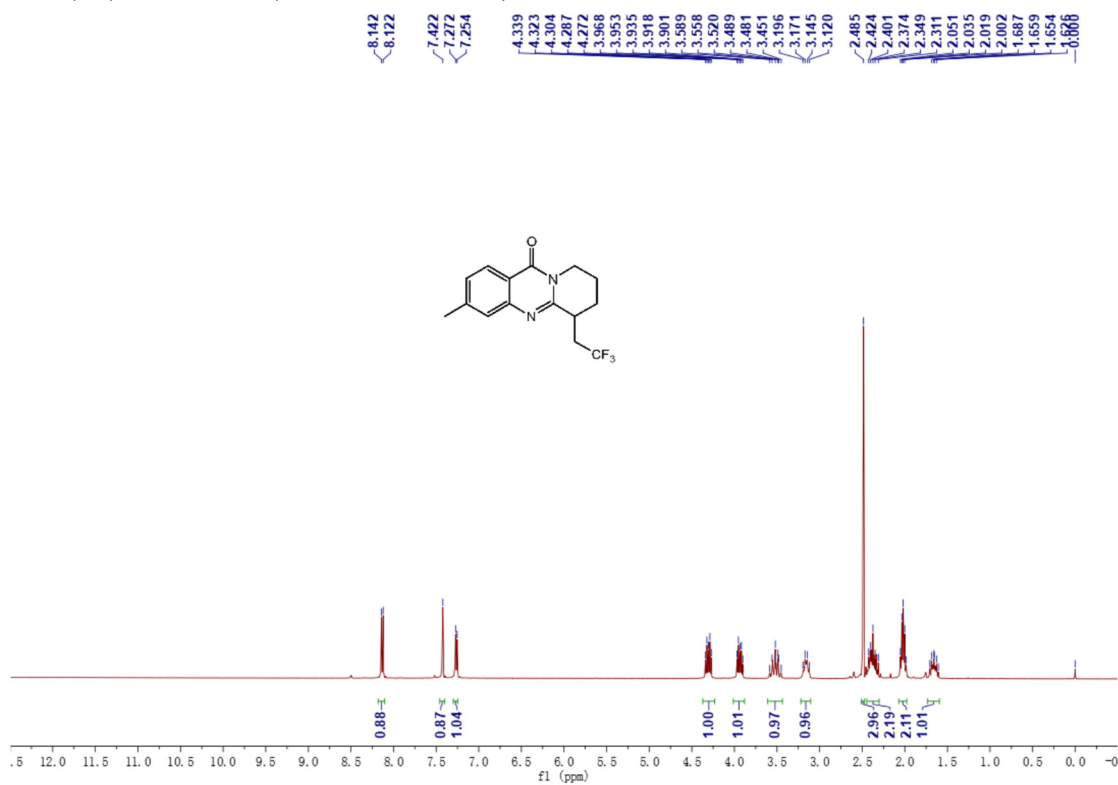
2-chloro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3g**): ¹³C NMR (150 MHz, CDCl₃)



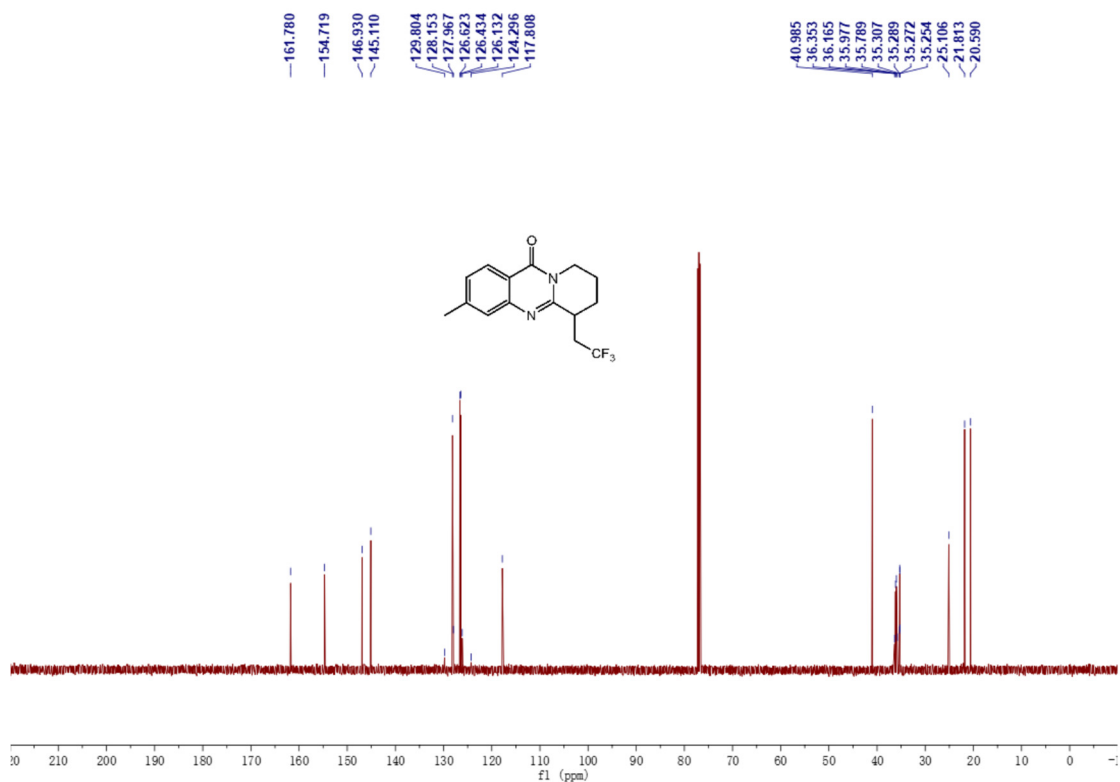
2-chloro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3g**): ¹⁹F NMR (376 MHz, CDCl₃)



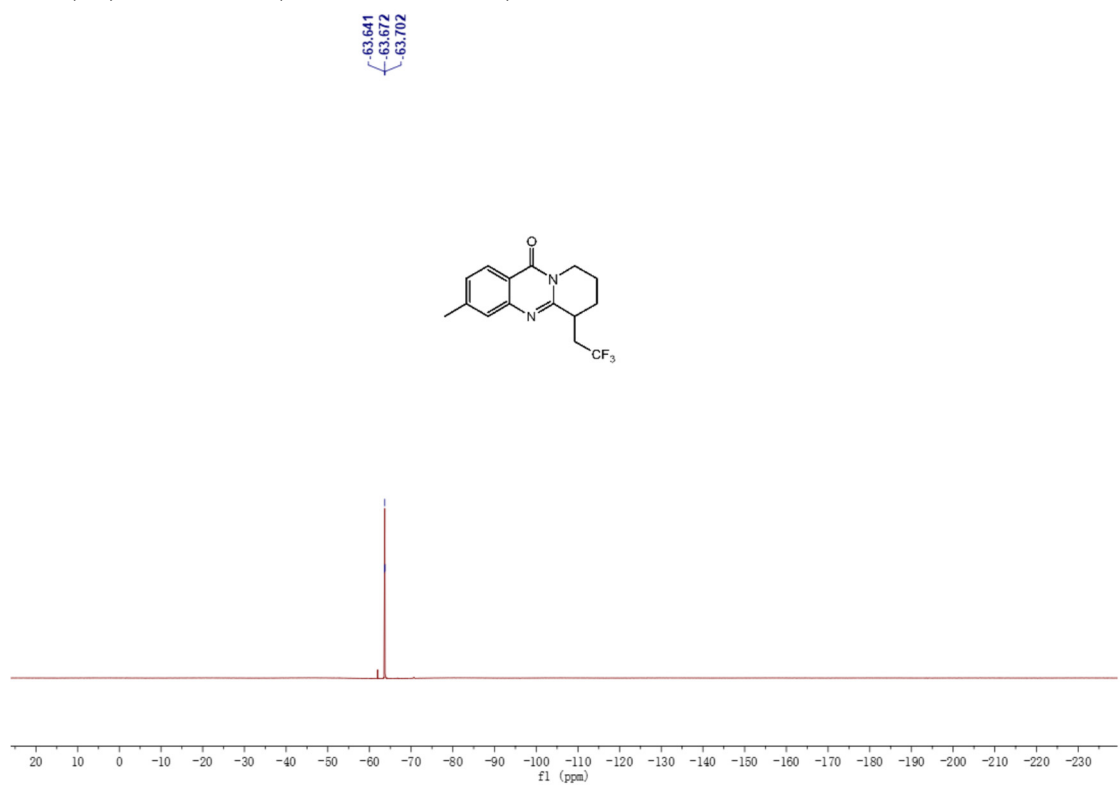
3-methyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-b]quinazolin-11-one (**3h**) : ^1H NMR (400 MHz, CDCl_3)



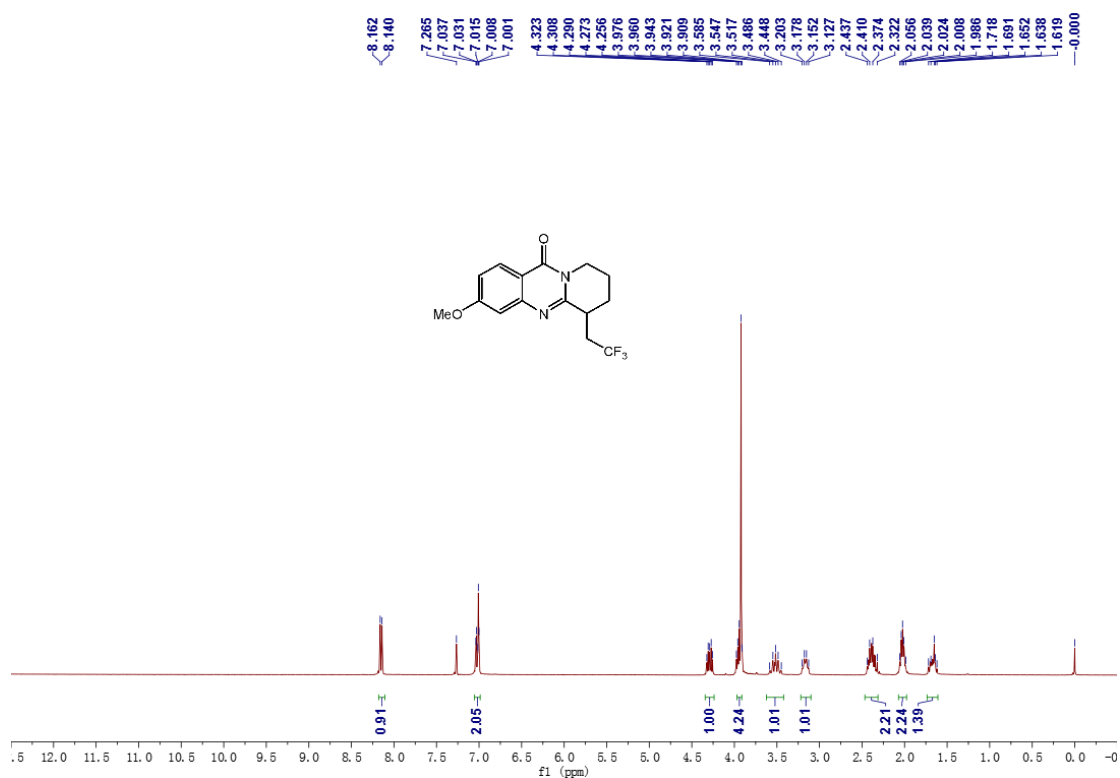
3-methyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-b]quinazolin-11-one (**3h**) : ^{13}C NMR (150 MHz, CDCl_3)



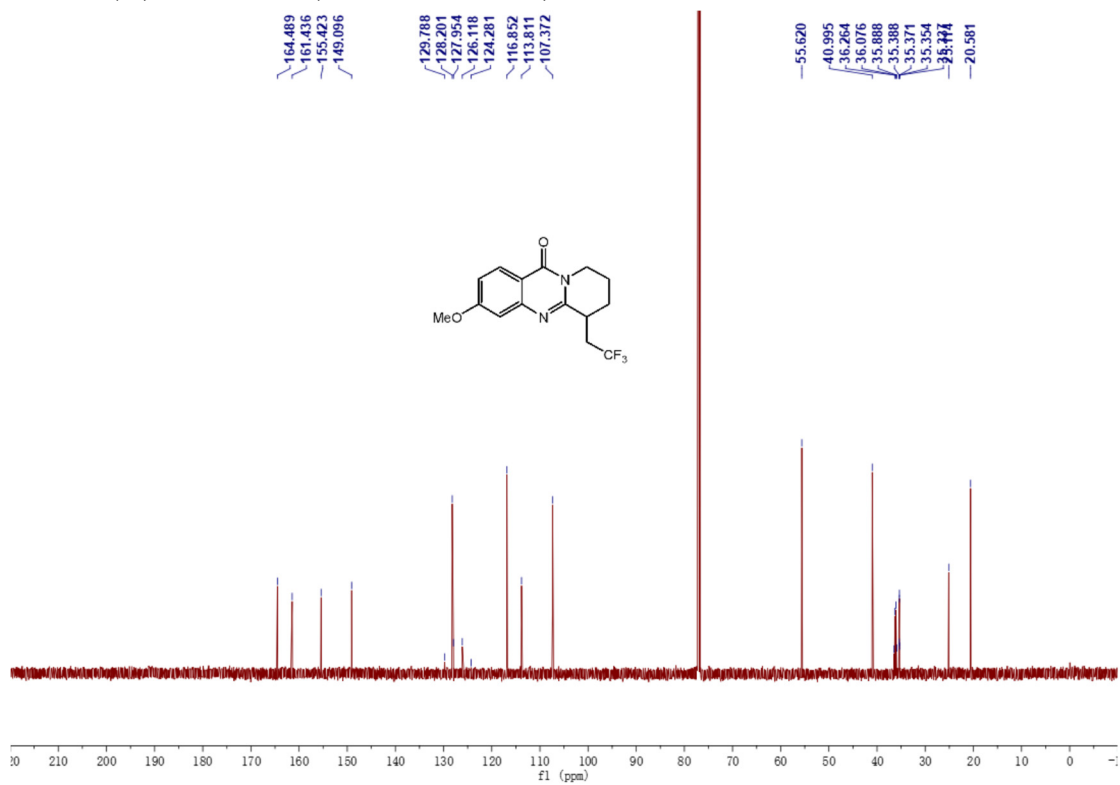
3-methyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-*b*]quinazolin-11-one (**3h**) : ^{19}F NMR (376 MHz, CDCl_3)



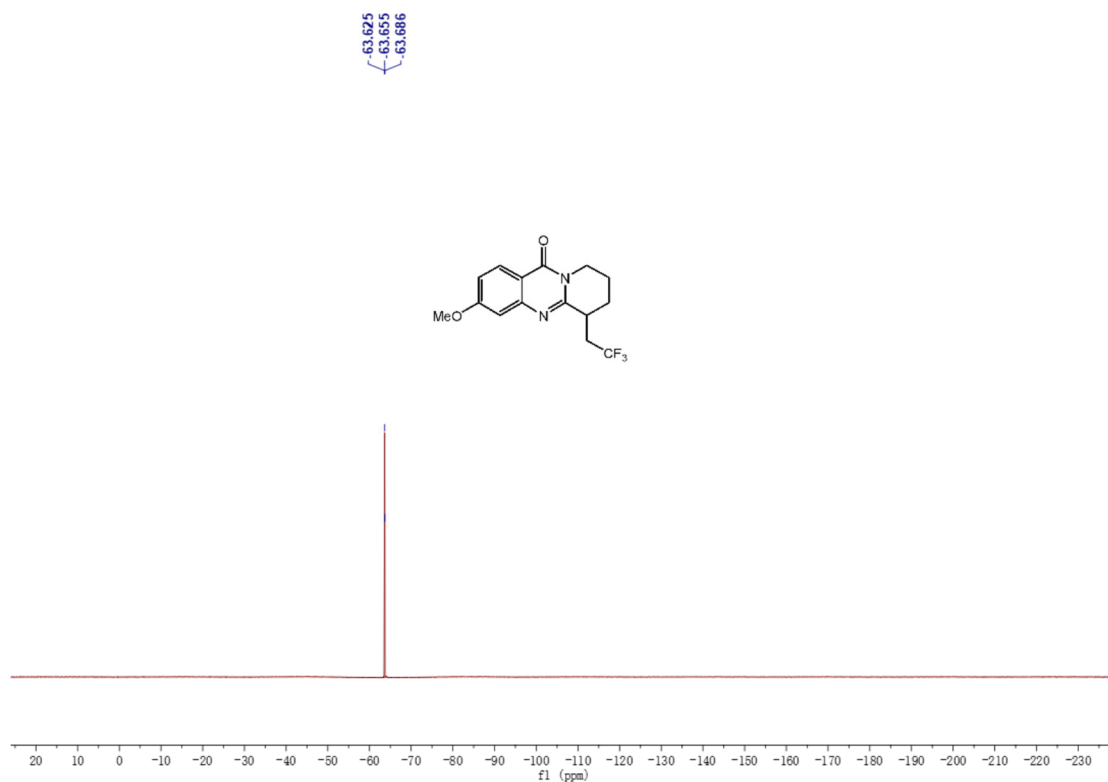
3-methoxy-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-*b*]quinazolin-11-one (**3i**) : ^{13}C NMR (400 MHz, CDCl_3)



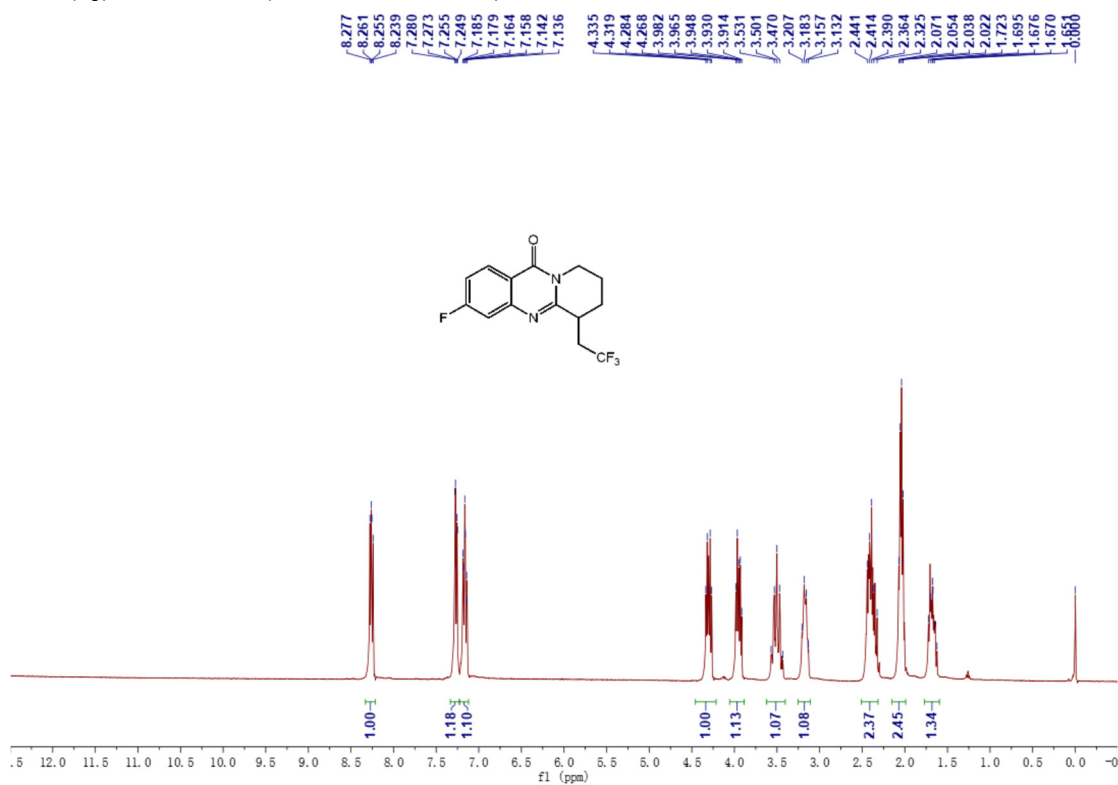
3-methoxy-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3i**) : ¹³C NMR (150 MHz, CDCl₃)



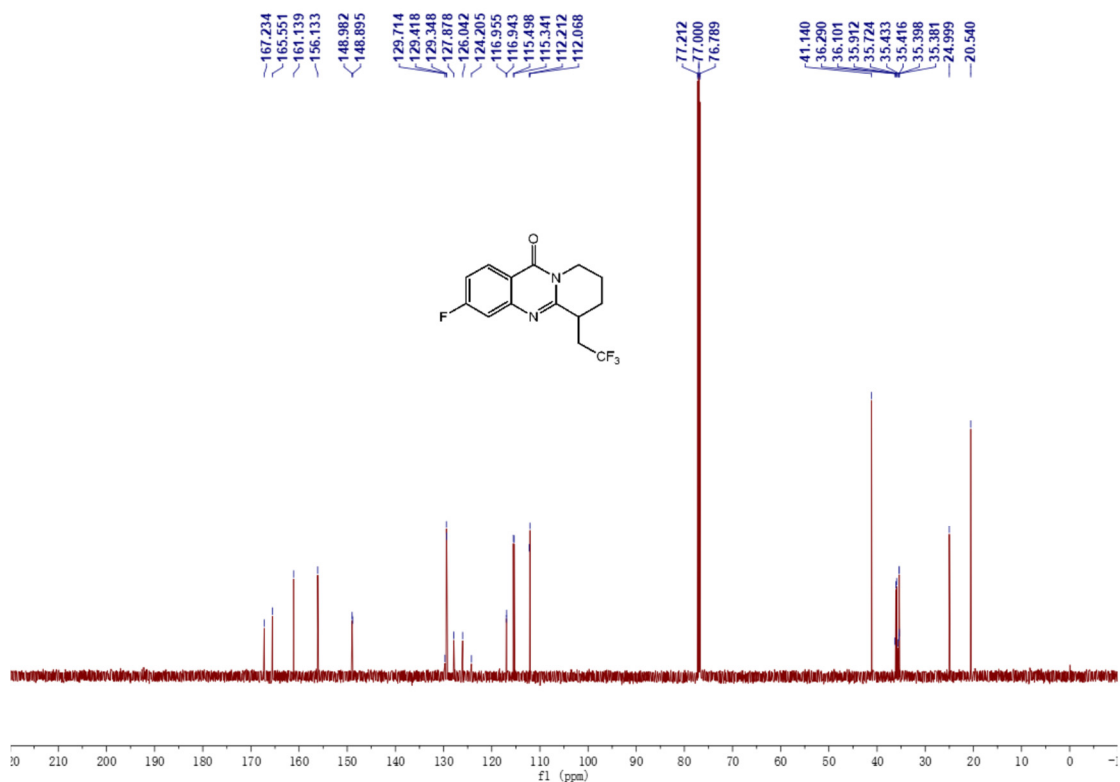
3-methoxy-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3i**) : ¹⁹F NMR (376 MHz, CDCl₃)



3-fluoro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-b]quinazolin-11-one (3j) : ^1H NMR (400 MHz, CDCl_3)



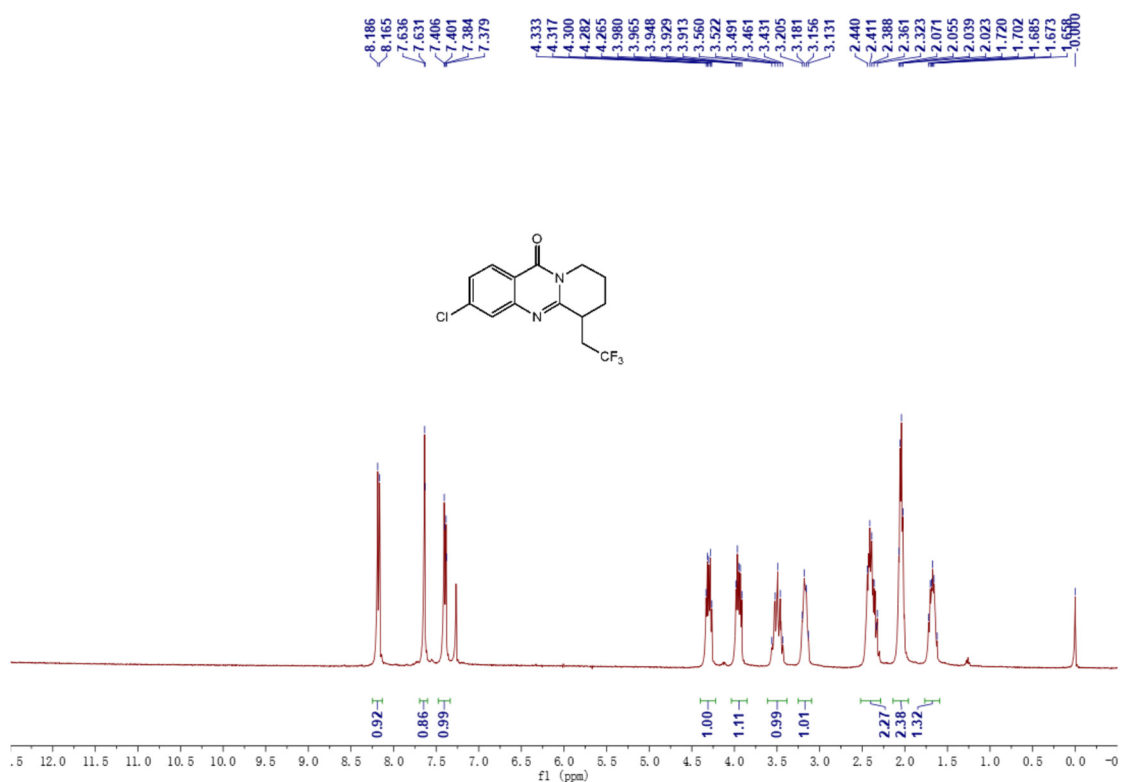
3-fluoro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-b]quinazolin-11-one (3j) : ^{13}C NMR (150 MHz, CDCl_3)



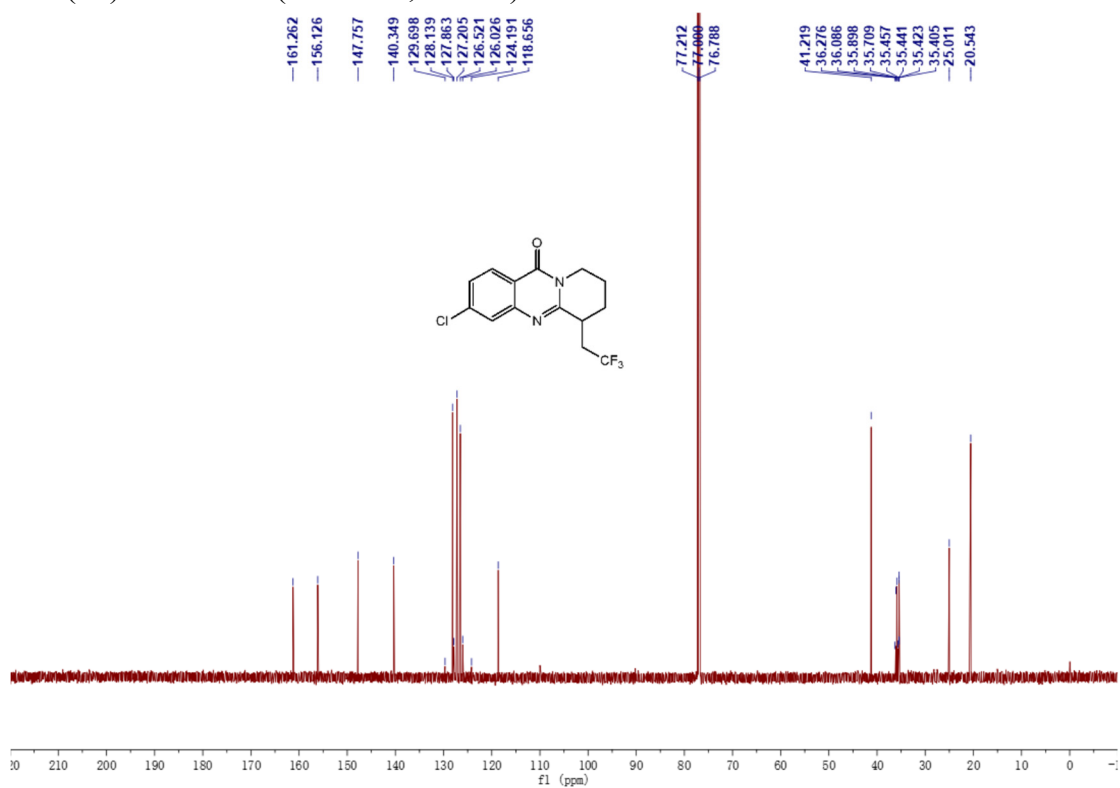
3-fluoro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*] quinazolin-11-one (**3j**) : ^{19}F NMR (376 MHz, CDCl_3)



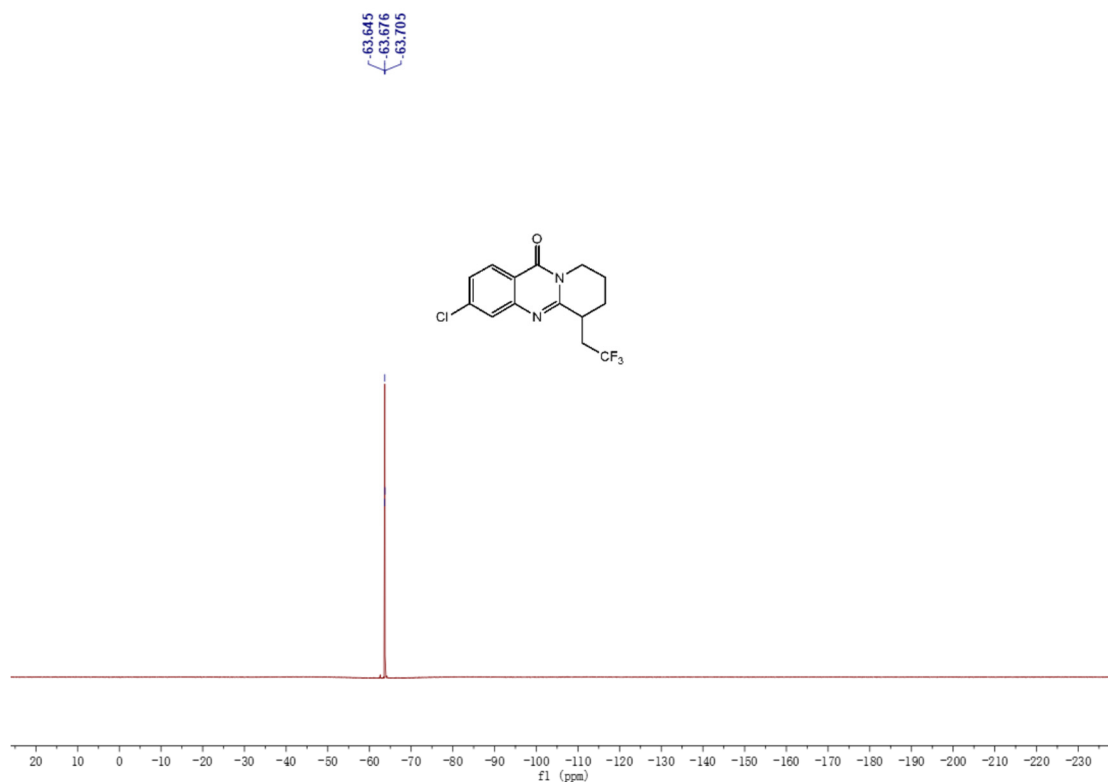
3-chloro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3k**) : ^1H NMR (400 MHz, CDCl_3)



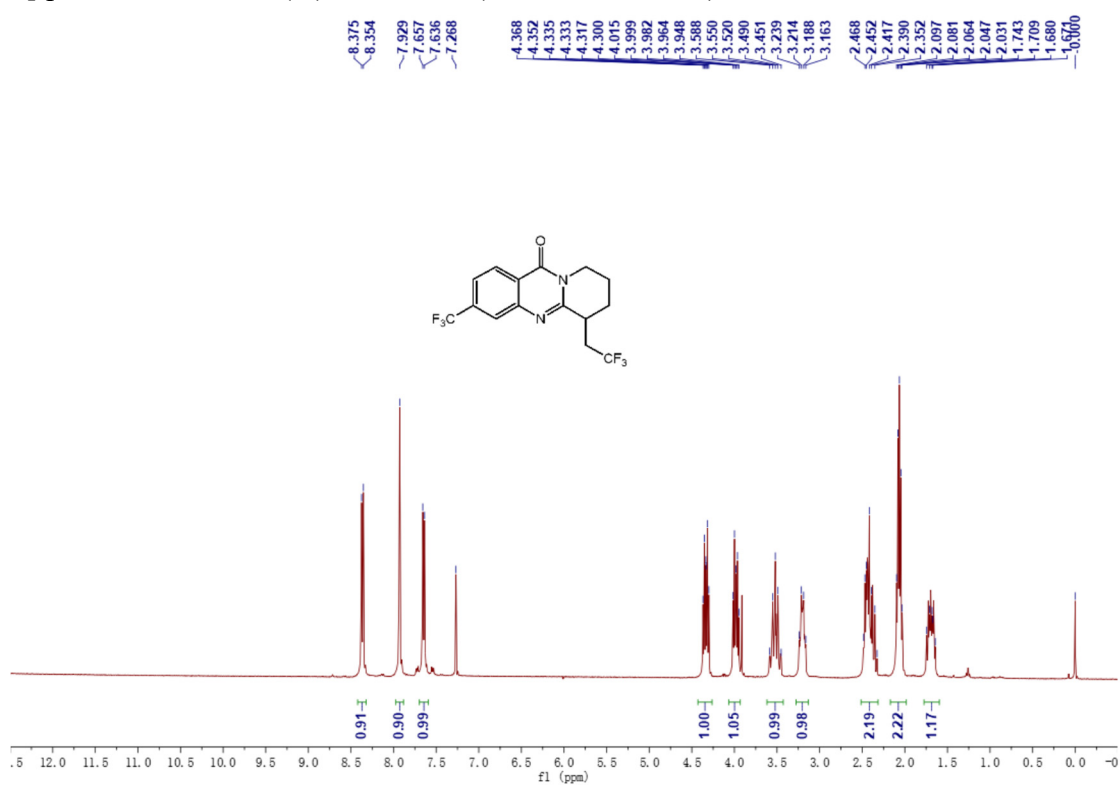
3-chloro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3k**): ^{13}C NMR (150 MHz, CDCl_3)



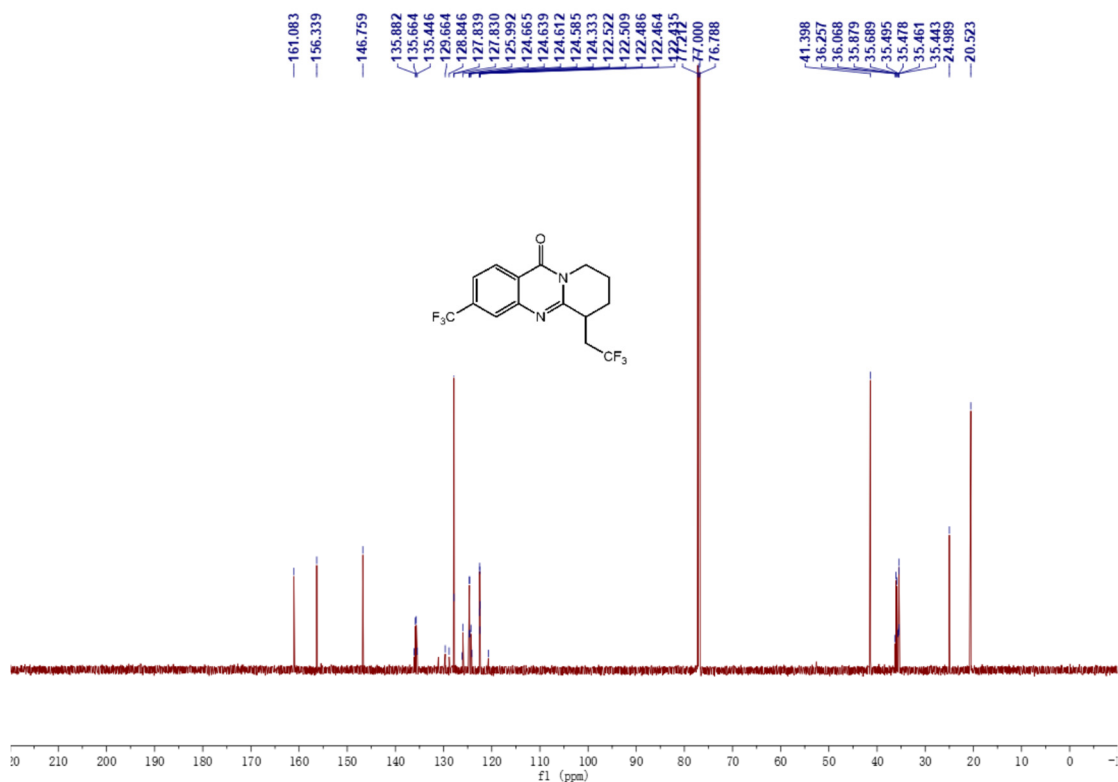
3-chloro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3k**) : ^{19}F NMR (376 MHz, CDCl_3)



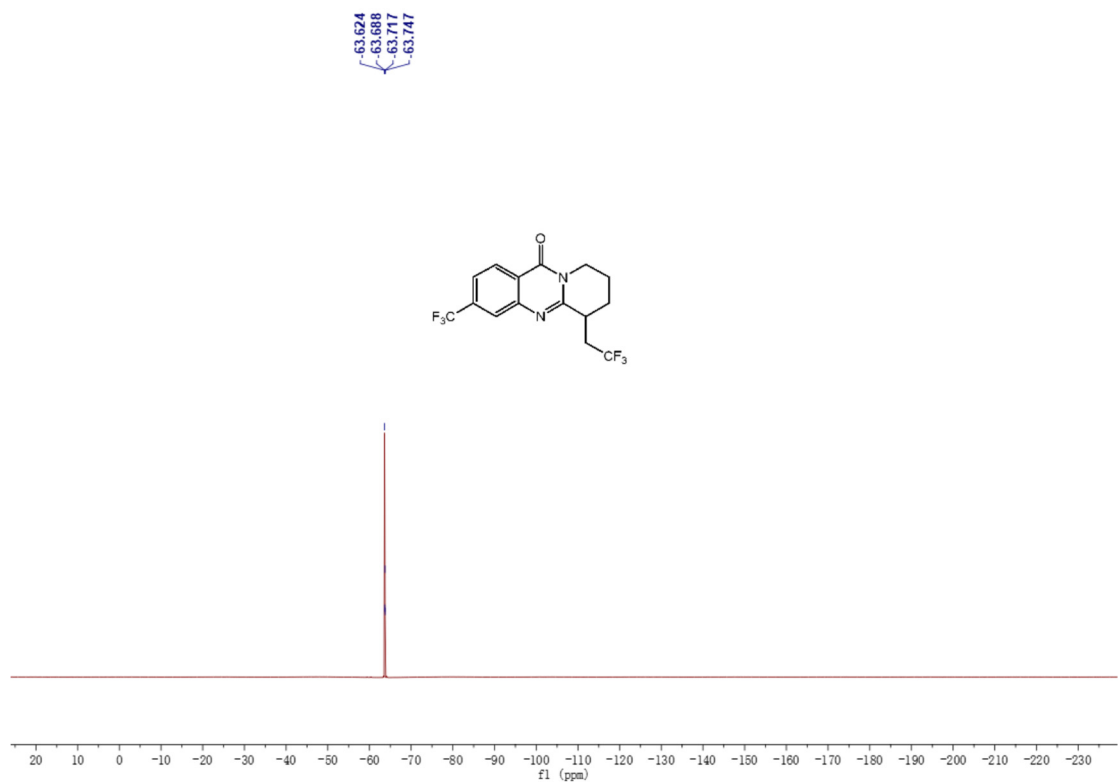
6-(2,2,2-trifluoroethyl)-3-(trifluoromethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3l**) : ^1H NMR (400 MHz, CDCl_3)

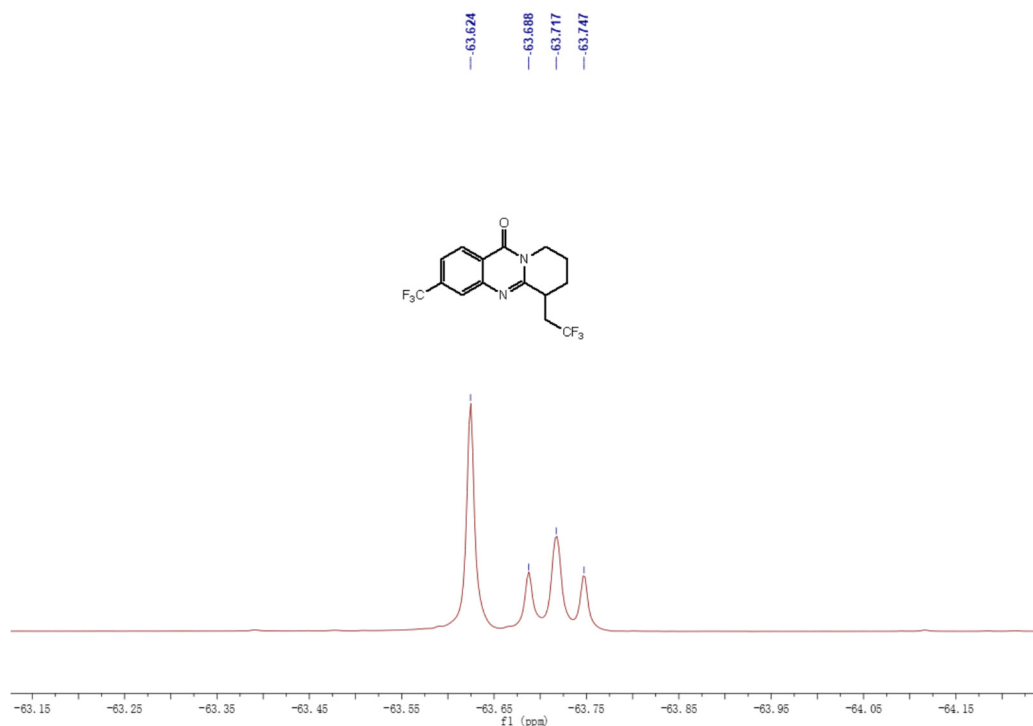


6-(2,2,2-trifluoroethyl)-3-(trifluoromethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-*b*]quinazolin-11-one (**3l**): ^{13}C NMR (150 MHz, CDCl_3)

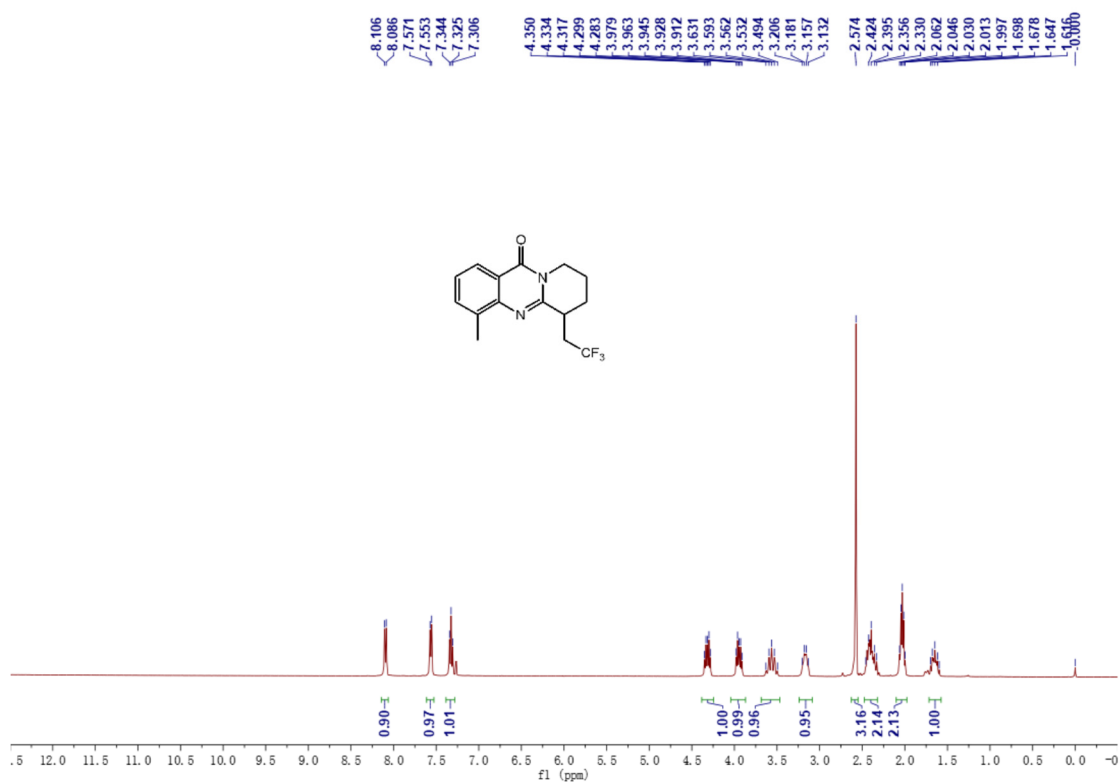


6-(2,2,2-trifluoroethyl)-3-(trifluoromethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-*b*]quinazolin-11-one (**3l**): ^{19}F NMR (376 MHz, CDCl_3)

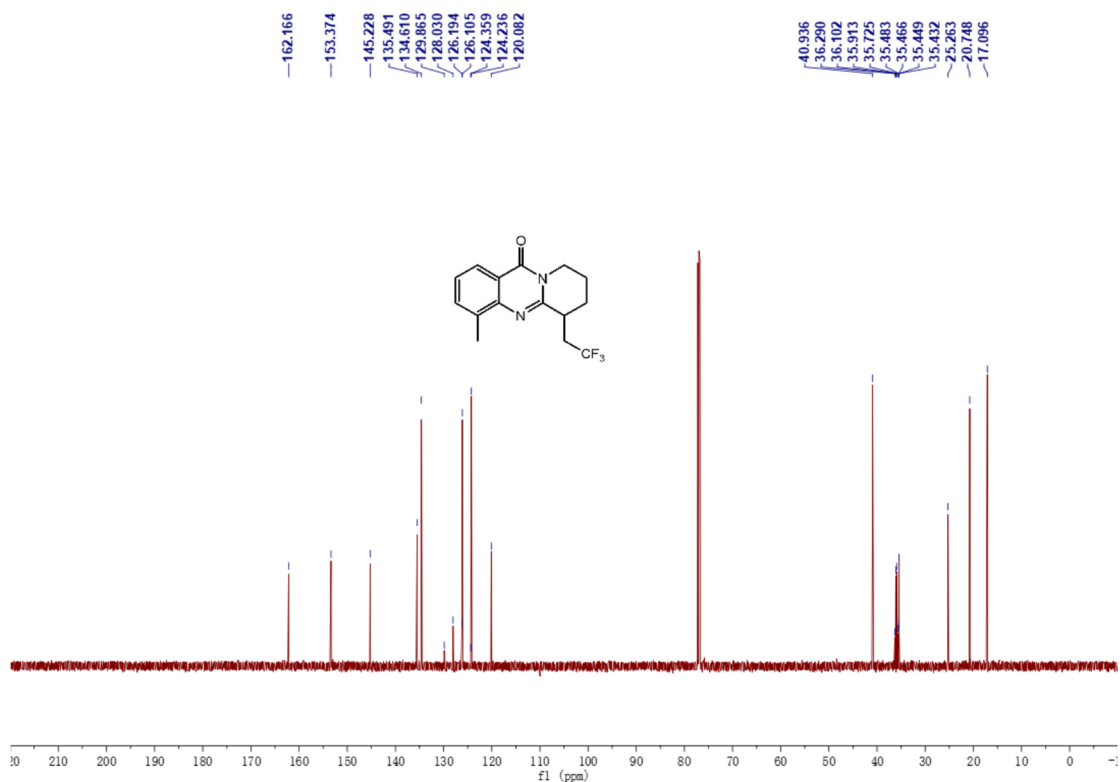




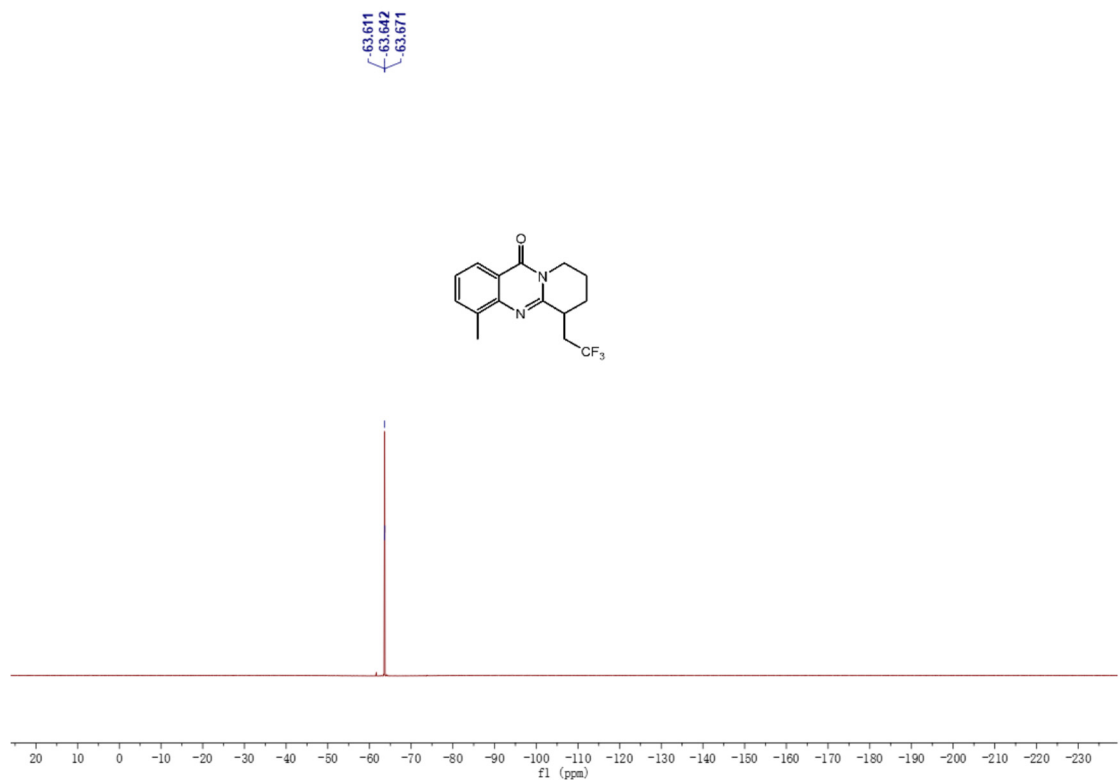
4-methyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-b]quinazolin-11-one (**3m**) : ^1H NMR (400 MHz, CDCl_3)



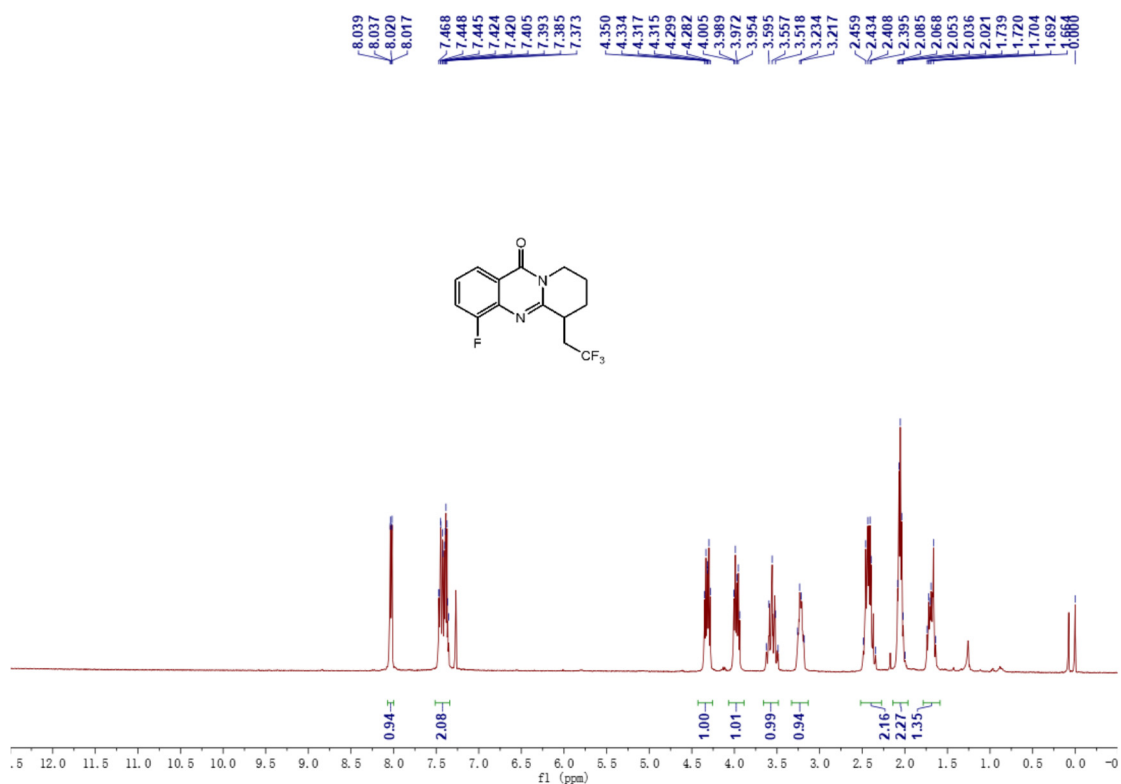
4-methyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-b]quinazolin-11-one (**3m**) : ^{13}C NMR (150 MHz, CDCl_3)



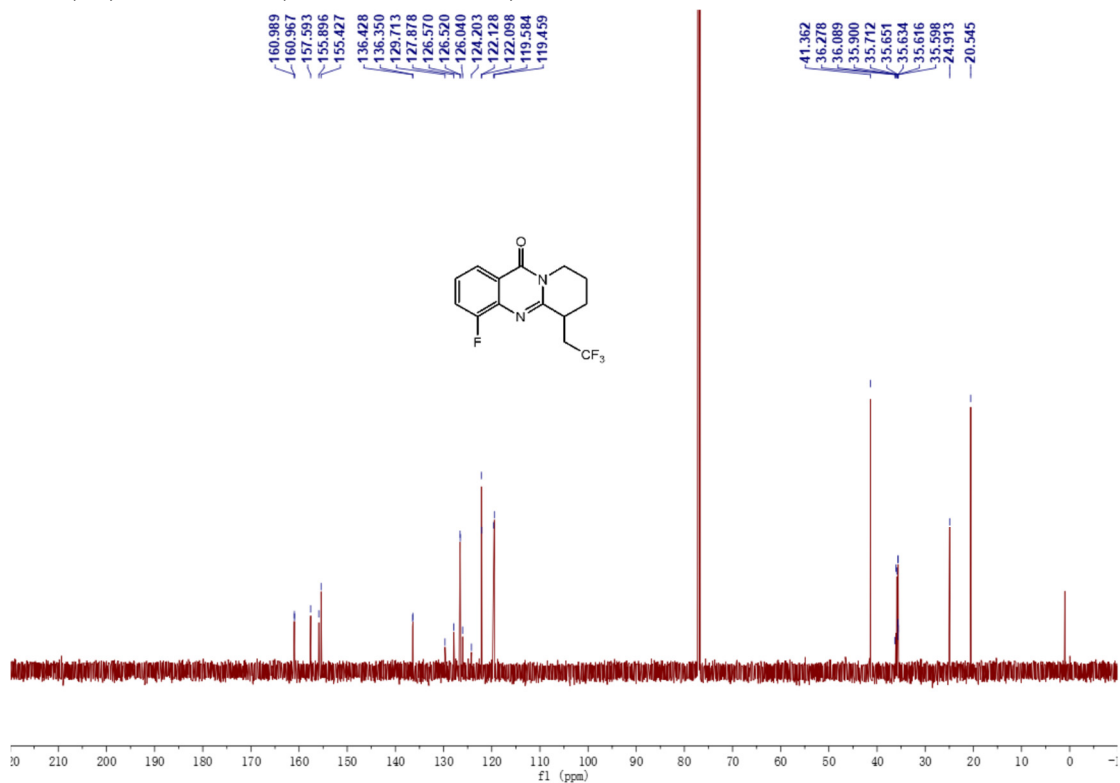
4-methyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-*b*]quinazolin-11-one (**3m**) : ¹⁹F NMR (376 MHz, CDCl₃)

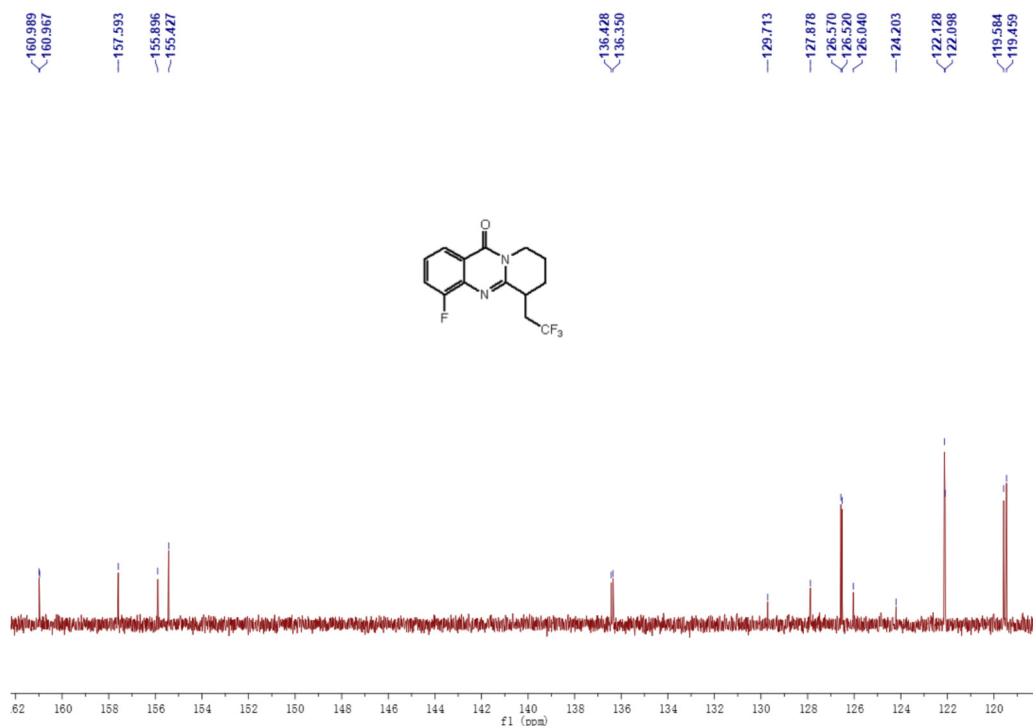


4-fluoro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-*b*]quinazolin-11-one (**3n**) : ¹H NMR (400 MHz, CDCl₃)



4-fluoro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-b]quinazolin-11-one (**3n**): ¹³C NMR (150 MHz, CDCl₃)

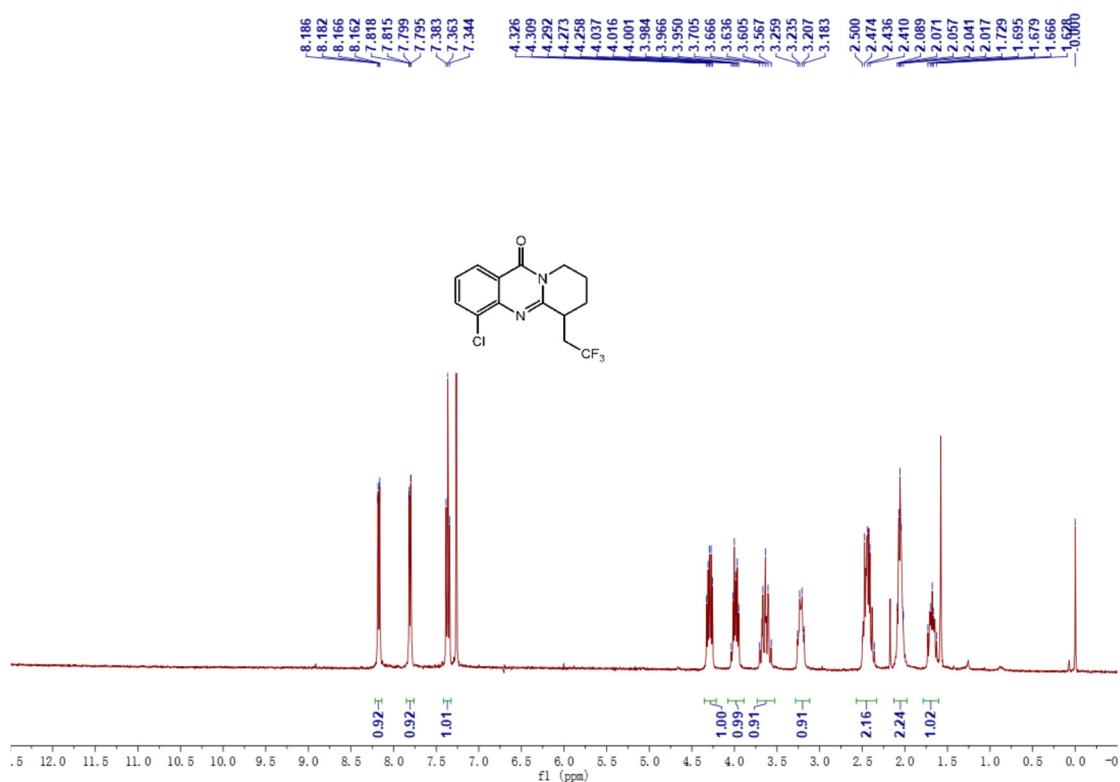




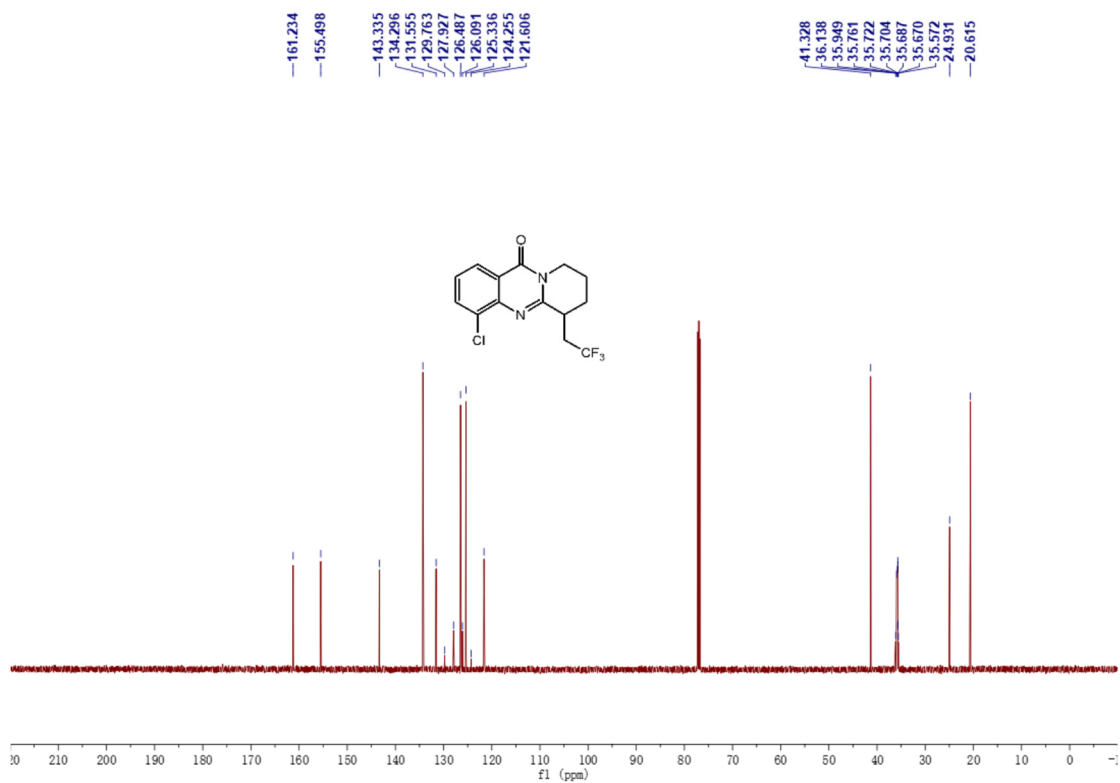
4-fluoro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3n**): ^{19}F NMR (376 MHz, CDCl_3)



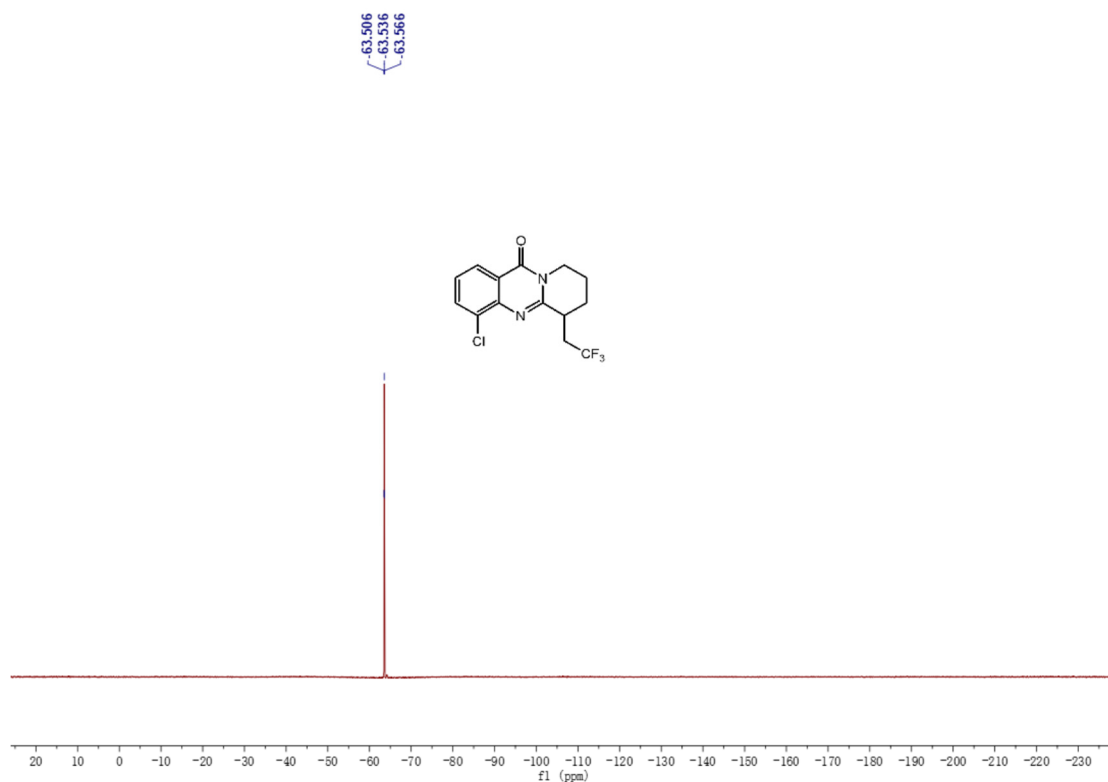
4-chloro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3o**): ^1H NMR (400 MHz, CDCl_3)



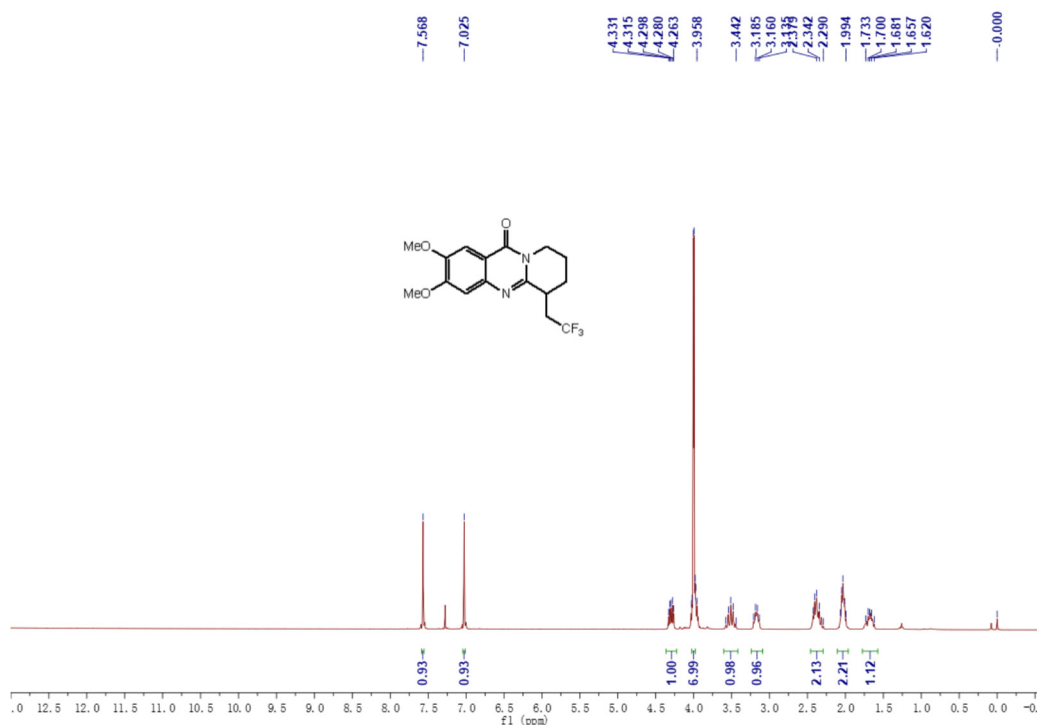
4-chloro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**30**) : ^{13}C NMR (150 MHz, CDCl_3)



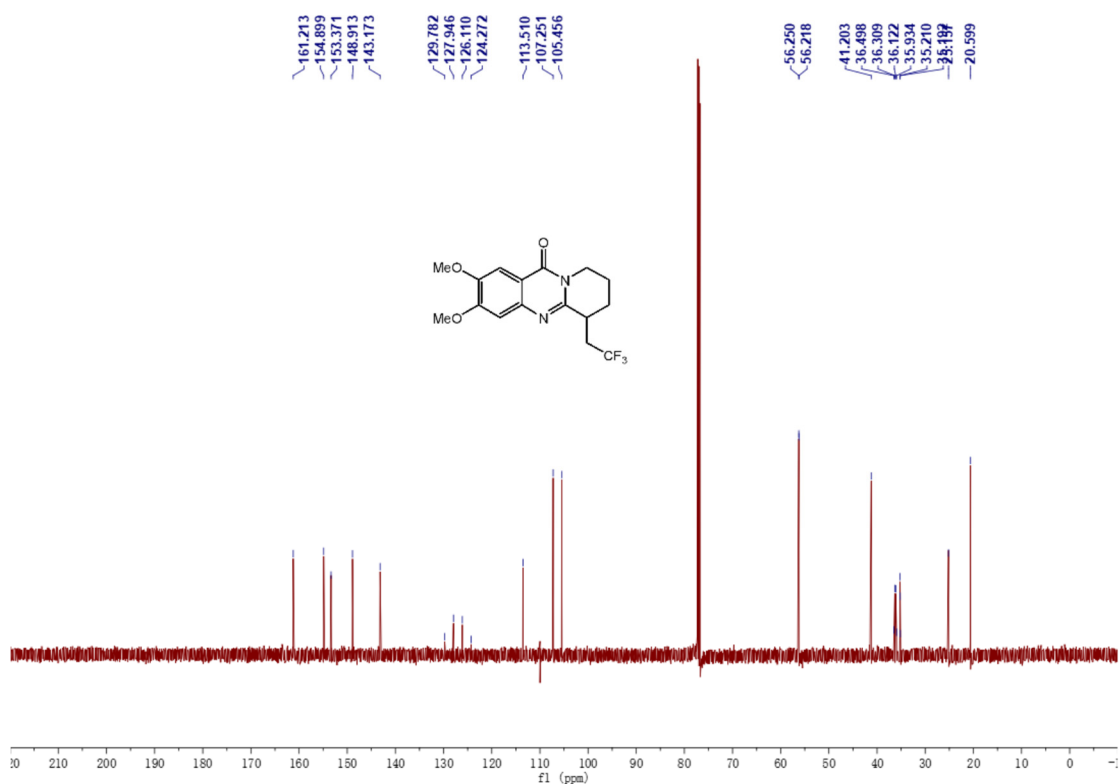
4-chloro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**30**) : ^{19}F NMR (376 MHz, CDCl_3)



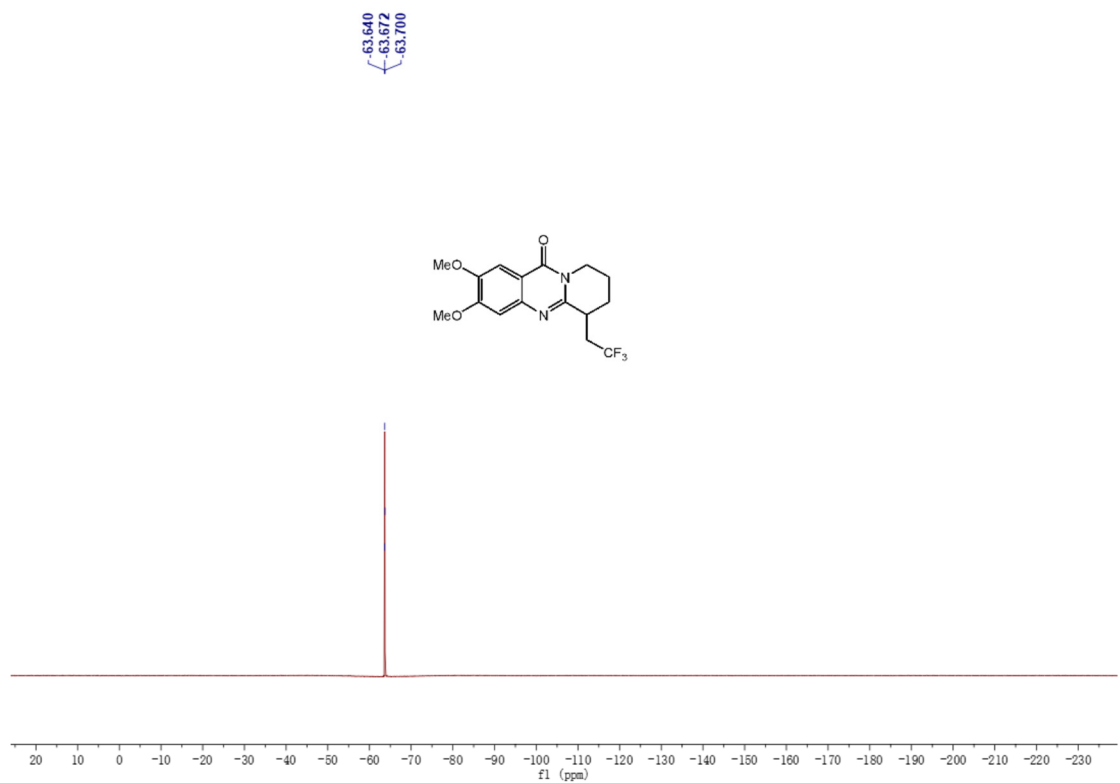
2,3-dimethoxy-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3p**) : ^1H NMR (400 MHz, CDCl_3)



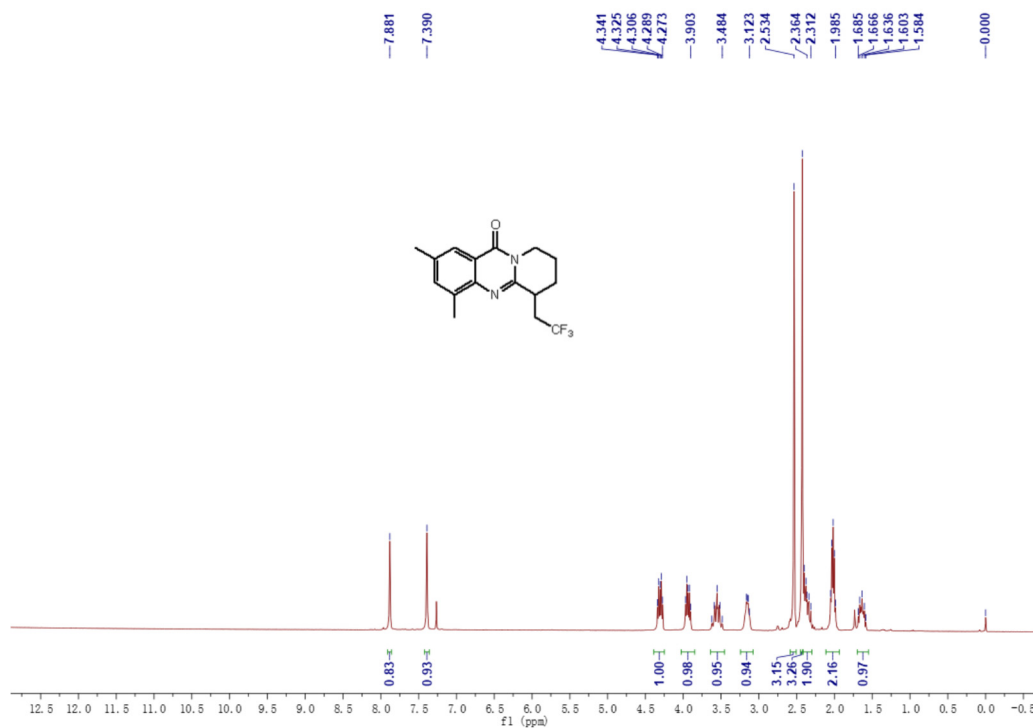
2,3-dimethoxy-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3p**) : ^{13}C NMR (150 MHz, CDCl_3)



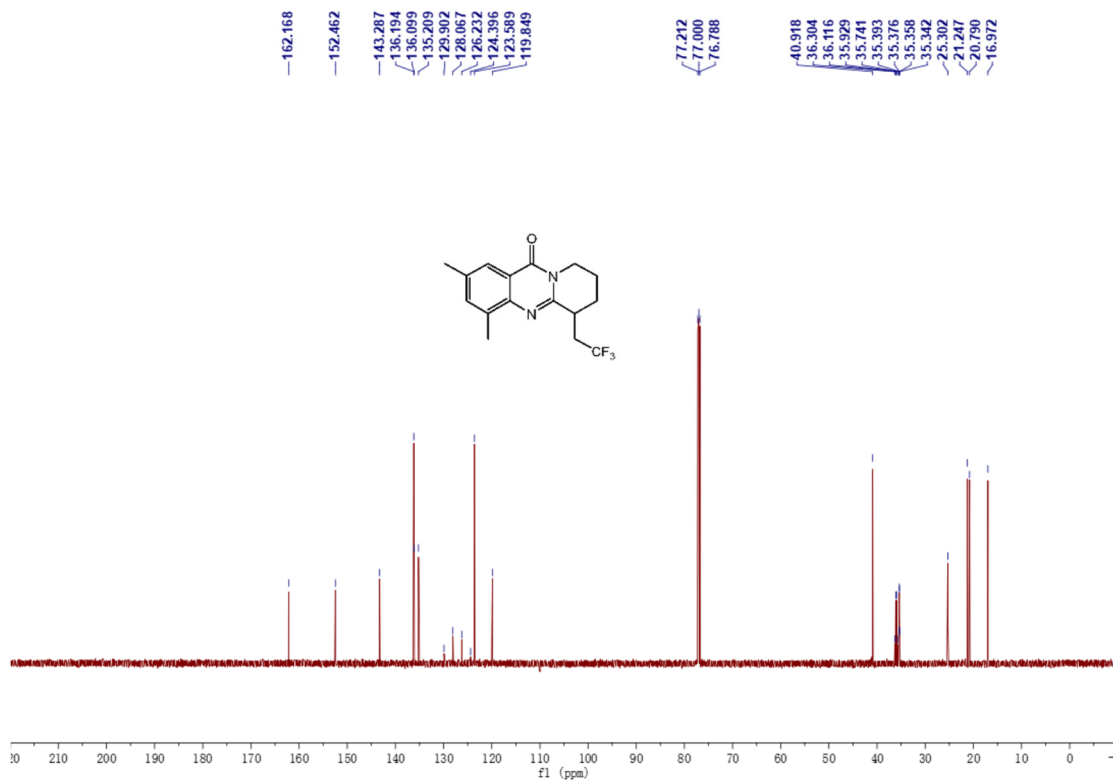
2,3-dimethoxy-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3p**) : ¹⁹F NMR (376 MHz, CDCl₃)



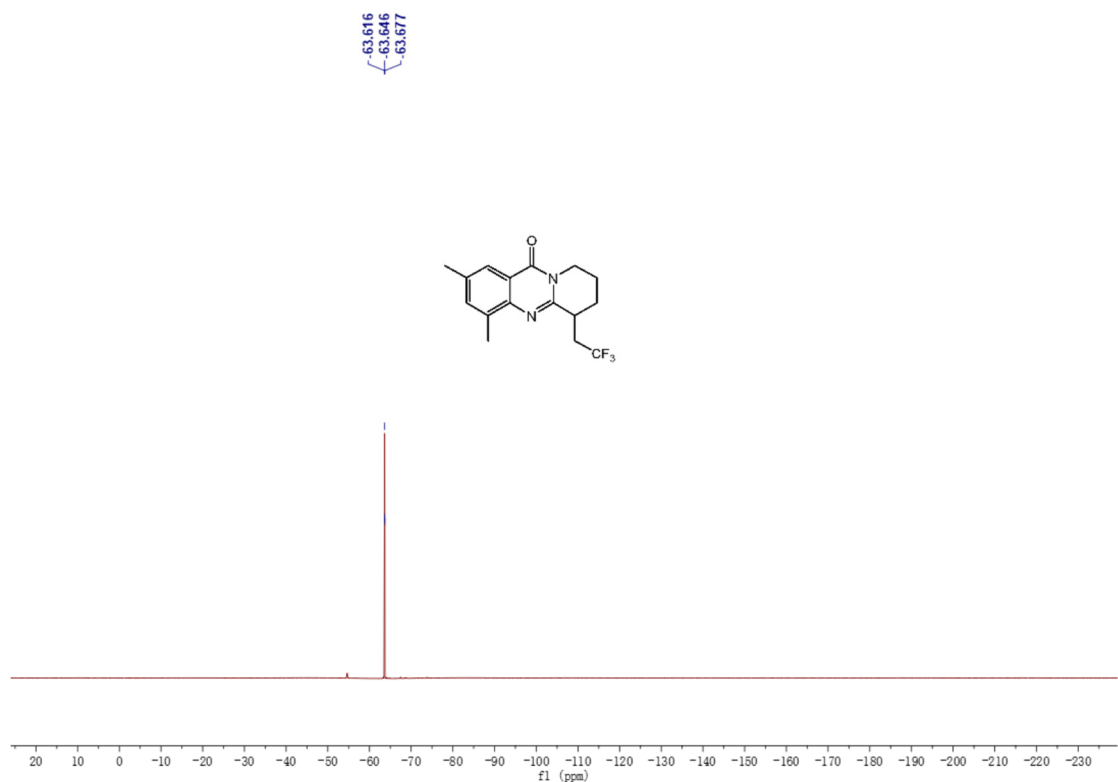
2,4-dimethyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-*b*]quinazolin-11-one (**3q**) : ¹H NMR (400 MHz, CDCl₃)



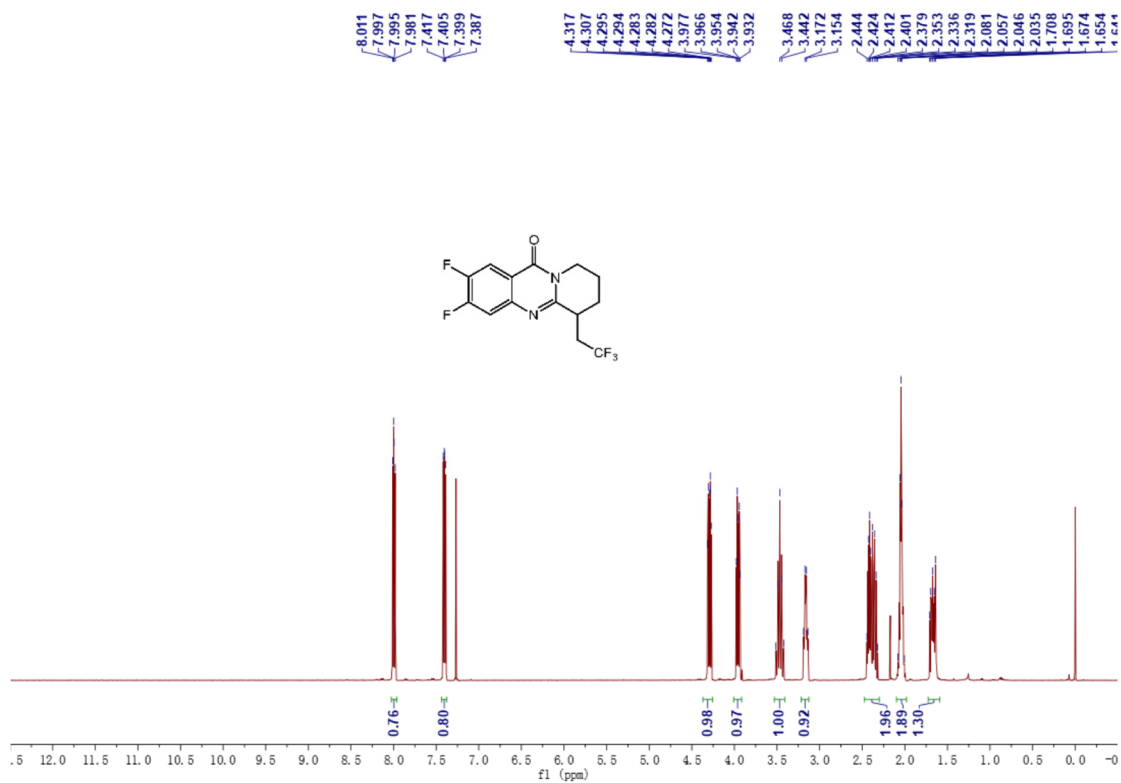
2,4-dimethyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-b]quinazolin-11-one (**3q**): ¹³C NMR (150 MHz, CDCl₃)



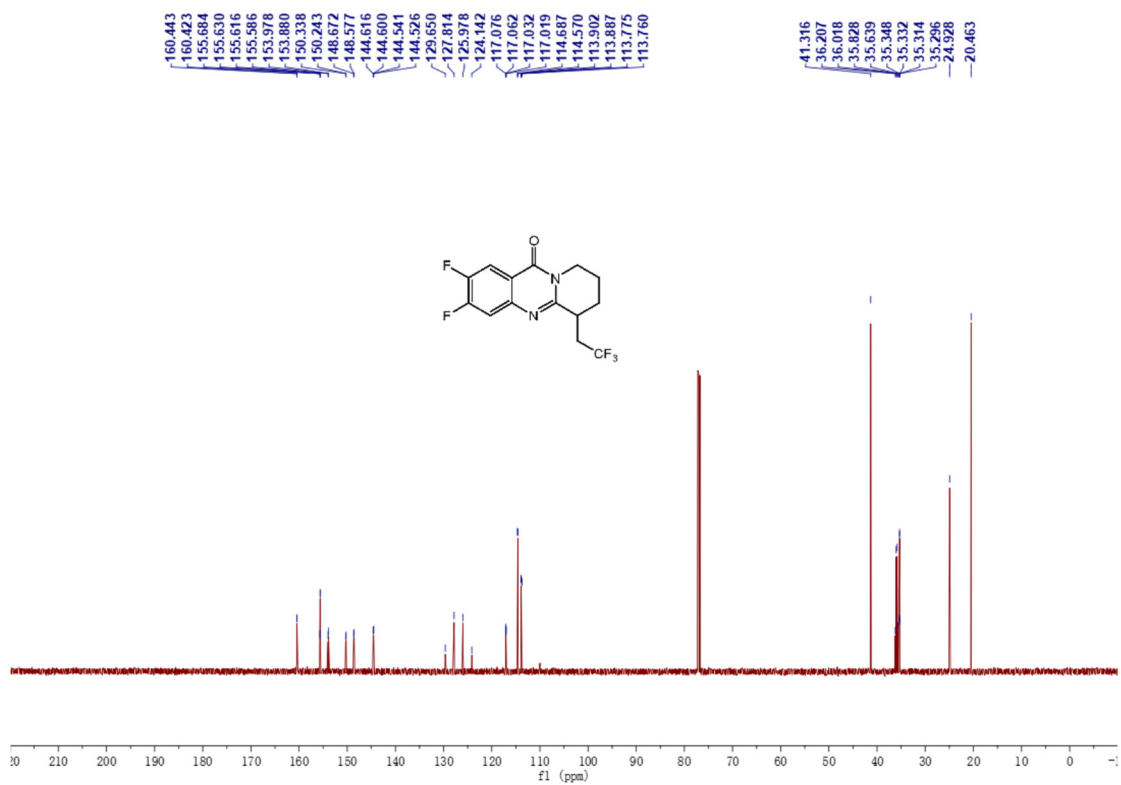
2,4-dimethyl-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-b]quinazolin-11-one (**3q**): ¹⁹F NMR (376 MHz, CDCl₃)

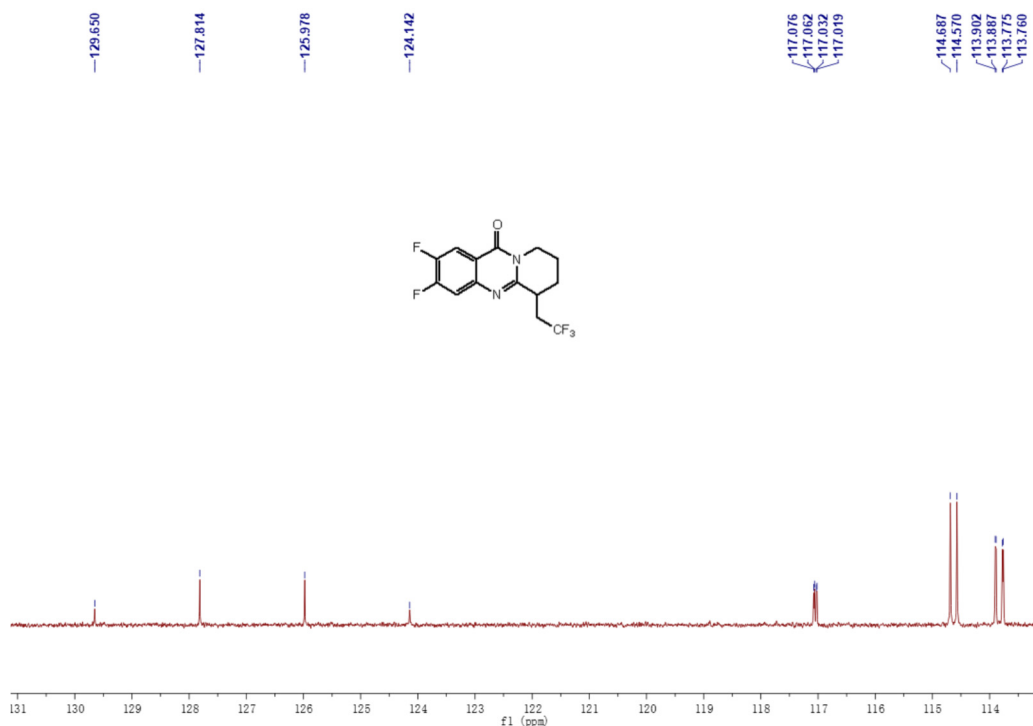


2,3-difluoro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-*b*]quinazolin-11-one (**3r**) : ¹H NMR (400 MHz, CDCl₃)

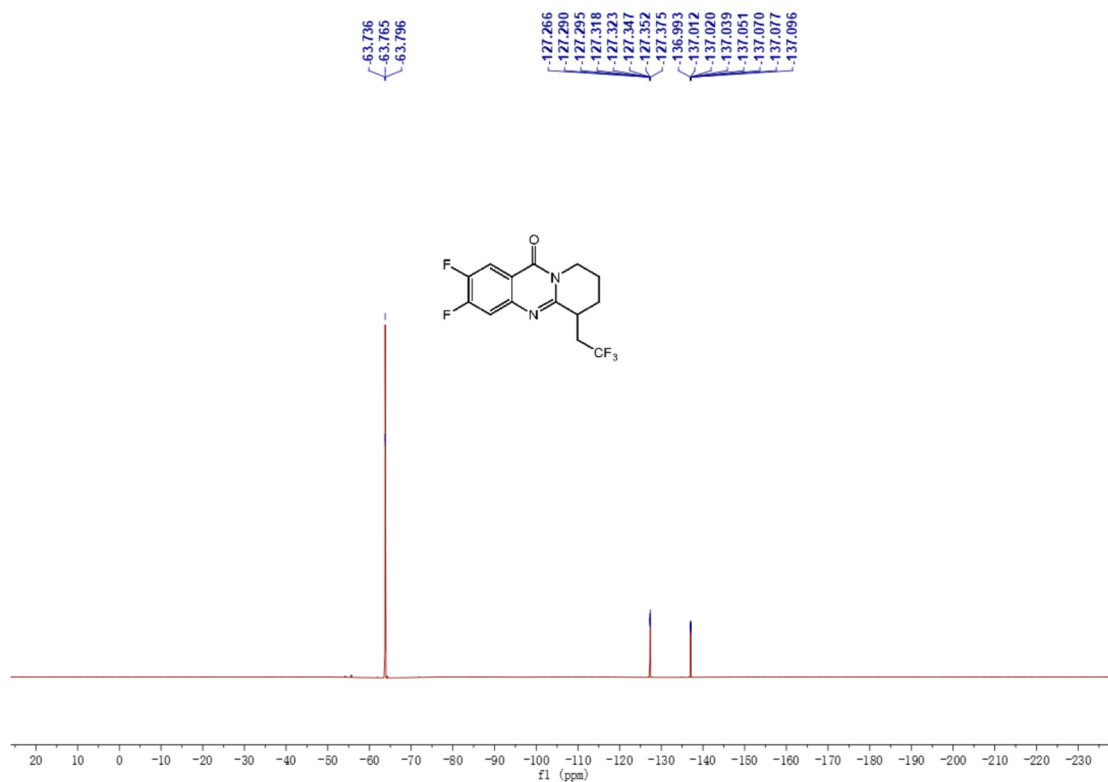


2,3-difluoro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-*b*]quinazolin-11-one (**3r**) : ¹³C NMR (150 MHz, CDCl₃)

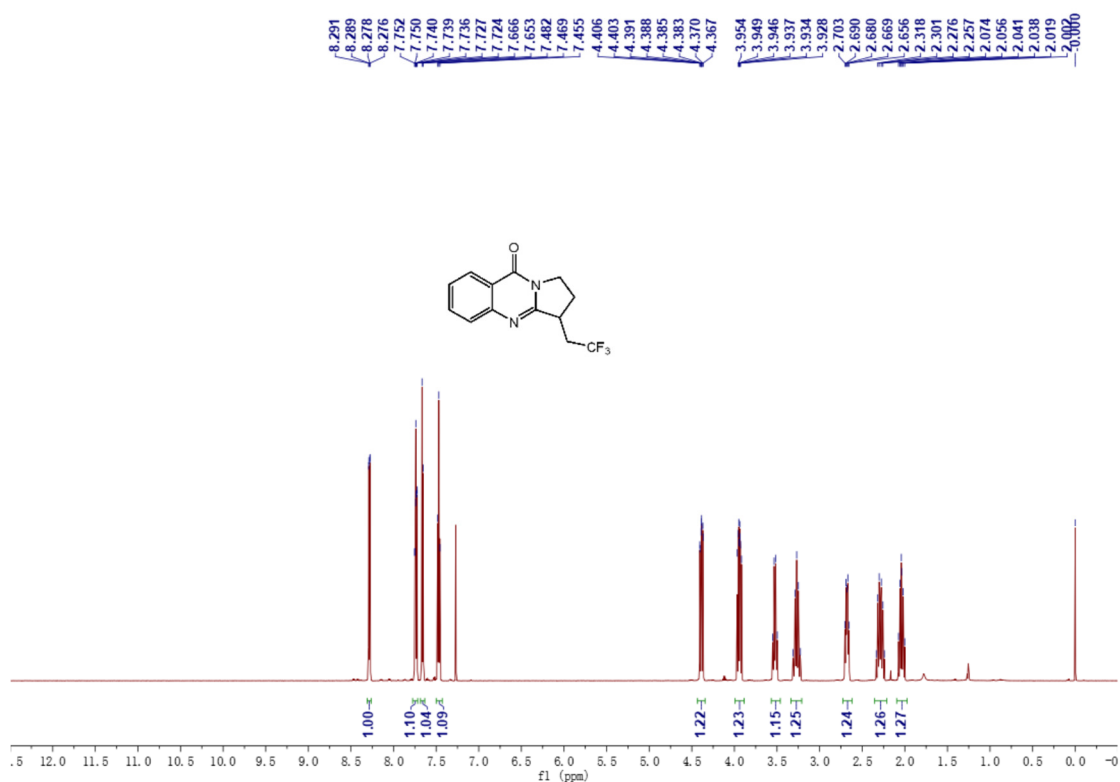




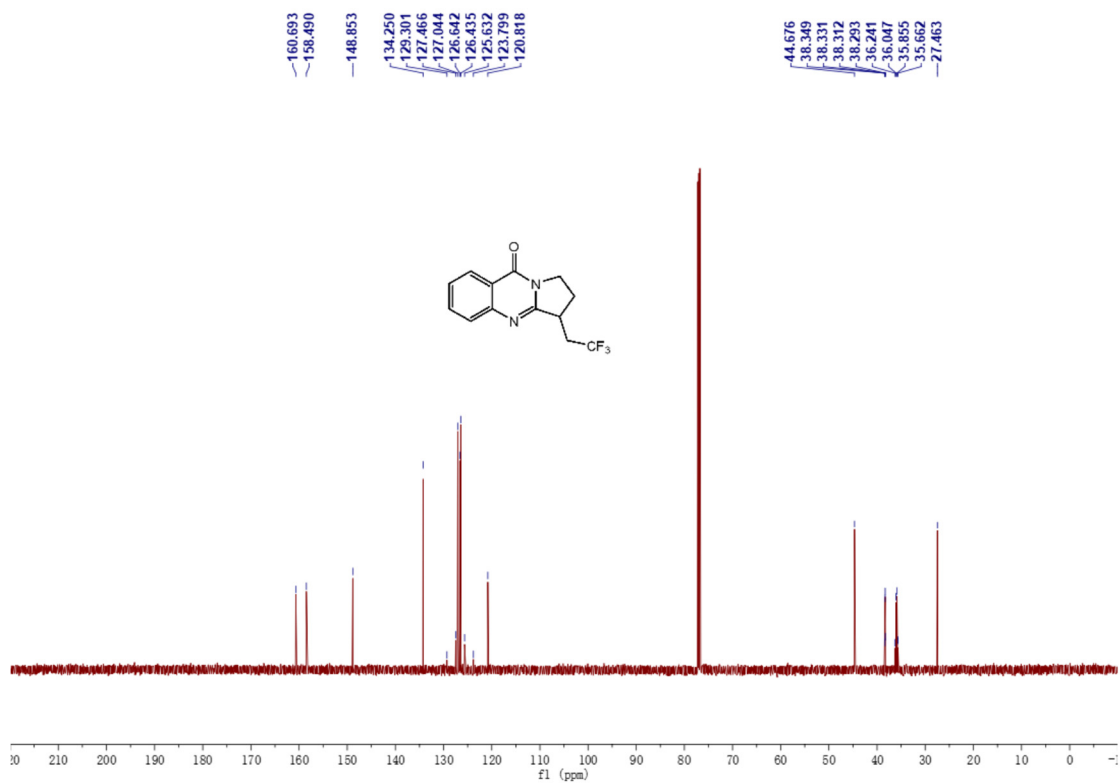
2,3-difluoro-6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-1H-pyrido[2,1-*b*]quinazolin-11-one (**3r**) : ¹⁹F NMR (376 MHz, CDCl₃)



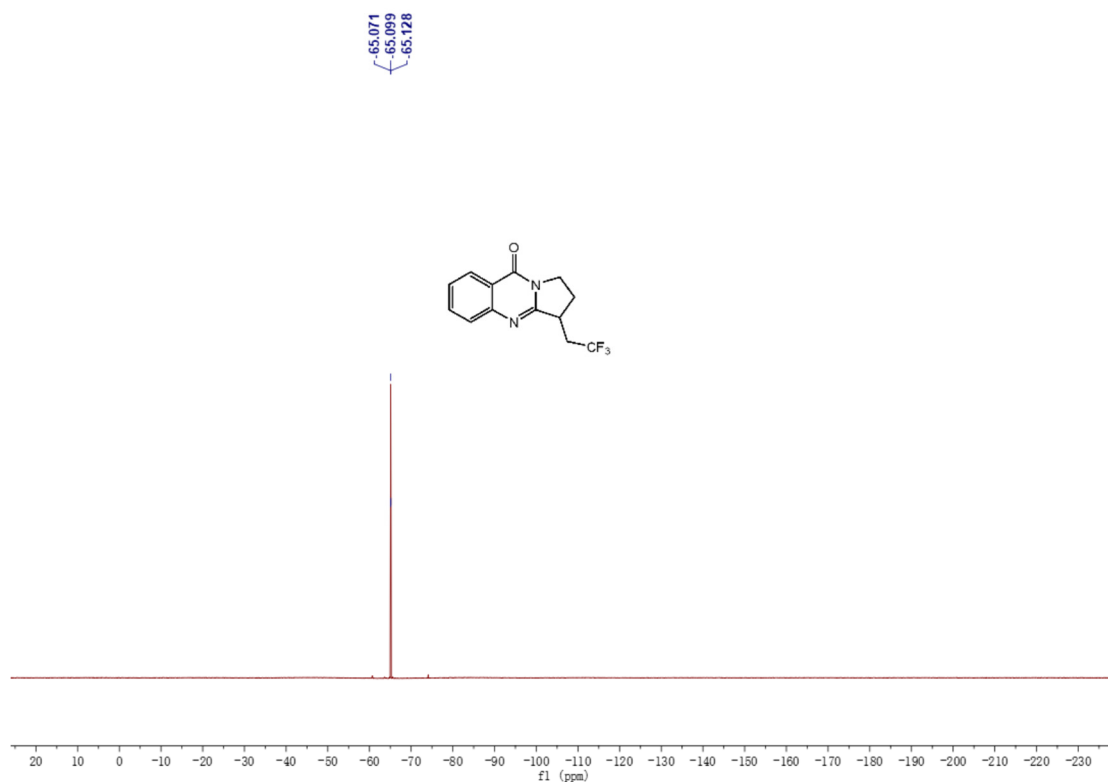
3-(2,2,2-trifluoroethyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1H)-one (**3s**) : ¹H NMR (400 MHz, CDCl₃)



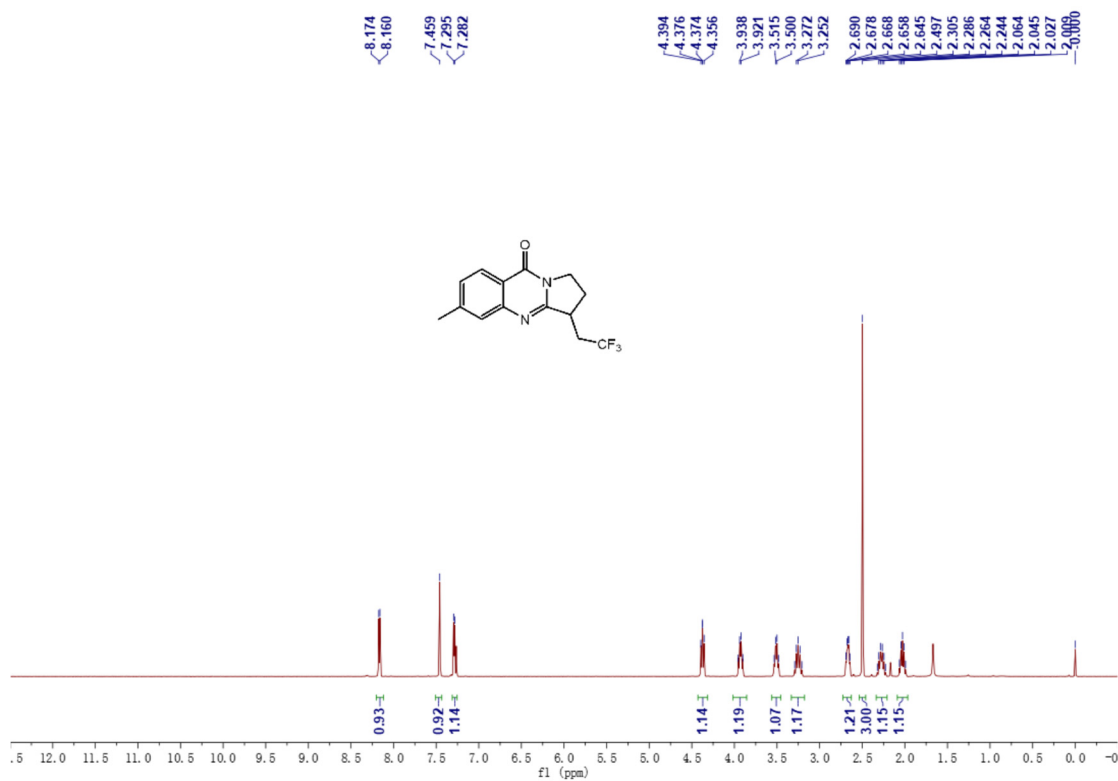
3-(2,2,2-trifluoroethyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1H)-one (**3s**) : ¹³C NMR (150 MHz, CDCl₃)



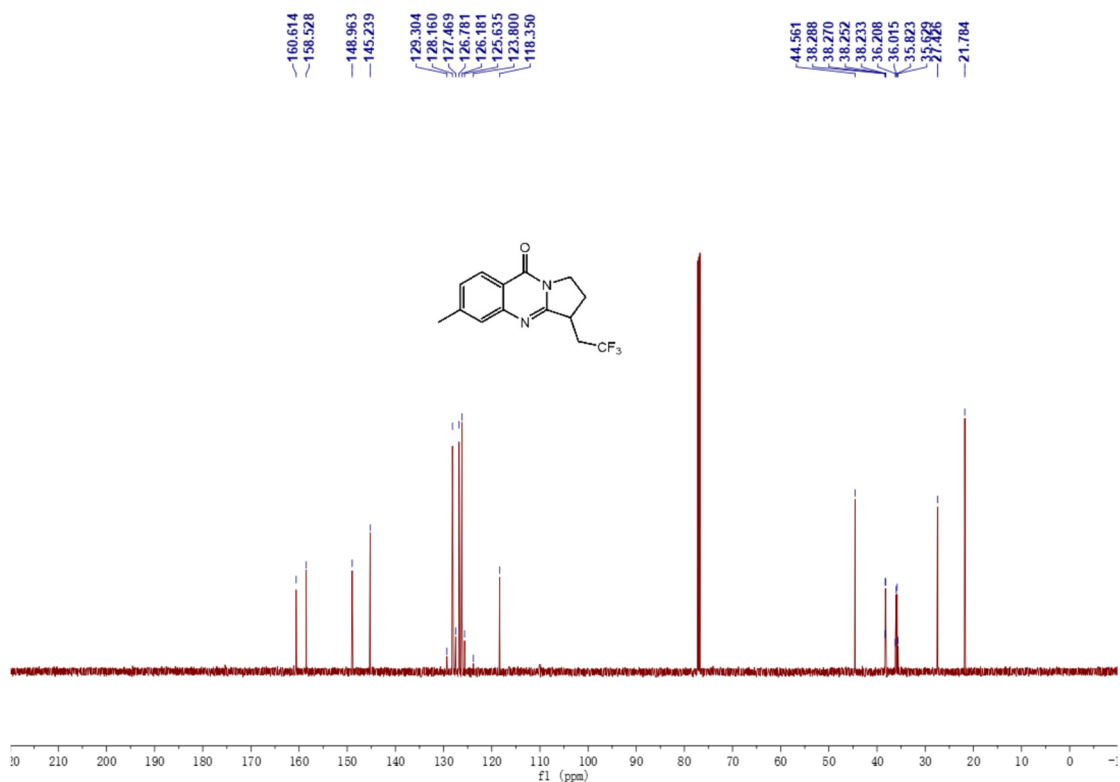
3-(2,2,2-trifluoroethyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1H)-one (**3s**) : ¹⁹F NMR (376 MHz, CDCl₃)



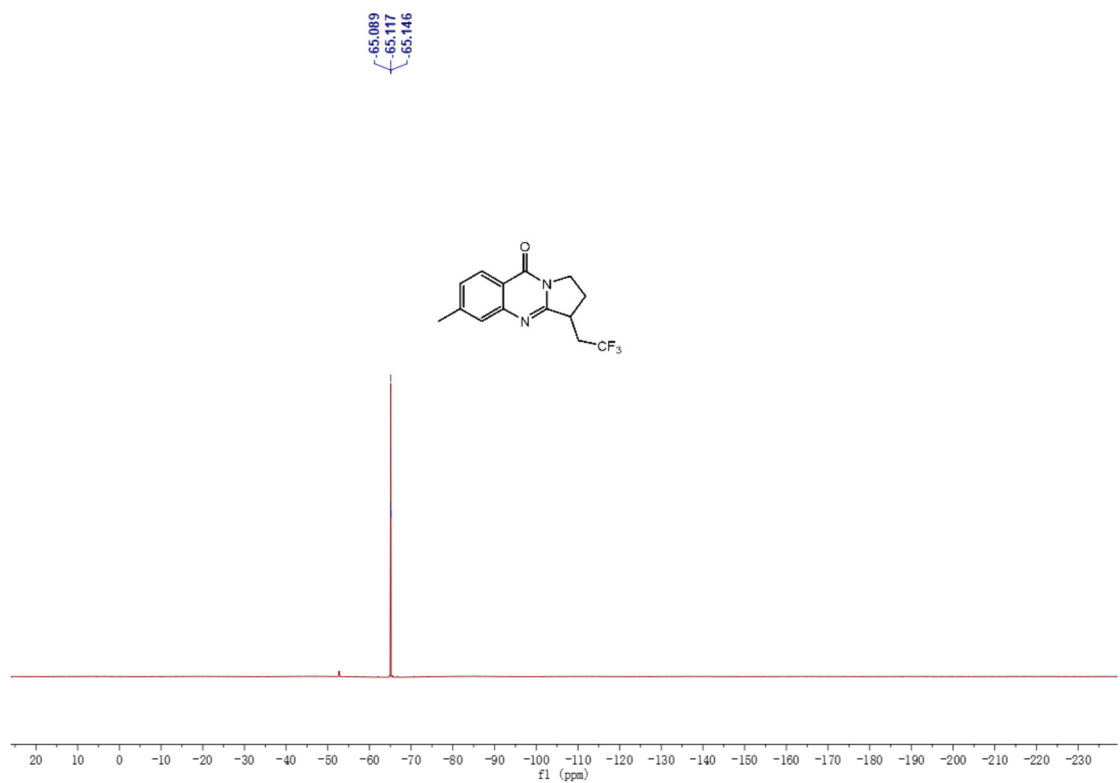
6-methyl-3-(2,2,2-trifluoroethyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1H)-one
(**3t**) : ^1H NMR (600 MHz, CDCl_3)



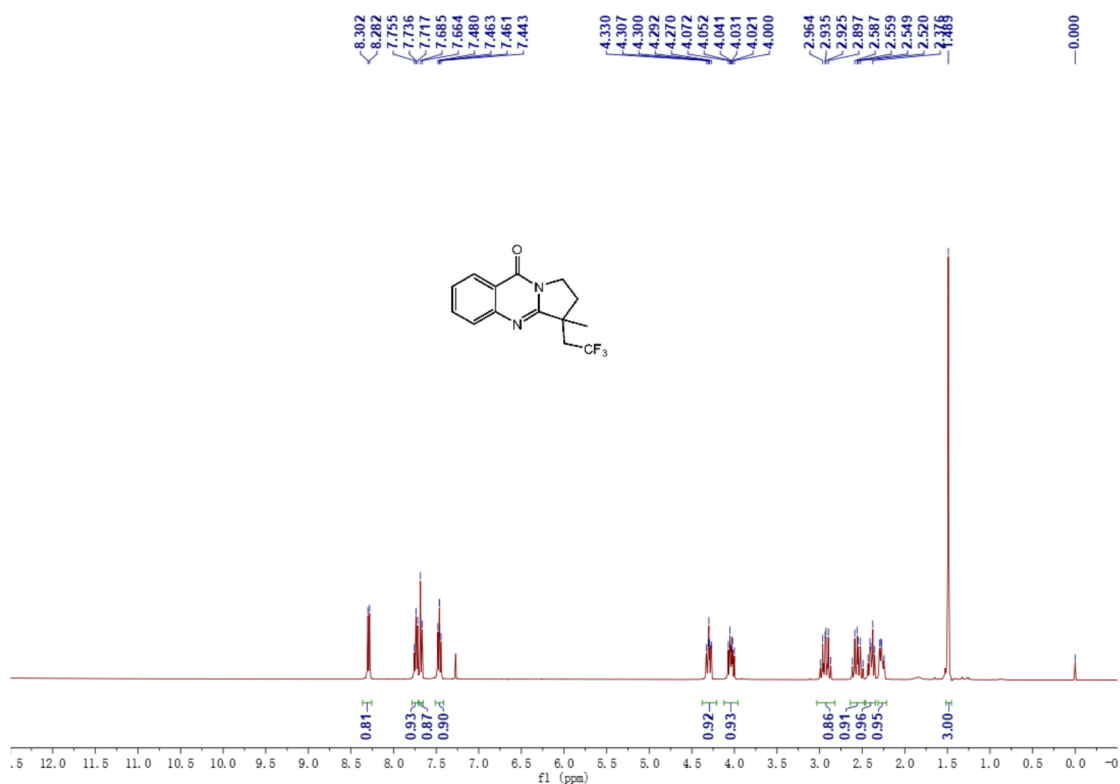
6-methyl-3-(2,2,2-trifluoroethyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1H)-one
(**3t**) : ^{13}C NMR (150 MHz, CDCl_3)



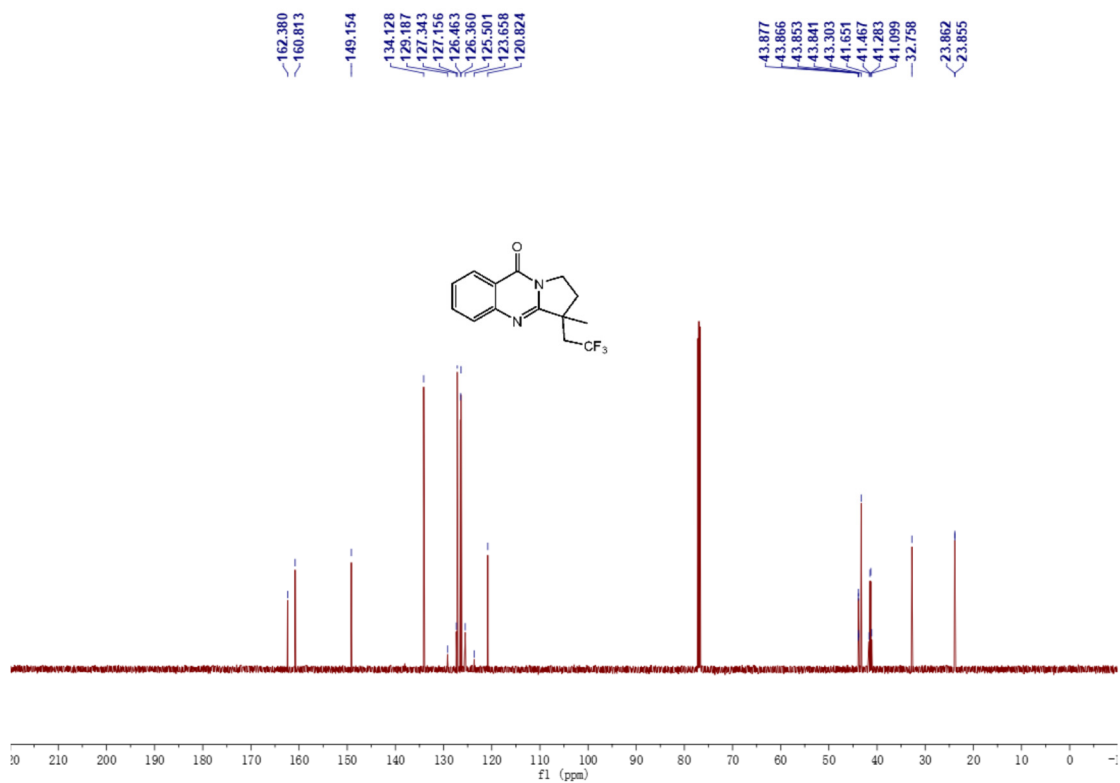
6-methyl-3-(2,2,2-trifluoroethyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1H)-one (**3t**) : ¹⁹F NMR (376 MHz, CDCl₃)



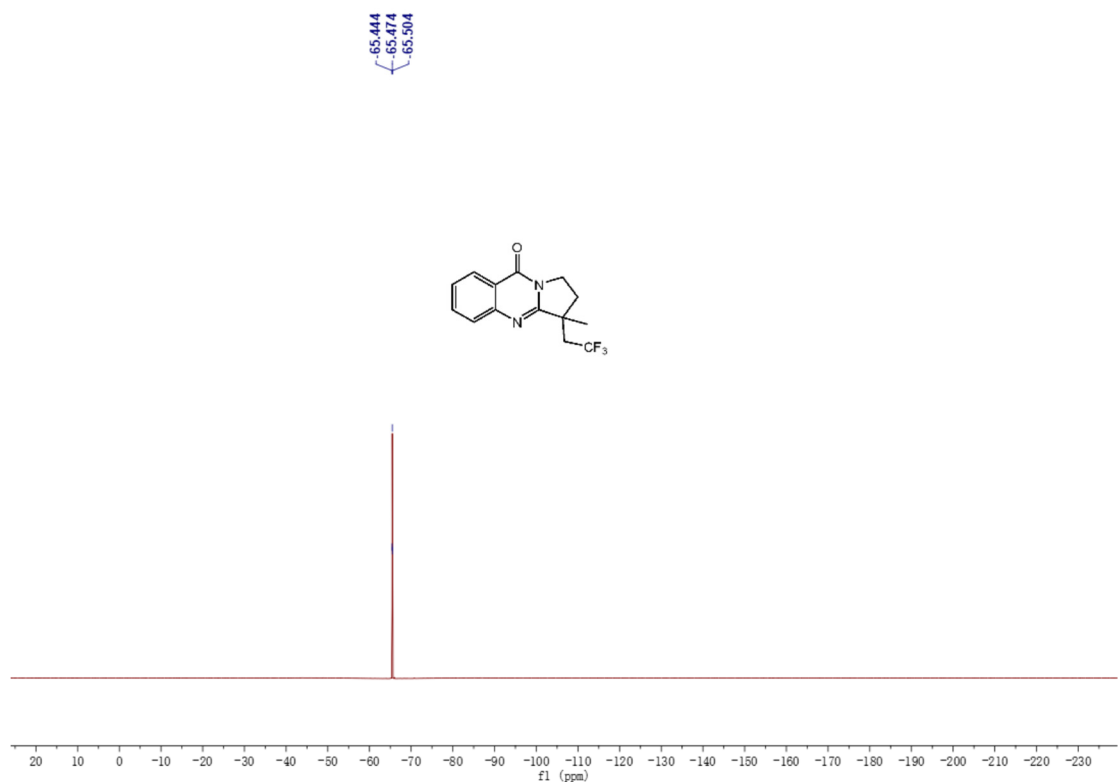
3-methyl-3-(2,2,2-trifluoroethyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1H)-one (**3u**) : ¹H NMR (400 MHz, CDCl₃)



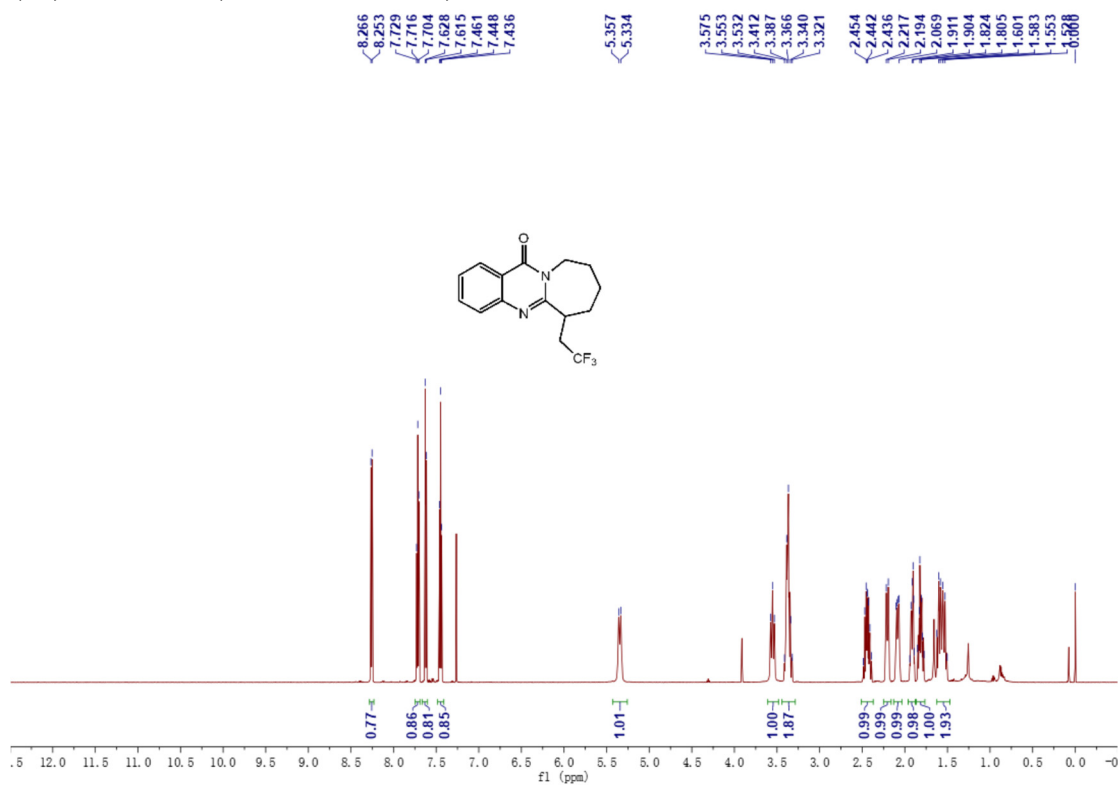
3-methyl-3-(2,2,2-trifluoroethyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1H)-one (**3u**) : ¹³C NMR (150 MHz, CDCl₃)



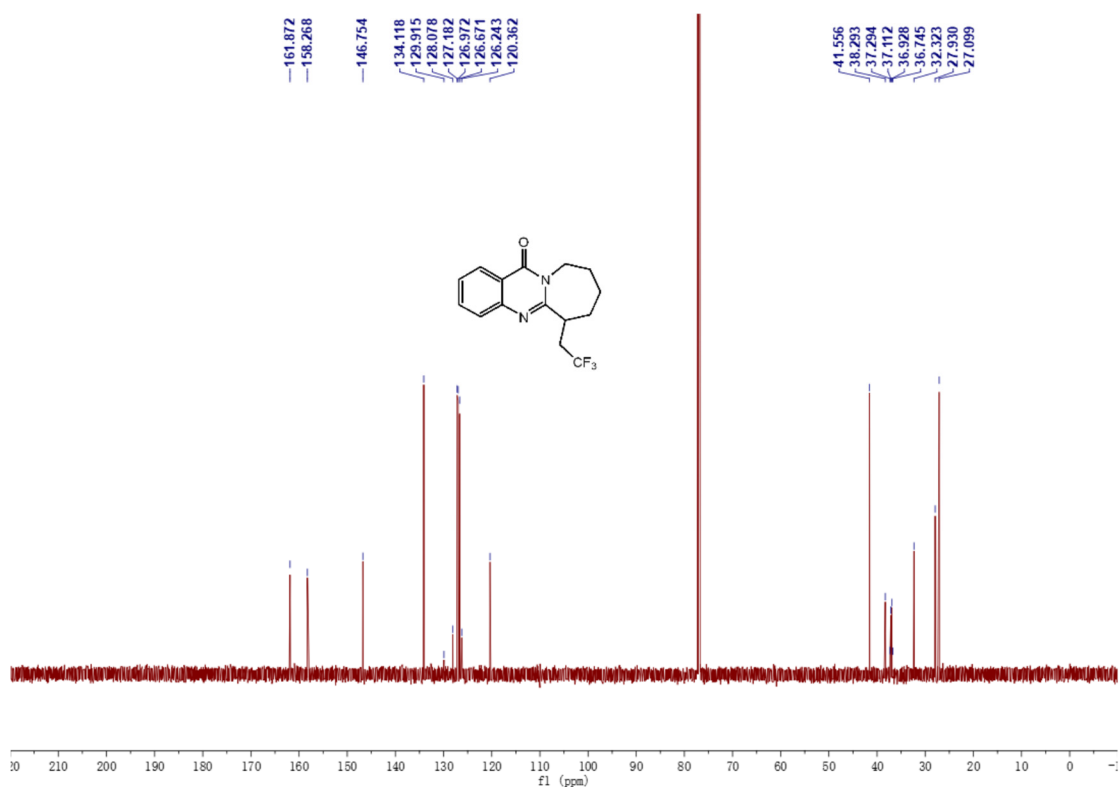
3-methyl-3-(2,2,2-trifluoroethyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1H)-one (**3u**) : ¹⁹F NMR (376 MHz, CDCl₃)



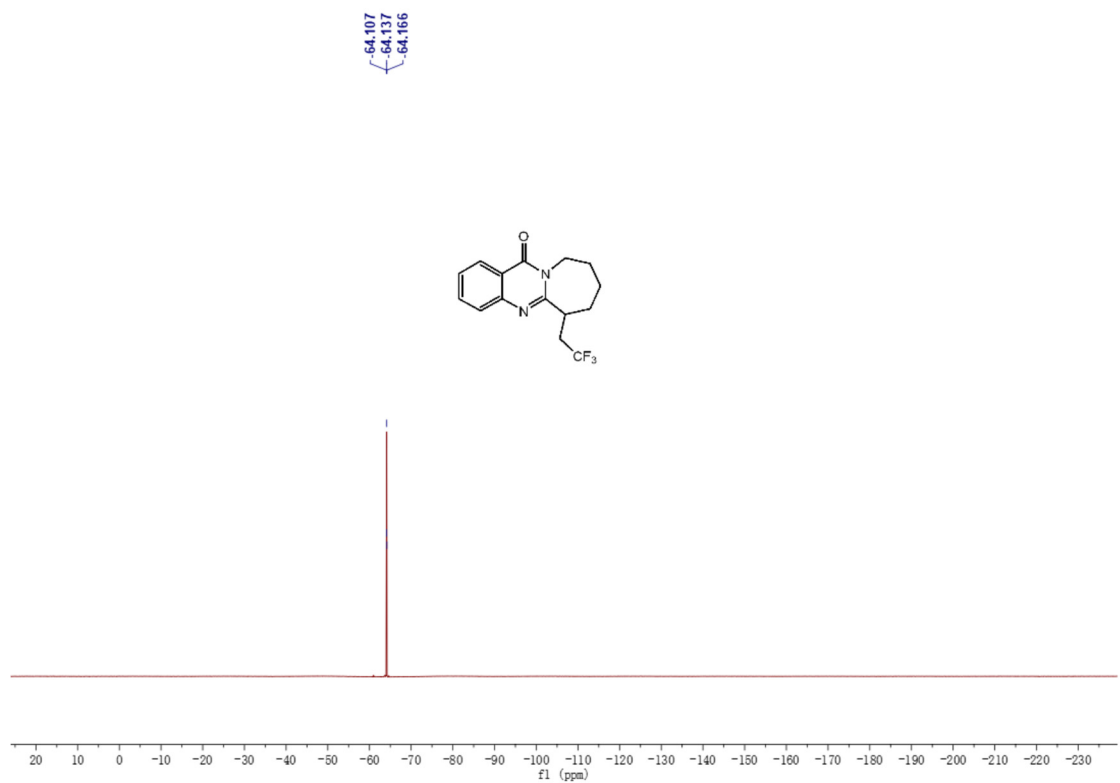
6-(2,2,2-trifluoroethyl)-7,8,9,10-tetrahydroazepino[2,1-*b*]quinazolin-12(6H)-one (**3v**) : ^1H NMR (400 MHz, CDCl_3)



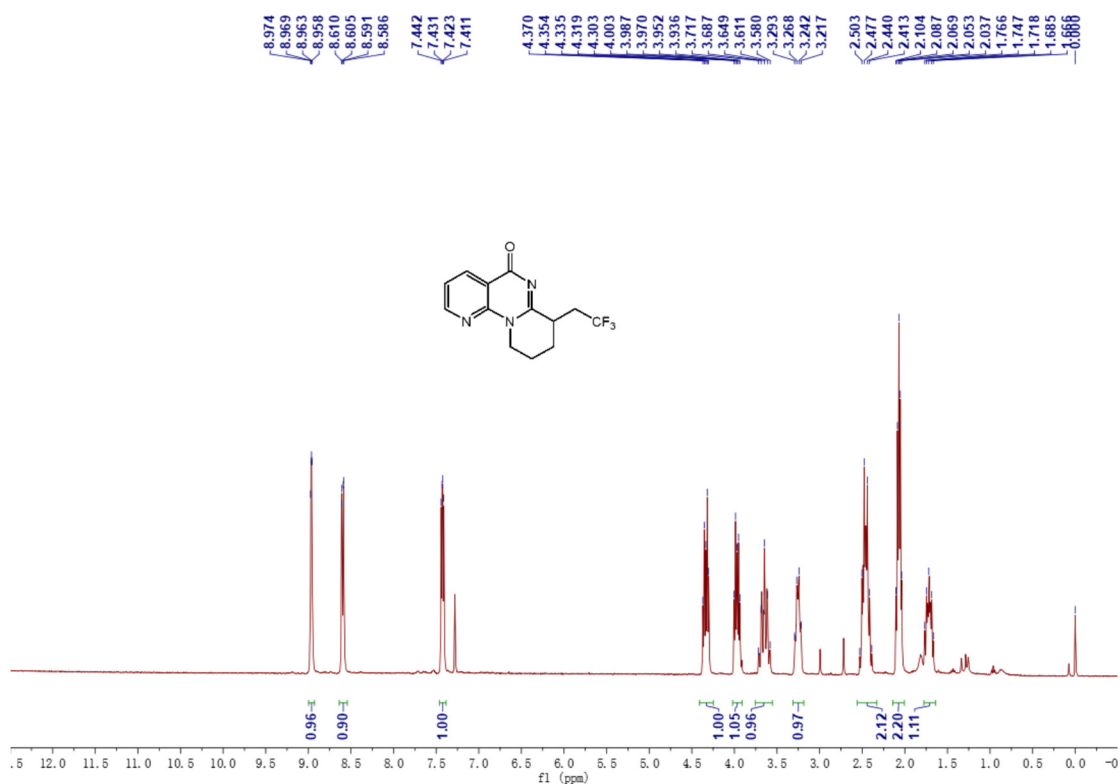
6-(2,2,2-trifluoroethyl)-7,8,9,10-tetrahydroazepino[2,1-*b*]quinazolin-12(6H)-one (**3v**) : ^{13}C NMR (150 MHz, CDCl_3)



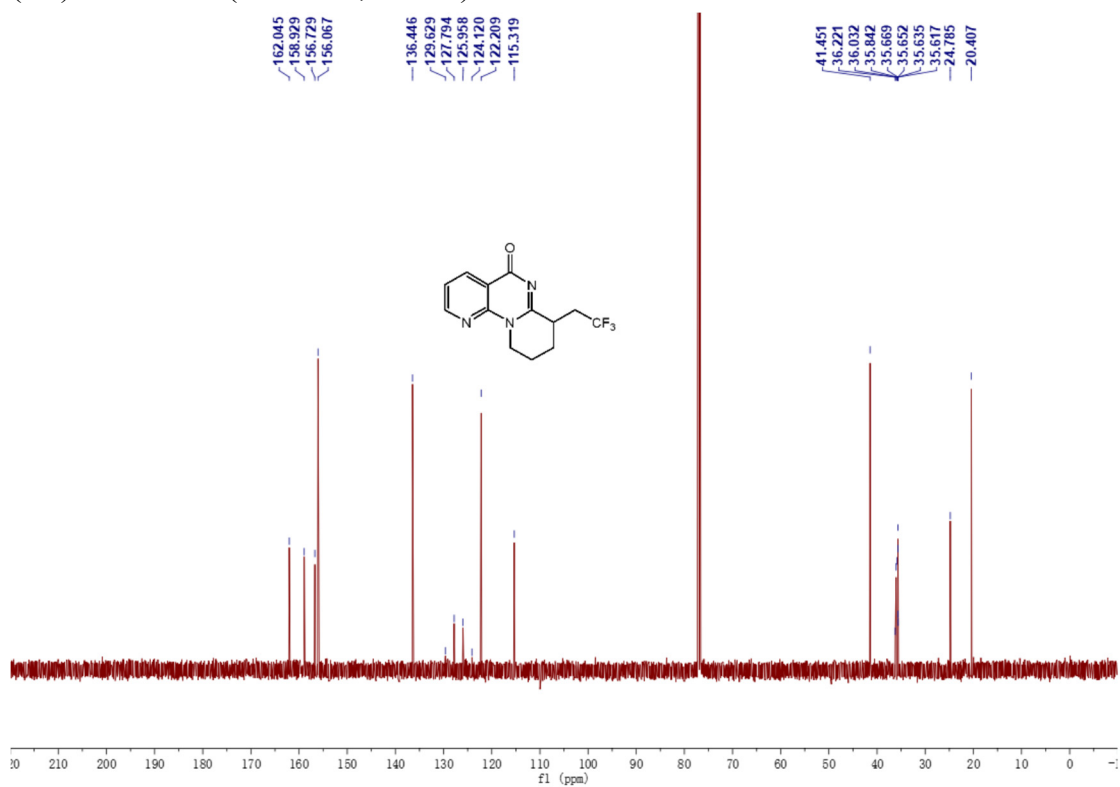
6-(2,2,2-trifluoroethyl)-7,8,9,10-tetrahydroazepino[2,1-*b*]quinazolin-12(6H)-one (**3v**) : ¹⁹F NMR (376 MHz, CDCl₃)



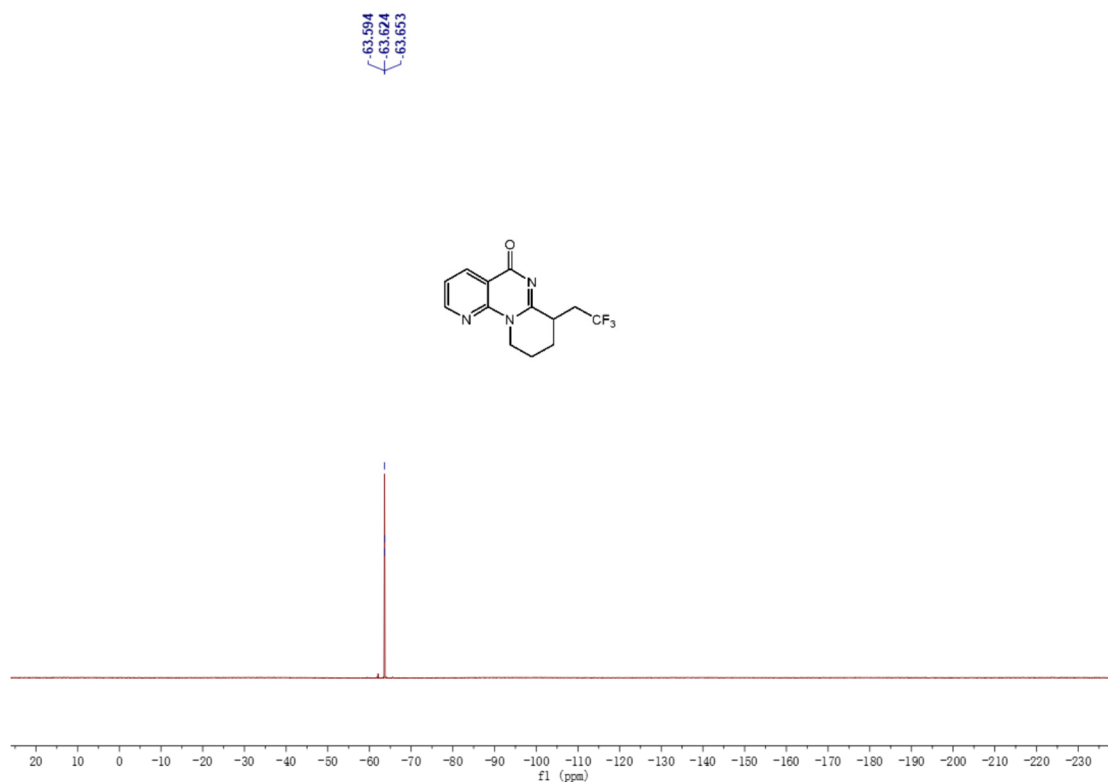
7-(2,2,2-trifluoroethyl)-7,8,9,10-tetrahydro-5H-dipyrido[1,2-*a*:3',2'-*e*]pyrimidin-5-one (**3w**) : ¹H NMR (400 MHz, CDCl₃)



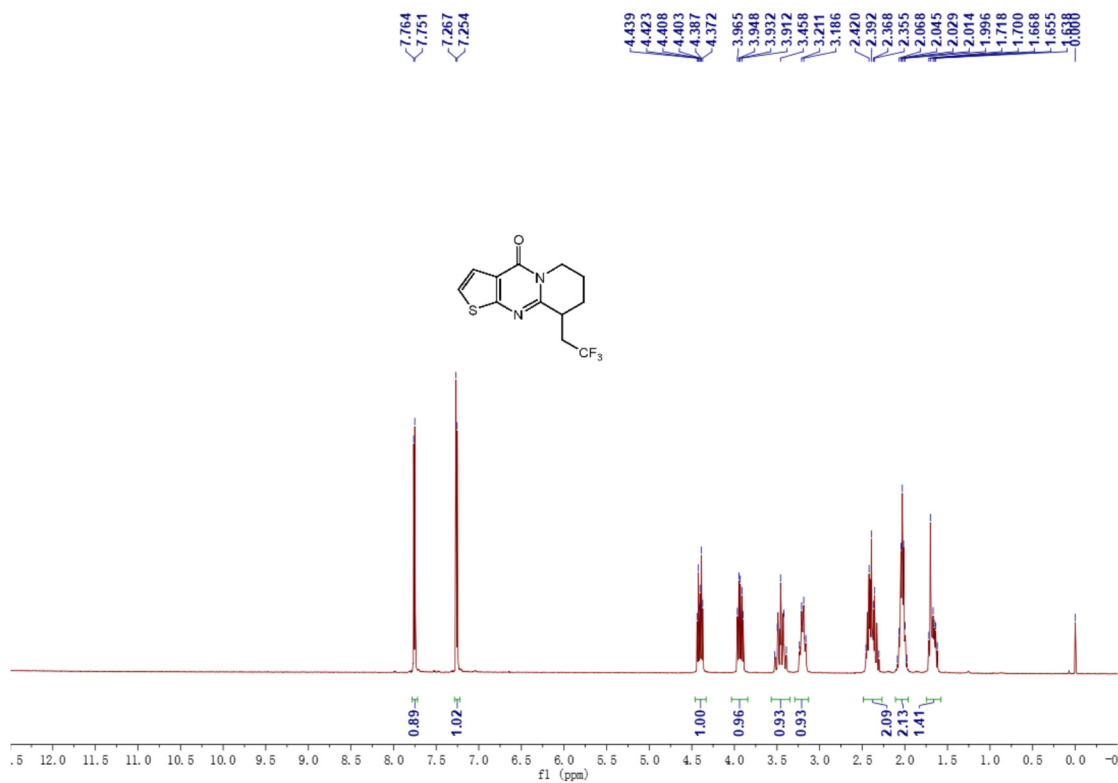
7-(2,2,2-trifluoroethyl)-7,8,9,10-tetrahydro-5H-dipyrido[1,2-*a*:3',2'-*e*]pyrimidin-5-one (**3w**) : ¹³C NMR (150 MHz, CDCl₃)



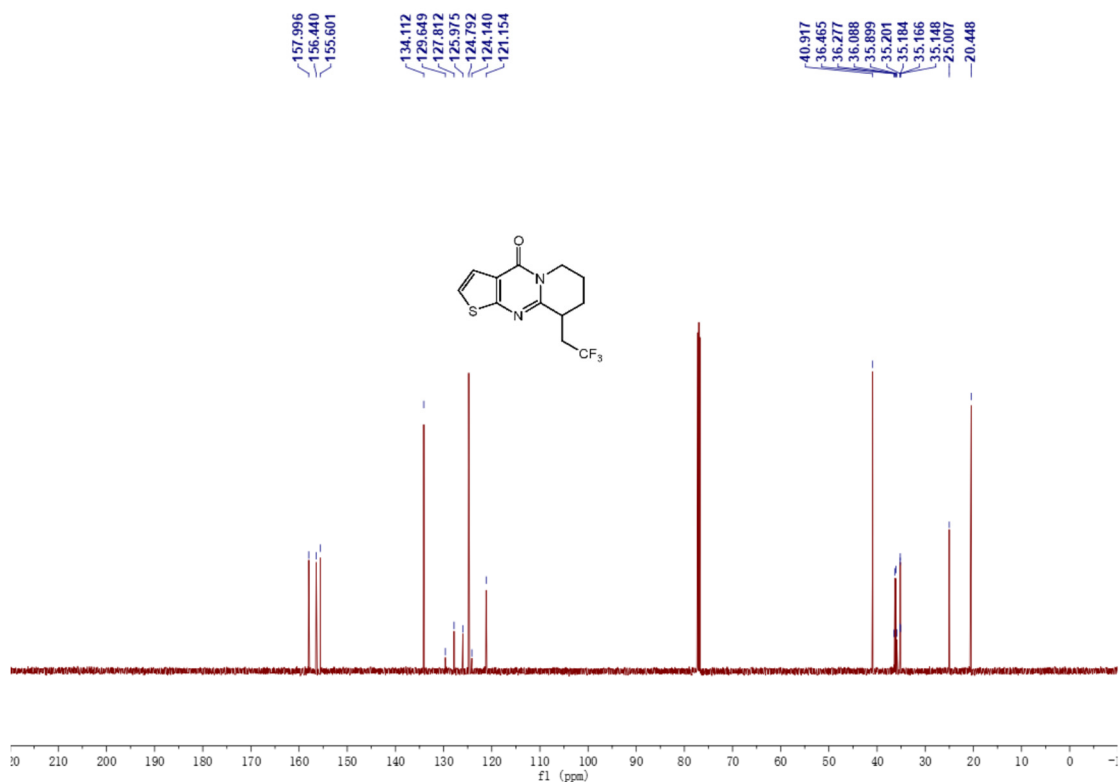
7-(2,2,2-trifluoroethyl)-7,8,9,10-tetrahydro-5H-dipyrido[1,2-*a*:3',2'-*e*]pyrimidin-5-one (**3w**) : ¹⁹F NMR (376 MHz, CDCl₃)



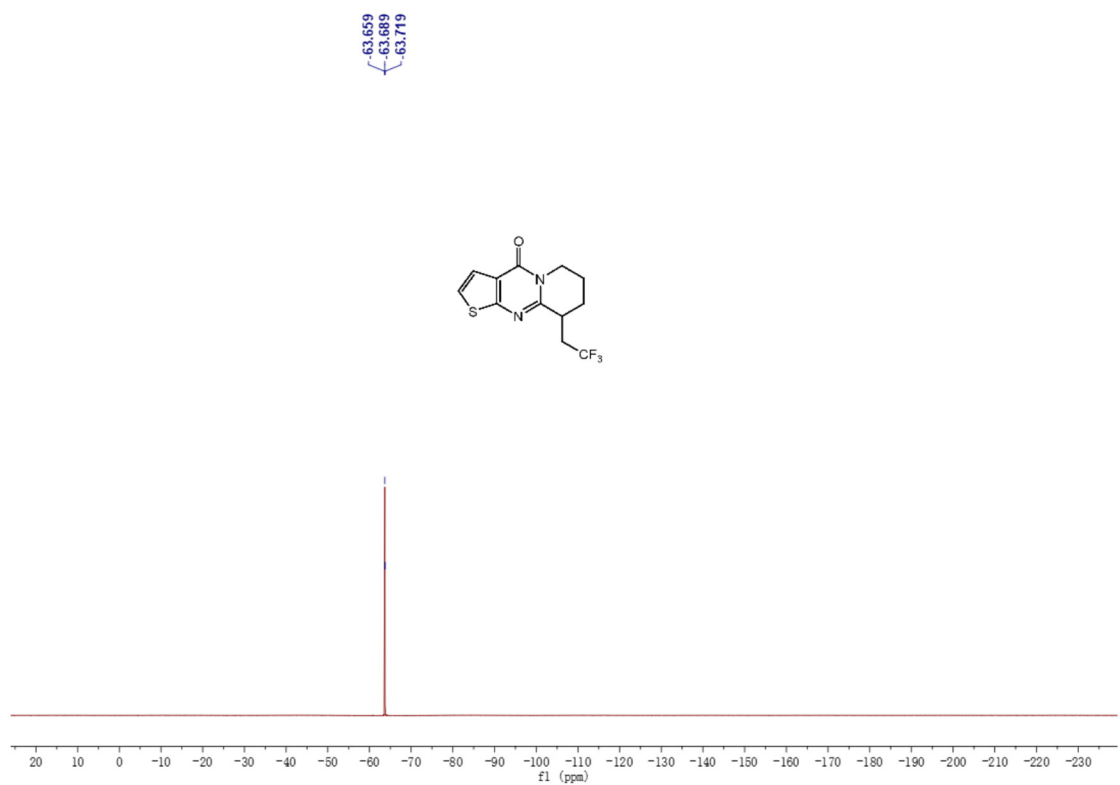
9-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-4H-pyrido[1,2-a]thieno[2,3-d]pyrimidin-4-one (**3x**) : ^1H NMR (400 MHz, CDCl_3)



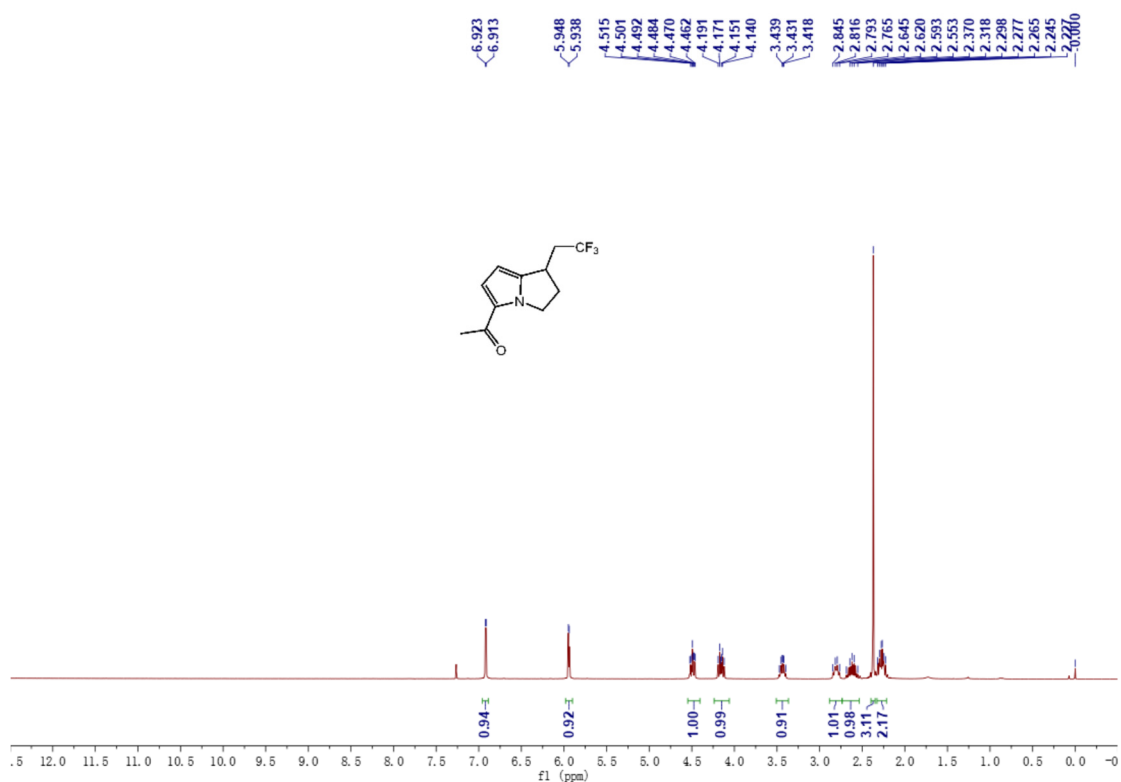
9-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-4H-pyrido[1,2-a]thieno[2,3-d]pyrimidin-4-one (**3x**) : ^{13}C NMR (150 MHz, CDCl_3)



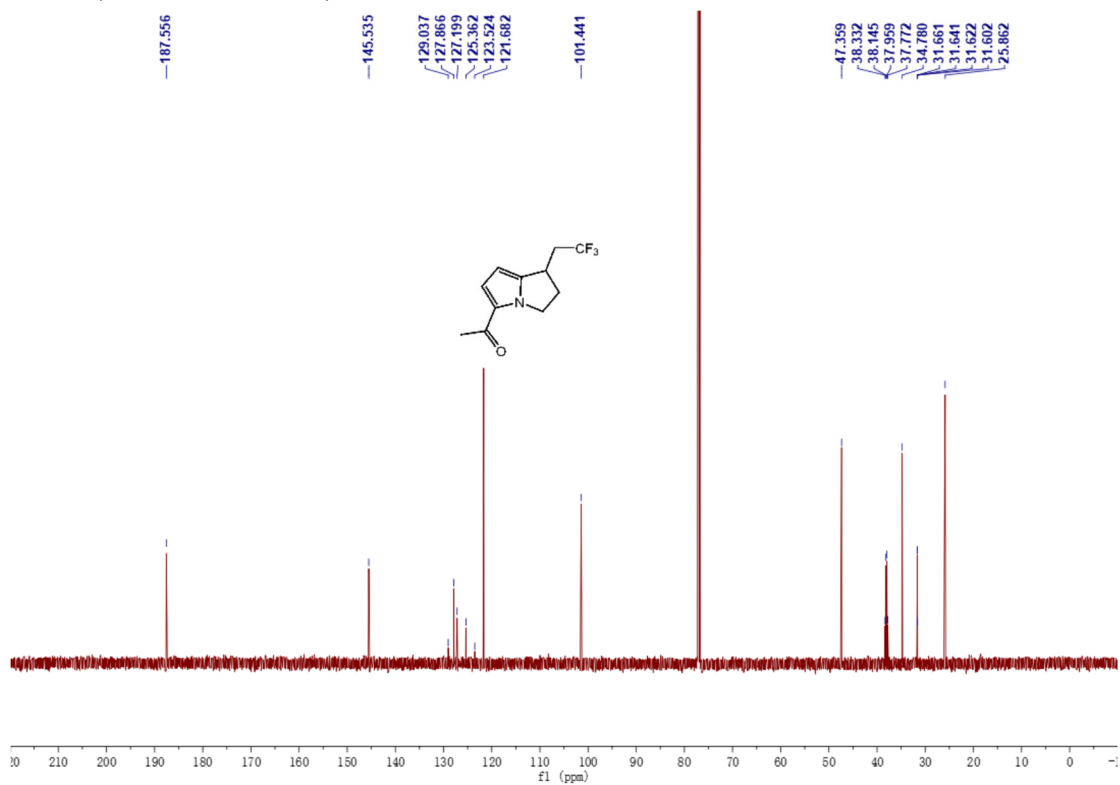
9-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydro-4H-pyrido[1,2-*a*]thieno[2,3-*d*]pyrimidin-4-one (**3x**) : ¹⁹F NMR (376 MHz, CDCl₃)



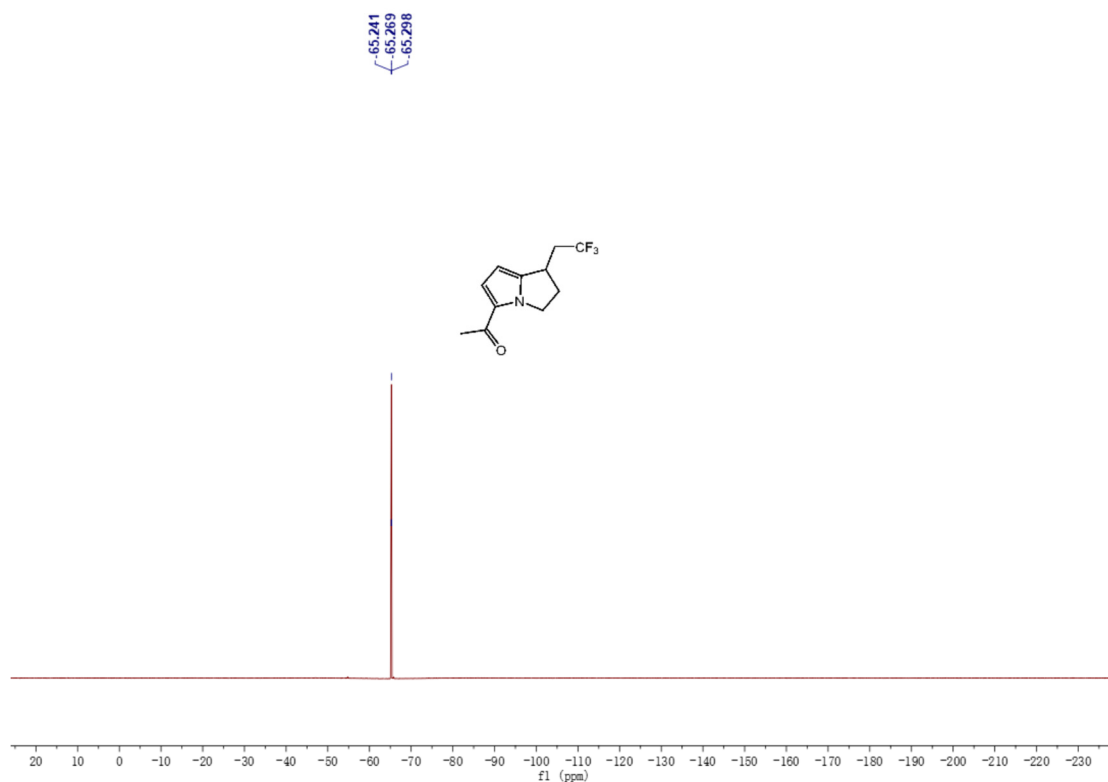
1-(1-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-pyrrolizin-5-yl)ethan-1-one (**5a**) : ¹H NMR (400 MHz, CDCl₃)



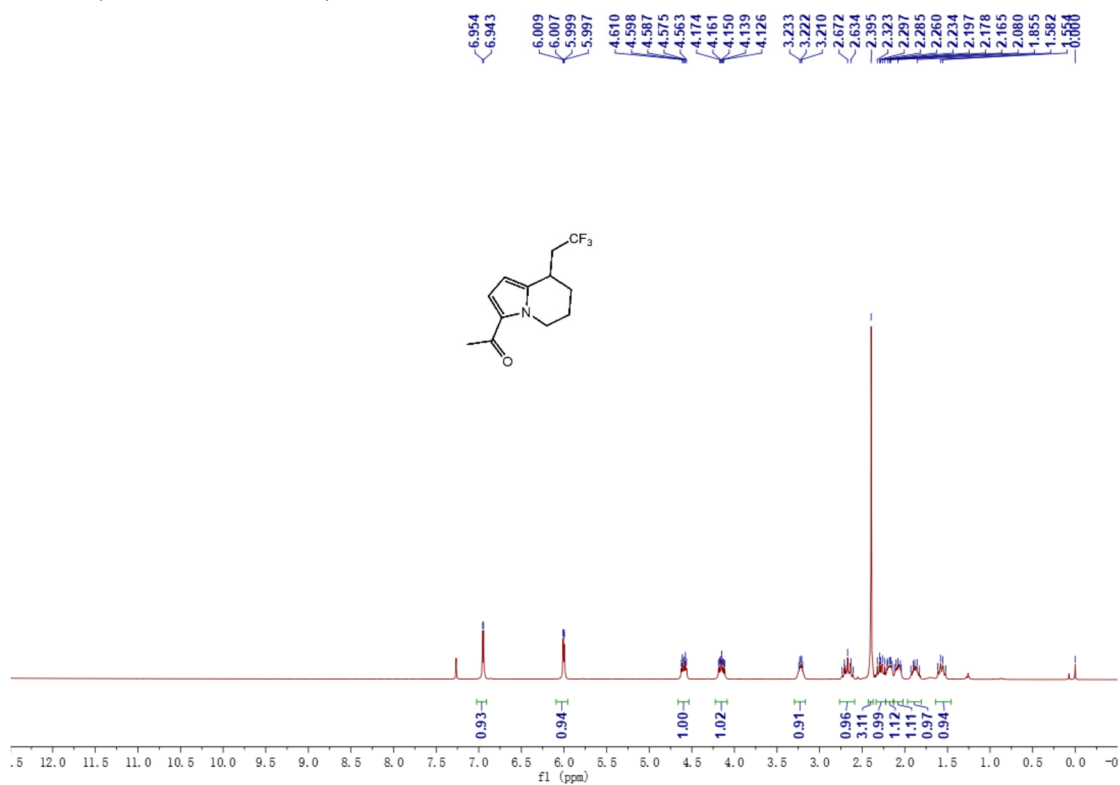
1-(1-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-pyrrolizin-5-yl)ethan-1-one (**5a**) : ¹³C
NMR (150 MHz, CDCl₃)



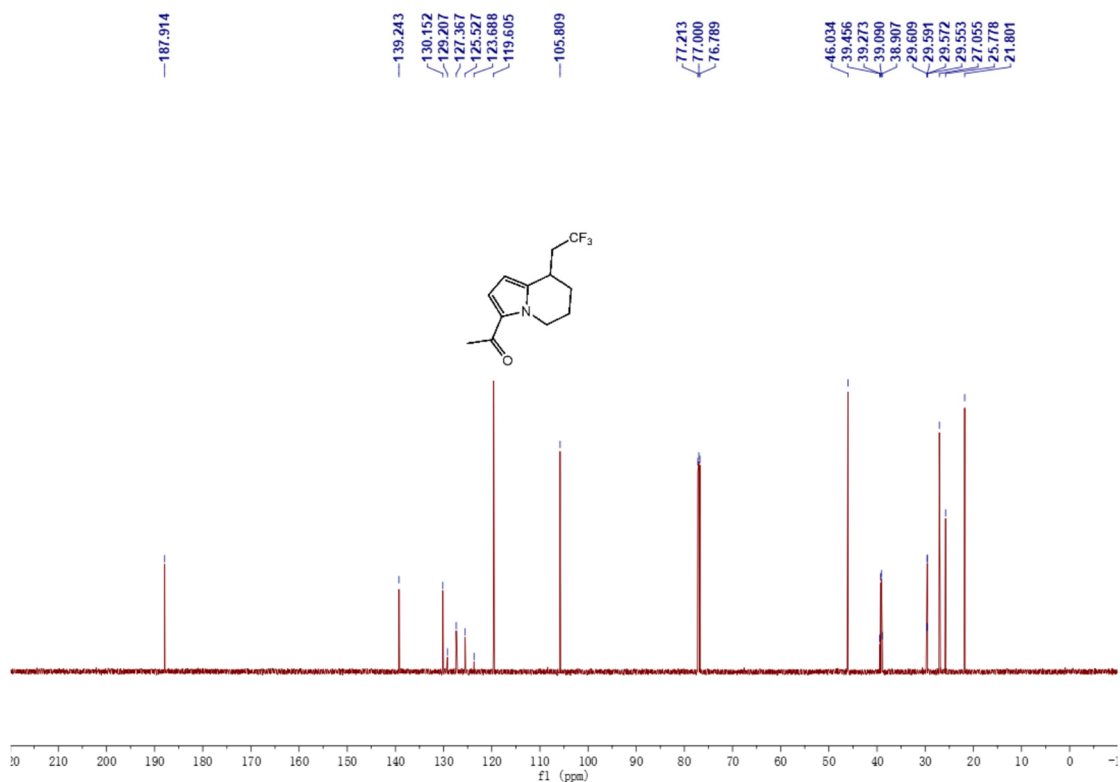
1-(1-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-pyrrolizin-5-yl)ethan-1-one (**5a**) : ¹⁹F
NMR (376 MHz, CDCl₃)



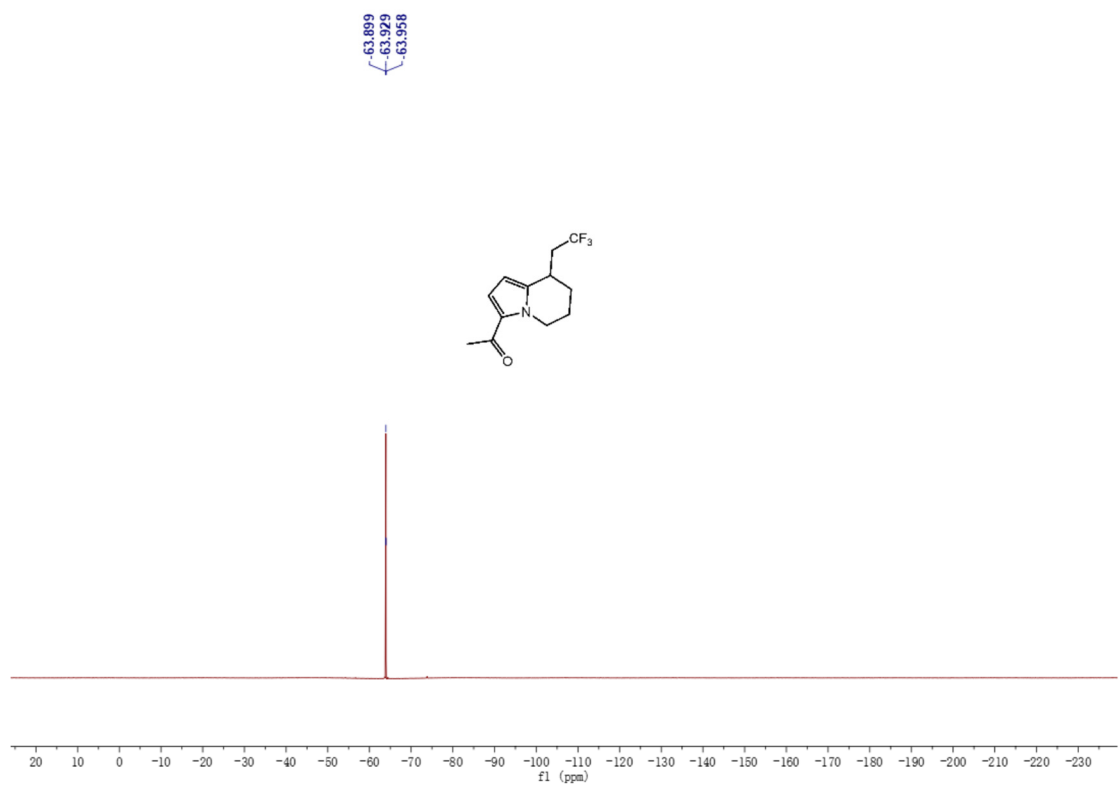
1-(8-(2,2,2-trifluoroethyl)-5,6,7,8-tetrahydroindolizin-3-yl)ethan-1-one (**5b**) : ¹H
NMR (400 MHz, CDCl₃)



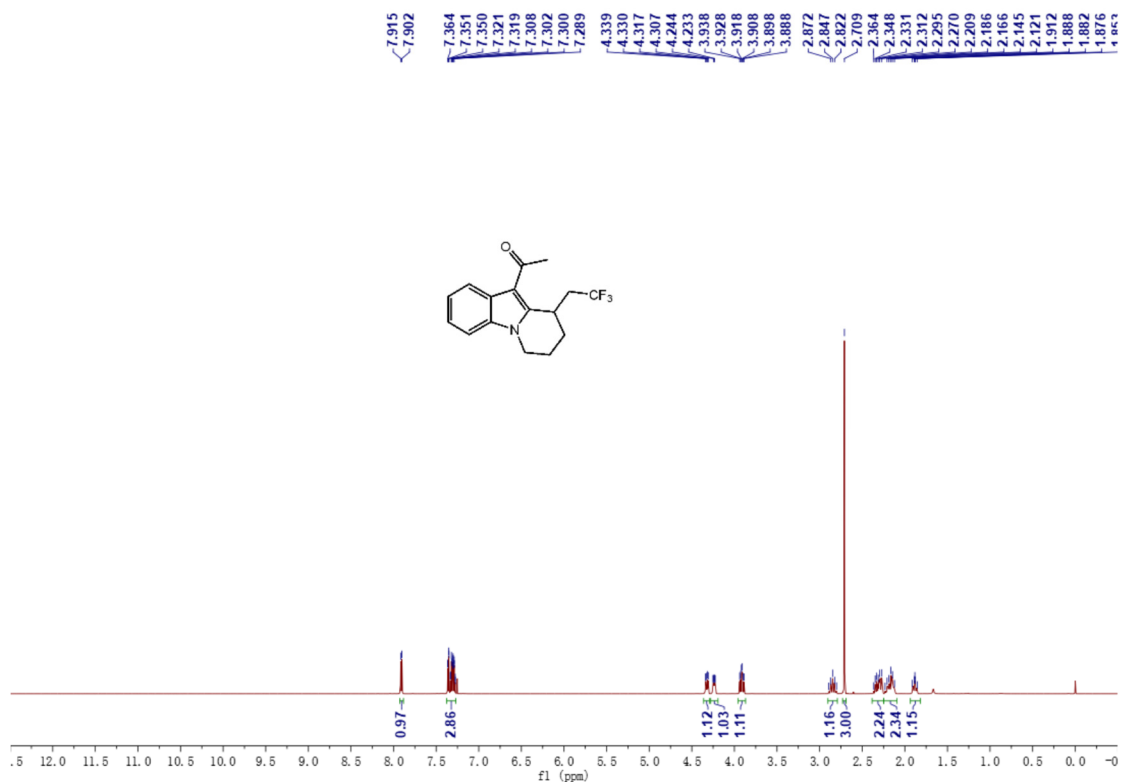
1-(8-(2,2,2-trifluoroethyl)-5,6,7,8-tetrahydroindolizin-3-yl)ethan-1-one (**5b**) : ¹³C
NMR (150 MHz, CDCl₃)



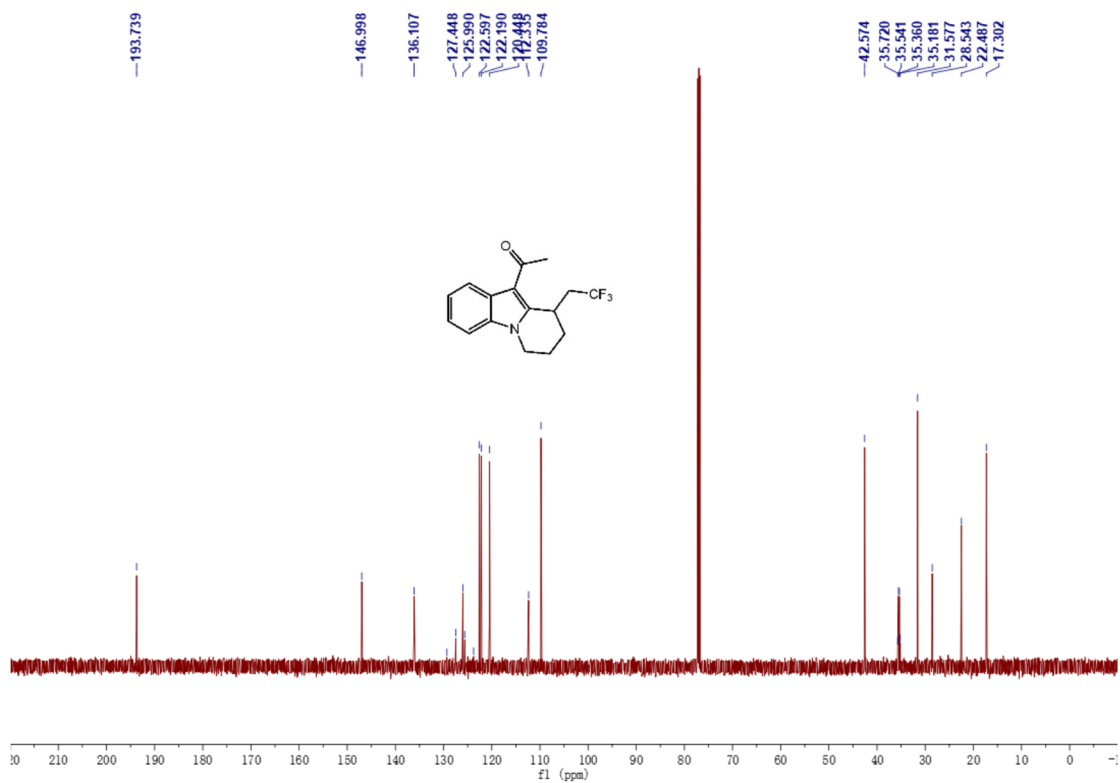
1-(8-(2,2,2-trifluoroethyl)-5,6,7,8-tetrahydroindolizin-3-yl)ethan-1-one (**5b**) : ¹⁹F
NMR (376 MHz, CDCl₃)



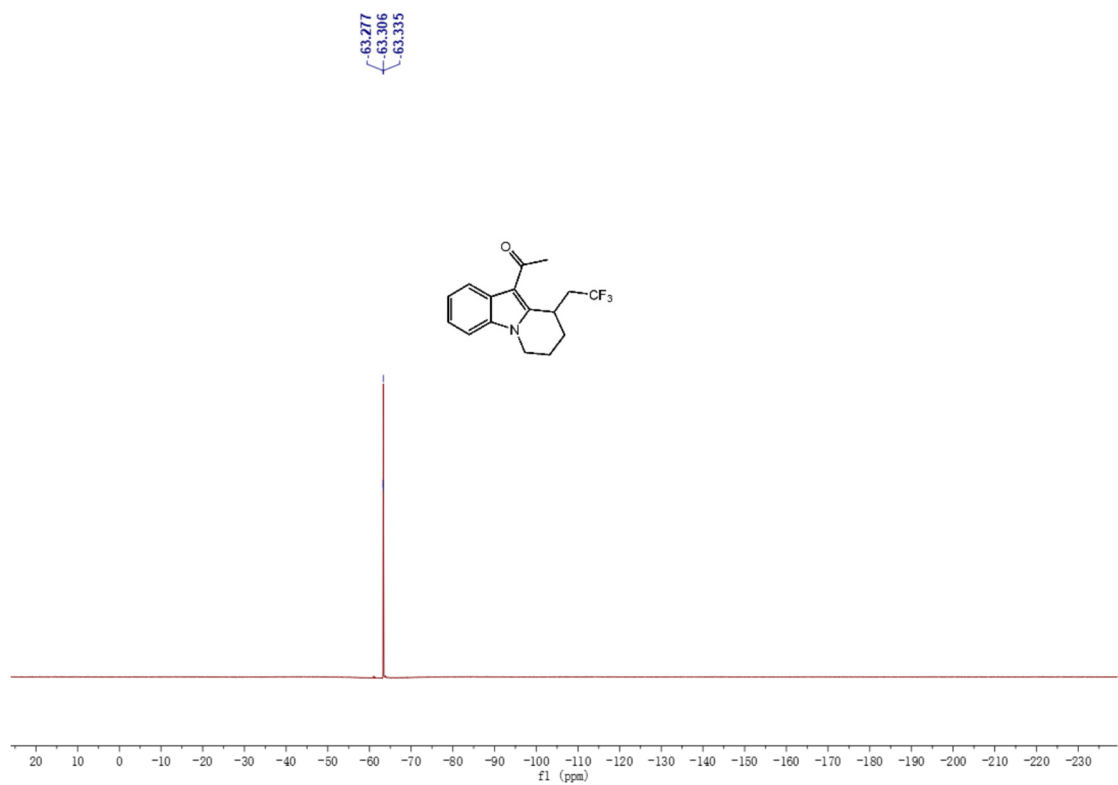
1-(9-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydropyrido[1,2-*a*]indol-10-yl)ethan-1-one (**5e**) : ¹H NMR (400 MHz, CDCl₃)



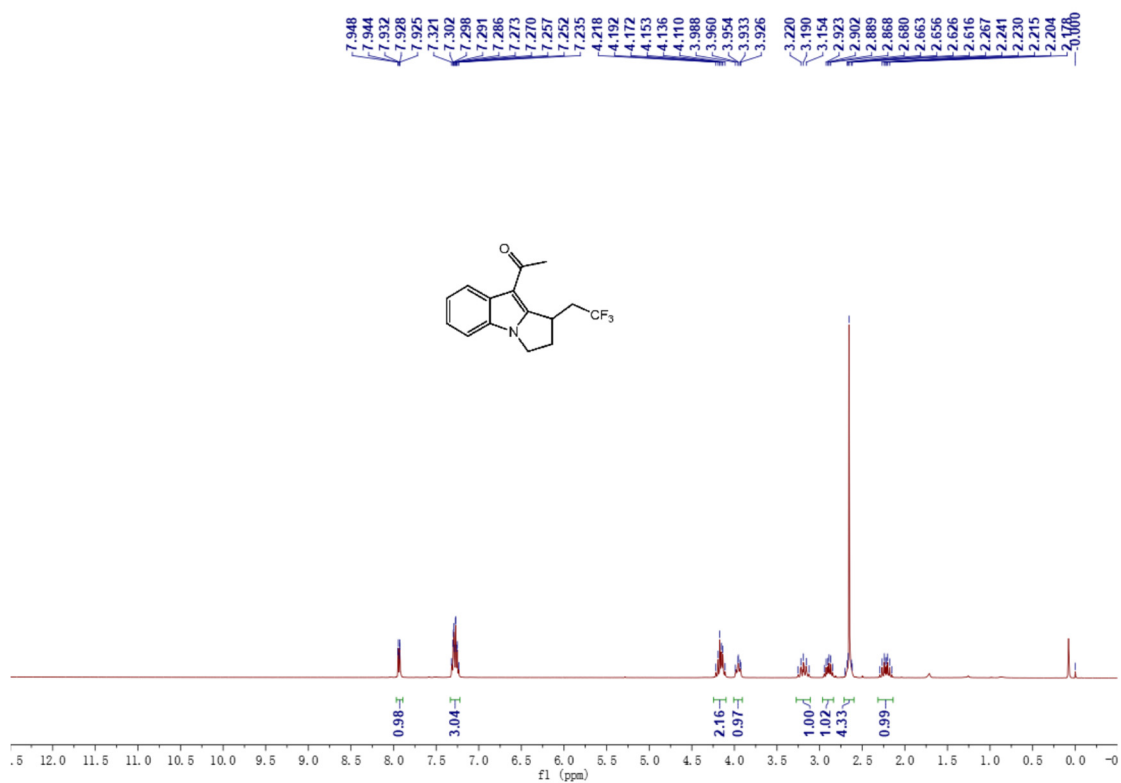
1-(9-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydropyrido[1,2-*a*]indol-10-yl)ethan-1-one (5e) : ¹³C NMR (150 MHz, CDCl₃)



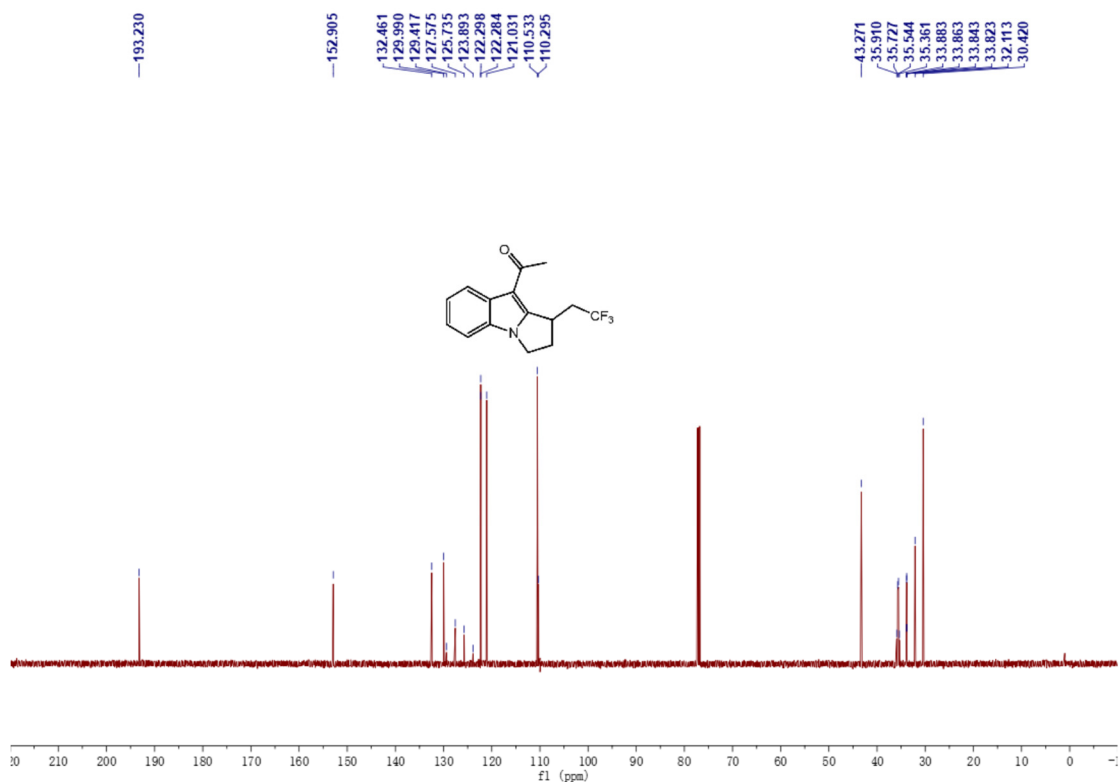
1-(9-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydropyrido[1,2-*a*]indol-10-yl)ethan-1-one (5e) : ¹⁹F NMR (376 MHz, CDCl₃)



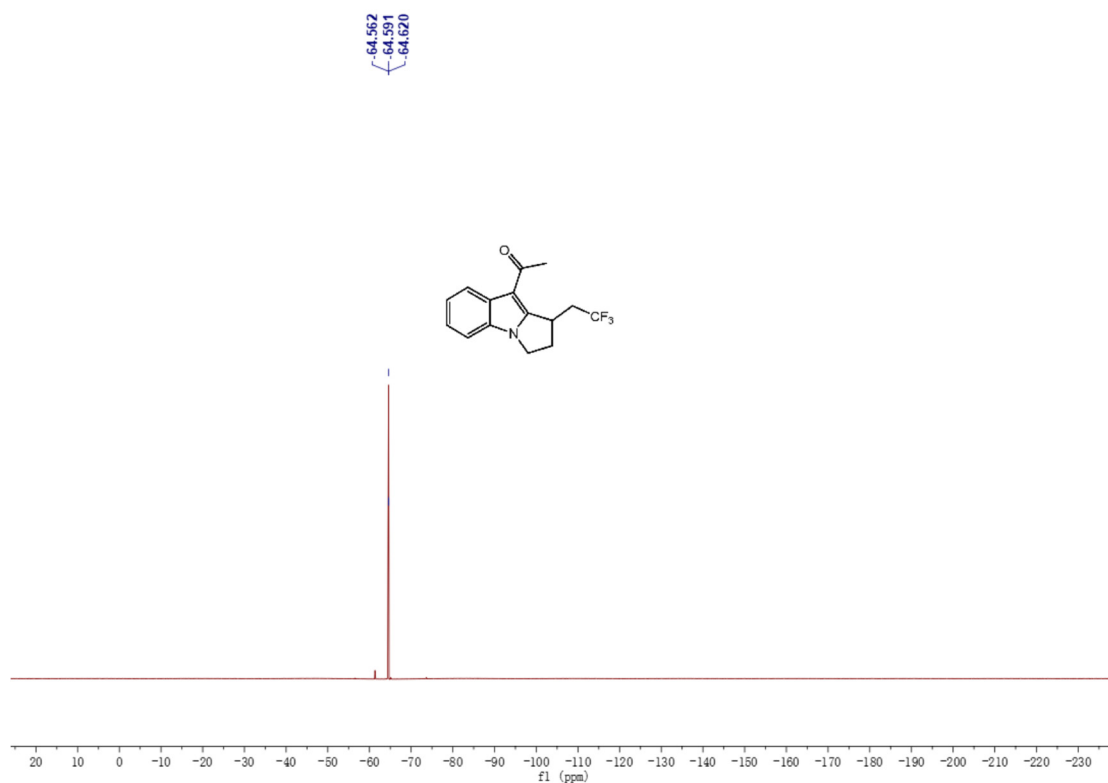
1-(1-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-pyrrolo[1,2-*a*]indol-9-yl)ethan-1-one (**5f**) :
¹H NMR (400 MHz, CDCl₃)



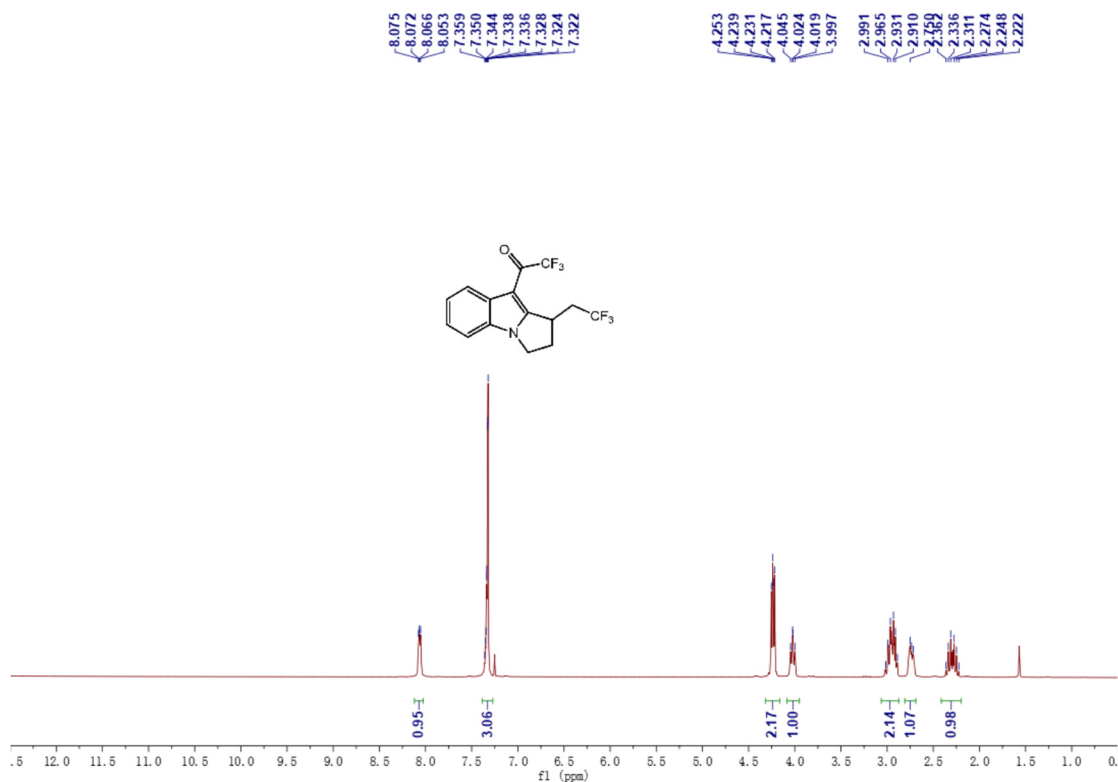
1-(1-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-pyrrolo[1,2-*a*]indol-9-yl)ethan-1-one (**5f**) :
¹³C NMR (150 MHz, CDCl₃)



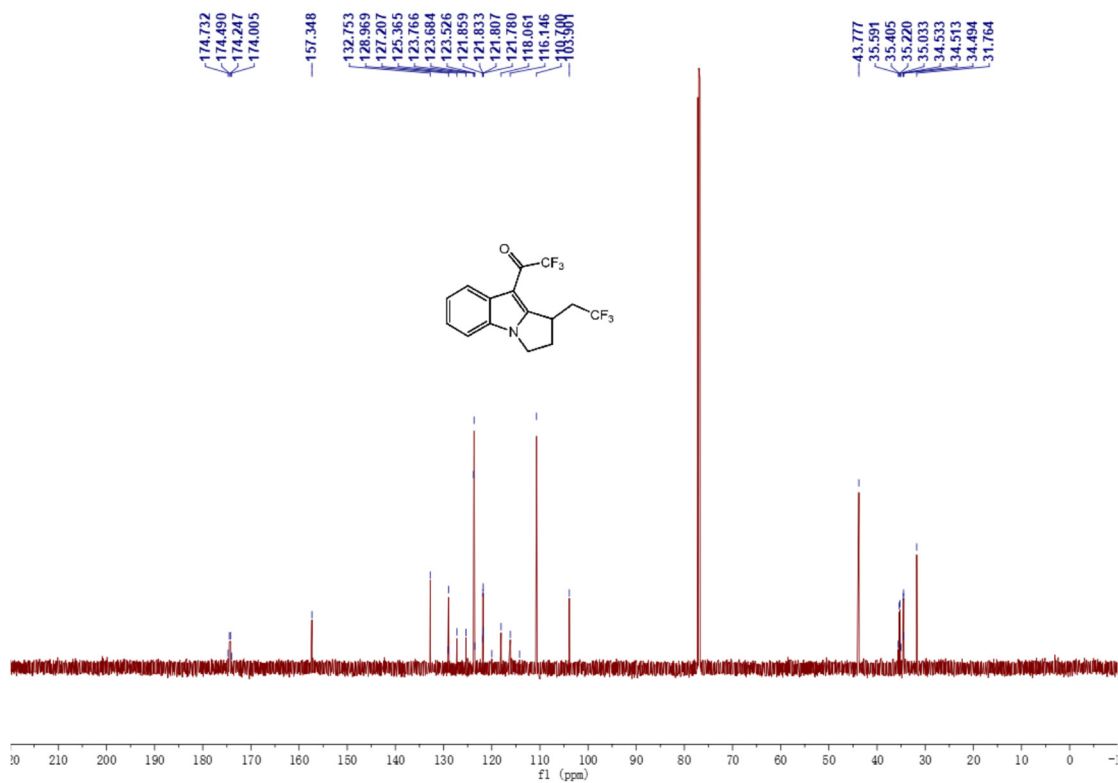
1-(1-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-pyrrolo[1,2-*a*]indol-9-yl)ethan-1-one (**5f**):
¹⁹F NMR (376 MHz, CDCl₃)



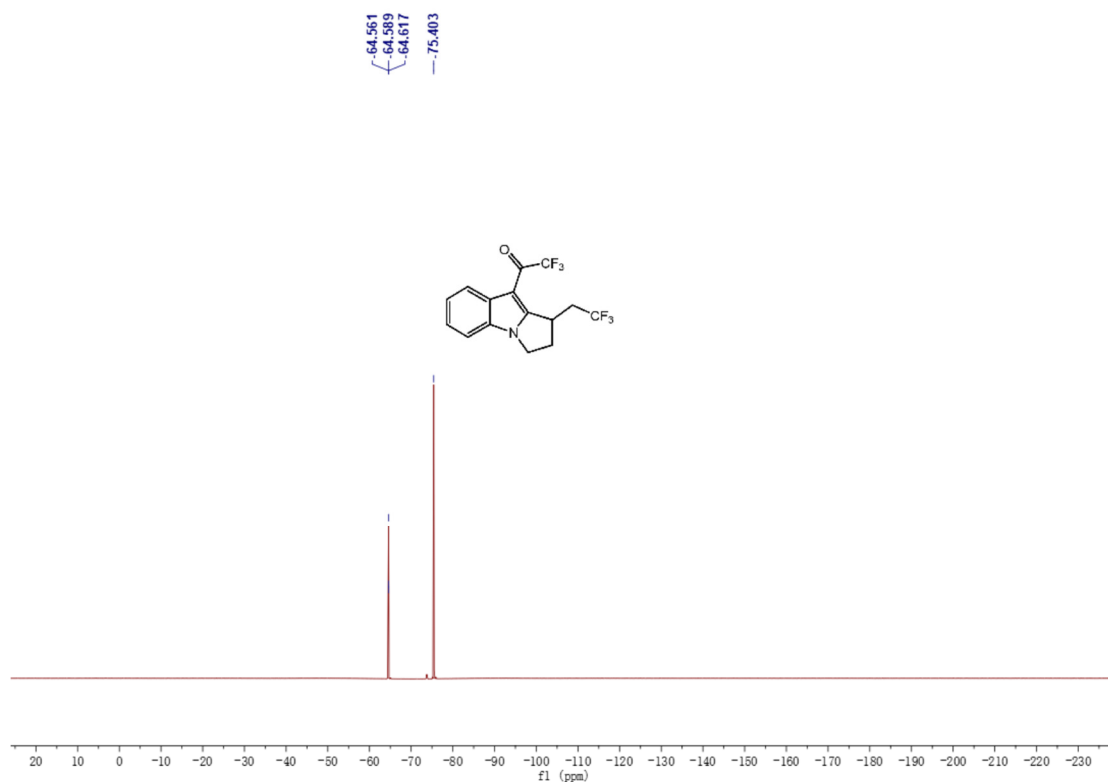
2,2,2-trifluoro-1-(1-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-pyrrolo[1,2-*a*]indol-9-yl)ethan-1-one (**5g**): ¹H NMR (400 MHz, CDCl₃)



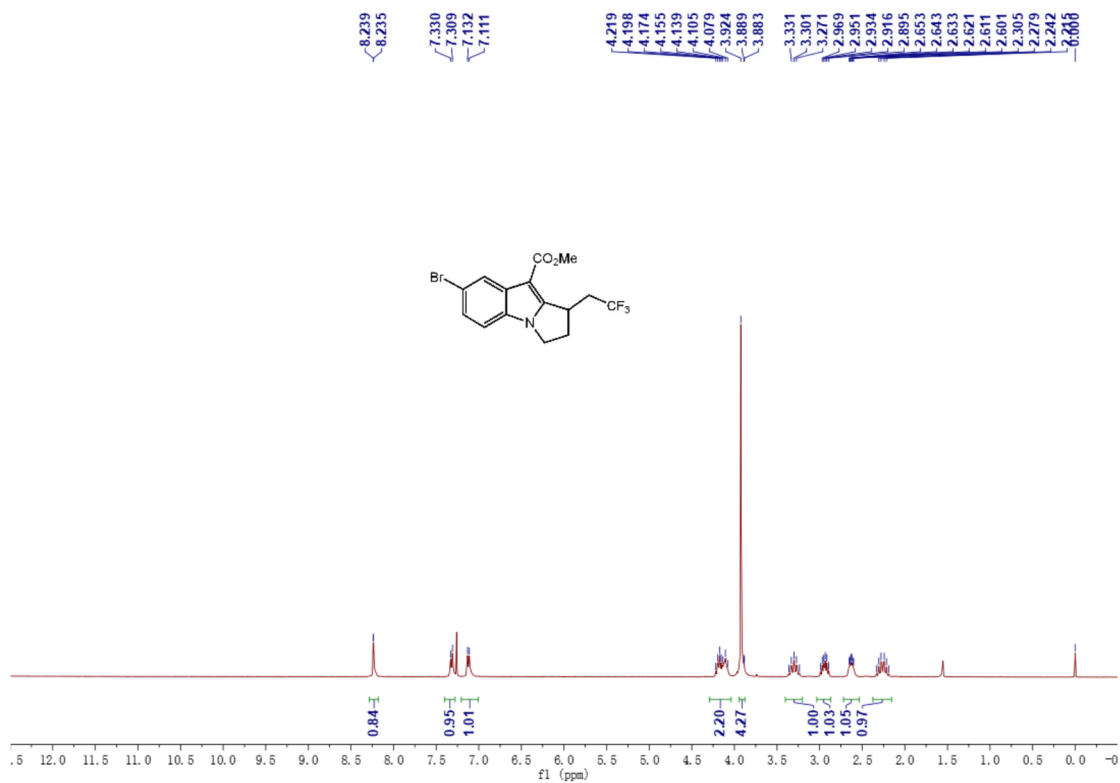
2,2,2-trifluoro-1-(1-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-pyrrolo[1,2-*a*]indol-9-yl)ethan-1-one (**5g**) : ¹³C NMR (150 MHz, CDCl₃)



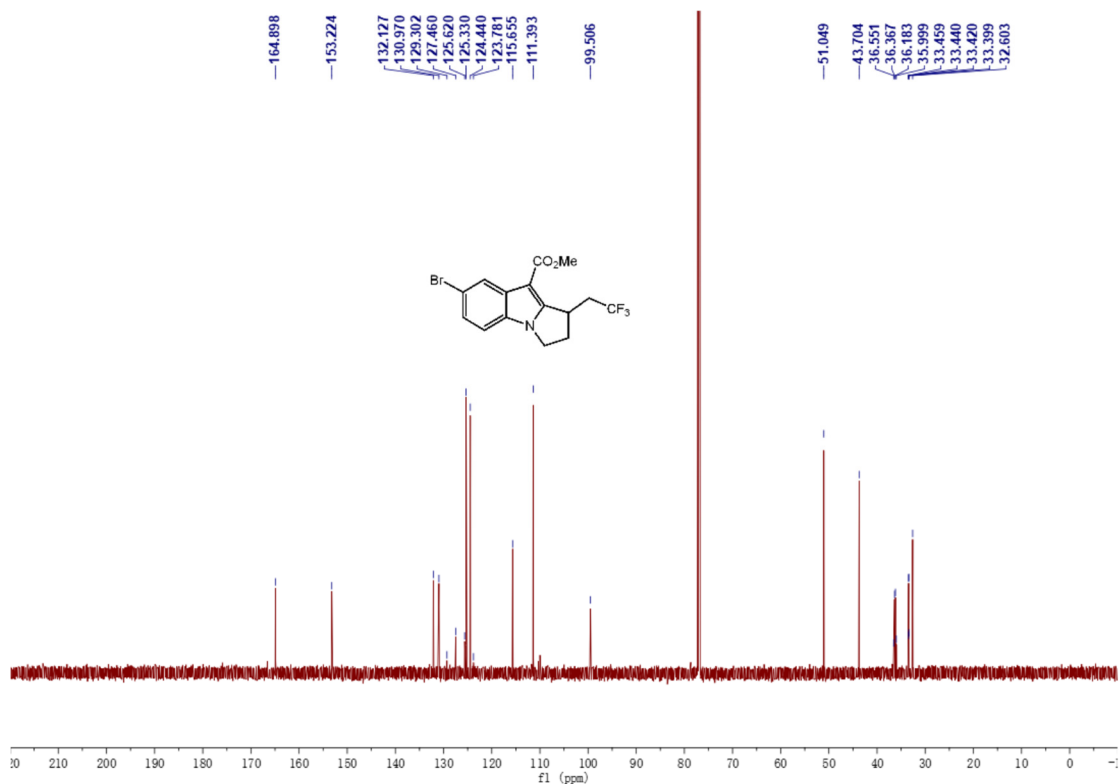
2,2,2-trifluoro-1-(1-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-pyrrolo[1,2-*a*]indol-9-yl)ethan-1-one (**5g**) : ¹⁹F NMR (376 MHz, CDCl₃)



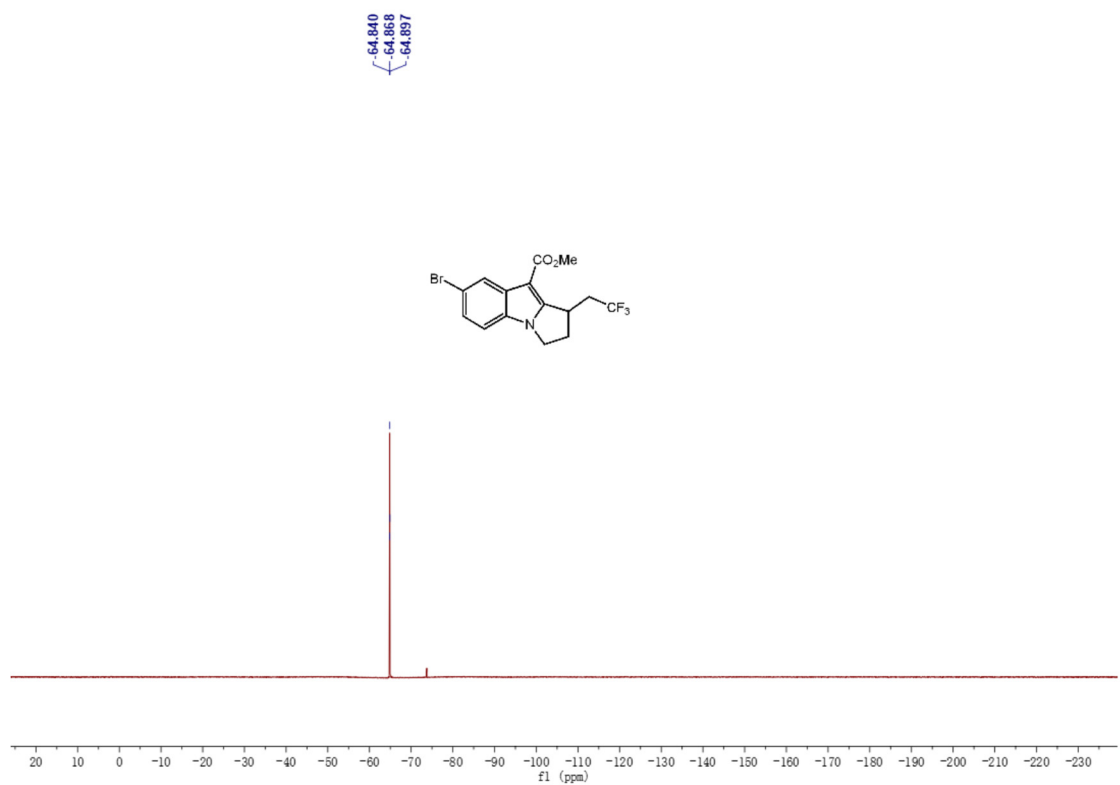
methyl 1-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-pyrrolo[1,2-*a*]indole-9-carboxylate (5h) : ^1H NMR (400 MHz, CDCl_3)



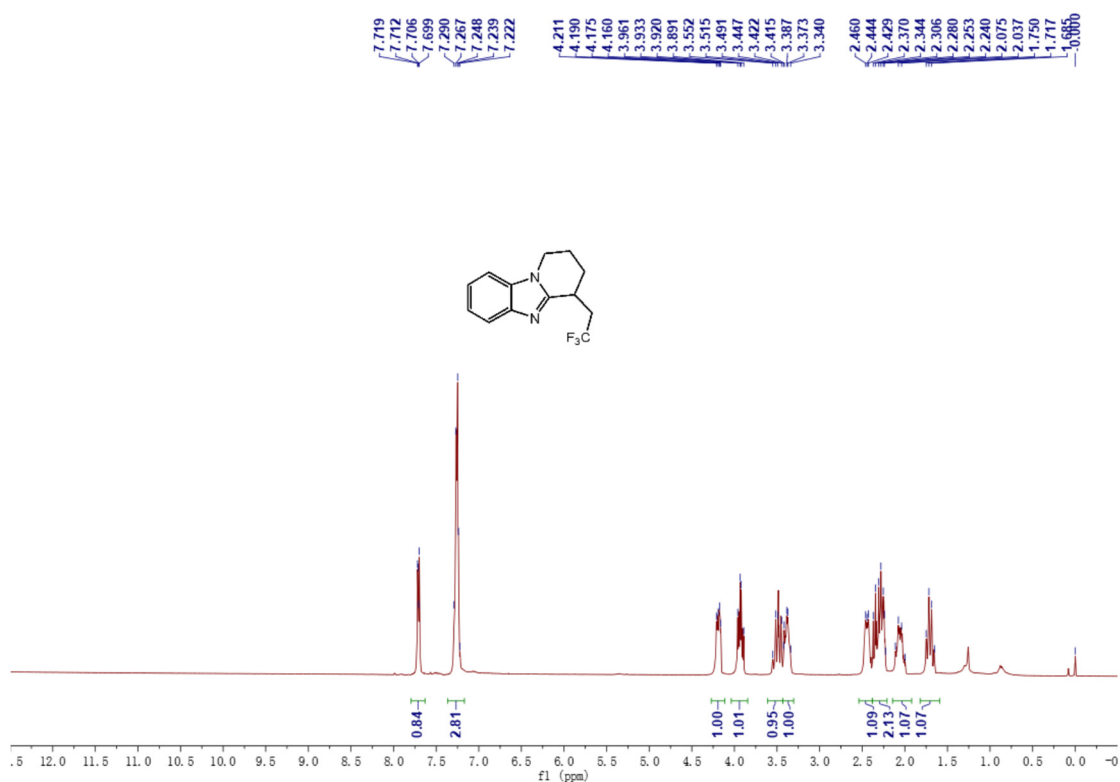
methyl 1-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-pyrrolo[1,2-*a*]indole-9-carboxylate (5h) : ^{13}C NMR (150 MHz, CDCl_3)



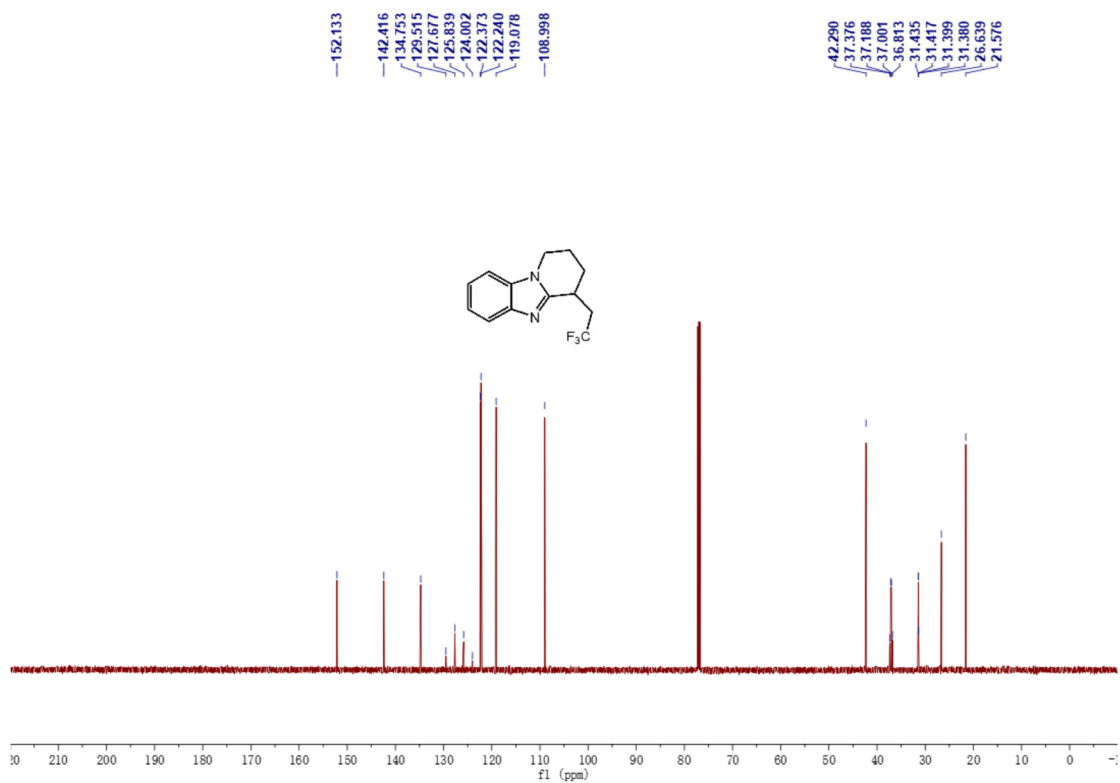
methyl 1-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-pyrrolo[1,2-*a*]indole-9-carboxylate
(**5h**) : ¹⁹F NMR (376 MHz, CDCl₃)



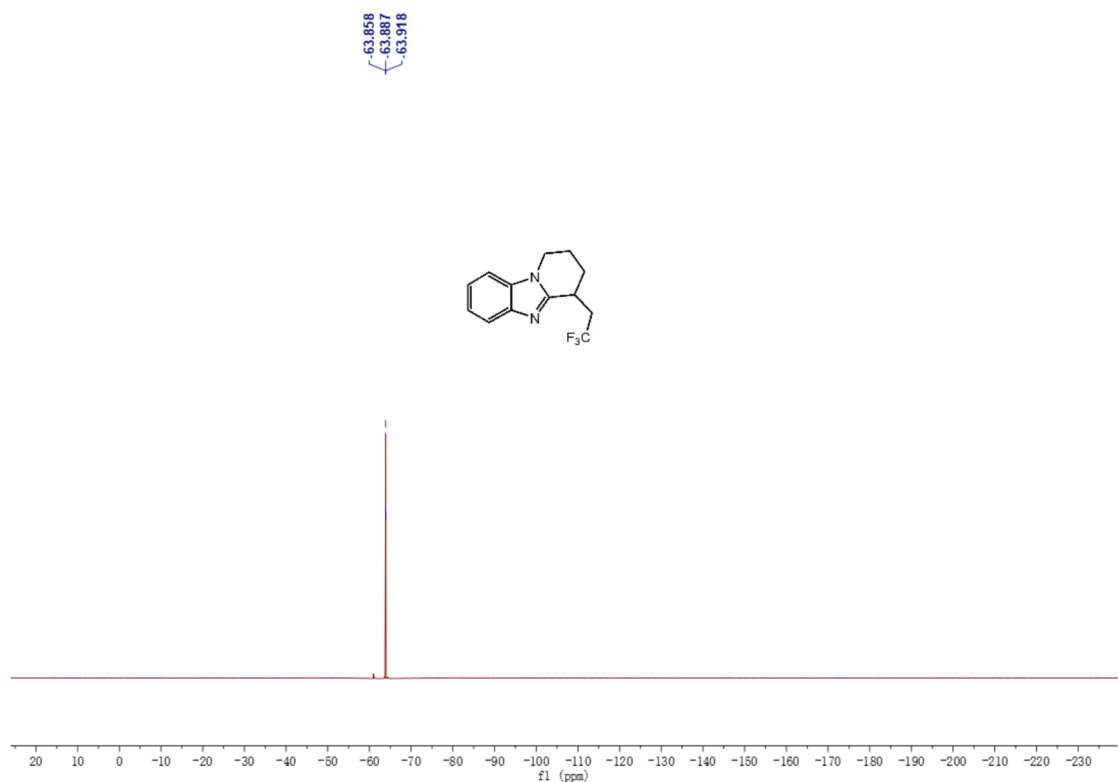
4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyridine (**7a**) : ¹H
NMR (400 MHz, CDCl₃)



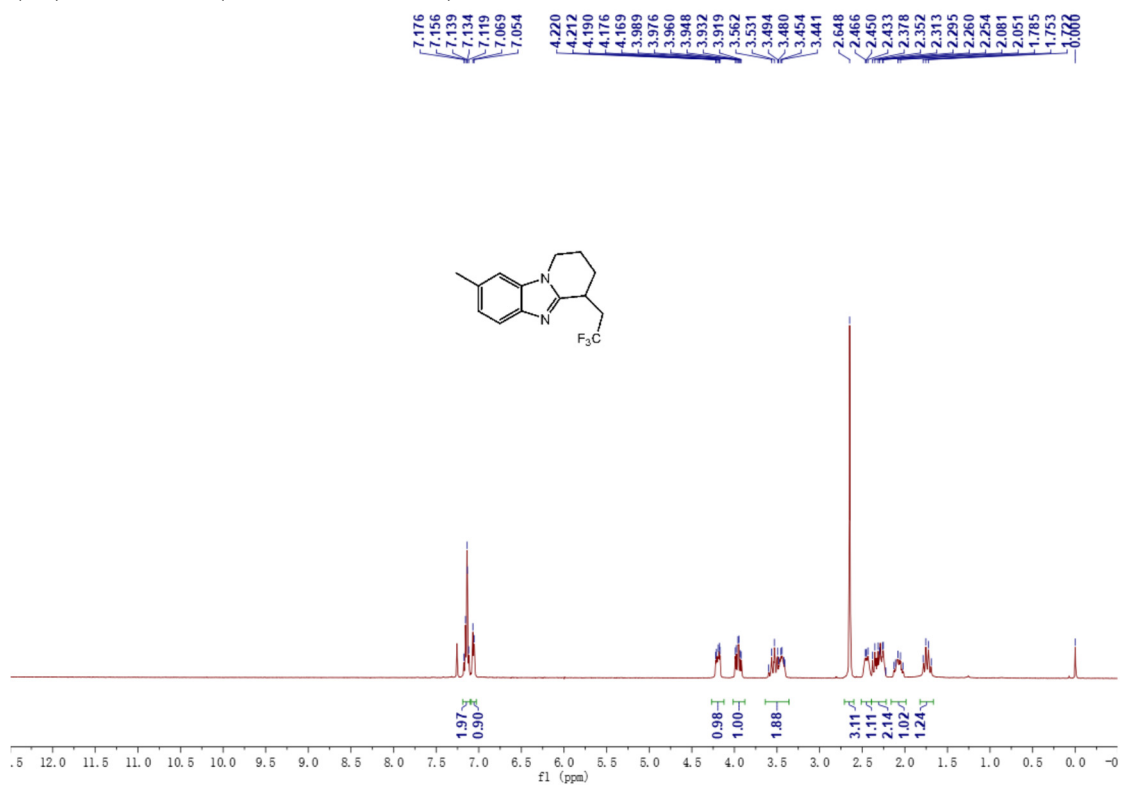
4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-a]pyridine (**7a**) : ¹³C NMR (150 MHz, CDCl₃)



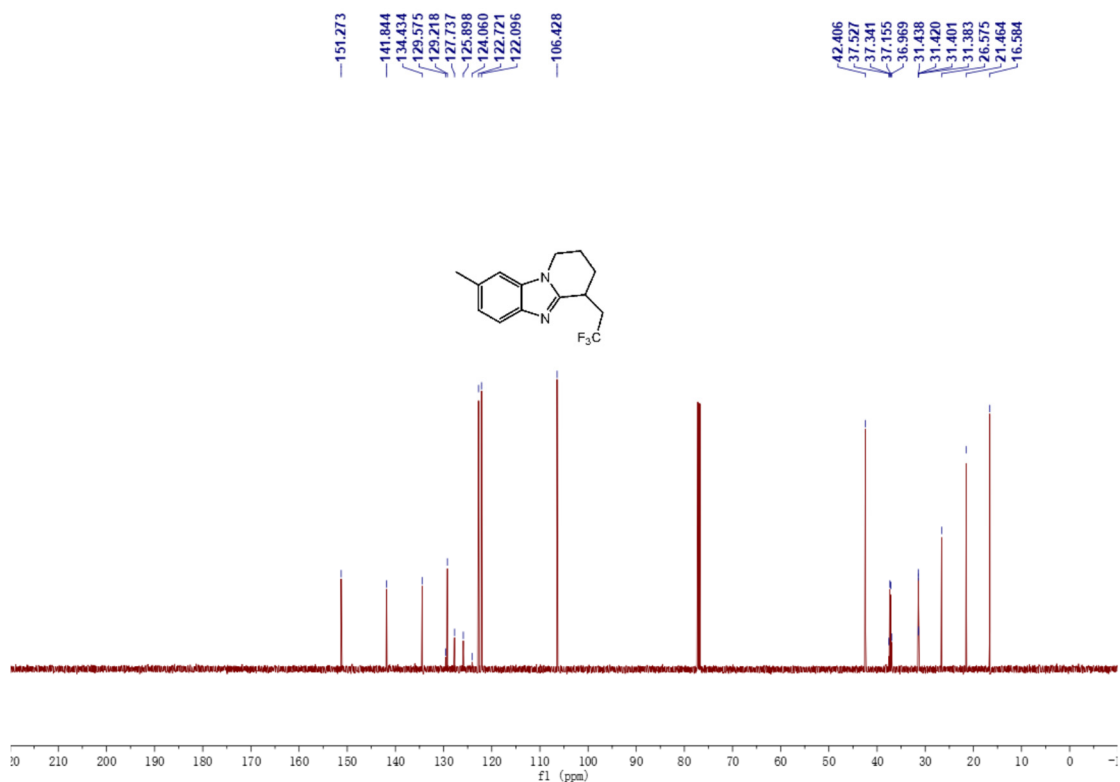
4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-a]pyridine (**7a**) : ¹⁹F NMR (376 MHz, CDCl₃)



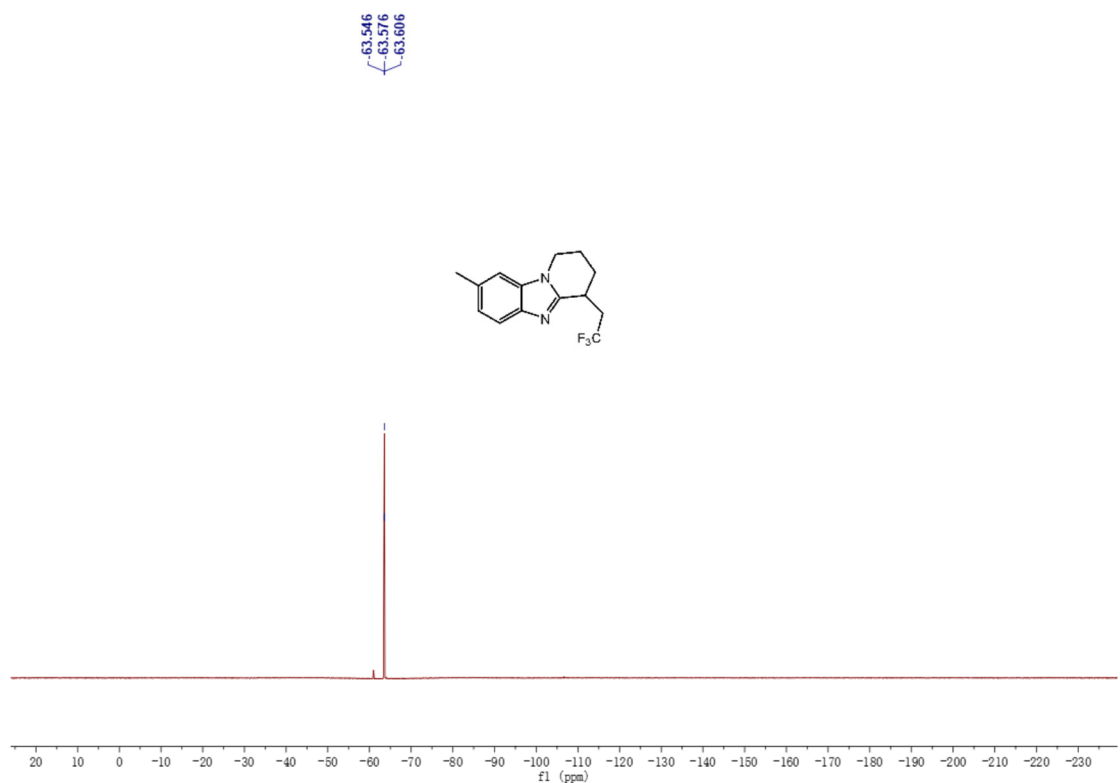
8-methyl-4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyridine (**7b**) : ¹H NMR (400 MHz, CDCl₃)



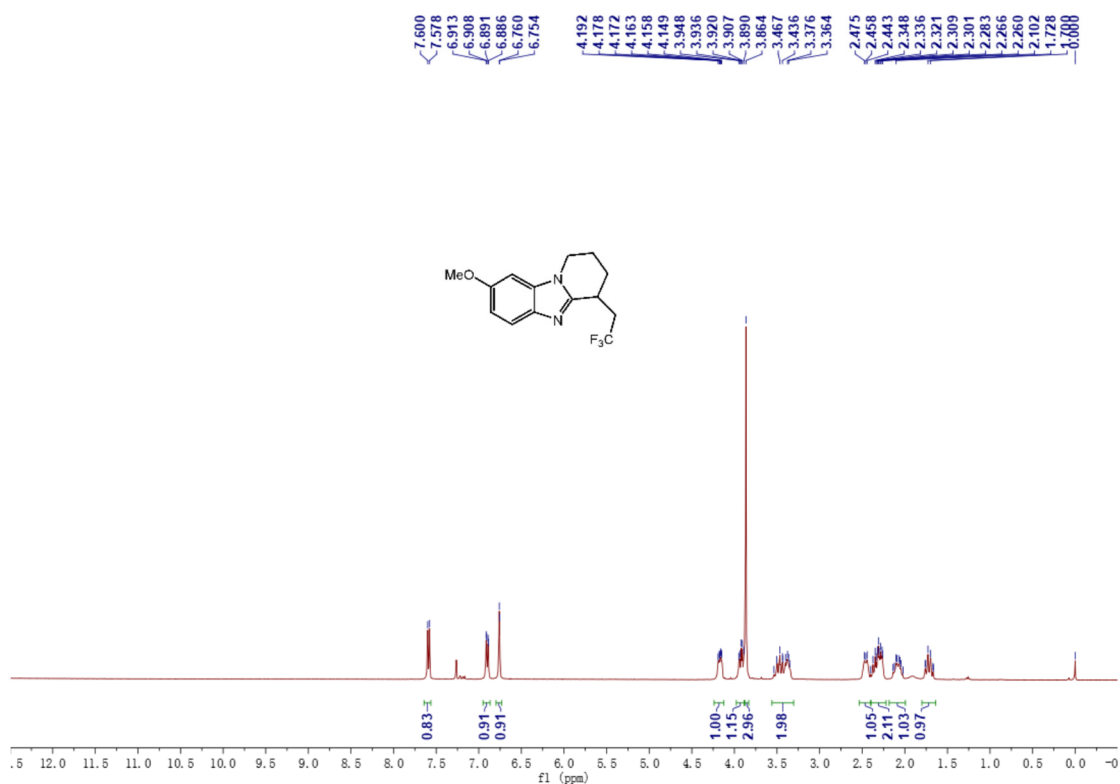
8-methyl-4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyridine (**7b**) : ¹³C NMR (150 MHz, CDCl₃)



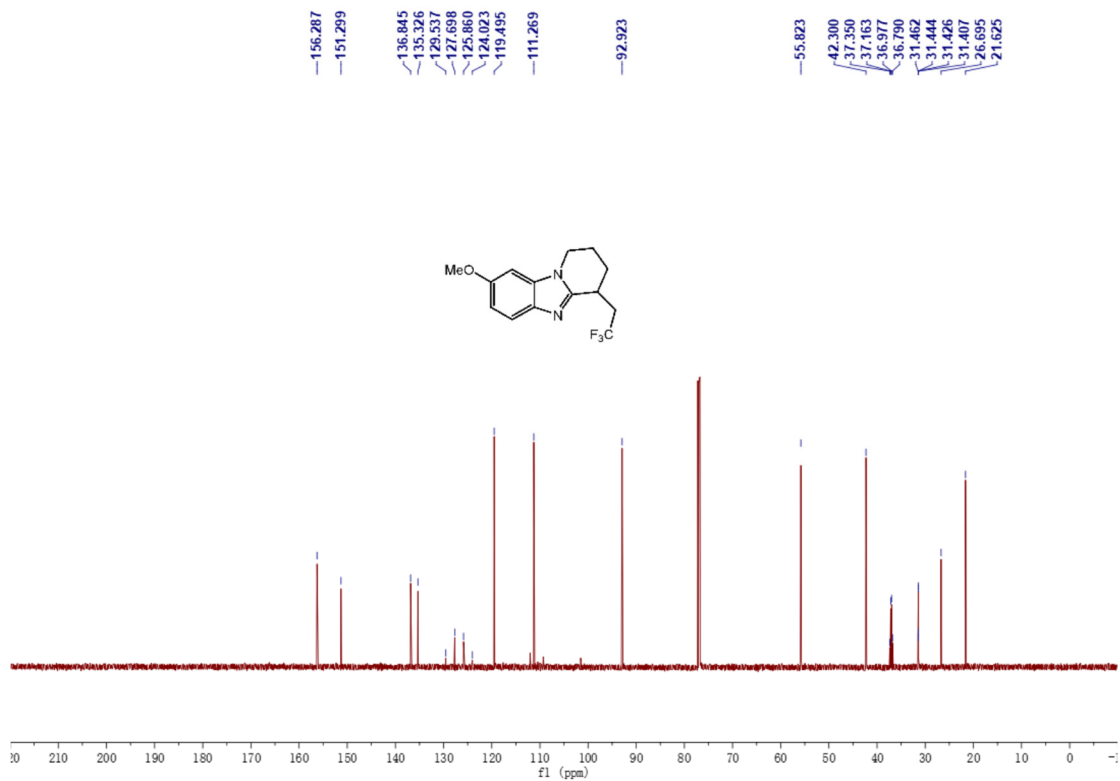
8-methyl-4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyridine
(7b) : ¹⁹F NMR (376 MHz, CDCl₃)



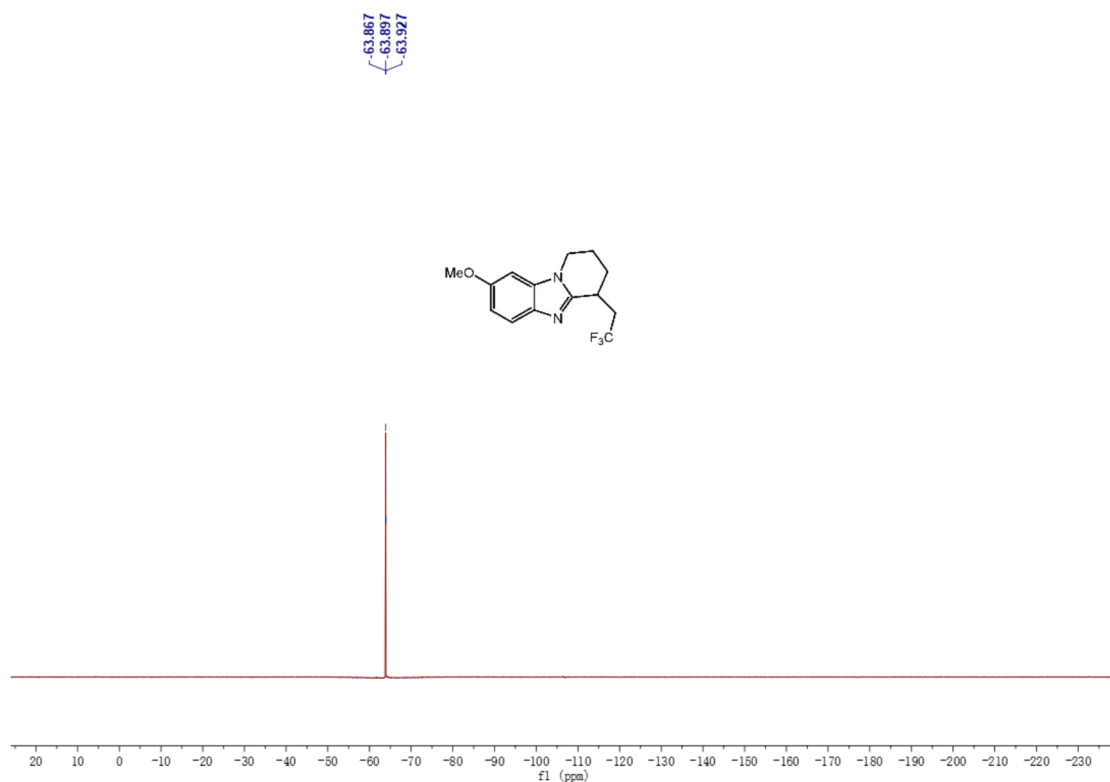
8-methoxy-4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyridine (7c) : ¹H NMR (400 MHz, CDCl₃)



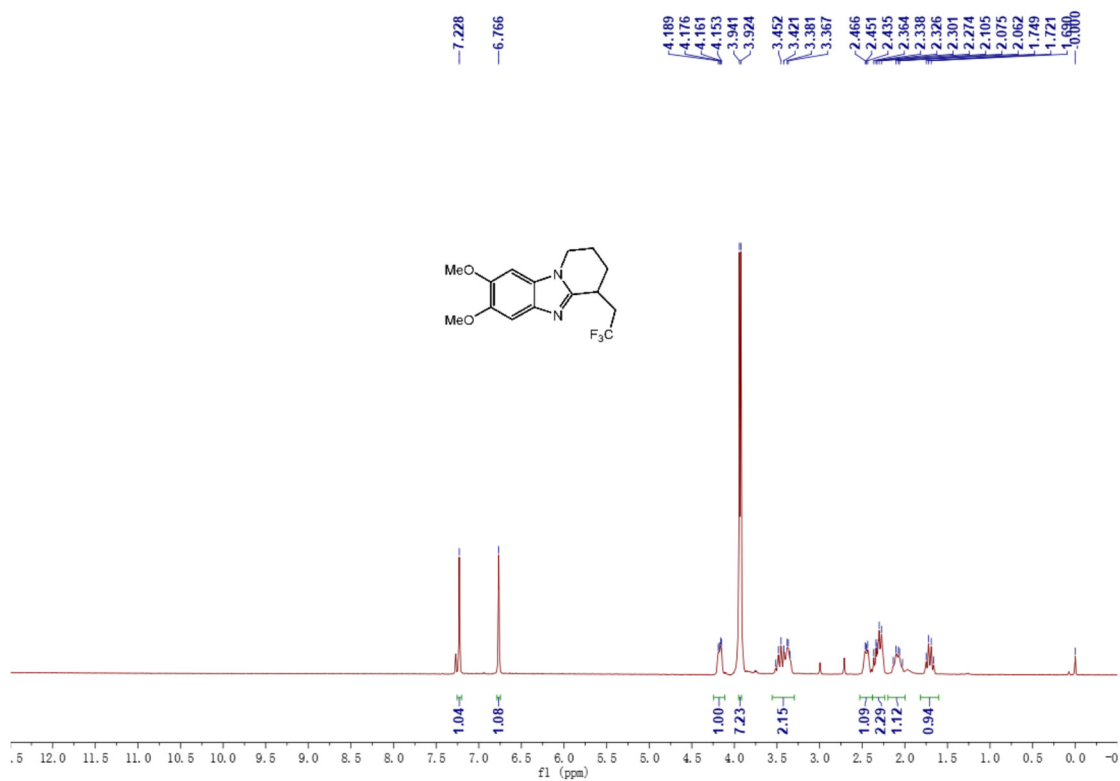
8-methoxy-4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyridine (7c): ^{13}C NMR (150 MHz, CDCl_3)



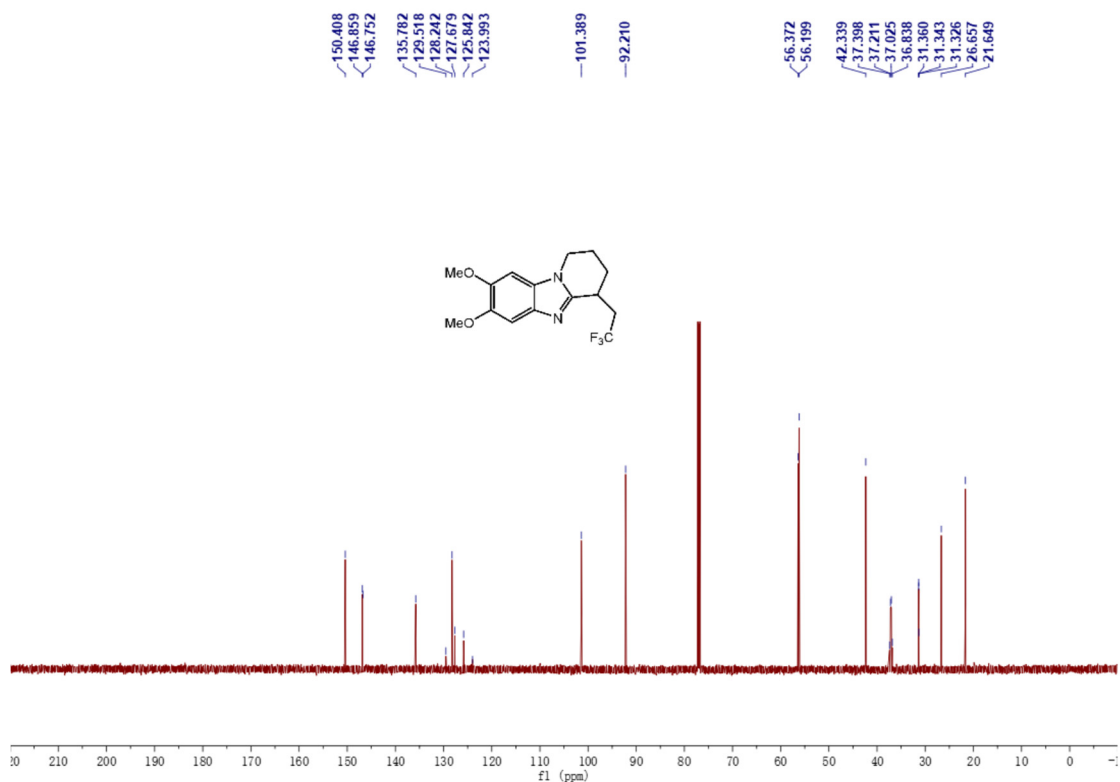
8-methoxy-4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyridine (7c): ^{19}F NMR (376 MHz, CDCl_3)



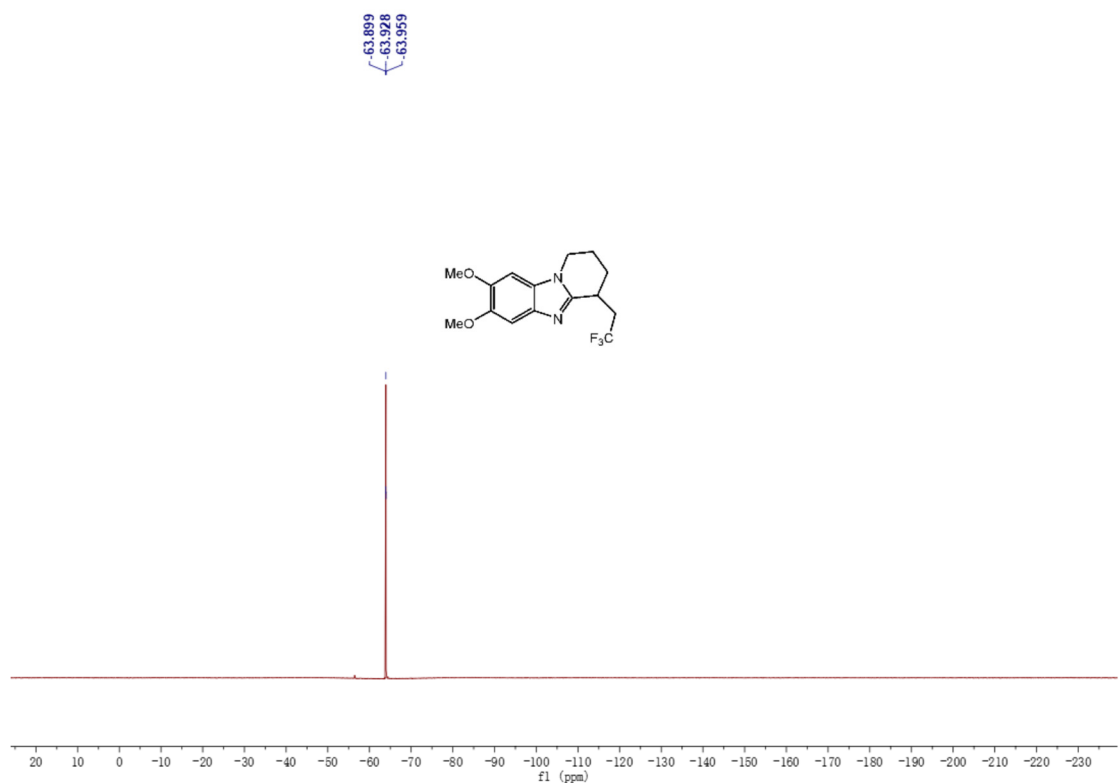
7,8-dimethoxy-4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-a]pyridine (**7d**) : ^1H NMR (400 MHz, CDCl_3)



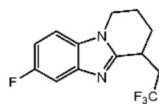
7,8-dimethoxy-4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-a]pyridine (**7d**) : ^{13}C NMR (150 MHz, CDCl_3)



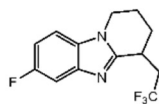
7,8-dimethoxy-4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-a]pyridine (**7d**) : ^{19}F NMR (376 MHz, CDCl_3)



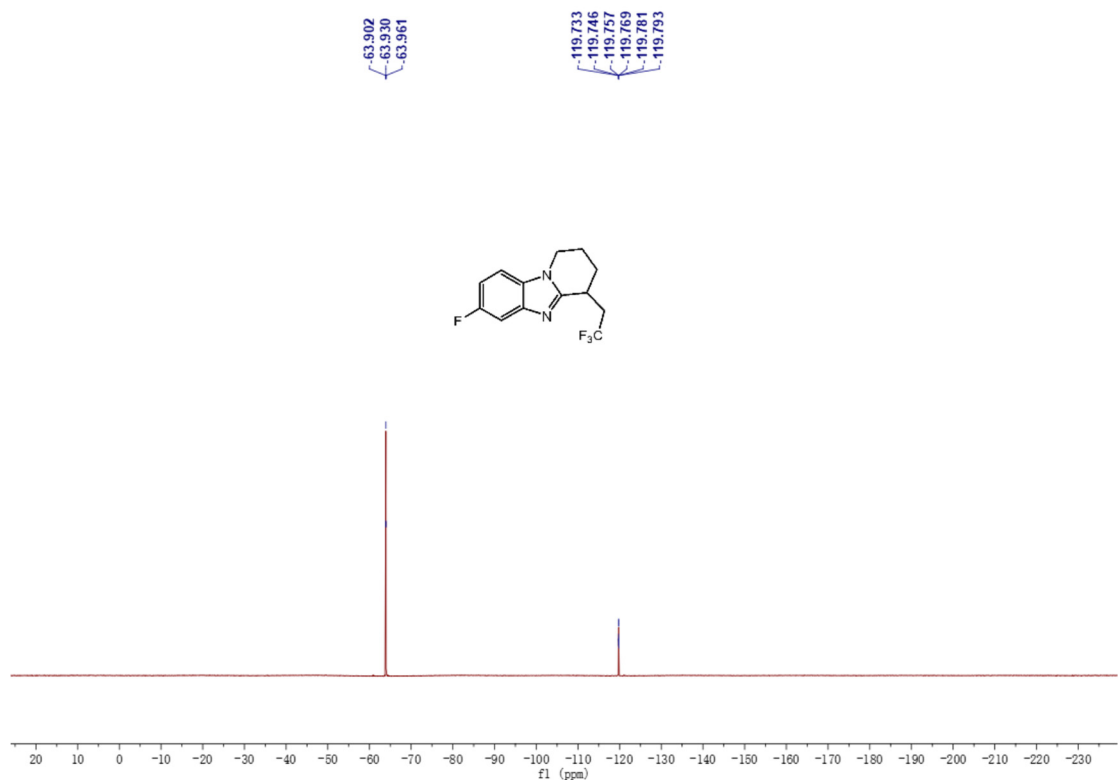
7-fluoro-4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-a]pyridine (**7e**) : ^1H NMR (400 MHz, CDCl_3)



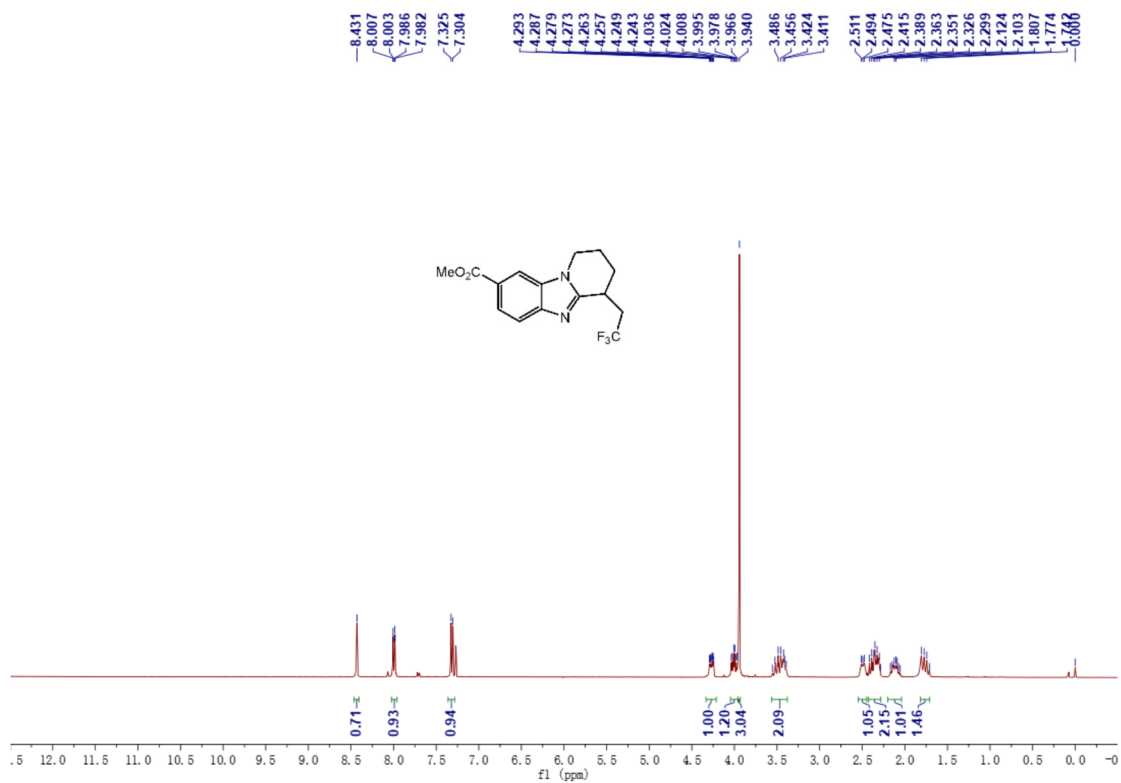
160.183	138.808	42.505
158.595	134.924	37.330
156.995	134.838	37.143
152.892	129.472	36.955
152.874	127.634	36.767
	125.797	31.549
	123.959	31.531
	119.825	31.512
	119.758	31.494
110.553		26.632
110.487		21.589
	95.341	
	95.760	



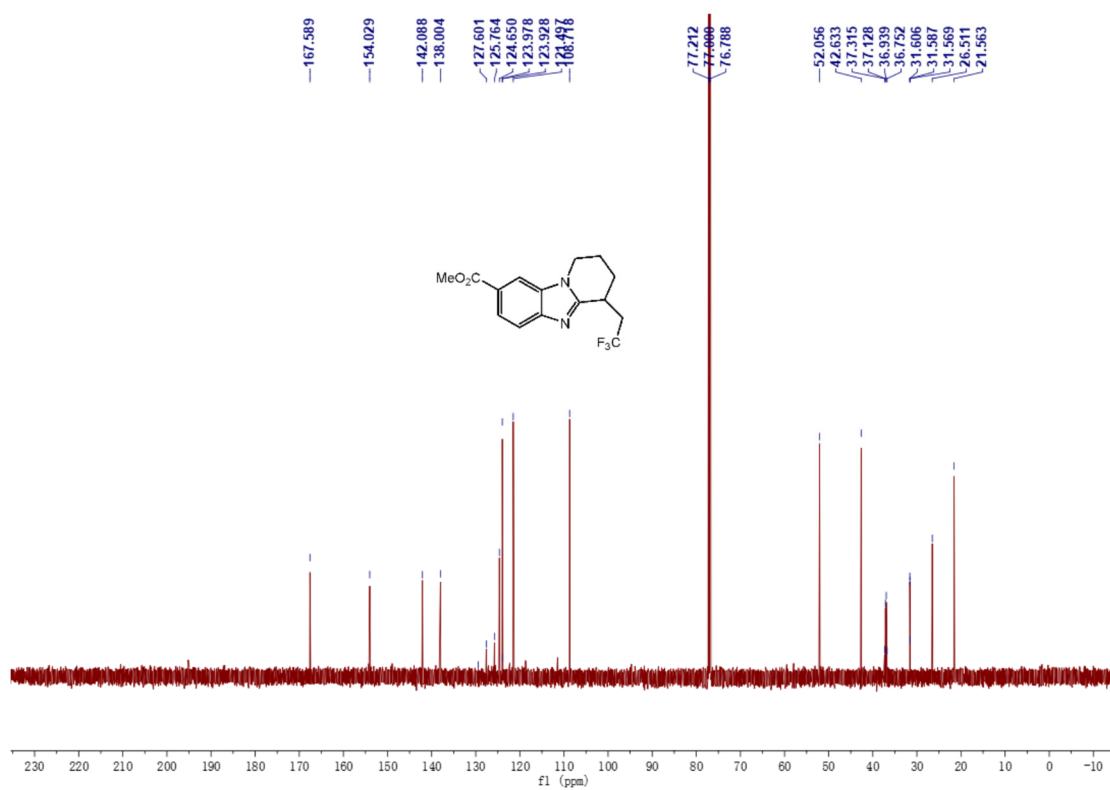
7-fluoro-4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-a]pyridine
(**7e**): ^{19}F NMR (376 MHz, CDCl_3)



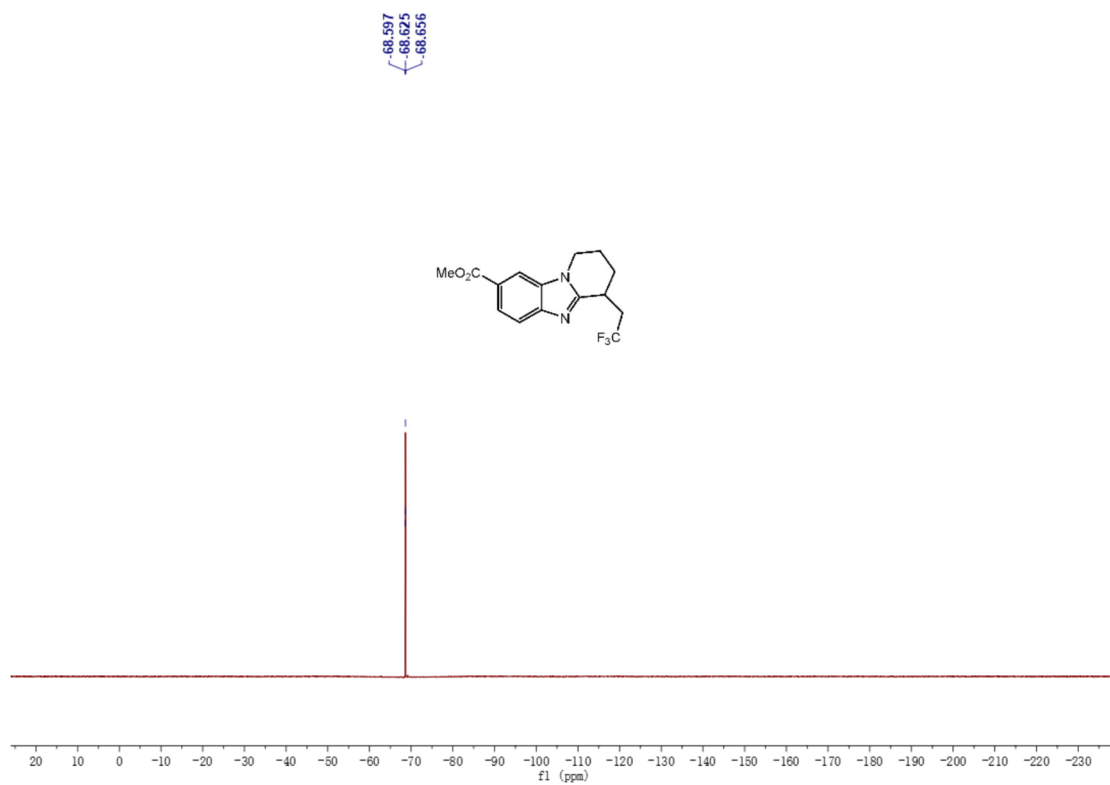
methyl 4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-a]pyridine-8-carboxylate (**7f**) : ^1H NMR (400 MHz, CDCl_3)



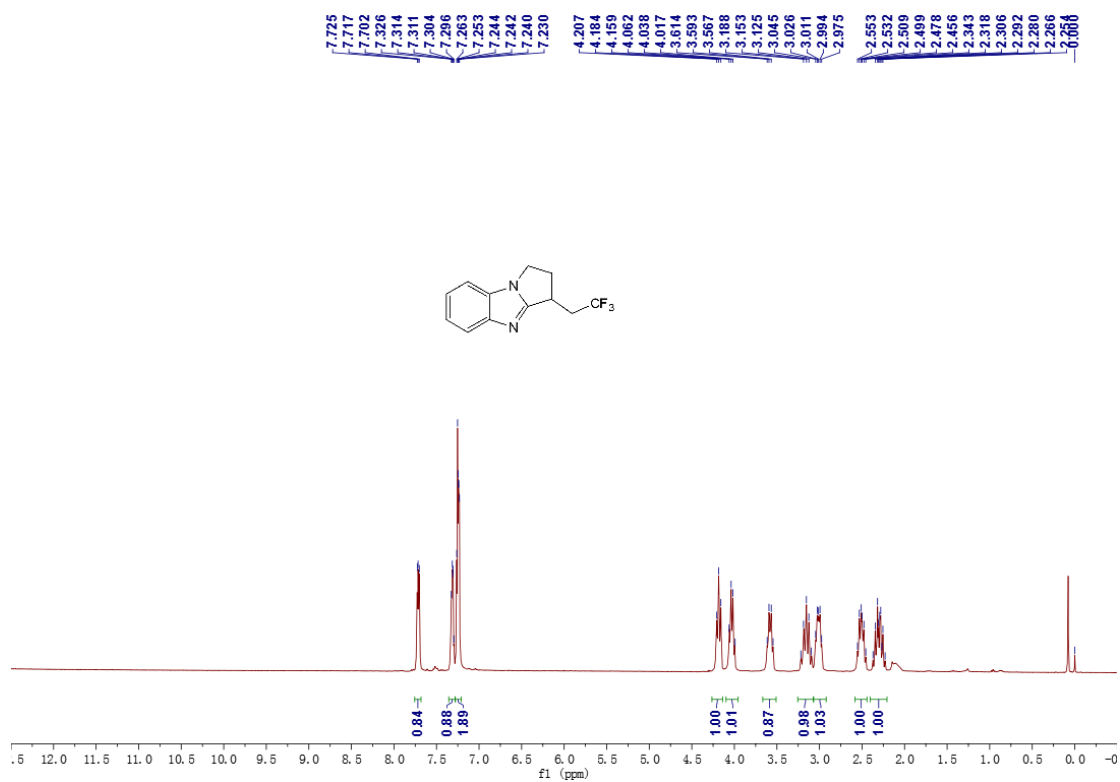
methyl 4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-a]pyridine-8-carboxylate (**7f**) : ^{13}C NMR (150 MHz, CDCl_3)



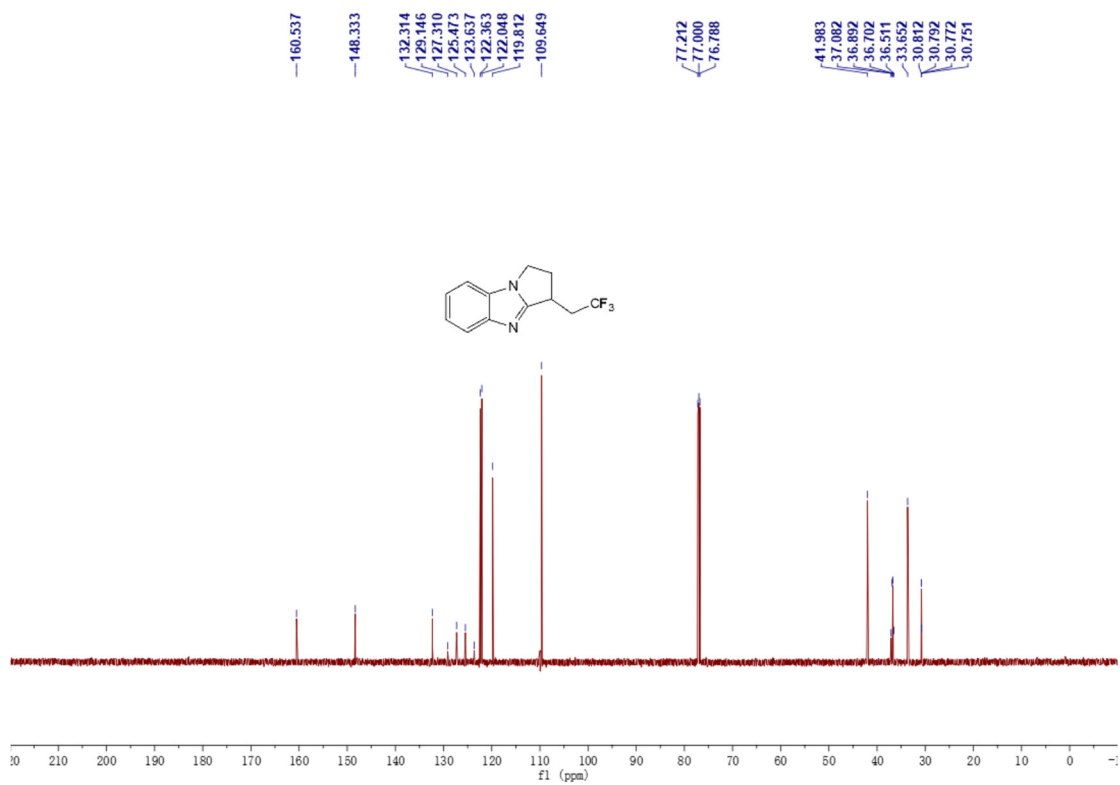
methyl 4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-a]pyridine-8-carboxylate (**7f**) : ¹⁹F NMR (376 MHz, CDCl₃)



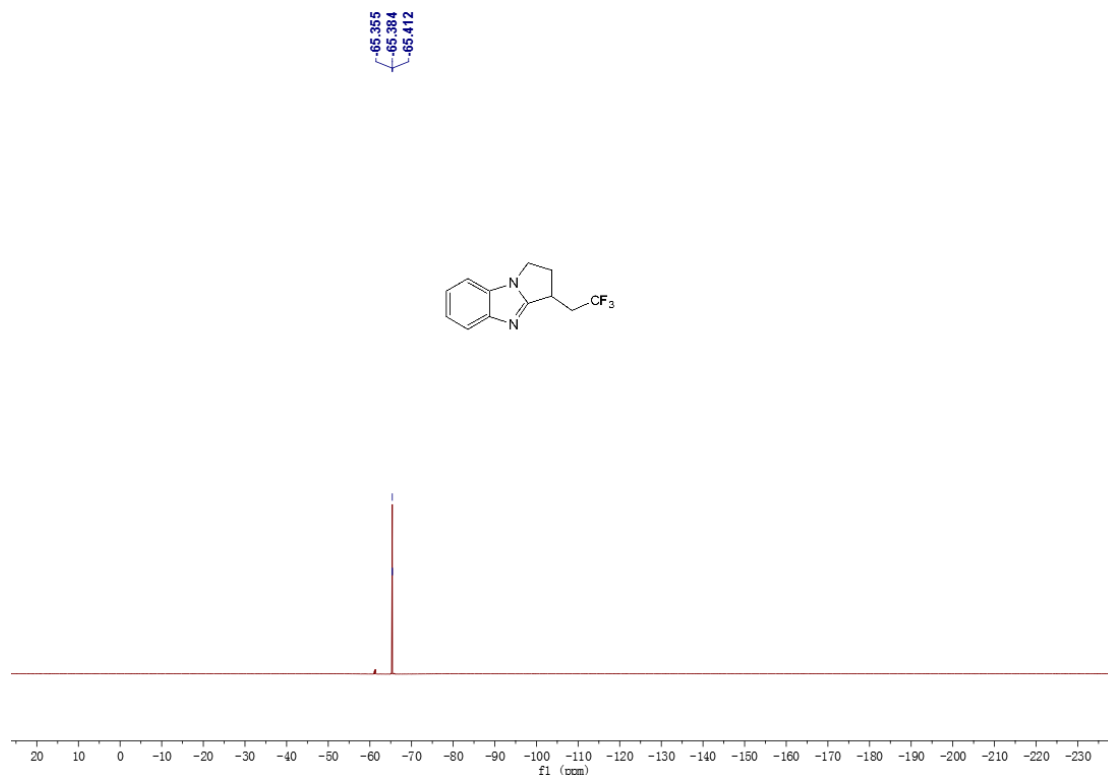
3-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-benzo[d]pyrrolo[1,2-*a*]imidazole (**7g**) : ^1H NMR (400 MHz, CDCl_3)



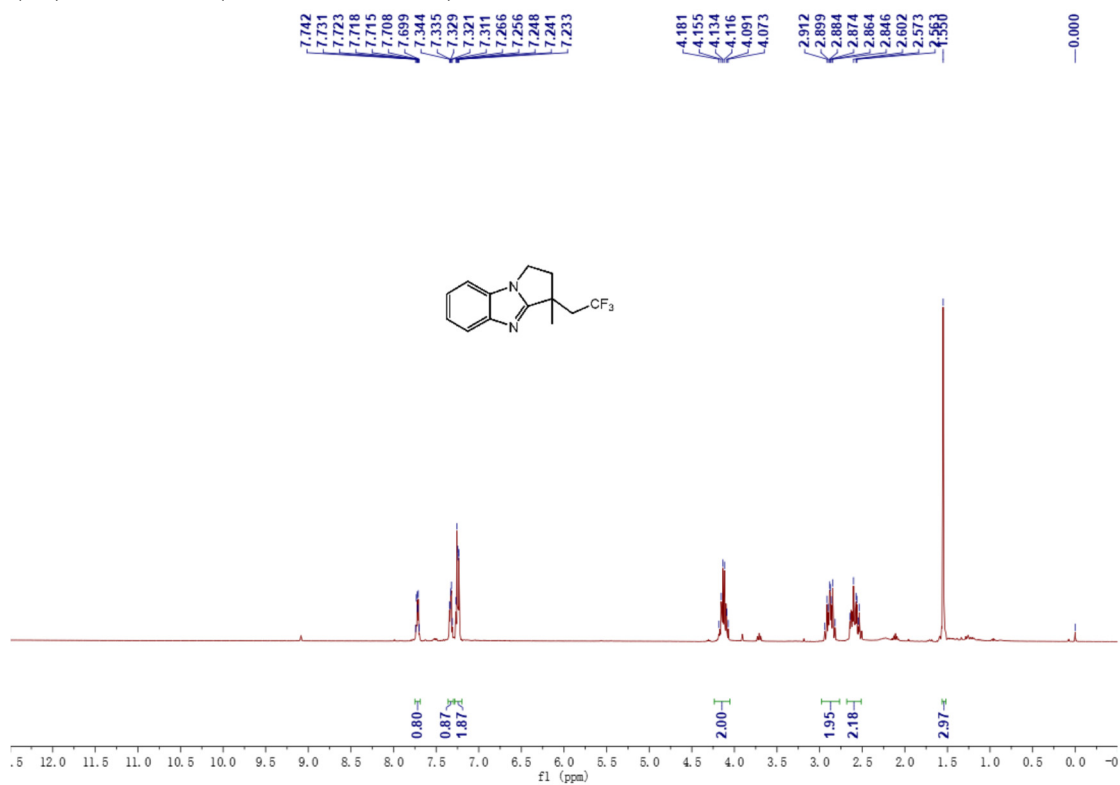
3-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-benzo[d]pyrrolo[1,2-*a*]imidazole (**7g**) : ^{13}C NMR (150 MHz, CDCl_3)



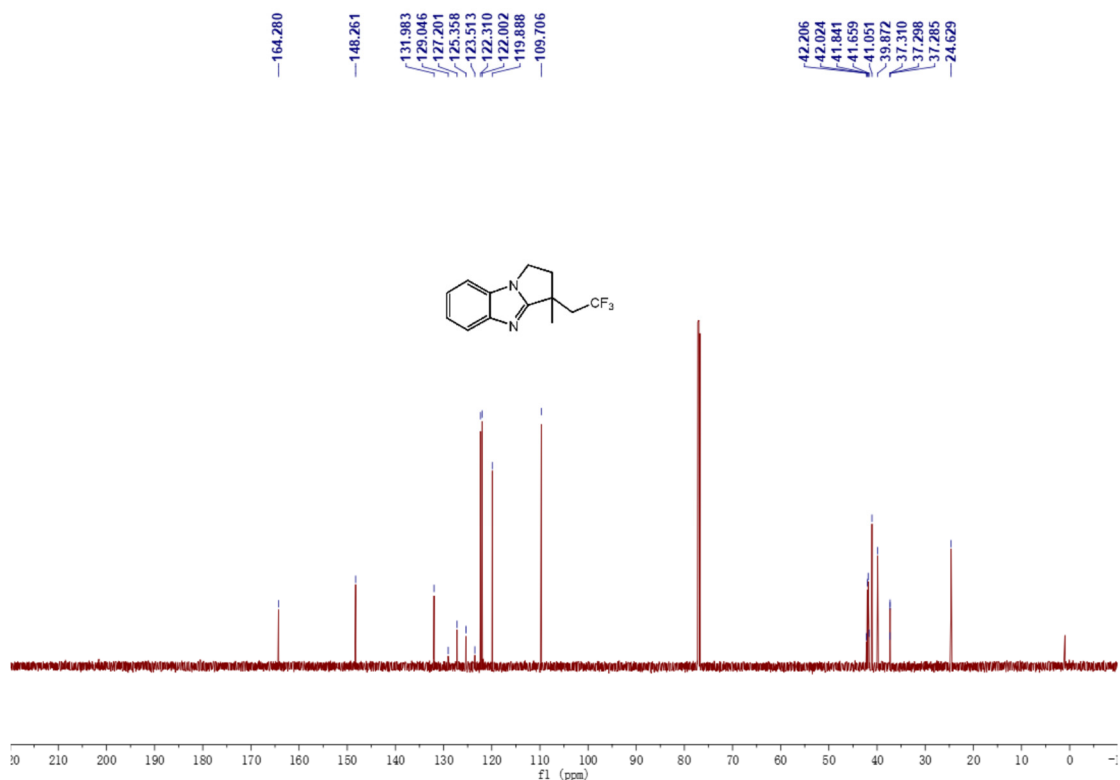
3-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-benzo[*d*]pyrrolo[1,2-*a*]imidazole (**7g**) : ^{19}F
NMR (376 MHz, CDCl_3)



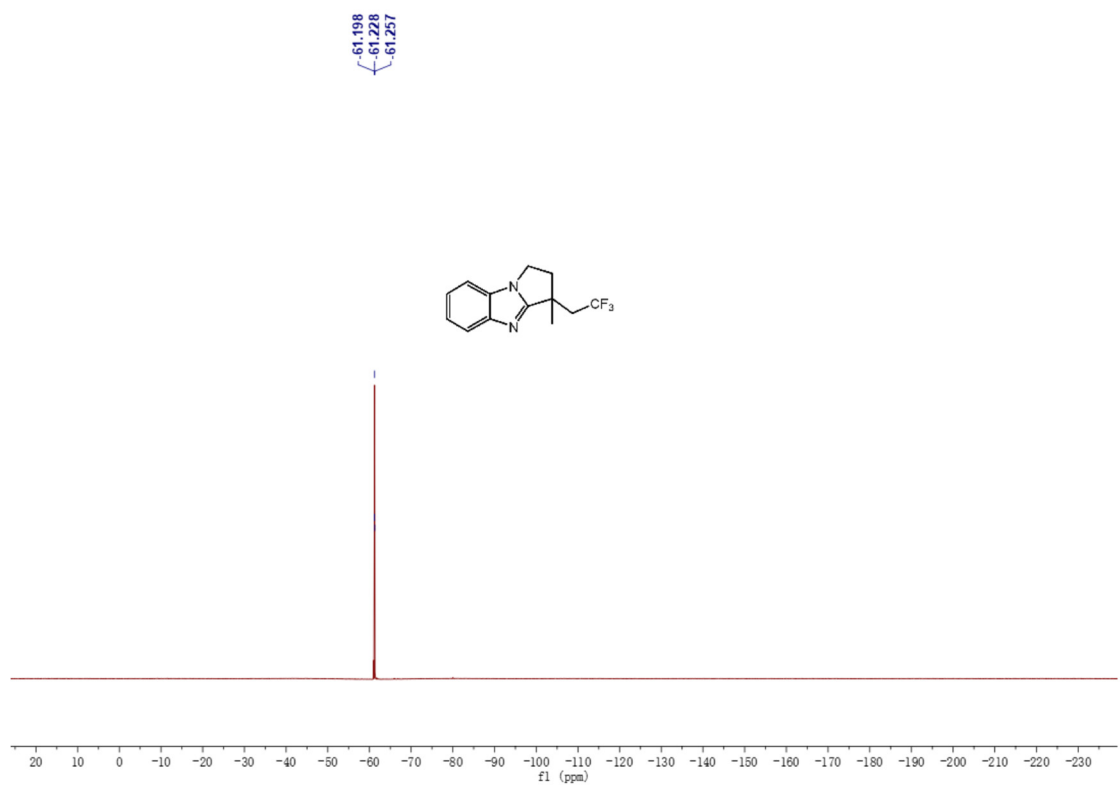
3-methyl-3-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-benzo[*d*]pyrrolo[1,2-*a*]imidazole (**7h**) : ^1H NMR (400 MHz, CDCl_3)



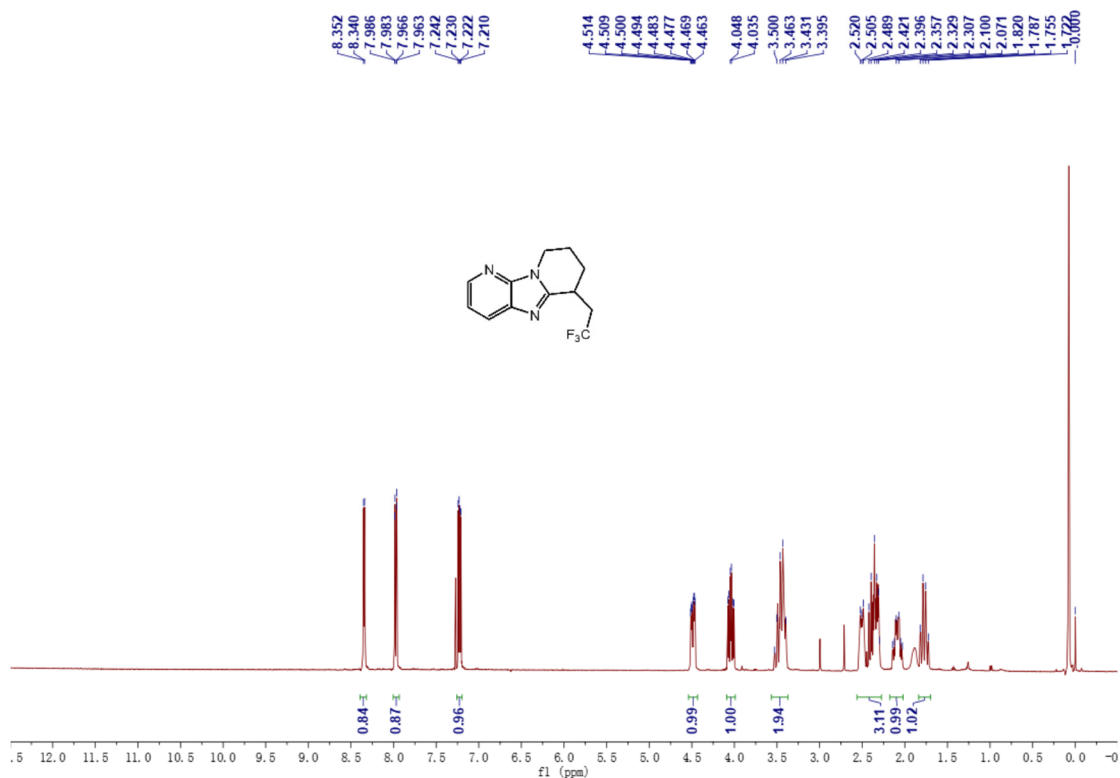
3-methyl-3-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-benzo[*d*]pyrrolo[1,2-*a*]imidazole
(**7h**) : ^{13}C NMR (150 MHz, CDCl_3)



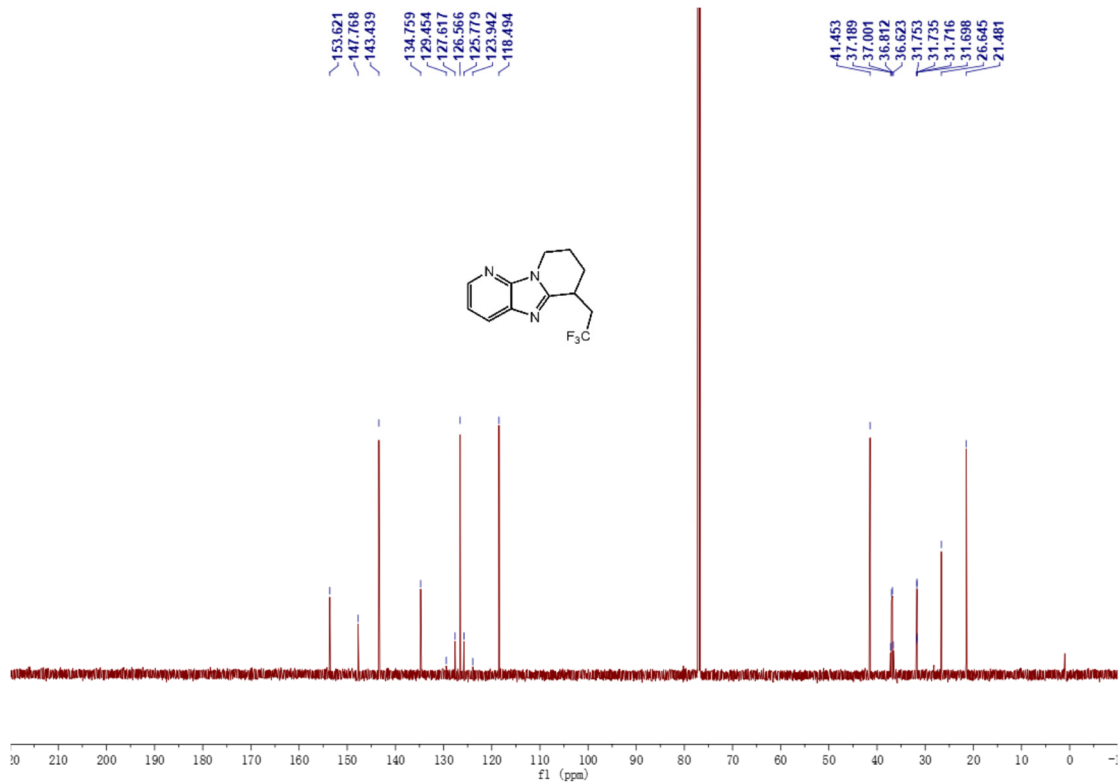
3-methyl-3-(2,2,2-trifluoroethyl)-2,3-dihydro-1H-benzo[*d*]pyrrolo[1,2-*a*]imidazole
(**7h**) : ^{19}F NMR (376 MHz, CDCl_3)



6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydroimidazo[1,2-*a*:5,4-*b'*]dipyridine (**7i**) : ^1H NMR (400 MHz, CDCl_3)

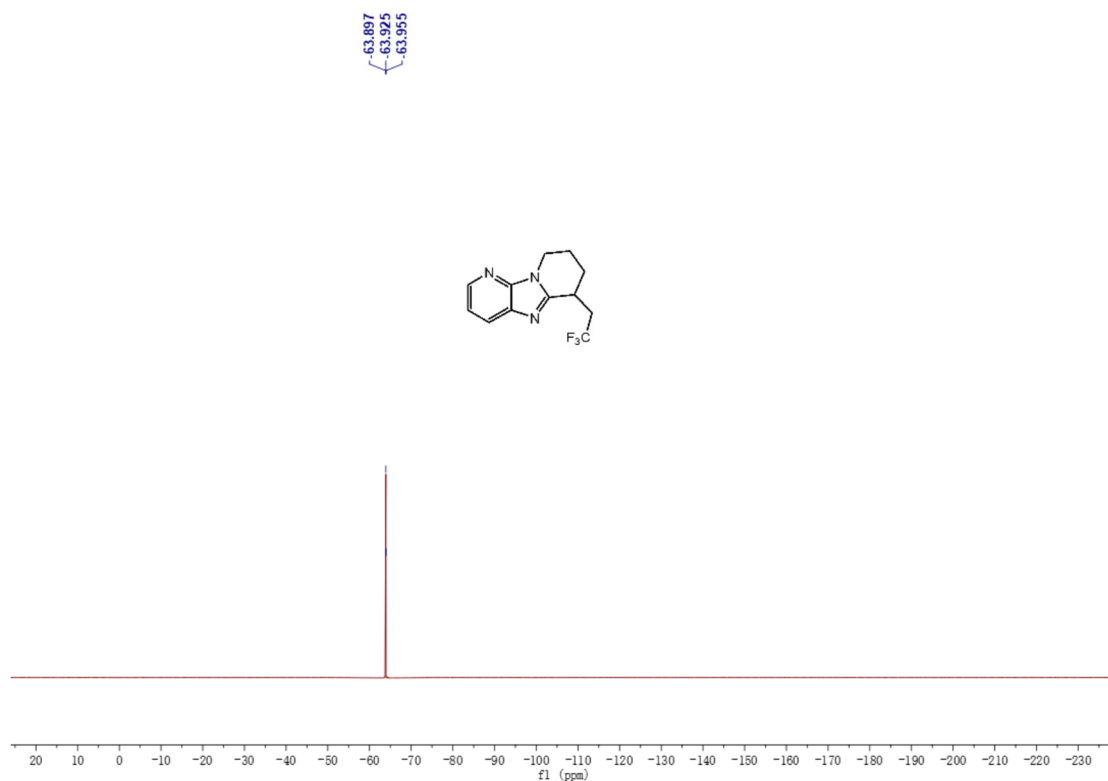


6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydroimidazo[1,2-*a*:5,4-*b'*]dipyridine (**7i**) : ^{13}C NMR (150 MHz, CDCl_3)

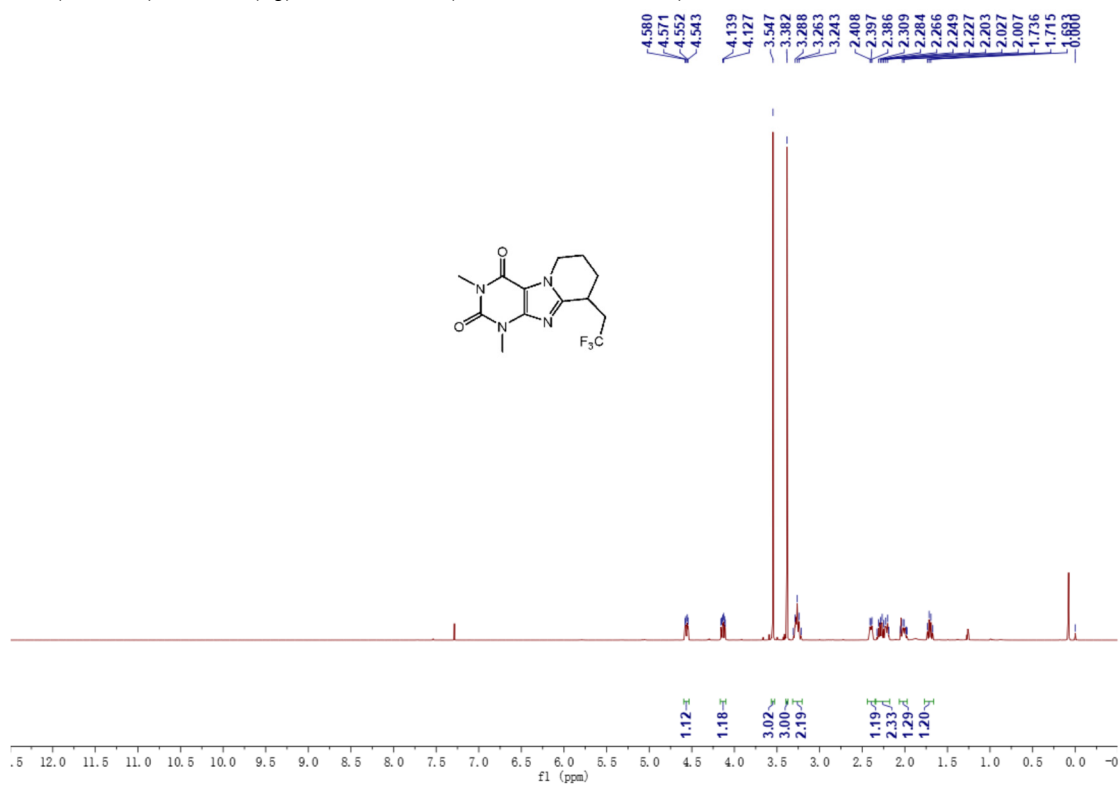


6-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydroimidazo[1,2-*a*:5,4-*b'*]dipyridine (**7i**) : ^{19}F

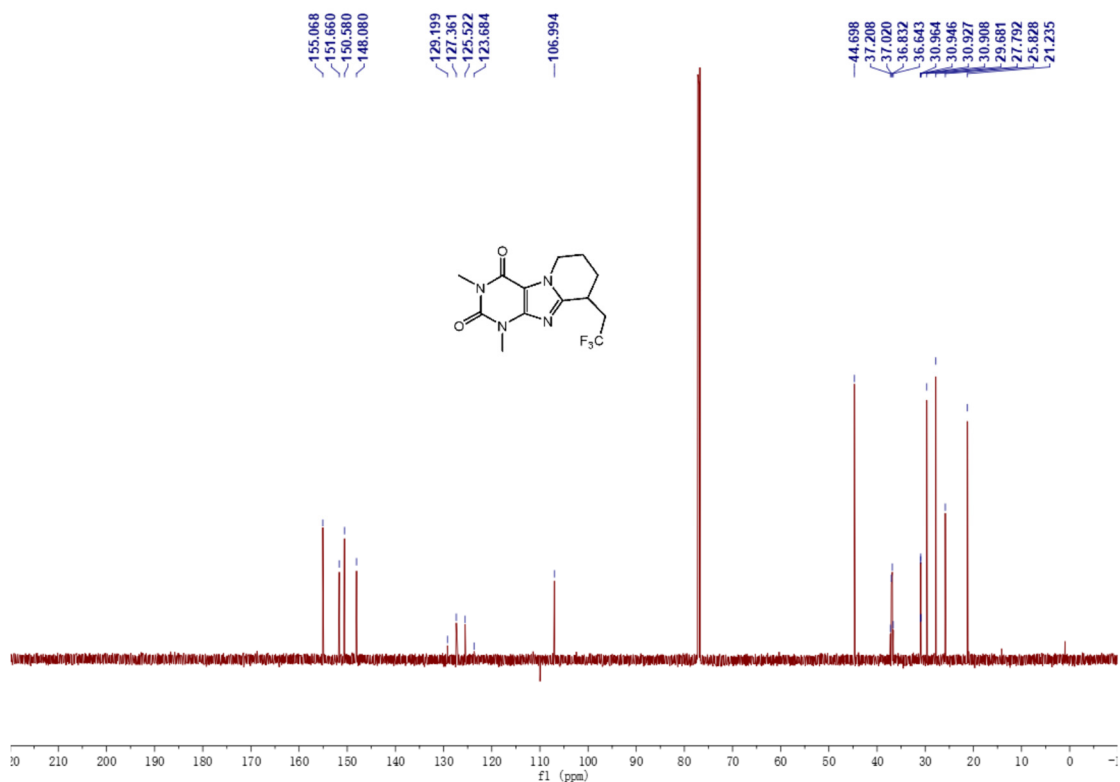
NMR (376 MHz, CDCl_3)



1,3-dimethyl-9-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydropyrido[2,1-*f*]purine-2,4(1H,3H)-dione (**7j**) : ^1H NMR (400 MHz, CDCl_3)



1,3-dimethyl-9-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydropyrido[2,1-*f*]purine-2,4(1*H*,3*H*)-dione (**7j**) : ^{13}C NMR (150 MHz, CDCl_3)



1,3-dimethyl-9-(2,2,2-trifluoroethyl)-6,7,8,9-tetrahydropyrido[2,1-*f*]purine-2,4(1*H*,3*H*)-dione (**7j**) : ^{19}F NMR (376 MHz, CDCl_3)

