One-pot Parallel Synthesis of 5-(Dialkylamino)tetrazoles

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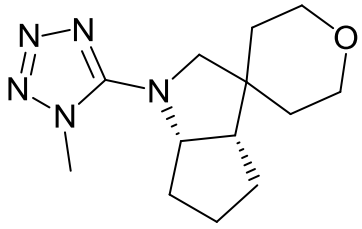
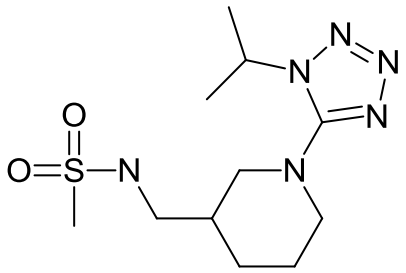
Library characterization data

General Methods. The solvents were purified according to the standard procedures. All starting materials were taken at Enamine Ltd. Reverse phase column chromatography was performed using C_{18}-modified silica gel as a stationary phase. ^{1}H, ^{19}F, and ^{13}C NMR spectra were recorded at 500 MHz, 470, and 126 MHz, respectively. Chemical shifts are reported in ppm downfield from TMS as internal standards. Mass spectra were recorded on an LC–MS instrument with chemical ionization (CI). LC–MS data were acquired on an Agilent 1200 HPLC system equipped with DAD/ELSD/LC–MS-6120 diodematrix and mass-selective detector. Melting points were measured on a MPA100 OptiMelt automated melting point system. Elemental analyses were performed at the Laboratory of Organic Analysis, Department of Chemistry, Taras Shevchenko National University of Kyiv.

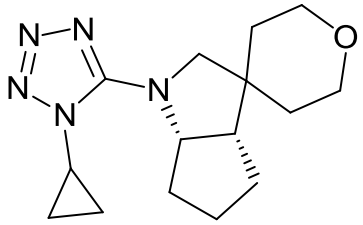
Products obtained by isothiocyanate-based method.



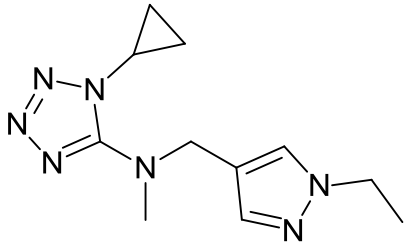
***rac*-(3*aR*,6*aR*)-1-(1-Methyl-1*H*-tetrazol-5-yl)decahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-3,4'-pyran] (8{*2,8*}).** Beige solid, mp = 137–139 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 4.46 (td, J = 6.7, 3.1 Hz, 1H), 3.92 (s, 3H), 3.67 – 3.54 (m, 4H), 3.51 – 3.44 (m, 1H), 3.36 (d, J = 9.9 Hz, 1H), 2.48 – 2.41 (m, 1H), 1.98 – 1.91 (m, 1H), 1.66 – 1.60 (m, 2H), 1.60 – 1.51 (m, 2H), 1.49 – 1.33 (m, 5H) ppm. $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO-d_6): δ 155.6, 64.6, 63.9, 63.6, 56.8, 51.8, 41.2, 36.1, 33.6, 33.1, 31.4, 26.1, 25.5 ppm. LC–MS (*m/z*): 264 ($M + H^+$). Anal. Calcd. for $C_{13}H_{21}N_5O$: C, 59.29; H, 8.04; N, 26.59. Found: C, 59.48; H, 8.19; N, 26.67.



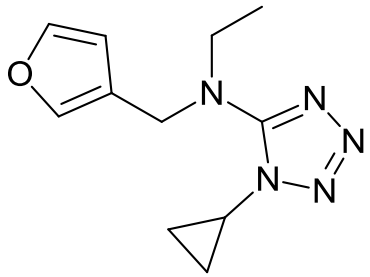
***N*-((1-(1-Isopropyl-1*H*-tetrazol-5-yl)piperidin-3-yl)methyl)methanesulfonamide (8{*10,50*}).** White solid, mp = 114–116 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.08 (s, 1H), 4.56 (hept, J = 6.5 Hz, 1H), 3.38 (dd, J = 12.3, 3.5 Hz, 1H), 3.28 (dt, J = 13.4, 3.9 Hz, 1H), 2.94 – 2.90 (m, 3H), 2.89 (s, 3H), 2.74 (dd, J = 12.2, 9.4 Hz, 1H), 1.94 – 1.80 (m, 1H), 1.80 – 1.70 (m, 2H), 1.68 – 1.56 (m, 1H), 1.47 (d, J = 6.4 Hz, 3H), 1.45 (d, J = 6.4 Hz, 3H), 1.26 – 1.17 (m, 1H) ppm. $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO-d_6): δ 158.5, 53.7, 50.9, 49.5, 45.2, 35.3, 27.1, 23.5, 22.22, 22.16 ppm. LC–MS (*m/z*): 303 ($M + H^+$). Anal. Calcd. for $C_{11}H_{22}N_6O_2S$: C, 43.69; H, 7.33; N, 27.79; S, 10.60. Found: C, 43.29; H, 7.54; N, 27.85; S, 10.82.



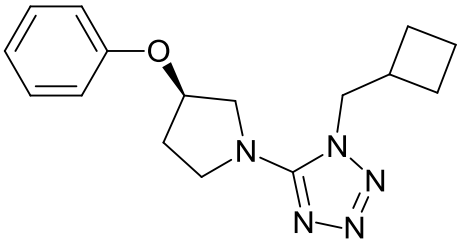
***rac*-(3a*R*,6a*R*)-1-(1-Cyclopropyl-1*H*-tetrazol-5-yl)decahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-3,4'-pyran] (8**{*15,8)*}**).** Yellow solid, mp = 92–95 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 4.53 (td, *J* = 6.8, 2.9 Hz, 1H), 3.75 (d, *J* = 10.1 Hz, 1H), 3.70 (tt, *J* = 7.1, 3.7 Hz, 1H), 3.66 – 3.52 (m, 3H), 3.51 – 3.44 (m, 1H), 3.40 (d, *J* = 10.1 Hz, 1H), 1.98 (dt, *J* = 11.4, 6.5 Hz, 1H), 1.69 – 1.55 (m, 4H), 1.54 – 1.40 (m, 5H), 1.39 – 1.29 (m, 1H), 1.25 – 1.06 (m, 3H), 1.05 – 0.96 (m, 1H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 156.2, 64.6, 64.2, 63.7, 56.6, 51.5, 41.2, 36.1, 33.2, 31.4, 27.6, 26.0, 25.5, 7.9, 7.4 ppm. LC–MS (*m/z*): 290 (M + H$^+$). Anal. Calcd. for $C_{15}H_{23}N_5O$: C, 62.26; H, 8.01; N, 24.20. Found: C, 62.12; H, 7.70; N, 23.94.



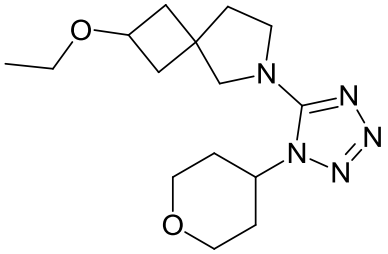
1-Cyclopropyl-*N*-((1-ethyl-1*H*-pyrazol-4-yl)methyl)-*N*-methyl-1*H*-tetrazol-5-amine (8{*15,71*}**).** Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.72 (s, 1H), 7.40 (s, 1H), 4.46 (s, 2H), 4.08 (q, *J* = 7.2 Hz, 2H), 3.73 – 3.67 (m, 1H), 2.99 (s, 3H), 1.33 (t, *J* = 7.2 Hz, 3H), 1.21 – 1.12 (m, 4H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 158.6, 138.5, 128.8, 115.3, 46.5, 46.1, 37.1, 28.5, 15.5, 7.7 ppm. LC–MS (*m/z*): = 248 (M + H$^+$). Anal. Calcd. for $C_{11}H_{17}N_7$: C, 53.42; H, 6.93; N, 39.65. Found: C, 53.28; H, 7.11; N, 39.43.



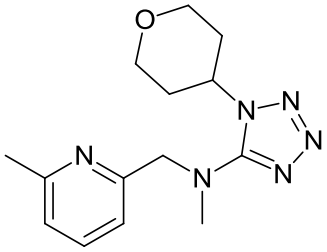
1-Cyclopropyl-*N*-ethyl-*N*-(furan-3-ylmethyl)-1*H*-tetrazol-5-amine (8{*15,72)*}**).** Beige solid, mp = 60–62 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.67 (s, 1H), 7.62 (s, 1H), 6.44 (s, 1H), 4.47 (s, 2H), 3.64 (quint, *J* = 5.3 Hz, 1H), 3.43 (q, *J* = 7.1 Hz, 2H), 1.15 (d, *J* = 5.3 Hz, 4H), 1.10 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 158.2, 143.7, 141.2, 121.0, 110.7, 44.0, 43.9, 28.4, 12.4, 7.4 ppm. LC–MS (*m/z*): 234 (M + H$^+$). Anal. Calcd. for $C_{11}H_{15}N_5O$: C, 56.64; H, 6.48; N, 30.02. Found: C, 56.98; H, 6.76; N, 29.86.



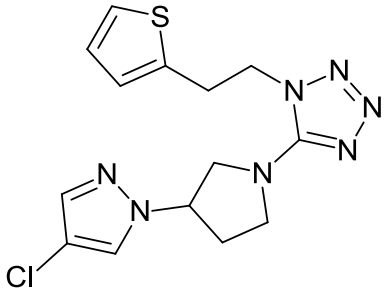
(*R*)-1-(Cyclobutylmethyl)-5-(3-phenoxypyrrolidin-1-yl)-1*H*-tetrazole (8{*36,164*}**).** White solid, mp = 52–54 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.30 (t, J = 7.8 Hz, 2H), 6.98 – 6.94 (m, 3H), 5.16 – 5.12 (m, 1H), 4.33 (d, J = 2.3 Hz, 1H), 4.32 (d, J = 2.2 Hz, 1H), 3.88 (dd, J = 11.2, 4.6 Hz, 1H), 3.70 – 3.62 (m, 3H), 2.74 (hept, J = 7.6 Hz, 1H), 2.33 – 2.23 (m, 1H), 2.20 – 2.12 (m, 1H), 1.98 – 1.91 (m, 2H), 1.86 – 1.73 (m, 4H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 156.8, 155.7, 129.6, 121.0, 115.5, 75.7, 54.7, 51.1, 47.4, 34.5, 30.9, 25.15, 25.12, 17.6 ppm. LC–MS (*m/z*): 300 (M + H$^+$). Anal. Calcd. for $C_{16}H_{21}N_5O$: C, 64.19; H, 7.07; N, 23.39. Found: C, 64.52; H, 6.87; N, 23.42.



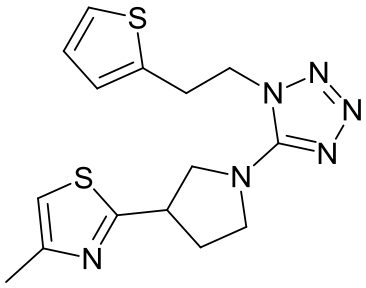
1-(1-(1-Methylcyclopropyl)-1*H*-tetrazol-5-yl)-4-((methylsulfonyl)methyl)piperidine (8{*40,188*}**).** Beige solid, mp = 66–69 °C. The compound existed as a *ca*. 3:2 mixture of rotamers. ^{1}H NMR (500 MHz, DMSO-d_6): δ 4.68 – 4.56 (m, 1H), 4.02 – 3.91 (m, 3H), 3.57 – 3.50 (m, 4H), 3.49 (s, 2H), 3.35 – 3.30 (m, 2H), 2.29 (ddd, J = 9.7, 7.0, 2.8 Hz, 0.8H), 2.23 (ddd, J = 9.6, 6.9, 2.9 Hz, 1.2H), 2.03 – 1.85 (m, 8H), 1.09 (t, J = 7.0 Hz, 3H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 155.8 and 155.5, 68.1 and 67.9, 65.73 and 65.70, 62.4, 60.5 and 59.9, 53.3, 48.5 and 47.9, 38.1, 37.4, 36.8 and 36.4, 32.85 and 32.76, 15.2 ppm. LC–MS (*m/z*): 308 (M + H$^+$). Anal. Calcd. for $C_{15}H_{25}N_5O_2$: C, 58.61; H, 8.20; N, 22.78. Found: C, 58.70; H, 8.00; N, 22.60.



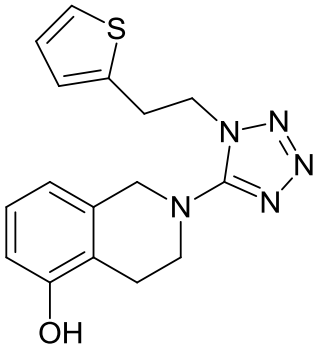
***N*-Methyl-*N*-((6-methylpyridin-2-yl)methyl)-1-(tetrahydro-2*H*-pyran-4-yl)-1*H*-tetrazol-5-amine (8**{*40,192*}**).** Brown solid, mp = 71–74 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.68 (t, J = 7.7 Hz, 1H), 7.20 (d, J = 7.7 Hz, 1H), 7.18 (d, J = 7.7 Hz, 1H), 4.82 (tt, J = 10.4, 5.3 Hz, 1H), 4.48 (s, 2H), 3.96 (d, J = 11.3 Hz, 2H), 3.42 (td, J = 11.4, 3.5 Hz, 2H), 3.00 (s, 3H), 2.43 (s, 3H), 2.05 – 1.96 (m, 4H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 158.1, 157.7, 155.8, 137.2, 122.0, 119.2, 65.9, 58.9, 53.6, 39.6, 32.5, 24.0 ppm. LC–MS (*m/z*): 289 (M + H$^+$). Anal. Calcd. for $C_{14}H_{20}N_6O$: C, 58.31; H, 6.99; N, 29.15. Found: C, 58.48; H, 7.31; N, 29.38.



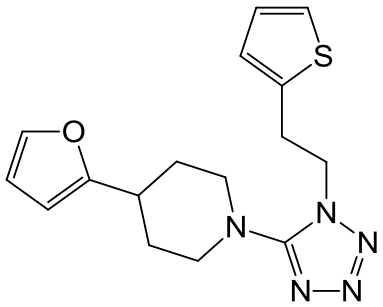
5-(3-(4-Chloro-1*H*-pyrazol-1-yl)pyrrolidin-1-yl)-1-(2-(thiophen-2-yl)ethyl)-1*H*-tetrazole (8{*41,147*}**).** Beige solid, mp = 92–94 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.08 (s, 1H), 7.58 (s, 1H), 7.33 (d, *J* = 5.1 Hz, 1H), 6.93 (dd, *J* = 5.1, 3.4 Hz, 1H), 6.81 (d, *J* = 3.4 Hz, 1H), 5.09 – 5.01 (m, 1H), 4.54 (t, *J* = 7.0 Hz, 2H), 3.91 (dd, *J* = 10.4, 6.3 Hz, 1H), 3.77 (dd, *J* = 10.4, 3.9 Hz, 1H), 3.67 (q, *J* = 7.9 Hz, 1H), 3.60 (dt, *J* = 9.0, 4.4 Hz, 1H), 3.35 – 3.29 (m, 2H), 2.44 – 2.32 (m, 2H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 155.6, 138.8, 137.2, 127.3, 127.1, 126.1, 124.8, 108.3, 60.3, 54.1, 47.8, 47.6, 31.0, 29.0 ppm. LC–MS (*m/z*): = 350 (M + H$^+$). Anal. Calcd. for $C_{14}H_{16}ClN_7S$: C, 48.07; H, 4.61; N, 28.03; S, 9.16; Cl, 10.13. Found: C, 47.96; H, 4.57; N, 28.14; S, 8.93; Cl, 9.87.



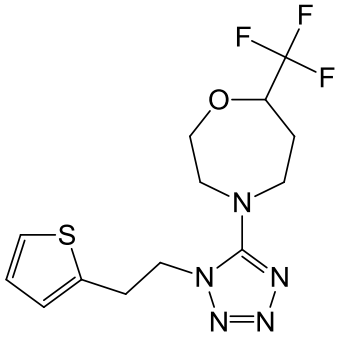
4-Methyl-2-(1-(1-(2-(thiophen-2-yl)ethyl)-1*H*-tetrazol-5-yl)pyrrolidin-3-yl)thiazole (8{*41,148*}**).** Brown oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.33 (d, *J* = 5.1 Hz, 1H), 7.17 (s, 1H), 6.92 (t, *J* = 5.1, 3.4 Hz, 1H), 6.81 (d, *J* = 3.4 Hz, 1H), 4.54 (t, *J* = 7.0 Hz, 2H), 3.90 – 3.82 (m, 2H), 3.69 – 3.52 (m, 3H), 3.33 (t, *J* = 6.9 Hz, 2H), 2.43 – 2.36 (m, 1H), 2.32 (s, 3H), 2.19 – 2.11 (m, 1H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 169.5, 155.7, 151.6, 138.8, 127.1, 126.2, 124.9, 113.7, 54.5, 48.5, 47.8, 41.6, 32.1, 29.0, 16.8 ppm. LC–MS (*m/z*): = 347 (M + H$^+$). Anal. Calcd. for $C_{15}H_{18}N_6S_2$: C, 52.00; H, 5.24; N, 24.26; S, 18.51. Found: C, 52.17; H, 5.34; N, 24.21; S, 18.37.



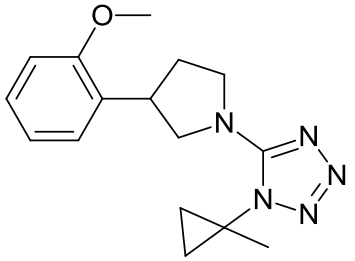
2-(1-(2-(Thiophen-2-yl)ethyl)-1*H*-tetrazol-5-yl)-1,2,3,4-tetrahydroisoquinolin-5-ol (8{*41*,*210*}**).** Beige solid, mp = 116–119 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 9.46 (s, 1H), 7.32 (dd, *J* = 5.1, 1.3 Hz, 1H), 6.98 (t, *J* = 7.8 Hz, 1H), 6.91 (t, *J* = 5.1, 3.4 Hz, 1H), 6.81 (d, *J* = 3.4 Hz, 1H), 6.67 (d, *J* = 7.9 Hz, 1H), 6.58 (d, *J* = 7.6 Hz, 1H), 4.53 (t, *J* = 6.8 Hz, 2H), 4.30 (s, 2H), 3.44 – 3.39 (m, 4H), 2.72 (t, *J* = 6.0 Hz, 2H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 158.7, 154.8, 138.9, 134.0, 127.1, 126.4, 126.1, 124.9, 120.4, 116.8, 112.4, 50.8, 48.2, 47.1, 27.8, 22.5 ppm. LC–MS (*m/z*): 328 (M + H$^+$). Anal. Calcd. for $C_{16}H_{17}N_5OS$: C, 58.70; H, 5.23; N, 21.39; S, 9.79. Found: C, 58.98; H, 5.44; N, 21.04; S, 9.56.



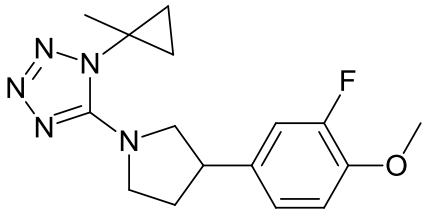
4-(Furan-2-yl)-1-(1-(2-(thiophen-2-yl)ethyl)-1*H*-tetrazol-5-yl)piperidine (8{*41*,*211*}**).** Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.53 (s, 1H), 7.32 (d, *J* = 5.2 Hz, 1H), 6.93 – 6.88 (m, 1H), 6.78 (d, *J* = 3.4 Hz, 1H), 6.37 (s, 1H), 6.12 (d, *J* = 3.1 Hz, 1H), 4.46 (t, *J* = 6.8 Hz, 2H), 3.42 – 3.36 (m, 4H), 3.00 (t, *J* = 12.2 Hz, 2H), 2.89 – 2.82 (m, 1H), 2.02 – 1.90 (m, 2H), 1.72 – 1.62 (m, 2H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 159.0, 158.2, 141.3, 138.9, 127.0, 126.1, 124.8, 110.2, 103.7, 49.2, 48.1, 33.8, 29.6, 27.8 ppm. LC–MS (*m/z*): 330 (M + H$^+$). Anal. Calcd. for $C_{16}H_{19}N_5OS$: C, 58.34; H, 5.81; N, 21.26; S, 9.73. Found: C, 58.07; H, 5.83; N, 21.40; S, 9.64.



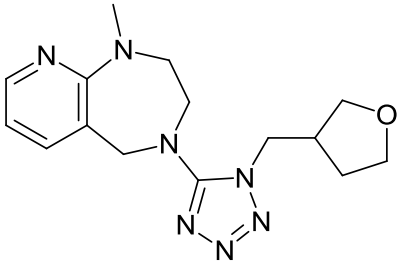
4-(1-(2-(Thiophen-2-yl)ethyl)-1*H*-tetrazol-5-yl)-7-(trifluoromethyl)-1,4-oxazepane (8{*41*,*212*}**).** Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.34 (d, *J* = 5.1 Hz, 1H), 6.94 – 6.90 (m, 1H), 6.83 – 6.77 (m, 1H), 4.54 – 4.43 (m, 2H), 4.31 – 4.24 (m, 1H), 4.02 (d, *J* = 12.9 Hz, 1H), 3.78 – 3.71 (m, 1H), 3.58 – 3.46 (m, 4H), 3.37 (t, *J* = 6.9 Hz, 2H), 2.13 – 2.05 (m, 1H), 2.01 – 1.94 (m, 1H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 157.9, 138.9, 127.1, 126.2, 124.9, 124.8 (q, *J* = 281.1 Hz), 75.4 (q, *J* = 29.8 Hz), 68.8, 53.1, 48.4, 48.3, 28.3, 28.1 ppm. ^{19}F{^{1}H} NMR (376 MHz, DMSO-d_6): δ –77.6 ppm. LC–MS (*m/z*): 348 (M + H$^+$). Anal. Calcd. for $C_{13}H_{16}F_3N_5OS$: C, 44.95; H, 4.64; N, 20.16; S, 9.23. Found: C, 44.92; H, 4.83; N, 19.96; S, 9.00.



5-(3-(2-Methoxyphenyl)pyrrolidin-1-yl)-1-(1-methylcyclopropyl)-1*H*-tetrazole (8{*42,193)*}**).** White solid, mp = 106–108 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.29 – 7.21 (m, 2H), 7.01 (d, *J* = 8.1 Hz, 1H), 6.93 (t, *J* = 7.5 Hz, 1H), 4.00 (dd, *J* = 9.5, 7.3 Hz, 1H), 3.82 (s, 3H), 3.78 – 3.65 (m, 3H), 3.54 – 3.49 (m, 1H), 2.33 – 2.24 (m, 1H), 2.11 (dq, *J* = 12.0, 8.6 Hz, 1H), 1.56 (s, 3H), 1.35 – 1.26 (m, 2H), 1.13 – 1.06 (m, 2H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 157.1, 156.0, 129.0, 127.9, 126.7, 120.5, 110.9, 55.4, 54.5, 49.2, 37.3, 34.2, 30.7, 23.9, 15.1, 14.9 ppm. LC–MS (*m/z*): 300 (M + H$^+$). Anal. Calcd. for $C_{16}H_{21}N_5O$: C, 64.19; H, 7.07; N, 23.39. Found: C, 64.57; H, 7.44; N, 23.30.

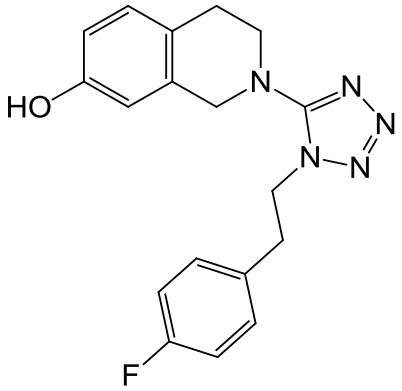


5-(3-(3-Fluoro-4-methoxyphenyl)pyrrolidin-1-yl)-1-(1-methylcyclopropyl)-1*H*-tetrazole (8{*42,227*}**).** White solid, mp = 95–97 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.24 (d, *J* = 13.1 Hz, 1H), 7.13 – 7.10 (m, 2H), 4.03 – 3.94 (m, 1H), 3.82 (s, 3H), 3.80 – 3.76 (m, 1H), 3.68 (td, *J* = 9.4, 6.9 Hz, 1H), 3.53 – 3.44 (m, 2H), 2.37 – 2.29 (m, 1H), 2.10 – 2.01 (m, 1H), 1.56 (s, 3H), 1.37 – 1.24 (m, 2H), 1.14 – 1.08 (m, 2H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 155.9, 151.4 (d, *J* = 243.4 Hz), 145.8 (d, *J* = 10.5 Hz), 134.3 (d, *J* = 6.0 Hz), 123.3 (d, *J* = 3.2 Hz), 114.8 (d, *J* = 18.0 Hz), 113.9 (d, *J* = 2.1 Hz), 56.0, 55.8, 49.6, 42.4, 34.2, 32.4, 23.9, 15.1, 14.8 ppm. ^{19}F NMR (470 MHz, DMSO-d_6): δ –135.2 – –135.3 (m) ppm. LC–MS (*m/z*): 318 (M + H$^+$). Anal. Calcd. for $C_{16}H_{20}FN_5O$: C, 60.55; H, 6.35; N, 22.07. Found: C, 60.54; H, 6.62; N, 21.69.

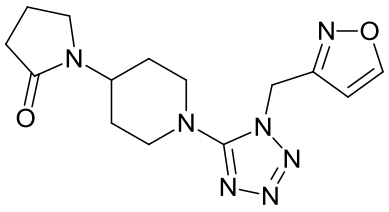


1-Methyl-4-(1-((tetrahydrofuran-3-yl)methyl)-1*H*-tetrazol-5-yl)-2,3,4,5-tetrahydro-1*H*-pyrido[2,3-e][1,4]diazepine (8{*51,251*}**).** Brownish oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.05 (dd, *J* = 4.8, 1.8 Hz, 1H), 7.50 (dd, *J* = 7.3, 1.8 Hz, 1H), 6.71 (dd, *J* = 7.3, 4.8 Hz, 1H), 4.53 (s, 2H), 4.22 (d, *J* = 7.6 Hz, 2H), 3.73 – 3.69 (m, 3H), 3.61 (td, *J* = 9.1, 7.1 Hz, 2H), 3.55 – 3.51 (m, 2H), 3.37 (dd, *J* = 8.8, 5.4 Hz, 1H), 2.99 (s, 3H), 2.77 – 2.65 (m, 1H), 1.94 – 1.83 (m, 1H), 1.57 – 1.46 (m, 1H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 160.2, 157.9, 146.2, 137.8, 119.9, 114.1, 70.0, 66.7, 52.5, 52.1, 51.4, 49.6,

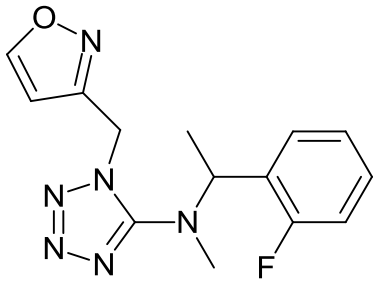
39.6, 37.9, 29.2 ppm. LC–MS (*m/z*): 316 (M + H^+). Anal. Calcd. for $C_{15}H_{21}N_7O$: C, 57.13; H, 6.71; N, 31.09. Found: C, 57.39; H, 7.08; N, 31.47.



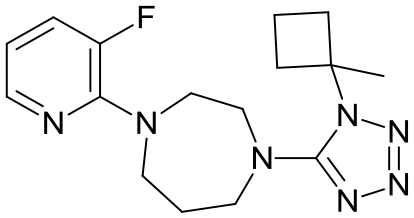
2-(1-(4-Fluorophenethyl)-1*H*-tetrazol-5-yl)-1,2,3,4-tetrahydroisoquinolin-7-ol (8{*53,236*}**).** Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 9.23 (s, 1H), 7.19 – 7.15 (m, 2H), 7.08 – 7.03 (m, 2H), 6.95 (d, *J* = 8.3 Hz, 1H), 6.61 (d, *J* = 8.3 Hz, 1H), 6.53 (s, 1H), 4.52 (t, *J* = 7.1 Hz, 2H), 4.28 (s, 2H), 3.40 (t, *J* = 6.0 Hz, 2H), 3.16 (t, *J* = 6.9 Hz, 2H), 2.77 (t, *J* = 6.0 Hz, 2H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 161.1 (d, *J* = 242.4 Hz), 158.5, 155.4, 133.7, 133.4 (d, *J* = 2.9 Hz), 130.6 (d, *J* = 8.0 Hz), 129.5, 123.5, 115.1 (d, *J* = 21.1 Hz), 114.1, 112.4, 50.6, 48.1, 47.4, 33.0, 26.8 ppm. ^{19}F{^{1}H} NMR (376 MHz, DMSO-d_6): δ –116.7 ppm. LC–MS (*m/z*): 340 (M + H^+). Anal. Calcd. for $C_{18}H_{18}FN_5O$: C, 63.70; H, 5.35; N, 20.64. Found: C, 64.08; H, 4.98; N, 20.68.



1-(1-(1-(Isoxazol-3-ylmethyl)-1*H*-tetrazol-5-yl)piperidin-4-yl)pyrrolidin-2-one (8{*56,108*}**).** Brown solid, mp = 88–92 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.98 (d, *J* = 1.7 Hz, 1H), 6.59 (d, *J* = 1.7 Hz, 1H), 5.68 (s, 2H), 3.96 (tt, *J* = 12.1, 4.1 Hz, 1H), 3.64 (d, *J* = 12.8 Hz, 2H), 3.27 (t, *J* = 7.0 Hz, 2H), 3.07 (td, *J* = 12.8, 2.4 Hz, 2H), 2.22 (t, *J* = 8.1 Hz, 2H), 1.90 (quint, *J* = 7.5 Hz, 2H), 1.78 – 1.66 (m, 2H), 1.61 – 1.53 (m, 2H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 173.4, 161.1, 158.2, 157.6, 104.3, 48.8, 47.7, 42.4, 42.4, 30.9, 28.0, 17.7 ppm. LC–MS (*m/z*): 318 (M + H^+). Anal. Calcd. for $C_{14}H_{19}N_7O_2$: C, 52.99; H, 6.03; N, 30.90. Found: C, 52.85; H, 6.07; N, 30.72.

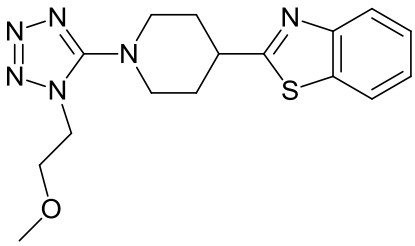


***N*-(1-(2-Fluorophenyl)ethyl)-1-(isoxazol-3-ylmethyl)-*N*-methyl-1*H*-tetrazol-5-amine (8**{*56,271*}**).** Brown oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.96 (s, 1H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.35 (q, *J* = 6.5 Hz, 1H), 7.20 (t, *J* = 7.5 Hz, 1H), 7.13 (dd, *J* = 10.8, 8.2 Hz, 1H), 6.52 (s, 1H), 5.76 (d, *J* = 16.8 Hz, 1H), 5.72 (d, *J* = 16.8 Hz, 1H), 5.23 (q, *J* = 6.9 Hz, 1H), 2.71 (s, 3H), 1.52 (d, *J* = 7.0 Hz, 3H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 161.1, 160.2 (d, *J* = 246.0 Hz), 158.2, 157.9, 129.8 (d, *J* = 8.6 Hz), 128.7 (d, *J* = 4.0 Hz), 126.5 (d, *J* = 13.7 Hz), 124.3 (d, *J* = 3.3 Hz), 115.4 (d, *J* = 22.1 Hz), 104.0, 53.1, 42.5, 32.8, 15.8 ppm. ^{19}F NMR (470 MHz, DMSO-d_6): δ –117.0 (dt, *J* = 11.8, 6.4 Hz) ppm. LC–MS (*m/z*): 303 (M + H$^+$). Anal. Calcd. for $C_{14}H_{15}FN_6O$: C, 55.62; H, 5.00; N, 27.80. Found: C, 55.77; H, 4.61; N, 27.73.



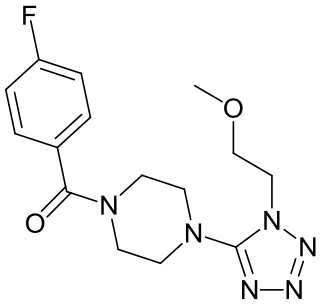
1-(3-Fluoropyridin-2-yl)-4-(1-(1-methylcyclobutyl)-1*H*-tetrazol-5-yl)-1,4-diazepane (8{*58,280*}**).** Brownish oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.90 – 7.87 (m, 1H), 7.41 (dd, *J* = 14.6, 7.8 Hz, 1H), 6.66 (ddd, *J* = 7.8, 4.7, 2.9 Hz, 1H), 3.85 (t, *J* = 5.2 Hz, 2H), 3.68 (t, *J* = 5.3 Hz, 2H), 3.51 (t, *J* = 5.3 Hz, 2H), 3.36 – 3.33 (m, 2H), 2.71 (qd, *J* = 10.0, 2.7 Hz, 2H), 2.25 (tt, *J* = 8.8, 2.6 Hz, 2H), 2.01 – 1.89 (m, 3H), 1.82 – 1.75 (m, 1H), 1.64 (s, 3H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 157.1, 148.0 (d, *J* = 126.3 Hz), 147.0 (d, *J* = 132.7 Hz), 142.9 (d, *J* = 5.0 Hz), 123.5 (d, *J* = 19.5 Hz), 113.5 (d, *J* = 2.1 Hz), 59.9, 52.7, 50.9, 49.4 (d, *J* = 4.7 Hz), 48.4 (d, *J* = 7.1 Hz), 33.9, 27.4, 24.9, 14.1 ppm. ^{19}F NMR (470 MHz, DMSO-d_6): δ –131.8 (d, *J* = 14.6 Hz) ppm. LC–MS (*m/z*): 332 (M + H$^+$). Anal. Calcd. for $C_{16}H_{22}FN_7$: C, 57.99; H, 6.69; N, 29.59. Found: C, 57.72; H, 6.69; N, 29.19.

Products obtained by BTTC-based method.

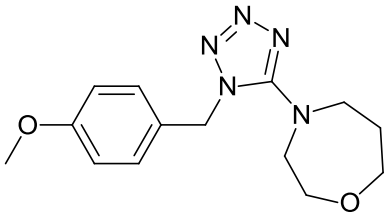


2-(1-(1-(2-Methoxyethyl)-1*H*-tetrazol-5-yl)piperidin-4-yl)benzo[*d*]thiazole (9{*4,289*}**).** Beige solid, mp = 90–93 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.08 (d, *J* = 8.0 Hz, 1H), 7.96 (d, *J* = 8.1 Hz, 1H),

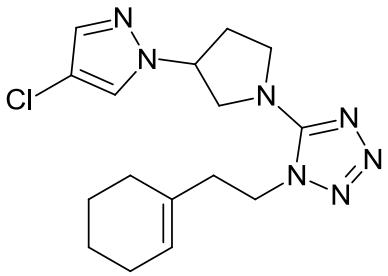
7.50 (t, *J* = 7.6 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 1H), 4.41 (t, *J* = 5.2 Hz, 2H), 3.82 (t, *J* = 5.2 Hz, 2H), 3.71 – 3.61 (m, 2H), 3.47 – 3.39 (m, 1H), 3.23 (s, 3H), 3.17 (t, *J* = 11.7 Hz, 2H), 2.23 – 2.17 (m, 2H), 2.00 (qd, *J* = 12.1, 3.8 Hz, 2H) ppm. $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO-d_6): δ 174.8, 159.1, 152.6, 134.1, 126.1, 124.9, 122.4, 122.2, 68.6, 58.1, 49.4, 46.6, 39.5, 31.0 ppm. LC–MS (*m/z*): 345 ($M + H^+$). Anal. Calcd. for $C_{16}H_{20}N_6OS$: C, 55.79; H, 5.85; N, 24.40; S, 9.31. Found: C, 55.42; H, 5.56; N, 24.75; S, 9.48.



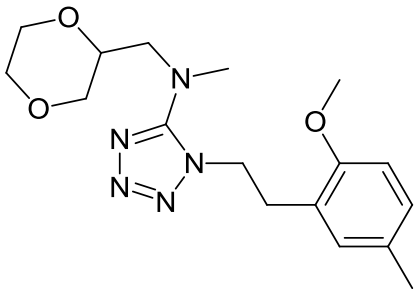
(4-Fluorophenyl)(4-(1-(2-methoxyethyl)-1*H*-tetrazol-5-yl)piperazin-1-yl)methanone (9{*4,291*}**).** Brown oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.52 (dd, *J* = 8.5, 5.6 Hz, 2H), 7.29 (t, *J* = 8.8 Hz, 2H), 4.41 (t, *J* = 5.2 Hz, 2H), 3.79 (t, *J* = 5.2 Hz, 2H), 3.74 – 3.40 (m, 4H), 3.33 – 3.24 (m, 4H), 3.21 (s, 3H) ppm. $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO-d_6): δ 168.3, 162.6 (d, *J* = 246.7 Hz), 158.6, 132.0 (d, *J* = 3.3 Hz), 129.7 (d, *J* = 8.7 Hz), 115.4 (d, *J* = 21.6 Hz), 68.7, 58.1, 49.3 (2C), 46.6 ppm. ^{19}F NMR (470 MHz, DMSO-d_6): δ –111.0 (tt, *J* = 9.3, 5.5 Hz) ppm. LC–MS (*m/z*): 335 ($M + H^+$). Anal. Calcd. for $C_{15}H_{19}FN_6O_2$: C, 53.88; H, 5.73; N, 25.14. Found: C, 53.61; H, 5.83; N, 24.93.



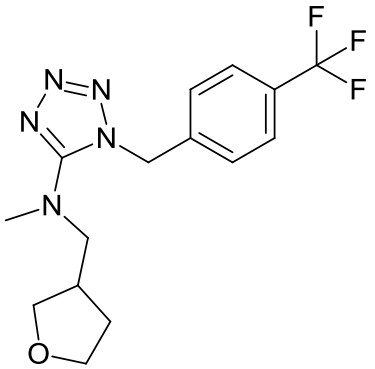
4-(1-(4-Methoxybenzyl)-1*H*-tetrazol-5-yl)-1,4-oxazepane (9{*18,300*}**).** Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.10 (d, *J* = 8.6 Hz, 2H), 6.93 (d, *J* = 8.6 Hz, 2H), 5.49 (s, 2H), 3.73 (s, 3H), 3.69 – 3.64 (m, 2H), 3.60 (t, *J* = 5.6 Hz, 2H), 3.57 – 3.50 (m, 4H), 1.81 (quint, *J* = 5.7 Hz, 2H) ppm. $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO-d_6): δ 158.9, 157.2, 128.1, 127.2, 114.3, 68.8, 68.8, 55.1, 52.8, 49.8, 49.3, 29.8 ppm. LC–MS (*m/z*): = 290 ($M + H^+$). Anal. Calcd. for $C_{14}H_{19}N_5O_2$: C, 58.12; H, 6.62; N, 24.21. Found: C, 58.43; H, 6.59; N, 24.32.



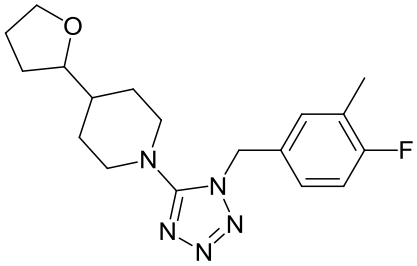
5-(3-(4-Chloro-1*H*-pyrazol-1-yl)pyrrolidin-1-yl)-1-(2-(cyclohex-1-en-1-yl)ethyl)-1*H*-tetrazole (9{*25*,*147*}**).** Brown oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.13 (s, 1H), 7.58 (s, 1H), 5.29 – 5.26 (m, 1H), 5.09 (tt, *J* = 6.3, 3.9 Hz, 1H), 4.35 (t, *J* = 7.3 Hz, 2H), 3.96 (dd, *J* = 10.5, 6.3 Hz, 1H), 3.83 (dd, *J* = 10.4, 3.7 Hz, 1H), 3.74 (q, *J* = 8.0 Hz, 1H), 3.66 (td, *J* = 8.6, 5.1 Hz, 1H), 2.47 – 2.39 (m, 2H), 2.34 (t, *J* = 7.3 Hz, 2H), 1.91 – 1.86 (m, 2H), 1.85 – 1.80 (m, 2H), 1.54 – 1.48 (m, 2H), 1.45 – 1.40 (m, 2H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 155.7, 137.2, 133.1, 127.4, 123.6, 108.3, 60.3, 54.3, 47.7, 45.3, 37.2, 30.9, 27.4, 24.6, 22.2, 21.7 ppm. LC–MS (*m/z*): 348 (M + H$^+$). Anal. Calcd. for $C_{16}H_{22}ClN_7$: C, 55.25; H, 6.38; N, 28.19; Cl, 10.19. Found: C, 54.89; H, 6.05; N, 28.50; Cl, 9.87.



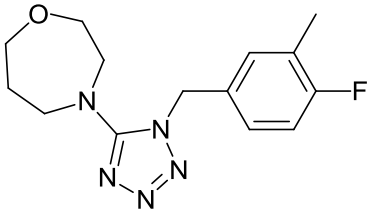
***N*-((1,4-Dioxan-2-yl)methyl)-1-(2-methoxy-5-methylphenethyl)-*N*-methyl-1*H*-tetrazol-5-amine (9**{*52*,*319*}**).** Brown oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.02 (d, *J* = 8.2 Hz, 1H), 6.88 – 6.83 (m, 2H), 4.42 (t, *J* = 7.4 Hz, 2H), 3.79 – 3.74 (m, 1H), 3.73 (s, 3H), 3.67 (d, *J* = 11.5 Hz, 2H), 3.62 (d, *J* = 11.3 Hz, 1H), 3.53 (td, *J* = 11.3, 2.5 Hz, 1H), 3.42 (td, *J* = 11.3, 2.5 Hz, 1H), 3.38 – 3.33 (m, 1H), 3.28 – 3.22 (m, 1H), 3.23 – 3.12 (m, 1H), 3.03 – 3.00 (m, 2H), 2.99 (s, 3H), 2.18 (s, 3H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 158.1, 155.2, 131.0, 128.9, 128.5, 124.5, 110.6, 72.7, 68.1, 65.9, 65.7, 55.3, 53.9, 46.7, 39.2, 30.0, 20.0 ppm. LC–MS (*m/z*): = 348 (M + H$^+$). Anal. Calcd. for $C_{17}H_{25}N_5O_3$: C, 58.77; H, 7.25; N, 20.16. Found: C, 58.97; H, 7.31; N, 20.05.



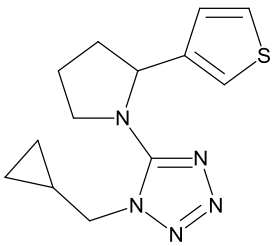
***N*-Methyl-*N*-((tetrahydrofuran-3-yl)methyl)-1-(4-(trifluoromethyl)benzyl)-1*H*-tetrazol-5-amine (9**{*55*,*337*}**).** Colorless oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.76 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 5.71 (s, 2H), 3.60 (td, *J* = 8.1, 5.3 Hz, 1H), 3.55 – 3.43 (m, 2H), 3.24 (qd, *J* = 13.6, 7.7 Hz, 2H), 3.17 (dd, *J* = 8.5, 5.7 Hz, 1H), 2.92 (s, 3H), 2.41 (dq, *J* = 14.1, 7.0 Hz, 1H), 1.78 – 1.69 (m, 1H), 1.34 – 1.25 (m, 1H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 158.3, 140.1, 128.6 (q, *J* = 31.9 Hz), 127.6, 125.8 (q, *J* = 3.8 Hz), 124.1 (q, *J* = 272.1 Hz), 70.0, 66.6, 55.6, 49.6, 38.7, 36.9, 29.1 ppm. ^{19}F NMR (470 MHz, DMSO-d_6): δ –61.1 ppm. LC–MS (*m/z*): = 342 (M + H$^+$). Anal. Calcd. for $C_{15}H_{18}F_3N_5O$: C, 52.78; H, 5.32; N, 20.52. Found: C, 52.49; H, 5.39; N, 20.39.



1-(1-(4-Fluoro-3-methylbenzyl)-1*H*-tetrazol-5-yl)-4-(tetrahydrofuran-2-yl)piperidine (9{*57,261*}**).** Beige solid, mp = 79–81 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.18 – 7.12 (m, 2H), 7.08 – 7.03 (m, 1H), 5.45 (s, 2H), 3.69 (q, *J* = 7.1 Hz, 1H), 3.58 (q, *J* = 7.2 Hz, 1H), 3.51 (d, *J* = 12.5 Hz, 2H), 3.44 (q, *J* = 7.2 Hz, 1H), 2.87 (dt, *J* = 12.8, 10.1 Hz, 2H), 2.21 (s, 3H), 1.90 – 1.82 (m, 1H), 1.81 – 1.74 (m, 3H), 1.54 (d, *J* = 13.5 Hz, 1H), 1.50 – 1.40 (m, 2H), 1.31 – 1.17 (m, 2H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 161.2, 159.3, 158.4, 130.6 (t, *J* = 4.7 Hz), 126.8 (d, *J* = 8.4 Hz), 124.7 (d, *J* = 17.7 Hz), 115.3 (d, *J* = 22.5 Hz), 82.0, 67.0, 49.37, 49.36, 49.28, 28.4, 27.8, 27.2, 25.3 (2C), 14.1 (d, *J* = 3.3 Hz) ppm. ^{19}F{^{1}H} NMR (470 MHz, DMSO-d_6): δ –118.6 ppm. LC–MS (*m/z*): 346 (M + H^{+}). Anal. Calcd. for $C_{18}H_{24}FN_5O$: C, 62.59; H, 7.00; N, 20.28. Found: C, 62.45; H, 6.88; N, 20.02.

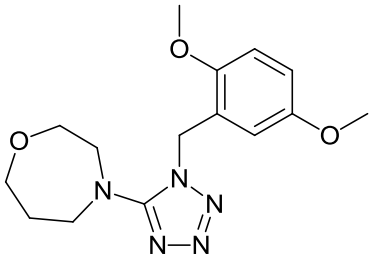


4-(1-(4-Fluoro-3-methylbenzyl)-1*H*-tetrazol-5-yl)-1,4-oxazepane (9{*57,300*}**).** White solid, mp = 107–109 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.14 (t, *J* = 9.1 Hz, 1H), 7.10 (d, *J* = 6.5 Hz, 1H), 7.02 – 6.95 (m, 1H), 5.52 (s, 2H), 3.66 (t, *J* = 4.9 Hz, 2H), 3.60 (t, *J* = 5.5 Hz, 2H), 3.58 – 3.52 (m, 4H), 2.20 (s, 3H), 1.85 – 1.78 (m, 2H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 160.2 (d, *J* = 243.4 Hz), 157.3, 131.2 (d, *J* = 3.4 Hz), 130.0 (d, *J* = 5.3 Hz), 126.1 (d, *J* = 8.4 Hz), 124.8 (d, *J* = 17.7 Hz), 115.4 (d, *J* = 22.6 Hz), 68.83, 68.77, 52.9, 49.6, 49.3, 29.8, 14.1 (d, *J* = 3.3 Hz) ppm. ^{19}F{^{1}H} NMR (470 MHz, DMSO-d_6): δ –118.63 ppm. LC–MS (*m/z*): = 292 (M + H^{+}). Anal. Calcd. for $C_{14}H_{18}FN_5O$: C, 57.72; H, 6.23; N, 24.04. Found: C, 57.59; H, 6.20; N, 24.18.

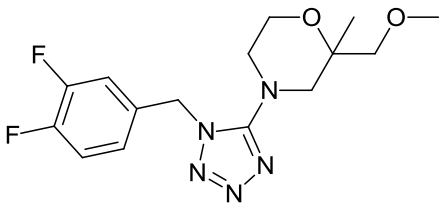


1-(Cyclopropylmethyl)-5-(2-(thiophen-3-yl)pyrrolidin-1-yl)-1*H*-tetrazole (9{*63,327*}**).** Beige solid, mp = 65–67 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.46 (dd, *J* = 4.9, 2.9 Hz, 1H), 7.27 – 7.25 (m, 1H), 7.03 (d, *J* = 4.9 Hz, 1H), 5.21 (dd, *J* = 7.5, 4.9 Hz, 1H), 4.07 (d, *J* = 7.1 Hz, 2H), 3.92 (dt, *J* = 9.4, 6.4 Hz, 1H), 3.54 (dt, *J* = 9.6, 7.2 Hz, 1H), 2.37 – 2.26 (m, 1H), 1.98 (quint, *J* = 6.7 Hz, 2H), 1.90 – 1.80 (m,

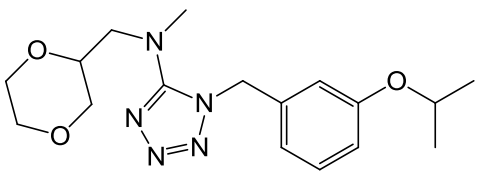
1H), 1.24 – 1.15 (m, 1H), 0.56 – 0.42 (m, 2H), 0.37 – 0.29 (m, 1H), 0.30 – 0.21 (m, 1H) ppm. $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO-d_6): δ 155.8, 144.5, 126.6, 126.1, 120.9, 60.2, 50.8, 50.4, 34.4, 23.9, 10.7, 3.9, 3.6 ppm. LC–MS (*m/z*): 276 (M + H^+). Anal. Calcd. for $C_{13}H_{17}N_5S$: C, 56.70; H, 6.22; N, 25.43; S, 11.64. Found: C, 56.81; H, 6.48; N, 25.60; S, 11.47.



4-(1-(2,5-Dimethoxybenzyl)-1*H*-tetrazol-5-yl)-1,4-oxazepane (9{*68,300*}**).** Yellow solid, mp = 78–81 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.00 (d, *J* = 8.9 Hz, 1H), 6.90 (dd, *J* = 8.9, 3.0 Hz, 1H), 6.40 (d, *J* = 3.0 Hz, 1H), 5.41 (s, 2H), 3.74 (s, 3H), 3.70 – 3.67 (m, 2H), 3.65 (s, 3H), 3.62 (t, *J* = 5.7 Hz, 2H), 3.57 – 3.53 (m, 4H), 1.84 (quint, *J* = 5.7 Hz, 2H) ppm. $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO-d_6): δ 157.6, 153.1, 150.2, 124.0, 114.2, 113.4, 112.3, 68.9, 68.9, 56.0, 55.4, 52.9, 49.2, 45.8, 29.9 ppm. LC–MS (*m/z*): = 320 (M + H^+). Anal. Calcd. for $C_{15}H_{21}N_5O_3$: C, 56.41; H, 6.63; N, 21.93. Found: C, 56.34; H, 6.61; N, 22.03.

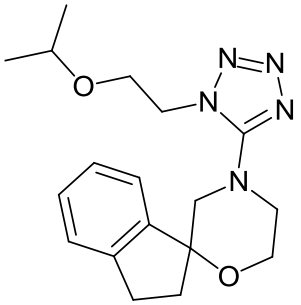


4-(1-(3,4-Difluorobenzyl)-1*H*-tetrazol-5-yl)-2-(methoxymethyl)-2-methylmorpholine (9{*77,363*}**).** Beige solid, mp = 89–91 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.48 (dt, *J* = 10.7, 8.5 Hz, 1H), 7.34 (ddd, *J* = 10.8, 7.8, 2.1 Hz, 1H), 7.08 – 7.01 (m, 1H), 5.57 (d, *J* = 16.4 Hz, 1H), 5.52 (d, *J* = 16.4 Hz, 1H), 3.70 (t, *J* = 5.0 Hz, 2H), 3.35 (d, *J* = 9.3 Hz, 1H), 3.21 (s, 3H), 3.20 – 3.16 (m, 3H), 3.15 (d, *J* = 12.4 Hz, 1H), 2.96 (d, *J* = 12.4 Hz, 1H), 1.07 (s, 3H) ppm. $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO-d_6): δ 158.3, 149.4 (dd, *J* = 246.7, 12.8 Hz), 149.2 (dd, *J* = 246.3, 12.4 Hz), 132.2 (d, *J* = 5.4 Hz), 124.4 (dd, *J* = 6.8, 3.5 Hz), 118.0 (d, *J* = 17.4 Hz), 116.8 (d, *J* = 18.1 Hz), 74.6, 72.1, 59.4, 58.8, 54.3, 48.8 (2C), 20.3 ppm. ^{19}F NMR (470 MHz, DMSO-d_6): δ –137.8 – –137.9 (m, 1F), –139.3 – –139.4 (m, 1F) ppm. LC–MS (*m/z*): 340 (M + H^+). Anal. Calcd. for $C_{15}H_{19}F_2N_5O_2$: C, 53.09; H, 5.64; N, 20.64. Found: C, 53.44; H, 5.96; N, 20.87.

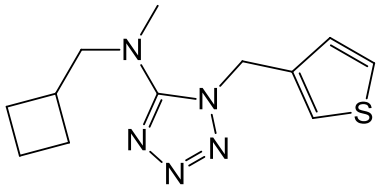


***N*-((1,4-Dioxan-2-yl)methyl)-1-(3-isopropoxybenzyl)-*N*-methyl-1*H*-tetrazol-5-amine (9{*84,319*}).** Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.27 (t, *J* = 7.8 Hz, 1H), 6.87 (d, *J* = 8.0 Hz, 1H), 6.66 (s,

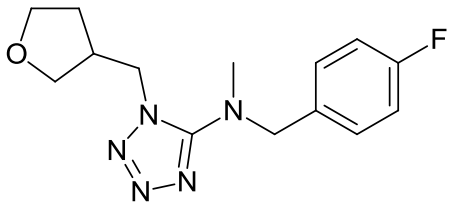
2H), 5.56 (s, 2H), 4.55 (sept, *J* = 6.0 Hz, 1H), 3.73 – 3.67 (m, 1H), 3.65 (d, *J* = 12.3 Hz, 1H), 3.58 (d, *J* = 11.4 Hz, 1H), 3.55 – 3.44 (m, 2H), 3.40 – 3.35 (m, 1H), 3.31 – 3.20 (m, 2H), 3.06 – 3.01 (m, 1H), 2.99 (s, 3H), 1.23 (d, *J* = 6.0 Hz, 6H) ppm. ^{13}C NMR{^{1}H} (126 MHz, DMSO-d_6): δ 158.0, 157.7, 137.2, 130.0, 118.4, 114.8, 114.0, 72.6, 69.2, 67.9, 65.9, 65.6, 53.7, 49.9, 39.2, 21.7 ppm. LC–MS (*m/z*): = 348 (M + H$^+$). Anal. Calcd. for $C_{17}H_{25}N_5O_3$: C, 58.77; H, 7.25; N, 20.16. Found: C, 58.76; H, 7.17; N, 20.10.



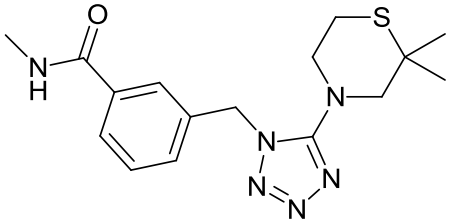
4'-(1-(2-Isopropoxyethyl)-1*H*-tetrazol-5-yl)-2,3-dihydrospiro[indene-1,2'-morpholine] (9{*90,371*}**).** Beige solid, mp = 104–106 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.48 (d, *J* = 7.5 Hz, 1H), 7.30 – 7.27 (m, 2H), 7.24 – 7.19 (m, 1H), 4.42 – 4.30 (m, 2H), 3.90 – 3.86 (m, 2H), 3.85 – 3.77 (m, 2H), 3.48 – 3.39 (m, 3H), 3.32 – 3.26 (m, 1H), 3.17 (d, *J* = 12.2 Hz, 1H), 3.02 – 2.94 (m, 1H), 2.90 – 2.82 (m, 1H), 2.56 – 2.52 (m, 1H), 2.12 (dt, *J* = 14.3, 7.6 Hz, 1H), 0.88 (d, *J* = 6.1 Hz, 3H), 0.85 (d, *J* = 6.1 Hz, 3H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 159.2, 143.7, 143.3, 128.7, 126.2, 124.8, 124.1, 83.3, 71.1, 64.8, 61.1, 56.4, 49.3, 47.3, 34.4, 28.8, 21.5 ppm. LC–MS (*m/z*): 344 (M + H$^+$). Anal. Calcd. for $C_{18}H_{25}N_5O_2$: C, 62.95; H, 7.34; N, 20.39. Found: C, 63.11; H, 6.95; N, 20.38.



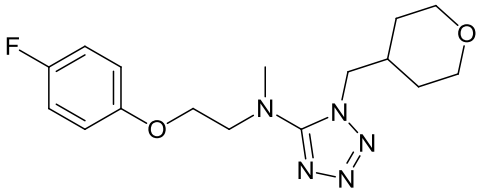
***N*-(Cyclobutylmethyl)-*N*-methyl-1-(thiophen-3-ylmethyl)-1*H*-tetrazol-5-amine (9**{*102,356*}**).** Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.61 – 7.54 (m, 1H), 7.37 (s, 1H), 6.95 (d, *J* = 5.1 Hz, 1H), 5.52 (s, 2H), 3.29 (d, *J* = 7.2 Hz, 2H), 2.92 (s, 3H), 2.50 – 2.44 (m, 1H), 1.88 – 1.80 (m, 2H), 1.80 – 1.72 (m, 1H), 1.71 – 1.62 (m, 1H), 1.58 – 1.47 (m, 2H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO) δ 158.0, 135.9, 127.5, 126.5, 123.3, 58.1, 46.1, 38.6, 33.3, 25.8, 18.1 ppm. LC–MS (*m/z*): = 264 (M + H$^+$). Anal. Calcd. for $C_{12}H_{17}N_5S$: C, 54.73; H, 6.51; N, 26.59; S, 12.17. Found: C, 54.63; H, 6.26; N, 26.55; S, 12.15.



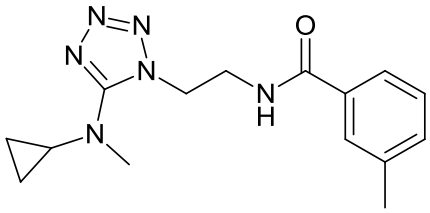
***N*-(4-Fluorobenzyl)-*N*-methyl-1-((tetrahydrofuran-3-yl)methyl)-1*H*-tetrazol-5-amine (9**{*103,386*}**).** Brownish oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.36 (t, J = 8.5, 5.7 Hz, 2H), 7.18 (t, J = 8.9 Hz, 2H), 4.47 (s, 2H), 4.25 (d, J = 7.8 Hz, 2H), 3.76 (td, J = 8.2, 5.5 Hz, 1H), 3.69 – 3.59 (m, 2H), 3.42 (dd, J = 8.9, 5.4 Hz, 1H), 2.91 (s, 3H), 2.81 – 2.73 (m, 1H), 1.98 – 1.88 (m, 1H), 1.59 – 1.51 (m, 1H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 161.5 (d, J = 243.2 Hz), 158.6, 132.9 (d, J = 3.0 Hz), 130.0 (d, J = 8.2 Hz), 115.3 (d, J = 21.3 Hz), 70.0, 66.7, 56.0, 49.3, 38.5, 38.3, 29.2 ppm. ^{19}F NMR (470 MHz, DMSO-d_6): δ –115.1 (tt, J = 9.6, 5.7 Hz) ppm. LC–MS (*m/z*): 292 (M + H$^+$). Anal. Calcd. for $C_{14}H_{18}FN_5O$: C, 57.72; H, 6.23; N, 24.04. Found: C, 57.45; H, 5.90; N, 24.30.



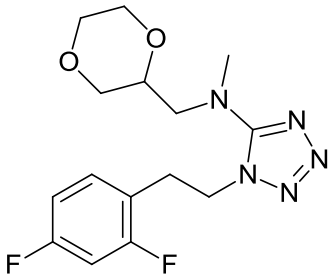
3-((5-(2,2-Dimethylthiomorpholino)-1*H*-tetrazol-1-yl)methyl)-*N*-methylbenzamide (9{*110,333*}**).** Yellow solid, mp = 72–75 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.51 – 8.42 (m, 1H), 7.80 (d, J = 7.7 Hz, 1H), 7.69 (s, 1H), 7.48 (t, J = 7.7 Hz, 1H), 7.35 (d, J = 7.7 Hz, 1H), 5.60 (s, 2H), 3.42 – 3.36 (m, 2H), 3.23 (s, 2H), 2.76 (d, J = 4.5 Hz, 3H), 2.73 – 2.69 (m, 2H), 1.12 (s, 6H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 166.0, 158.7, 135.0, 134.8, 129.9, 128.9, 126.6, 126.3, 62.4, 51.0, 49.9, 38.9, 26.6, 26.2, 24.0 ppm. LC–MS (*m/z*): = 347 (M + H$^+$). Anal. Calcd. for $C_{16}H_{22}N_6OS$: C, 55.47; H, 6.40; N, 24.26; S, 9.25. Found: C, 55.29; H, 6.21; N, 24.59; S, 9.65.



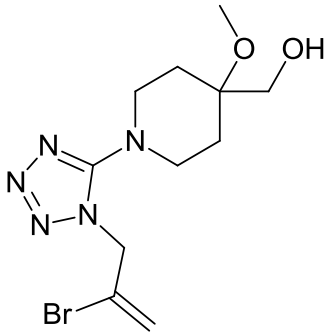
***N*-(2-(4-Fluorophenoxy)ethyl)-*N*-methyl-1-((tetrahydro-2*H*-pyran-4-yl)methyl)-1*H*-tetrazol-5-amine (9**{*121,302*}**).** Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.10 (t, J = 8.8 Hz, 2H), 6.87 (dd, J = 9.1, 4.2 Hz, 2H), 4.19 (d, J = 7.3 Hz, 2H), 4.15 (t, J = 5.1 Hz, 2H), 3.76 (dd, J = 11.3, 3.1 Hz, 2H), 3.69 (t, J = 5.1 Hz, 2H), 3.16 (td, J = 11.8, 2.2 Hz, 2H), 3.07 (s, 3H), 2.14 – 2.01 (m, 1H), 1.41 – 1.31 (m, 2H), 1.29 – 1.17 (m, 2H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 158.5, 156.6 (d, J = 236.0 Hz), 154.5 (d, J = 1.7 Hz), 115.9 (d, J = 23.0 Hz), 115.6 (d, J = 8.1 Hz), 66.3, 65.4, 52.4, 52.0, 39.1, 34.4, 29.7 ppm. ^{19}F NMR (470 MHz, DMSO-d_6): δ –123.7 (tt, J = 8.8, 4.5 Hz) ppm. LC–MS (*m/z*): = 336 (M + H$^+$). Anal. Calcd. for $C_{16}H_{22}FN_5O_2$: C, 57.30; H, 6.61; N, 20.88. Found: C, 57.12; H, 6.84; N, 20.61.



***N*-(2-(5-(Cyclopropyl(methyl)amino)-1*H*-tetrazol-1-yl)ethyl)-3-methylbenzamide (9**{*146,322*}**).** White solid, mp = 75–77 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.60 (t, *J* = 5.8 Hz, 1H), 7.60 (s, 1H), 7.56 (t, *J* = 5.0 Hz, 1H), 7.34 (d, *J* = 4.6 Hz, 2H), 4.54 (t, *J* = 6.1 Hz, 2H), 3.63 (dt, *J* = 5.8, 6.1 Hz, 2H), 2.93 (s, 3H), 2.84 (tt, *J* = 6.9, 3.6 Hz, 1H), 2.35 (s, 3H), 0.75 – 0.70 (m, 2H), 0.54 – 0.50 (m, 2H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 166.7, 158.6, 137.5, 134.0, 131.9, 128.2, 127.6, 124.2, 46.1, 39.4, 38.8, 33.4, 20.9, 8.2 ppm. LC–MS (*m/z*): = 301 (M + H$^+$). Anal. Calcd. for $C_{15}H_{20}N_6O$: C, 59.98; H, 6.71; N, 27.98. Found: C, 60.24; H, 6.96; N, 28.09.

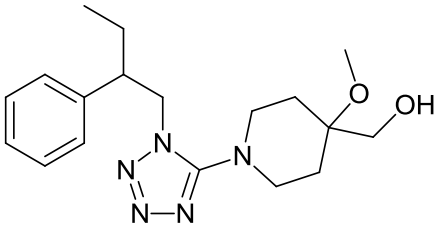


***N*-((1,4-Dioxan-2-yl)methyl)-1-(2,4-difluorophenethyl)-*N*-methyl-1*H*-tetrazol-5-amine (9**{*151,319*}**).** Beige solid, mp = 41–44 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.26 (q, *J* = 8.5 Hz, 1H), 7.19 (td, *J* = 9.9, 2.6 Hz, 1H), 7.01 (td, *J* = 8.6, 2.6 Hz, 1H), 4.52 (t, *J* = 7.1 Hz, 2H), 3.79 – 3.72 (m, 1H), 3.67 (d, *J* = 11.4 Hz, 2H), 3.62 (d, *J* = 11.2 Hz, 1H), 3.53 (td, *J* = 11.3, 2.5 Hz, 1H), 3.42 (td, *J* = 11.2, 2.7 Hz, 1H), 3.31 – 3.21 (m, 2H), 3.18 (dd, *J* = 11.4, 9.9 Hz, 1H), 3.12 (t, *J* = 7.0 Hz, 2H), 2.98 (s, 3H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 161.3 (dd, *J* = 245.3, 12.2 Hz), 160.6 (dd, *J* = 246.6, 12.2 Hz), 158.3, 132.3 (dd, *J* = 9.7, 6.2 Hz), 120.3 (dd, *J* = 15.9, 3.7 Hz), 111.5 (dd, *J* = 21.0, 3.6 Hz), 103.7 (t, *J* = 26.1 Hz), 72.6, 68.1, 65.9, 65.7, 54.1, 46.7, 39.3, 27.5 ppm. ^{19}F NMR (470 MHz, DMSO-d_6): δ –111.9 (quint, *J* = 7.9 Hz), –114.4 (q, *J* = 8.9 Hz) ppm. LC–MS (*m/z*): = 340 (M + H$^+$). Anal. Calcd. for $C_{15}H_{19}F_2N_5O_2$: C, 53.09; H, 5.64; N, 20.64. Found: C, 53.37; H, 5.60; N, 20.31.

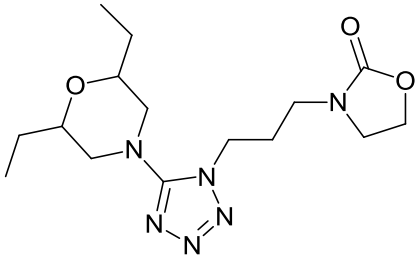


(1-(1-(2-Bromoallyl)-1*H*-tetrazol-5-yl)-4-methoxypiperidin-4-yl)methanol (9{*165,299*}**).** Brown oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 6.05 (d, *J* = 2.6 Hz, 1H), 5.82 (d, *J* = 2.6 Hz, 1H), 5.25 (s, 2H), 3.36 (s, 2H), 3.35 – 3.31 (m, 2H), 3.17 – 3.12 (m, 5H), 1.75 – 1.66 (m, 2H), 1.63 – 1.55 (m, 2H) ppm.

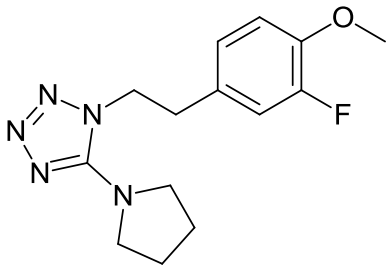
$^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO-d_6): δ 158.4, 124.8, 121.9, 72.9, 64.0, 53.8, 48.6, 45.1, 29.2 ppm. LC–MS (*m/z*): = 332/334 ($M + H^+$). Anal. Calcd. for $C_{11}H_{18}BrN_5O_2$: C, 39.77; H, 5.46; N, 21.08; Br, 24.05. Found: C, 39.41; H, 5.73; N, 20.96; Br, 24.22.



(4-Methoxy-1-(1-(2-phenylbutyl)-1*H*-tetrazol-5-yl)piperidin-4-yl)methanol (9{*175,299*}**).** Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.23 (t, *J* = 7.5 Hz, 2H), 7.17 (t, *J* = 7.2 Hz, 1H), 7.11 (d, *J* = 7.0 Hz, 2H), 4.63 (t, *J* = 5.6 Hz, 1H), 4.49 (dd, *J* = 14.2, 6.0 Hz, 1H), 4.36 (dd, *J* = 14.2, 9.2 Hz, 1H), 3.37 (s, 1H), 3.36 (s, 1H), 3.14 (s, 3H), 3.12 – 3.06 (m, 1H), 3.04 – 2.91 (m, 3H), 1.75 – 1.62 (m, 4H), 1.61 – 1.48 (m, 2H), 0.75 (t, *J* = 7.3 Hz, 3H) ppm. $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO-d_6): δ 158.9, 140.7, 128.3, 127.7, 126.8, 72.8, 64.1, 51.8, 48.6, 45.9, 45.4, 45.1, 29.34, 29.31, 25.6, 11.7 ppm. LC–MS (*m/z*): = 346 ($M + H^+$). Anal. Calcd. for $C_{18}H_{27}N_5O_2$: C, 62.58; H, 7.88; N, 20.27. Found: C, 62.77; H, 7.62; N, 20.08.

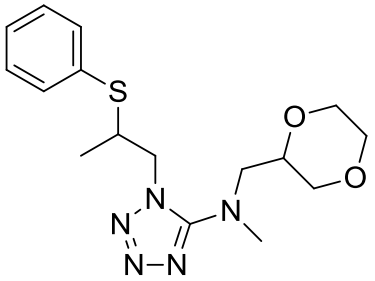


3-(3-(5-(2,6-Diethylmorpholino)-1*H*-tetrazol-1-yl)propyl)oxazolidin-2-one (9{*188,338*}**).** White solid, mp = 79–81 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 4.25 (d, *J* = 6.9 Hz, 2H), 4.23 (t, *J* = 7.9 Hz, 2H), 3.53 – 3.48 (m, 4H), 3.37 (d, *J* = 12.1 Hz, 2H), 3.17 (t, *J* = 6.9 Hz, 2H), 2.65 (t, *J* = 12.1, 10.5 Hz, 2H), 2.09 (quint, *J* = 6.9 Hz, 2H), 1.53 – 1.37 (m, 4H), 0.92 (t, *J* = 7.4 Hz, 6H) ppm. $^{13}C\ \{^{1}H\}$ NMR (126 MHz, DMSO-d_6): δ 158.7, 158.4, 76.1, 62.2, 53.7, 44.8, 44.5, 41.3, 26.2, 26.1, 10.0 ppm. LC–MS (*m/z*): = 339 ($M + H^+$). Anal. Calcd. for $C_{15}H_{26}N_6O_3$: C, 53.24; H, 7.74; N, 24.83. Found: C, 53.56; H, 8.04; N, 24.88.

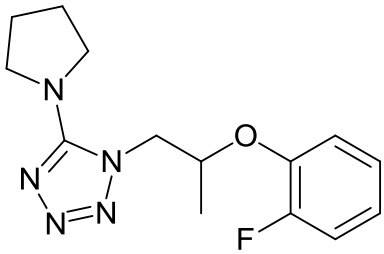


1-(3-Fluoro-4-methoxyphenethyl)-5-(pyrrolidin-1-yl)-1*H*-tetrazole (9{*190,341*}**).** Whire solid, mp = 70–72 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.07 – 7.01 (m, 2H), 6.87 (d, *J* = 8.5 Hz, 1H), 4.48 (t, *J* = 7.2 Hz, 2H), 3.78 (s, 3H), 3.43 – 3.38 (m, 4H), 3.01 (t, *J* = 7.2 Hz, 2H), 1.90 – 1.83 (m, 4H) ppm.

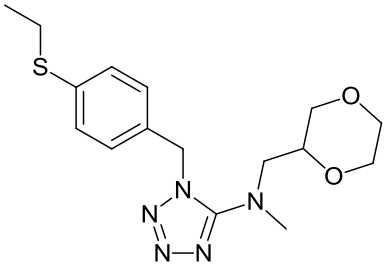
$^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO-d_6): δ 155.9, 151.2 (d, J = 243.5 Hz), 145.8 (d, J = 10.4 Hz), 130.2 (d, J = 6.2 Hz), 125.0 (d, J = 3.3 Hz), 116.3 (d, J = 17.7 Hz), 113.7, 55.9, 49.0, 47.5, 34.1, 25.1 ppm. ^{19}F NMR (470 MHz, DMSO-d_6): δ –135.6 (dd, J = 12.5, 9.2 Hz) ppm. LC–MS (*m/z*): = 292 ($M + H^+$). Anal. Calcd. for $C_{14}H_{18}FN_5O$: C, 57.72; H, 6.23; N, 24.04. Found: C, 58.04; H, 6.03; N, 23.88.



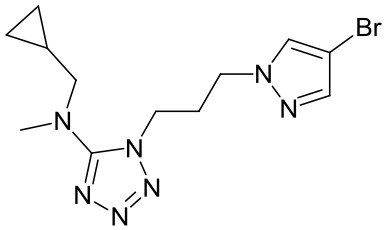
***N*-((1,4-Dioxan-2-yl)methyl)-*N*-methyl-1-(2-(phenylthio)propyl)-1*H*-tetrazol-5-amine (9**{*262,319*}**).** Yellow oil. The compound existed as *ca.* 1:1 mixture of diastereomers. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.43 (t, J = 8.3 Hz, 2H), 7.40 – 7.29 (m, 3H), 4.44 – 4.32 (m, 2H), 3.79 – 3.69 (m, 2H), 3.67 – 3.59 (m, 3H), 3.50 (t, J = 11.4 Hz, 1H), 3.44 – 3.36 (m, 1H), 3.28 – 3.08 (m, 3H), 2.92 (s, 1.5H) and 2.91 (s, 1.5H), 1.23 (d, J = 6.8 Hz, 1.5H) and 1.19 (d, J = 6.8 Hz, 1.5H) ppm. $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO-d_6): δ 158.5 and 158.4, 132.57 and 132.55, 132.4 and 132.3, 129.3 and 129.2, 127.8 and 127.7, 72.7, 72.5, 68.1 and 68.0, 65.9, 65.7, 54.02 and 53.95, 51.9 and 51.8, 41.64 and 41.56, 18.4 and 18.3 ppm. LC–MS (*m/z*): = 350 ($M + H^+$). Anal. Calcd. for $C_{16}H_{23}N_5O_2S$: C, 54.99; H, 6.63; N, 20.04; S, 9.17. Found: C, 54.87; H, 6.82; N, 20.09; S, 8.90.



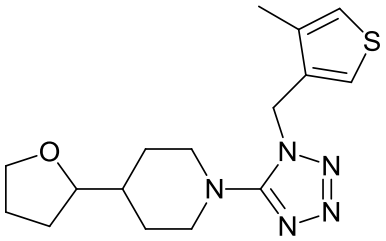
1-(2-(2-Fluorophenoxy)propyl)-5-(pyrrolidin-1-yl)-1*H*-tetrazole (9{*263,341*}**).** Beige solid, mp = 78–80 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.15 (dd, J = 11.7, 8.1 Hz, 1H), 7.06 – 7.02 (m, 2H), 6.94 – 6.87 (m, 1H), 4.85 (sext, J = 6.2 Hz, 1H), 4.62 – 4.56 (m, 2H), 3.63 – 3.55 (m, 2H), 3.51 – 3.43 (m, 2H), 1.94 – 1.88 (m, 4H), 1.34 (d, J = 6.2 Hz, 3H) ppm. $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO-d_6): δ 155.9, 152.3 (d, J = 243.6 Hz), 144.7 (d, J = 10.4 Hz), 124.7 (d, J = 3.7 Hz), 121.8 (d, J = 7.0 Hz), 116.4, 116.2 (d, J = 18.2 Hz), 73.8, 51.0, 48.9, 25.2, 17.0 ppm. ^{19}F NMR (470 MHz, DMSO-d_6): δ –134.51 – –134.66 (m) ppm. LC–MS (*m/z*): = 292 ($M + H^+$). Anal. Calcd. for $C_{14}H_{18}FN_5O$: C, 57.72; H, 6.23; N, 24.04. Found: C, 57.44; H, 6.51; N, 24.32.



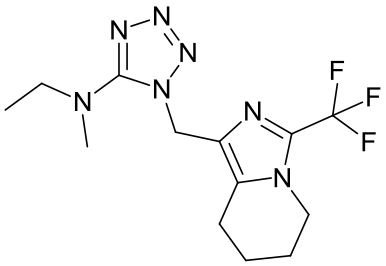
***N*-((1,4-Dioxan-2-yl)methyl)-1-(4-(ethylthio)benzyl)-*N*-methyl-1*H*-tetrazol-5-amine (9{*272,319*}).** Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.31 (d, J = 8.3 Hz, 2H), 7.10 (d, J = 8.3 Hz, 2H), 5.56 (s, 2H), 3.72 – 3.67 (m, 1H), 3.65 (d, J = 11.3 Hz, 1H), 3.58 (d, J = 11.1 Hz, 1H), 3.53 (dd, J = 11.4, 2.6 Hz, 1H), 3.48 (td, J = 11.3, 2.6 Hz, 1H), 3.36 (td, J = 11.3, 2.7 Hz, 1H), 3.32 – 3.21 (m, 2H), 3.03 (dd, J = 11.4, 9.9 Hz, 1H), 2.98 (s, 3H), 2.96 (q, J = 7.3 Hz, 2H), 1.21 (t, J = 7.3 Hz, 3H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 158.0, 136.3, 132.7, 128.0, 127.5, 72.5, 67.9, 65.8, 65.6, 53.7, 49.6, 39.3, 25.9, 14.1 ppm. LC–MS (*m/z*): = 350 (M + H$^+$). Anal. Calcd. for $C_{16}H_{23}N_5O_2S$: C, 54.99; H, 6.63; N, 20.04; S, 9.17. Found: C, 54.79; H, 6.72; N, 19.85; S, 9.54.



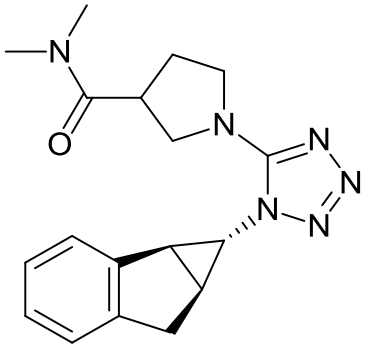
1-(3-(4-Bromo-1*H*-pyrazol-1-yl)propyl)-*N*-(cyclopropylmethyl)-*N*-methyl-1*H*-tetrazol-5-amine (9{*280,391*}). Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.98 (s, 1H), 7.56 (s, 1H), 4.17 (q, J = 6.8 Hz, 4H), 3.05 (d, J = 6.8 Hz, 2H), 2.95 (s, 3H), 2.31 (quint, J = 6.8 Hz, 2H), 0.98 – 0.90 (m, 1H), 0.48 – 0.39 (m, 2H), 0.15 (dt, J = 5.8, 4.3 Hz, 2H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 158.9, 139.7, 130.9, 92.0, 57.9, 49.3, 44.7, 38.8, 29.3, 9.0, 3.5 ppm. LC–MS (*m/z*): = 340/342 (M + H$^+$). Anal. Calcd. for $C_{12}H_{18}BrN_7$: C, 42.36; H, 5.33; N, 28.82; Br, 23.49. Found: C, 42.26; H, 5.31; N, 28.73; Br, 23.52.



1-(1-((4-Methylthiophen-3-yl)methyl)-1*H*-tetrazol-5-yl)-4-(tetrahydrofuran-2-yl)piperidine (9{*306,261*}). Brown solid, mp = 64–66 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.24 (d, J = 3.1 Hz, 1H), 7.19 (d, J = 3.1 Hz, 1H), 5.39 (s, 2H), 3.70 (dt, J = 8.1, 6.7 Hz, 1H), 3.59 (q, J = 7.3 Hz, 1H), 3.54 – 3.49 (m, 2H), 3.45 (q, J = 7.3 Hz, 1H), 2.94 – 2.83 (m, 2H), 2.04 (s, 3H), 1.88 – 1.83 (m, 1H), 1.82 – 1.75 (m, 3H), 1.58 – 1.53 (m, 1H), 1.51 – 1.43 (m, 2H), 1.33 – 1.20 (m, 2H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 158.5, 135.8, 134.2, 124.6, 122.8, 82.1, 66.9, 49.5, 49.4, 45.3, 39.9, 28.5, 27.9, 27.3, 25.3, 13.7 ppm. LC–MS (*m/z*): 334 (M + H$^+$). Anal. Calcd. for $C_{16}H_{23}N_5OS$: C, 57.63; H, 6.95; N, 21.00; S, 9.61. Found: C, 57.86; H, 6.58; N, 20.84; S, 9.37.

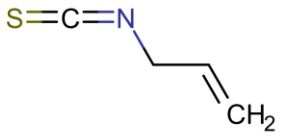
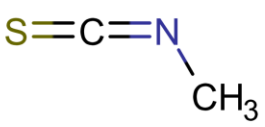
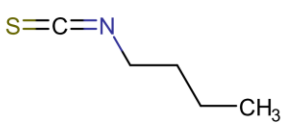
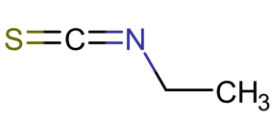


***N*-Ethyl-*N*-methyl-1-((3-(trifluoromethyl)-5,6,7,8-tetrahydroimidazo[1,5-*a*]pyridin-1-yl)methyl)-1*H*-tetrazol-5-amine (9**{*341*,*346*}**).** Beige solid, mp = 60–62 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 5.35 (s, 2H), 4.08 (t, *J* = 6.1 Hz, 2H), 3.41 (q, *J* = 7.1 Hz, 2H), 3.02 (s, 3H), 2.75 (t, *J* = 6.5 Hz, 2H), 1.94 – 1.88 (m, 2H), 1.80 – 1.74 (m, 2H), 1.07 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 157.8, 131.7 (q, *J* = 38.4 Hz), 131.2, 130.0, 119.0 (q, *J* = 268.8 Hz), 47.9, 43.6, 43.5, 37.8, 21.7, 20.0, 18.6, 11.7 ppm. ^{19}F NMR (470 MHz, DMSO-d_6): δ –60.9 ppm. LC–MS (*m/z*): = 330 (M + H$^+$). Anal. Calcd. for $C_{13}H_{18}F_3N_7$: C, 47.41; H, 5.51; N, 29.77. Found: C, 47.53; H, 5.82; N, 29.58.



***rac*-*N*,*N*-dimethyl-1-(1-((1*R*,1*aS*,6*aS*)-1,1*a*,6,6*a*-tetrahydrocyclopropa[*a*]inden-1-yl)-1*H*-tetrazol-5-yl)pyrrolidine-3-carboxamide (9**{*375*,*511*}**).** Brown solid, mp = 60–63 °C. The compound existed as *ca.* 1:1 mixture of diastereomers. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.49 – 7.41 (m, 1H), 7.29 – 7.24 (m, 1H), 7.21 – 7.17 (m, 2H), 3.88 (dd, *J* = 9.5, 7.8 Hz, 0.5H), 3.81 (d, *J* = 7.5 Hz, 1H), 3.79 – 3.72 (m, 0.5H), 3.71 – 3.57 (m, 2H), 3.56 – 3.47 (m, 1H), 3.30 (dd, *J* = 7.0, 3.8 Hz, 0.5H), 3.22 – 3.12 (m, 3.5H), 3.06 (s, 1.5H) and 3.03 (s, 1.5H), 2.87 (s, 1.5H) and 2.85 (s, 1.5H), 2.70 (t, *J* = 6.9 Hz, 0.5H) and 2.66 (t, *J* = 5.9 Hz, 0.5H), 2.25 – 2.14 (m, 1H), 2.10 – 1.97 (m, 1H) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ 171.4, 156.32 and 156.27, 142.1 and 142.0, 141.4 and 141.3, 126.8, 126.52 and 126.49, 125.25 and 125.23, 124.0, 51.5 and 51.4, 48.9 and 48.8, 40.4, 39.8, 36.72 and 36.70, 35.2 and 35.1, 34.1 and 34.0, 33.0, 28.73 and 28.70, 24.81 and 24.77 ppm. LC–MS (*m/z*): = 339 (M + H$^+$). Anal. Calcd. for $C_{18}H_{22}N_6O$: C, 63.89; H, 6.55; N, 24.83. Found: C, 63.66; H, 6.18; N, 24.49.

Figure S1. Structures of the reagents **10**{*1–58*}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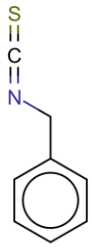	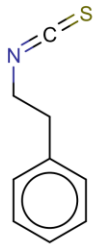	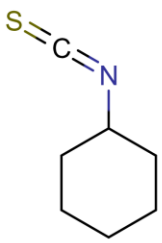	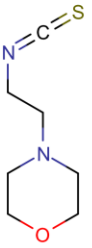
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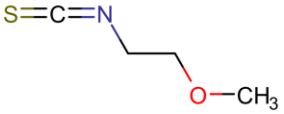	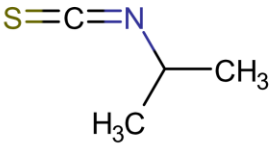	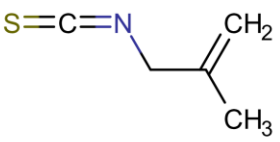	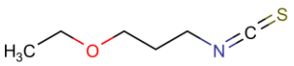
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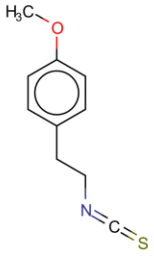	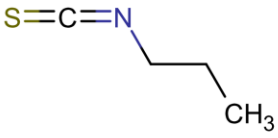	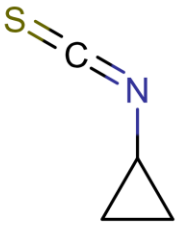	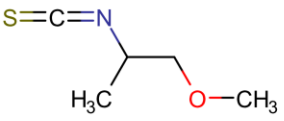
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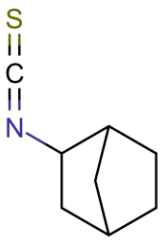	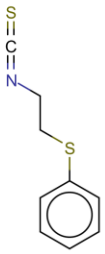	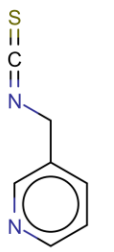	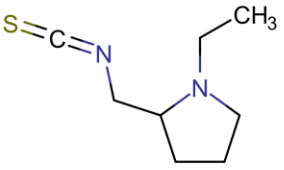
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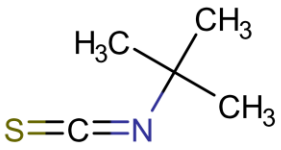	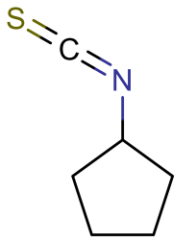	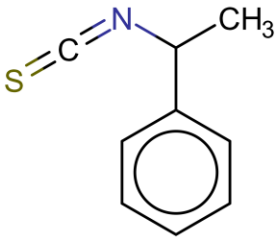	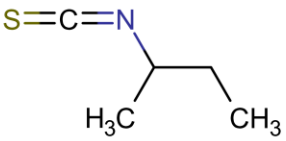
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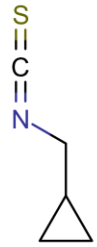	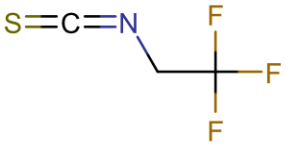	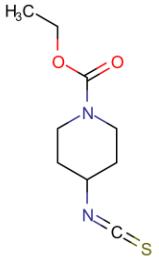	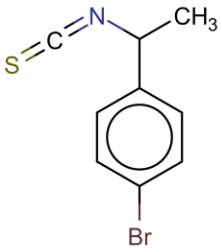
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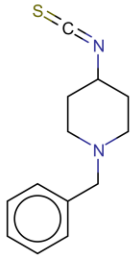	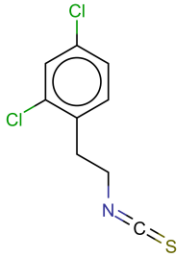	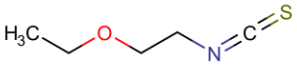	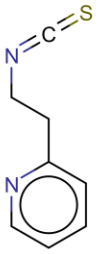
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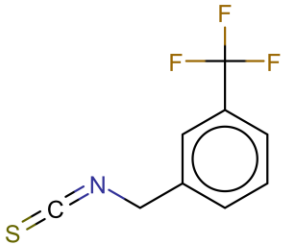	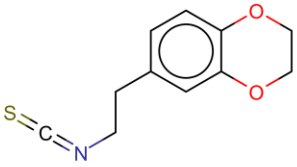	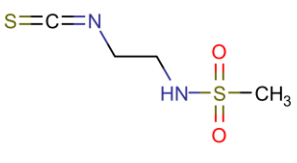	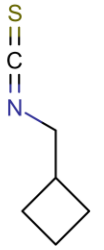
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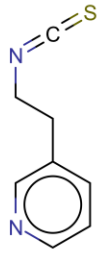	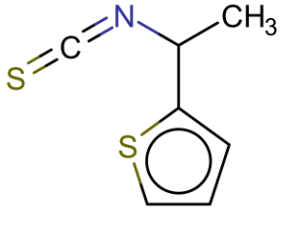	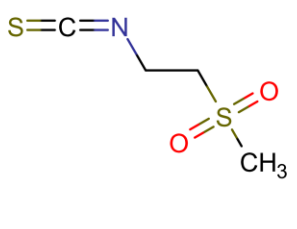	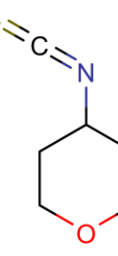
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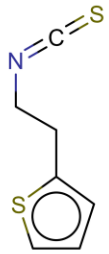	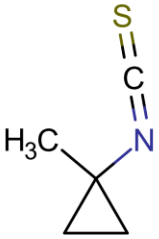	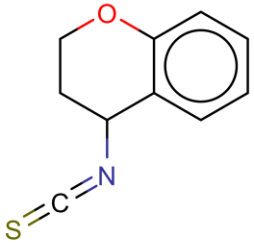	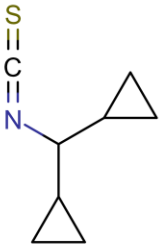
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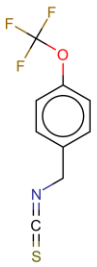	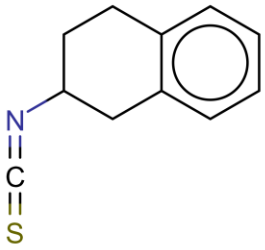	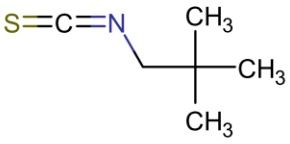	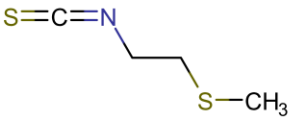
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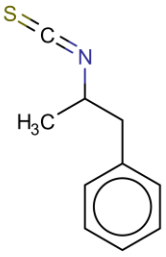	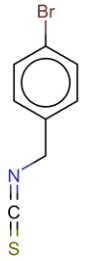	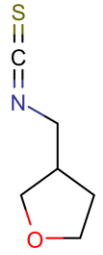	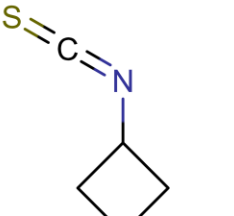
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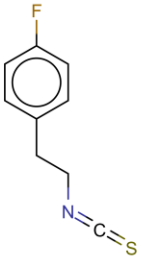	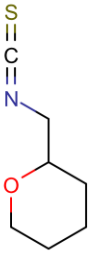	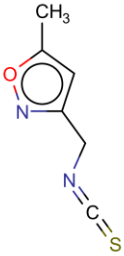	
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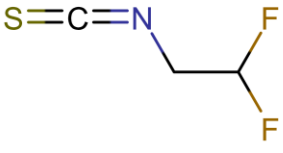	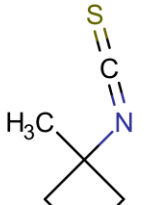		
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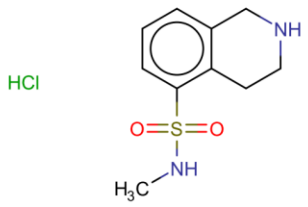
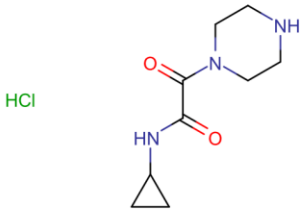
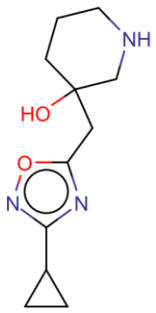
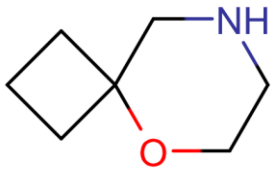
Figure S2. Structures of the reagents **11**{*1–511*}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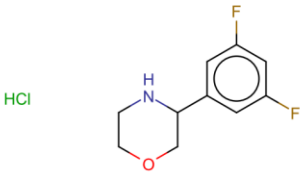	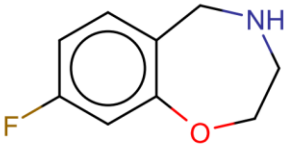	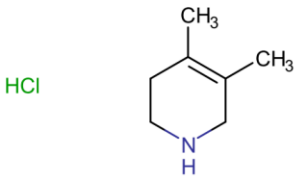	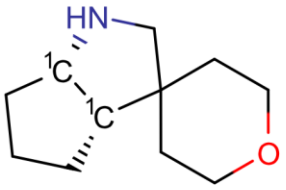
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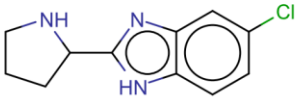	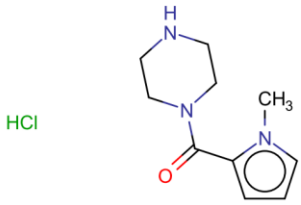	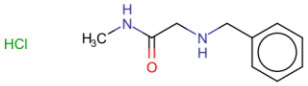	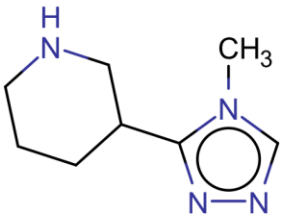
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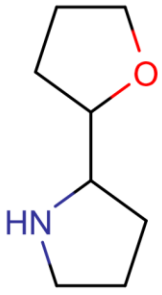	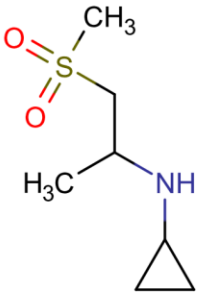	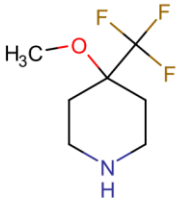	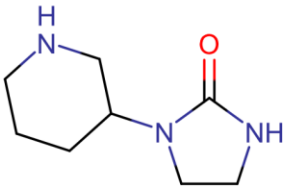
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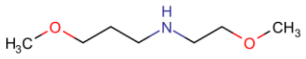	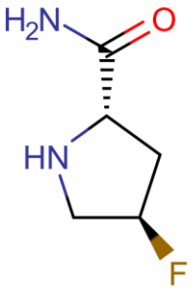	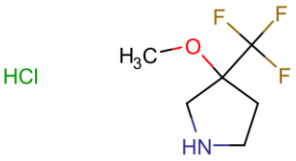	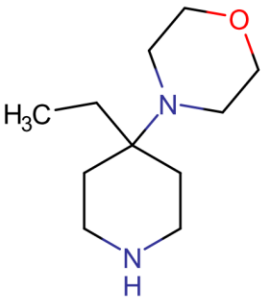
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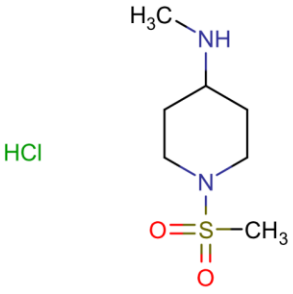	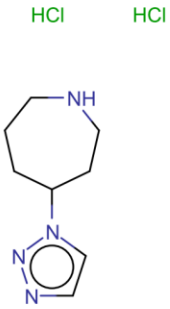	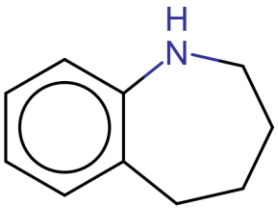	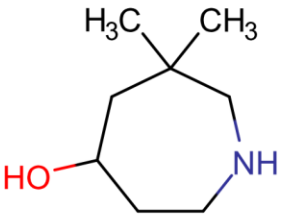
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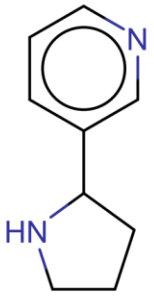	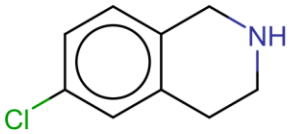	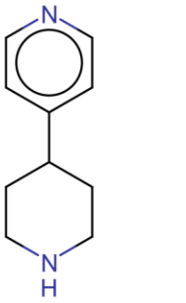	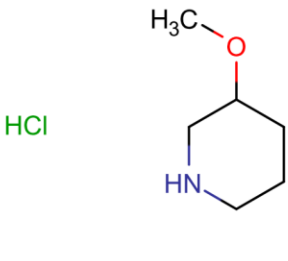
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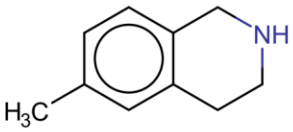	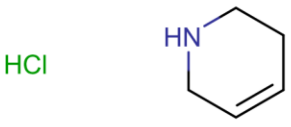	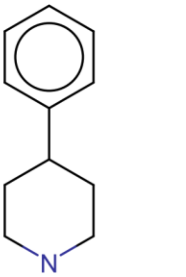	
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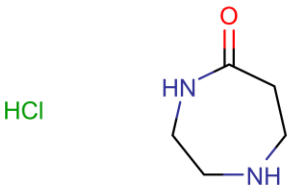	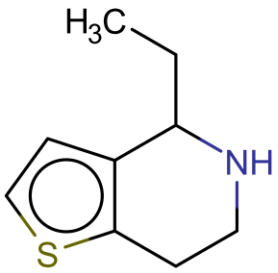	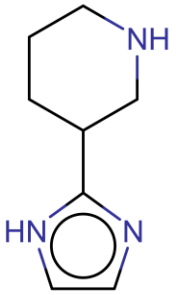	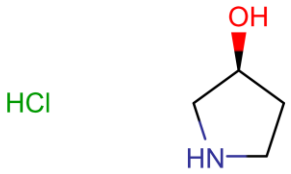
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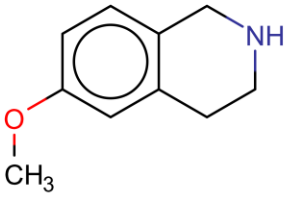	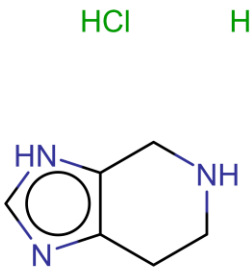	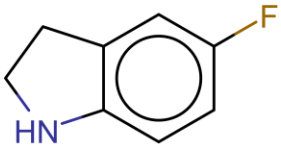	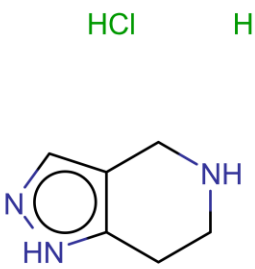
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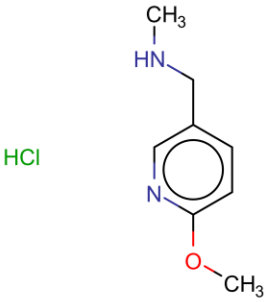	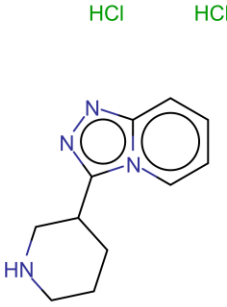	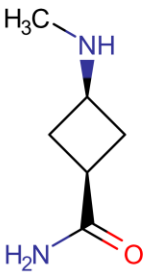	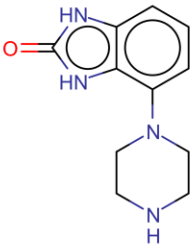
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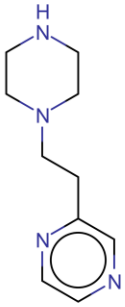	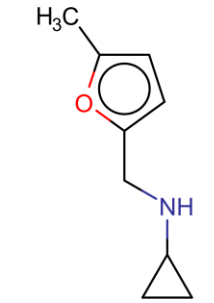		
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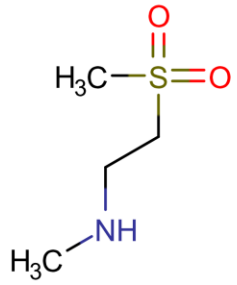	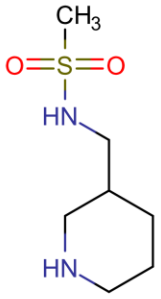	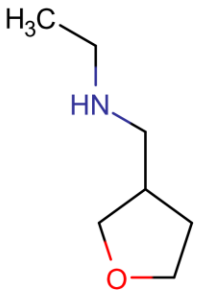	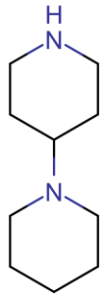
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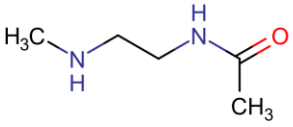	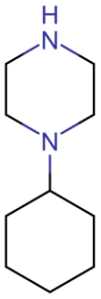	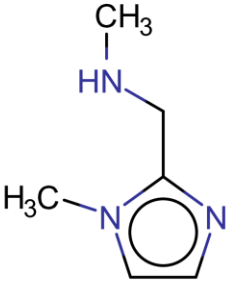	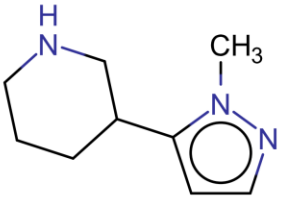
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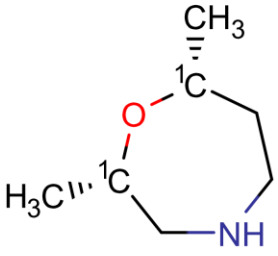
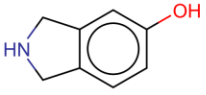
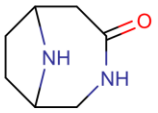
		HBr 	HCl 
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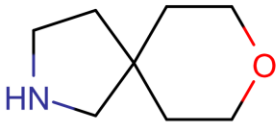
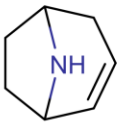
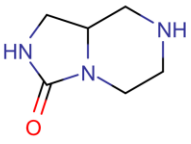
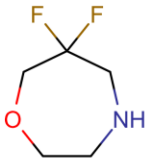
	HCl 	HCl 	HCl 
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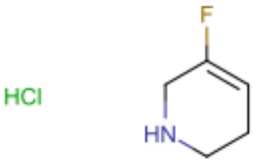	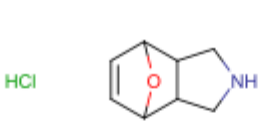	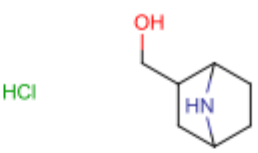	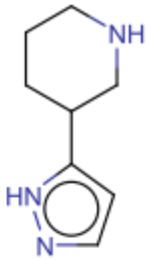
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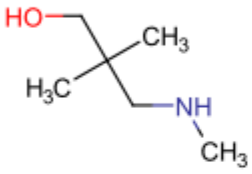	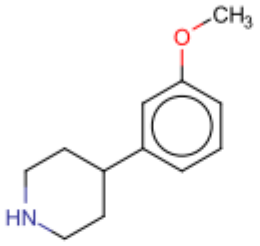	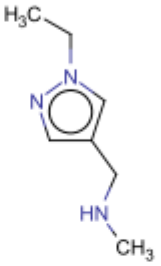	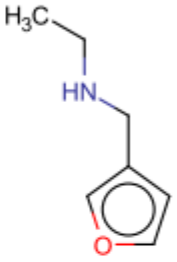
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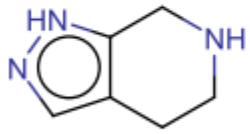	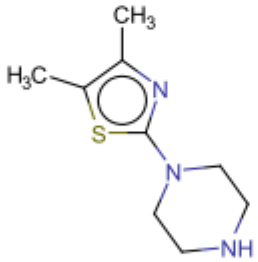	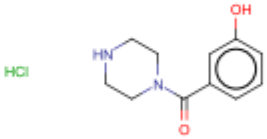	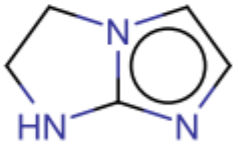
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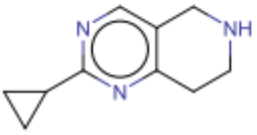	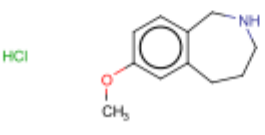	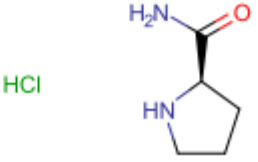	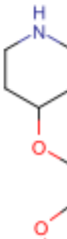
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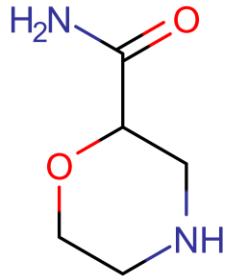	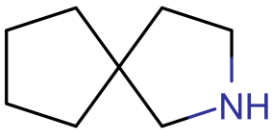	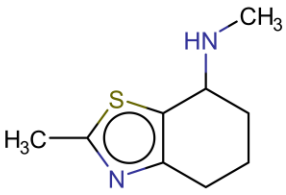	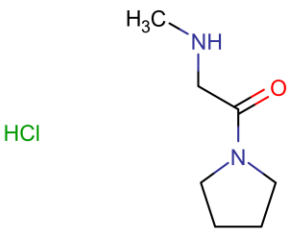
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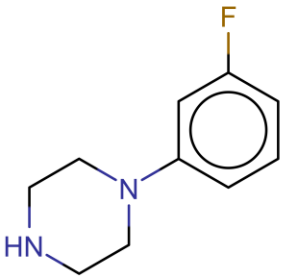	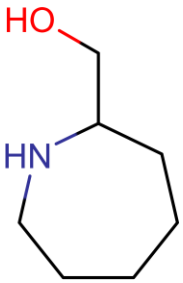	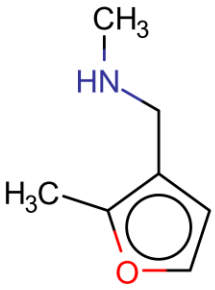	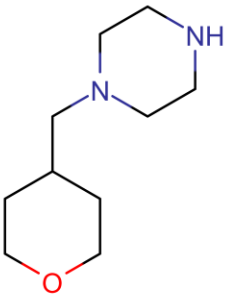
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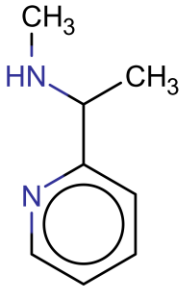	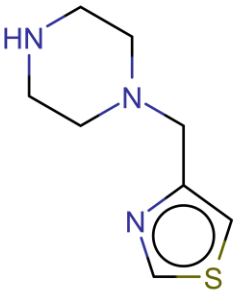	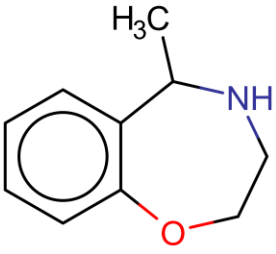	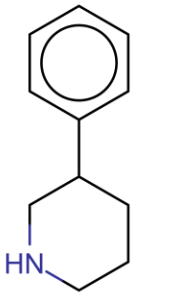
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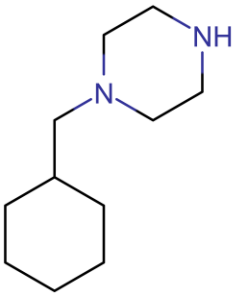	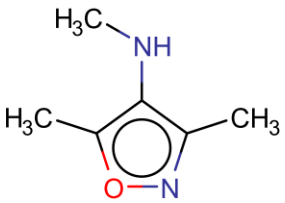	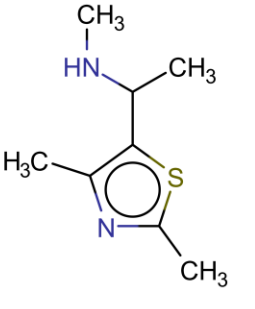	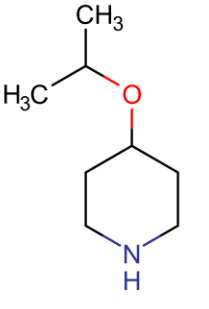
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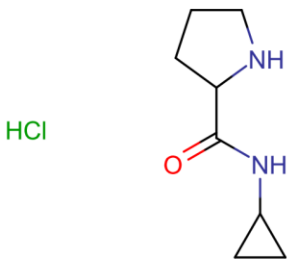	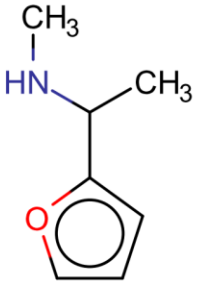	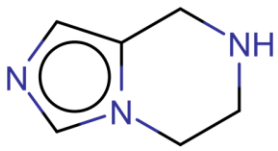	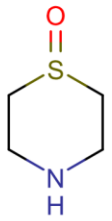
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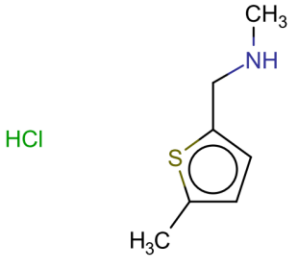	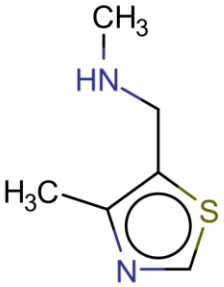	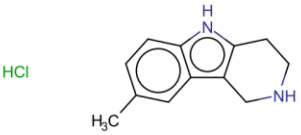	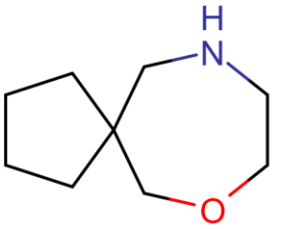
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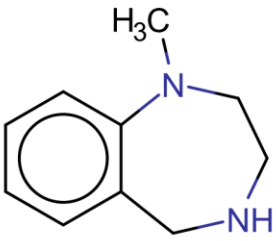	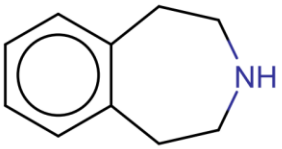	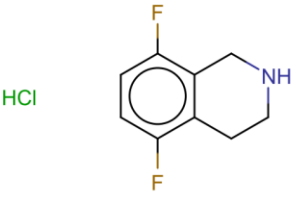	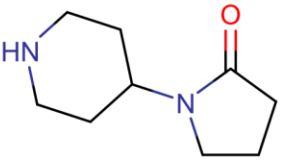
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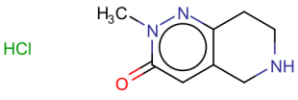	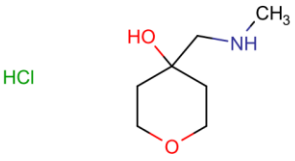	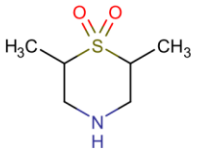	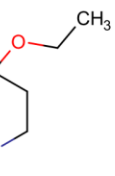
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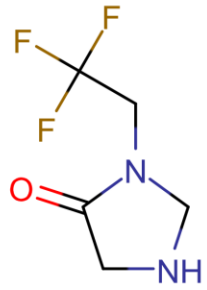
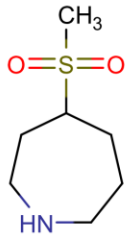
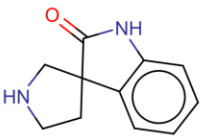
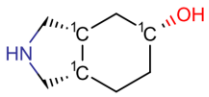
	HCl 	HCl 	HCl 
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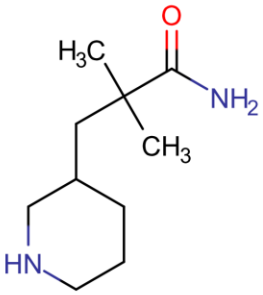
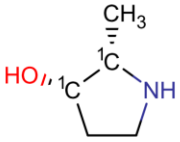
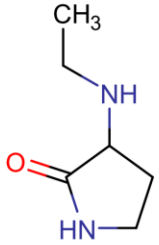
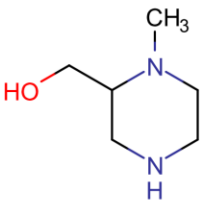
	HCl 	HCl 	HCl HCl 
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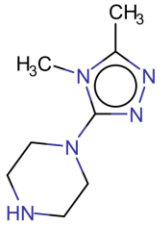
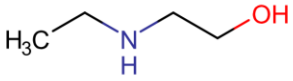
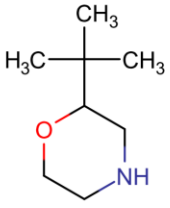
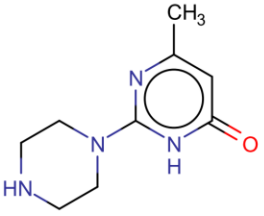
HI HI 		HCl 	HCl HCl 
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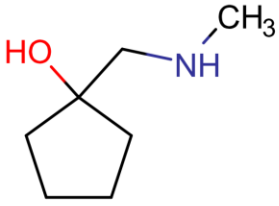
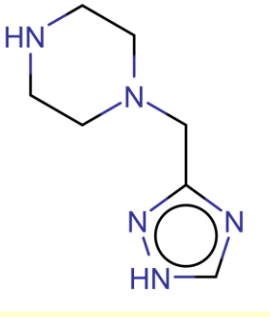
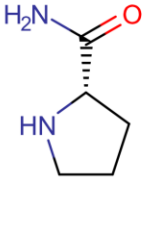
		HCl 	HCl 
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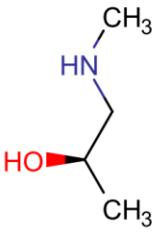
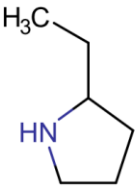
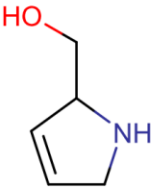
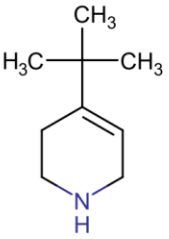
HCl 	HCl 	HCl 	HCl 
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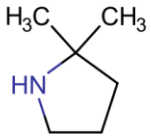
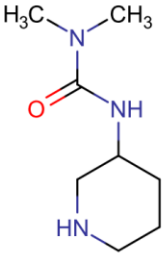
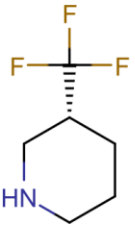
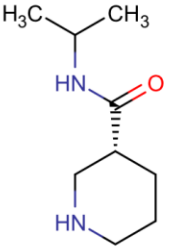
HCl 	HCl 	HCl 	HCl 
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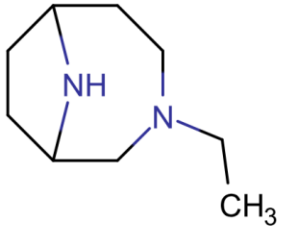
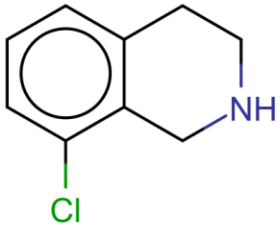
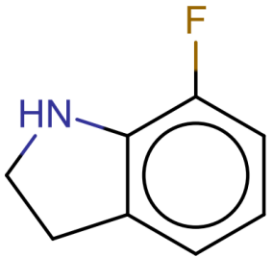
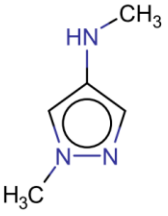
			HCl 
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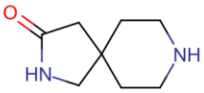
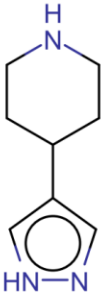
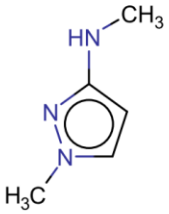
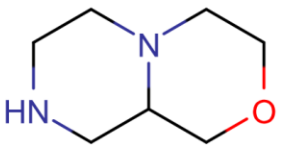
HCl 		HCl 	
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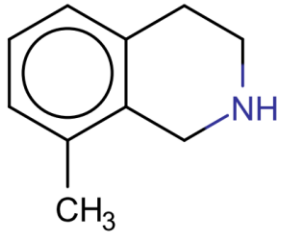	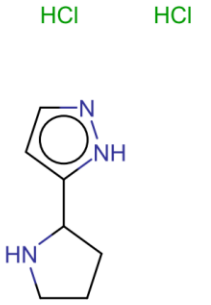	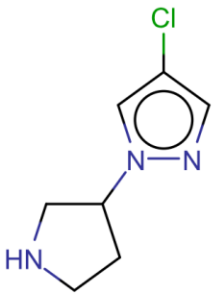	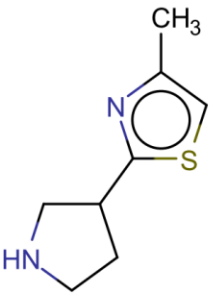
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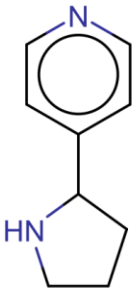	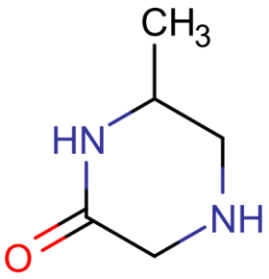	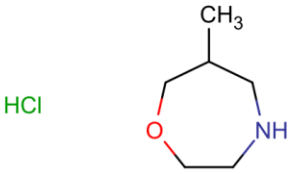	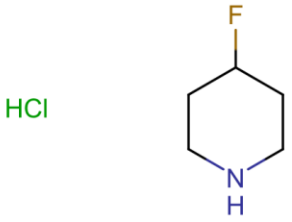
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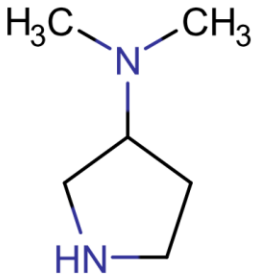	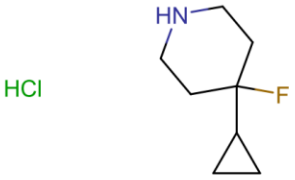	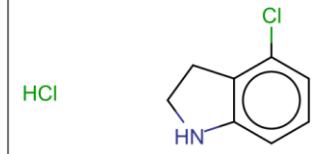	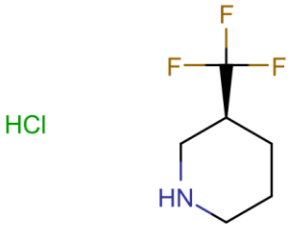
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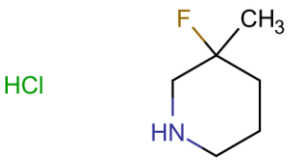	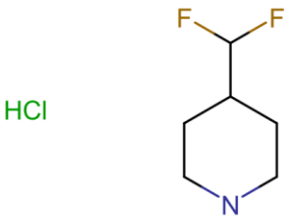	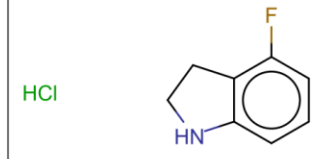	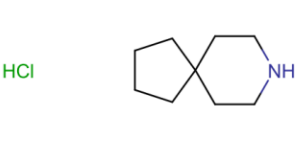
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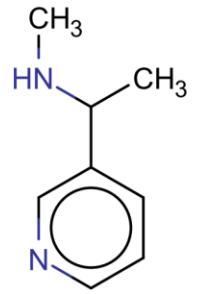	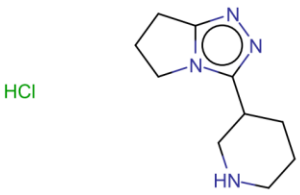	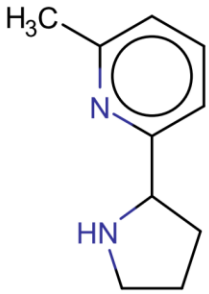	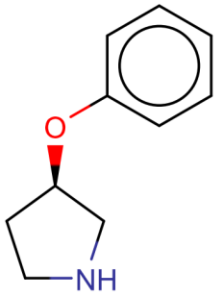
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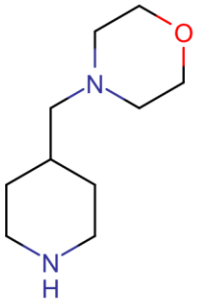	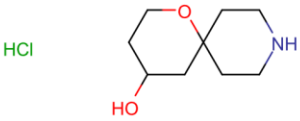	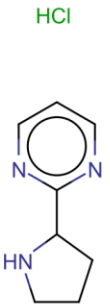	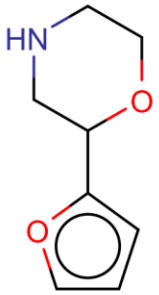
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	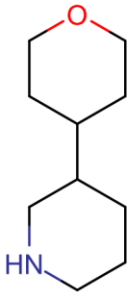	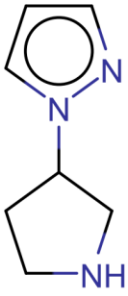	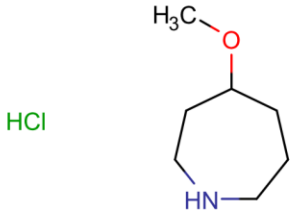
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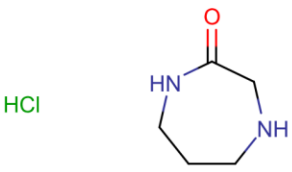	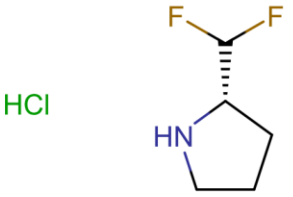	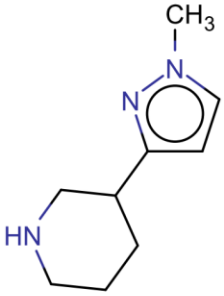	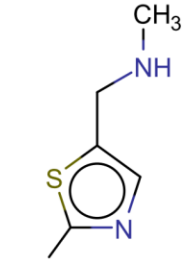
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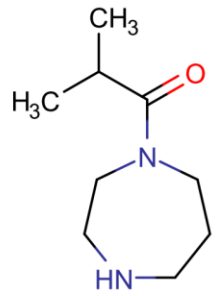	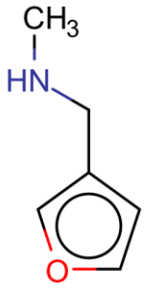	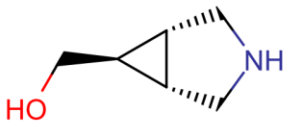	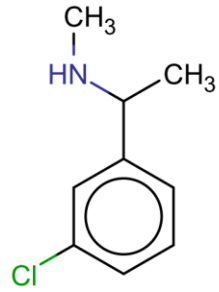
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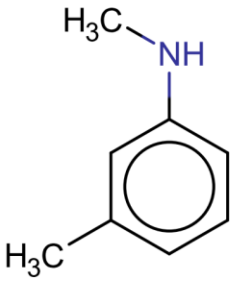	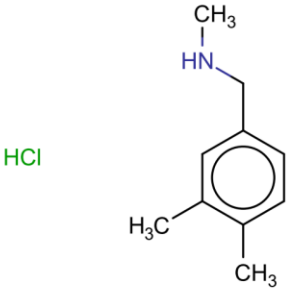	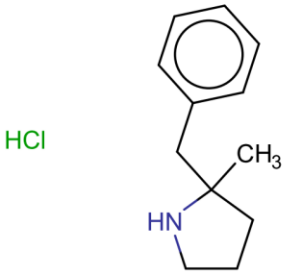	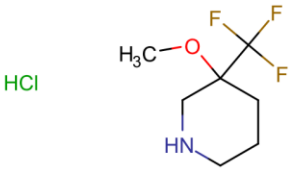
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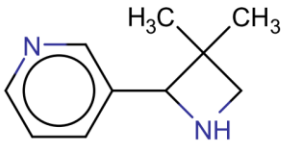	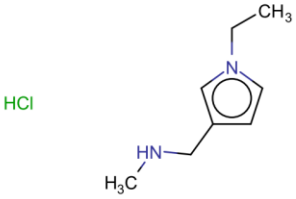	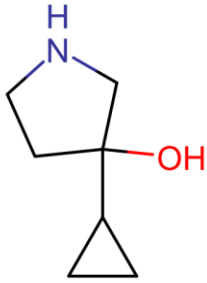	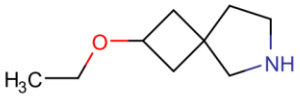
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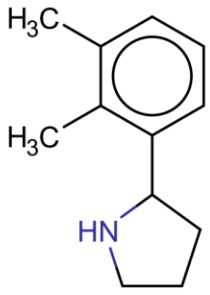	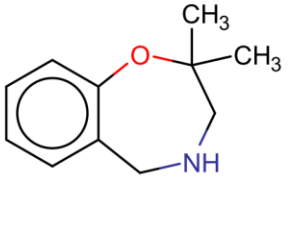	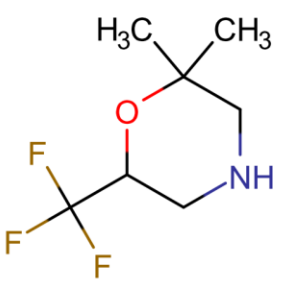	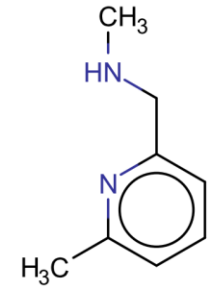
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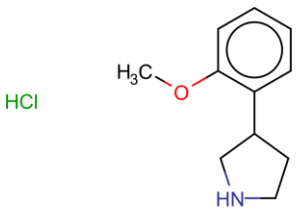	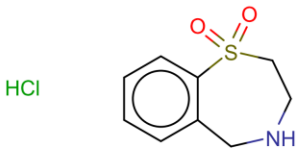	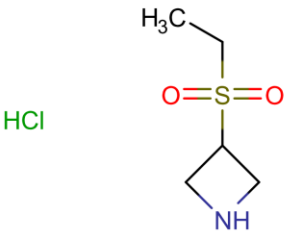	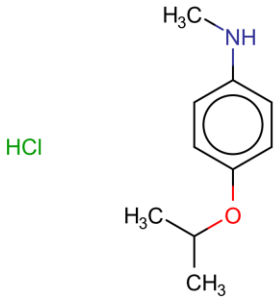
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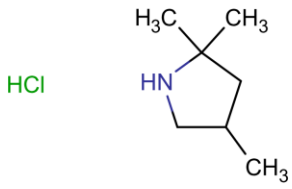	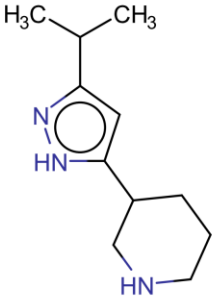	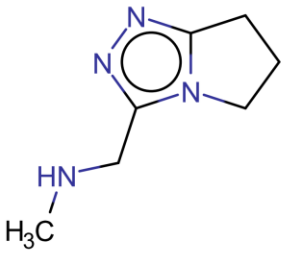	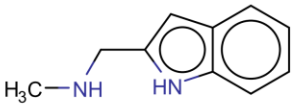
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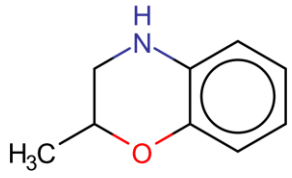	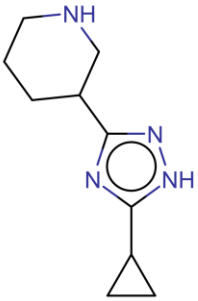	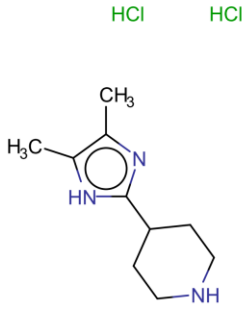	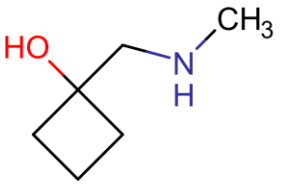
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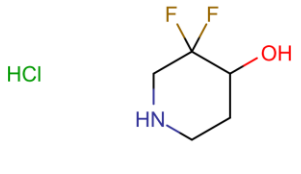	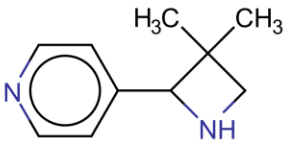	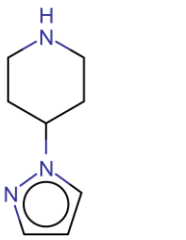	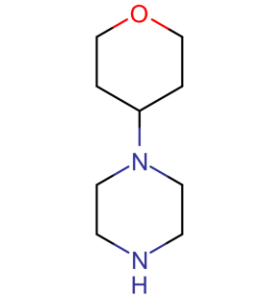
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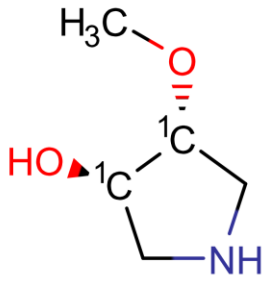	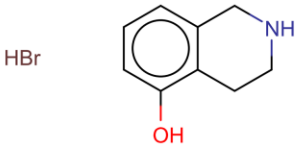	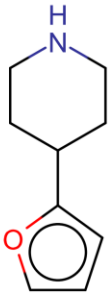	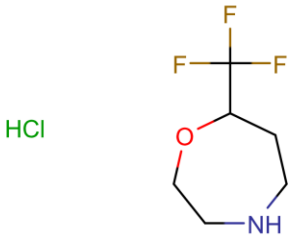
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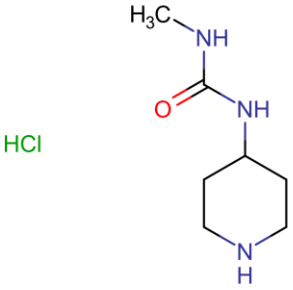	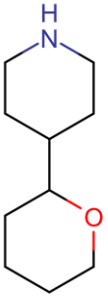	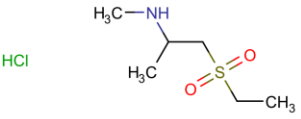	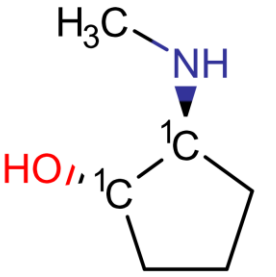
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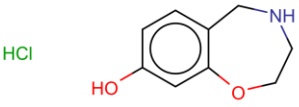	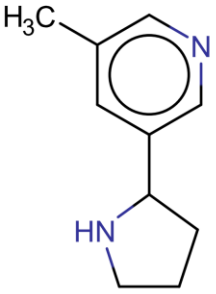	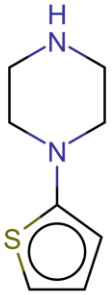	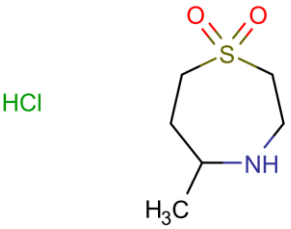
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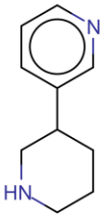	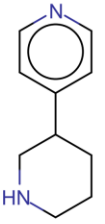	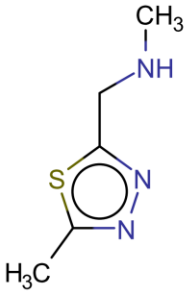	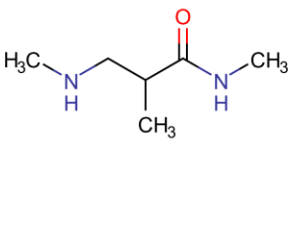
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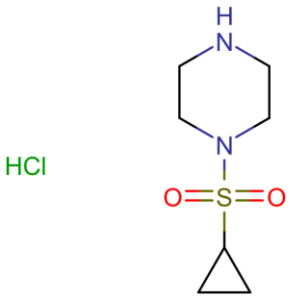	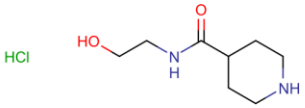	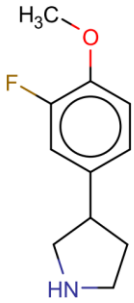	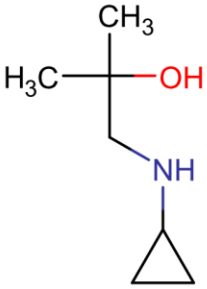
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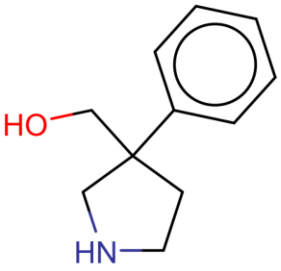	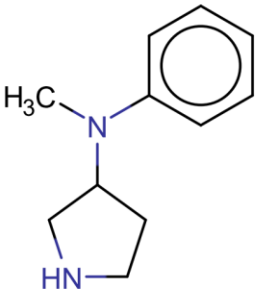	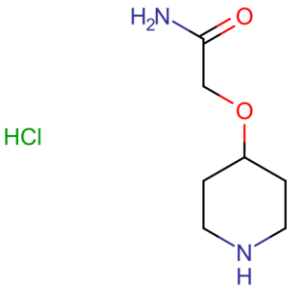	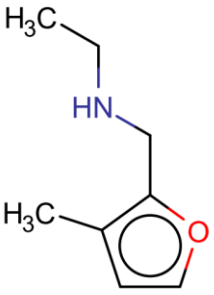
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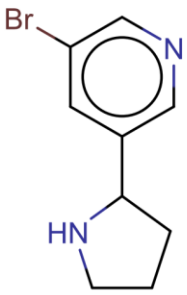	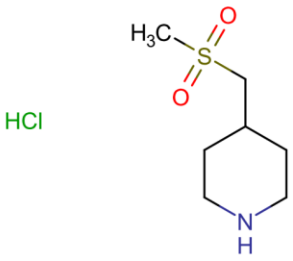	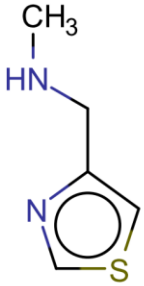	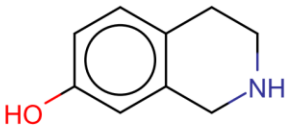
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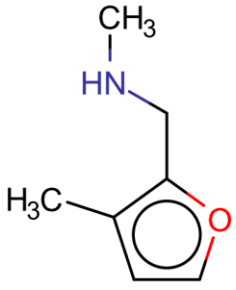	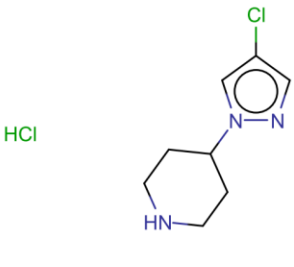	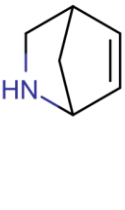	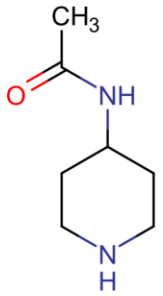
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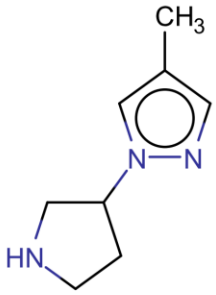	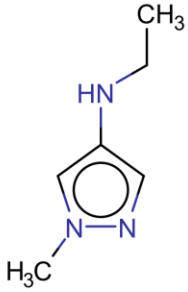	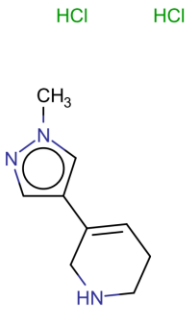	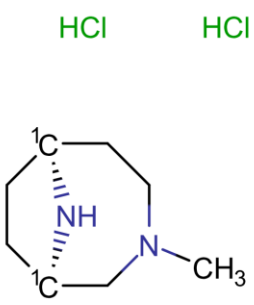
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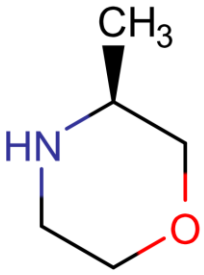	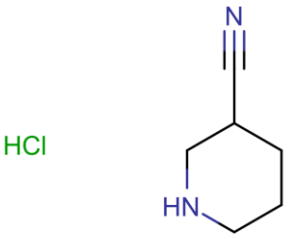	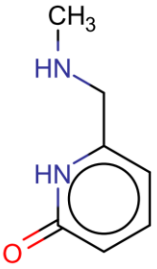	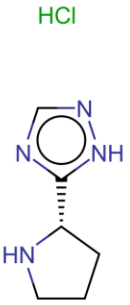
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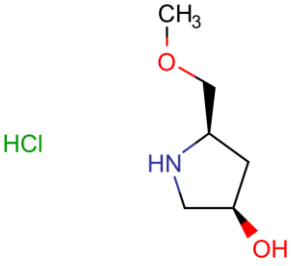	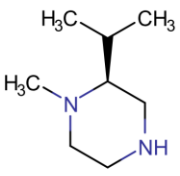	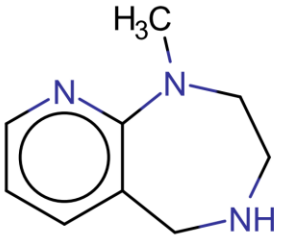	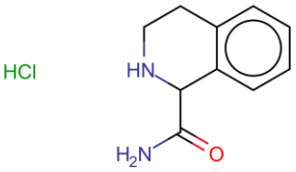
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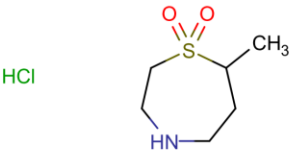	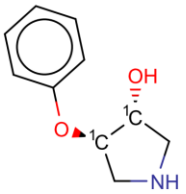		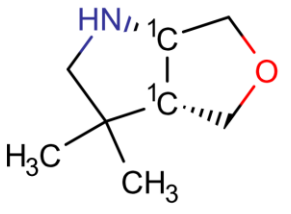
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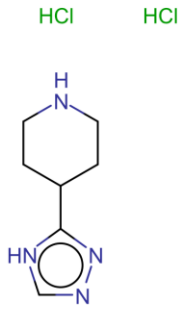	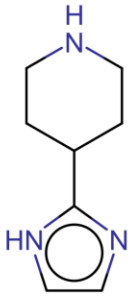	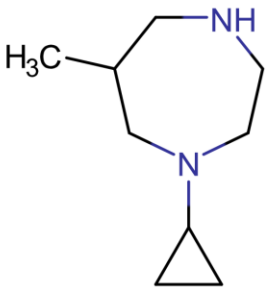	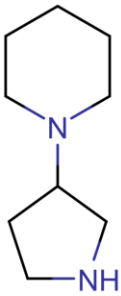
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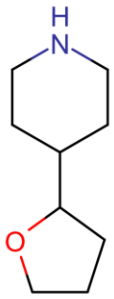	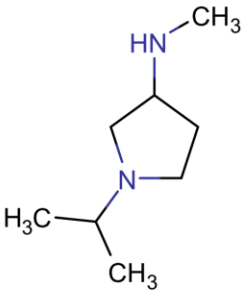	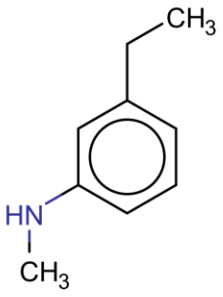	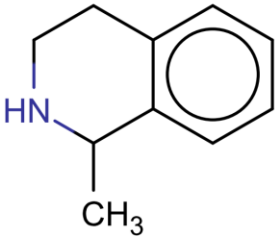
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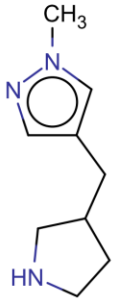	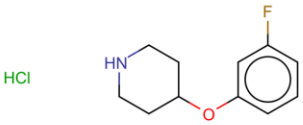	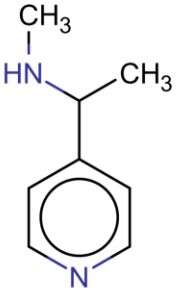	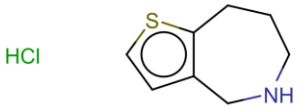
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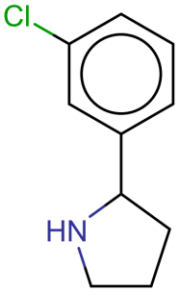	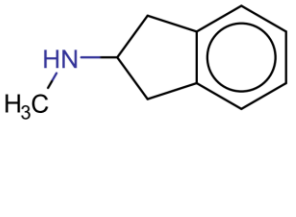	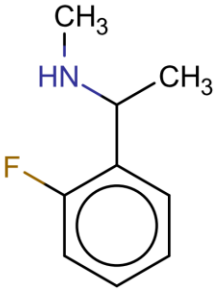	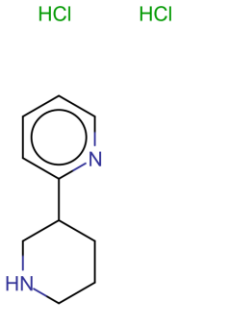
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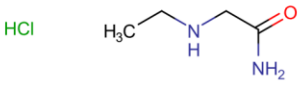	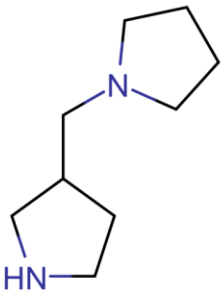	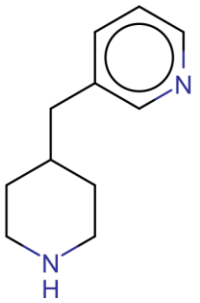	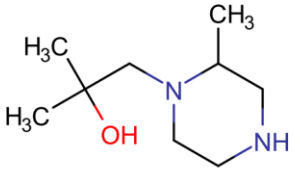
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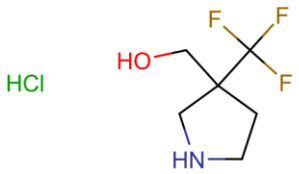	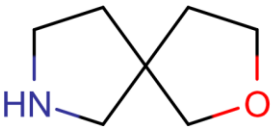	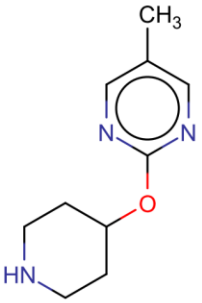	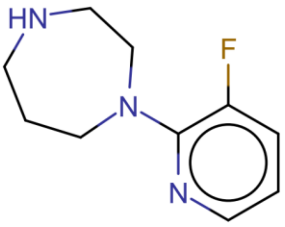
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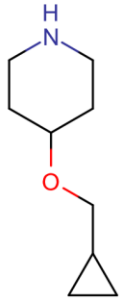	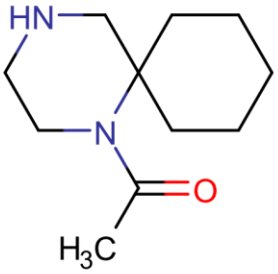	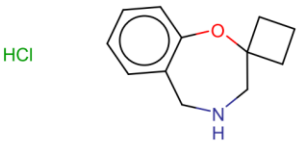	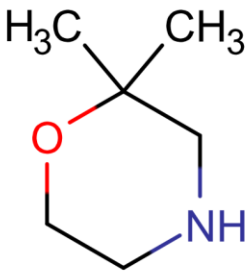
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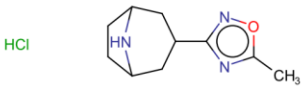	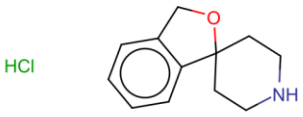	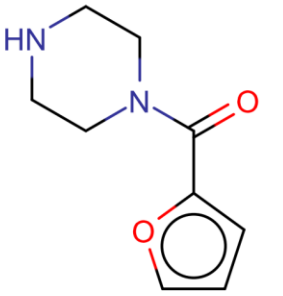	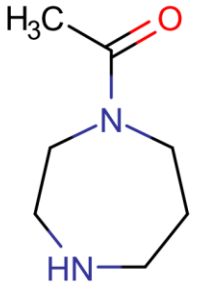
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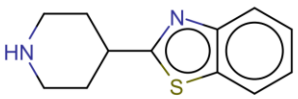	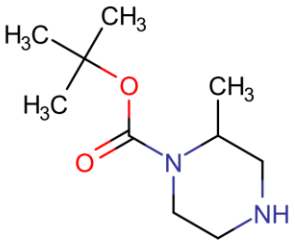	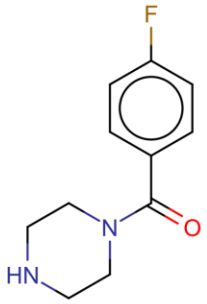	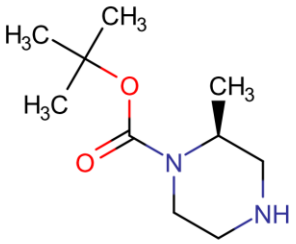
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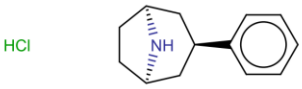	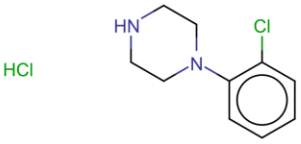	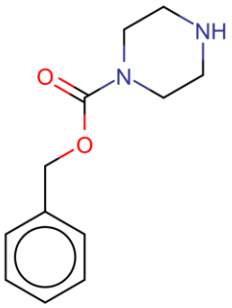	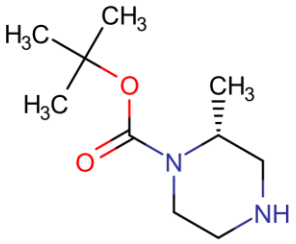
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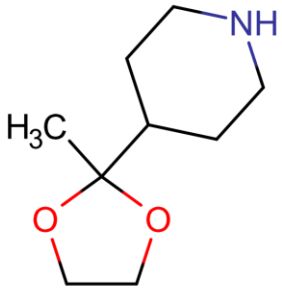	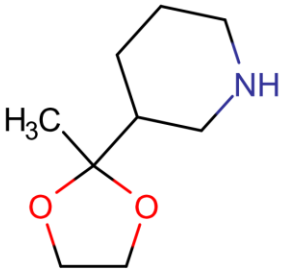	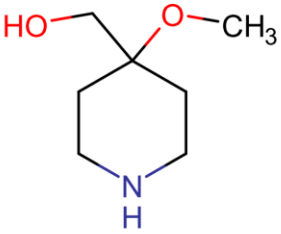	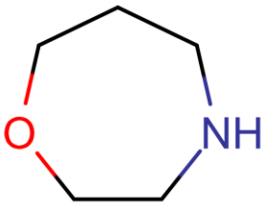
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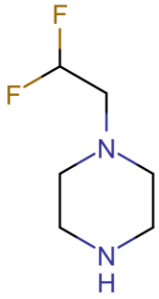	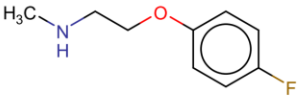	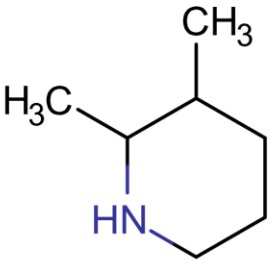	
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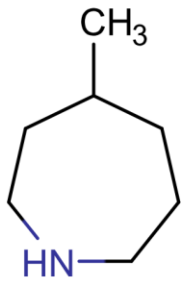	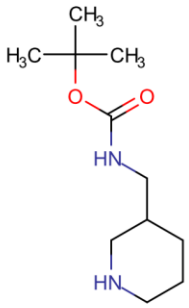	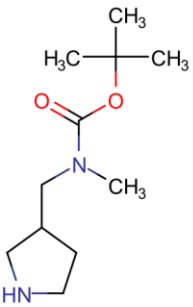	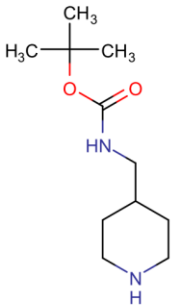
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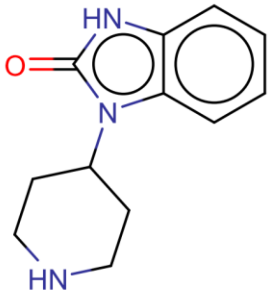	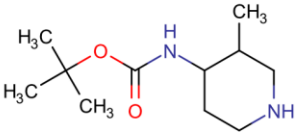	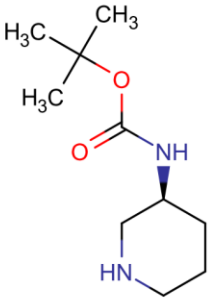	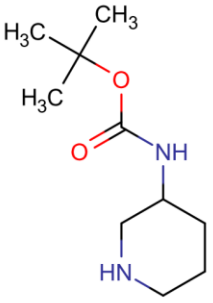
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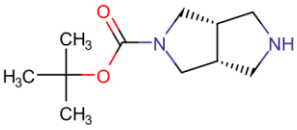	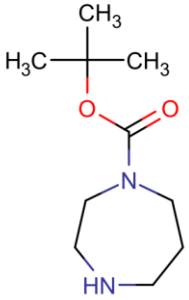	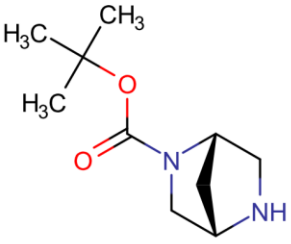	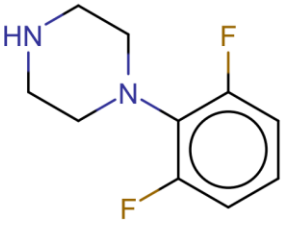
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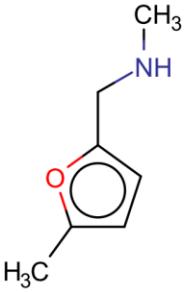	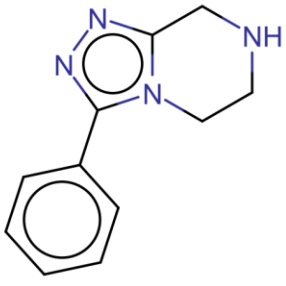	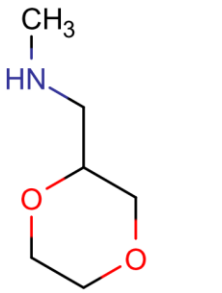	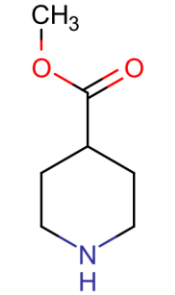
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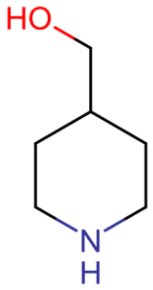	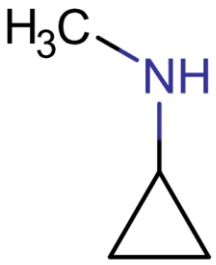	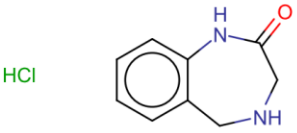	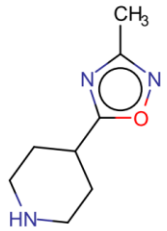
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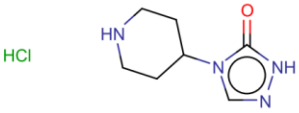	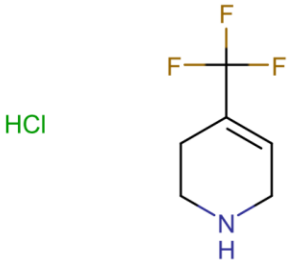	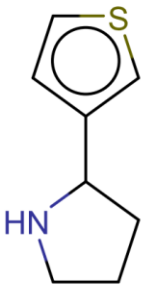	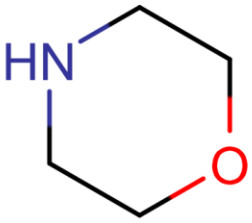
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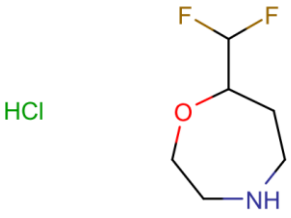	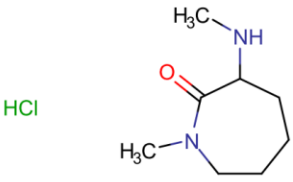	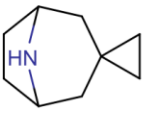	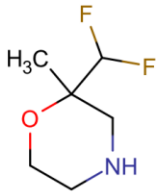
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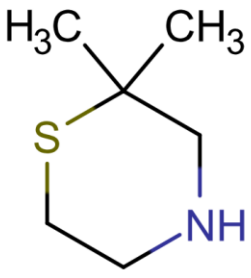	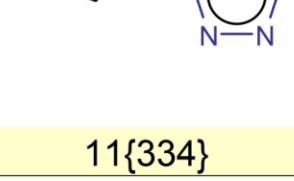	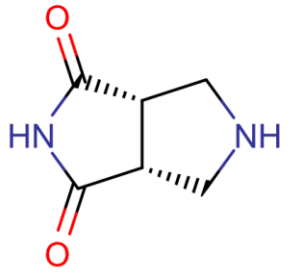	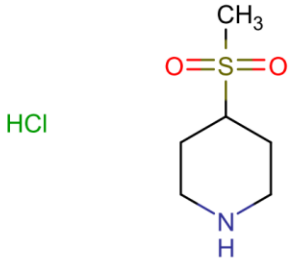
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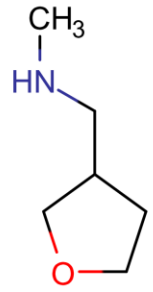	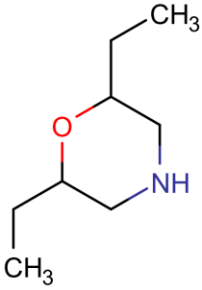	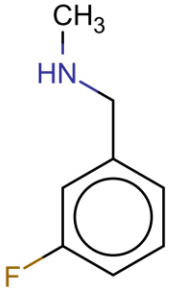	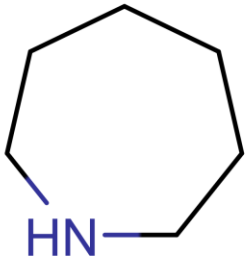
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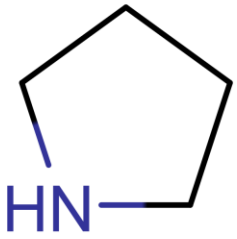	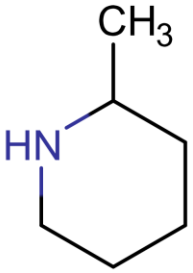	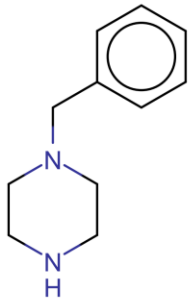	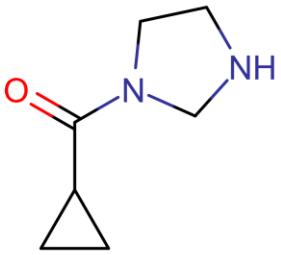
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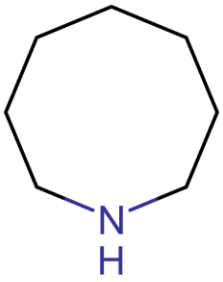	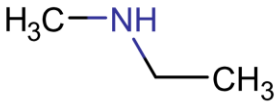	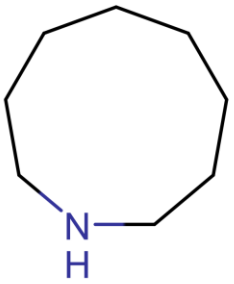	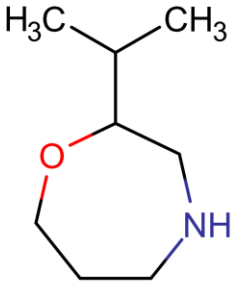
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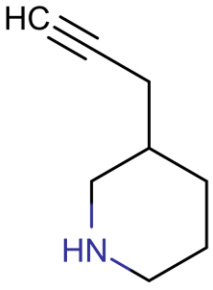	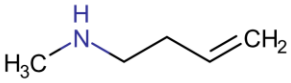	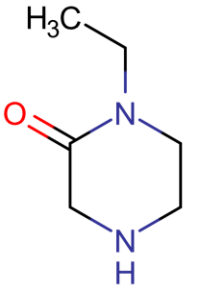	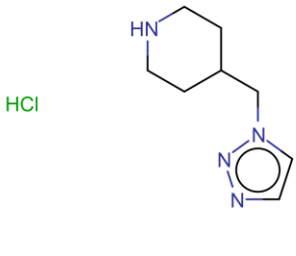
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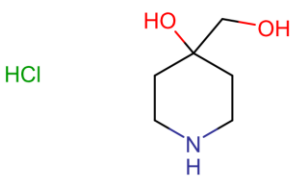	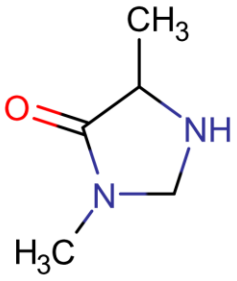	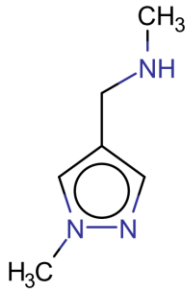	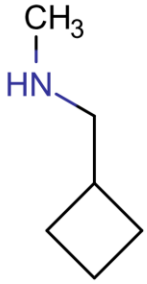
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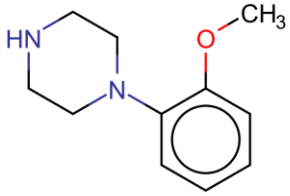	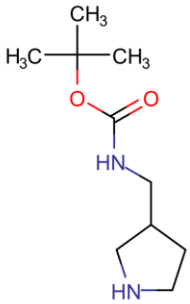	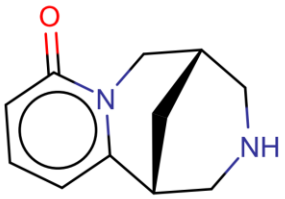	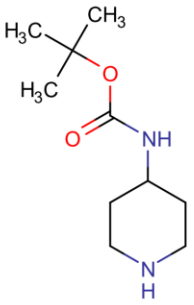
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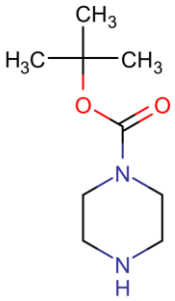	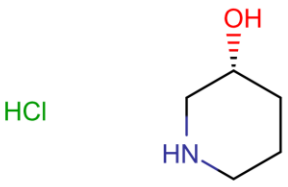	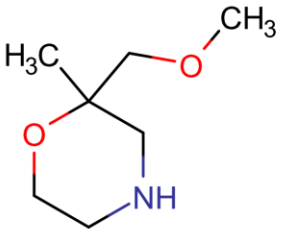	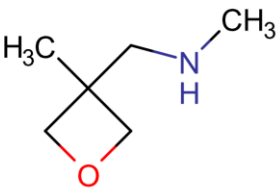
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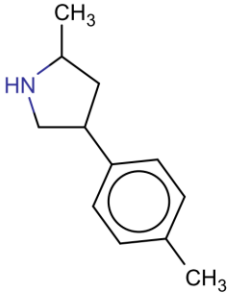	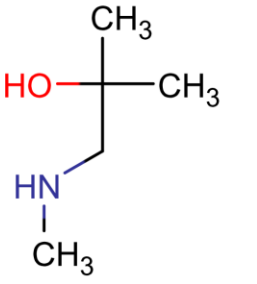	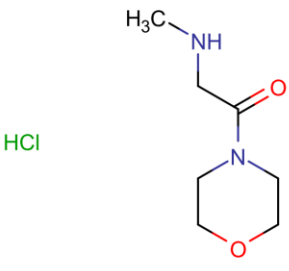	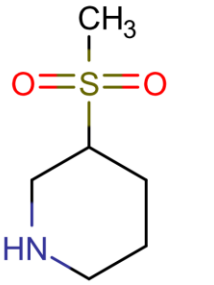
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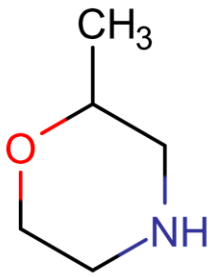
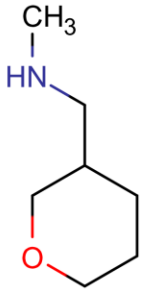
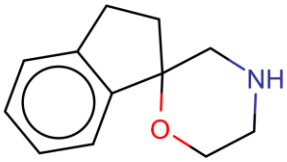
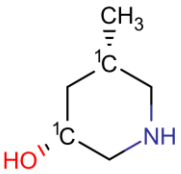
			HCl 
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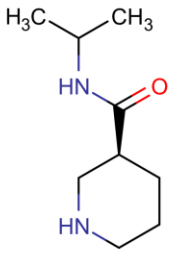
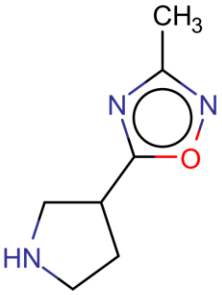
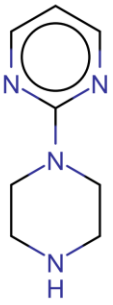
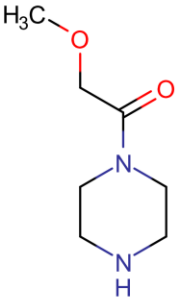
HCl 			
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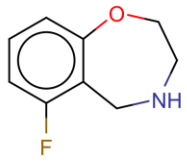
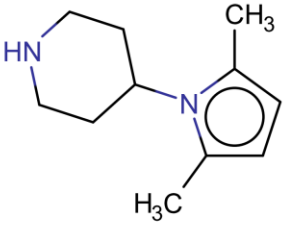
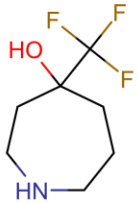
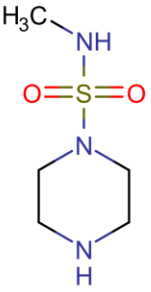
HCl 		HCl 	HCl 
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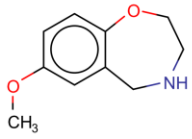
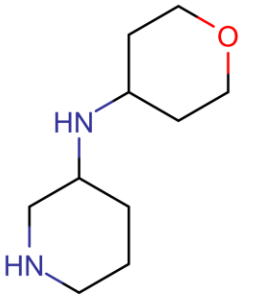
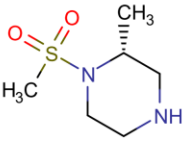
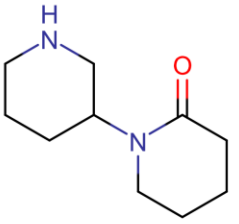
HCl 		HCl 	HCl HCl 
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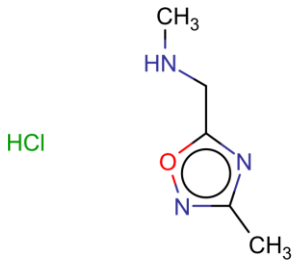	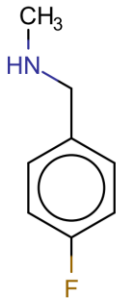	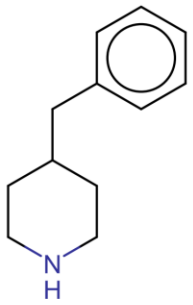	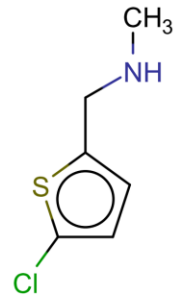
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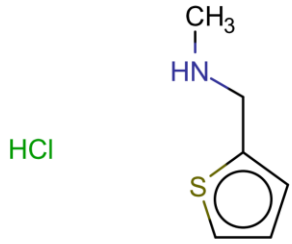	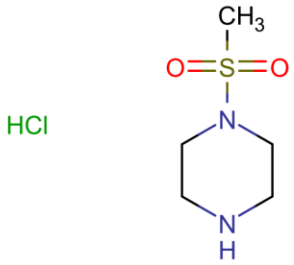	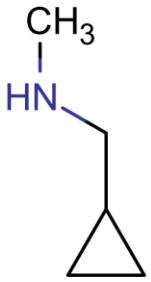	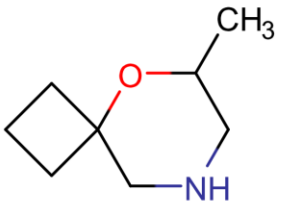
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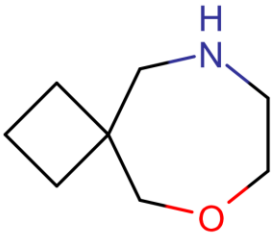	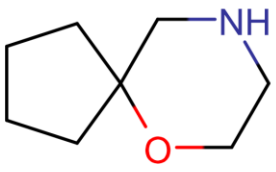	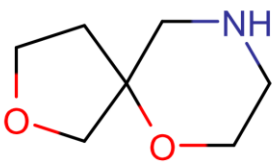	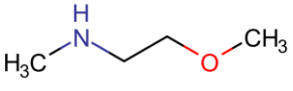
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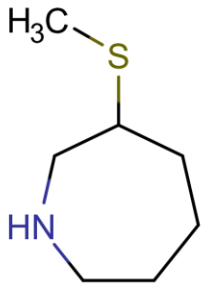	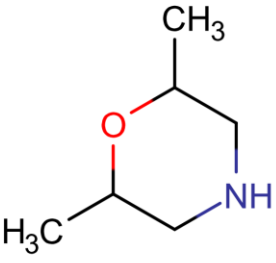	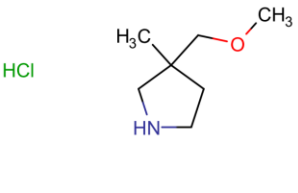	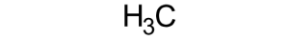
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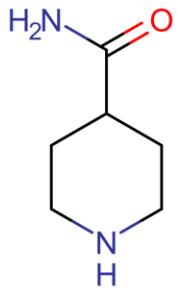	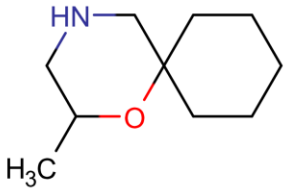	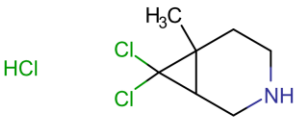	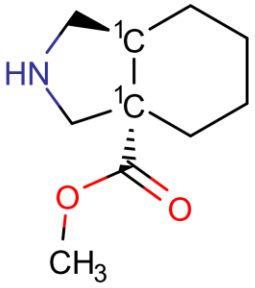
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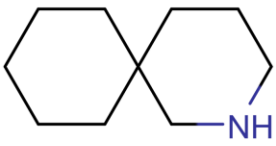	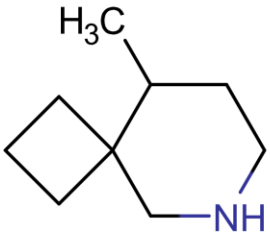		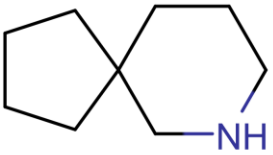
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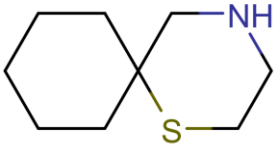	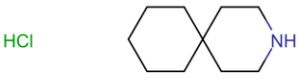	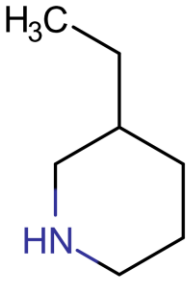	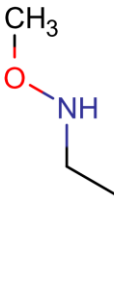
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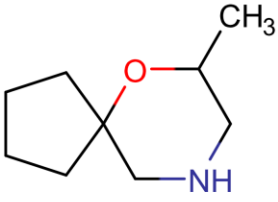	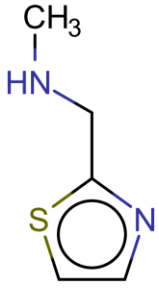	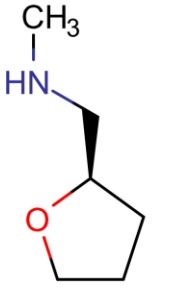	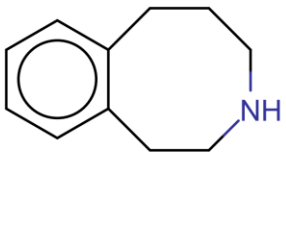
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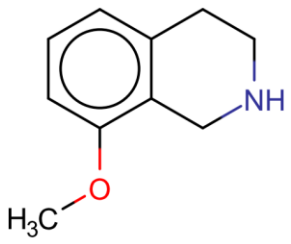	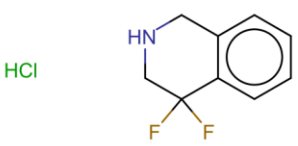	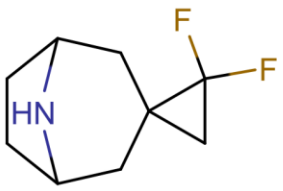	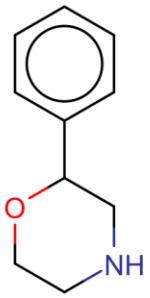
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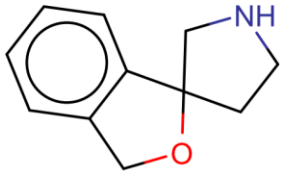	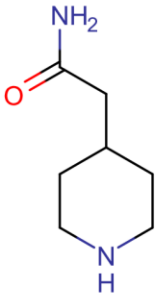	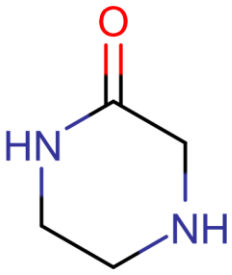	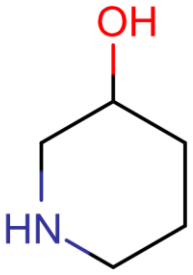
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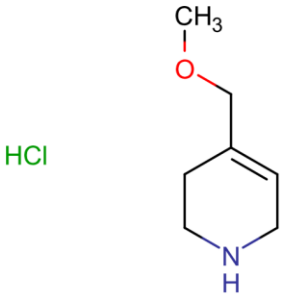	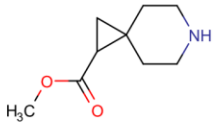	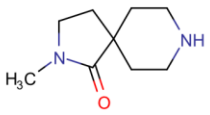	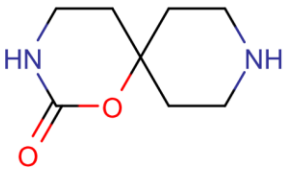
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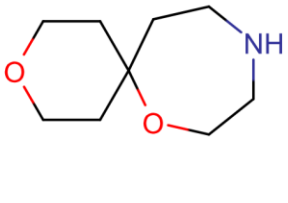	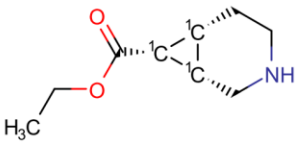		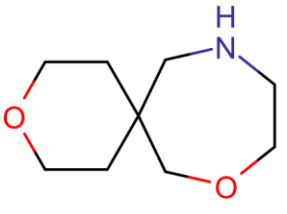
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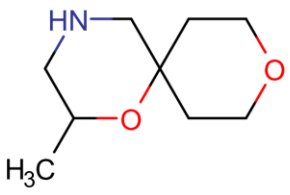	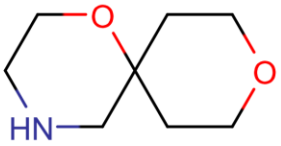	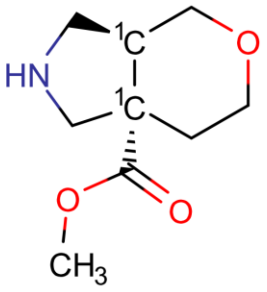	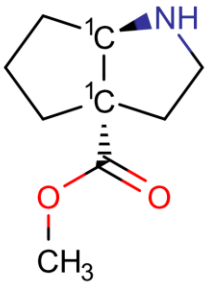
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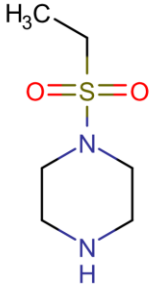
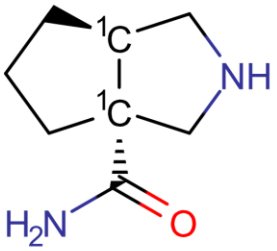
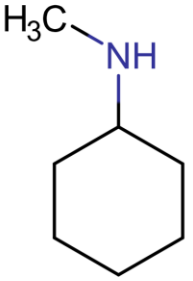
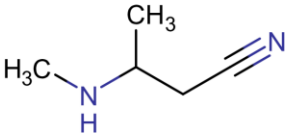
HCl 			
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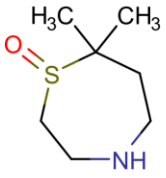
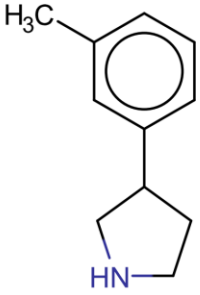
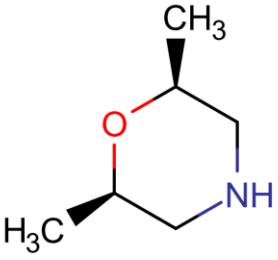
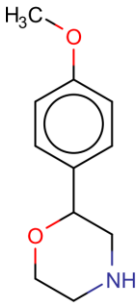
HCl 			
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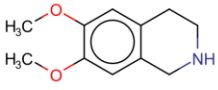
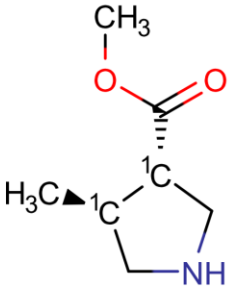
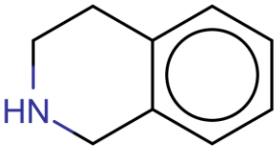
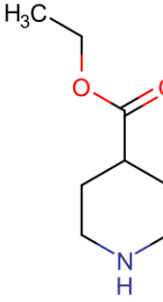
HCl 			
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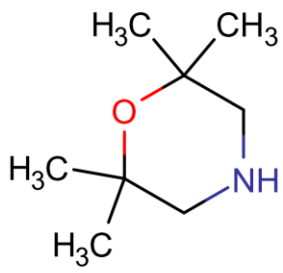	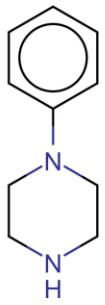	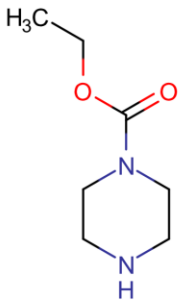	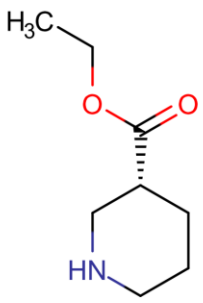
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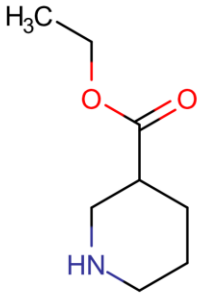	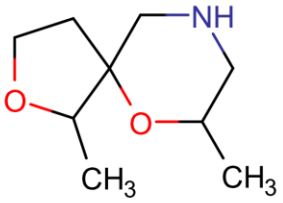	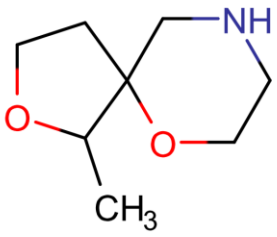	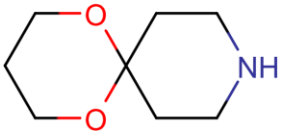
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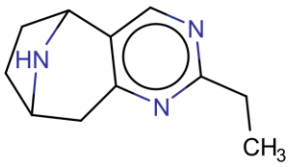	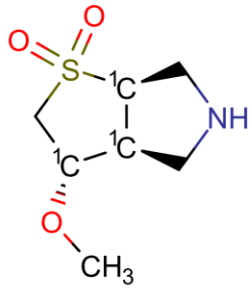	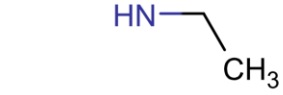	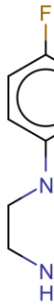
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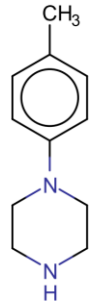	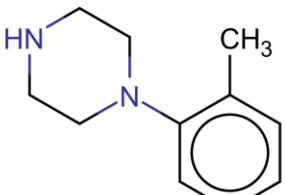	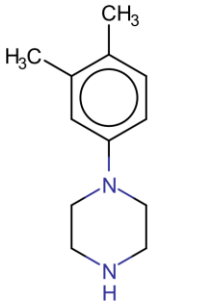	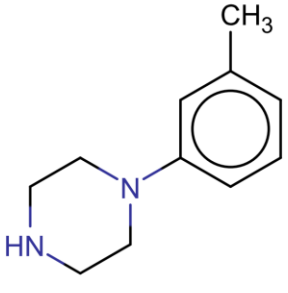
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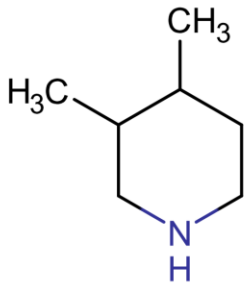	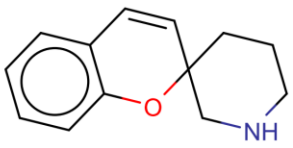	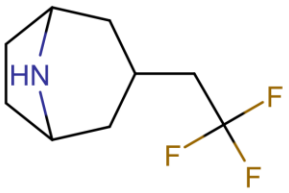	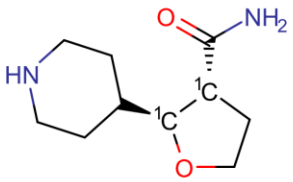
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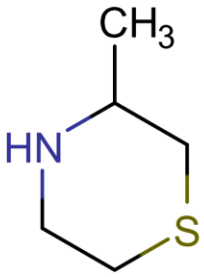	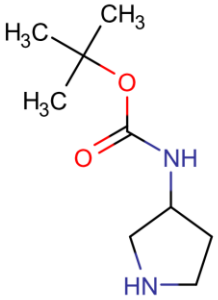	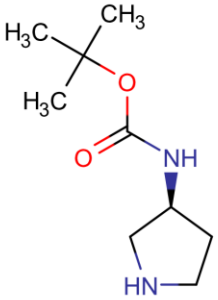	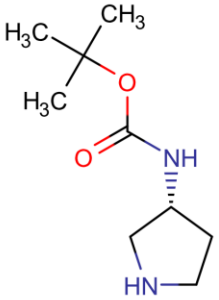
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	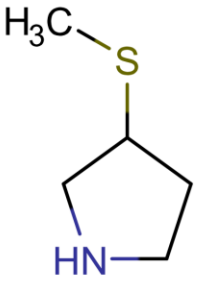	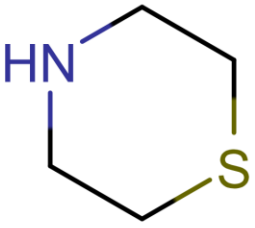	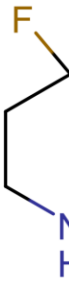
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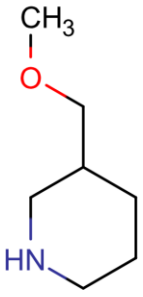	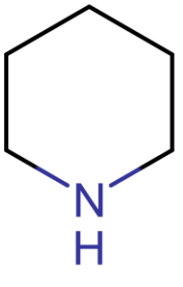	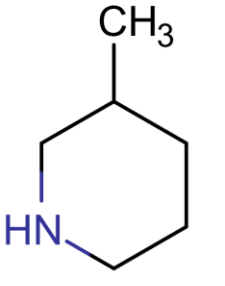	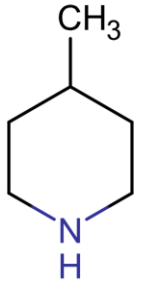
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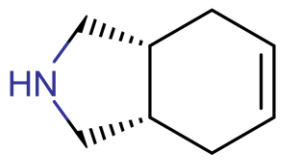	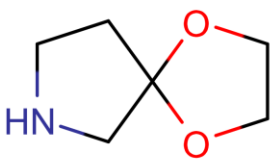	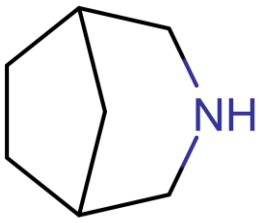	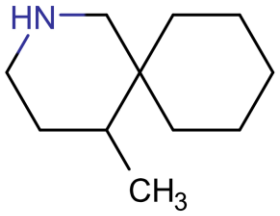
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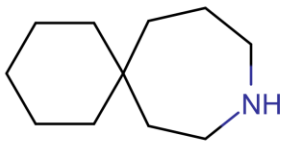	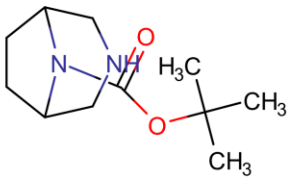	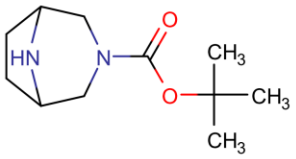	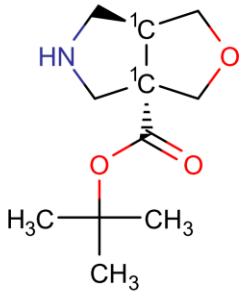
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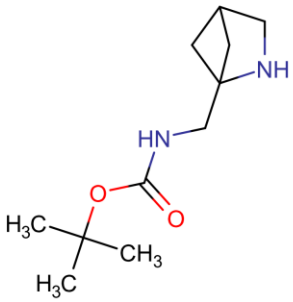	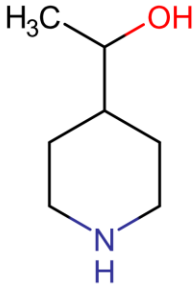	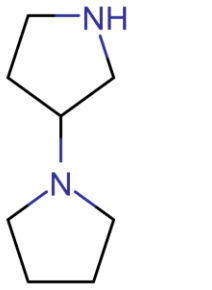	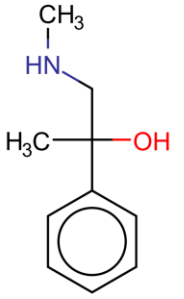
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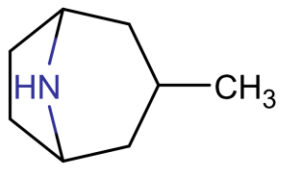	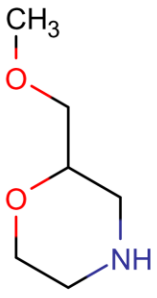	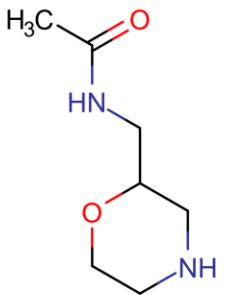	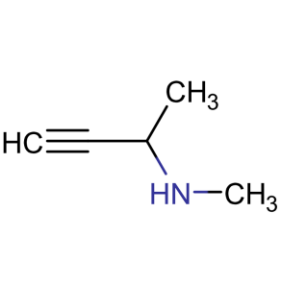
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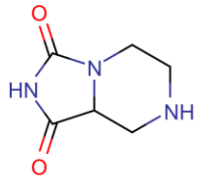
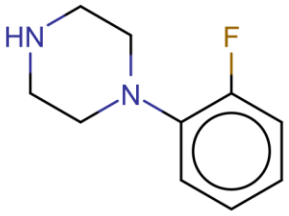
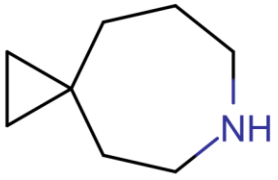
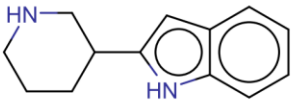
HCl 			
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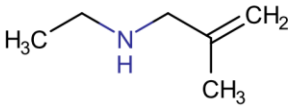	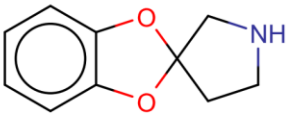	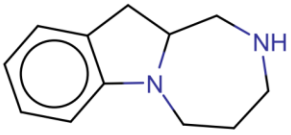	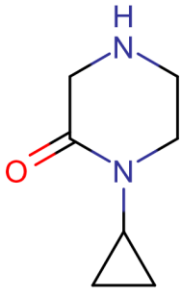
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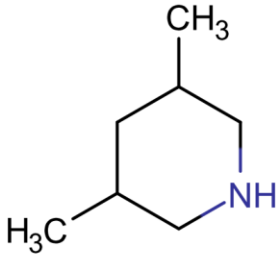
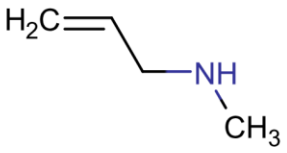
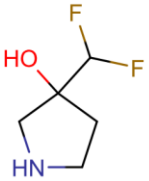
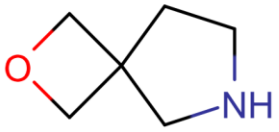
		HCl 	
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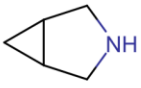
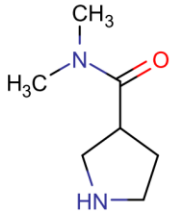
HCl 	HCl 	HCl 	
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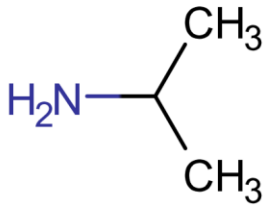
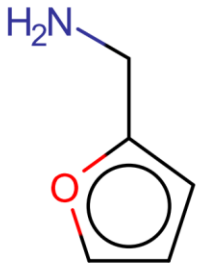
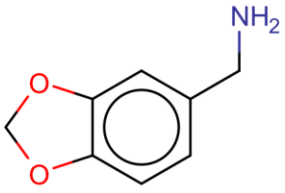
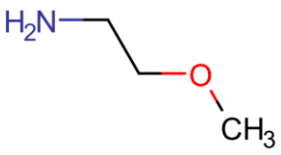
Figure S3. Structures of the reagents **15**{*1–378*}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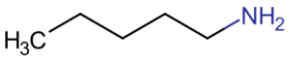	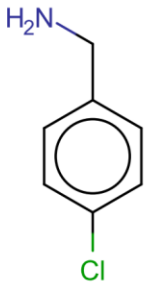	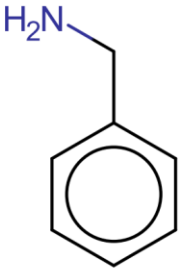	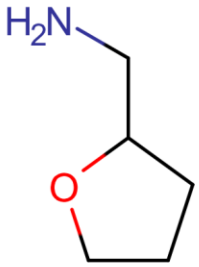
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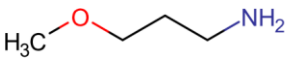	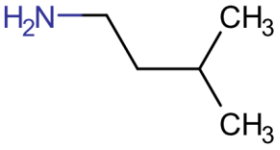	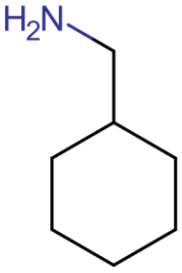	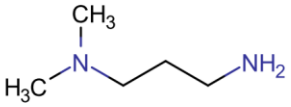
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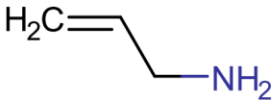	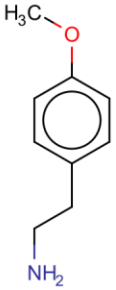	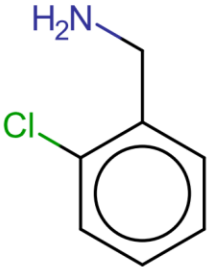	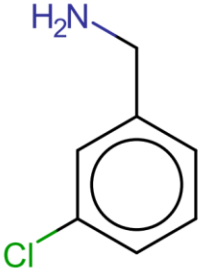
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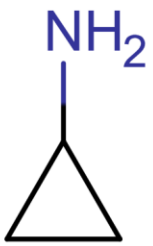	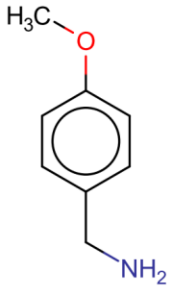	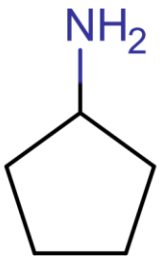	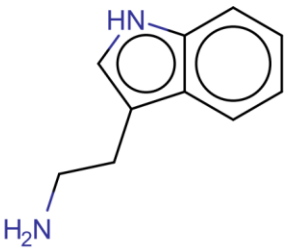
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	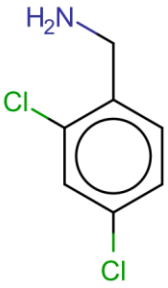	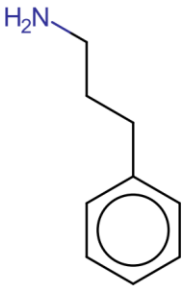	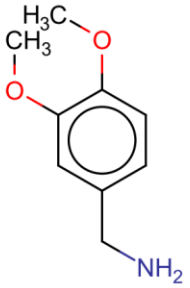
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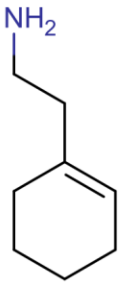	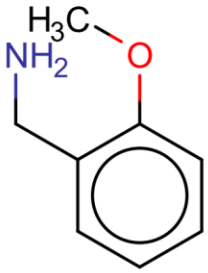	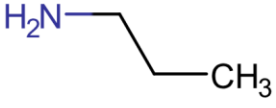	
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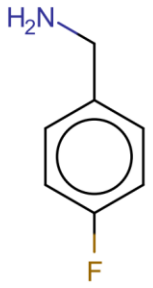	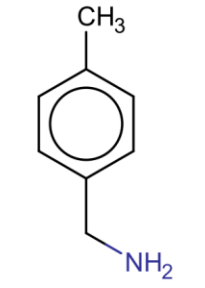	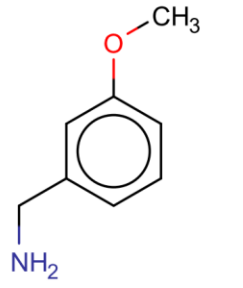	
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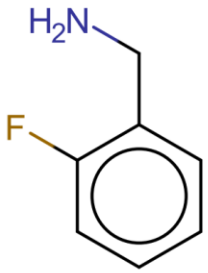	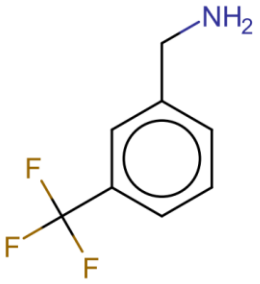	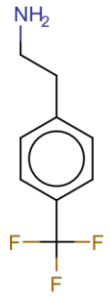	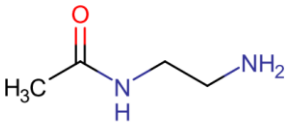
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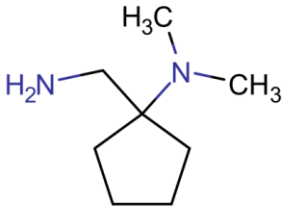	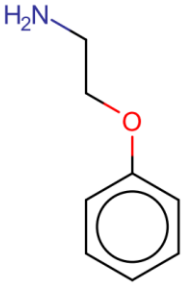	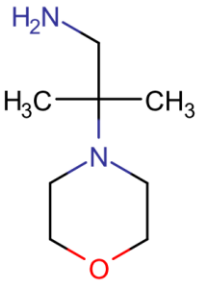	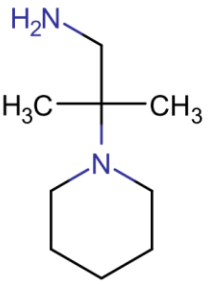
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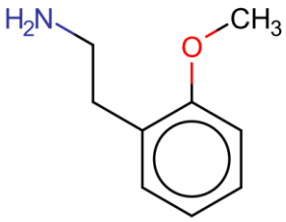	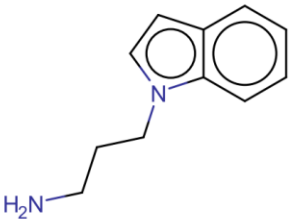	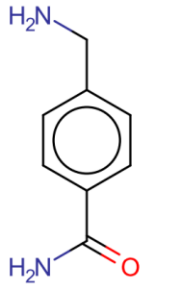	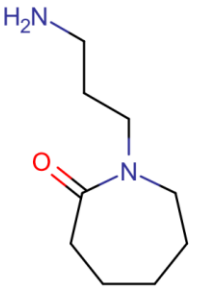
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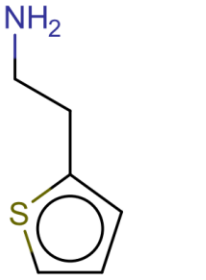	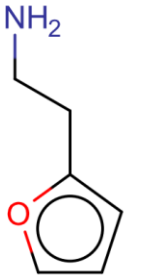	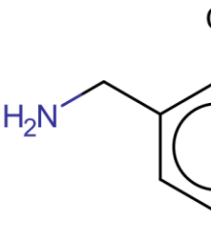	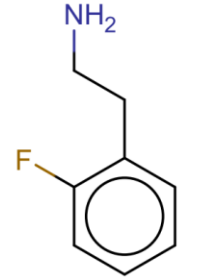
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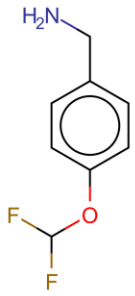	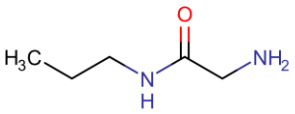	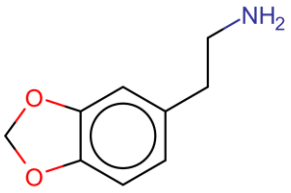	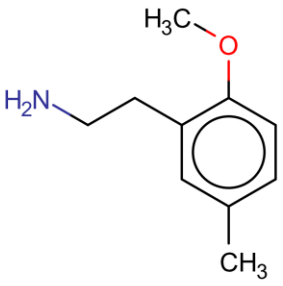
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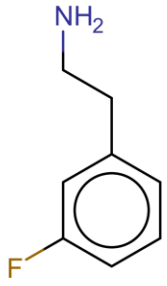	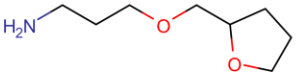	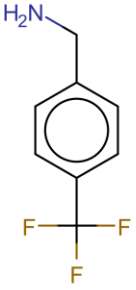	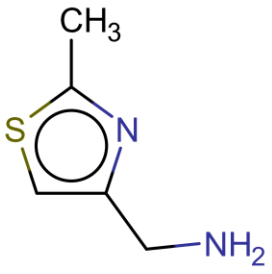
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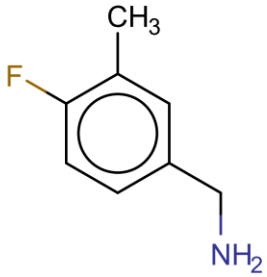	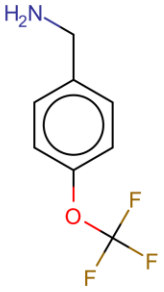	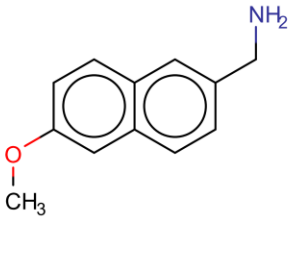	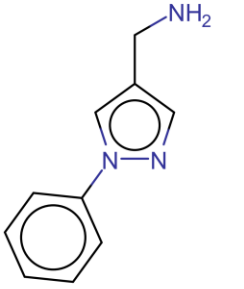
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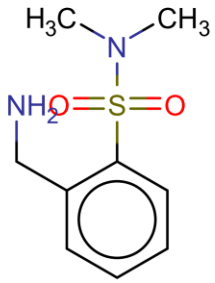	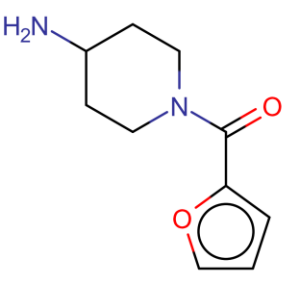	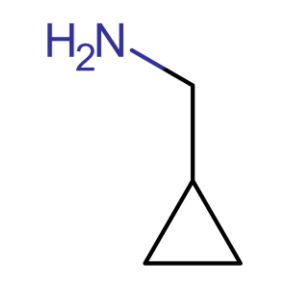	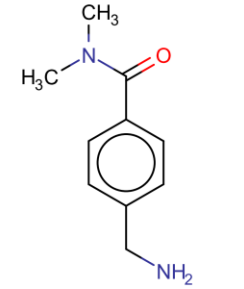
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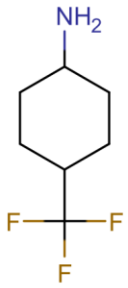	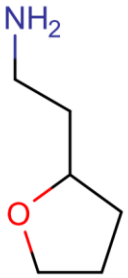	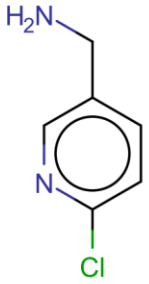	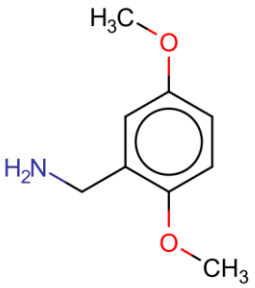
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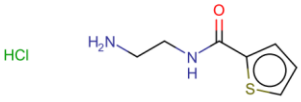	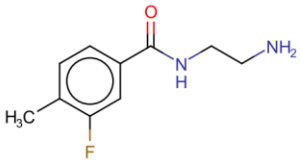	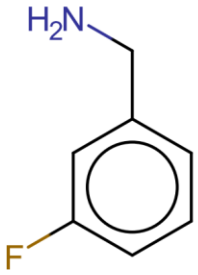	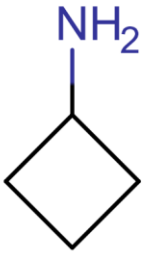
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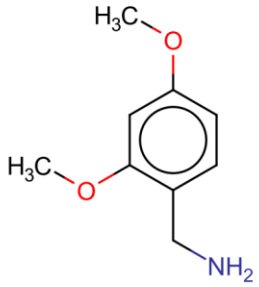	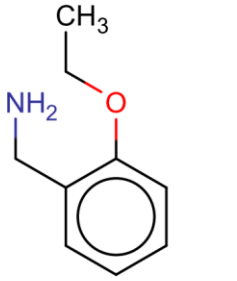	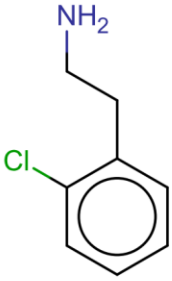	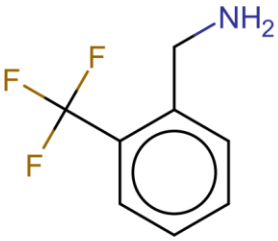
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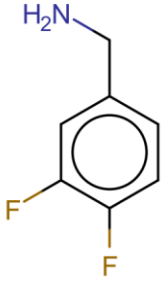	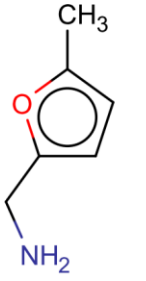	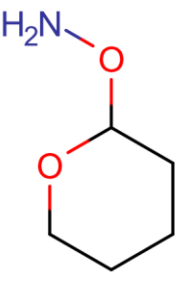	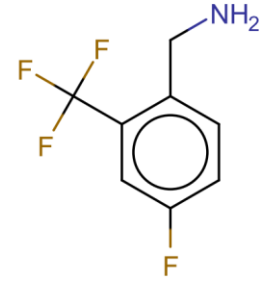
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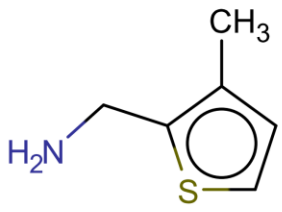	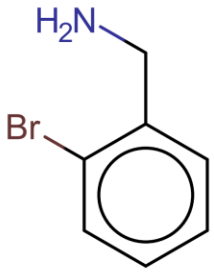	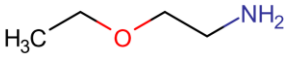	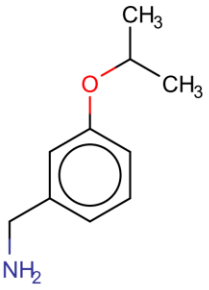
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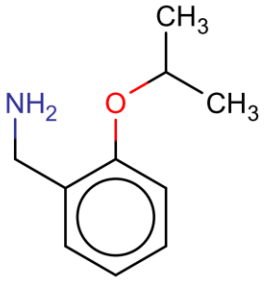	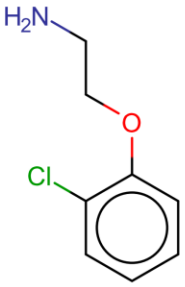	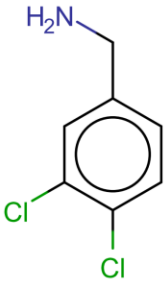	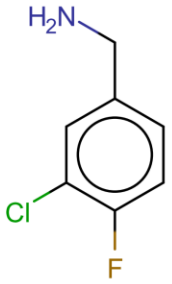
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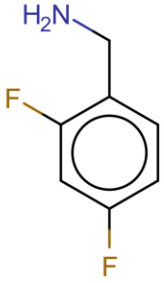	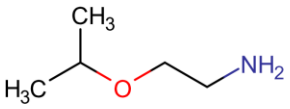	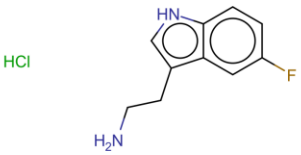	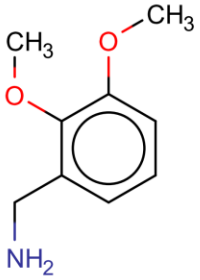
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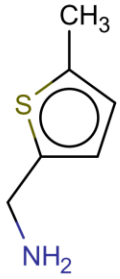	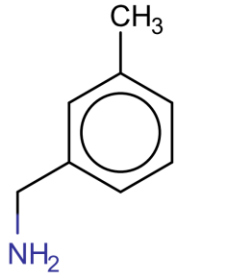	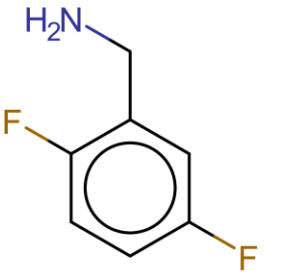	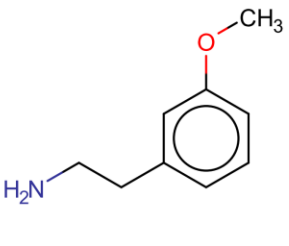
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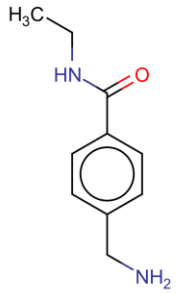	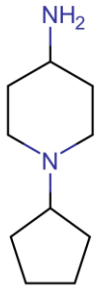	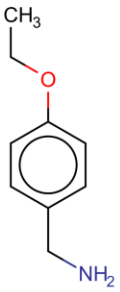	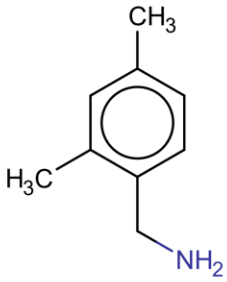
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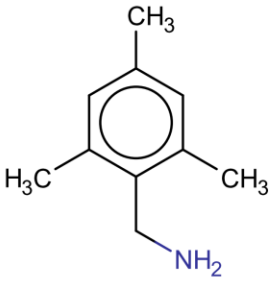	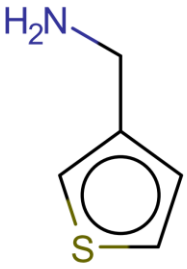	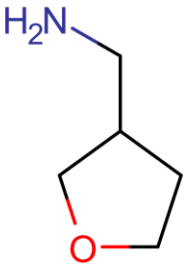	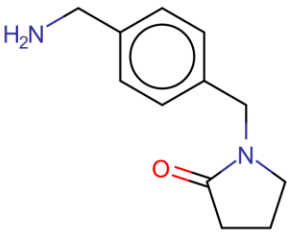
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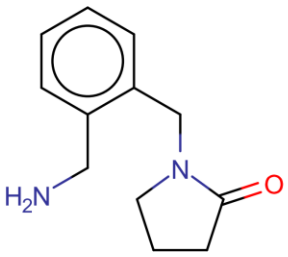	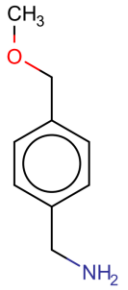	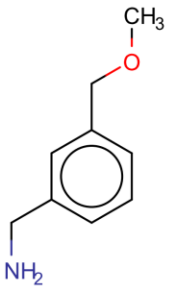	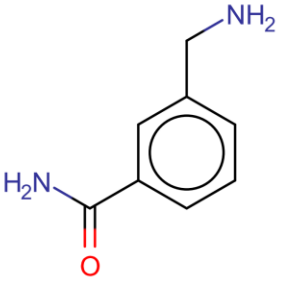
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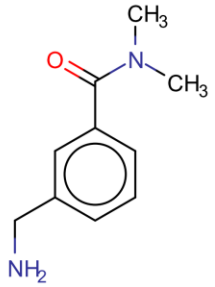	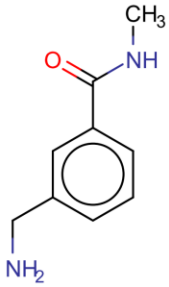	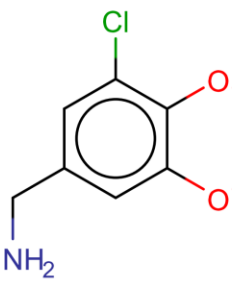	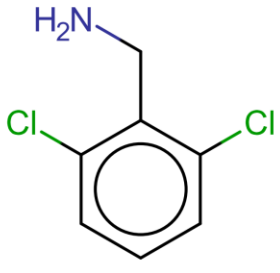
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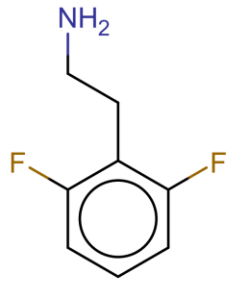	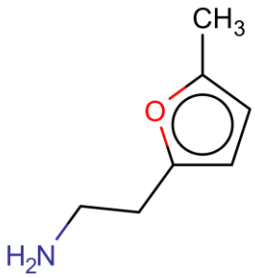	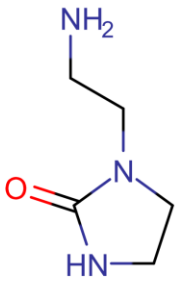	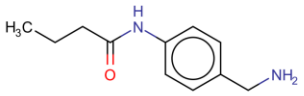
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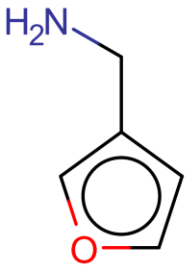	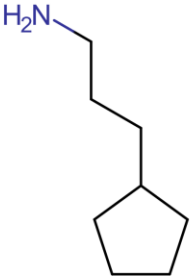	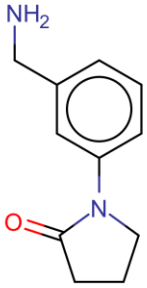	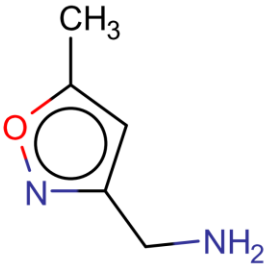
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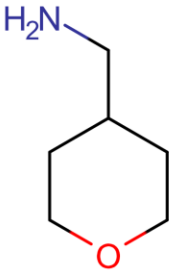	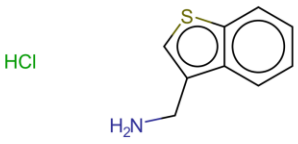	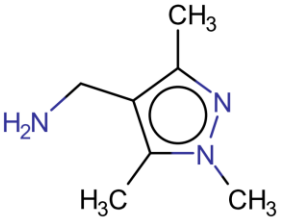	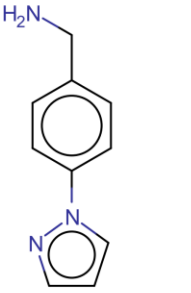
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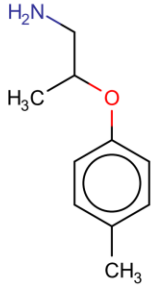	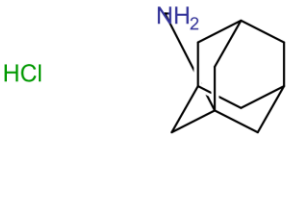	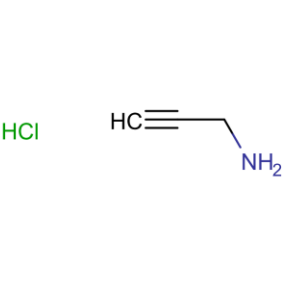	
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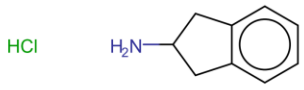	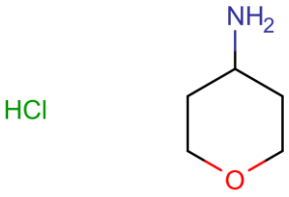	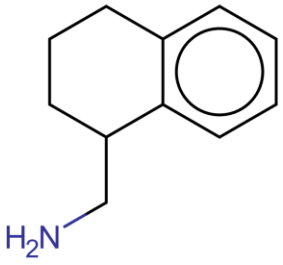	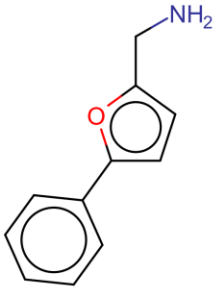
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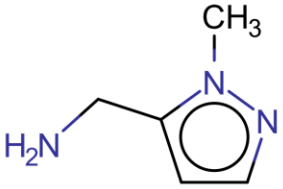	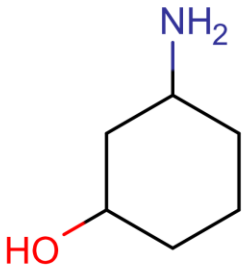	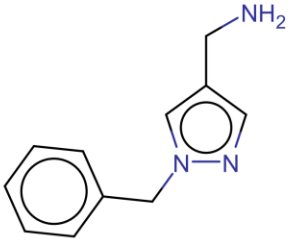	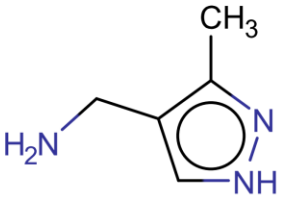
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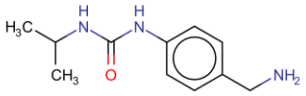	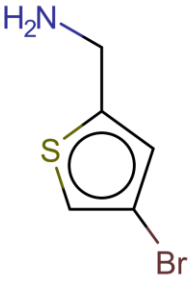	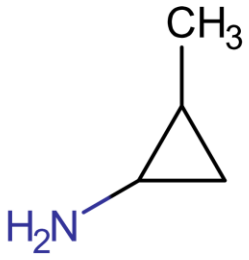	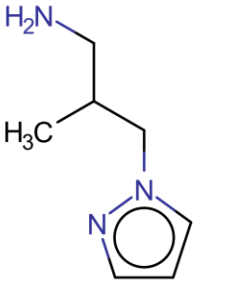
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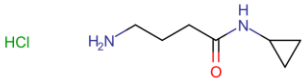	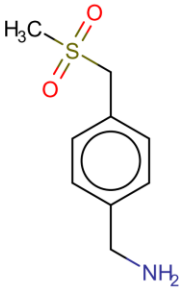	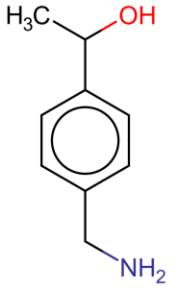	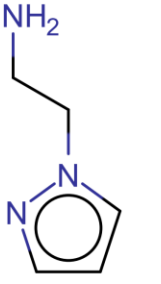
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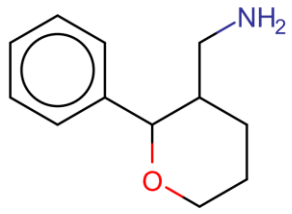	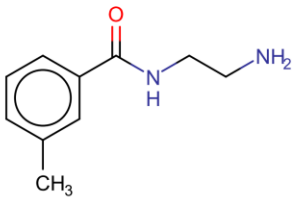	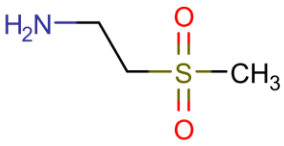	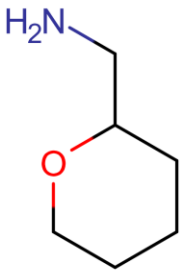
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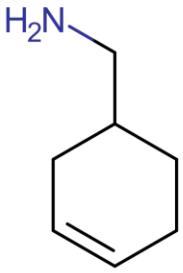	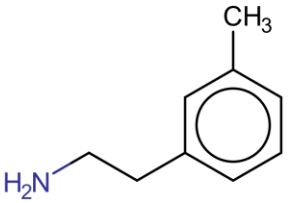	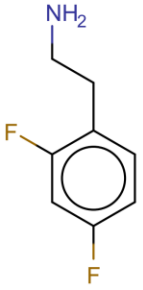	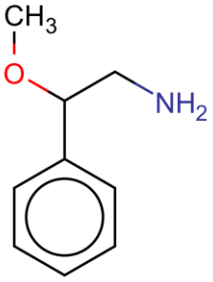
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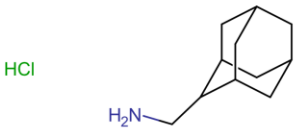	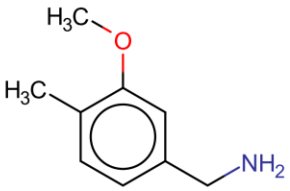	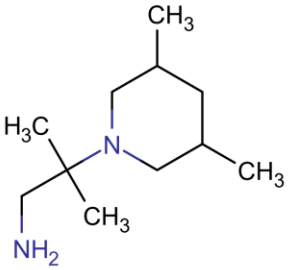	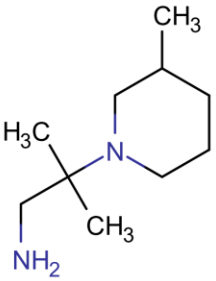
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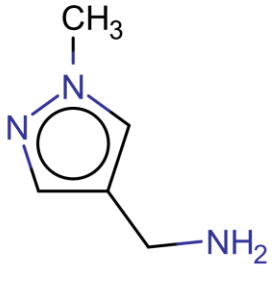	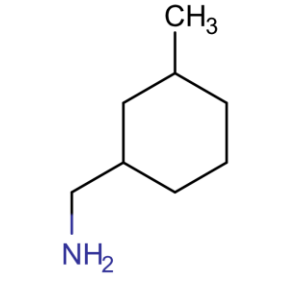	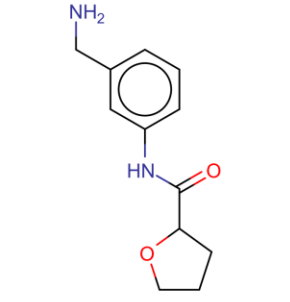	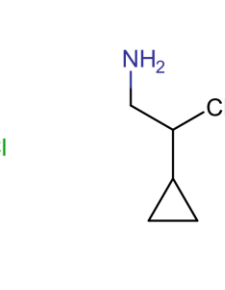
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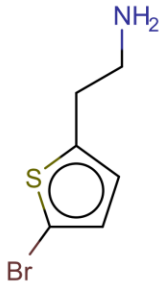	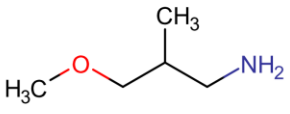	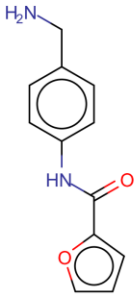	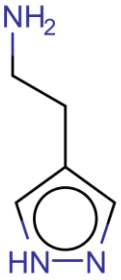
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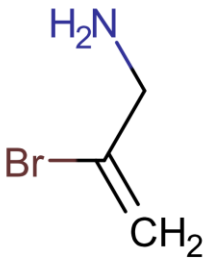	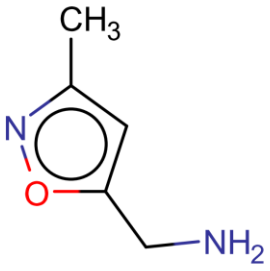	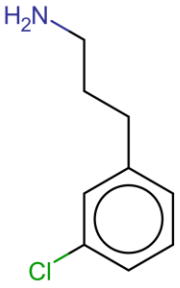	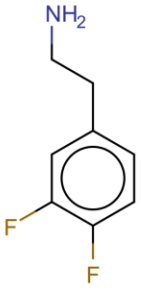
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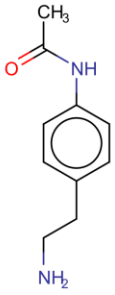	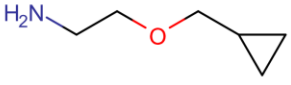	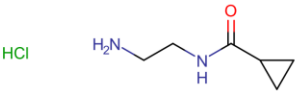	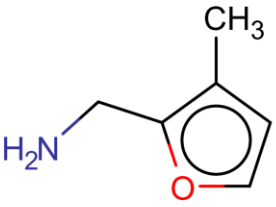
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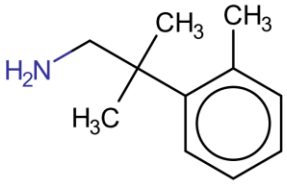	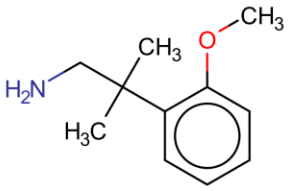	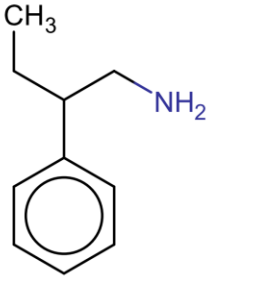	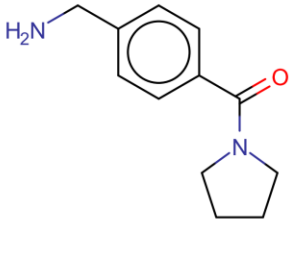
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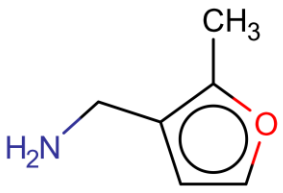	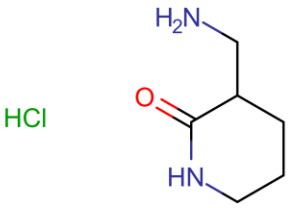	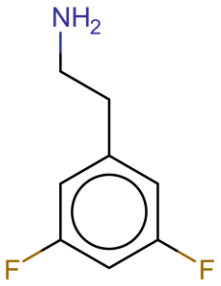	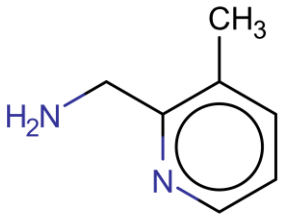
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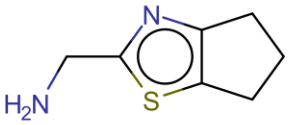	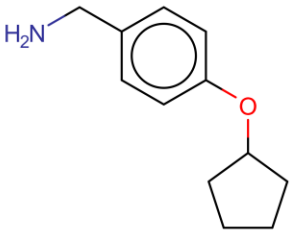	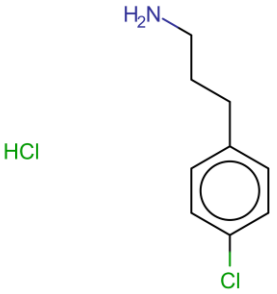	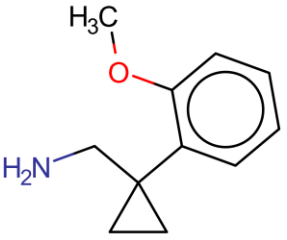
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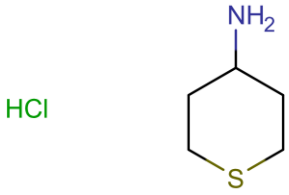	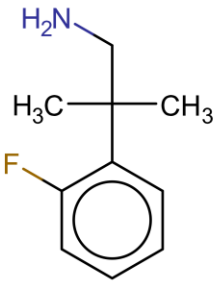	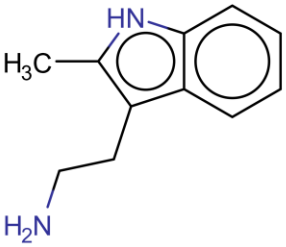	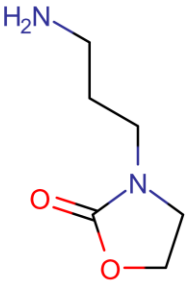
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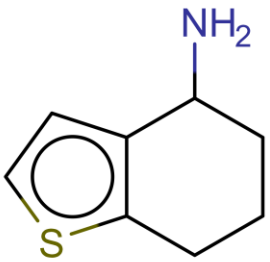	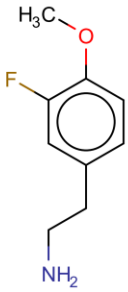	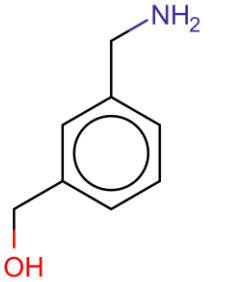	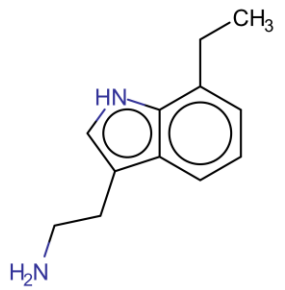
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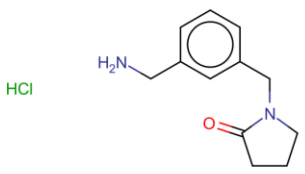	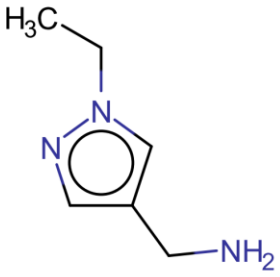	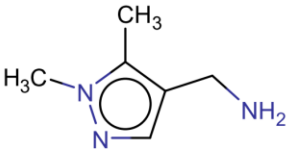	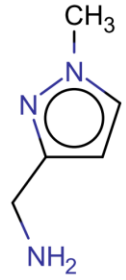
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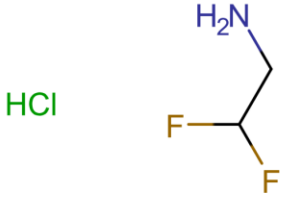	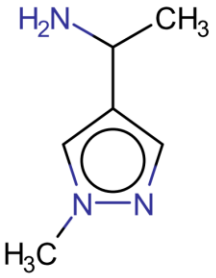	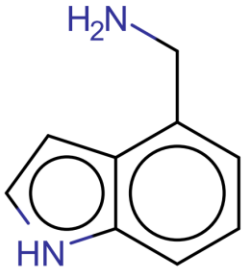	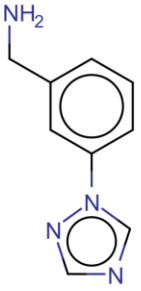
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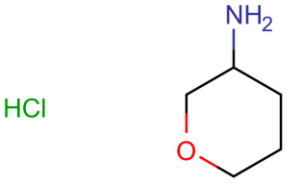	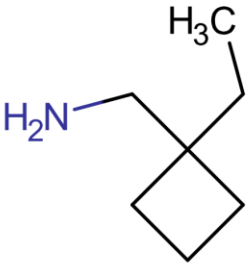	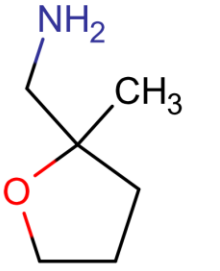	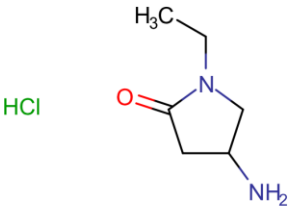
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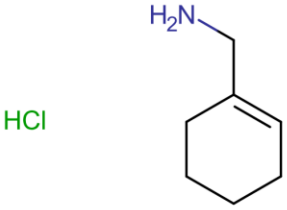	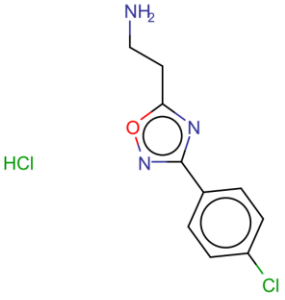	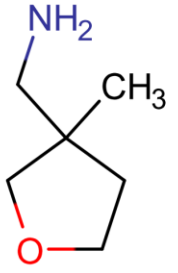	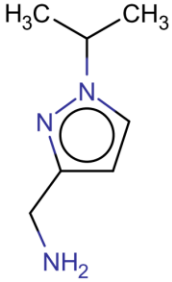
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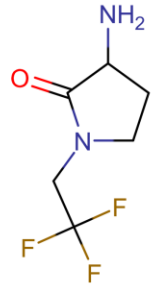
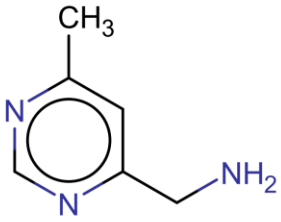
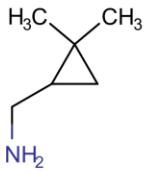
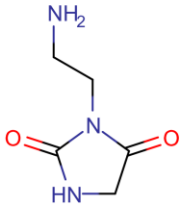
		HCl 	HCl 
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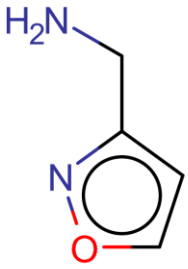	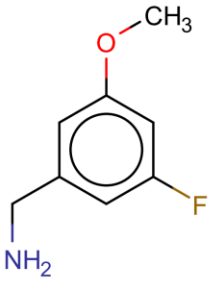	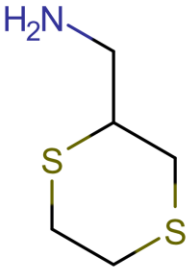	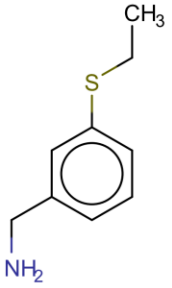
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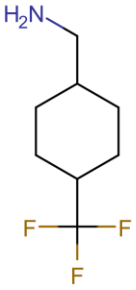
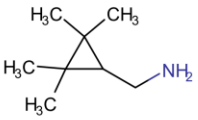
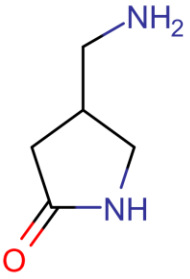
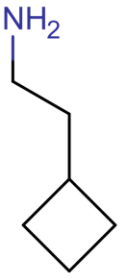
	HCl 		
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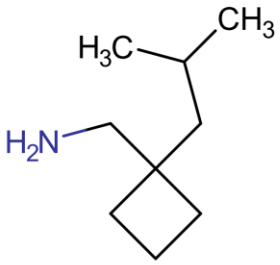	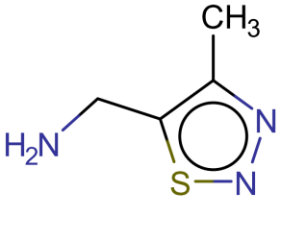		
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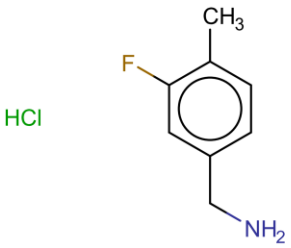	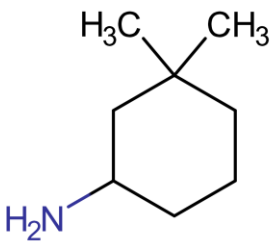	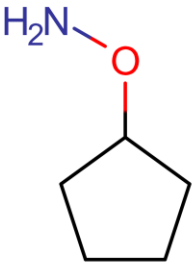	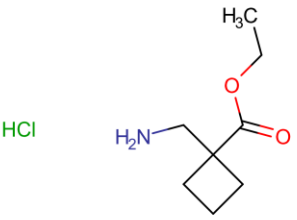
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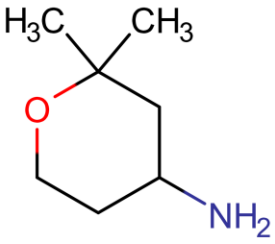	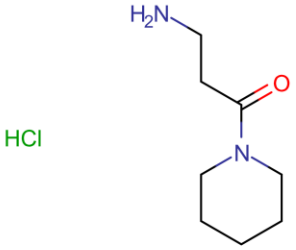	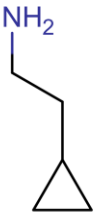	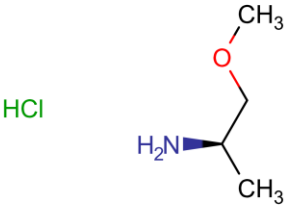
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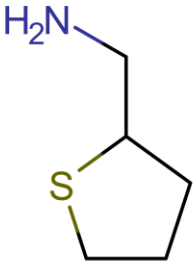	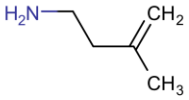	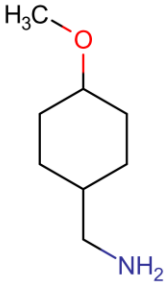	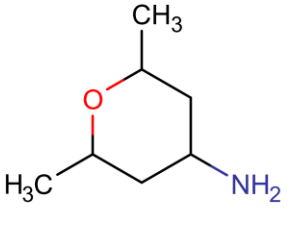
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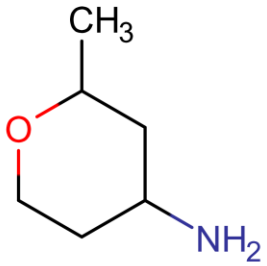	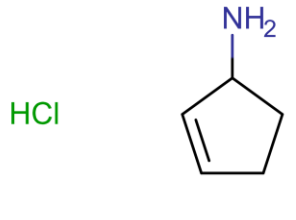	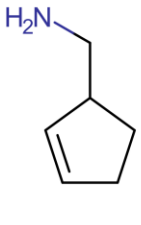	
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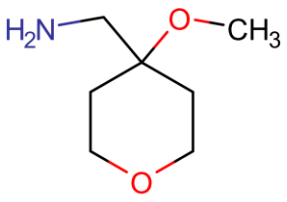	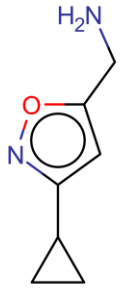	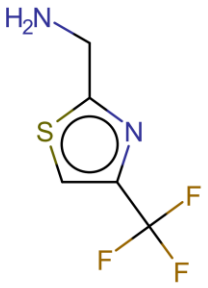	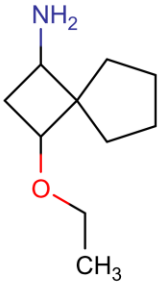
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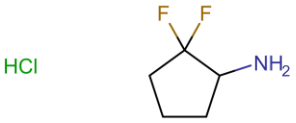	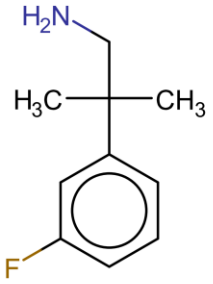	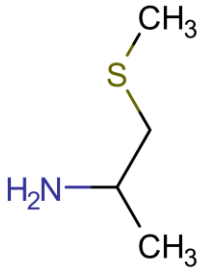	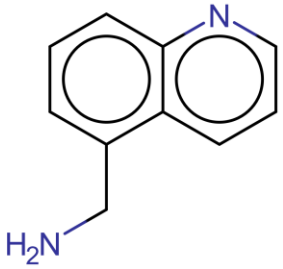
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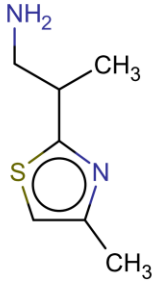	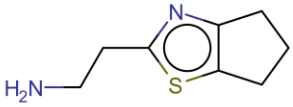	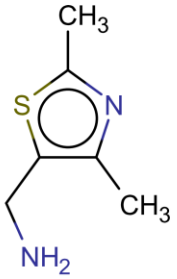	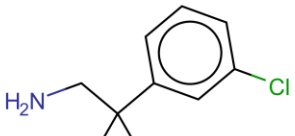
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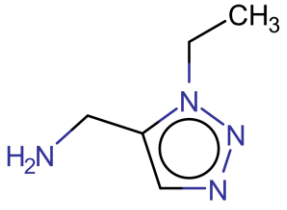	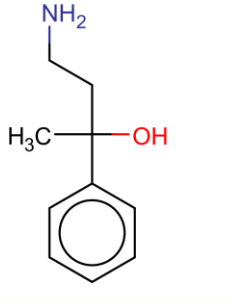	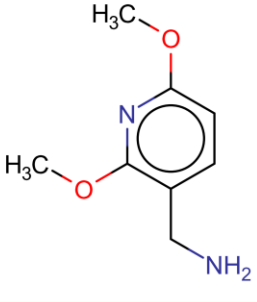	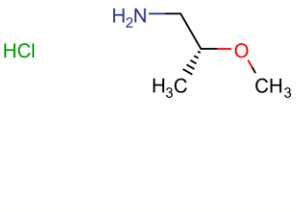
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	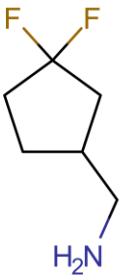	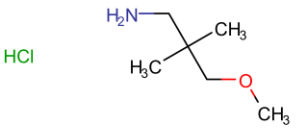	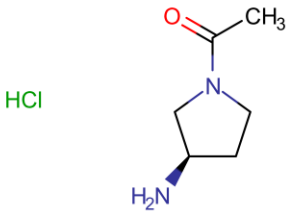
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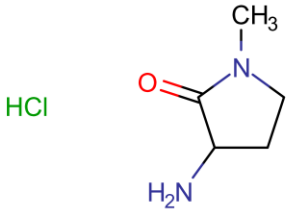	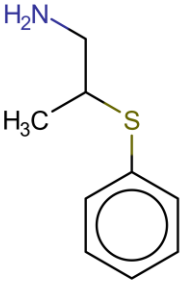	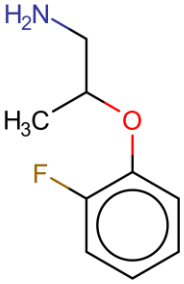	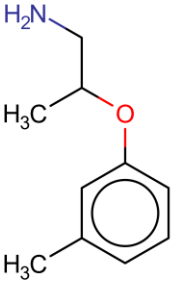
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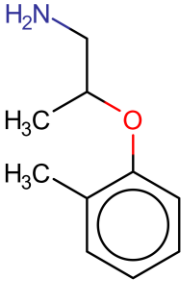	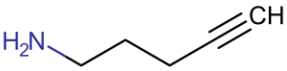	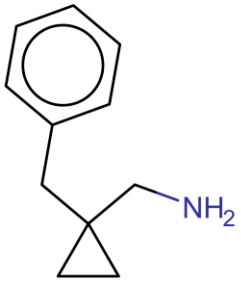	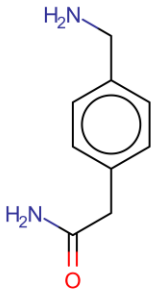
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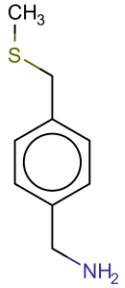	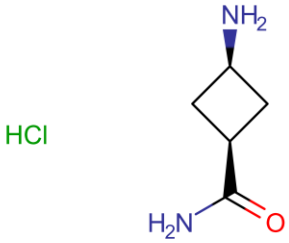	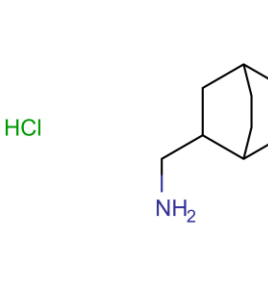	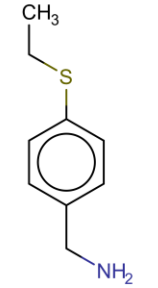
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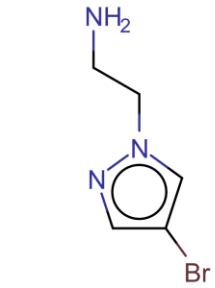	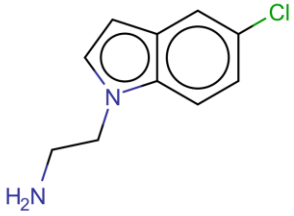	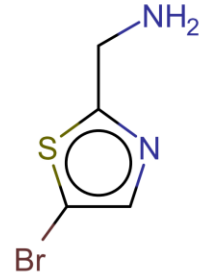	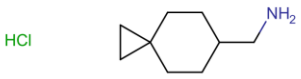
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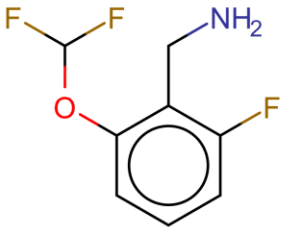	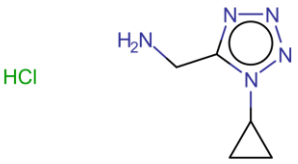	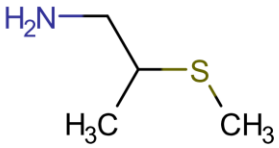	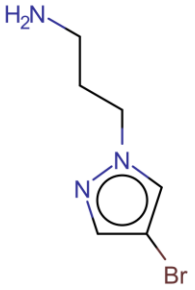
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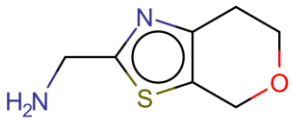	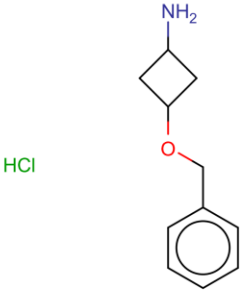	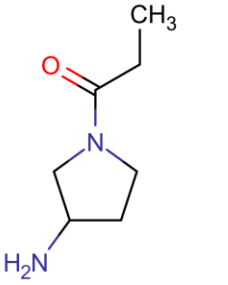	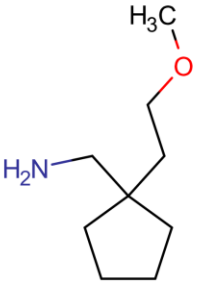
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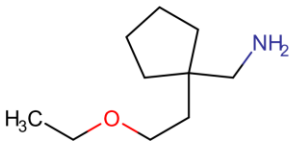	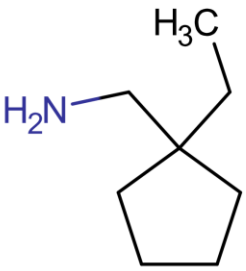	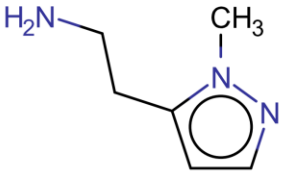	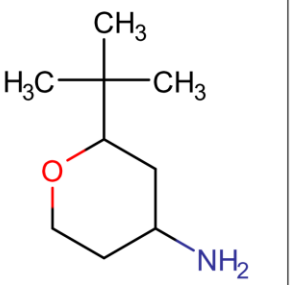
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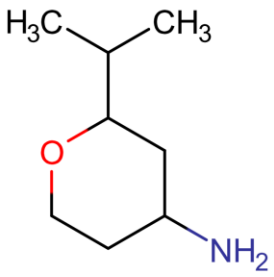	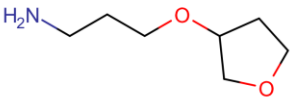	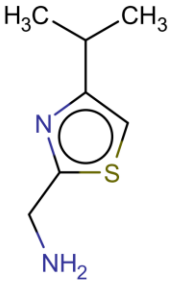	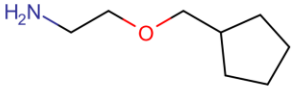
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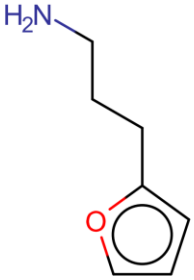	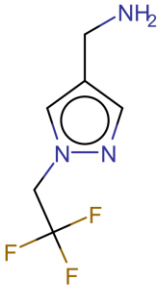	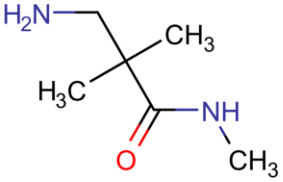	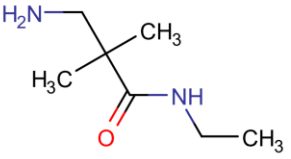
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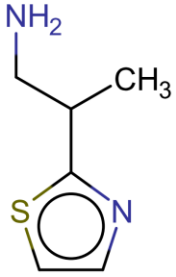	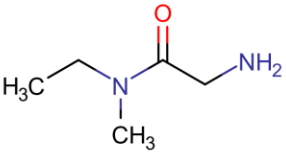	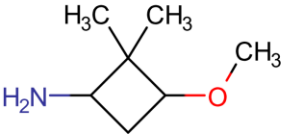	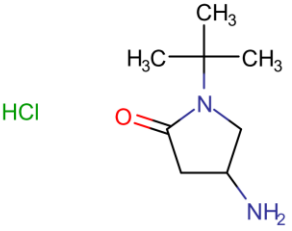
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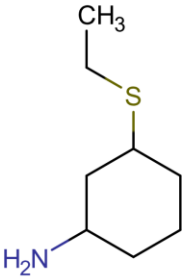	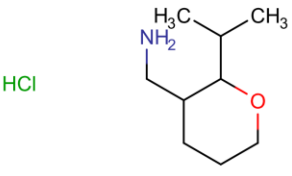	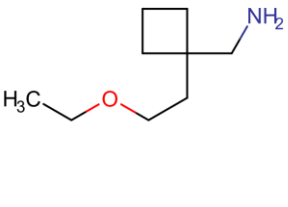	
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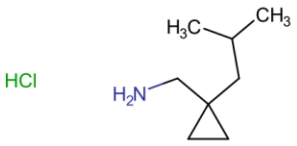	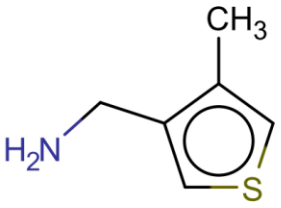	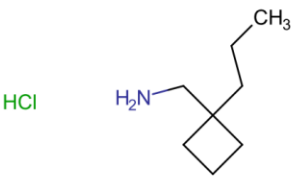	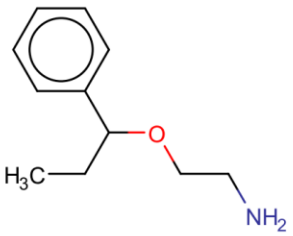
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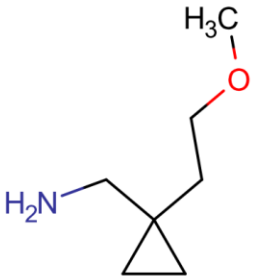	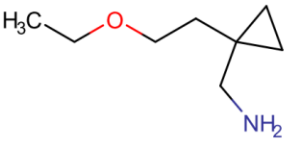	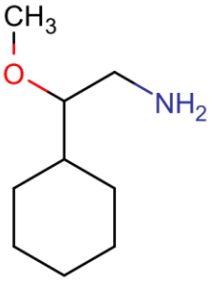	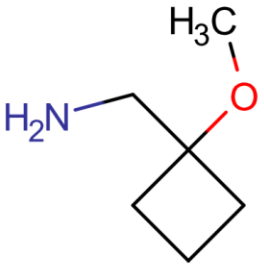
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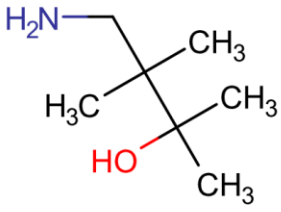	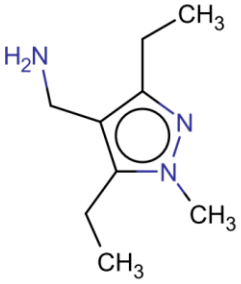	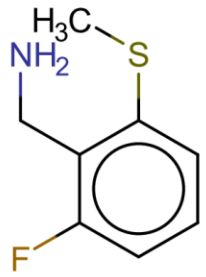	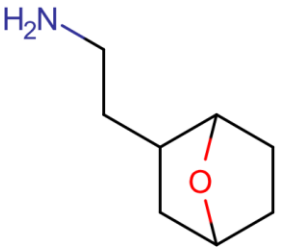
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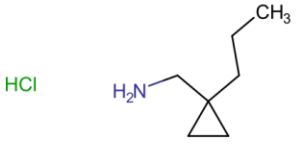	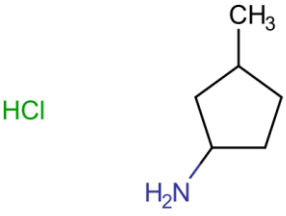	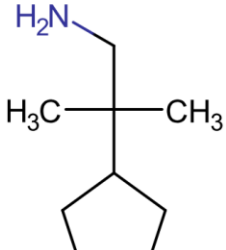	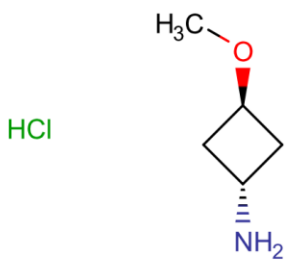
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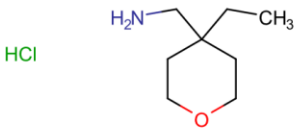	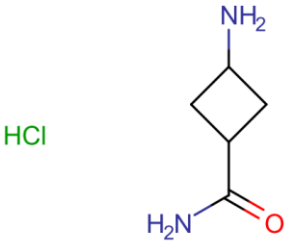	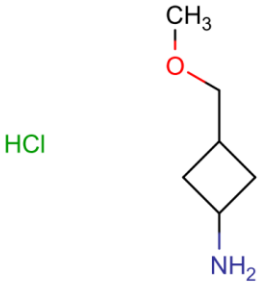	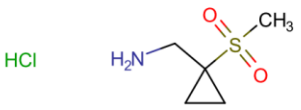
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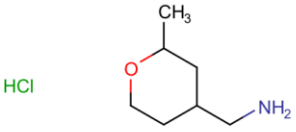	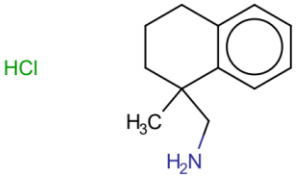	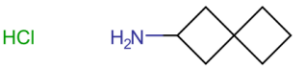	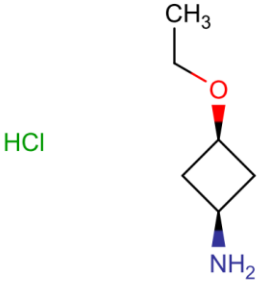
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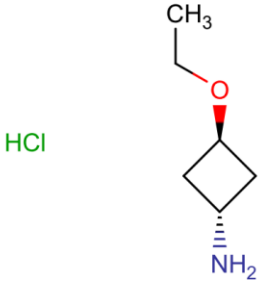	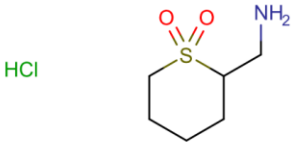	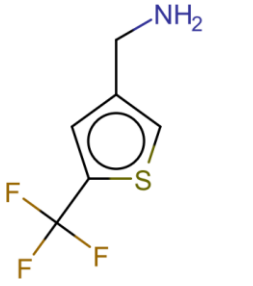	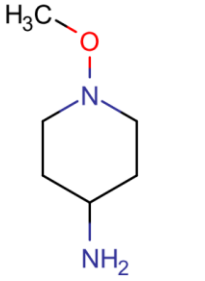
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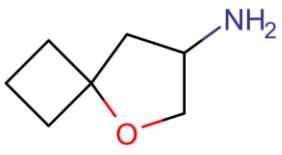	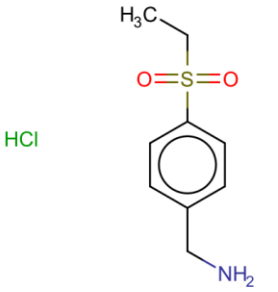	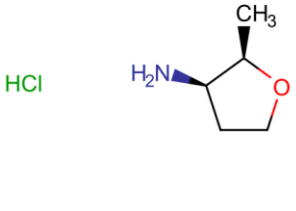	
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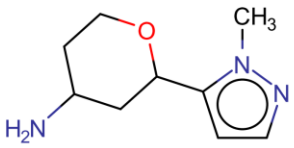	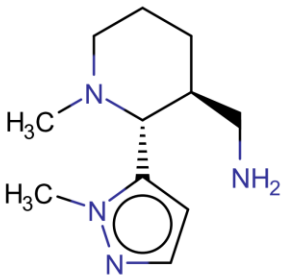	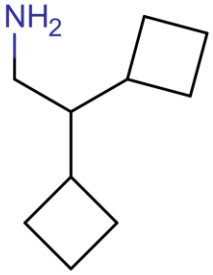	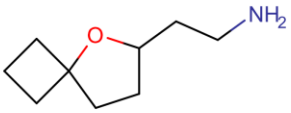
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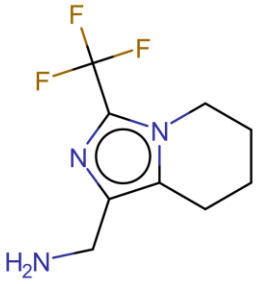	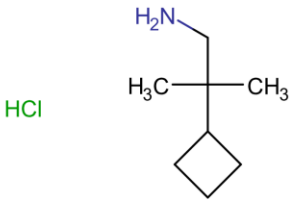	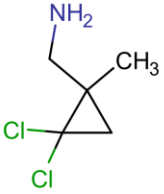	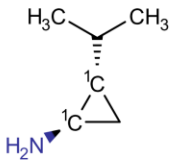
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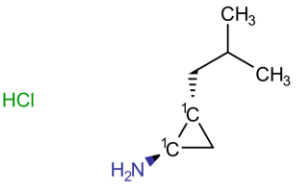	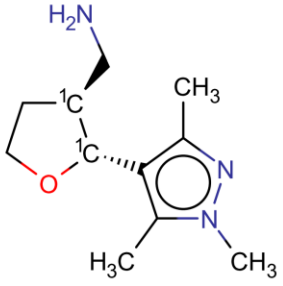	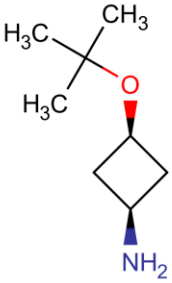	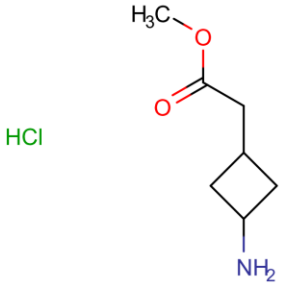
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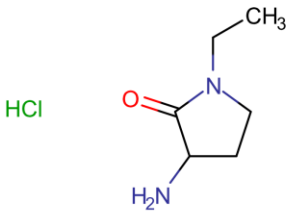	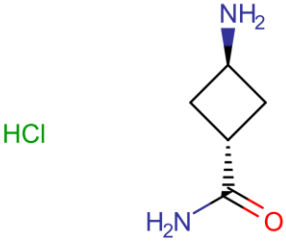	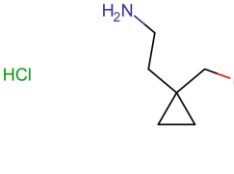	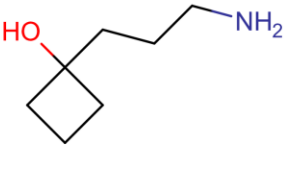
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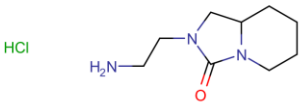	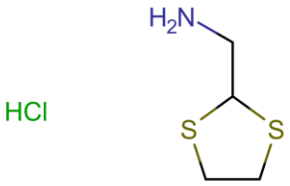	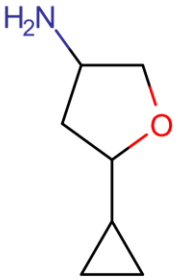	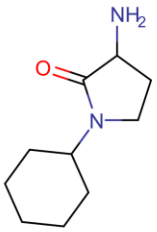
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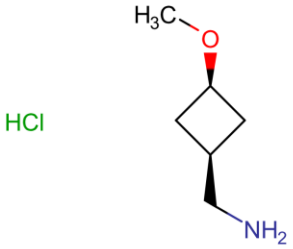	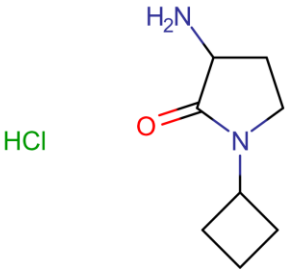	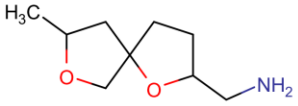	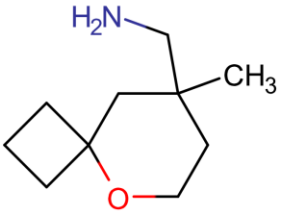
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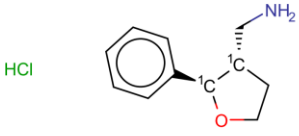	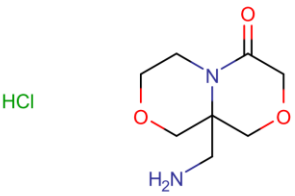	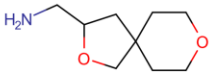	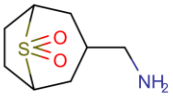
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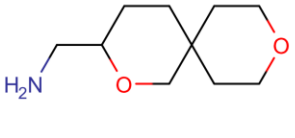
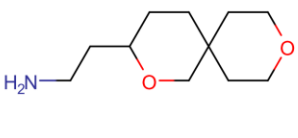
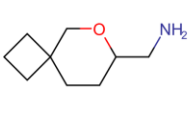
			
15{365}	15{366}	15{367}	15{368}

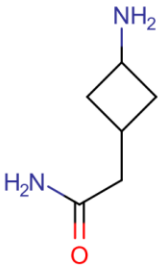
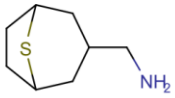
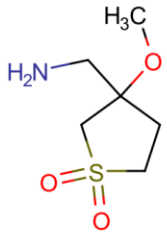
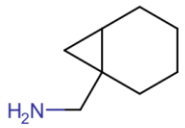
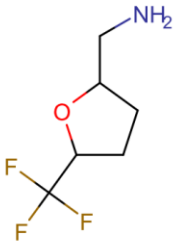
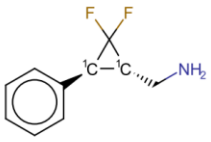
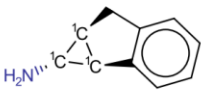
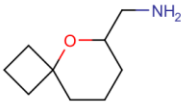
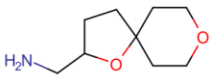
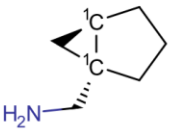
HCl 	HCl 	HCl 	HCl 
15{369}	15{370}	15{371}	15{372}
HCl 	HCl 	HCl 	HCl 
15{373}	15{374}	15{375}	15{376}
HCl 	HCl 		
15{377}	15{378}		

Table S1. SMILES strings for the regents **10**.

#	Reagent **10**	SMILE
1	**10**{*1*}	C=CCN=C=S
2	**10**{*2*}	CN=C=S
3	**10**{*3*}	CCCCN=C=S
4	**10**{*4*}	CCN=C=S
5	**10**{*5*}	S=C=NCc1ccccc1
6	**10**{*6*}	S=C=NCCc1ccccc1
7	**10**{*7*}	S=C=NC1CCCCC1
8	**10**{*8*}	S=C=NCCN1CCOCC1
9	**10**{*9*}	COCCN=C=S
10	**10**{10}	CC(C)N=C=S
11	**10**{*11*}	CC(=C)CN=C=S
12	**10**{*12*}	CCOCCCN=C=S
13	**10**{*13*}	COc1ccc(CCN=C=S)cc1
14	**10**{*14*}	CCCN=C=S
15	**10**{*15*}	S=C=NC1CC1
16	**10**{*16*}	COCC(C)N=C=S
17	**10**{*17*}	S=C=NC1CC2CCC1C2
18	**10**{*18*}	S=C=NCCSc1ccccc1
19	**10**{*19*}	S=C=NCc1cccnc1
20	**10**{*20*}	CCN1CCCC1CN=C=S
21	**10**{*21*}	CC(C)(C)N=C=S
22	**10**{*22*}	S=C=NC1CCCC1
23	**10**{*23*}	CC(N=C=S)c1ccccc1
24	**10**{*24*}	CCC(C)N=C=S
25	**10**{*25*}	S=C=NCC1CC1

26	**10**{*26*}	FC(F)(F)CN=C=S
27	**10**{*27*}	CCOC(=O)N1CCC(CC1)N=C=S
28	**10**{*28*}	CC(N=C=S)c1ccc(Br)cc1
29	**10**{*29*}	S=C=NC1CCN(Cc2ccccc2)CC1
30	**10**{*30*}	Clc1ccc(CCN=C=S)c(Cl)c1
31	**10**{*31*}	CCOCCN=C=S
32	**10**{*32*}	S=C=NCCc1ccccn1
33	**10**{*33*}	FC(F)(F)c1cccc(CN=C=S)c1
34	**10**{*34*}	S=C=NCCc1ccc2OCCOc2c1
35	**10**{*35*}	CS(=O)(=O)NCCN=C=S
36	**10**{*36*}	S=C=NCC1CCC1
37	**10**{*37*}	S=C=NCCc1cccnc1
38	**10**{*38*}	CC(N=C=S)c1cccs1
39	**10**{*39*}	CS(=O)(=O)CCN=C=S
40	**10**{*40*}	S=C=NC1CCOCC1
41	**10**{*41*}	S=C=NCCc1cccs1
42	**10**{*42*}	CC1(CC1)N=C=S
43	**10**{*43*}	S=C=NC1CCOc2ccccc12
44	**10**{*44*}	S=C=NC(C1CC1)C1CC1
45	**10**{*45*}	FC(F)(F)Oc1ccc(CN=C=S)cc1
46	**10**{*46*}	S=C=NC1CCc2ccccc2C1
47	**10**{*47*}	CC(C)(C)CN=C=S
48	**10**{*48*}	CSCCN=C=S
49	**10**{*49*}	CC(Cc1ccccc1)N=C=S
50	**10**{*50*}	Brc1ccc(CN=C=S)cc1
51	**10**{*51*}	S=C=NCC1CCOC1
52	**10**{*52*}	S=C=NC1CCC1
53	**10**{*53*}	Fc1ccc(CCN=C=S)cc1

54	**10**{*54*}	S=C=NCC1CCCCO1
55	**10**{*55*}	Cc1cc(CN=C=S)no1
56	**10**{*56*}	S=C=NCc1ccon1
57	**10**{*57*}	FC(F)CN=C=S
58	**10**{*58*}	CC1(CCC1)N=C=S

Table S2. SMILES strings for the regents **11**.

#	Reagent **11**	SMILE
1	**11**{*1*}	Cl.CNS(=O)(=O)c1cccc2CNCCc12
2	**11**{*2*}	Cl.O=C(NC1CC1)C(=O)N1CCNCC1
3	**11**{*3*}	OC1(Cc2nc(no2)C2CC2)CCCNC1
4	**11**{*4*}	C1CC2(C1)CNCCO2
5	**11**{*5*}	Cl.Fc1cc(F)cc(c1)C1COCCN1
6	**11**{*6*}	Fc1ccc2CNCCOc2c1
7	**11**{*7*}	Cl.CC1=C(C)CNCC1
8	**11**{*8*}	C1C[1C@@H]2NCC3(CCOCC3)[1C@@H]2C1
9	**11**{*9*}	Clc1ccc2[nH]c(nc2c1)C1CCCN1
10	**11**{*10*}	Cl.Cn1cccc1C(=O)N1CCNCC1
11	**11**{*11*}	Cl.CNC(=O)CNCc1ccccc1
12	**11**{*12*}	Cn1cnnc1C1CCCNC1
13	**11**{*13*}	C1CNC(C1)C1CCCO1
14	**11**{*14*}	CC(CS(C)(=O)=O)NC1CC1
15	**11**{*15*}	Cl.COC1(CCNCC1)C(F)(F)F
16	**11**{*16*}	O=C1NCCN1C1CCCNC1
17	**11**{*17*}	COCCCNCCOC
18	**11**{*18*}	NC(=O)[C@@H]1C[C@@H](F)CN1
19	**11**{*19*}	Cl.COC1(CCNC1)C(F)(F)F
20	**11**{*20*}	CCC1(CCNCC1)N1CCOCC1
21	**11**{*21*}	Cl.CNC1CCN(CC1)S(C)(=O)=O
22	**11**{*22*}	Cl.Cl.C1CNCCC(C1)n1ccnn1
23	**11**{*23*}	C1CCc2ccccc2NC1
24	**11**{*24*}	CC1(C)CNCCC(O)C1
25	**11**{*25*}	C1CNC(C1)c1cccnc1

26	**11**{*26*}	Clc1ccc2CNCCc2c1
27	**11**{*27*}	C1CC(CCN1)c1ccncc1
28	**11**{*28*}	Cl.COC1CCCNC1
29	**11**{*29*}	Cc1ccc2CNCCc2c1
30	**11**{*30*}	Cl.C1CC=CCN1
31	**11**{*31*}	C1CC(CCN1)c1ccccc1
32	**11**{*32*}	CC1NCCc2cccc(F)c12
33	**11**{*33*}	Cl.O=C1CCNCCN1
34	**11**{*34*}	CCC1NCCc2sccc12
35	**11**{*35*}	C1CNCC(C1)c1ncc[nH]1
36	**11**{*36*}	Cl.O[C@H]1CCNC1
37	**11**{*37*}	COc1ccc2CNCCc2c1
38	**11**{*38*}	Cl.Cl.C1Cc2nc[nH]c2CN1
39	**11**{*39*}	Fc1ccc2NCCc2c1
40	**11**{*40*}	Cl.Cl.C1Cc2[nH]ncc2CN1
41	**11**{*41*}	Cl.CNCc1ccc(OC)nc1
42	**11**{*42*}	Cl.Cl.C1CNCC(C1)c1nnc2ccccn12
43	**11**{*43*}	Cl.CN[C@H]1C[C@H](C1)C(N)=O
44	**11**{*44*}	Cl.O=c1[nH]c2cccc(N3CCNCC3)c2[nH]1
45	**11**{*45*}	C(Cc1cnccn1)N1CCNCC1
46	**11**{*46*}	Cc1ccc(CNC2CC2)o1
47	**11**{*47*}	Cl.CC12CNCC1(C)C(=O)NC2=O
48	**11**{*48*}	Cc1ccnc(c1)N1CCNCC1
49	**11**{*49*}	CNCCS(C)(=O)=O
50	**11**{*50*}	CS(=O)(=O)NCC1CCCNC1
51	**11**{*51*}	CCNCC1CCOC1
52	**11**{*52*}	C1CCN(CC1)C1CCNCC1
53	**11**{*53*}	CNCCNC(C)=O

54	**11**{*54*}	C1CCC(CC1)N1CCNCC1
55	**11**{*55*}	CNCc1nccn1C
56	**11**{*56*}	Cn1nccc1C1CCCNC1
57	**11**{*57*}	C1CNc2c[nH]nc2C1
58	**11**{*58*}	C[1C@@H]1CCNC[1C@H](C)O1
59	**11**{*59*}	Br.Oc1ccc2CNCc2c1
60	**11**{*60*}	Cl.O=C1CC2CCC(CN1)N2
61	**11**{*61*}	C1CC2(CN1)CCOCC2
62	**11**{*62*}	Cl.C1CC2NC1CC=C2
63	**11**{*63*}	Cl.O=C1NCC2CNCCN12
64	**11**{*64*}	Cl.FC1(F)CNCCOC1
65	**11**{*65*}	Cl.FC1=CCCNC1
66	**11**{*66*}	Cl.C1NCC2C1C1OC2C=C1
67	**11**{*67*}	Cl.OCC1CC2CCC1N2
68	**11**{*68*}	C1CNCC(C1)c1ccn[nH]1
69	**11**{*69*}	CNCC(C)(C)CO
70	**11**{*70*}	COc1cccc(c1)C1CCNCC1
71	**11**{*71*}	CCn1cc(CNC)cn1
72	**11**{*72*}	CCNCc1ccoc1
73	**11**{*73*}	C1Cc2cn[nH]c2CN1
74	**11**{*74*}	Cc1nc(sc1C)N1CCNCC1
75	**11**{*75*}	Cl.Oc1cccc(c1)C(=O)N1CCNCC1
76	**11**{*76*}	C1Cn2ccnc2N1
77	**11**{*77*}	C1CC1c1ncc2CNCCc2n1
78	**11**{*78*}	Cl.COc1ccc2CNCCCc2c1
79	**11**{*79*}	Cl.NC(=O)[C@H]1CCCN1
80	**11**{*80*}	Cl.C(OC1CCNCC1)C1CCCO1
81	**11**{*81*}	NC(=O)C1CNCCO1

82	**11**{*82*}	C1CCC2(C1)CCNC2
83	**11**{*83*}	CNC1CCCc2nc(C)sc12
84	**11**{*84*}	Cl.CNCC(=O)N1CCCC1
85	**11**{*85*}	Fc1cccc(c1)N1CCNCC1
86	**11**{*86*}	OCC1CCCCCN1
87	**11**{*87*}	CNCc1ccoc1C
88	**11**{*88*}	C(C1CCOCC1)N1CCNCC1
89	**11**{*89*}	CNC(C)c1ccccn1
90	**11**{*90*}	C(N1CCNCC1)c1cscn1
91	**11**{*91*}	CC1NCCOc2ccccc12
92	**11**{*92*}	C1CNCC(C1)c1ccccc1
93	**11**{*93*}	C(C1CCCCC1)N1CCNCC1
94	**11**{*94*}	CNc1c(C)noc1C
95	**11**{*95*}	CNC(C)c1sc(C)nc1C
96	**11**{*96*}	CC(C)OC1CCNCC1
97	**11**{*97*}	Cl.O=C(NC1CC1)C1CCCN1
98	**11**{*98*}	CNC(C)c1ccco1
99	**11**{*99*}	C1Cn2cncc2CN1
100	**11**{*100*}	Cl.O=S1CCNCC1
101	**11**{*101*}	Cl.CNCc1ccc(C)s1
102	**11**{*102*}	CNCc1scnc1C
103	**11**{*103*}	Cl.Cc1ccc2[nH]c3CCNCc3c2c1
104	**11**{*104*}	C1CCC2(C1)CNCCOC2
105	**11**{*105*}	CN1CCNCc2ccccc12
106	**11**{*106*}	C1Cc2ccccc2CCN1
107	**11**{*107*}	Cl.Fc1ccc(F)c2CNCCc12
108	**11**{*108*}	O=C1CCCN1C1CCNCC1
109	**11**{*109*}	Cl.Cn1nc2CCNCc2cc1=O

110	**11**{*110*}	Cl.CNCC1(O)CCOCC1
111	**11**{*111*}	Cl.CC1CNCC(C)S1(=O)=O
112	**11**{*112*}	Cl.CCOC1(C)CCNCC1
113	**11**{*113*}	FC(F)(F)CN1CNCC1=O
114	**11**{*114*}	Cl.CS(=O)(=O)C1CCCNCC1
115	**11**{*115*}	Cl.O=C1Nc2ccccc2C11CCNC1
116	**11**{*116*}	Cl.O[1C@@H]1CC[1C@@H]2CNC[1C@@H]2C1
117	**11**{*117*}	CC(C)(CC1CCCNC1)C(N)=O
118	**11**{*118*}	Cl.C[1C@@H]1NCC[1C@@H]1O
119	**11**{*119*}	Cl.CCNC1CCNC1=O
120	**11**{*120*}	Cl.Cl.CN1CCNCC1CO
121	**11**{*121*}	I.I.Cc1nnc(N2CCNCC2)n1C
122	**11**{*122*}	CCNCCO
123	**11**{*123*}	Cl.CC(C)(C)C1CNCCO1
124	**11**{*124*}	Cl.Cl.Cc1cc(=O)[nH]c(n1)N1CCNCC1
125	**11**{*125*}	CNCC1(O)CCCC1
126	**11**{*126*}	C(N1CCNCC1)c1nc[nH]n1
127	**11**{*127*}	Cl.NC(=O)[C@@H]1CCCN1
128	**11**{*128*}	Cl.C1CC1C1CCCNC1
129	**11**{*129*}	Cl.CNC[C@@H](C)O
130	**11**{*130*}	Cl.CCC1CCCN1
131	**11**{*131*}	Cl.OCC1NCC=C1
132	**11**{*132*}	Cl.CC(C)(C)C1=CCNCC1
133	**11**{*133*}	Cl.CC1(C)CCCN1
134	**11**{*134*}	Cl.CN(C)C(=O)NC1CCCNC1
135	**11**{*135*}	Cl.FC(F)(F)[C@@H]1CCCNC1
136	**11**{*136*}	Cl.CC(C)NC(=O)[C@@H]1CCCNC1
137	**11**{*137*}	CCN1CCC2CCC(C1)N2

138	**11**{*138*}	Clc1cccc2CCNCc12
139	**11**{*139*}	Fc1cccc2CCNc12
140	**11**{*140*}	Cl.CNc1cnn(C)c1
141	**11**{*141*}	Cl.O=C1CC2(CN1)CCNCC2
142	**11**{*142*}	C1CC(CCN1)c1cn[nH]c1
143	**11**{*143*}	Cl.CNc1ccn(C)n1
144	**11**{*144*}	C1CN2CCOCC2CN1
145	**11**{*145*}	Cc1cccc2CCNCc12
146	**11**{*146*}	Cl.Cl.C1CNC(C1)c1ccn[nH]1
147	**11**{*147*}	Clc1cnn(c1)C1CCNC1
148	**11**{*148*}	Cc1csc(n1)C1CCNC1
149	**11**{*149*}	C1CNC(C1)c1ccncc1
150	**11**{*150*}	CC1CNCC(=O)N1
151	**11**{*151*}	Cl.CC1CNCCOC1
152	**11**{*152*}	Cl.FC1CCNCC1
153	**11**{*153*}	CN(C)C1CCNC1
154	**11**{*154*}	Cl.FC1(CCNCC1)C1CC1
155	**11**{*155*}	Cl.Clc1cccc2NCCc12
156	**11**{*156*}	Cl.FC(F)(F)[C@H]1CCCNC1
157	**11**{*157*}	Cl.CC1(F)CCCNC1
158	**11**{*158*}	Cl.FC(F)C1CCNCC1
159	**11**{*159*}	Cl.Fc1cccc2NCCc12
160	**11**{*160*}	Cl.C1CCC2(C1)CCNCC2
161	**11**{*161*}	CNC(C)c1cccnc1
162	**11**{*162*}	Cl.C1Cc2nnc(C3CCCNC3)n2C1
163	**11**{*163*}	Cc1cccc(n1)C1CCCN1
164	**11**{*164*}	C1C[C@H](CN1)Oc1ccccc1
165	**11**{*165*}	C(C1CCNCC1)N1CCOCC1

166	**11**{*166*}	Cl.OC1CCOC2(CCNCC2)C1
167	**11**{*167*}	Cl.Cl.C1CNC(C1)c1ncccn1
168	**11**{*168*}	C1COC(CN1)c1ccco1
169	**11**{*169*}	Cl.C1CC2(C1)CCNC2
170	**11**{*170*}	C1CNCC(C1)C1CCOCC1
171	**11**{*171*}	C1CC(CN1)n1cccn1
172	**11**{*172*}	Cl.COC1CCCNCC1
173	**11**{*173*}	Cl.O=C1CNCCCN1
174	**11**{*174*}	Cl.FC(F)[C@@H]1CCCN1
175	**11**{*175*}	Cn1ccc(n1)C1CCCNC1
176	**11**{*176*}	CNCc1cnc(C)s1
177	**11**{*177*}	CC(C)C(=O)N1CCCNCC1
178	**11**{*178*}	CNCc1ccoc1
179	**11**{*179*}	OC[C@H]1[C@@H]2CNC[C@H]12
180	**11**{*180*}	CNC(C)c1cccc(Cl)c1
181	**11**{*181*}	CNc1cccc(C)c1
182	**11**{*182*}	Cl.CNCc1ccc(C)c(C)c1
183	**11**{*183*}	Cl.CC1(Cc2ccccc2)CCCN1
184	**11**{*184*}	Cl.COC1(CCCNC1)C(F)(F)F
185	**11**{*185*}	CC1(C)CNC1c1cccnc1
186	**11**{*186*}	Cl.CCn1ccc(CNC)c1
187	**11**{*187*}	OC1(CCNC1)C1CC1
188	**11**{*188*}	CCOC1CC2(C1)CCNC2
189	**11**{*189*}	Cc1cccc(C2CCCN2)c1C
190	**11**{*190*}	CC1(C)CNCc2ccccc2O1
191	**11**{*191*}	CC1(C)CNCC(O1)C(F)(F)F
192	**11**{*192*}	CNCc1cccc(C)n1
193	**11**{*193*}	Cl.COc1ccccc1C1CCNC1

194	**11**{*194*}	Cl.O=S1(=O)CCNCc2ccccc12
195	**11**{*195*}	Cl.CCS(=O)(=O)C1CNC1
196	**11**{*196*}	Cl.CNc1ccc(OC(C)C)cc1
197	**11**{*197*}	Cl.CC1CNC(C)(C)C1
198	**11**{*198*}	CC(C)c1cc([nH]n1)C1CCCNC1
199	**11**{*199*}	CNCc1nnc2CCCn12
200	**11**{*200*}	CNCc1cc2ccccc2[nH]1
201	**11**{*201*}	CC1CNc2ccccc2O1
202	**11**{*202*}	C1CC1c1nc(n[nH]1)C1CCCNC1
203	**11**{*203*}	Cl.Cl.Cc1nc([nH]c1C)C1CCNCC1
204	**11**{*204*}	CNCC1(O)CCC1
205	**11**{*205*}	Cl.OC1CCNCC1(F)F
206	**11**{*206*}	CC1(C)CNC1c1ccncc1
207	**11**{*207*}	Cl.Cl.C1CC(CCN1)n1cccn1
208	**11**{*208*}	C1CN(CCN1)C1CCOCC1
209	**11**{*209*}	CO[1C@@H]1CNC[1C@H]1O
210	**11**{*210*}	Br.Oc1cccc2CNCCc12
211	**11**{*211*}	C1CC(CCN1)c1ccco1
212	**11**{*212*}	Cl.FC(F)(F)C1CCNCCO1
213	**11**{*213*}	Cl.CNC(=O)NC1CCNCC1
214	**11**{*214*}	C1CCC(OC1)C1CCNCC1
215	**11**{*215*}	Cl.CCS(=O)(=O)CC(C)NC
216	**11**{*216*}	CN[1C@H]1CCC[1C@@H]1O
217	**11**{*217*}	Cl.Oc1ccc2CNCCOc2c1
218	**11**{*218*}	Cc1cncc(c1)C1CCCN1
219	**11**{*219*}	C1CN(CCN1)c1cccs1
220	**11**{*220*}	Cl.CC1CCS(=O)(=O)CCN1
221	**11**{*221*}	Cl.Cl.C1CNCC(C1)c1cccnc1

222	**11**{*222*}	Cl.Cl.C1CNCC(C1)c1ccncc1
223	**11**{*223*}	CNCc1nnc(C)s1
224	**11**{*224*}	CNCC(C)C(=O)NC
225	**11**{*225*}	Cl.O=S(=O)(C1CC1)N1CCNCC1
226	**11**{*226*}	Cl.OCCNC(=O)C1CCNCC1
227	**11**{*227*}	COc1ccc(cc1F)C1CCNC1
228	**11**{*228*}	CC(C)(O)CNC1CC1
229	**11**{*229*}	OCC1(CCNC1)c1ccccc1
230	**11**{*230*}	CN(C1CCNC1)c1ccccc1
231	**11**{*231*}	Cl.NC(=O)COC1CCNCC1
232	**11**{*232*}	CCNCc1occc1C
233	**11**{*233*}	Brc1cncc(c1)C1CCCN1
234	**11**{*234*}	Cl.CS(=O)(=O)CC1CCNCC1
235	**11**{*235*}	CNCc1cscn1
236	**11**{*236*}	Oc1ccc2CCNCc2c1
237	**11**{*237*}	CNCc1occc1C
238	**11**{*238*}	Cl.Clc1cnn(c1)C1CCNCC1
239	**11**{*239*}	Cl.C1NC2CC1C=C2
240	**11**{*240*}	Cl.CC(=O)NC1CCNCC1
241	**11**{*241*}	Cc1cnn(c1)C1CCNC1
242	**11**{*242*}	CCNc1cnn(C)c1
243	**11**{*243*}	Cl.Cl.Cn1cc(cn1)C1=CCCNC1
244	**11**{*244*}	Cl.Cl.CN1CC[1C@@H]2CC[1C@H](C1)N2
245	**11**{*245*}	C[C@H]1COCCN1
246	**11**{*246*}	Cl.N#CC1CCCNC1
247	**11**{*247*}	Br.CNCc1cccc(=O)[nH]1
248	**11**{*248*}	Cl.Cl.C1CN[C@@H](C1)c1ncn[nH]1
249	**11**{*249*}	Cl.COC[C@H]1C[C@@H](O)CN1

250	**11**{*250*}	Cl.CC(C)[C@H]1CNCCN1C
251	**11**{*251*}	CN1CCNCc2cccnc12
252	**11**{*252*}	Cl.NC(=O)C1NCCc2ccccc12
253	**11**{*253*}	Cl.CC1CCNCCS1(=O)=O
254	**11**{*254*}	Cl.O[1C@@H]1CNC[1C@H]1Oc1ccccc1
255	**11**{*255*}	Cl.CC1CNCCS(=O)(=O)C1
256	**11**{*256*}	CC1(C)CN[1C@@H]2COC[1C@H]12
257	**11**{*257*}	Cl.Cl.C1CC(CCN1)c1nnc[nH]1
258	**11**{*258*}	C1CC(CCN1)c1ncc[nH]1
259	**11**{*259*}	CC1CNCCN(C1)C1CC1
260	**11**{*260*}	C1CC(CN1)N1CCCCC1
261	**11**{*261*}	C1COC(C1)C1CCNCC1
262	**11**{*262*}	CNC1CCN(C1)C(C)C
263	**11**{*263*}	CCc1cccc(NC)c1
264	**11**{*264*}	CC1NCCc2ccccc12
265	**11**{*265*}	Cn1cc(CC2CCNC2)cn1
266	**11**{*266*}	Cl.Fc1cccc(OC2CCNCC2)c1
267	**11**{*267*}	CNC(C)c1ccncc1
268	**11**{*268*}	Cl.C1CNCc2ccsc2C1
269	**11**{*269*}	Clc1cccc(c1)C1CCCN1
270	**11**{*270*}	CNC1Cc2ccccc2C1
271	**11**{*271*}	CNC(C)c1ccccc1F
272	**11**{*272*}	Cl.Cl.C1CNCC(C1)c1ccccn1
273	**11**{*273*}	Cl.CCNCC(N)=O
274	**11**{*274*}	C(C1CCNC1)N1CCCC1
275	**11**{*275*}	C(C1CCNCC1)c1cccnc1
276	**11**{*276*}	CC1CNCCN1CC(C)(C)O
277	**11**{*277*}	Cl.OCC1(CCNC1)C(F)(F)F

278	**11**{*278*}	C1CC2(CCOC2)CN1
279	**11**{*279*}	Cc1cnc(OC2CCNCC2)nc1
280	**11**{*280*}	Fc1cccnc1N1CCCNCC1
281	**11**{*281*}	C(OC1CCNCC1)C1CC1
282	**11**{*282*}	CC(=O)N1CCNCC11CCCCC1
283	**11**{*283*}	Cl.C1CC2(C1)CNCc1ccccc1O2
284	**11**{*284*}	CC1(C)CNCCO1
285	**11**{*285*}	Cl.Cc1nc(no1)C1CC2CCC(C1)N2
286	**11**{*286*}	Cl.C1OC2(CCNCC2)c2ccccc12
287	**11**{*287*}	O=C(N1CCNCC1)c1ccco1
288	**11**{*288*}	CC(=O)N1CCCNCC1
289	**11**{*289*}	C1CC(CCN1)c1nc2ccccc2s1
290	**11**{*290*}	CC1CNCCN1C(=O)OC(C)(C)C
291	**11**{*291*}	Fc1ccc(cc1)C(=O)N1CCNCC1
292	**11**{*292*}	C[C@H]1CNCCN1C(=O)OC(C)(C)C
293	**11**{*293*}	Cl.C1C[C@@H]2C[C@@H](C[C@H]1N2)c1ccccc1
294	**11**{*294*}	Cl.Clc1ccccc1N1CCNCC1
295	**11**{*295*}	O=C(OCc1ccccc1)N1CCNCC1
296	**11**{*296*}	C[C@@H]1CNCCN1C(=O)OC(C)(C)C
297	**11**{*297*}	CC1(OCCO1)C1CCNCC1
298	**11**{*298*}	CC1(OCCO1)C1CCCNC1
299	**11**{*299*}	COC1(CO)CCNCC1
300	**11**{*300*}	C1CNCCOC1
301	**11**{*301*}	FC(F)CN1CCNCC1
302	**11**{*302*}	CNCCOc1ccc(F)cc1
303	**11**{*303*}	CC1CCCNC1C
304	**11**{*304*}	CC(C)C(=O)NCC1CCCNC1
305	**11**{*305*}	CC1CCCNCC1

306	**11**{*306*}	CC(C)(C)OC(=O)NCC1CCCNC1
307	**11**{*307*}	CN(CC1CCNC1)C(=O)OC(C)(C)C
308	**11**{*308*}	CC(C)(C)OC(=O)NCC1CCNCC1
309	**11**{*309*}	O=c1[nH]c2ccccc2n1C1CCNCC1
310	**11**{*310*}	CC1CNCCC1NC(=O)OC(C)(C)C
311	**11**{*311*}	CC(C)(C)OC(=O)N[C@H]1CCCNC1
312	**11**{*312*}	CC(C)(C)OC(=O)NC1CCCNC1
313	**11**{*313*}	CC(C)(C)OC(=O)N1C[C@@H]2CNC[C@@H]2C1
314	**11**{*314*}	CC(C)(C)OC(=O)N1CCCNCC1
315	**11**{*315*}	CC(C)(C)OC(=O)N1C[C@@H]2C[C@H]1CN2
316	**11**{*316*}	Fc1cccc(F)c1N1CCNCC1
317	**11**{*317*}	CNCc1ccc(C)o1
318	**11**{*318*}	C1Cn2c(CN1)nnc2-c1ccccc1
319	**11**{*319*}	CNCC1COCCO1
320	**11**{*320*}	COC(=O)C1CCNCC1
321	**11**{*321*}	OCC1CCNCC1
322	**11**{*322*}	CNC1CC1
323	**11**{*323*}	Cl.O=C1CNCc2ccccc2N1
324	**11**{*324*}	Cl.Cc1noc(n1)C1CCNCC1
325	**11**{*325*}	Cl.O=c1[nH]ncn1C1CCNCC1
326	**11**{*326*}	Cl.FC(F)(F)C1=CCNCC1
327	**11**{*327*}	C1CNC(C1)c1ccsc1
328	**11**{*328*}	C1COCCN1
329	**11**{*329*}	Cl.FC(F)C1CCNCCO1
330	**11**{*330*}	Cl.CNC1CCCCN(C)C1=O
331	**11**{*331*}	Cl.C1CC11CC2CCC(C1)N2
332	**11**{*332*}	Cl.CC1(CNCCO1)C(F)F
333	**11**{*333*}	CC1(C)CNCCS1

334	**11**{*334*}	Cn1cnnc1N1CCNCC1
335	**11**{*335*}	O=C1NC(=O)[C@@H]2CNC[C@H]12
336	**11**{*336*}	Cl.CS(=O)(=O)C1CCNCC1
337	**11**{*337*}	CNCC1CCOC1
338	**11**{*338*}	CCC1CNCC(CC)O1
339	**11**{*339*}	CNCc1cccc(F)c1
340	**11**{*340*}	C1CCCNCC1
341	**11**{*341*}	C1CCNC1
342	**11**{*342*}	CC1CCCCN1
343	**11**{*343*}	C(N1CCNCC1)c1ccccc1
344	**11**{*344*}	O=C(C1CC1)N1CCNC1
345	**11**{*345*}	C1CCCNCCC1
346	**11**{*346*}	CCNC
347	**11**{*347*}	C1CCCCNCCC1
348	**11**{*348*}	CC(C)C1CNCCCO1
349	**11**{*349*}	C#CCC1CCCNC1
350	**11**{*350*}	CNCCC=C
351	**11**{*351*}	CCN1CCNCC1=O
352	**11**{*352*}	Cl.C(C1CCNCC1)n1ccnn1
353	**11**{*353*}	Cl.OCC1(O)CCNCC1
354	**11**{*354*}	CC1NCN(C)C1=O
355	**11**{*355*}	CNCc1cnn(C)c1
356	**11**{*356*}	CNCC1CCC1
357	**11**{*357*}	COc1ccccc1N1CCNCC1
358	**11**{*358*}	CC(C)(C)OC(=O)NCC1CCNC1
359	**11**{*359*}	O=c1cccc2[C@H]3CNC[C@H](C3)Cn12
360	**11**{*360*}	CC(C)(C)OC(=O)NC1CCNCC1
361	**11**{*361*}	CC(C)(C)OC(=O)N1CCNCC1

362	**11**{*362*}	Cl.O[C@@H]1CCCNC1
363	**11**{*363*}	COCC1(C)CNCCO1
364	**11**{*364*}	CNCC1(C)COC1
365	**11**{*365*}	CC1CC(CN1)c1ccc(C)cc1
366	**11**{*366*}	CNCC(C)(C)O
367	**11**{*367*}	Cl.CNCC(=O)N1CCOCC1
368	**11**{*368*}	CS(=O)(=O)C1CCCNC1
369	**11**{*369*}	CC1CNCCO1
370	**11**{*370*}	CNCC1CCCOC1
371	**11**{*371*}	C1CC2(CNCCO2)c2ccccc12
372	**11**{*372*}	Cl.C[1C@@H]1CNC[1C@H](O)C1
373	**11**{*373*}	Cl.CC(C)NC(=O)[C@H]1CCCNC1
374	**11**{*374*}	Cc1noc(n1)C1CCNC1
375	**11**{*375*}	C1CN(CCN1)c1ncccn1
376	**11**{*376*}	COCC(=O)N1CCNCC1
377	**11**{*377*}	Cl.Fc1cccc2OCCNCc12
378	**11**{*378*}	Cc1ccc(C)n1C1CCNCC1
379	**11**{*379*}	Cl.OC1(CCCNCC1)C(F)(F)F
380	**11**{*380*}	Cl.CNS(=O)(=O)N1CCNCC1
381	**11**{*381*}	Cl.COc1ccc2OCCNCc2c1
382	**11**{*382*}	C1CNCC(C1)NC1CCOCC1
383	**11**{*383*}	Cl.C[C@@H]1CNCCN1S(C)(=O)=O
384	**11**{*384*}	Cl.Cl.O=C1CCCCN1C1CCCNC1
385	**11**{*385*}	Cl.CNCc1nc(C)no1
386	**11**{*386*}	CNCc1ccc(F)cc1
387	**11**{*387*}	C(C1CCNCC1)c1ccccc1
388	**11**{*388*}	CNCc1ccc(Cl)s1
389	**11**{*389*}	Cl.CNCc1cccs1

390	**11**{*390*}	Cl.CS(=O)(=O)N1CCNCC1
391	**11**{*391*}	CNCC1CC1
392	**11**{*392*}	CC1CNCC2(CCC2)O1
393	**11**{*393*}	C1CC2(C1)CNCCOC2
394	**11**{*394*}	C1CCC2(C1)CNCCO2
395	**11**{*395*}	C1CC2(CO1)CNCCO2
396	**11**{*396*}	CNCCOC
397	**11**{*397*}	CSC1CCCCNC1
398	**11**{*398*}	CC1CNCC(C)O1
399	**11**{*399*}	Cl.COCC1(C)CCNC1
400	**11**{*400*}	CNC1CCS(=O)(=O)C1
401	**11**{*401*}	NC(=O)C1CCNCC1
402	**11**{*402*}	CC1CNCC2(CCCCC2)O1
403	**11**{*403*}	Cl.CC12CCNCC1C2(Cl)Cl
404	**11**{*404*}	COC(=O)[1C@]12CNC[1C@H]1CCCC2
405	**11**{*405*}	C1CCC2(CC1)CCCNC2
406	**11**{*406*}	CC1CCNCC11CCC1
407	**11**{*407*}	C1CC2(CN1)CCCCC2
408	**11**{*408*}	C1CCC2(C1)CCCNC2
409	**11**{*409*}	C1CCC2(CC1)CNCCS2
410	**11**{*410*}	Cl.C1CCC2(CC1)CCNCC2
411	**11**{*411*}	CCC1CCCNC1
412	**11**{*412*}	CONCC1CC2CCC1C2
413	**11**{*413*}	CC1CNCC2(CCCC2)O1
414	**11**{*414*}	CNCc1nccs1
415	**11**{*415*}	CNC[C@H]1CCCO1
416	**11**{*416*}	C1CNCCc2ccccc2C1
417	**11**{*417*}	COc1cccc2CCNCc12

418	**11**{*418*}	Cl.FC1(F)CNCc2ccccc12
419	**11**{*419*}	FC1(F)CC11CC2CCC(C1)N2
420	**11**{*420*}	C1COC(CN1)c1ccccc1
421	**11**{*421*}	C1CC2(CN1)OCc1ccccc21
422	**11**{*422*}	NC(=O)CC1CCNCC1
423	**11**{*423*}	O=C1CNCCN1
424	**11**{*424*}	OC1CCCNC1
425	**11**{*425*}	Cl.COCC1=CCNCC1
426	**11**{*426*}	Cl.COC(=O)C1CC11CCNCC1
427	**11**{*427*}	Cl.CN1CCC2(CCNCC2)C1=O
428	**11**{*428*}	O=C1NCCC2(CCNCC2)O1
429	**11**{*429*}	C1CC2(CCO1)CCNCCO2
430	**11**{*430*}	CCOC(=O)[1C@@H]1[1C@@H]2CCNC[1C@H]12
431	**11**{*431*}	C1CC2(CS1)CNCCO2
432	**11**{*432*}	C1CC2(CCO1)CNCCOC2
433	**11**{*433*}	CC1CNCC2(CCOCC2)O1
434	**11**{*434*}	C1COC2(CCOCC2)CN1
435	**11**{*435*}	COC(=O)[1C@]12CNC[1C@H]1COCC2
436	**11**{*436*}	COC(=O)[1C@]12CCC[1C@H]1NCC2
437	**11**{*437*}	Cl.CCS(=O)(=O)N1CCNCC1
438	**11**{*438*}	NC(=O)[1C@]12CCC[1C@H]1CNC2
439	**11**{*439*}	CNC1CCCCC1
440	**11**{*440*}	CNC(C)CC#N
441	**11**{*441*}	Cl.CC1(C)CCNCCS1=O
442	**11**{*442*}	Cc1cccc(c1)C1CCNC1
443	**11**{*443*}	C[C@H]1CNC[C@@H](C)O1
444	**11**{*444*}	COc1ccc(cc1)C1CNCCO1
445	**11**{*445*}	Cl.COc1cc2CCNCc2cc1OC

446	**11**{*446*}	COC(=O)[1C@@H]1CNC[1C@H]1C
447	**11**{*447*}	C1Cc2ccccc2CN1
448	**11**{*448*}	CCOC(=O)C1CCNCC1
449	**11**{*449*}	CC1(C)CNCC(C)(C)O1
450	**11**{*450*}	C1CN(CCN1)c1ccccc1
451	**11**{*451*}	CCOC(=O)N1CCNCC1
452	**11**{*452*}	CCOC(=O)[C@@H]1CCCNC1
453	**11**{*453*}	CCOC(=O)C1CCCNC1
454	**11**{*454*}	CC1OCCC11CNCC(C)O1
455	**11**{*455*}	CC1OCCC11CNCCO1
456	**11**{*456*}	C1COC2(CCNCC2)OC1
457	**11**{*457*}	CCc1ncc2C3CCC(Cc2n1)N3
458	**11**{*458*}	CO[1C@@H]1CS(=O)(=O)[1C@H]2CNC[1C@@H]12
459	**11**{*459*}	CCNCC
460	**11**{*460*}	Fc1ccc(cc1)N1CCNCC1
461	**11**{*461*}	Cc1ccc(cc1)N1CCNCC1
462	**11**{*462*}	Cc1ccccc1N1CCNCC1
463	**11**{*463*}	Cc1ccc(cc1C)N1CCNCC1
464	**11**{*464*}	Cc1cccc(c1)N1CCNCC1
465	**11**{*465*}	CC1CCNCC1C
466	**11**{*466*}	C1CNCC2(C1)Oc1ccccc1C=C2
467	**11**{*467*}	FC(F)(F)CC1CC2CCC(C1)N2
468	**11**{*468*}	NC(=O)[1C@@H]1CCO[1C@H]1C1CCNCC1
469	**11**{*469*}	CC1CSCCN1
470	**11**{*470*}	CC(C)(C)OC(=O)NC1CCNC1
471	**11**{*471*}	CC(C)(C)OC(=O)N[C@H]1CCNC1
472	**11**{*472*}	CC(C)(C)OC(=O)N[C@@H]1CCNC1
473	**11**{*473*}	CCO[C@H]1CCNC1

474	**11**{*474*}	CSC1CCNC1
475	**11**{*475*}	C1CSCCN1
476	**11**{*476*}	FC1(F)CCNCC1
477	**11**{*477*}	COCC1CCCNC1
478	**11**{*478*}	C1CCNCC1
479	**11**{*479*}	CC1CCCNC1
480	**11**{*480*}	CC1CCNCC1
481	**11**{*481*}	C1NC[C@@H]2CC=CC[C@H]12
482	**11**{*482*}	C1CC2(CN1)OCCO2
483	**11**{*483*}	C1CC2CC1CNC2
484	**11**{*484*}	CC1CCNCC11CCCCC1
485	**11**{*485*}	C1CCC2(CC1)CCCNCC2
486	**11**{*486*}	CC(C)(C)OC(=O)N1C2CCC1CNC2
487	**11**{*487*}	CC(C)(C)OC(=O)N1CC2CCC(C1)N2
488	**11**{*488*}	CC(C)(C)OC(=O)[1C@]12CNC[1C@H]1COC2
489	**11**{*489*}	CC(C)(C)OC(=O)NCC12CC(C1)CN2
490	**11**{*490*}	CC(O)C1CCNCC1
491	**11**{*491*}	C1CCN(C1)C1CCNC1
492	**11**{*492*}	CNCC(C)(O)c1ccccc1
493	**11**{*493*}	CC1CC2CCC(C1)N2
494	**11**{*494*}	COCC1CNCCO1
495	**11**{*495*}	CC(=O)NCC1CNCCO1
496	**11**{*496*}	CNC(C)C#C
497	**11**{*497*}	Cl.O=C1NC(=O)N2CCNCC12
498	**11**{*498*}	Fc1ccccc1N1CCNCC1
499	**11**{*499*}	C1CC11CCCNCC1
500	**11**{*500*}	C1CNCC(C1)c1cc2ccccc2[nH]1
501	**11**{*501*}	CCNCC(C)=C

502	**11**{*502*}	C1CC2(CN1)Oc1ccccc1O2
503	**11**{*503*}	C1C2CNCCCN2c2ccccc12
504	**11**{*504*}	O=C1CNCCN1C1CC1
505	**11**{*505*}	CC1CNCC(C)C1
506	**11**{*506*}	CNCC=C
507	**11**{*507*}	Cl.OC1(CCNC1)C(F)F
508	**11**{*508*}	C1OCC11CCNC1
509	**11**{*509*}	Cl.C1CC2CCC1N2
510	**11**{*510*}	Cl.C1C2CNCC12
511	**11**{*511*}	Cl.CN(C)C(=O)C1CCNC1

Table S3. SMILES strings for the regents **15**.

#	Reagent **15**	SMILE
1	**15**{*1*}	CC(C)N
2	**15**{*2*}	NCc1ccco1
3	**15**{*3*}	NCc1ccc2OCOc2c1
4	**15**{*4*}	COCCN
5	**15**{*5*}	CCCCCN
6	**15**{*6*}	NCc1ccc(Cl)cc1
7	**15**{*7*}	NCc1ccccc1
8	**15**{*8*}	NCC1CCCO1
9	**15**{*9*}	COCCCN
10	**15**{*10*}	CC(C)CCN
11	**15**{*11*}	NCC1CCCCC1
12	**15**{*12*}	CN(C)CCCN
13	**15**{*13*}	NCC=C
14	**15**{*14*}	COc1ccc(CCN)cc1
15	**15**{*15*}	NCc1ccccc1Cl
16	**15**{*16*}	NCc1cccc(Cl)c1
17	**15**{*17*}	NC1CC1
18	**15**{*18*}	COc1ccc(CN)cc1
19	**15**{*19*}	NC1CCCC1
20	**15**{*20*}	NCCc1c[nH]c2ccccc12
21	**15**{*21*}	NCCc1ccc(Cl)cc1
22	**15**{*22*}	NCc1ccc(Cl)cc1Cl
23	**15**{*23*}	NCCCc1ccccc1
24	**15**{*24*}	COc1ccc(CN)cc1OC
25	**15**{*25*}	NCCC1=CCCCC1

26	**15**{*26*}	COc1ccccc1CN
27	**15**{*27*}	CCCN
28	**15**{*28*}	NCCc1ccc(F)cc1
29	**15**{*29*}	NCc1ccc(F)cc1
30	**15**{*30*}	Cc1ccc(CN)cc1
31	**15**{*31*}	COc1cccc(CN)c1
32	**15**{*32*}	NCc1cccs1
33	**15**{*33*}	NCc1ccccc1F
34	**15**{*34*}	NCc1cccc(c1)C(F)(F)F
35	**15**{*35*}	NCCc1ccc(cc1)C(F)(F)F
36	**15**{*36*}	CC(=O)NCCN
37	**15**{*37*}	CN(C)C1(CN)CCCC1
38	**15**{*38*}	NCCOc1ccccc1
39	**15**{*39*}	CC(C)(CN)N1CCOCC1
40	**15**{*40*}	CC(C)(CN)N1CCCCC1
41	**15**{*41*}	COc1ccccc1CCN
42	**15**{*42*}	NCCCn1ccc2ccccc12
43	**15**{*43*}	NCc1ccc(cc1)C(N)=O
44	**15**{*44*}	NCCCN1CCCCCC1=O
45	**15**{*45*}	NCCc1cccs1
46	**15**{*46*}	NCCc1ccco1
47	**15**{*47*}	Cc1ccccc1CN
48	**15**{*48*}	NCCc1ccccc1F
49	**15**{*49*}	NCc1ccc(OC(F)F)cc1
50	**15**{*50*}	CCCNC(=O)CN
51	**15**{*51*}	NCCc1ccc2OCOc2c1
52	**15**{*52*}	COc1ccc(C)cc1CCN
53	**15**{*53*}	NCCc1cccc(F)c1

54	**15**{*54*}	NCCCOCC1CCCO1
55	**15**{*55*}	NCc1ccc(cc1)C(F)(F)F
56	**15**{*56*}	Cc1nc(CN)cs1
57	**15**{*57*}	Cc1cc(CN)ccc1F
58	**15**{*58*}	NCc1ccc(OC(F)(F)F)cc1
59	**15**{*59*}	COc1ccc2cc(CN)ccc2c1
60	**15**{*60*}	NCc1cnn(c1)-c1ccccc1
61	**15**{*61*}	CN(C)S(=O)(=O)c1ccccc1CN
62	**15**{*62*}	NC1CCN(CC1)C(=O)c1ccco1
63	**15**{*63*}	NCC1CC1
64	**15**{*64*}	CN(C)C(=O)c1ccc(CN)cc1
65	**15**{*65*}	NC1CCC(CC1)C(F)(F)F
66	**15**{*66*}	NCCC1CCCO1
67	**15**{*67*}	NCc1ccc(Cl)nc1
68	**15**{*68*}	COc1ccc(OC)c(CN)c1
69	**15**{*69*}	Cl.NCCNC(=O)c1cccs1
70	**15**{*70*}	Cc1ccc(cc1F)C(=O)NCCN
71	**15**{*71*}	NCc1cccc(F)c1
72	**15**{*72*}	NC1CCC1
73	**15**{*73*}	COc1ccc(CN)c(OC)c1
74	**15**{*74*}	CCOc1ccccc1CN
75	**15**{*75*}	NCCc1ccccc1Cl
76	**15**{*76*}	NCc1ccccc1C(F)(F)F
77	**15**{*77*}	NCc1ccc(F)c(F)c1
78	**15**{*78*}	Cc1ccc(CN)o1
79	**15**{*79*}	NOC1CCCCO1
80	**15**{*80*}	NCc1ccc(F)cc1C(F)(F)F
81	**15**{*81*}	Cc1ccsc1CN

82	**15**{*82*}	NCc1ccccc1Br
83	**15**{*83*}	CCOCCN
84	**15**{*84*}	CC(C)Oc1cccc(CN)c1
85	**15**{*85*}	CC(C)Oc1ccccc1CN
86	**15**{*86*}	NCCOc1ccccc1Cl
87	**15**{*87*}	NCc1ccc(Cl)c(Cl)c1
88	**15**{*88*}	NCc1ccc(F)c(Cl)c1
89	**15**{*89*}	NCc1ccc(F)cc1F
90	**15**{*90*}	CC(C)OCCN
91	**15**{*91*}	Cl.NCCc1c[nH]c2ccc(F)cc12
92	**15**{*92*}	COc1cccc(CN)c1OC
93	**15**{*93*}	Cc1ccc(CN)s1
94	**15**{*94*}	Cc1cccc(CN)c1
95	**15**{*95*}	NCc1cc(F)ccc1F
96	**15**{*96*}	COc1cccc(CCN)c1
97	**15**{*97*}	CCNC(=O)c1ccc(CN)cc1
98	**15**{*98*}	NC1CCN(CC1)C1CCCC1
99	**15**{*99*}	CCOc1ccc(CN)cc1
100	**15**{*100*}	Cc1ccc(CN)c(C)c1
101	**15**{*101*}	Cc1cc(C)c(CN)c(C)c1
102	**15**{*102*}	NCc1ccsc1
103	**15**{*103*}	NCC1CCOC1
104	**15**{*104*}	NCc1ccc(CN2CCCC2=O)cc1
105	**15**{*105*}	NCc1ccccc1CN1CCCC1=O
106	**15**{*106*}	COCc1ccc(CN)cc1
107	**15**{*107*}	COCc1cccc(CN)c1
108	**15**{*108*}	NCc1cccc(c1)C(N)=O
109	**15**{*109*}	CN(C)C(=O)c1cccc(CN)c1

110	**15**{*110*}	CNC(=O)c1cccc(CN)c1
111	**15**{*111*}	NCc1cc(Cl)c2OCCOc2c1
112	**15**{*112*}	NCc1c(Cl)cccc1Cl
113	**15**{*113*}	NCCc1c(F)cccc1F
114	**15**{*114*}	Cc1ccc(CCN)o1
115	**15**{*115*}	NCCN1CCNC1=O
116	**15**{*116*}	CCCC(=O)Nc1ccc(CN)cc1
117	**15**{*117*}	NCc1ccoc1
118	**15**{*118*}	NCCCC1CCCC1
119	**15**{*119*}	NCc1cccc(c1)N1CCCC1=O
120	**15**{*120*}	Cc1cc(CN)no1
121	**15**{*121*}	NCC1CCOCC1
122	**15**{*122*}	Cl.NCc1csc2ccccc12
123	**15**{*123*}	Cc1nn(C)c(C)c1CN
124	**15**{*124*}	NCc1ccc(cc1)-n1cccn1
125	**15**{*125*}	CC(CN)Oc1ccc(C)cc1
126	**15**{*126*}	Cl.NCC12CC3CC(CC(C3)C1)C2
127	**15**{*127*}	Cl.NCC#C
128	**15**{*128*}	NCc1ccc(Cn2cccn2)cc1
129	**15**{*129*}	Cl.NC1Cc2ccccc2C1
130	**15**{*130*}	Cl.NC1CCOCC1
131	**15**{*131*}	NCC1CCCc2ccccc12
132	**15**{*132*}	NCc1ccc(o1)-c1ccccc1
133	**15**{*133*}	Cn1nccc1CN
134	**15**{*134*}	NC1CCCC(O)C1
135	**15**{*135*}	NCc1cnn(Cc2ccccc2)c1
136	**15**{*136*}	Cc1n[nH]cc1CN
137	**15**{*137*}	CC(C)NC(=O)Nc1ccc(CN)cc1

138	**15**{*138*}	NCc1cc(Br)cs1
139	**15**{*139*}	CC1CC1N
140	**15**{*140*}	CC(CN)Cn1cccn1
141	**15**{*141*}	Cl.NCCCC(=O)NC1CC1
142	**15**{*142*}	CS(=O)(=O)Cc1ccc(CN)cc1
143	**15**{*143*}	CC(O)c1ccc(CN)cc1
144	**15**{*144*}	NCCn1cccn1
145	**15**{*145*}	NCC1CCCOC1c1ccccc1
146	**15**{*146*}	Cc1cccc(c1)C(=O)NCCN
147	**15**{*147*}	CS(=O)(=O)CCN
148	**15**{*148*}	NCC1CCCCO1
149	**15**{*149*}	NCC1CCC=CC1
150	**15**{*150*}	Cc1cccc(CCN)c1
151	**15**{*151*}	NCCc1ccc(F)cc1F
152	**15**{*152*}	COC(CN)c1ccccc1
153	**15**{*153*}	Cl.NCC1C2CC3CC(C2)CC1C3
154	**15**{*154*}	COc1cc(CN)ccc1C
155	**15**{*155*}	CC1CC(C)CN(C1)C(C)(C)CN
156	**15**{*156*}	CC1CCCN(C1)C(C)(C)CN
157	**15**{*157*}	Cn1cc(CN)cn1
158	**15**{*158*}	CC1CCCC(CN)C1
159	**15**{*159*}	NCc1cccc(NC(=O)C2CCCO2)c1
160	**15**{*160*}	Cl.CC(CN)C1CC1
161	**15**{*161*}	NCCc1ccc(Br)s1
162	**15**{*162*}	COCC(C)CN
163	**15**{*163*}	NCc1ccc(NC(=O)c2ccco2)cc1
164	**15**{*164*}	NCCc1cn[nH]c1
165	**15**{*165*}	NCC(Br)=C

166	**15**{*166*}	Cc1cc(CN)on1
167	**15**{*167*}	NCCCc1cccc(Cl)c1
168	**15**{*168*}	NCCc1ccc(F)c(F)c1
169	**15**{*169*}	CC(=O)Nc1ccc(CCN)cc1
170	**15**{*170*}	NCCOCC1CC1
171	**15**{*171*}	Cl.NCCNC(=O)C1CC1
172	**15**{*172*}	Cc1ccoc1CN
173	**15**{*173*}	Cc1ccccc1C(C)(C)CN
174	**15**{*174*}	COc1ccccc1C(C)(C)CN
175	**15**{*175*}	CCC(CN)c1ccccc1
176	**15**{*176*}	NCc1ccc(cc1)C(=O)N1CCCC1
177	**15**{*177*}	Cc1occc1CN
178	**15**{*178*}	Cl.NCC1CCCNC1=O
179	**15**{*179*}	NCCc1cc(F)cc(F)c1
180	**15**{*180*}	Cc1cccnc1CN
181	**15**{*181*}	NCc1nc2CCCc2s1
182	**15**{*182*}	NCc1ccc(OC2CCCC2)cc1
183	**15**{*183*}	Cl.NCCCc1ccc(Cl)cc1
184	**15**{*184*}	COc1ccccc1C1(CN)CC1
185	**15**{*185*}	Cl.NC1CCSCC1
186	**15**{*186*}	CC(C)(CN)c1ccccc1F
187	**15**{*187*}	Cc1[nH]c2ccccc2c1CCN
188	**15**{*188*}	NCCCN1CCOC1=O
189	**15**{*189*}	NC1CCCc2sccc12
190	**15**{*190*}	COc1ccc(CCN)cc1F
191	**15**{*191*}	NCc1cccc(CO)c1
192	**15**{*192*}	CCc1cccc2c(CCN)c[nH]c12
193	**15**{*193*}	Cl.NCc1cccc(CN2CCCC2=O)c1

194	**15**{*194*}	CCn1cc(CN)cn1
195	**15**{*195*}	Cc1c(CN)cnn1C
196	**15**{*196*}	Cn1ccc(CN)n1
197	**15**{*197*}	Cl.NCC(F)F
198	**15**{*198*}	CC(N)c1cnn(C)c1
199	**15**{*199*}	NCc1cccc2[nH]ccc12
200	**15**{*200*}	NCc1cccc(c1)-n1cncn1
201	**15**{*201*}	Cl.NC1CCCOC1
202	**15**{*202*}	CCC1(CN)CCC1
203	**15**{*203*}	CC1(CN)CCCO1
204	**15**{*204*}	Cl.CCN1CC(N)CC1=O
205	**15**{*205*}	Cl.NCC1=CCCCC1
206	**15**{*206*}	Cl.NCCc1nc(no1)-c1ccc(Cl)cc1
207	**15**{*207*}	CC1(CN)CCOC1
208	**15**{*208*}	CC(C)n1ccc(CN)n1
209	**15**{*209*}	NC1CCN(CC(F)(F)F)C1=O
210	**15**{*210*}	Cc1cc(CN)ncn1
211	**15**{*211*}	Cl.CC1(C)CC1CN
212	**15**{*212*}	Cl.NCCN1C(=O)CNC1=O
213	**15**{*213*}	NCc1ccon1
214	**15**{*214*}	COc1cc(F)cc(CN)c1
215	**15**{*215*}	NCC1CSCCS1
216	**15**{*216*}	CCSc1cccc(CN)c1
217	**15**{*217*}	NCC1CCC(CC1)C(F)(F)F
218	**15**{*218*}	Cl.CC1(C)C(CN)C1(C)C
219	**15**{*219*}	NCC1CNC(=O)C1
220	**15**{*220*}	NCCC1CCC1
221	**15**{*221*}	CC(C)CC1(CN)CCC1

222	**15**{*222*}	Cc1nnsc1CN
223	**15**{*223*}	NCc1ccc(F)cn1
224	**15**{*224*}	Cc1nnc(CN)s1
225	**15**{*225*}	Cl.Cc1ccc(CN)cc1F
226	**15**{*226*}	CC1(C)CCCC(N)C1
227	**15**{*227*}	NOC1CCCC1
228	**15**{*228*}	Cl.CCOC(=O)C1(CN)CCC1
229	**15**{*229*}	CC1(C)CC(N)CCO1
230	**15**{*230*}	Cl.NCCC(=O)N1CCCCC1
231	**15**{*231*}	Cl.NCCC1CC1
232	**15**{*232*}	Cl.COC[C@@H](C)N
233	**15**{*233*}	NCC1CCCS1
234	**15**{*234*}	Cl.CC(=C)CCN
235	**15**{*235*}	COC1CCC(CN)CC1
236	**15**{*236*}	CC1CC(N)CC(C)O1
237	**15**{*237*}	CC1CC(N)CCO1
238	**15**{*238*}	Cl.NC1CCC=C1
239	**15**{*239*}	Cl.NCC1CCC=C1
240	**15**{*240*}	NCCCCC1CC1
241	**15**{*241*}	COC1(CN)CCOCC1
242	**15**{*242*}	NCc1cc(no1)C1CC1
243	**15**{*243*}	NCc1nc(cs1)C(F)(F)F
244	**15**{*244*}	CCOC1CC(N)C11CCCC1
245	**15**{*245*}	Cl.NC1CCCC1(F)F
246	**15**{*246*}	CC(C)(CN)c1cccc(F)c1
247	**15**{*247*}	CSCC(C)N
248	**15**{*248*}	NCc1cccc2ncccc12
249	**15**{*249*}	CC(CN)c1nc(C)cs1

250	**15**{*250*}	NCCc1nc2CCCc2s1
251	**15**{*251*}	Cc1nc(C)c(CN)s1
252	**15**{*252*}	NCC1(CC1)c1cccc(Cl)c1
253	**15**{*253*}	CCn1nncc1CN
254	**15**{*254*}	CC(O)(CCN)c1ccccc1
255	**15**{*255*}	COc1ccc(CN)c(OC)n1
256	**15**{*256*}	Cl.CO[C@H](C)CN
257	**15**{*257*}	Cl.NC1CCC2(CCCC2)CC1
258	**15**{*258*}	NCC1CCC(F)(F)C1
259	**15**{*259*}	Cl.COCC(C)(C)CN
260	**15**{*260*}	Cl.CC(=O)N1CC[C@@H](N)C1
261	**15**{*261*}	Cl.CN1CCC(N)C1=O
262	**15**{*262*}	CC(CN)Sc1ccccc1
263	**15**{*263*}	CC(CN)Oc1ccccc1F
264	**15**{*264*}	CC(CN)Oc1cccc(C)c1
265	**15**{*265*}	CC(CN)Oc1ccccc1C
266	**15**{*266*}	NCCCC#C
267	**15**{*267*}	NCC1(Cc2ccccc2)CC1
268	**15**{*268*}	NCc1ccc(CC(N)=O)cc1
269	**15**{*269*}	CSCc1ccc(CN)cc1
270	**15**{*270*}	Cl.N[C@H]1C[C@H](C1)C(N)=O
271	**15**{*271*}	Cl.NCC1CC2CCC1CC2
272	**15**{*272*}	CCSc1ccc(CN)cc1
273	**15**{*273*}	NCCn1cc(Br)cn1
274	**15**{*274*}	NCCn1ccc2cc(Cl)ccc12
275	**15**{*275*}	NCc1ncc(Br)s1
276	**15**{*276*}	Cl.NCC1CCC2(CC2)CC1
277	**15**{*277*}	NCc1c(F)cccc1OC(F)F

278	**15**{*278*}	Cl.NCc1nnnn1C1CC1
279	**15**{*279*}	CSC(C)CN
280	**15**{*280*}	NCCCn1cc(Br)cn1
281	**15**{*281*}	NCc1nc2CCOCc2s1
282	**15**{*282*}	Cl.NC1CC(C1)OCc1ccccc1
283	**15**{*283*}	CCC(=O)N1CCC(N)C1
284	**15**{*284*}	COCCC1(CN)CCCC1
285	**15**{*285*}	CCOCCC1(CN)CCCC1
286	**15**{*286*}	CCC1(CN)CCCC1
287	**15**{*287*}	Cn1nccc1CCN
288	**15**{*288*}	CC(C)(C)C1CC(N)CCO1
289	**15**{*289*}	CC(C)C1CC(N)CCO1
290	**15**{*290*}	NCCCOC1CCOC1
291	**15**{*291*}	CC(C)c1csc(CN)n1
292	**15**{*292*}	NCCOCC1CCCC1
293	**15**{*293*}	NCCCc1ccco1
294	**15**{*294*}	NCc1cnn(CC(F)(F)F)c1
295	**15**{*295*}	CNC(=O)C(C)(C)CN
296	**15**{*296*}	CCNC(=O)C(C)(C)CN
297	**15**{*297*}	CC(CN)c1nccs1
298	**15**{*298*}	CCN(C)C(=O)CN
299	**15**{*299*}	COC1CC(N)C1(C)C
300	**15**{*300*}	Cl.CC(C)(C)N1CC(N)CC1=O
301	**15**{*301*}	CCSC1CCCC(N)C1
302	**15**{*302*}	Cl.CC(C)C1OCCCC1CN
303	**15**{*303*}	CCOCCC1(CN)CCC1
304	**15**{*304*}	COCCC1(CN)CCC1
305	**15**{*305*}	Cl.CC(C)CC1(CN)CC1

306	**15**{*306*}	Cc1cscc1CN
307	**15**{*307*}	Cl.CCCC1(CN)CCC1
308	**15**{*308*}	CCC(OCCN)c1ccccc1
309	**15**{*309*}	COCCC1(CN)CC1
310	**15**{*310*}	CCOCCC1(CN)CC1
311	**15**{*311*}	COC(CN)C1CCCCC1
312	**15**{*312*}	COC1(CN)CCC1
313	**15**{*313*}	CC(C)(O)C(C)(C)CN
314	**15**{*314*}	CCc1nn(C)c(CC)c1CN
315	**15**{*315*}	CSc1cccc(F)c1CN
316	**15**{*316*}	NCCC1CC2CCC1O2
317	**15**{*317*}	Cl.CCCC1(CN)CC1
318	**15**{*318*}	Cl.CC1CCC(N)C1
319	**15**{*319*}	CC(C)(CN)C1CCCC1
320	**15**{*320*}	Cl.CO[C@H]1C[C@H](N)C1
321	**15**{*321*}	Cl.CCC1(CN)CCOCC1
322	**15**{*322*}	Cl.NC1CC(C1)C(N)=O
323	**15**{*323*}	Cl.COCC1CC(N)C1
324	**15**{*324*}	Cl.CS(=O)(=O)C1(CN)CC1
325	**15**{*325*}	Cl.CC1CC(CN)CCO1
326	**15**{*326*}	Cl.CC1(CN)CCCc2ccccc12
327	**15**{*327*}	Cl.NC1CC2(CCC2)C1
328	**15**{*328*}	Cl.CCO[C@@H]1C[C@H](N)C1
329	**15**{*329*}	Cl.CCO[C@H]1C[C@H](N)C1
330	**15**{*330*}	Cl.NCC1CCCCS1(=O)=O
331	**15**{*331*}	NCc1csc(c1)C(F)(F)F
332	**15**{*332*}	CON1CCC(N)CC1
333	**15**{*333*}	NC1COC2(CCC2)C1

334	**15**{*334*}	Cl.CCS(=O)(=O)c1ccc(CN)cc1
335	**15**{*335*}	Cl.C[C@H]1OCC[C@H]1N
336	**15**{*336*}	Cl.CCC[1C@@H]1C[1C@H]1N
337	**15**{*337*}	Cn1nccc1C1CC(N)CCO1
338	**15**{*338*}	CN1CCC[C@@H](CN)[C@@H]1c1ccnn1C
339	**15**{*339*}	NCC(C1CCC1)C1CCC1
340	**15**{*340*}	NCCC1CCC2(CCC2)O1
341	**15**{*341*}	NCc1nc(n2CCCCc12)C(F)(F)F
342	**15**{*342*}	Cl.CC(C)(CN)C1CCC1
343	**15**{*343*}	Cl.CC1(CN)CC1(Cl)Cl
344	**15**{*344*}	Cl.CC(C)[1C@@H]1C[1C@H]1N
345	**15**{*345*}	Cl.CC(C)C[1C@@H]1C[1C@H]1N
346	**15**{*346*}	Cc1nn(C)c(C)c1[1C@@H]1OCC[1C@H]1CN
347	**15**{*347*}	CC(C)(C)O[C@@H]1C[C@H](N)C1
348	**15**{*348*}	Cl.COC(=O)CC1CC(N)C1
349	**15**{*349*}	Cl.CCN1CCC(N)C1=O
350	**15**{*350*}	Cl.N[C@H]1C[C@@H](C1)C(N)=O
351	**15**{*351*}	Cl.COCC1(CCN)CC1
352	**15**{*352*}	NCCCC1(O)CCC1
353	**15**{*353*}	Cl.NCCN1CC2CCCCN2C1=O
354	**15**{*354*}	Cl.NCC1SCCS1
355	**15**{*355*}	NC1COC(C1)C1CC1
356	**15**{*356*}	Cl.NC1CCN(C2CCCCC2)C1=O
357	**15**{*357*}	Cl.CO[C@@H]1C[C@H](CN)C1
358	**15**{*358*}	Cl.NC1CCN(C2CCC2)C1=O
359	**15**{*359*}	CC1CC2(CCC(CN)O2)CO1
360	**15**{*360*}	CC1(CN)CCOC2(CCC2)C1
361	**15**{*361*}	Cl.NC[1C@@H]1CCO[1C@H]1c1ccccc1

362	**15**{*362*}	Cl.NCC12COCCN1C(=O)COC2
363	**15**{*363*}	Cl.NCC1CC2(CO1)CCOCC2
364	**15**{*364*}	Cl.NCC1CC2CCC(C1)S2(=O)=O
365	**15**{*365*}	NCC1CCC2(CCOCC2)CO1
366	**15**{*366*}	NCCC1CCC2(CCOCC2)CO1
367	**15**{*367*}	Cl.NCCC1CCCC1(F)F
368	**15**{*368*}	Cl.NCC1CCC2(CCC2)CO1
369	**15**{*369*}	Cl.NC1CC(CC(N)=O)C1
370	**15**{*370*}	Cl.NCC1CC2CCC(C1)S2
371	**15**{*371*}	Cl.COC1(CN)CCS(=O)(=O)C1
372	**15**{*372*}	Cl.NCC12CC1CCCC2
373	**15**{*373*}	Cl.NCC1CCC(O1)C(F)(F)F
374	**15**{*374*}	Cl.NC[1C@@H]1[1C@@H](c2ccccc2)C1(F)F
375	**15**{*375*}	Cl.N[1C@@H]1[1C@H]2Cc3ccccc3[1C@@H]12
376	**15**{*376*}	Cl.NCC1CCCC2(CCC2)O1
377	**15**{*377*}	Cl.NCC1CCC2(CCOCC2)O1
378	**15**{*378*}	Cl.NC[1C@]12C[1C@H]1CCC2

Table S4. Parallel synthesis of 5-aminotetrazoles **8**

#	Isothio-cyanate	Secondary amine	Product	SMILE	Yield, mg	Yield, %
1	**10**{*1*}	**11**{*1*}	**8**{*1,1*}	CNS(=O)(=O)c1cccc2CN(CCc12)c1nnnn1CC=C	27	22
2	**10**{*1*}	**11**{*2*}	**8**{*1,2*}	C=CCn1nnnc1N1CCN(CC1)C(=O)C(=O)NC1CC1	13	15
3	**10**{*1*}	**11**{*3*}	**8**{*1,3*}	OC1(Cc2nc(no2)C2CC2)CCCN(C1)c1nnnn1CC=C	0	0
4	**10**{*2*}	**11**{*4*}	**8**{*2,4*}	Cn1nnnc1N1CCOC2(CCC2)C1	0	0
5	**10**{*2*}	**11**{*5*}	**8**{*2,5*}	Cn1nnnc1N1CCOCC1c1cc(F)cc(F)c1	0	0
6	**10**{*2*}	**11**{*6*}	**8**{*2,6*}	Cn1nnnc1N1CCOc2cc(F)ccc2C1	0	0
7	**10**{*2*}	**11**{*7*}	**8**{*2,7*}	CC1=C(C)CN(CC1)c1nnnn1C	0	0
8	**10**{*2*}	**11**{*8*}	**8**{*2,8*}	Cn1nnnc1N1CC2(CCOCC2)[1C@@H]2CCC[1C@H]12	43	34
9	**10**{*2*}	**11**{*9*}	**8**{*2,9*}	Cn1nnnc1N1CCCC1c1nc2cc(Cl)ccc2[nH]1	43	21
10	**10**{*3*}	**11**{*10*}	**8**{*3,10*}	CCCCn1nnnc1N1CCN(CC1)C(=O)c1cccn1C	27	31
11	**10**{*3*}	**11**{*2*}	**8**{*3,2*}	CCCCn1nnnc1N1CCN(CC1)C(=O)C(=O)NC1CC1	16	21
12	**10**{*3*}	**11**{*8*}	**8**{*3,8*}	CCCCn1nnnc1N1CC2(CCOCC2)[1C@@H]2CCC[1C@H]12	21	24
13	**10**{*3*}	**11**{*3*}	**8**{*3,3*}	CCCCn1nnnc1N1CCCC(O)(Cc2nc(no2)C2CC2)C1	0	0
14	**10**{*3*}	**11**{*11*}	**8**{*3,11*}	CCCCn1nnnc1N(CC(=O)NC)Cc1ccccc1	0	0
15	**10**{*3*}	**11**{*12*}	**8**{*3,12*}	CCCCn1nnnc1N1CCCC(C1)c1nncn1C	0	0
16	**10**{*4*}	**11**{*7*}	**8**{*4,7*}	CCn1nnnc1N1CCC(C)=C(C)C1	0	0
17	**10**{*4*}	**11**{*8*}	**8**{*4,8*}	CCn1nnnc1N1CC2(CCOCC2)[1C@@H]2CCC[1C@H]12	26	29

18	**10**{*4*}	**11**{*2*}	**8**{*4,2*}	CCn1nnnc1N1CCN(CC1)C(=O)C(=O)NC1CC1	29	30
19	**10**{*5*}	**11**{*13*}	**8**{*5,13*}	C(c1ccccc1)n1nnnc1N1CCCC1C1CCCO1	35	34
20	**10**{*5*}	**11**{*14*}	**8**{*5,14*}	CC(CS(C)(=O)=O)N(C1CC1)c1nnnn1Cc1ccccc1	15	18
21	**10**{*5*}	**11**{*15*}	**8**{*5,15*}	COC1(CCN(CC1)c1nnnn1Cc1ccccc1)C(F)(F)F	0	0
22	**10**{*5*}	**11**{*8*}	**8**{*5,8*}	C(c1ccccc1)n1nnnc1N1CC2(CCOCC2)[1C@@H]2CCC[1C@H]12	0	0
23	**10**{*5*}	**11**{*12*}	**8**{*5,12*}	Cn1cnnc1C1CCCN(C1)c1nnnn1Cc1ccccc1	0	0
24	**10**{*6*}	**11**{*16*}	**8**{*6,16*}	O=C1NCCN1C1CCCN(C1)c1nnnn1CCc1ccccc1	29	30
25	**10**{*6*}	**11**{*13*}	**8**{*6,13*}	C(Cn1nnnc1N1CCCC1C1CCCO1)c1ccccc1	5	5
26	**10**{*6*}	**11**{*14*}	**8**{*6,14*}	CC(CS(C)(=O)=O)N(C1CC1)c1nnnn1CCc1ccccc1	0	0
27	**10**{*6*}	**11**{*17*}	**8**{*6,17*}	COCCCN(CCOC)c1nnnn1CCc1ccccc1	0	0
28	**10**{*6*}	**11**{*18*}	**8**{*6,18*}	NC(=O)[C@@H]1C[C@@H](F)CN1c1nnnn1CCc1ccccc1	0	0
29	**10**{*6*}	**11**{*12*}	**8**{*6,12*}	Cn1cnnc1C1CCCN(C1)c1nnnn1CCc1ccccc1	0	0
30	**10**{*6*}	**11**{*4*}	**8**{*6,4*}	C(Cn1nnnc1N1CCOC2(CCC2)C1)c1ccccc1	0	0
31	**10**{*7*}	**11**{*19*}	**8**{*7,19*}	COC1(CCN(C1)c1nnnn1C1CCCCC1)C(F)(F)F	14	7
32	**10**{*7*}	**11**{*20*}	**8**{*7,20*}	CCC1(CCN(CC1)c1nnnn1C1CCCCC1)N1CCOCC1	20	10
33	**10**{*7*}	**11**{*21*}	**8**{*7,21*}	CN(C1CCN(CC1)S(C)(=O)=O)c1nnnn1C1CCCCC1	26	13
34	**10**{*7*}	**11**{*22*}	**8**{*7,22*}	C1CCC(CC1)n1nnnc1N1CCCC(CC1)n1ccnn1	0	0
35	**10**{*8*}	**11**{*23*}	**8**{*8,23*}	C(Cn1nnnc1N1CCCCc2ccccc12)N1CCOCC1	19	9
36	**10**{*8*}	**11**{*24*}	**8**{*8,24*}	CC1(C)CC(O)CCN(C1)c1nnnn1CCN1CCOCC1	0	0
37	**10**{*8*}	**11**{*25*}	**8**{*8,25*}	C(Cn1nnnc1N1CCCC1c1cccnc1)N1CCOCC1	0	0
38	**10**{*8*}	**11**{*26*}	**8**{*8,26*}	Clc1ccc2CN(CCc2c1)c1nnnn1CCN1CCOCC1	0	0

39	**10**{*8*}	**11**{*27*}	**8**{*8,27*}	C(Cn1nnnc1N1CCC(CC1)c1ccncc1)N1CCOCC1	0	0
40	**10**{*8*}	**11**{*28*}	**8**{*8,28*}	COC1CCCN(C1)c1nnnn1CCN1CCOCC1	0	0
41	**10**{*8*}	**11**{*29*}	**8**{*8,29*}	Cc1ccc2CN(CCc2c1)c1nnnn1CCN1CCOCC1	0	0
42	**10**{*8*}	**11**{*30*}	**8**{*8,30*}	C(Cn1nnnc1N1CCC=CC1)N1CCOCC1	0	0
43	**10**{*8*}	**11**{*31*}	**8**{*8,31*}	C(Cn1nnnc1N1CCC(CC1)c1ccccc1)N1CCOCC1	0	0
44	**10**{*8*}	**11**{*32*}	**8**{*8,32*}	CC1N(CCc2cccc(F)c12)c1nnnn1CCN1CCOCC1	0	0
45	**10**{*8*}	**11**{*33*}	**8**{*8,33*}	O=C1CCN(CCN1)c1nnnn1CCN1CCOCC1	0	0
46	**10**{*8*}	**11**{*34*}	**8**{*8,34*}	CCC1N(CCc2sccc12)c1nnnn1CCN1CCOCC1	0	0
47	**10**{*8*}	**11**{*35*}	**8**{*8,35*}	C(Cn1nnnc1N1CCCC(C1)c1ncc[nH]1)N1CCOCC1	0	0
48	**10**{*8*}	**11**{*36*}	**8**{*8,36*}	O[C@H]1CCN(C1)c1nnnn1CCN1CCOCC1	0	0
49	**10**{*8*}	**11**{*37*}	**8**{*8,37*}	COc1ccc2CN(CCc2c1)c1nnnn1CCN1CCOCC1	0	0
50	**10**{*8*}	**11**{*38*}	**8**{*8,38*}	C(Cn1nnnc1N1CCc2nc[nH]c2C1)N1CCOCC1	0	0
51	**10**{*8*}	**11**{*39*}	**8**{*8,39*}	Fc1ccc2N(CCc2c1)c1nnnn1CCN1CCOCC1	0	0
52	**10**{*9*}	**11**{*4*}	**8**{*9,4*}	COCCn1nnnc1N1CCOC2(CCC2)C1	29	35
53	**10**{*9*}	**11**{*7*}	**8**{*9,7*}	COCCn1nnnc1N1CCC(C)=C(C)C1	21	22
54	**10**{*9*}	**11**{*5*}	**8**{*9,5*}	COCCn1nnnc1N1CCOCC1c1cc(F)cc(F)c1	0	0
55	**10**{*9*}	**11**{*6*}	**8**{*9,6*}	COCCn1nnnc1N1CCOc2cc(F)ccc2C1	0	0
56	**10**{*10*}	**11**{*40*}	**8**{*10,40*}	CC(C)n1nnnc1N1CCc2[nH]ncc2C1	0	0
57	**10**{*10*}	**11**{*41*}	**8**{*10,41*}	COc1ccc(CN(C)c2nnnn2C(C)C)cn1	0	0
58	**10**{*10*}	**11**{*42*}	**8**{*10,42*}	CC(C)n1nnnc1N1CCCC(C1)c1nnc2ccccn12	0	0
59	**10**{*10*}	**11**{*43*}	**8**{*10,43*}	CC(C)n1nnnc1N(C)[C@H]1C[C@H](C1)C(N)=O	16	8

60	**10**{*10*}	**11**{*2*}	**8**{*10,2*}	CC(C)n1nnnc1N1CCN(CC1)C(=O)C(=O)NC1CC1	19	18
61	**10**{*10*}	**11**{*44*}	**8**{*10,44*}	CC(C)n1nnnc1N1CCN(CC1)c1cccc2[nH]c(=O)[nH]c12	5	3
62	**10**{*10*}	**11**{*45*}	**8**{*10,45*}	CC(C)n1nnnc1N1CCN(CCc2cnccn2)CC1	16	8
63	**10**{*10*}	**11**{*46*}	**8**{*10,46*}	CC(C)n1nnnc1N(Cc1ccc(C)o1)C1CC1	15	7
64	**10**{*10*}	**11**{*47*}	**8**{*10,47*}	CC(C)n1nnnc1N1CC2(C)C(=O)NC(=O)C2(C)C1	26	13
65	**10**{*10*}	**11**{*1*}	**8**{*10,1*}	CNS(=O)(=O)c1cccc2CN(CCc12)c1nnnn1C(C)C	17	13
66	**10**{*10*}	**11**{*48*}	**8**{*10,48*}	CC(C)n1nnnc1N1CCN(CC1)c1cc(C)ccn1	9	4
67	**10**{*10*}	**11**{*49*}	**8**{*10,49*}	CC(C)n1nnnc1N(C)CCS(C)(=O)=O	11	5
68	**10**{*10*}	**11**{*50*}	**8**{*10,50*}	CC(C)n1nnnc1N1CCCC(CNS(C)(=O)=O)C1	51	29
69	**10**{*10*}	**11**{*51*}	**8**{*10,51*}	CCN(CC1CCOC1)c1nnnn1C(C)C	43	22
70	**10**{*10*}	**11**{*52*}	**8**{*10,52*}	CC(C)n1nnnc1N1CCC(CC1)N1CCCCC1	16	8
71	**10**{*10*}	**11**{*53*}	**8**{*10,53*}	CC(C)n1nnnc1N(C)CCNC(C)=O	19	10
72	**10**{*10*}	**11**{*54*}	**8**{*10,54*}	CC(C)n1nnnc1N1CCN(CC1)C1CCCCC1	0	0
73	**10**{*10*}	**11**{*55*}	**8**{*10,55*}	CC(C)n1nnnc1N(C)Cc1nccn1C	0	0
74	**10**{*10*}	**11**{*56*}	**8**{*10,56*}	CC(C)n1nnnc1N1CCCC(C1)c1ccnn1C	0	0
75	**10**{*11*}	**11**{*2*}	**8**{*11,2*}	CC(=C)Cn1nnnc1N1CCN(CC1)C(=O)C(=O)NC1CC1	17	19
76	**10**{*11*}	**11**{*12*}	**8**{*11,12*}	CC(=C)Cn1nnnc1N1CCCC(C1)c1nncn1C	0	0
77	**10**{*12*}	**11**{*6*}	**8**{*12,6*}	CCOCCCn1nnnc1N1CCOc2cc(F)ccc2C1	29	27
78	**10**{*12*}	**11**{*8*}	**8**{*12,8*}	CCOCCCn1nnnc1N1CC2(CCOCC2)[1C@@H]2CCC[1C@H]12	9	10
79	**10**{*12*}	**11**{*7*}	**8**{*12,7*}	CCOCCCn1nnnc1N1CCC(C)=C(C)C1	11	12
80	**10**{*12*}	**11**{*10*}	**8**{*12,10*}	CCOCCCn1nnnc1N1CCN(CC1)C(=O)c1cccn1C	0	0

81	**10**{*13*}	**11**{*57*}	**8**{*13,57*}	COc1ccc(CCn2nnnc2N2CCCc3n[nH]cc23)cc1	5	3
82	**10**{*13*}	**11**{*58*}	**8**{*13,58*}	COc1ccc(CCn2nnnc2N2CC[1C@@H](C)O[1C@@H](C)C2)cc1	34	16
83	**10**{*13*}	**11**{*59*}	**8**{*13,59*}	COc1ccc(CCn2nnnc2N2Cc3ccc(O)cc3C2)cc1	11	5
84	**10**{*13*}	**11**{*60*}	**8**{*13,60*}	COc1ccc(CCn2nnnc2N2C3CCC2CC(=O)NC3)cc1	7	4
85	**10**{*13*}	**11**{*61*}	**8**{*13,61*}	COc1ccc(CCn2nnnc2N2CCC3(C2)CCOCC3)cc1	48	22
86	**10**{*13*}	**11**{*62*}	**8**{*13,62*}	COc1ccc(CCn2nnnc2N2C3CCC2C=CC3)cc1	30	16
87	**10**{*13*}	**11**{*63*}	**8**{*13,63*}	COc1ccc(CCn2nnnc2N2CCN3C(CNC3=O)C2)cc1	10	4
88	**10**{*13*}	**11**{*17*}	**8**{*13,17*}	COCCCN(CCOC)c1nnnn1CCc1ccc(OC)cc1	8	8
89	**10**{*13*}	**11**{*64*}	**8**{*13,64*}	COc1ccc(CCn2nnnc2N2CCOCC(F)(F)C2)cc1	0	0
90	**10**{*13*}	**11**{*65*}	**8**{*13,65*}	COc1ccc(CCn2nnnc2N2CCC=C(F)C2)cc1	0	0
91	**10**{*13*}	**11**{*66*}	**8**{*13,66*}	COc1ccc(CCn2nnnc2N2CC3C4OC(C=C4)C3C2)cc1	0	0
92	**10**{*13*}	**11**{*13*}	**8**{*13,13*}	COc1ccc(CCn2nnnc2N2CCCC2C2CCCO2)cc1	0	0
93	**10**{*13*}	**11**{*67*}	**8**{*13,67*}	COc1ccc(CCn2nnnc2N2C3CCC2C(CO)C3)cc1	0	0
94	**10**{*14*}	**11**{*8*}	**8**{*14,8*}	CCCn1nnnc1N1CC2(CCOCC2)[1C@@H]2CCC[1C@H]12	0	0
95	**10**{*14*}	**11**{*7*}	**8**{*14,7*}	CCCn1nnnc1N1CCC(C)=C(C)C1	0	0
96	**10**{*14*}	**11**{*12*}	**8**{*14,12*}	CCCn1nnnc1N1CCCC(C1)c1nncn1C	4	4
97	**10**{*14*}	**11**{*2*}	**8**{*14,2*}	CCCn1nnnc1N1CCN(CC1)C(=O)C(=O)NC1CC1	30	32
98	**10**{*15*}	**11**{*68*}	**8**{*15,68*}	C1CC1n1nnnc1N1CCCC(C1)c1ccn[nH]1	0	0
99	**10**{*15*}	**11**{*1*}	**8**{*15,1*}	CNS(=O)(=O)c1cccc2CN(CCc12)c1nnnn1C1CC1	8	10
100	**10**{*15*}	**11**{*69*}	**8**{*15,69*}	CN(CC(C)(C)CO)c1nnnn1C1CC1	10	5
101	**10**{*15*}	**11**{*70*}	**8**{*15,70*}	COc1cccc(c1)C1CCN(CC1)c1nnnn1C1CC1	13	6

102	**10**{*15*}	**11**{*7*}	**8**{*15,7*}	CC1=C(C)CN(CC1)c1nnnn1C1CC1	36	30
103	**10**{*15*}	**11**{*2*}	**8**{*15,2*}	O=C(NC1CC1)C(=O)N1CCN(CC1)c1nnnn1C1CC1	20	22
104	**10**{*15*}	**11**{*8*}	**8**{*15,8*}	C1CC1n1nnnc1N1CC2(CCOCC2)[1C@@H]2CCC[1C@H]12	66	81
105	**10**{*15*}	**11**{*71*}	**8**{*15,71*}	CCn1cc(CN(C)c2nnnn2C2CC2)cn1	62	31
106	**10**{*15*}	**11**{*72*}	**8**{*15,72*}	CCN(Cc1ccoc1)c1nnnn1C1CC1	87	42
107	**10**{*16*}	**11**{*73*}	**8**{*16,73*}	COCC(C)n1nnnc1N1CCc2cn[nH]c2C1	0	0
108	**10**{*16*}	**11**{*74*}	**8**{*16,74*}	COCC(C)n1nnnc1N1CCN(CC1)c1nc(C)c(C)s1	0	0
109	**10**{*16*}	**11**{*75*}	**8**{*16,75*}	COCC(C)n1nnnc1N1CCN(CC1)C(=O)c1cccc(O)c1	7	3
110	**10**{*16*}	**11**{*76*}	**8**{*16,76*}	COCC(C)n1nnnc1N1CCn2ccnc12	8	4
111	**10**{*16*}	**11**{*77*}	**8**{*16,77*}	COCC(C)n1nnnc1N1CCc2nc(ncc2C1)C1CC1	17	9
112	**10**{*16*}	**11**{*48*}	**8**{*16,48*}	COCC(C)n1nnnc1N1CCN(CC1)c1cc(C)ccn1	8	4
113	**10**{*16*}	**11**{*78*}	**8**{*16,78*}	COCC(C)n1nnnc1N1CCCc2cc(OC)ccc2C1	0	0
114	**10**{*16*}	**11**{*79*}	**8**{*16,79*}	COCC(C)n1nnnc1N1CCC[C@@H]1C(N)=O	0	0
115	**10**{*17*}	**11**{*15*}	**8**{*17,15*}	COC1(CCN(CC1)c1nnnn1C1CC2CCC1C2)C(F)(F)F	29	35
116	**10**{*17*}	**11**{*80*}	**8**{*17,80*}	C(OC1CCN(CC1)c1nnnn1C1CC2CCC1C2)C1CCCO1	33	40
117	**10**{*18*}	**11**{*81*}	**8**{*18,81*}	NC(=O)C1CN(CCO1)c1nnnn1CCSc1ccccc1	0	0
118	**10**{*19*}	**11**{*36*}	**8**{*19,36*}	O[C@H]1CCN(C1)c1nnnn1Cc1cccnc1	0	0
119	**10**{*19*}	**11**{*82*}	**8**{*19,82*}	C(c1cccnc1)n1nnnc1N1CCC2(CCCC2)C1	0	0
120	**10**{*19*}	**11**{*83*}	**8**{*19,83*}	CN(C1CCCc2nc(C)sc12)c1nnnn1Cc1cccnc1	0	0
121	**10**{*19*}	**11**{*84*}	**8**{*19,84*}	CN(CC(=O)N1CCCC1)c1nnnn1Cc1cccnc1	0	0
122	**10**{*19*}	**11**{*85*}	**8**{*19,85*}	Fc1cccc(c1)N1CCN(CC1)c1nnnn1Cc1cccnc1	0	0

123	**10**{*19*}	**11**{*86*}	**8**{*19,86*}	OCC1CCCCCN1c1nnnn1Cc1cccnc1	0	0
124	**10**{*19*}	**11**{*87*}	**8**{*19,87*}	CN(Cc1ccoc1C)c1nnnn1Cc1cccnc1	0	0
125	**10**{*19*}	**11**{*88*}	**8**{*19,88*}	C(C1CCOCC1)N1CCN(CC1)c1nnnn1Cc1cccnc1	0	0
126	**10**{*19*}	**11**{*78*}	**8**{*19,78*}	COc1ccc2CN(CCCc2c1)c1nnnn1Cc1cccnc1	0	0
127	**10**{*19*}	**11**{*89*}	**8**{*19,89*}	CC(N(C)c1nnnn1Cc1cccnc1)c1ccccn1	0	0
128	**10**{*19*}	**11**{*90*}	**8**{*19,90*}	C(N1CCN(CC1)c1nnnn1Cc1cccnc1)c1cscn1	0	0
129	**10**{*19*}	**11**{*91*}	**8**{*19,91*}	CC1N(CCOc2ccccc12)c1nnnn1Cc1cccnc1	0	0
130	**10**{*19*}	**11**{*92*}	**8**{*19,92*}	C(c1cccnc1)n1nnnc1N1CCCC(C1)c1ccccc1	0	0
131	**10**{*19*}	**11**{*93*}	**8**{*19,93*}	C(C1CCCCC1)N1CCN(CC1)c1nnnn1Cc1cccnc1	0	0
132	**10**{*19*}	**11**{*94*}	**8**{*19,94*}	CN(c1nnnn1Cc1cccnc1)c1c(C)noc1C	0	0
133	**10**{*19*}	**11**{*95*}	**8**{*19,95*}	CC(N(C)c1nnnn1Cc1cccnc1)c1sc(C)nc1C	0	0
134	**10**{*19*}	**11**{*96*}	**8**{*19,96*}	CC(C)OC1CCN(CC1)c1nnnn1Cc1cccnc1	0	0
135	**10**{*19*}	**11**{*97*}	**8**{*19,97*}	O=C(NC1CC1)C1CCCN1c1nnnn1Cc1cccnc1	0	0
136	**10**{*19*}	**11**{*98*}	**8**{*19,98*}	CC(N(C)c1nnnn1Cc1cccnc1)c1ccco1	0	0
137	**10**{*19*}	**11**{*99*}	**8**{*19,99*}	C(c1cccnc1)n1nnnc1N1CCn2cncc2C1	0	0
138	**10**{*19*}	**11**{*100*}	**8**{*19,100*}	O=S1CCN(CC1)c1nnnn1Cc1cccnc1	0	0
139	**10**{*19*}	**11**{*101*}	**8**{*19,101*}	CN(Cc1ccc(C)s1)c1nnnn1Cc1cccnc1	0	0
140	**10**{*19*}	**11**{*102*}	**8**{*19,102*}	CN(Cc1scnc1C)c1nnnn1Cc1cccnc1	0	0
141	**10**{*19*}	**11**{*103*}	**8**{*19,103*}	Cc1ccc2[nH]c3CCN(Cc3c2c1)c1nnnn1Cc1cccnc1	0	0
142	**10**{*20*}	**11**{*79*}	**8**{*20,79*}	CCN1CCCC1Cn1nnnc1N1CCC[C@@H]1C(N)=O	0	0
143	**10**{*20*}	**11**{*104*}	**8**{*20,104*}	CCN1CCCC1Cn1nnnc1N1CCOCC2(CCCC2)C1	0	0

144	**10**{*20*}	**11**{*105*}	**8**{*20,105*}	CCN1CCCC1Cn1nnnc1N1CCN(C)c2ccccc2C1	0	0
145	**10**{*20*}	**11**{*38*}	**8**{*20,38*}	CCN1CCCC1Cn1nnnc1N1CCc2nc[nH]c2C1	0	0
146	**10**{*20*}	**11**{*106*}	**8**{*20,106*}	CCN1CCCC1Cn1nnnc1N1CCc2ccccc2CC1	0	0
147	**10**{*20*}	**11**{*40*}	**8**{*20,40*}	CCN1CCCC1Cn1nnnc1N1CCc2[nH]ncc2C1	0	0
148	**10**{*20*}	**11**{*107*}	**8**{*20,107*}	CCN1CCCC1Cn1nnnc1N1CCc2c(F)ccc(F)c2C1	0	0
149	**10**{*20*}	**11**{*108*}	**8**{*20,108*}	CCN1CCCC1Cn1nnnc1N1CCC(CC1)N1CCCC1=O	0	0
150	**10**{*20*}	**11**{*109*}	**8**{*20,109*}	CCN1CCCC1Cn1nnnc1N1CCc2nn(C)c(=O)cc2C1	0	0
151	**10**{*21*}	**11**{*110*}	**8**{*21,110*}	CN(CC1(O)CCOCC1)c1nnnn1C(C)(C)C	0	0
152	**10**{*21*}	**11**{*111*}	**8**{*21,111*}	CC1CN(CC(C)S1(=O)=O)c1nnnn1C(C)(C)C	0	0
153	**10**{*21*}	**11**{*112*}	**8**{*21,112*}	CCOC1(C)CCN(CC1)c1nnnn1C(C)(C)C	0	0
154	**10**{*21*}	**11**{*113*}	**8**{*21,113*}	CC(C)(C)n1nnnc1N1CN(CC(F)(F)F)C(=O)C1	0	0
155	**10**{*21*}	**11**{*114*}	**8**{*21,114*}	CC(C)(C)n1nnnc1N1CCCC(CC1)S(C)(=O)=O	0	0
156	**10**{*21*}	**11**{*115*}	**8**{*21,115*}	CC(C)(C)n1nnnc1N1CCC2(C1)C(=O)Nc1ccccc21	28	13
157	**10**{*21*}	**11**{*116*}	**8**{*21,116*}	CC(C)(C)n1nnnc1N1C[1C@@H]2CC[1C@H](O)C[1C@@H]2C1	31	16
158	**10**{*21*}	**11**{*117*}	**8**{*21,117*}	CC(C)(C)n1nnnc1N1CCCC(CC(C)(C)C(N)=O)C1	8	4
159	**10**{*21*}	**11**{*118*}	**8**{*21,118*}	C[1C@@H]1[1C@H](O)CCN1c1nnnn1C(C)(C)C	38	19
160	**10**{*21*}	**11**{*119*}	**8**{*21,119*}	CCN(C1CCNC1=O)c1nnnn1C(C)(C)C	0	0
161	**10**{*21*}	**11**{*120*}	**8**{*21,120*}	CN1CCN(CC1CO)c1nnnn1C(C)(C)C	0	0
162	**10**{*21*}	**11**{*121*}	**8**{*21,121*}	Cc1nnc(N2CCN(CC2)c2nnnn2C(C)(C)C)n1C	0	0
163	**10**{*21*}	**11**{*122*}	**8**{*21,122*}	CCN(CCO)c1nnnn1C(C)(C)C	0	0
164	**10**{*21*}	**11**{*123*}	**8**{*21,123*}	CC(C)(C)C1CN(CCO1)c1nnnn1C(C)(C)C	0	0

165	**10**{*21*}	**11**{*124*}	**8**{*21,124*}	Cc1cc(=O)[nH]c(n1)N1CCN(CC1)c1nnnn1C(C)(C)C	0	0
166	**10**{*22*}	**11**{*12*}	**8**{*22,12*}	Cn1cnnc1C1CCCN(C1)c1nnnn1C1CCCC1	0	0
167	**10**{*22*}	**11**{*2*}	**8**{*22,2*}	O=C(NC1CC1)C(=O)N1CCN(CC1)c1nnnn1C1CCCC1	24	22
168	**10**{*22*}	**11**{*10*}	**8**{*22,10*}	Cn1cccc1C(=O)N1CCN(CC1)c1nnnn1C1CCCC1	9	10
169	**10**{*22*}	**11**{*100*}	**8**{*22,100*}	O=S1CCN(CC1)c1nnnn1C1CCCC1	0	0
170	**10**{*23*}	**11**{*38*}	**8**{*23,38*}	CC(c1ccccc1)n1nnnc1N1CCc2nc[nH]c2C1	0	0
171	**10**{*23*}	**11**{*125*}	**8**{*23,125*}	CC(c1ccccc1)n1nnnc1N(C)CC1(O)CCCC1	0	0
172	**10**{*23*}	**11**{*94*}	**8**{*23,94*}	CC(c1ccccc1)n1nnnc1N(C)c1c(C)noc1C	33	18
173	**10**{*23*}	**11**{*126*}	**8**{*23,126*}	CC(c1ccccc1)n1nnnc1N1CCN(Cc2nc[nH]n2)CC1	21	11
174	**10**{*23*}	**11**{*108*}	**8**{*23,108*}	CC(c1ccccc1)n1nnnc1N1CCC(CC1)N1CCCC1=O	45	22
175	**10**{*23*}	**11**{*99*}	**8**{*23,99*}	CC(c1ccccc1)n1nnnc1N1CCn2cncc2C1	0	0
176	**10**{*23*}	**11**{*127*}	**8**{*23,127*}	CC(c1ccccc1)n1nnnc1N1CCC[C@H]1C(N)=O	0	0
177	**10**{*24*}	**11**{*12*}	**8**{*24,12*}	CCC(C)n1nnnc1N1CCCC(C1)c1nncn1C	0	0
178	**10**{*25*}	**11**{*8*}	**8**{*25,8*}	C(C1CC1)n1nnnc1N1CC2(CCOCC2)[1C@@H]2CCC[1C@H]12	0	0
179	**10**{*25*}	**11**{*1*}	**8**{*25,1*}	CNS(=O)(=O)c1cccc2CN(CCc12)c1nnnn1CC1CC1	26	24
180	**10**{*26*}	**11**{*7*}	**8**{*26,7*}	CC1=C(C)CN(CC1)c1nnnn1CC(F)(F)F	0	0
181	**10**{*26*}	**11**{*4*}	**8**{*26,4*}	FC(F)(F)Cn1nnnc1N1CCOC2(CCC2)C1	0	0
182	**10**{*26*}	**11**{*10*}	**8**{*26,10*}	Cn1cccc1C(=O)N1CCN(CC1)c1nnnn1CC(F)(F)F	0	0
183	**10**{*26*}	**11**{*5*}	**8**{*26,5*}	Fc1cc(F)cc(c1)C1COCCN1c1nnnn1CC(F)(F)F	0	0
184	**10**{*26*}	**11**{*6*}	**8**{*26,6*}	Fc1ccc2CN(CCOc2c1)c1nnnn1CC(F)(F)F	0	0
185	**10**{*26*}	**11**{*8*}	**8**{*26,8*}	FC(F)(F)Cn1nnnc1N1CC2(CCOCC2)[1C@@H]2CCC[1C@H]12	27	29

186	**10**{*27*}	**11**{*128*}	**8**{*27,128*}	CCOC(=O)N1CCC(CC1)n1nnnc1N1CCCC(C1)C1CC1	13	15
187	**10**{*27*}	**11**{*7*}	**8**{*27,7*}	CCOC(=O)N1CCC(CC1)n1nnnc1N1CCC(C)=C(C)C1	0	0
188	**10**{*28*}	**11**{*129*}	**8**{*28,129*}	C[C@@H](O)CN(C)c1nnnn1C(C)c1ccc(Br)cc1	13	7
189	**10**{*29*}	**11**{*130*}	**8**{*29,130*}	CCC1CCCN1c1nnnn1C1CCN(Cc2ccccc2)CC1	21	11
190	**10**{*30*}	**11**{*36*}	**8**{*30,36*}	O[C@H]1CCN(C1)c1nnnn1CCc1ccc(Cl)cc1Cl	24	12
191	**10**{*30*}	**11**{*131*}	**8**{*30,131*}	OCC1C=CCN1c1nnnn1CCc1ccc(Cl)cc1Cl	0	0
192	**10**{*31*}	**11**{*7*}	**8**{*31,7*}	CCOCCn1nnnc1N1CCC(C)=C(C)C1	0	0
193	**10**{*32*}	**11**{*132*}	**8**{*32,132*}	CC(C)(C)C1=CCN(CC1)c1nnnn1CCc1ccccn1	0	0
194	**10**{*32*}	**11**{*133*}	**8**{*32,133*}	CC1(C)CCCN1c1nnnn1CCc1ccccn1	16	9
195	**10**{*32*}	**11**{*104*}	**8**{*32,104*}	C(Cn1nnnc1N1CCOCC2(CCCC2)C1)c1ccccn1	0	0
196	**10**{*32*}	**11**{*134*}	**8**{*32,134*}	CN(C)C(=O)NC1CCCN(C1)c1nnnn1CCc1ccccn1	0	0
197	**10**{*32*}	**11**{*135*}	**8**{*32,135*}	FC(F)(F)[C@@H]1CCCN(C1)c1nnnn1CCc1ccccn1	0	0
198	**10**{*32*}	**11**{*136*}	**8**{*32,136*}	CC(C)NC(=O)[C@@H]1CCCN(C1)c1nnnn1CCc1ccccn1	0	0
199	**10**{*32*}	**11**{*137*}	**8**{*32,137*}	CCN1CCC2CCC(C1)N2c1nnnn1CCc1ccccn1	0	0
200	**10**{*32*}	**11**{*99*}	**8**{*32,99*}	C(Cn1nnnc1N1CCn2cncc2C1)c1ccccn1	0	0
201	**10**{*32*}	**11**{*116*}	**8**{*32,116*}	O[1C@@H]1CC[1C@@H]2CN(C[1C@@H]2C1)c1nnnn1CCc1ccccn1	0	0
202	**10**{*32*}	**11**{*138*}	**8**{*32,138*}	Clc1cccc2CCN(Cc12)c1nnnn1CCc1ccccn1	0	0
203	**10**{*32*}	**11**{*139*}	**8**{*32,139*}	Fc1cccc2CCN(c3nnnn3CCc3ccccn3)c12	0	0
204	**10**{*32*}	**11**{*140*}	**8**{*32,140*}	CN(c1cnn(C)c1)c1nnnn1CCc1ccccn1	0	0
205	**10**{*32*}	**11**{*141*}	**8**{*32,141*}	O=C1CC2(CN1)CCN(CC2)c1nnnn1CCc1ccccn1	0	0
206	**10**{*32*}	**11**{*142*}	**8**{*32,142*}	C(Cn1nnnc1N1CCC(CC1)c1cn[nH]c1)c1ccccn1	0	0

207	**10**{*32*}	**11**{*143*}	**8**{*32,143*}	CN(c1ccn(C)n1)c1nnnn1CCc1ccccn1	0	0
208	**10**{*32*}	**11**{*144*}	**8**{*32,144*}	C(Cn1nnnc1N1CCN2CCOCC2C1)c1ccccn1	0	0
209	**10**{*32*}	**11**{*145*}	**8**{*32,145*}	Cc1cccc2CCN(Cc12)c1nnnn1CCc1ccccn1	0	0
210	**10**{*32*}	**11**{*4*}	**8**{*32,4*}	C(Cn1nnnc1N1CCOC2(CCC2)C1)c1ccccn1	0	0
211	**10**{*32*}	**11**{*146*}	**8**{*32,146*}	C(Cn1nnnc1N1CCCC1c1ccn[nH]1)c1ccccn1	0	0
212	**10**{*32*}	**11**{*147*}	**8**{*32,147*}	Clc1cnn(c1)C1CCN(C1)c1nnnn1CCc1ccccn1	0	0
213	**10**{*32*}	**11**{*148*}	**8**{*32,148*}	Cc1csc(n1)C1CCN(C1)c1nnnn1CCc1ccccn1	0	0
214	**10**{*32*}	**11**{*149*}	**8**{*32,149*}	C(Cn1nnnc1N1CCCC1c1ccncc1)c1ccccn1	0	0
215	**10**{*33*}	**11**{*150*}	**8**{*33,150*}	CC1CN(CC(=O)N1)c1nnnn1Cc1cccc(c1)C(F)(F)F	19	9
216	**10**{*33*}	**11**{*143*}	**8**{*33,143*}	CN(c1ccn(C)n1)c1nnnn1Cc1cccc(c1)C(F)(F)F	0	0
217	**10**{*33*}	**11**{*99*}	**8**{*33,99*}	FC(F)(F)c1cccc(Cn2nnnc2N2CCn3cncc3C2)c1	0	0
218	**10**{*33*}	**11**{*140*}	**8**{*33,140*}	CN(c1cnn(C)c1)c1nnnn1Cc1cccc(c1)C(F)(F)F	0	0
219	**10**{*33*}	**11**{*73*}	**8**{*33,73*}	FC(F)(F)c1cccc(Cn2nnnc2N2CCc3cn[nH]c3C2)c1	0	0
220	**10**{*34*}	**11**{*151*}	**8**{*34,151*}	CC1COCCN(C1)c1nnnn1CCc1ccc2OCCOc2c1	24	11
221	**10**{*34*}	**11**{*152*}	**8**{*34,152*}	FC1CCN(CC1)c1nnnn1CCc1ccc2OCCOc2c1	21	11
222	**10**{*34*}	**11**{*153*}	**8**{*34,153*}	CN(C)C1CCN(C1)c1nnnn1CCc1ccc2OCCOc2c1	0	0
223	**10**{*35*}	**11**{*154*}	**8**{*35,154*}	CS(=O)(=O)NCCn1nnnc1N1CCC(F)(CC1)C1CC1	0	0
224	**10**{*35*}	**11**{*155*}	**8**{*35,155*}	CS(=O)(=O)NCCn1nnnc1N1CCc2c1cccc2Cl	10	4
225	**10**{*35*}	**11**{*156*}	**8**{*35,156*}	CS(=O)(=O)NCCn1nnnc1N1CCC[C@@H](C1)C(F)(F)F	0	0
226	**10**{*35*}	**11**{*157*}	**8**{*35,157*}	CC1(F)CCCN(C1)c1nnnn1CCNS(C)(=O)=O	0	0
227	**10**{*35*}	**11**{*158*}	**8**{*35,158*}	CS(=O)(=O)NCCn1nnnc1N1CCC(CC1)C(F)F	0	0

228	**10**{*35*}	**11**{*159*}	**8**{*35,159*}	CS(=O)(=O)NCCn1nnnc1N1CCc2c1cccc2F	0	0
229	**10**{*35*}	**11**{*133*}	**8**{*35,133*}	CC1(C)CCCN1c1nnnn1CCNS(C)(=O)=O	0	0
230	**10**{*35*}	**11**{*160*}	**8**{*35,160*}	CS(=O)(=O)NCCn1nnnc1N1CCC2(CCCC2)CC1	0	0
231	**10**{*36*}	**11**{*161*}	**8**{*36,161*}	CC(N(C)c1nnnn1CC1CCC1)c1cccnc1	0	0
232	**10**{*36*}	**11**{*162*}	**8**{*36,162*}	C(C1CCC1)n1nnnc1N1CCCC(C1)c1nnc2CCCn12	0	0
233	**10**{*36*}	**11**{*163*}	**8**{*36,163*}	Cc1cccc(n1)C1CCCN1c1nnnn1CC1CCC1	15	7
234	**10**{*36*}	**11**{*164*}	**8**{*36,164*}	C(C1CCC1)n1nnnc1N1CC[C@H](C1)Oc1ccccc1	117	64
235	**10**{*36*}	**11**{*165*}	**8**{*36,165*}	C(C1CCN(CC1)c1nnnn1CC1CCC1)N1CCOCC1	53	28
236	**10**{*36*}	**11**{*94*}	**8**{*36,94*}	CN(c1nnnn1CC1CCC1)c1c(C)noc1C	15	8
237	**10**{*37*}	**11**{*166*}	**8**{*37,166*}	OC1CCOC2(CCN(CC2)c2nnnn2CCc2cccnc2)C1	0	0
238	**10**{*37*}	**11**{*59*}	**8**{*37,59*}	Oc1ccc2CN(Cc2c1)c1nnnn1CCc1cccnc1	0	0
239	**10**{*37*}	**11**{*167*}	**8**{*37,167*}	C(Cn1nnnc1N1CCCC1c1ncccn1)c1cccnc1	0	0
240	**10**{*37*}	**11**{*168*}	**8**{*37,168*}	C(Cn1nnnc1N1CCOC(C1)c1ccco1)c1cccnc1	0	0
241	**10**{*37*}	**11**{*169*}	**8**{*37,169*}	C(Cn1nnnc1N1CCC2(CCC2)C1)c1cccnc1	7	4
242	**10**{*37*}	**11**{*64*}	**8**{*37,64*}	FC1(F)COCCN(C1)c1nnnn1CCc1cccnc1	0	0
243	**10**{*37*}	**11**{*104*}	**8**{*37,104*}	C(Cn1nnnc1N1CCOCC2(CCCC2)C1)c1cccnc1	0	0
244	**10**{*37*}	**11**{*170*}	**8**{*37,170*}	C(Cn1nnnc1N1CCCC(C1)C1CCOCC1)c1cccnc1	0	0
245	**10**{*37*}	**11**{*171*}	**8**{*37,171*}	C(Cn1nnnc1N1CCC(C1)n1cccn1)c1cccnc1	0	0
246	**10**{*37*}	**11**{*135*}	**8**{*37,135*}	FC(F)(F)[C@@H]1CCCN(C1)c1nnnn1CCc1cccnc1	0	0
247	**10**{*37*}	**11**{*172*}	**8**{*37,172*}	COC1CCCN(CC1)c1nnnn1CCc1cccnc1	0	0
248	**10**{*37*}	**11**{*109*}	**8**{*37,109*}	Cn1nc2CCN(Cc2cc1=O)c1nnnn1CCc1cccnc1	0	0

249	**10**{*37*}	**11**{*173*}	**8**{*37,173*}	O=C1CN(CCCN1)c1nnnn1CCc1cccnc1	0	0
250	**10**{*37*}	**11**{*174*}	**8**{*37,174*}	FC(F)[C@@H]1CCCN1c1nnnn1CCc1cccnc1	0	0
251	**10**{*37*}	**11**{*175*}	**8**{*37,175*}	Cn1ccc(n1)C1CCCN(C1)c1nnnn1CCc1cccnc1	0	0
252	**10**{*38*}	**11**{*176*}	**8**{*38,176*}	CC(c1cccs1)n1nnnc1N(C)Cc1cnc(C)s1	0	0
253	**10**{*38*}	**11**{*177*}	**8**{*38,177*}	CC(C)C(=O)N1CCCN(CC1)c1nnnn1C(C)c1cccs1	0	0
254	**10**{*38*}	**11**{*178*}	**8**{*38,178*}	CC(c1cccs1)n1nnnc1N(C)Cc1ccoc1	0	0
255	**10**{*38*}	**11**{*142*}	**8**{*38,142*}	CC(c1cccs1)n1nnnc1N1CCC(CC1)c1cn[nH]c1	0	0
256	**10**{*38*}	**11**{*179*}	**8**{*38,179*}	CC(c1cccs1)n1nnnc1N1C[C@H]2[C@H](CO)[C@H]2C1	0	0
257	**10**{*38*}	**11**{*84*}	**8**{*38,84*}	CC(c1cccs1)n1nnnc1N(C)CC(=O)N1CCCC1	0	0
258	**10**{*39*}	**11**{*7*}	**8**{*39,7*}	CC1=C(C)CN(CC1)c1nnnn1CCS(C)(=O)=O	0	0
259	**10**{*39*}	**11**{*180*}	**8**{*39,180*}	CC(N(C)c1nnnn1CCS(C)(=O)=O)c1cccc(Cl)c1	0	0
260	**10**{*39*}	**11**{*181*}	**8**{*39,181*}	CN(c1nnnn1CCS(C)(=O)=O)c1cccc(C)c1	0	0
261	**10**{*39*}	**11**{*182*}	**8**{*39,182*}	CN(Cc1ccc(C)c(C)c1)c1nnnn1CCS(C)(=O)=O	0	0
262	**10**{*39*}	**11**{*183*}	**8**{*39,183*}	CC1(Cc2ccccc2)CCCN1c1nnnn1CCS(C)(=O)=O	0	0
263	**10**{*39*}	**11**{*6*}	**8**{*39,6*}	CS(=O)(=O)CCn1nnnc1N1CCOc2cc(F)ccc2C1	0	0
264	**10**{*40*}	**11**{*184*}	**8**{*40,184*}	COC1(CCCN(C1)c1nnnn1C1CCOCC1)C(F)(F)F	0	0
265	**10**{*40*}	**11**{*185*}	**8**{*40,185*}	CC1(C)CN(C1c1cccnc1)c1nnnn1C1CCOCC1	0	0
266	**10**{*40*}	**11**{*186*}	**8**{*40,186*}	CCn1ccc(CN(C)c2nnnn2C2CCOCC2)c1	0	0
267	**10**{*40*}	**11**{*187*}	**8**{*40,187*}	OC1(CCN(C1)c1nnnn1C1CCOCC1)C1CC1	32	16
268	**10**{*40*}	**11**{*188*}	**8**{*40,188*}	CCOC1CC2(C1)CCN(C2)c1nnnn1C1CCOCC1	112	57
269	**10**{*40*}	**11**{*189*}	**8**{*40,189*}	Cc1cccc(C2CCCN2c2nnnn2C2CCOCC2)c1C	66	31

270	**10**{*40*}	**11**{*115*}	**8**{*40,115*}	O=C1Nc2ccccc2C11CCN(C1)c1nnnn1C1CCOCC1	27	13
271	**10**{*40*}	**11**{*190*}	**8**{*40,190*}	CC1(C)CN(Cc2ccccc2O1)c1nnnn1C1CCOCC1	41	21
272	**10**{*40*}	**11**{*191*}	**8**{*40,191*}	CC1(C)CN(CC(O1)C(F)(F)F)c1nnnn1C1CCOCC1	35	16
273	**10**{*40*}	**11**{*192*}	**8**{*40,192*}	CN(Cc1cccc(C)n1)c1nnnn1C1CCOCC1	84	41
274	**10**{*40*}	**11**{*193*}	**8**{*40,193*}	COc1ccccc1C1CCN(C1)c1nnnn1C1CCOCC1	45	22
275	**10**{*40*}	**11**{*194*}	**8**{*40,194*}	O=S1(=O)CCN(Cc2ccccc12)c1nnnn1C1CCOCC1	113	54
276	**10**{*40*}	**11**{*195*}	**8**{*40,195*}	CCS(=O)(=O)C1CN(C1)c1nnnn1C1CCOCC1	18	9
277	**10**{*40*}	**11**{*196*}	**8**{*40,196*}	CC(C)Oc1ccc(cc1)N(C)c1nnnn1C1CCOCC1	0	0
278	**10**{*40*}	**11**{*197*}	**8**{*40,197*}	CC1CN(c2nnnn2C2CCOCC2)C(C)(C)C1	0	0
279	**10**{*40*}	**11**{*198*}	**8**{*40,198*}	CC(C)c1cc([nH]n1)C1CCCN(C1)c1nnnn1C1CCOCC1	0	0
280	**10**{*40*}	**11**{*199*}	**8**{*40,199*}	CN(Cc1nnc2CCCn12)c1nnnn1C1CCOCC1	0	0
281	**10**{*40*}	**11**{*143*}	**8**{*40,143*}	CN(c1ccn(C)n1)c1nnnn1C1CCOCC1	0	0
282	**10**{*40*}	**11**{*200*}	**8**{*40,200*}	CN(Cc1cc2ccccc2[nH]1)c1nnnn1C1CCOCC1	0	0
283	**10**{*40*}	**11**{*201*}	**8**{*40,201*}	CC1CN(c2nnnn2C2CCOCC2)c2ccccc2O1	0	0
284	**10**{*40*}	**11**{*202*}	**8**{*40,202*}	C1CC1c1nc(n[nH]1)C1CCCN(C1)c1nnnn1C1CCOCC1	0	0
285	**10**{*40*}	**11**{*203*}	**8**{*40,203*}	Cc1nc([nH]c1C)C1CCN(CC1)c1nnnn1C1CCOCC1	0	0
286	**10**{*40*}	**11**{*204*}	**8**{*40,204*}	CN(CC1(O)CCC1)c1nnnn1C1CCOCC1	0	0
287	**10**{*41*}	**11**{*205*}	**8**{*41,205*}	OC1CCN(CC1(F)F)c1nnnn1CCc1cccs1	0	0
288	**10**{*41*}	**11**{*206*}	**8**{*41,206*}	CC1(C)CN(C1c1ccncc1)c1nnnn1CCc1cccs1	0	0
289	**10**{*41*}	**11**{*207*}	**8**{*41,207*}	C(Cn1nnnc1N1CCC(CC1)n1cccn1)c1cccs1	0	0
290	**10**{*41*}	**11**{*208*}	**8**{*41,208*}	C(Cn1nnnc1N1CCN(CC1)C1CCOCC1)c1cccs1	36	16

291	**10**{*41*}	**11**{*147*}	**8**{*41,147*}	Clc1cnn(c1)C1CCN(C1)c1nnnn1CCc1cccs1	70	32
292	**10**{*41*}	**11**{*148*}	**8**{*41,148*}	Cc1csc(n1)C1CCN(C1)c1nnnn1CCc1cccs1	62	28
293	**10**{*41*}	**11**{*209*}	**8**{*41,209*}	CO[1C@@H]1CN(C[1C@H]1O)c1nnnn1CCc1cccs1	48	23
294	**10**{*41*}	**11**{*210*}	**8**{*41,210*}	Oc1cccc2CN(CCc12)c1nnnn1CCc1cccs1	71	36
295	**10**{*41*}	**11**{*211*}	**8**{*41,211*}	C(Cn1nnnc1N1CCC(CC1)c1ccco1)c1cccs1	40	20
296	**10**{*41*}	**11**{*212*}	**8**{*41,212*}	FC(F)(F)C1CCN(CCO1)c1nnnn1CCc1cccs1	41	22
297	**10**{*41*}	**11**{*213*}	**8**{*41,213*}	CNC(=O)NC1CCN(CC1)c1nnnn1CCc1cccs1	46	22
298	**10**{*41*}	**11**{*214*}	**8**{*41,214*}	C(Cn1nnnc1N1CCC(CC1)C1CCCCO1)c1cccs1	54	28
299	**10**{*41*}	**11**{*215*}	**8**{*41,215*}	CCS(=O)(=O)CC(C)N(C)c1nnnn1CCc1cccs1	14	16
300	**10**{*41*}	**11**{*216*}	**8**{*41,216*}	CN([1C@@H]1CCC[1C@H]1O)c1nnnn1CCc1cccs1	18	9
301	**10**{*41*}	**11**{*217*}	**8**{*41,217*}	Oc1ccc2CN(CCOc2c1)c1nnnn1CCc1cccs1	37	20
302	**10**{*41*}	**11**{*218*}	**8**{*41,218*}	Cc1cncc(c1)C1CCCN1c1nnnn1CCc1cccs1	0	0
303	**10**{*41*}	**11**{*16*}	**8**{*41,16*}	O=C1NCCN1C1CCCN(C1)c1nnnn1CCc1cccs1	0	0
304	**10**{*41*}	**11**{*219*}	**8**{*41,219*}	C(Cn1nnnc1N1CCN(CC1)c1cccs1)c1cccs1	0	0
305	**10**{*41*}	**11**{*146*}	**8**{*41,146*}	C(Cn1nnnc1N1CCCC1c1ccn[nH]1)c1cccs1	0	0
306	**10**{*41*}	**11**{*220*}	**8**{*41,220*}	CC1CCS(=O)(=O)CCN1c1nnnn1CCc1cccs1	0	0
307	**10**{*41*}	**11**{*68*}	**8**{*41,68*}	C(Cn1nnnc1N1CCCC(C1)c1ccn[nH]1)c1cccs1	0	0
308	**10**{*41*}	**11**{*221*}	**8**{*41,221*}	C(Cn1nnnc1N1CCCC(C1)c1cccnc1)c1cccs1	0	0
309	**10**{*41*}	**11**{*222*}	**8**{*41,222*}	C(Cn1nnnc1N1CCCC(C1)c1ccncc1)c1cccs1	0	0
310	**10**{*42*}	**11**{*223*}	**8**{*42,223*}	CN(Cc1nnc(C)s1)c1nnnn1C1(C)CC1	0	0
311	**10**{*42*}	**11**{*224*}	**8**{*42,224*}	CNC(=O)C(C)CN(C)c1nnnn1C1(C)CC1	0	0

312	**10**{*42*}	**11**{*225*}	**8**{*42,225*}	CC1(CC1)n1nnnc1N1CCN(CC1)S(=O)(=O)C1CC1	10	4
313	**10**{*42*}	**11**{*226*}	**8**{*42,226*}	CC1(CC1)n1nnnc1N1CCC(CC1)C(=O)NCCO	41	19
314	**10**{*42*}	**11**{*227*}	**8**{*42,227*}	COc1ccc(cc1F)C1CCN(C1)c1nnnn1C1(C)CC1	93	46
315	**10**{*42*}	**11**{*228*}	**8**{*42,228*}	CC(C)(O)CN(C1CC1)c1nnnn1C1(C)CC1	4	2
316	**10**{*42*}	**11**{*229*}	**8**{*42,229*}	CC1(CC1)n1nnnc1N1CCC(CO)(C1)c1ccccc1	6	3
317	**10**{*42*}	**11**{*230*}	**8**{*42,230*}	CN(C1CCN(C1)c1nnnn1C1(C)CC1)c1ccccc1	24	13
318	**10**{*42*}	**11**{*193*}	**8**{*42,193*}	COc1ccccc1C1CCN(C1)c1nnnn1C1(C)CC1	51	27
319	**10**{*42*}	**11**{*231*}	**8**{*42,231*}	CC1(CC1)n1nnnc1N1CCC(CC1)OCC(N)=O	83	45
320	**10**{*42*}	**11**{*232*}	**8**{*42,232*}	CCN(Cc1occc1C)c1nnnn1C1(C)CC1	29	15
321	**10**{*42*}	**11**{*233*}	**8**{*42,233*}	CC1(CC1)n1nnnc1N1CCCC1c1cncc(Br)c1	6	3
322	**10**{*42*}	**11**{*234*}	**8**{*42,234*}	CC1(CC1)n1nnnc1N1CCC(CS(C)(=O)=O)CC1	75	34
323	**10**{*43*}	**11**{*235*}	**8**{*43,235*}	CN(Cc1cscn1)c1nnnn1C1CCOc2ccccc12	0	0
324	**10**{*43*}	**11**{*178*}	**8**{*43,178*}	CN(Cc1ccoc1)c1nnnn1C1CCOc2ccccc12	0	0
325	**10**{*43*}	**11**{*176*}	**8**{*43,176*}	CN(Cc1cnc(C)s1)c1nnnn1C1CCOc2ccccc12	0	0
326	**10**{*43*}	**11**{*236*}	**8**{*43,236*}	Oc1ccc2CCN(Cc2c1)c1nnnn1C1CCOc2ccccc12	25	12
327	**10**{*43*}	**11**{*237*}	**8**{*43,237*}	CN(Cc1occc1C)c1nnnn1C1CCOc2ccccc12	26	14
328	**10**{*43*}	**11**{*99*}	**8**{*43,99*}	C1CC(c2ccccc2O1)n1nnnc1N1CCn2cncc2C1	0	0
329	**10**{*43*}	**11**{*94*}	**8**{*43,94*}	CN(c1nnnn1C1CCOc2ccccc12)c1c(C)noc1C	0	0
330	**10**{*44*}	**11**{*238*}	**8**{*44,238*}	Clc1cnn(c1)C1CCN(CC1)c1nnnn1C(C1CC1)C1CC1	0	0
331	**10**{*44*}	**11**{*73*}	**8**{*44,73*}	C1CC1C(C1CC1)n1nnnc1N1CCc2cn[nH]c2C1	0	0
332	**10**{*44*}	**11**{*142*}	**8**{*44,142*}	C1CC1C(C1CC1)n1nnnc1N1CCC(CC1)c1cn[nH]c1	0	0

333	**10**{*44*}	**11**{*148*}	**8**{*44,148*}	Cc1csc(n1)C1CCN(C1)c1nnnn1C(C1CC1)C1CC1	19	11
334	**10**{*45*}	**11**{*239*}	**8**{*45,239*}	FC(F)(F)Oc1ccc(Cn2nnnc2N2CC3CC2C=C3)cc1	0	0
335	**10**{*46*}	**11**{*240*}	**8**{*46,240*}	CC(=O)NC1CCN(CC1)c1nnnn1C1CCc2ccccc2C1	24	12
336	**10**{*46*}	**11**{*84*}	**8**{*46,84*}	CN(CC(=O)N1CCCC1)c1nnnn1C1CCc2ccccc2C1	0	0
337	**10**{*46*}	**11**{*79*}	**8**{*46,79*}	NC(=O)[C@H]1CCCN1c1nnnn1C1CCc2ccccc2C1	0	0
338	**10**{*46*}	**11**{*40*}	**8**{*46,40*}	C1Cc2ccccc2CC1n1nnnc1N1CCc2[nH]ncc2C1	0	0
339	**10**{*46*}	**11**{*241*}	**8**{*46,241*}	Cc1cnn(c1)C1CCN(C1)c1nnnn1C1CCc2ccccc2C1	0	0
340	**10**{*46*}	**11**{*116*}	**8**{*46,116*}	O[1C@@H]1CC[1C@@H]2CN(C[1C@@H]2C1)c1nnnn1C1CCc2ccccc2C1	0	0
341	**10**{*46*}	**11**{*143*}	**8**{*46,143*}	CN(c1ccn(C)n1)c1nnnn1C1CCc2ccccc2C1	0	0
342	**10**{*46*}	**11**{*81*}	**8**{*46,81*}	NC(=O)C1CN(CCO1)c1nnnn1C1CCc2ccccc2C1	0	0
343	**10**{*47*}	**11**{*10*}	**8**{*47,10*}	Cn1cccc1C(=O)N1CCN(CC1)c1nnnn1CC(C)(C)C	0	0
344	**10**{*47*}	**11**{*12*}	**8**{*47,12*}	Cn1cnnc1C1CCCN(C1)c1nnnn1CC(C)(C)C	0	0
345	**10**{*48*}	**11**{*7*}	**8**{*48,7*}	CSCCn1nnnc1N1CCC(C)=C(C)C1	0	0
346	**10**{*48*}	**11**{*8*}	**8**{*48,8*}	CSCCn1nnnc1N1CC2(CCOCC2)[1C@@H]2CCC[1C@H]12	20	20
347	**10**{*49*}	**11**{*81*}	**8**{*49,81*}	CC(Cc1ccccc1)n1nnnc1N1CCOC(C1)C(N)=O	0	0
348	**10**{*49*}	**11**{*143*}	**8**{*49,143*}	CC(Cc1ccccc1)n1nnnc1N(C)c1ccn(C)n1	22	11
349	**10**{*49*}	**11**{*242*}	**8**{*49,242*}	CCN(c1cnn(C)c1)c1nnnn1C(C)Cc1ccccc1	12	6
350	**10**{*49*}	**11**{*143*}	**8**{*49,143*}	CC(Cc1ccccc1)n1nnnc1N(C)c1ccn(C)n1	12	6
351	**10**{*49*}	**11**{*242*}	**8**{*49,242*}	CCN(c1cnn(C)c1)c1nnnn1C(C)Cc1ccccc1	29	14
352	**10**{*49*}	**11**{*242*}	**8**{*49,242*}	CCN(c1cnn(C)c1)c1nnnn1C(C)Cc1ccccc1	0	0
353	**10**{*49*}	**11**{*140*}	**8**{*49,140*}	CC(Cc1ccccc1)n1nnnc1N(C)c1cnn(C)c1	0	0

354	**10**{*49*}	**11**{*243*}	**8**{*49,243*}	CC(Cc1ccccc1)n1nnnc1N1CCC=C(C1)c1cnn(C)c1	0	0
355	**10**{*49*}	**11**{*143*}	**8**{*49,143*}	CC(Cc1ccccc1)n1nnnc1N(C)c1ccn(C)n1	0	0
356	**10**{*49*}	**11**{*73*}	**8**{*49,73*}	CC(Cc1ccccc1)n1nnnc1N1CCc2cn[nH]c2C1	0	0
357	**10**{*49*}	**11**{*99*}	**8**{*49,99*}	CC(Cc1ccccc1)n1nnnc1N1CCn2cncc2C1	0	0
358	**10**{*49*}	**11**{*79*}	**8**{*49,79*}	CC(Cc1ccccc1)n1nnnc1N1CCC[C@@H]1C(N)=O	0	0
359	**10**{*49*}	**11**{*244*}	**8**{*49,244*}	CC(Cc1ccccc1)n1nnnc1N1[1C@@H]2CC[1C@H]1CN(C)CC2	0	0
360	**10**{*49*}	**11**{*140*}	**8**{*49,140*}	CC(Cc1ccccc1)n1nnnc1N(C)c1cnn(C)c1	0	0
361	**10**{*50*}	**11**{*245*}	**8**{*50,245*}	C[C@H]1COCCN1c1nnnn1Cc1ccc(Br)cc1	7	7
362	**10**{*50*}	**11**{*118*}	**8**{*50,118*}	C[1C@@H]1[1C@H](O)CCN1c1nnnn1Cc1ccc(Br)cc1	15	15
363	**10**{*50*}	**11**{*246*}	**8**{*50,246*}	Brc1ccc(Cn2nnnc2N2CCCC(C2)C#N)cc1	0	0
364	**10**{*51*}	**11**{*247*}	**8**{*51,247*}	CN(Cc1cccc(=O)[nH]1)c1nnnn1CC1CCOC1	0	0
365	**10**{*51*}	**11**{*248*}	**8**{*51,248*}	C(C1CCOC1)n1nnnc1N1CCC[C@H]1c1ncn[nH]1	0	0
366	**10**{*51*}	**11**{*249*}	**8**{*51,249*}	COC[C@H]1C[C@@H](O)CN1c1nnnn1CC1CCOC1	0	0
367	**10**{*51*}	**11**{*244*}	**8**{*51,244*}	CN1CC[1C@@H]2CC[1C@H](C1)N2c1nnnn1CC1CCOC1	0	0
368	**10**{*51*}	**11**{*250*}	**8**{*51,250*}	CC(C)[C@H]1CN(CCN1C)c1nnnn1CC1CCOC1	0	0
369	**10**{*51*}	**11**{*43*}	**8**{*51,43*}	CN([C@H]1C[C@H](C1)C(N)=O)c1nnnn1CC1CCOC1	39	19
370	**10**{*51*}	**11**{*251*}	**8**{*51,251*}	CN1CCN(Cc2cccnc12)c1nnnn1CC1CCOC1	93	46
371	**10**{*52*}	**11**{*252*}	**8**{*52,252*}	NC(=O)C1N(CCc2ccccc12)c1nnnn1C1CCC1	0	0
372	**10**{*52*}	**11**{*222*}	**8**{*52,222*}	C1CC(C1)n1nnnc1N1CCCC(C1)c1ccncc1	0	0
373	**10**{*52*}	**11**{*1*}	**8**{*52,1*}	CNS(=O)(=O)c1cccc2CN(CCc12)c1nnnn1C1CCC1	14	16
374	**10**{*52*}	**11**{*253*}	**8**{*52,253*}	CC1CCN(CCS1(=O)=O)c1nnnn1C1CCC1	18	9

375	**10**{*52*}	**11**{*254*}	**8**{*52,254*}	O[1C@@H]1CN(C[1C@H]1Oc1ccccc1)c1nnnn1C1CCC1	27	14
376	**10**{*52*}	**11**{*255*}	**8**{*52,255*}	CC1CN(CCS(=O)(=O)C1)c1nnnn1C1CCC1	21	10
377	**10**{*52*}	**11**{*256*}	**8**{*52,256*}	CC1(C)CN([1C@@H]2COC[1C@H]12)c1nnnn1C1CCC1	43	22
378	**10**{*52*}	**11**{*220*}	**8**{*52,220*}	CC1CCS(=O)(=O)CCN1c1nnnn1C1CCC1	8	4
379	**10**{*53*}	**11**{*127*}	**8**{*53,127*}	NC(=O)[C@@H]1CCCN1c1nnnn1CCc1ccc(F)cc1	0	0
380	**10**{*53*}	**11**{*257*}	**8**{*53,257*}	Fc1ccc(CCn2nnnc2N2CCC(CC2)c2nnc[nH]2)cc1	0	0
381	**10**{*53*}	**11**{*258*}	**8**{*53,258*}	Fc1ccc(CCn2nnnc2N2CCC(CC2)c2ncc[nH]2)cc1	0	0
382	**10**{*53*}	**11**{*259*}	**8**{*53,259*}	CC1CN(CCN(C1)c1nnnn1CCc1ccc(F)cc1)C1CC1	0	0
383	**10**{*53*}	**11**{*260*}	**8**{*53,260*}	Fc1ccc(CCn2nnnc2N2CCC(C2)N2CCCCC2)cc1	0	0
384	**10**{*53*}	**11**{*205*}	**8**{*53,205*}	OC1CCN(CC1(F)F)c1nnnn1CCc1ccc(F)cc1	6	3
385	**10**{*53*}	**11**{*68*}	**8**{*53,68*}	Fc1ccc(CCn2nnnc2N2CCCC(C2)c2ccn[nH]2)cc1	0	0
386	**10**{*53*}	**11**{*236*}	**8**{*53,236*}	Oc1ccc2CCN(Cc2c1)c1nnnn1CCc1ccc(F)cc1	47	23
387	**10**{*53*}	**11**{*4*}	**8**{*53,4*}	Fc1ccc(CCn2nnnc2N2CCOC3(CCC3)C2)cc1	0	0
388	**10**{*53*}	**11**{*57*}	**8**{*53,57*}	Fc1ccc(CCn2nnnc2N2CCCc3n[nH]cc23)cc1	0	0
389	**10**{*53*}	**11**{*261*}	**8**{*53,261*}	Fc1ccc(CCn2nnnc2N2CCC(CC2)C2CCCO2)cc1	41	19
390	**10**{*53*}	**11**{*140*}	**8**{*53,140*}	CN(c1cnn(C)c1)c1nnnn1CCc1ccc(F)cc1	0	0
391	**10**{*53*}	**11**{*73*}	**8**{*53,73*}	Fc1ccc(CCn2nnnc2N2CCc3cn[nH]c3C2)cc1	6	3
392	**10**{*53*}	**11**{*116*}	**8**{*53,116*}	O[1C@@H]1CC[1C@@H]2CN(C[1C@@H]2C1)c1nnnn1CCc1ccc(F)cc1	23	12
393	**10**{*53*}	**11**{*249*}	**8**{*53,249*}	COC[C@H]1C[C@@H](O)CN1c1nnnn1CCc1ccc(F)cc1	11	12
394	**10**{*54*}	**11**{*27*}	**8**{*54,27*}	C(C1CCCCO1)n1nnnc1N1CCC(CC1)c1ccncc1	0	0
395	**10**{*54*}	**11**{*90*}	**8**{*54,90*}	C(N1CCN(CC1)c1nnnn1CC1CCCCO1)c1cscn1	12	5

396	**10**{*55*}	**11**{*262*}	**8**{*55,262*}	CC(C)N1CCC(C1)N(C)c1nnnn1Cc1cc(C)on1	0	0
397	**10**{*55*}	**11**{*156*}	**8**{*55,156*}	Cc1cc(Cn2nnnc2N2CCC[C@@H](C2)C(F)(F)F)no1	0	0
398	**10**{*55*}	**11**{*263*}	**8**{*55,263*}	CCc1cccc(c1)N(C)c1nnnn1Cc1cc(C)on1	41	20
399	**10**{*55*}	**11**{*264*}	**8**{*55,264*}	CC1N(CCc2ccccc12)c1nnnn1Cc1cc(C)on1	35	18
400	**10**{*55*}	**11**{*265*}	**8**{*55,265*}	Cc1cc(Cn2nnnc2N2CCC(Cc3cnn(C)c3)C2)no1	25	12
401	**10**{*56*}	**11**{*266*}	**8**{*56,266*}	Fc1cccc(OC2CCN(CC2)c2nnnn2Cc2ccon2)c1	0	0
402	**10**{*56*}	**11**{*101*}	**8**{*56,101*}	CN(Cc1ccc(C)s1)c1nnnn1Cc1ccon1	0	0
403	**10**{*56*}	**11**{*267*}	**8**{*56,267*}	CC(N(C)c1nnnn1Cc1ccon1)c1ccncc1	0	0
404	**10**{*56*}	**11**{*268*}	**8**{*56,268*}	C(c1ccon1)n1nnnc1N1CCCc2sccc2C1	0	0
405	**10**{*56*}	**11**{*94*}	**8**{*56,94*}	CN(c1nnnn1Cc1ccon1)c1c(C)noc1C	0	0
406	**10**{*56*}	**11**{*176*}	**8**{*56,176*}	CN(Cc1cnc(C)s1)c1nnnn1Cc1ccon1	0	0
407	**10**{*56*}	**11**{*269*}	**8**{*56,269*}	Clc1cccc(c1)C1CCCN1c1nnnn1Cc1ccon1	0	0
408	**10**{*56*}	**11**{*6*}	**8**{*56,6*}	Fc1ccc2CN(CCOc2c1)c1nnnn1Cc1ccon1	0	0
409	**10**{*56*}	**11**{*270*}	**8**{*56,270*}	CN(C1Cc2ccccc2C1)c1nnnn1Cc1ccon1	21	9
410	**10**{*56*}	**11**{*165*}	**8**{*56,165*}	C(C1CCN(CC1)c1nnnn1Cc1ccon1)N1CCOCC1	20	10
411	**10**{*56*}	**11**{*48*}	**8**{*56,48*}	Cc1ccnc(c1)N1CCN(CC1)c1nnnn1Cc1ccon1	8	4
412	**10**{*56*}	**11**{*271*}	**8**{*56,271*}	CC(N(C)c1nnnn1Cc1ccon1)c1ccccc1F	59	28
413	**10**{*56*}	**11**{*4*}	**8**{*56,4*}	C(c1ccon1)n1nnnc1N1CCOC2(CCC2)C1	18	19
414	**10**{*56*}	**11**{*108*}	**8**{*56,108*}	O=C1CCCN1C1CCN(CC1)c1nnnn1Cc1ccon1	89	43
415	**10**{*57*}	**11**{*7*}	**8**{*57,7*}	CC1=C(C)CN(CC1)c1nnnn1CC(F)F	0	0
416	**10**{*57*}	**11**{*4*}	**8**{*57,4*}	FC(F)Cn1nnnc1N1CCOC2(CCC2)C1	0	0

417	**10**{*57*}	**11**{*2*}	**8**{*57,2*}	FC(F)Cn1nnnc1N1CCN(CC1)C(=O)C(=O)NC1CC1	0	0
418	**10**{*57*}	**11**{*8*}	**8**{*57,8*}	FC(F)Cn1nnnc1N1CC2(CCOCC2)[1C@@H]2CCC[1C@H]12	28	27
419	**10**{*58*}	**11**{*272*}	**8**{*58,272*}	CC1(CCC1)n1nnnc1N1CCCC(C1)c1ccccn1	0	0
420	**10**{*58*}	**11**{*273*}	**8**{*58,273*}	CCN(CC(N)=O)c1nnnn1C1(C)CCC1	0	0
421	**10**{*58*}	**11**{*274*}	**8**{*58,274*}	CC1(CCC1)n1nnnc1N1CCC(CN2CCCC2)C1	0	0
422	**10**{*58*}	**11**{*127*}	**8**{*58,127*}	CC1(CCC1)n1nnnc1N1CCC[C@H]1C(N)=O	0	0
423	**10**{*58*}	**11**{*275*}	**8**{*58,275*}	CC1(CCC1)n1nnnc1N1CCC(Cc2cccnc2)CC1	0	0
424	**10**{*58*}	**11**{*276*}	**8**{*58,276*}	CC1CN(CCN1CC(C)(C)O)c1nnnn1C1(C)CCC1	17	8
425	**10**{*58*}	**11**{*277*}	**8**{*58,277*}	CC1(CCC1)n1nnnc1N1CCC(CO)(C1)C(F)(F)F	38	19
426	**10**{*58*}	**11**{*278*}	**8**{*58,278*}	CC1(CCC1)n1nnnc1N1CCC2(CCOC2)C1	21	11
427	**10**{*58*}	**11**{*187*}	**8**{*58,187*}	CC1(CCC1)n1nnnc1N1CCC(O)(C1)C1CC1	15	7
428	**10**{*58*}	**11**{*279*}	**8**{*58,279*}	Cc1cnc(OC2CCN(CC2)c2nnnn2C2(C)CCC2)nc1	19	10
429	**10**{*58*}	**11**{*280*}	**8**{*58,280*}	CC1(CCC1)n1nnnc1N1CCCN(CC1)c1ncccc1F	106	52
430	**10**{*58*}	**11**{*192*}	**8**{*58,192*}	CN(Cc1cccc(C)n1)c1nnnn1C1(C)CCC1	51	22

Table S5. Parallel synthesis of 5-aminotetrazoles **9**

#	Primary amine	Secondary amine	Product	SMILE	Yield, mg	Yield, %
1	**15**{*1*}	**11**{*281*}	**9**{*1,281*}	CC(C)n1nnnc1N1CCC(CC1)OCC1CC1	11	5
2	**15**{*2*}	**11**{*282*}	**9**{*2,282*}	CC(=O)N1CCN(CC11CCCCC1)c1nnnn1Cc1ccco1	0	0
3	**15**{*2*}	**11**{*283*}	**9**{*2,283*}	C(c1ccco1)n1nnnc1N1Cc2ccccc2OC2(CCC2)C1	0	0
4	**15**{*2*}	**11**{*284*}	**9**{*2,284*}	CC1(C)CN(CCO1)c1nnnn1Cc1ccco1	9	4
5	**15**{*2*}	**11**{*285*}	**9**{*2,285*}	Cc1nc(no1)C1CC2CCC(C1)N2c1nnnn1Cc1ccco1	0	0
6	**15**{*2*}	**11**{*286*}	**9**{*2,286*}	C(c1ccco1)n1nnnc1N1CCC2(CC1)OCc1ccccc21	0	0
7	**15**{*2*}	**11**{*287*}	**9**{*2,287*}	O=C(N1CCN(CC1)c1nnnn1Cc1ccco1)c1ccco1	0	0
8	**15**{*3*}	**11**{*288*}	**9**{*3,288*}	CC(=O)N1CCCN(CC1)c1nnnn1Cc1ccc2OCOc2c1	0	0
9	**15**{*4*}	**11**{*289*}	**9**{*4,289*}	COCCn1nnnc1N1CCC(CC1)c1nc2ccccc2s1	111	46
10	**15**{*4*}	**11**{*290*}	**9**{*4,290*}	COCCn1nnnc1N1CCN(C(C)C1)C(=O)OC(C)(C)C	18	10
11	**15**{*4*}	**11**{*291*}	**9**{*4,291*}	COCCn1nnnc1N1CCN(CC1)C(=O)c1ccc(F)cc1	70	33
12	**15**{*4*}	**11**{*292*}	**9**{*4,292*}	COCCn1nnnc1N1CCN([C@@H](C)C1)C(=O)OC(C)(C)C	26	12
13	**15**{*4*}	**11**{*293*}	**9**{*4,293*}	COCCn1nnnc1N1[C@H]2CC[C@@H]1C[C@@H](C2)c1ccccc1	0	0
14	**15**{*4*}	**11**{*287*}	**9**{*4,287*}	COCCn1nnnc1N1CCN(CC1)C(=O)c1ccco1	40	22
15	**15**{*4*}	**11**{*294*}	**9**{*4,294*}	COCCn1nnnc1N1CCN(CC1)c1ccccc1Cl	6	3
16	**15**{*4*}	**11**{*295*}	**9**{*4,295*}	COCCn1nnnc1N1CCN(CC1)C(=O)OCc1ccccc1	38	17
17	**15**{*4*}	**11**{*296*}	**9**{*4,296*}	COCCn1nnnc1N1CCN([C@H](C)C1)C(=O)OC(C)(C)C	12	6

18	**15**{*5*}	**11**{*297*}	**9**{*5,297*}	CCCCCn1nnnc1N1CCC(CC1)C1(C)OCCO1	7	4
19	**15**{*5*}	**11**{*298*}	**9**{*5,298*}	CCCCCn1nnnc1N1CCCC(C1)C1(C)OCCO1	8	4
20	**15**{*6*}	**11**{*299*}	**9**{*6,299*}	COC1(CO)CCN(CC1)c1nnnn1Cc1ccc(Cl)cc1	46	24
21	**15**{*6*}	**11**{*300*}	**9**{*6,300*}	Clc1ccc(Cn2nnnc2N2CCCOCC2)cc1	54	28
22	**15**{*7*}	**11**{*301*}	**9**{*7,301*}	FC(F)CN1CCN(CC1)c1nnnn1Cc1ccccc1	15	7
23	**15**{*8*}	**11**{*302*}	**9**{*8,302*}	CN(CCOc1ccc(F)cc1)c1nnnn1CC1CCCO1	56	28
24	**15**{*8*}	**11**{*303*}	**9**{*8,303*}	CC1CCCN(C1C)c1nnnn1CC1CCCO1	26	13
25	**15**{*9*}	**11**{*297*}	**9**{*9,297*}	COCCCn1nnnc1N1CCC(CC1)C1(C)OCCO1	26	13
26	**15**{*9*}	**11**{*298*}	**9**{*9,298*}	COCCCn1nnnc1N1CCCC(C1)C1(C)OCCO1	24	13
27	**15**{*10*}	**11**{*298*}	**9**{*10,298*}	CC(C)CCn1nnnc1N1CCCC(C1)C1(C)OCCO1	29	15
28	**15**{*10*}	**11**{*297*}	**9**{*10,297*}	CC(C)CCn1nnnc1N1CCC(CC1)C1(C)OCCO1	34	18
29	**15**{*11*}	**11**{*304*}	**9**{*11,304*}	CC(C)C(=O)NCC1CCCN(C1)c1nnnn1CC1CCCCC1	20	10
30	**15**{*12*}	**11**{*305*}	**9**{*12,305*}	CC1CCCN(CC1)c1nnnn1CCCN(C)C	0	0
31	**15**{*13*}	**11**{*306*}	**9**{*13,306*}	CC(C)(C)OC(=O)NCC1CCCN(C1)c1nnnn1CC=C	0	0
32	**15**{*13*}	**11**{*307*}	**9**{*13,307*}	CN(CC1CCN(C1)c1nnnn1CC=C)C(=O)OC(C)(C)C	19	10
33	**15**{*13*}	**11**{*308*}	**9**{*13,308*}	CC(C)(C)OC(=O)NCC1CCN(CC1)c1nnnn1CC=C	0	0
34	**15**{*13*}	**11**{*307*}	**9**{*13,307*}	CN(CC1CCN(C1)c1nnnn1CC=C)C(=O)OC(C)(C)C	0	0
35	**15**{*13*}	**11**{*309*}	**9**{*13,309*}	C=CCn1nnnc1N1CCC(CC1)n1c2ccccc2[nH]c1=O	56	30
36	**15**{*13*}	**11**{*310*}	**9**{*13,310*}	CC1CN(CCC1NC(=O)OC(C)(C)C)c1nnnn1CC=C	0	0
37	**15**{*13*}	**11**{*309*}	**9**{*13,309*}	C=CCn1nnnc1N1CCC(CC1)n1c2ccccc2[nH]c1=	0	0

				O		
38	**15**{*13*}	**11**{*311*}	**9**{*13,311*}	CC(C)(C)OC(=O)N[C@H]1CCCN(C1)c1nnnn1CC=C	0	0
39	**15**{*13*}	**11**{*306*}	**9**{*13,306*}	CC(C)(C)OC(=O)NCC1CCCN(C1)c1nnnn1CC=C	16	9
40	**15**{*13*}	**11**{*311*}	**9**{*13,311*}	CC(C)(C)OC(=O)N[C@H]1CCCN(C1)c1nnnn1CC=C	25	14
41	**15**{*13*}	**11**{*312*}	**9**{*13,312*}	CC(C)(C)OC(=O)NC1CCCN(C1)c1nnnn1CC=C	0	0
42	**15**{*13*}	**11**{*313*}	**9**{*13,313*}	CC(C)(C)OC(=O)N1C[C@H]2CN(C[C@H]2C1)c1nnnn1CC=C	0	0
43	**15**{*13*}	**11**{*313*}	**9**{*13,313*}	CC(C)(C)OC(=O)N1C[C@H]2CN(C[C@H]2C1)c1nnnn1CC=C	30	16
44	**15**{*13*}	**11**{*314*}	**9**{*13,314*}	CC(C)(C)OC(=O)N1CCCN(CC1)c1nnnn1CC=C	0	0
45	**15**{*13*}	**11**{*315*}	**9**{*13,315*}	CC(C)(C)OC(=O)N1C[C@@H]2C[C@H]1CN2c1nnnn1CC=C	0	0
46	**15**{*13*}	**11**{*314*}	**9**{*13,314*}	CC(C)(C)OC(=O)N1CCCN(CC1)c1nnnn1CC=C	9	4
47	**15**{*14*}	**11**{*300*}	**9**{*14,300*}	COc1ccc(CCn2nnnc2N2CCCOCC2)cc1	53	25
48	**15**{*14*}	**11**{*299*}	**9**{*14,299*}	COc1ccc(CCn2nnnc2N2CCC(CO)(CC2)OC)cc1	32	16
49	**15**{*15*}	**11**{*110*}	**9**{*15,110*}	CN(CC1(O)CCOCC1)c1nnnn1Cc1ccccc1Cl	0	0
50	**15**{*15*}	**11**{*102*}	**9**{*15,102*}	CN(Cc1scnc1C)c1nnnn1Cc1ccccc1Cl	0	0
51	**15**{*15*}	**11**{*299*}	**9**{*15,299*}	COC1(CO)CCN(CC1)c1nnnn1Cc1ccccc1Cl	52	24
52	**15**{*15*}	**11**{*213*}	**9**{*15,213*}	CNC(=O)NC1CCN(CC1)c1nnnn1Cc1ccccc1Cl	0	0
53	**15**{*15*}	**11**{*300*}	**9**{*15,300*}	Clc1ccccc1Cn1nnnc1N1CCCOCC1	27	13
54	**15**{*16*}	**11**{*299*}	**9**{*16,299*}	COC1(CO)CCN(CC1)c1nnnn1Cc1cccc(Cl)c1	53	23
55	**15**{*16*}	**11**{*300*}	**9**{*16,300*}	Clc1cccc(Cn2nnnc2N2CCCOCC2)c1	45	23
56	**15**{*17*}	**11**{*316*}	**9**{*17,316*}	Fc1cccc(F)c1N1CCN(CC1)c1nnnn1C1CC1	18	7

57	**15**{*18*}	**11**{*299*}	**9**{*18,299*}	COc1ccc(Cn2nnnc2N2CCC(CO)(CC2)OC)cc1	46	22
58	**15**{*18*}	**11**{*300*}	**9**{*18,300*}	COc1ccc(Cn2nnnc2N2CCCOCC2)cc1	63	31
59	**15**{*19*}	**11**{*317*}	**9**{*19,317*}	CN(Cc1ccc(C)o1)c1nnnn1C1CCCC1	18	10
60	**15**{*19*}	**11**{*288*}	**9**{*19,288*}	CC(=O)N1CCCN(CC1)c1nnnn1C1CCCC1	29	14
61	**15**{*19*}	**11**{*318*}	**9**{*19,318*}	C1CCC(C1)n1nnnc1N1CCn2c(C1)nnc2-c1ccccc1	0	0
62	**15**{*20*}	**11**{*319*}	**9**{*20,319*}	CN(CC1COCCO1)c1nnnn1CCc1c[nH]c2ccccc12	20	9
63	**15**{*20*}	**11**{*300*}	**9**{*20,300*}	C(Cn1nnnc1N1CCCOCC1)c1c[nH]c2ccccc12	0	0
64	**15**{*21*}	**11**{*300*}	**9**{*21,300*}	Clc1ccc(CCn2nnnc2N2CCCOCC2)cc1	52	26
65	**15**{*21*}	**11**{*320*}	**9**{*21,320*}	COC(=O)C1CCN(CC1)c1nnnn1CCc1ccc(Cl)cc1	38	19
66	**15**{*22*}	**11**{*321*}	**9**{*22,321*}	OCC1CCN(CC1)c1nnnn1Cc1ccc(Cl)cc1Cl	11	6
67	**15**{*22*}	**11**{*300*}	**9**{*22,300*}	Clc1ccc(Cn2nnnc2N2CCCOCC2)c(Cl)c1	39	21
68	**15**{*23*}	**11**{*300*}	**9**{*23,300*}	C(Cc1ccccc1)Cn1nnnc1N1CCCOCC1	32	15
69	**15**{*23*}	**11**{*299*}	**9**{*23,299*}	COC1(CO)CCN(CC1)c1nnnn1CCCc1ccccc1	47	23
70	**15**{*24*}	**11**{*322*}	**9**{*24,322*}	COc1ccc(Cn2nnnc2N(C)C2CC2)cc1OC	13	6
71	**15**{*24*}	**11**{*300*}	**9**{*24,300*}	COc1ccc(Cn2nnnc2N2CCCOCC2)cc1OC	11	6
72	**15**{*25*}	**11**{*147*}	**9**{*25,147*}	Clc1cnn(c1)C1CCN(C1)c1nnnn1CCC1=CCCCC1	63	30
73	**15**{*25*}	**11**{*323*}	**9**{*25,323*}	O=C1CN(Cc2ccccc2N1)c1nnnn1CCC1=CCCCC1	0	0
74	**15**{*25*}	**11**{*324*}	**9**{*25,324*}	Cc1noc(n1)C1CCN(CC1)c1nnnn1CCC1=CCCCC1	20	10
75	**15**{*25*}	**11**{*325*}	**9**{*25,325*}	O=c1[nH]ncn1C1CCN(CC1)c1nnnn1CCC1=CCCCC1	0	0
76	**15**{*25*}	**11**{*288*}	**9**{*25,288*}	CC(=O)N1CCCN(CC1)c1nnnn1CCC1=CCCCC1	26	12

77	**15**{*26*}	**11**{*326*}	**9**{*26,326*}	COc1ccccc1Cn1nnnc1N1CCC(=CC1)C(F)(F)F	13	5
78	**15**{*26*}	**11**{*299*}	**9**{*26,299*}	COc1ccccc1Cn1nnnc1N1CCC(CO)(CC1)OC	45	22
79	**15**{*26*}	**11**{*300*}	**9**{*26,300*}	COc1ccccc1Cn1nnnc1N1CCCOCC1	49	23
80	**15**{*27*}	**11**{*327*}	**9**{*27,327*}	CCCn1nnnc1N1CCCC1c1ccsc1	35	18
81	**15**{*28*}	**11**{*299*}	**9**{*28,299*}	COC1(CO)CCN(CC1)c1nnnn1CCc1ccc(F)cc1	0	0
82	**15**{*28*}	**11**{*300*}	**9**{*28,300*}	Fc1ccc(CCn2nnnc2N2CCCOCC2)cc1	28	13
83	**15**{*29*}	**11**{*328*}	**9**{*29,328*}	Fc1ccc(Cn2nnnc2N2CCOCC2)cc1	41	20
84	**15**{*30*}	**11**{*299*}	**9**{*30,299*}	COC1(CO)CCN(CC1)c1nnnn1Cc1ccc(C)cc1	26	14
85	**15**{*30*}	**11**{*300*}	**9**{*30,300*}	Cc1ccc(Cn2nnnc2N2CCCOCC2)cc1	50	26
86	**15**{*31*}	**11**{*329*}	**9**{*31,329*}	COc1cccc(Cn2nnnc2N2CCOC(CC2)C(F)F)c1	13	7
87	**15**{*31*}	**11**{*330*}	**9**{*31,330*}	COc1cccc(Cn2nnnc2N(C)C2CCCCN(C)C2=O)c1	0	0
88	**15**{*31*}	**11**{*331*}	**9**{*31,331*}	COc1cccc(Cn2nnnc2N2C3CCC2CC2(CC2)C3)c1	0	0
89	**15**{*31*}	**11**{*299*}	**9**{*31,299*}	COc1cccc(Cn2nnnc2N2CCC(CO)(CC2)OC)c1	39	18
90	**15**{*31*}	**11**{*332*}	**9**{*31,332*}	COc1cccc(Cn2nnnc2N2CCOC(C)(C2)C(F)F)c1	0	0
91	**15**{*31*}	**11**{*300*}	**9**{*31,300*}	COc1cccc(Cn2nnnc2N2CCCOCC2)c1	54	28
92	**15**{*32*}	**11**{*287*}	**9**{*32,287*}	O=C(N1CCN(CC1)c1nnnn1Cc1cccs1)c1ccco1	0	0
93	**15**{*32*}	**11**{*333*}	**9**{*32,333*}	CC1(C)CN(CCS1)c1nnnn1Cc1cccs1	23	12
94	**15**{*33*}	**11**{*334*}	**9**{*33,334*}	Cn1cnnc1N1CCN(CC1)c1nnnn1Cc1ccccc1F	0	0
95	**15**{*33*}	**11**{*335*}	**9**{*33,335*}	Fc1ccccc1Cn1nnnc1N1C[C@H]2[C@@H](C1)C(=O)NC2=O	0	0
96	**15**{*33*}	**11**{*336*}	**9**{*33,336*}	CS(=O)(=O)C1CCN(CC1)c1nnnn1Cc1ccccc1F	0	0

97	**15**{*33*}	**11**{*109*}	**9**{*33,109*}	Cn1nc2CCN(Cc2cc1=O)c1nnnn1Cc1ccccc1F	0	0
98	**15**{*33*}	**11**{*321*}	**9**{*33,321*}	OCC1CCN(CC1)c1nnnn1Cc1ccccc1F	29	14
99	**15**{*34*}	**11**{*337*}	**9**{*34,337*}	CN(CC1CCOC1)c1nnnn1Cc1cccc(c1)C(F)(F)F	31	16
100	**15**{*34*}	**11**{*300*}	**9**{*34,300*}	FC(F)(F)c1cccc(Cn2nnnc2N2CCCOCC2)c1	66	35
101	**15**{*35*}	**11**{*328*}	**9**{*35,328*}	FC(F)(F)c1ccc(CCn2nnnc2N2CCOCC2)cc1	39	20
102	**15**{*36*}	**11**{*338*}	**9**{*36,338*}	CCC1CN(CC(CC)O1)c1nnnn1CCNC(C)=O	42	22
103	**15**{*36*}	**11**{*339*}	**9**{*36,339*}	CN(Cc1cccc(F)c1)c1nnnn1CCNC(C)=O	44	20
104	**15**{*37*}	**11**{*340*}	**9**{*37,340*}	CN(C)C1(Cn2nnnc2N2CCCCCC2)CCCC1	0	0
105	**15**{*38*}	**11**{*341*}	**9**{*38,341*}	C(Cn1nnnc1N1CCCC1)Oc1ccccc1	0	0
106	**15**{*38*}	**11**{*342*}	**9**{*38,342*}	CC1CCCCN1c1nnnn1CCOc1ccccc1	20	10
107	**15**{*38*}	**11**{*343*}	**9**{*38,343*}	C(Cn1nnnc1N1CCN(Cc2ccccc2)CC1)Oc1ccccc1	0	0
108	**15**{*38*}	**11**{*343*}	**9**{*38,343*}	C(Cn1nnnc1N1CCN(Cc2ccccc2)CC1)Oc1ccccc1	17	9
109	**15**{*38*}	**11**{*341*}	**9**{*38,341*}	C(Cn1nnnc1N1CCCC1)Oc1ccccc1	36	16
110	**15**{*39*}	**11**{*158*}	**9**{*39,158*}	CC(C)(Cn1nnnc1N1CCC(CC1)C(F)F)N1CCOCC1	13	5
111	**15**{*39*}	**11**{*344*}	**9**{*39,344*}	CC(C)(Cn1nnnc1N1CCN(C1)C(=O)C1CC1)N1CCOCC1	0	0
112	**15**{*39*}	**11**{*345*}	**9**{*39,345*}	CC(C)(Cn1nnnc1N1CCCCCCC1)N1CCOCC1	0	0
113	**15**{*40*}	**11**{*346*}	**9**{*40,346*}	CCN(C)c1nnnn1CC(C)(C)N1CCCCC1	0	0
114	**15**{*41*}	**11**{*299*}	**9**{*41,299*}	COc1ccccc1CCn1nnnc1N1CCC(CO)(CC1)OC	35	19
115	**15**{*41*}	**11**{*300*}	**9**{*41,300*}	COc1ccccc1CCn1nnnc1N1CCCOCC1	56	28
116	**15**{*42*}	**11**{*300*}	**9**{*42,300*}	C(Cn1nnnc1N1CCCOCC1)Cn1ccc2ccccc12	7	3
117	**15**{*42*}	**11**{*337*}	**9**{*42,337*}	CN(CC1CCOC1)c1nnnn1CCCn1ccc2ccccc12	5	2

118	**15**{*43*}	**11**{*347*}	**9**{*43,347*}	NC(=O)c1ccc(Cn2nnnc2N2CCCCCCCC2)cc1	32	17
119	**15**{*43*}	**11**{*106*}	**9**{*43,106*}	NC(=O)c1ccc(Cn2nnnc2N2CCc3ccccc3CC2)cc1	49	24
120	**15**{*43*}	**11**{*320*}	**9**{*43,320*}	COC(=O)C1CCN(CC1)c1nnnn1Cc1ccc(cc1)C(N)=O	17	8
121	**15**{*43*}	**11**{*348*}	**9**{*43,348*}	CC(C)C1CN(CCCO1)c1nnnn1Cc1ccc(cc1)C(N)=O	0	0
122	**15**{*43*}	**11**{*338*}	**9**{*43,338*}	CCC1CN(CC(CC)O1)c1nnnn1Cc1ccc(cc1)C(N)=O	31	15
123	**15**{*44*}	**11**{*349*}	**9**{*44,349*}	O=C1CCCCCN1CCCn1nnnc1N1CCCC(CC#C)C1	43	22
124	**15**{*44*}	**11**{*350*}	**9**{*44,350*}	CN(CCC=C)c1nnnn1CCCN1CCCCCC1=O	53	24
125	**15**{*44*}	**11**{*351*}	**9**{*44,351*}	CCN1CCN(CC1=O)c1nnnn1CCCN1CCCCCC1=O	36	18
126	**15**{*45*}	**11**{*297*}	**9**{*45,297*}	CC1(OCCO1)C1CCN(CC1)c1nnnn1CCc1cccs1	39	19
127	**15**{*45*}	**11**{*298*}	**9**{*45,298*}	CC1(OCCO1)C1CCCN(C1)c1nnnn1CCc1cccs1	23	12
128	**15**{*46*}	**11**{*297*}	**9**{*46,297*}	CC1(OCCO1)C1CCN(CC1)c1nnnn1CCc1ccco1	0	0
129	**15**{*46*}	**11**{*298*}	**9**{*46,298*}	CC1(OCCO1)C1CCCN(C1)c1nnnn1CCc1ccco1	26	13
130	**15**{*47*}	**11**{*343*}	**9**{*47,343*}	Cc1ccccc1Cn1nnnc1N1CCN(Cc2ccccc2)CC1	0	0
131	**15**{*47*}	**11**{*341*}	**9**{*47,341*}	Cc1ccccc1Cn1nnnc1N1CCCC1	36	17
132	**15**{*47*}	**11**{*352*}	**9**{*47,352*}	Cc1ccccc1Cn1nnnc1N1CCC(Cn2ccnn2)CC1	0	0
133	**15**{*47*}	**11**{*341*}	**9**{*47,341*}	Cc1ccccc1Cn1nnnc1N1CCCC1	0	0
134	**15**{*47*}	**11**{*343*}	**9**{*47,343*}	Cc1ccccc1Cn1nnnc1N1CCN(Cc2ccccc2)CC1	0	0
135	**15**{*48*}	**11**{*299*}	**9**{*48,299*}	COC1(CO)CCN(CC1)c1nnnn1CCc1ccccc1F	33	17
136	**15**{*48*}	**11**{*300*}	**9**{*48,300*}	Fc1ccccc1CCn1nnnc1N1CCCOCC1	49	24
137	**15**{*48*}	**11**{*353*}	**9**{*48,353*}	OCC1(O)CCN(CC1)c1nnnn1CCc1ccccc1F	27	13

138	**15**{*49*}	**11**{*354*}	**9**{*49,354*}	CC1N(CN(C)C1=O)c1nnnn1Cc1ccc(OC(F)F)cc1	0	0
139	**15**{*50*}	**11**{*298*}	**9**{*50,298*}	CCCNC(=O)Cn1nnnc1N1CCCC(C1)C1(C)OCCO1	0	0
140	**15**{*50*}	**11**{*297*}	**9**{*50,297*}	CCCNC(=O)Cn1nnnc1N1CCC(CC1)C1(C)OCCO1	0	0
141	**15**{*51*}	**11**{*355*}	**9**{*51,355*}	CN(Cc1cnn(C)c1)c1nnnn1CCc1ccc2OCOc2c1	44	21
142	**15**{*52*}	**11**{*300*}	**9**{*52,300*}	COc1ccc(C)cc1CCn1nnnc1N1CCCOCC1	56	27
143	**15**{*52*}	**11**{*319*}	**9**{*52,319*}	COc1ccc(C)cc1CCn1nnnc1N(C)CC1COCCO1	67	35
144	**15**{*53*}	**11**{*300*}	**9**{*53,300*}	Fc1cccc(CCn2nnnc2N2CCCOCC2)c1	37	17
145	**15**{*53*}	**11**{*299*}	**9**{*53,299*}	COC1(CO)CCN(CC1)c1nnnn1CCc1cccc(F)c1	45	23
146	**15**{*54*}	**11**{*319*}	**9**{*54,319*}	CN(CC1COCCO1)c1nnnn1CCCOCC1CCCO1	38	19
147	**15**{*55*}	**11**{*300*}	**9**{*55,300*}	FC(F)(F)c1ccc(Cn2nnnc2N2CCCOCC2)cc1	64	31
148	**15**{*55*}	**11**{*337*}	**9**{*55,337*}	CN(CC1CCOC1)c1nnnn1Cc1ccc(cc1)C(F)(F)F	60	28
149	**15**{*56*}	**11**{*338*}	**9**{*56,338*}	CCC1CN(CC(CC)O1)c1nnnn1Cc1csc(C)n1	28	13
150	**15**{*57*}	**11**{*300*}	**9**{*57,300*}	Cc1cc(Cn2nnnc2N2CCCOCC2)ccc1F	65	32
151	**15**{*57*}	**11**{*261*}	**9**{*57,261*}	Cc1cc(Cn2nnnc2N2CCC(CC2)C2CCCO2)ccc1F	65	29
152	**15**{*57*}	**11**{*299*}	**9**{*57,299*}	COC1(CO)CCN(CC1)c1nnnn1Cc1ccc(F)c(C)c1	54	27
153	**15**{*58*}	**11**{*328*}	**9**{*58,328*}	FC(F)(F)Oc1ccc(Cn2nnnc2N2CCOCC2)cc1	39	19
154	**15**{*58*}	**11**{*300*}	**9**{*58,300*}	FC(F)(F)Oc1ccc(Cn2nnnc2N2CCCOCC2)cc1	24	12
155	**15**{*59*}	**11**{*300*}	**9**{*59,300*}	COc1ccc2cc(Cn3nnnc3N3CCCOCC3)ccc2c1	59	28
156	**15**{*60*}	**11**{*346*}	**9**{*60,346*}	CCN(C)c1nnnn1Cc1cnn(c1)-c1ccccc1	0	0
157	**15**{*60*}	**11**{*354*}	**9**{*60,354*}	CC1N(CN(C)C1=O)c1nnnn1Cc1cnn(c1)-c1ccccc1	0	0

158	**15**{*61*}	**11**{*322*}	**9**{*61,322*}	CN(C)S(=O)(=O)c1ccccc1Cn1nnnc1N(C)C1CC1	37	18
159	**15**{*61*}	**11**{*346*}	**9**{*61,346*}	CCN(C)c1nnnn1Cc1ccccc1S(=O)(=O)N(C)C	40	19
160	**15**{*62*}	**11**{*322*}	**9**{*62,322*}	CN(C1CC1)c1nnnn1C1CCN(CC1)C(=O)c1ccco1	40	20
161	**15**{*62*}	**11**{*356*}	**9**{*62,356*}	CN(CC1CCC1)c1nnnn1C1CCN(CC1)C(=O)c1ccco1	38	20
162	**15**{*63*}	**11**{*318*}	**9**{*63,318*}	C(C1CC1)n1nnnc1N1CCn2c(C1)nnc2-c1ccccc1	0	0
163	**15**{*63*}	**11**{*357*}	**9**{*63,357*}	COc1ccccc1N1CCN(CC1)c1nnnn1CC1CC1	40	19
164	**15**{*63*}	**11**{*311*}	**9**{*63,311*}	CC(C)(C)OC(=O)N[C@H]1CCCN(C1)c1nnnn1CC1CC1	0	0
165	**15**{*63*}	**11**{*307*}	**9**{*63,307*}	CN(CC1CCN(C1)c1nnnn1CC1CC1)C(=O)OC(C)(C)C	4	2
166	**15**{*63*}	**11**{*309*}	**9**{*63,309*}	O=c1[nH]c2ccccc2n1C1CCN(CC1)c1nnnn1CC1CC1	0	0
167	**15**{*63*}	**11**{*358*}	**9**{*63,358*}	CC(C)(C)OC(=O)NCC1CCN(C1)c1nnnn1CC1CC1	39	14
168	**15**{*63*}	**11**{*313*}	**9**{*63,313*}	CC(C)(C)OC(=O)N1C[C@H]2CN(C[C@H]2C1)c1nnnn1CC1CC1	22	9
169	**15**{*63*}	**11**{*314*}	**9**{*63,314*}	CC(C)(C)OC(=O)N1CCCN(CC1)c1nnnn1CC1CC1	43	17
170	**15**{*63*}	**11**{*310*}	**9**{*63,310*}	CC1CN(CCC1NC(=O)OC(C)(C)C)c1nnnn1CC1CC1	32	13
171	**15**{*63*}	**11**{*315*}	**9**{*63,315*}	CC(C)(C)OC(=O)N1C[C@@H]2C[C@H]1CN2c1nnnn1CC1CC1	0	0
172	**15**{*63*}	**11**{*312*}	**9**{*63,312*}	CC(C)(C)OC(=O)NC1CCCN(C1)c1nnnn1CC1CC1	0	0
173	**15**{*63*}	**11**{*359*}	**9**{*63,359*}	O=c1cccc2[C@@H]3C[C@@H](CN(C3)c3nnnn3CC3CC3)Cn12	0	0
174	**15**{*63*}	**11**{*360*}	**9**{*63,360*}	CC(C)(C)OC(=O)NC1CCN(CC1)c1nnnn1CC1CC1	22	9
175	**15**{*63*}	**11**{*361*}	**9**{*63,361*}	CC(C)(C)OC(=O)N1CCN(CC1)c1nnnn1CC1CC1	0	0

176	**15**{*63*}	**11**{*327*}	**9**{*63,327*}	C(C1CC1)n1nnnc1N1CCCC1c1ccsc1	106	50
177	**15**{*63*}	**11**{*306*}	**9**{*63,306*}	CC(C)(C)OC(=O)NCC1CCCN(C1)c1nnnn1CC1CC1	37	16
178	**15**{*63*}	**11**{*308*}	**9**{*63,308*}	CC(C)(C)OC(=O)NCC1CCN(CC1)c1nnnn1CC1CC1	21	8
179	**15**{*64*}	**11**{*322*}	**9**{*64,322*}	CN(C)C(=O)c1ccc(Cn2nnnc2N(C)C2CC2)cc1	26	12
180	**15**{*64*}	**11**{*356*}	**9**{*64,356*}	CN(C)C(=O)c1ccc(Cn2nnnc2N(C)CC2CCC2)cc1	32	16
181	**15**{*65*}	**11**{*355*}	**9**{*65,355*}	CN(Cc1cnn(C)c1)c1nnnn1C1CCC(CC1)C(F)(F)F	17	9
182	**15**{*66*}	**11**{*338*}	**9**{*66,338*}	CCC1CN(CC(CC)O1)c1nnnn1CCC1CCCO1	62	31
183	**15**{*67*}	**11**{*300*}	**9**{*67,300*}	Clc1ccc(Cn2nnnc2N2CCCOCC2)cn1	11	6
184	**15**{*67*}	**11**{*338*}	**9**{*67,338*}	CCC1CN(CC(CC)O1)c1nnnn1Cc1ccc(Cl)nc1	26	13
185	**15**{*68*}	**11**{*322*}	**9**{*68,322*}	COc1ccc(OC)c(Cn2nnnc2N(C)C2CC2)c1	43	20
186	**15**{*68*}	**11**{*300*}	**9**{*68,300*}	COc1ccc(OC)c(Cn2nnnc2N2CCCOCC2)c1	72	34
187	**15**{*69*}	**11**{*65*}	**9**{*69,65*}	FC1=CCCN(C1)c1nnnn1CCNC(=O)c1cccs1	0	0
188	**15**{*70*}	**11**{*362*}	**9**{*70,362*}	Cc1ccc(cc1F)C(=O)NCCn1nnnc1N1CCC[C@@H](O)C1	0	0
189	**15**{*71*}	**11**{*297*}	**9**{*71,297*}	CC1(OCCO1)C1CCN(CC1)c1nnnn1Cc1cccc(F)c1	0	0
190	**15**{*71*}	**11**{*298*}	**9**{*71,298*}	CC1(OCCO1)C1CCCN(C1)c1nnnn1Cc1cccc(F)c1	25	13
191	**15**{*72*}	**11**{*318*}	**9**{*72,318*}	C1CC(C1)n1nnnc1N1CCn2c(C1)nnc2-c1ccccc1	0	0
192	**15**{*73*}	**11**{*322*}	**9**{*73,322*}	COc1ccc(Cn2nnnc2N(C)C2CC2)c(OC)c1	0	0
193	**15**{*73*}	**11**{*300*}	**9**{*73,300*}	COc1ccc(Cn2nnnc2N2CCCOCC2)c(OC)c1	0	0
194	**15**{*74*}	**11**{*299*}	**9**{*74,299*}	CCOc1ccccc1Cn1nnnc1N1CCC(CO)(CC1)OC	41	19
195	**15**{*74*}	**11**{*300*}	**9**{*74,300*}	CCOc1ccccc1Cn1nnnc1N1CCCOCC1	44	21

196	**15**{*75*}	**11**{*320*}	**9**{*75,320*}	COC(=O)C1CCN(CC1)c1nnnn1CCc1ccccc1Cl	54	26
197	**15**{*75*}	**11**{*335*}	**9**{*75,335*}	Clc1ccccc1CCn1nnnc1N1C[C@H]2[C@@H](C1)C(=O)NC2=O	0	0
198	**15**{*75*}	**11**{*300*}	**9**{*75,300*}	Clc1ccccc1CCn1nnnc1N1CCCOCC1	42	22
199	**15**{*76*}	**11**{*337*}	**9**{*76,337*}	CN(CC1CCOC1)c1nnnn1Cc1ccccc1C(F)(F)F	42	22
200	**15**{*77*}	**11**{*363*}	**9**{*77,363*}	COCC1(C)CN(CCO1)c1nnnn1Cc1ccc(F)c(F)c1	72	33
201	**15**{*77*}	**11**{*364*}	**9**{*77,364*}	CN(CC1(C)COC1)c1nnnn1Cc1ccc(F)c(F)c1	0	0
202	**15**{*77*}	**11**{*299*}	**9**{*77,299*}	COC1(CO)CCN(CC1)c1nnnn1Cc1ccc(F)c(F)c1	50	24
203	**15**{*78*}	**11**{*298*}	**9**{*78,298*}	Cc1ccc(Cn2nnnc2N2CCCC(C2)C2(C)OCCO2)o1	31	16
204	**15**{*78*}	**11**{*297*}	**9**{*78,297*}	Cc1ccc(Cn2nnnc2N2CCC(CC2)C2(C)OCCO2)o1	23	12
205	**15**{*79*}	**11**{*365*}	**9**{*79,365*}	CC1CC(CN1c1nnnn1OC1CCCCO1)c1ccc(C)cc1	0	0
206	**15**{*79*}	**11**{*327*}	**9**{*79,327*}	C1CC(N(C1)c1nnnn1OC1CCCCO1)c1ccsc1	0	0
207	**15**{*80*}	**11**{*328*}	**9**{*80,328*}	Fc1ccc(Cn2nnnc2N2CCOCC2)c(c1)C(F)(F)F	18	9
208	**15**{*81*}	**11**{*298*}	**9**{*81,298*}	Cc1ccsc1Cn1nnnc1N1CCCC(C1)C1(C)OCCO1	23	12
209	**15**{*81*}	**11**{*366*}	**9**{*81,366*}	CN(CC(C)(C)O)c1nnnn1Cc1sccc1C	0	0
210	**15**{*81*}	**11**{*297*}	**9**{*81,297*}	Cc1ccsc1Cn1nnnc1N1CCC(CC1)C1(C)OCCO1	38	19
211	**15**{*81*}	**11**{*367*}	**9**{*81,367*}	CN(CC(=O)N1CCOCC1)c1nnnn1Cc1sccc1C	0	0
212	**15**{*81*}	**11**{*368*}	**9**{*81,368*}	Cc1ccsc1Cn1nnnc1N1CCCC(C1)S(C)(=O)=O	0	0
213	**15**{*82*}	**11**{*369*}	**9**{*82,369*}	CC1CN(CCO1)c1nnnn1Cc1ccccc1Br	33	16
214	**15**{*83*}	**11**{*298*}	**9**{*83,298*}	CCOCCn1nnnc1N1CCCC(C1)C1(C)OCCO1	41	22
215	**15**{*83*}	**11**{*297*}	**9**{*83,297*}	CCOCCn1nnnc1N1CCC(CC1)C1(C)OCCO1	28	14

216	**15**{*84*}	**11**{*319*}	**9**{*84,319*}	CC(C)Oc1cccc(Cn2nnnc2N(C)CC2COCCO2)c1	70	31
217	**15**{*85*}	**11**{*319*}	**9**{*85,319*}	CC(C)Oc1ccccc1Cn1nnnc1N(C)CC1COCCO1	56	26
218	**15**{*86*}	**11**{*337*}	**9**{*86,337*}	CN(CC1CCOC1)c1nnnn1CCOc1ccccc1Cl	0	0
219	**15**{*87*}	**11**{*321*}	**9**{*87,321*}	OCC1CCN(CC1)c1nnnn1Cc1ccc(Cl)c(Cl)c1	44	22
220	**15**{*88*}	**11**{*319*}	**9**{*88,319*}	CN(CC1COCCO1)c1nnnn1Cc1ccc(F)c(Cl)c1	41	21
221	**15**{*89*}	**11**{*110*}	**9**{*89,110*}	CN(CC1(O)CCOCC1)c1nnnn1Cc1ccc(F)cc1F	0	0
222	**15**{*89*}	**11**{*370*}	**9**{*89,370*}	CN(CC1CCCOC1)c1nnnn1Cc1ccc(F)cc1F	35	25
223	**15**{*89*}	**11**{*299*}	**9**{*89,299*}	COC1(CO)CCN(CC1)c1nnnn1Cc1ccc(F)cc1F	33	15
224	**15**{*90*}	**11**{*371*}	**9**{*90,371*}	CC(C)OCCn1nnnc1N1CCOC2(CCc3ccccc23)C1	73	33
225	**15**{*91*}	**11**{*372*}	**9**{*91,372*}	C[1C@@H]1C[1C@H](O)CN(C1)c1nnnn1CCc1c[nH]c2ccc(F)cc12	0	0
226	**15**{*92*}	**11**{*322*}	**9**{*92,322*}	COc1cccc(Cn2nnnc2N(C)C2CC2)c1OC	43	22
227	**15**{*93*}	**11**{*344*}	**9**{*93,344*}	Cc1ccc(Cn2nnnc2N2CCN(C2)C(=O)C2CC2)s1	0	0
228	**15**{*93*}	**11**{*367*}	**9**{*93,367*}	CN(CC(=O)N1CCOCC1)c1nnnn1Cc1ccc(C)s1	0	0
229	**15**{*93*}	**11**{*297*}	**9**{*93,297*}	Cc1ccc(Cn2nnnc2N2CCC(CC2)C2(C)OCCO2)s1	39	19
230	**15**{*93*}	**11**{*373*}	**9**{*93,373*}	CC(C)NC(=O)[C@H]1CCCN(C1)c1nnnn1Cc1ccc(C)s1	0	0
231	**15**{*93*}	**11**{*298*}	**9**{*93,298*}	Cc1ccc(Cn2nnnc2N2CCCC(C2)C2(C)OCCO2)s1	0	0
232	**15**{*93*}	**11**{*374*}	**9**{*93,374*}	Cc1noc(n1)C1CCN(C1)c1nnnn1Cc1ccc(C)s1	0	0
233	**15**{*94*}	**11**{*299*}	**9**{*94,299*}	COC1(CO)CCN(CC1)c1nnnn1Cc1cccc(C)c1	34	18
234	**15**{*94*}	**11**{*375*}	**9**{*94,375*}	Cc1cccc(Cn2nnnc2N2CCN(CC2)c2ncccn2)c1	48	24
235	**15**{*95*}	**11**{*299*}	**9**{*95,299*}	COC1(CO)CCN(CC1)c1nnnn1Cc1cc(F)ccc1F	17	9

236	**15**{*96*}	**11**{*299*}	**9**{*96,299*}	COc1cccc(CCn2nnnc2N2CCC(CO)(CC2)OC)c1	42	21
237	**15**{*97*}	**11**{*356*}	**9**{*97,356*}	CCNC(=O)c1ccc(Cn2nnnc2N(C)CC2CCC2)cc1	0	0
238	**15**{*98*}	**11**{*349*}	**9**{*98,349*}	C#CCC1CCCN(C1)c1nnnn1C1CCN(CC1)C1CCCC1	0	0
239	**15**{*98*}	**11**{*350*}	**9**{*98,350*}	CN(CCC=C)c1nnnn1C1CCN(CC1)C1CCCC1	0	0
240	**15**{*99*}	**11**{*299*}	**9**{*99,299*}	CCOc1ccc(Cn2nnnc2N2CCC(CO)(CC2)OC)cc1	58	24
241	**15**{*100*}	**11**{*299*}	**9**{*100,299*}	COC1(CO)CCN(CC1)c1nnnn1Cc1ccc(C)cc1C	31	16
242	**15**{*100*}	**11**{*376*}	**9**{*100,376*}	COCC(=O)N1CCN(CC1)c1nnnn1Cc1ccc(C)cc1C	11	6
243	**15**{*101*}	**11**{*299*}	**9**{*101,299*}	COC1(CO)CCN(CC1)c1nnnn1Cc1c(C)cc(C)cc1C	14	7
244	**15**{*102*}	**11**{*377*}	**9**{*102,377*}	Fc1cccc2OCCN(Cc12)c1nnnn1Cc1ccsc1	0	0
245	**15**{*102*}	**11**{*378*}	**9**{*102,378*}	Cc1ccc(C)n1C1CCN(CC1)c1nnnn1Cc1ccsc1	0	0
246	**15**{*102*}	**11**{*255*}	**9**{*102,255*}	CC1CN(CCS(=O)(=O)C1)c1nnnn1Cc1ccsc1	0	0
247	**15**{*102*}	**11**{*379*}	**9**{*102,379*}	OC1(CCCN(CC1)c1nnnn1Cc1ccsc1)C(F)(F)F	0	0
248	**15**{*102*}	**11**{*184*}	**9**{*102,184*}	COC1(CCCN(C1)c1nnnn1Cc1ccsc1)C(F)(F)F	0	0
249	**15**{*102*}	**11**{*380*}	**9**{*102,380*}	CNS(=O)(=O)N1CCN(CC1)c1nnnn1Cc1ccsc1	0	0
250	**15**{*102*}	**11**{*381*}	**9**{*102,381*}	COc1ccc2OCCN(Cc2c1)c1nnnn1Cc1ccsc1	0	0
251	**15**{*102*}	**11**{*382*}	**9**{*102,382*}	C(c1ccsc1)n1nnnc1N1CCCC(C1)NC1CCOCC1	0	0
252	**15**{*102*}	**11**{*287*}	**9**{*102,287*}	O=C(N1CCN(CC1)c1nnnn1Cc1ccsc1)c1ccco1	65	23
253	**15**{*102*}	**11**{*383*}	**9**{*102,383*}	C[C@@H]1CN(CCN1S(C)(=O)=O)c1nnnn1Cc1ccsc1	11	5
254	**15**{*102*}	**11**{*384*}	**9**{*102,384*}	O=C1CCCCN1C1CCCN(C1)c1nnnn1Cc1ccsc1	0	0
255	**15**{*102*}	**11**{*385*}	**9**{*102,385*}	CN(Cc1nc(C)no1)c1nnnn1Cc1ccsc1	0	0

256	**15**{*102*}	**11**{*356*}	**9**{*102,356*}	CN(CC1CCC1)c1nnnn1Cc1ccsc1	58	28
257	**15**{*103*}	**11**{*293*}	**9**{*103,293*}	C(C1CCOC1)n1nnnc1N1[C@H]2CC[C@@H]1C[C@@H](C2)c1ccccc1	0	0
258	**15**{*103*}	**11**{*386*}	**9**{*103,386*}	CN(Cc1ccc(F)cc1)c1nnnn1CC1CCOC1	80	37
259	**15**{*103*}	**11**{*387*}	**9**{*103,387*}	C(C1CCOC1)n1nnnc1N1CCC(Cc2ccccc2)CC1	0	0
260	**15**{*103*}	**11**{*388*}	**9**{*103,388*}	CN(Cc1ccc(Cl)s1)c1nnnn1CC1CCOC1	0	0
261	**15**{*103*}	**11**{*317*}	**9**{*103,317*}	CN(Cc1ccc(C)o1)c1nnnn1CC1CCOC1	0	0
262	**15**{*103*}	**11**{*389*}	**9**{*103,389*}	CN(Cc1cccs1)c1nnnn1CC1CCOC1	22	11
263	**15**{*103*}	**11**{*390*}	**9**{*103,390*}	CS(=O)(=O)N1CCN(CC1)c1nnnn1CC1CCOC1	7	3
264	**15**{*104*}	**11**{*391*}	**9**{*104,391*}	CN(CC1CC1)c1nnnn1Cc1ccc(CN2CCCC2=O)cc1	41	22
265	**15**{*104*}	**11**{*322*}	**9**{*104,322*}	CN(C1CC1)c1nnnn1Cc1ccc(CN2CCCC2=O)cc1	53	25
266	**15**{*105*}	**11**{*322*}	**9**{*105,322*}	CN(C1CC1)c1nnnn1Cc1ccccc1CN1CCCC1=O	19	10
267	**15**{*105*}	**11**{*391*}	**9**{*105,391*}	CN(CC1CC1)c1nnnn1Cc1ccccc1CN1CCCC1=O	41	21
268	**15**{*106*}	**11**{*392*}	**9**{*106,392*}	COCc1ccc(Cn2nnnc2N2CC(C)OC3(CCC3)C2)cc1	48	23
269	**15**{*106*}	**11**{*61*}	**9**{*106,61*}	COCc1ccc(Cn2nnnc2N2CCC3(C2)CCOCC3)cc1	23	12
270	**15**{*106*}	**11**{*393*}	**9**{*106,393*}	COCc1ccc(Cn2nnnc2N2CCOCC3(CCC3)C2)cc1	37	18
271	**15**{*106*}	**11**{*394*}	**9**{*106,394*}	COCc1ccc(Cn2nnnc2N2CCOC3(CCCC3)C2)cc1	37	18
272	**15**{*106*}	**11**{*395*}	**9**{*106,395*}	COCc1ccc(Cn2nnnc2N2CCOC3(CCOC3)C2)cc1	20	9
273	**15**{*107*}	**11**{*299*}	**9**{*107,299*}	COCc1cccc(Cn2nnnc2N2CCC(CO)(CC2)OC)c1	14	6
274	**15**{*108*}	**11**{*338*}	**9**{*108,338*}	CCC1CN(CC(CC)O1)c1nnnn1Cc1cccc(c1)C(N)=O	32	17
275	**15**{*108*}	**11**{*320*}	**9**{*108,320*}	COC(=O)C1CCN(CC1)c1nnnn1Cc1cccc(c1)C(N)=O	27	13

276	**15**{*109*}	**11**{*322*}	**9**{*109,322*}	CN(C)C(=O)c1cccc(Cn2nnnc2N(C)C2CC2)c1	26	13
277	**15**{*109*}	**11**{*356*}	**9**{*109,356*}	CN(C)C(=O)c1cccc(Cn2nnnc2N(C)CC2CCC2)c1	44	21
278	**15**{*110*}	**11**{*333*}	**9**{*110,333*}	CNC(=O)c1cccc(Cn2nnnc2N2CCSC(C)(C)C2)c1	87	42
279	**15**{*111*}	**11**{*328*}	**9**{*111,328*}	Clc1cc(Cn2nnnc2N2CCOCC2)cc2OCCOc12	57	29
280	**15**{*111*}	**11**{*396*}	**9**{*111,396*}	COCCN(C)c1nnnn1Cc1cc(Cl)c2OCCOc2c1	55	27
281	**15**{*112*}	**11**{*321*}	**9**{*112,321*}	OCC1CCN(CC1)c1nnnn1Cc1c(Cl)cccc1Cl	42	20
282	**15**{*113*}	**11**{*319*}	**9**{*113,319*}	CN(CC1COCCO1)c1nnnn1CCc1c(F)cccc1F	0	0
283	**15**{*114*}	**11**{*297*}	**9**{*114,297*}	Cc1ccc(CCn2nnnc2N2CCC(CC2)C2(C)OCCO2)o1	20	10
284	**15**{*114*}	**11**{*298*}	**9**{*114,298*}	Cc1ccc(CCn2nnnc2N2CCCC(C2)C2(C)OCCO2)o1	29	13
285	**15**{*115*}	**11**{*302*}	**9**{*115,302*}	CN(CCOc1ccc(F)cc1)c1nnnn1CCN1CCNC1=O	40	19
286	**15**{*115*}	**11**{*327*}	**9**{*115,327*}	O=C1NCCN1CCn1nnnc1N1CCCC1c1ccsc1	27	13
287	**15**{*115*}	**11**{*349*}	**9**{*115,349*}	O=C1NCCN1CCn1nnnc1N1CCCC(CC#C)C1	25	11
288	**15**{*116*}	**11**{*322*}	**9**{*116,322*}	CCCC(=O)Nc1ccc(Cn2nnnc2N(C)C2CC2)cc1	32	17
289	**15**{*117*}	**11**{*340*}	**9**{*117,340*}	C(c1ccoc1)n1nnnc1N1CCCCCC1	33	16
290	**15**{*117*}	**11**{*397*}	**9**{*117,397*}	CSC1CCCCN(C1)c1nnnn1Cc1ccoc1	48	21
291	**15**{*118*}	**11**{*288*}	**9**{*118,288*}	CC(=O)N1CCCN(CC1)c1nnnn1CCCC1CCCC1	52	24
292	**15**{*119*}	**11**{*322*}	**9**{*119,322*}	CN(C1CC1)c1nnnn1Cc1cccc(c1)N1CCCC1=O	48	24
293	**15**{*120*}	**11**{*344*}	**9**{*120,344*}	Cc1cc(Cn2nnnc2N2CCN(C2)C(=O)C2CC2)no1	0	0
294	**15**{*120*}	**11**{*298*}	**9**{*120,298*}	Cc1cc(Cn2nnnc2N2CCCC(C2)C2(C)OCCO2)no1	0	0
295	**15**{*120*}	**11**{*297*}	**9**{*120,297*}	Cc1cc(Cn2nnnc2N2CCC(CC2)C2(C)OCCO2)no1	22	11

296	**15**{*121*}	**11**{*398*}	**9**{*121,398*}	CC1CN(CC(C)O1)c1nnnn1CC1CCOCC1	29	14
297	**15**{*121*}	**11**{*302*}	**9**{*121,302*}	CN(CCOc1ccc(F)cc1)c1nnnn1CC1CCOCC1	71	29
298	**15**{*121*}	**11**{*114*}	**9**{*121,114*}	CS(=O)(=O)C1CCCN(CC1)c1nnnn1CC1CCOCC1	22	10
299	**15**{*121*}	**11**{*349*}	**9**{*121,349*}	C#CCC1CCCN(C1)c1nnnn1CC1CCOCC1	45	22
300	**15**{*121*}	**11**{*399*}	**9**{*121,399*}	COCC1(C)CCN(C1)c1nnnn1CC1CCOCC1	28	24
301	**15**{*122*}	**11**{*385*}	**9**{*122,385*}	CN(Cc1nc(C)no1)c1nnnn1Cc1csc2ccccc12	0	0
302	**15**{*123*}	**11**{*400*}	**9**{*123,400*}	CN(C1CCS(=O)(=O)C1)c1nnnn1Cc1c(C)nn(C)c1C	0	0
303	**15**{*124*}	**11**{*322*}	**9**{*124,322*}	CN(C1CC1)c1nnnn1Cc1ccc(cc1)-n1cccn1	41	20
304	**15**{*125*}	**11**{*319*}	**9**{*125,319*}	CC(Cn1nnnc1N(C)CC1COCCO1)Oc1ccc(C)cc1	40	20
305	**15**{*126*}	**11**{*401*}	**9**{*126,401*}	NC(=O)C1CCN(CC1)c1nnnn1CC12CC3CC(CC(C3)C1)C2	0	0
306	**15**{*127*}	**11**{*290*}	**9**{*127,290*}	CC1CN(CCN1C(=O)OC(C)(C)C)c1nnnn1CC#C	0	0
307	**15**{*127*}	**11**{*295*}	**9**{*127,295*}	O=C(OCc1ccccc1)N1CCN(CC1)c1nnnn1CC#C	0	0
308	**15**{*127*}	**11**{*292*}	**9**{*127,292*}	C[C@H]1CN(CCN1C(=O)OC(C)(C)C)c1nnnn1CC#C	0	0
309	**15**{*127*}	**11**{*296*}	**9**{*127,296*}	C[C@@H]1CN(CCN1C(=O)OC(C)(C)C)c1nnnn1CC#C	0	0
310	**15**{*127*}	**11**{*289*}	**9**{*127,289*}	C#CCn1nnnc1N1CCC(CC1)c1nc2ccccc2s1	0	0
311	**15**{*128*}	**11**{*322*}	**9**{*128,322*}	CN(C1CC1)c1nnnn1Cc1ccc(Cn2cccn2)cc1	41	21
312	**15**{*129*}	**11**{*288*}	**9**{*129,288*}	CC(=O)N1CCCN(CC1)c1nnnn1C1Cc2ccccc2C1	29	14
313	**15**{*130*}	**11**{*302*}	**9**{*130,302*}	CN(CCOc1ccc(F)cc1)c1nnnn1C1CCOCC1	0	0
314	**15**{*130*}	**11**{*327*}	**9**{*130,327*}	C1CC(N(C1)c1nnnn1C1CCOCC1)c1ccsc1	30	14
315	**15**{*130*}	**11**{*365*}	**9**{*130,365*}	CC1CC(CN1c1nnnn1C1CCOCC1)c1ccc(C)cc1	27	13

316	**15**{*131*}	**11**{*401*}	**9**{*131,401*}	NC(=O)C1CCN(CC1)c1nnnn1CC1CCCc2ccccc12	0	0
317	**15**{*132*}	**11**{*321*}	**9**{*132,321*}	OCC1CCN(CC1)c1nnnn1Cc1ccc(o1)-c1ccccc1	0	0
318	**15**{*133*}	**11**{*402*}	**9**{*133,402*}	CC1CN(CC2(CCCCC2)O1)c1nnnn1Cc1ccnn1C	8	4
319	**15**{*133*}	**11**{*403*}	**9**{*133,403*}	Cn1nccc1Cn1nnnc1N1CCC2(C)C(C1)C2(Cl)Cl	5	3
320	**15**{*133*}	**11**{*404*}	**9**{*133,404*}	COC(=O)[1C@]12CN(C[1C@H]1CCCC2)c1nnnn1Cc1ccnn1C	45	24
321	**15**{*133*}	**11**{*405*}	**9**{*133,405*}	Cn1nccc1Cn1nnnc1N1CCCC2(CCCCC2)C1	30	14
322	**15**{*133*}	**11**{*406*}	**9**{*133,406*}	CC1CCN(CC11CCC1)c1nnnn1Cc1ccnn1C	36	17
323	**15**{*133*}	**11**{*407*}	**9**{*133,407*}	Cn1nccc1Cn1nnnc1N1CCC2(C1)CCCCC2	50	23
324	**15**{*133*}	**11**{*408*}	**9**{*133,408*}	Cn1nccc1Cn1nnnc1N1CCCC2(CCCC2)C1	36	17
325	**15**{*133*}	**11**{*409*}	**9**{*133,409*}	Cn1nccc1Cn1nnnc1N1CCSC2(CCCCC2)C1	11	6
326	**15**{*133*}	**11**{*410*}	**9**{*133,410*}	Cn1nccc1Cn1nnnc1N1CCC2(CCCCC2)CC1	11	6
327	**15**{*133*}	**11**{*411*}	**9**{*133,411*}	CCC1CCCN(C1)c1nnnn1Cc1ccnn1C	39	19
328	**15**{*133*}	**11**{*412*}	**9**{*133,412*}	CON(CC1CC2CCC1C2)c1nnnn1Cc1ccnn1C	0	0
329	**15**{*133*}	**11**{*413*}	**9**{*133,413*}	CC1CN(CC2(CCCC2)O1)c1nnnn1Cc1ccnn1C	17	9
330	**15**{*134*}	**11**{*414*}	**9**{*134,414*}	CN(Cc1nccs1)c1nnnn1C1CCCC(O)C1	2	1
331	**15**{*135*}	**11**{*322*}	**9**{*135,322*}	CN(C1CC1)c1nnnn1Cc1cnn(Cc2ccccc2)c1	9	4
332	**15**{*136*}	**11**{*284*}	**9**{*136,284*}	Cc1n[nH]cc1Cn1nnnc1N1CCOC(C)(C)C1	0	0
333	**15**{*137*}	**11**{*391*}	**9**{*137,391*}	CC(C)NC(=O)Nc1ccc(Cn2nnnc2N(C)CC2CC2)cc1	0	0
334	**15**{*137*}	**11**{*322*}	**9**{*137,322*}	CC(C)NC(=O)Nc1ccc(Cn2nnnc2N(C)C2CC2)cc1	0	0
335	**15**{*138*}	**11**{*321*}	**9**{*138,321*}	OCC1CCN(CC1)c1nnnn1Cc1cc(Br)cs1	34	16

336	**15**{*139*}	**11**{*415*}	**9**{*139,415*}	CC1CC1n1nnnc1N(C)C[C@H]1CCCO1	11	5
337	**15**{*139*}	**11**{*318*}	**9**{*139,318*}	CC1CC1n1nnnc1N1CCn2c(C1)nnc2-c1ccccc1	23	12
338	**15**{*140*}	**11**{*338*}	**9**{*140,338*}	CCC1CN(CC(CC)O1)c1nnnn1CC(C)Cn1cccn1	50	24
339	**15**{*141*}	**11**{*349*}	**9**{*141,349*}	O=C(CCCn1nnnc1N1CCCC(CC#C)C1)NC1CC1	12	6
340	**15**{*142*}	**11**{*322*}	**9**{*142,322*}	CN(C1CC1)c1nnnn1Cc1ccc(CS(C)(=O)=O)cc1	30	15
341	**15**{*142*}	**11**{*356*}	**9**{*142,356*}	CN(CC1CCC1)c1nnnn1Cc1ccc(CS(C)(=O)=O)cc1	47	23
342	**15**{*143*}	**11**{*338*}	**9**{*143,338*}	CCC1CN(CC(CC)O1)c1nnnn1Cc1ccc(cc1)C(C)O	30	15
343	**15**{*144*}	**11**{*298*}	**9**{*144,298*}	CC1(OCCO1)C1CCCN(C1)c1nnnn1CCn1cccn1	10	5
344	**15**{*144*}	**11**{*297*}	**9**{*144,297*}	CC1(OCCO1)C1CCN(CC1)c1nnnn1CCn1cccn1	31	14
345	**15**{*145*}	**11**{*322*}	**9**{*145,322*}	CN(C1CC1)c1nnnn1CC1CCCOC1c1ccccc1	27	13
346	**15**{*146*}	**11**{*322*}	**9**{*146,322*}	CN(C1CC1)c1nnnn1CCNC(=O)c1cccc(C)c1	66	31
347	**15**{*147*}	**11**{*416*}	**9**{*147,416*}	CS(=O)(=O)CCn1nnnc1N1CCCc2ccccc2CC1	0	0
348	**15**{*147*}	**11**{*417*}	**9**{*147,417*}	COc1cccc2CCN(Cc12)c1nnnn1CCS(C)(=O)=O	0	0
349	**15**{*147*}	**11**{*405*}	**9**{*147,405*}	CS(=O)(=O)CCn1nnnc1N1CCCC2(CCCCC2)C1	0	0
350	**15**{*147*}	**11**{*418*}	**9**{*147,418*}	CS(=O)(=O)CCn1nnnc1N1Cc2ccccc2C(F)(F)C1	0	0
351	**15**{*147*}	**11**{*419*}	**9**{*147,419*}	CS(=O)(=O)CCn1nnnc1N1C2CCC1CC1(CC1(F)F)C2	0	0
352	**15**{*147*}	**11**{*420*}	**9**{*147,420*}	CS(=O)(=O)CCn1nnnc1N1CCOC(C1)c1ccccc1	0	0
353	**15**{*147*}	**11**{*421*}	**9**{*147,421*}	CS(=O)(=O)CCn1nnnc1N1CCC2(C1)OCc1ccccc21	24	14
354	**15**{*147*}	**11**{*387*}	**9**{*147,387*}	CS(=O)(=O)CCn1nnnc1N1CCC(Cc2ccccc2)CC1	35	18
355	**15**{*148*}	**11**{*349*}	**9**{*148,349*}	C#CCC1CCCN(C1)c1nnnn1CC1CCCCO1	45	22

356	**15**{*149*}	**11**{*304*}	**9**{*149,304*}	CC(C)C(=O)NCC1CCCN(C1)c1nnnn1CC1CCC=CC1	26	14
357	**15**{*150*}	**11**{*299*}	**9**{*150,299*}	COC1(CO)CCN(CC1)c1nnnn1CCc1cccc(C)c1	31	13
358	**15**{*151*}	**11**{*319*}	**9**{*151,319*}	CN(CC1COCCO1)c1nnnn1CCc1ccc(F)cc1F	74	36
359	**15**{*152*}	**11**{*299*}	**9**{*152,299*}	COC(Cn1nnnc1N1CCC(CO)(CC1)OC)c1ccccc1	0	0
360	**15**{*153*}	**11**{*401*}	**9**{*153,401*}	NC(=O)C1CCN(CC1)c1nnnn1CC1C2CC3CC(C2)CC1C3	0	0
361	**15**{*154*}	**11**{*299*}	**9**{*154,299*}	COc1cc(Cn2nnnc2N2CCC(CO)(CC2)OC)ccc1C	36	17
362	**15**{*155*}	**11**{*328*}	**9**{*155,328*}	CC1CC(C)CN(C1)C(C)(C)Cn1nnnc1N1CCOCC1	0	0
363	**15**{*156*}	**11**{*355*}	**9**{*156,355*}	CC1CCCN(C1)C(C)(C)Cn1nnnc1N(C)Cc1cnn(C)c1	0	0
364	**15**{*157*}	**11**{*298*}	**9**{*157,298*}	Cn1cc(Cn2nnnc2N2CCCC(C2)C2(C)OCCO2)cn1	35	18
365	**15**{*157*}	**11**{*297*}	**9**{*157,297*}	Cn1cc(Cn2nnnc2N2CCC(CC2)C2(C)OCCO2)cn1	25	13
366	**15**{*158*}	**11**{*422*}	**9**{*158,422*}	CC1CCCC(Cn2nnnc2N2CCC(CC(N)=O)CC2)C1	0	0
367	**15**{*158*}	**11**{*321*}	**9**{*158,321*}	CC1CCCC(Cn2nnnc2N2CCC(CO)CC2)C1	37	18
368	**15**{*158*}	**11**{*401*}	**9**{*158,401*}	CC1CCCC(Cn2nnnc2N2CCC(CC2)C(N)=O)C1	23	11
369	**15**{*158*}	**11**{*328*}	**9**{*158,328*}	CC1CCCC(Cn2nnnc2N2CCOCC2)C1	37	17
370	**15**{*158*}	**11**{*423*}	**9**{*158,423*}	CC1CCCC(Cn2nnnc2N2CCNC(=O)C2)C1	0	0
371	**15**{*158*}	**11**{*424*}	**9**{*158,424*}	CC1CCCC(Cn2nnnc2N2CCCC(O)C2)C1	0	0
372	**15**{*158*}	**11**{*299*}	**9**{*158,299*}	COC1(CO)CCN(CC1)c1nnnn1CC1CCCC(C)C1	12	6
373	**15**{*159*}	**11**{*346*}	**9**{*159,346*}	CCN(C)c1nnnn1Cc1cccc(NC(=O)C2CCCO2)c1	31	15
374	**15**{*160*}	**11**{*304*}	**9**{*160,304*}	CC(Cn1nnnc1N1CCCC(CNC(=O)C(C)C)C1)C1CC1	27	14

375	**15**{*161*}	**11**{*328*}	**9**{*161,328*}	Brc1ccc(CCn2nnnc2N2CCOCC2)s1	34	17
376	**15**{*162*}	**11**{*298*}	**9**{*162,298*}	COCC(C)Cn1nnnc1N1CCCC(C1)C1(C)OCCO1	20	10
377	**15**{*162*}	**11**{*297*}	**9**{*162,297*}	COCC(C)Cn1nnnc1N1CCC(CC1)C1(C)OCCO1	26	13
378	**15**{*163*}	**11**{*322*}	**9**{*163,322*}	CN(C1CC1)c1nnnn1Cc1ccc(NC(=O)c2ccco2)cc1	22	11
379	**15**{*163*}	**11**{*346*}	**9**{*163,346*}	CCN(C)c1nnnn1Cc1ccc(NC(=O)c2ccco2)cc1	0	0
380	**15**{*164*}	**11**{*284*}	**9**{*164,284*}	CC1(C)CN(CCO1)c1nnnn1CCc1cn[nH]c1	13	6
381	**15**{*165*}	**11**{*299*}	**9**{*165,299*}	COC1(CO)CCN(CC1)c1nnnn1CC(Br)=C	66	30
382	**15**{*166*}	**11**{*78*}	**9**{*166,78*}	COc1ccc2CN(CCCc2c1)c1nnnn1Cc1cc(C)no1	0	0
383	**15**{*166*}	**11**{*340*}	**9**{*166,340*}	Cc1cc(Cn2nnnc2N2CCCCCC2)on1	44	21
384	**15**{*166*}	**11**{*103*}	**9**{*166,103*}	Cc1cc(Cn2nnnc2N2CCc3[nH]c4ccc(C)cc4c3C2)on1	0	0
385	**15**{*166*}	**11**{*425*}	**9**{*166,425*}	COCC1=CCN(CC1)c1nnnn1Cc1cc(C)no1	11	5
386	**15**{*167*}	**11**{*401*}	**9**{*167,401*}	NC(=O)C1CCN(CC1)c1nnnn1CCCc1cccc(Cl)c1	25	12
387	**15**{*168*}	**11**{*319*}	**9**{*168,319*}	CN(CC1COCCO1)c1nnnn1CCc1ccc(F)c(F)c1	59	30
388	**15**{*169*}	**11**{*322*}	**9**{*169,322*}	CN(C1CC1)c1nnnn1CCc1ccc(NC(C)=O)cc1	32	16
389	**15**{*170*}	**11**{*338*}	**9**{*170,338*}	CCC1CN(CC(CC)O1)c1nnnn1CCOCC1CC1	35	17
390	**15**{*171*}	**11**{*302*}	**9**{*171,302*}	CN(CCOc1ccc(F)cc1)c1nnnn1CCNC(=O)C1CC1	0	0
391	**15**{*171*}	**11**{*349*}	**9**{*171,349*}	O=C(NCCn1nnnc1N1CCCC(CC#C)C1)C1CC1	0	0
392	**15**{*172*}	**11**{*426*}	**9**{*172,426*}	COC(=O)C1CC11CCN(CC1)c1nnnn1Cc1occc1C	0	0
393	**15**{*172*}	**11**{*427*}	**9**{*172,427*}	CN1CCC2(CCN(CC2)c2nnnn2Cc2occc2C)C1=O	0	0
394	**15**{*172*}	**11**{*428*}	**9**{*172,428*}	Cc1ccoc1Cn1nnnc1N1CCC2(CCNC(=O)O2)CC1	27	13

395	**15**{*172*}	**11**{*429*}	**9**{*172,429*}	Cc1ccoc1Cn1nnnc1N1CCOC2(CCOCC2)CC1	32	16
396	**15**{*172*}	**11**{*430*}	**9**{*172,430*}	CCOC(=O)[1C@@H]1[1C@@H]2CCN(C[1C@H]12)c1nnnn1Cc1occc1C	27	14
397	**15**{*172*}	**11**{*419*}	**9**{*172,419*}	Cc1ccoc1Cn1nnnc1N1C2CCC1CC1(CC1(F)F)C2	39	21
398	**15**{*172*}	**11**{*63*}	**9**{*172,63*}	Cc1ccoc1Cn1nnnc1N1CCN2C(CNC2=O)C1	0	0
399	**15**{*172*}	**11**{*431*}	**9**{*172,431*}	Cc1ccoc1Cn1nnnc1N1CCOC2(CCSC2)C1	0	0
400	**15**{*172*}	**11**{*432*}	**9**{*172,432*}	Cc1ccoc1Cn1nnnc1N1CCOCC2(CCOCC2)C1	33	16
401	**15**{*172*}	**11**{*433*}	**9**{*172,433*}	CC1CN(CC2(CCOCC2)O1)c1nnnn1Cc1occc1C	32	16
402	**15**{*172*}	**11**{*434*}	**9**{*172,434*}	Cc1ccoc1Cn1nnnc1N1CCOC2(CCOCC2)C1	29	14
403	**15**{*172*}	**11**{*435*}	**9**{*172,435*}	COC(=O)[1C@]12CN(C[1C@H]1COCC2)c1nnnn1Cc1occc1C	25	13
404	**15**{*172*}	**11**{*436*}	**9**{*172,436*}	COC(=O)[1C@]12CCC[1C@H]1N(CC2)c1nnnn1Cc1occc1C	25	12
405	**15**{*172*}	**11**{*437*}	**9**{*172,437*}	CCS(=O)(=O)N1CCN(CC1)c1nnnn1Cc1occc1C	0	0
406	**15**{*172*}	**11**{*438*}	**9**{*172,438*}	Cc1ccoc1Cn1nnnc1N1C[1C@@H]2CCC[1C@@]2(C1)C(N)=O	31	15
407	**15**{*172*}	**11**{*421*}	**9**{*172,421*}	Cc1ccoc1Cn1nnnc1N1CCC2(C1)OCc1ccccc21	34	17
408	**15**{*172*}	**11**{*104*}	**9**{*172,104*}	Cc1ccoc1Cn1nnnc1N1CCOCC2(CCCC2)C1	0	0
409	**15**{*173*}	**11**{*321*}	**9**{*173,321*}	Cc1ccccc1C(C)(C)Cn1nnnc1N1CCC(CO)CC1	21	10
410	**15**{*173*}	**11**{*401*}	**9**{*173,401*}	Cc1ccccc1C(C)(C)Cn1nnnc1N1CCC(CC1)C(N)=O	33	17
411	**15**{*174*}	**11**{*321*}	**9**{*174,321*}	COc1ccccc1C(C)(C)Cn1nnnc1N1CCC(CO)CC1	19	10
412	**15**{*175*}	**11**{*299*}	**9**{*175,299*}	CCC(Cn1nnnc1N1CCC(CO)(CC1)OC)c1ccccc1	64	29
413	**15**{*176*}	**11**{*391*}	**9**{*176,391*}	CN(CC1CC1)c1nnnn1Cc1ccc(cc1)C(=O)N1CCCC1	22	11
414	**15**{*176*}	**11**{*322*}	**9**{*176,322*}	CN(C1CC1)c1nnnn1Cc1ccc(cc1)C(=O)N1CCCC	39	20

415	**15**{*177*}	**11**{*298*}	**9**{*177,298*}	Cc1occc1Cn1nnnc1N1CCCC(C1)C1(C)OCCO1	13	7
416	**15**{*177*}	**11**{*297*}	**9**{*177,297*}	Cc1occc1Cn1nnnc1N1CCC(CC1)C1(C)OCCO1	0	0
417	**15**{*178*}	**11**{*302*}	**9**{*178,302*}	CN(CCOc1ccc(F)cc1)c1nnnn1CC1CCCNC1=O	16	7
418	**15**{*179*}	**11**{*319*}	**9**{*179,319*}	CN(CC1COCCO1)c1nnnn1CCc1cc(F)cc(F)c1	45	24
419	**15**{*180*}	**11**{*439*}	**9**{*180,439*}	CN(C1CCCCC1)c1nnnn1Cc1ncccc1C	0	0
420	**15**{*181*}	**11**{*338*}	**9**{*181,338*}	CCC1CN(CC(CC)O1)c1nnnn1Cc1nc2CCCc2s1	0	0
421	**15**{*182*}	**11**{*328*}	**9**{*182,328*}	C(c1ccc(OC2CCCC2)cc1)n1nnnc1N1CCOCC1	0	0
422	**15**{*183*}	**11**{*328*}	**9**{*183,328*}	Clc1ccc(CCCn2nnnc2N2CCOCC2)cc1	0	0
423	**15**{*183*}	**11**{*328*}	**9**{*183,328*}	Clc1ccc(CCCn2nnnc2N2CCOCC2)cc1	0	0
424	**15**{*184*}	**11**{*337*}	**9**{*184,337*}	COc1ccccc1C1(Cn2nnnc2N(C)CC2CCOC2)CC1	47	24
425	**15**{*185*}	**11**{*349*}	**9**{*185,349*}	C#CCC1CCCN(C1)c1nnnn1C1CCSCC1	32	16
426	**15**{*185*}	**11**{*338*}	**9**{*185,338*}	CCC1CN(CC(CC)O1)c1nnnn1C1CCSCC1	0	0
427	**15**{*185*}	**11**{*327*}	**9**{*185,327*}	C1CC(N(C1)c1nnnn1C1CCSCC1)c1ccsc1	37	17
428	**15**{*186*}	**11**{*401*}	**9**{*186,401*}	CC(C)(Cn1nnnc1N1CCC(CC1)C(N)=O)c1ccccc1F	24	11
429	**15**{*187*}	**11**{*337*}	**9**{*187,337*}	CN(CC1CCOC1)c1nnnn1CCc1c(C)[nH]c2ccccc12	26	13
430	**15**{*188*}	**11**{*349*}	**9**{*188,349*}	O=C1OCCN1CCCn1nnnc1N1CCCC(CC#C)C1	29	15
431	**15**{*188*}	**11**{*338*}	**9**{*188,338*}	CCC1CN(CC(CC)O1)c1nnnn1CCCN1CCOC1=O	60	27
432	**15**{*189*}	**11**{*440*}	**9**{*189,440*}	CC(CC#N)N(C)c1nnnn1C1CCCc2sccc12	0	0
433	**15**{*190*}	**11**{*341*}	**9**{*190,341*}	COc1ccc(CCn2nnnc2N2CCCC2)cc1F	78	37

434	**15**{*191*}	**11**{*338*}	**9**{*191,338*}	CCC1CN(CC(CC)O1)c1nnnn1Cc1cccc(CO)c1	20	10
435	**15**{*192*}	**11**{*328*}	**9**{*192,328*}	CCc1cccc2c(CCn3nnnc3N3CCOCC3)c[nH]c12	9	4
436	**15**{*193*}	**11**{*350*}	**9**{*193,350*}	CN(CCC=C)c1nnnn1Cc1cccc(CN2CCCC2=O)c1	23	12
437	**15**{*194*}	**11**{*297*}	**9**{*194,297*}	CCn1cc(Cn2nnnc2N2CCC(CC2)C2(C)OCCO2)cn1	33	16
438	**15**{*194*}	**11**{*298*}	**9**{*194,298*}	CCn1cc(Cn2nnnc2N2CCCC(C2)C2(C)OCCO2)cn1	26	13
439	**15**{*195*}	**11**{*441*}	**9**{*195,441*}	Cc1c(Cn2nnnc2N2CCS(=O)C(C)(C)CC2)cnn1C	0	0
440	**15**{*195*}	**11**{*326*}	**9**{*195,326*}	Cc1c(Cn2nnnc2N2CCC(=CC2)C(F)(F)F)cnn1C	0	0
441	**15**{*195*}	**11**{*442*}	**9**{*195,442*}	Cc1c(Cn2nnnc2N2CCC(C2)c2cccc(C)c2)cnn1C	0	0
442	**15**{*195*}	**11**{*182*}	**9**{*195,182*}	CN(Cc1ccc(C)c(C)c1)c1nnnn1Cc1cnn(C)c1C	0	0
443	**15**{*195*}	**11**{*443*}	**9**{*195,443*}	C[C@H]1CN(C[C@@H](C)O1)c1nnnn1Cc1cnn(C)c1C	17	8
444	**15**{*196*}	**11**{*297*}	**9**{*196,297*}	Cn1ccc(Cn2nnnc2N2CCC(CC2)C2(C)OCCO2)n1	0	0
445	**15**{*196*}	**11**{*298*}	**9**{*196,298*}	Cn1ccc(Cn2nnnc2N2CCCC(C2)C2(C)OCCO2)n1	42	21
446	**15**{*197*}	**11**{*105*}	**9**{*197,105*}	CN1CCN(Cc2ccccc12)c1nnnn1CC(F)F	0	0
447	**15**{*197*}	**11**{*444*}	**9**{*197,444*}	COc1ccc(cc1)C1CN(CCO1)c1nnnn1CC(F)F	0	0
448	**15**{*197*}	**11**{*445*}	**9**{*197,445*}	COc1cc2CCN(Cc2cc1OC)c1nnnn1CC(F)F	0	0
449	**15**{*198*}	**11**{*297*}	**9**{*198,297*}	CC(c1cnn(C)c1)n1nnnc1N1CCC(CC1)C1(C)OCCO1	0	0
450	**15**{*198*}	**11**{*298*}	**9**{*198,298*}	CC(c1cnn(C)c1)n1nnnc1N1CCCC(C1)C1(C)OCCO1	0	0
451	**15**{*199*}	**11**{*446*}	**9**{*199,446*}	COC(=O)[1C@@H]1CN(C[1C@H]1C)c1nnnn1Cc1cccc2[nH]ccc12	16	8
452	**15**{*199*}	**11**{*96*}	**9**{*199,96*}	CC(C)OC1CCN(CC1)c1nnnn1Cc1cccc2[nH]ccc12	20	10

453	**15**{*199*}	**11**{*299*}	**9**{*199,299*}	COC1(CO)CCN(CC1)c1nnnn1Cc1cccc2[nH]ccc12	3	2
454	**15**{*199*}	**11**{*320*}	**9**{*199,320*}	COC(=O)C1CCN(CC1)c1nnnn1Cc1cccc2[nH]ccc12	12	6
455	**15**{*200*}	**11**{*356*}	**9**{*200,356*}	CN(CC1CCC1)c1nnnn1Cc1cccc(c1)-n1cncn1	35	18
456	**15**{*201*}	**11**{*327*}	**9**{*201,327*}	C1CC(N(C1)c1nnnn1C1CCCOC1)c1ccsc1	10	5
457	**15**{*201*}	**11**{*302*}	**9**{*201,302*}	CN(CCOc1ccc(F)cc1)c1nnnn1C1CCCOC1	0	0
458	**15**{*201*}	**11**{*349*}	**9**{*201,349*}	C#CCC1CCCN(C1)c1nnnn1C1CCCOC1	35	17
459	**15**{*202*}	**11**{*304*}	**9**{*202,304*}	CCC1(Cn2nnnc2N2CCCC(CNC(=O)C(C)C)C2)CCC1	34	16
460	**15**{*203*}	**11**{*338*}	**9**{*203,338*}	CCC1CN(CC(CC)O1)c1nnnn1CC1(C)CCCO1	15	9
461	**15**{*203*}	**11**{*339*}	**9**{*203,339*}	CN(Cc1cccc(F)c1)c1nnnn1CC1(C)CCCO1	29	14
462	**15**{*204*}	**11**{*447*}	**9**{*204,447*}	CCN1CC(CC1=O)n1nnnc1N1CCc2ccccc2C1	9	4
463	**15**{*204*}	**11**{*448*}	**9**{*204,448*}	CCOC(=O)C1CCN(CC1)c1nnnn1C1CN(CC)C(=O)C1	22	10
464	**15**{*204*}	**11**{*449*}	**9**{*204,449*}	CCN1CC(CC1=O)n1nnnc1N1CC(C)(C)OC(C)(C)C1	0	0
465	**15**{*204*}	**11**{*106*}	**9**{*204,106*}	CCN1CC(CC1=O)n1nnnc1N1CCc2ccccc2CC1	0	0
466	**15**{*204*}	**11**{*450*}	**9**{*204,450*}	CCN1CC(CC1=O)n1nnnc1N1CCN(CC1)c1ccccc1	0	0
467	**15**{*204*}	**11**{*451*}	**9**{*204,451*}	CCOC(=O)N1CCN(CC1)c1nnnn1C1CN(CC)C(=O)C1	0	0
468	**15**{*204*}	**11**{*349*}	**9**{*204,349*}	CCN1CC(CC1=O)n1nnnc1N1CCCC(CC#C)C1	0	0
469	**15**{*204*}	**11**{*452*}	**9**{*204,452*}	CCOC(=O)[C@@H]1CCCN(C1)c1nnnn1C1CN(CC)C(=O)C1	0	0
470	**15**{*204*}	**11**{*453*}	**9**{*204,453*}	CCOC(=O)C1CCCN(C1)c1nnnn1C1CN(CC)C(=O)C1	0	0
471	**15**{*204*}	**11**{*302*}	**9**{*204,302*}	CCN1CC(CC1=O)n1nnnc1N(C)CCOc1ccc(F)cc1	16	8

472	**15**{*204*}	**11**{*327*}	**9**{*204,327*}	CCN1CC(CC1=O)n1nnnc1N1CCCC1c1ccsc1	32	16
473	**15**{*205*}	**11**{*435*}	**9**{*205,435*}	COC(=O)[1C@]12CN(C[1C@H]1COCC2)c1nnnn1CC1=CCCCC1	15	7
474	**15**{*205*}	**11**{*454*}	**9**{*205,454*}	CC1OCCC11CN(CC(C)O1)c1nnnn1CC1=CCCCC1	12	6
475	**15**{*205*}	**11**{*438*}	**9**{*205,438*}	NC(=O)[1C@]12CCC[1C@H]1CN(C2)c1nnnn1CC1=CCCCC1	28	14
476	**15**{*205*}	**11**{*433*}	**9**{*205,433*}	CC1CN(CC2(CCOCC2)O1)c1nnnn1CC1=CCCCC1	31	16
477	**15**{*205*}	**11**{*455*}	**9**{*205,455*}	CC1OCCC11CN(CCO1)c1nnnn1CC1=CCCCC1	0	0
478	**15**{*205*}	**11**{*335*}	**9**{*205,335*}	O=C1NC(=O)[C@@H]2CN(C[C@H]12)c1nnnn1CC1=CCCCC1	0	0
479	**15**{*205*}	**11**{*432*}	**9**{*205,432*}	C(C1=CCCCC1)n1nnnc1N1CCOCC2(CCOCC2)C1	25	13
480	**15**{*205*}	**11**{*429*}	**9**{*205,429*}	C(C1=CCCCC1)n1nnnc1N1CCOC2(CCOCC2)CC1	0	0
481	**15**{*205*}	**11**{*188*}	**9**{*205,188*}	CCOC1CC2(C1)CCN(C2)c1nnnn1CC1=CCCCC1	32	16
482	**15**{*205*}	**11**{*431*}	**9**{*205,431*}	C(C1=CCCCC1)n1nnnc1N1CCOC2(CCSC2)C1	12	6
483	**15**{*205*}	**11**{*428*}	**9**{*205,428*}	O=C1NCCC2(CCN(CC2)c2nnnn2CC2=CCCCC2)O1	16	8
484	**15**{*205*}	**11**{*434*}	**9**{*205,434*}	C(C1=CCCCC1)n1nnnc1N1CCOC2(CCOCC2)C1	10	5
485	**15**{*205*}	**11**{*304*}	**9**{*205,304*}	CC(C)C(=O)NCC1CCCN(C1)c1nnnn1CC1=CCCCC1	8	4
486	**15**{*205*}	**11**{*456*}	**9**{*205,456*}	C(C1=CCCCC1)n1nnnc1N1CCC2(CC1)OCCCO2	29	14
487	**15**{*206*}	**11**{*341*}	**9**{*206,341*}	Clc1ccc(cc1)-c1noc(CCn2nnnc2N2CCCC2)n1	25	12
488	**15**{*207*}	**11**{*302*}	**9**{*207,302*}	CN(CCOc1ccc(F)cc1)c1nnnn1CC1(C)CCOC1	17	8
489	**15**{*208*}	**11**{*338*}	**9**{*208,338*}	CCC1CN(CC(CC)O1)c1nnnn1Cc1ccn(n1)C(C)C	61	31
490	**15**{*209*}	**11**{*350*}	**9**{*209,350*}	CN(CCC=C)c1nnnn1C1CCN(CC(F)(F)F)C1=O	18	9

491	**15**{*210*}	**11**{*298*}	**9**{*210,298*}	Cc1cc(Cn2nnnc2N2CCCC(C2)C2(C)OCCO2)ncn1	0	0
492	**15**{*210*}	**11**{*297*}	**9**{*210,297*}	Cc1cc(Cn2nnnc2N2CCC(CC2)C2(C)OCCO2)ncn1	0	0
493	**15**{*211*}	**11**{*457*}	**9**{*211,457*}	CCc1ncc2C3CCC(Cc2n1)N3c1nnnn1CC1CC1(C)C	8	4
494	**15**{*211*}	**11**{*359*}	**9**{*211,359*}	CC1(C)CC1Cn1nnnc1N1C[C@@H]2C[C@H](C1)c1cccc(=O)n1C2	27	13
495	**15**{*211*}	**11**{*458*}	**9**{*211,458*}	CO[1C@@H]1CS(=O)(=O)[1C@H]2CN(C[1C@@H]12)c1nnnn1CC1CC1(C)C	20	10
496	**15**{*212*}	**11**{*327*}	**9**{*212,327*}	O=C1CNC(=O)N1CCn1nnnc1N1CCCC1c1ccsc1	57	26
497	**15**{*212*}	**11**{*349*}	**9**{*212,349*}	O=C1CNC(=O)N1CCn1nnnc1N1CCCC(CC#C)C1	21	10
498	**15**{*213*}	**11**{*297*}	**9**{*213,297*}	CC1(OCCO1)C1CCN(CC1)c1nnnn1Cc1ccon1	0	0
499	**15**{*213*}	**11**{*298*}	**9**{*213,298*}	CC1(OCCO1)C1CCCN(C1)c1nnnn1Cc1ccon1	0	0
500	**15**{*214*}	**11**{*320*}	**9**{*214,320*}	COC(=O)C1CCN(CC1)c1nnnn1Cc1cc(F)cc(OC)c1	43	20
501	**15**{*215*}	**11**{*369*}	**9**{*215,369*}	CC1CN(CCO1)c1nnnn1CC1CSCCS1	30	15
502	**15**{*216*}	**11**{*319*}	**9**{*216,319*}	CCSc1cccc(Cn2nnnc2N(C)CC2COCCO2)c1	57	27
503	**15**{*217*}	**11**{*337*}	**9**{*217,337*}	CN(CC1CCOC1)c1nnnn1CC1CCC(CC1)C(F)(F)F	49	24
504	**15**{*218*}	**11**{*288*}	**9**{*218,288*}	CC(=O)N1CCCN(CC1)c1nnnn1CC1C(C)(C)C1(C)C	12	6
505	**15**{*218*}	**11**{*395*}	**9**{*218,395*}	CC1(C)C(Cn2nnnc2N2CCOC3(CCOC3)C2)C1(C)C	0	0
506	**15**{*219*}	**11**{*327*}	**9**{*219,327*}	O=C1CC(Cn2nnnc2N2CCCC2c2ccsc2)CN1	32	14
507	**15**{*219*}	**11**{*365*}	**9**{*219,365*}	CC1CC(CN1c1nnnn1CC1CNC(=O)C1)c1ccc(C)cc1	12	6
508	**15**{*219*}	**11**{*302*}	**9**{*219,302*}	CN(CCOc1ccc(F)cc1)c1nnnn1CC1CNC(=O)C1	0	0
509	**15**{*220*}	**11**{*304*}	**9**{*220,304*}	CC(C)C(=O)NCC1CCCN(C1)c1nnnn1CCC1CCC1	28	13

510	**15**{*220*}	**11**{*288*}	**9**{*220,288*}	CC(=O)N1CCCN(CC1)c1nnnn1CCC1CCC1	32	16
511	**15**{*221*}	**11**{*288*}	**9**{*221,288*}	CC(C)CC1(Cn2nnnc2N2CCCN(CC2)C(C)=O)CCC1	27	13
512	**15**{*221*}	**11**{*395*}	**9**{*221,395*}	CC(C)CC1(Cn2nnnc2N2CCOC3(CCOC3)C2)CCC1	0	0
513	**15**{*222*}	**11**{*411*}	**9**{*222,411*}	CCC1CCCN(C1)c1nnnn1Cc1snnc1C	10	5
514	**15**{*223*}	**11**{*333*}	**9**{*223,333*}	CC1(C)CN(CCS1)c1nnnn1Cc1ccc(F)cn1	12	6
515	**15**{*224*}	**11**{*459*}	**9**{*224,459*}	CCN(CC)c1nnnn1Cc1nnc(C)s1	9	4
516	**15**{*225*}	**11**{*366*}	**9**{*225,366*}	CN(CC(C)(C)O)c1nnnn1Cc1ccc(C)c(F)c1	0	0
517	**15**{*225*}	**11**{*399*}	**9**{*225,399*}	COCC1(C)CCN(C1)c1nnnn1Cc1ccc(C)c(F)c1	33	15
518	**15**{*225*}	**11**{*367*}	**9**{*225,367*}	CN(CC(=O)N1CCOCC1)c1nnnn1Cc1ccc(C)c(F)c1	0	0
519	**15**{*226*}	**11**{*288*}	**9**{*226,288*}	CC(=O)N1CCCN(CC1)c1nnnn1C1CCCC(C)(C)C1	21	9
520	**15**{*227*}	**11**{*460*}	**9**{*227,460*}	Fc1ccc(cc1)N1CCN(CC1)c1nnnn1OC1CCCC1	0	0
521	**15**{*227*}	**11**{*446*}	**9**{*227,446*}	COC(=O)[1C@@H]1CN(C[1C@H]1C)c1nnnn1OC1CCCC1	0	0
522	**15**{*227*}	**11**{*461*}	**9**{*227,461*}	Cc1ccc(cc1)N1CCN(CC1)c1nnnn1OC1CCCC1	0	0
523	**15**{*227*}	**11**{*462*}	**9**{*227,462*}	Cc1ccccc1N1CCN(CC1)c1nnnn1OC1CCCC1	0	0
524	**15**{*227*}	**11**{*463*}	**9**{*227,463*}	Cc1ccc(cc1C)N1CCN(CC1)c1nnnn1OC1CCCC1	0	0
525	**15**{*227*}	**11**{*464*}	**9**{*227,464*}	Cc1cccc(c1)N1CCN(CC1)c1nnnn1OC1CCCC1	0	0
526	**15**{*227*}	**11**{*465*}	**9**{*227,465*}	CC1CCN(CC1C)c1nnnn1OC1CCCC1	0	0
527	**15**{*228*}	**11**{*355*}	**9**{*228,355*}	CCOC(=O)C1(Cn2nnnc2N(C)Cc2cnn(C)c2)CCC1	21	11
528	**15**{*229*}	**11**{*327*}	**9**{*229,327*}	CC1(C)CC(CCO1)n1nnnc1N1CCCC1c1ccsc1	180	92
529	**15**{*229*}	**11**{*349*}	**9**{*229,349*}	CC1(C)CC(CCO1)n1nnnc1N1CCCC(CC#C)C1	37	18

530	**15**{*229*}	**11**{*338*}	**9**{*229,338*}	CCC1CN(CC(CC)O1)c1nnnn1C1CCOC(C)(C)C1	42	19
531	**15**{*230*}	**11**{*349*}	**9**{*230,349*}	O=C(CCn1nnnc1N1CCCC(CC#C)C1)N1CCCCC1	29	13
532	**15**{*230*}	**11**{*350*}	**9**{*230,350*}	CN(CCC=C)c1nnnn1CCC(=O)N1CCCCC1	18	9
533	**15**{*231*}	**11**{*349*}	**9**{*231,349*}	C#CCC1CCCN(C1)c1nnnn1CCC1CC1	37	17
534	**15**{*231*}	**11**{*288*}	**9**{*231,288*}	CC(=O)N1CCCN(CC1)c1nnnn1CCC1CC1	25	12
535	**15**{*231*}	**11**{*318*}	**9**{*231,318*}	C(Cn1nnnc1N1CCn2c(C1)nnc2-c1ccccc1)C1CC1	0	0
536	**15**{*232*}	**11**{*466*}	**9**{*232,466*}	COC[C@@H](C)n1nnnc1N1CCCC2(C1)Oc1ccccc1C=C2	26	12
537	**15**{*232*}	**11**{*315*}	**9**{*232,315*}	COC[C@@H](C)n1nnnc1N1C[C@@H]2C[C@H]1CN2C(=O)OC(C)(C)C	20	10
538	**15**{*232*}	**11**{*467*}	**9**{*232,467*}	COC[C@@H](C)n1nnnc1N1C2CCC1CC(CC(F)(F)F)C2	33	15
539	**15**{*233*}	**11**{*349*}	**9**{*233,349*}	C#CCC1CCCN(C1)c1nnnn1CC1CCCS1	29	14
540	**15**{*234*}	**11**{*468*}	**9**{*234,468*}	CC(=C)CCn1nnnc1N1CCC(CC1)[1C@@H]1OCC[1C@H]1C(N)=O	21	10
541	**15**{*235*}	**11**{*469*}	**9**{*235,469*}	COC1CCC(Cn2nnnc2N2CCSCC2C)CC1	12	6
542	**15**{*236*}	**11**{*349*}	**9**{*236,349*}	CC1CC(CC(C)O1)n1nnnc1N1CCCC(CC#C)C1	0	0
543	**15**{*236*}	**11**{*327*}	**9**{*236,327*}	CC1CC(CC(C)O1)n1nnnc1N1CCCC1c1ccsc1	40	21
544	**15**{*236*}	**11**{*338*}	**9**{*236,338*}	CCC1CN(CC(CC)O1)c1nnnn1C1CC(C)OC(C)C1	34	15
545	**15**{*237*}	**11**{*302*}	**9**{*237,302*}	CC1CC(CCO1)n1nnnc1N(C)CCOc1ccc(F)cc1	31	14
546	**15**{*238*}	**11**{*318*}	**9**{*238,318*}	C1CC(C=C1)n1nnnc1N1CCn2c(C1)nnc2-c1ccccc1	0	0
547	**15**{*239*}	**11**{*298*}	**9**{*239,298*}	CC1(OCCO1)C1CCCN(C1)c1nnnn1CC1CCC=C1	28	14
548	**15**{*239*}	**11**{*468*}	**9**{*239,468*}	NC(=O)[1C@@H]1CCO[1C@H]1C1CCN(CC1)c1nnnn1CC1CCC=C1	43	20

549	**15**{*239*}	**11**{*470*}	**9**{*239,470*}	CC(C)(C)OC(=O)NC1CCN(C1)c1nnnn1CC1CCC=C1	52	25
550	**15**{*239*}	**11**{*471*}	**9**{*239,471*}	CC(C)(C)OC(=O)N[C@H]1CCN(C1)c1nnnn1CC1CCC=C1	0	0
551	**15**{*239*}	**11**{*360*}	**9**{*239,360*}	CC(C)(C)OC(=O)NC1CCN(CC1)c1nnnn1CC1CCC=C1	35	17
552	**15**{*239*}	**11**{*297*}	**9**{*239,297*}	CC1(OCCO1)C1CCN(CC1)c1nnnn1CC1CCC=C1	53	26
553	**15**{*239*}	**11**{*287*}	**9**{*239,287*}	O=C(N1CCN(CC1)c1nnnn1CC1CCC=C1)c1ccco1	22	12
554	**15**{*239*}	**11**{*359*}	**9**{*239,359*}	O=c1cccc2[C@@H]3C[C@@H](CN(C3)c3nnnn3CC3CCC=C3)Cn12	17	8
555	**15**{*239*}	**11**{*320*}	**9**{*239,320*}	COC(=O)C1CCN(CC1)c1nnnn1CC1CCC=C1	20	10
556	**15**{*239*}	**11**{*358*}	**9**{*239,358*}	CC(C)(C)OC(=O)NCC1CCN(C1)c1nnnn1CC1CCC=C1	108	56
557	**15**{*239*}	**11**{*472*}	**9**{*239,472*}	CC(C)(C)OC(=O)N[C@@H]1CCN(C1)c1nnnn1CC1CCC=C1	44	22
558	**15**{*239*}	**11**{*375*}	**9**{*239,375*}	C(C1CCC=C1)n1nnnc1N1CCN(CC1)c1ncccn1	26	13
559	**15**{*240*}	**11**{*304*}	**9**{*240,304*}	CC(C)C(=O)NCC1CCCN(C1)c1nnnn1CCCCC1CC1	16	7
560	**15**{*241*}	**11**{*349*}	**9**{*241,349*}	COC1(Cn2nnnc2N2CCCC(CC#C)C2)CCOCC1	33	17
561	**15**{*241*}	**11**{*327*}	**9**{*241,327*}	COC1(Cn2nnnc2N2CCCC2c2ccsc2)CCOCC1	61	29
562	**15**{*241*}	**11**{*338*}	**9**{*241,338*}	CCC1CN(CC(CC)O1)c1nnnn1CC1(CCOCC1)OC	49	25
563	**15**{*242*}	**11**{*338*}	**9**{*242,338*}	CCC1CN(CC(CC)O1)c1nnnn1Cc1cc(no1)C1CC1	55	23
564	**15**{*243*}	**11**{*322*}	**9**{*243,322*}	CN(C1CC1)c1nnnn1Cc1nc(cs1)C(F)(F)F	43	20
565	**15**{*244*}	**11**{*473*}	**9**{*244,473*}	CCOC1CC(n2nnnc2N2CC[C@@H](C2)OCC)C11CCCC1	43	21
566	**15**{*244*}	**11**{*474*}	**9**{*244,474*}	CCOC1CC(n2nnnc2N2CCC(C2)SC)C11CCCC1	45	23
567	**15**{*245*}	**11**{*288*}	**9**{*245,288*}	CC(=O)N1CCCN(CC1)c1nnnn1C1CCCC1(F)F	0	0

568	**15**{*246*}	**11**{*401*}	**9**{*246,401*}	CC(C)(Cn1nnnc1N1CCC(CC1)C(N)=O)c1cccc(F)c1	0	0
569	**15**{*247*}	**11**{*298*}	**9**{*247,298*}	CSCC(C)n1nnnc1N1CCCC(C1)C1(C)OCCO1	12	7
570	**15**{*247*}	**11**{*297*}	**9**{*247,297*}	CSCC(C)n1nnnc1N1CCC(CC1)C1(C)OCCO1	14	6
571	**15**{*248*}	**11**{*284*}	**9**{*248,284*}	CC1(C)CN(CCO1)c1nnnn1Cc1cccc2ncccc12	5	3
572	**15**{*248*}	**11**{*351*}	**9**{*248,351*}	CCN1CCN(CC1=O)c1nnnn1Cc1cccc2ncccc12	0	0
573	**15**{*248*}	**11**{*475*}	**9**{*248,475*}	C(c1cccc2ncccc12)n1nnnc1N1CCSCC1	11	5
574	**15**{*248*}	**11**{*476*}	**9**{*248,476*}	FC1(F)CCN(CC1)c1nnnn1Cc1cccc2ncccc12	6	3
575	**15**{*248*}	**11**{*477*}	**9**{*248,477*}	COCC1CCCN(C1)c1nnnn1Cc1cccc2ncccc12	14	7
576	**15**{*248*}	**11**{*478*}	**9**{*248,478*}	C(c1cccc2ncccc12)n1nnnc1N1CCCCC1	9	5
577	**15**{*248*}	**11**{*401*}	**9**{*248,401*}	NC(=O)C1CCN(CC1)c1nnnn1Cc1cccc2ncccc12	13	6
578	**15**{*248*}	**11**{*443*}	**9**{*248,443*}	C[C@H]1CN(C[C@@H](C)O1)c1nnnn1Cc1cccc2ncccc12	10	5
579	**15**{*249*}	**11**{*479*}	**9**{*249,479*}	CC(Cn1nnnc1N1CCCC(C)C1)c1nc(C)cs1	29	14
580	**15**{*249*}	**11**{*422*}	**9**{*249,422*}	CC(Cn1nnnc1N1CCC(CC(N)=O)CC1)c1nc(C)cs1	32	17
581	**15**{*249*}	**11**{*341*}	**9**{*249,341*}	CC(Cn1nnnc1N1CCCC1)c1nc(C)cs1	22	11
582	**15**{*249*}	**11**{*478*}	**9**{*249,478*}	CC(Cn1nnnc1N1CCCCC1)c1nc(C)cs1	19	10
583	**15**{*249*}	**11**{*443*}	**9**{*249,443*}	CC(Cn1nnnc1N1C[C@H](C)O[C@H](C)C1)c1nc(C)cs1	38	19
584	**15**{*249*}	**11**{*480*}	**9**{*249,480*}	CC(Cn1nnnc1N1CCC(C)CC1)c1nc(C)cs1	28	14
585	**15**{*249*}	**11**{*284*}	**9**{*249,284*}	CC(Cn1nnnc1N1CCOC(C)(C)C1)c1nc(C)cs1	13	7
586	**15**{*250*}	**11**{*278*}	**9**{*250,278*}	C(Cn1nnnc1N1CCC2(CCOC2)C1)c1nc2CCCc2s1	22	11
587	**15**{*250*}	**11**{*4*}	**9**{*250,4*}	C(Cn1nnnc1N1CCOC2(CCC2)C1)c1nc2CCCc2s1	0	0

588	**15**{*250*}	**11**{*179*}	**9**{*250,179*}	OC[C@H]1[C@@H]2CN(C[C@H]12)c1nnnn1CCc1nc2CCCc2s1	0	0
589	**15**{*250*}	**11**{*481*}	**9**{*250,481*}	C(Cn1nnnc1N1C[C@H]2CC=CC[C@H]2C1)c1nc2CCCc2s1	21	11
590	**15**{*250*}	**11**{*482*}	**9**{*250,482*}	C(Cn1nnnc1N1CCC2(C1)OCCO2)c1nc2CCCc2s1	0	0
591	**15**{*250*}	**11**{*483*}	**9**{*250,483*}	C(Cn1nnnc1N1CC2CCC(C2)C1)c1nc2CCCc2s1	0	0
592	**15**{*251*}	**11**{*338*}	**9**{*251,338*}	CCC1CN(CC(CC)O1)c1nnnn1Cc1sc(C)nc1C	22	11
593	**15**{*252*}	**11**{*321*}	**9**{*252,321*}	OCC1CCN(CC1)c1nnnn1CC1(CC1)c1cccc(Cl)c1	19	10
594	**15**{*252*}	**11**{*328*}	**9**{*252,328*}	Clc1cccc(c1)C1(Cn2nnnc2N2CCOCC2)CC1	0	0
595	**15**{*253*}	**11**{*405*}	**9**{*253,405*}	CCn1nncc1Cn1nnnc1N1CCCC2(CCCCC2)C1	10	5
596	**15**{*254*}	**11**{*355*}	**9**{*254,355*}	CN(Cc1cnn(C)c1)c1nnnn1CCC(C)(O)c1ccccc1	0	0
597	**15**{*254*}	**11**{*355*}	**9**{*254,355*}	CN(Cc1cnn(C)c1)c1nnnn1CCC(C)(O)c1ccccc1	0	0
598	**15**{*255*}	**11**{*322*}	**9**{*255,322*}	COc1ccc(Cn2nnnc2N(C)C2CC2)c(OC)n1	0	0
599	**15**{*256*}	**11**{*466*}	**9**{*256,466*}	CO[C@H](C)Cn1nnnc1N1CCCC2(C1)Oc1ccccc1C=C2	18	9
600	**15**{*257*}	**11**{*288*}	**9**{*257,288*}	CC(=O)N1CCCN(CC1)c1nnnn1C1CCC2(CCCC2)CC1	23	11
601	**15**{*258*}	**11**{*322*}	**9**{*258,322*}	CN(C1CC1)c1nnnn1CC1CCC(F)(F)C1	43	20
602	**15**{*258*}	**11**{*391*}	**9**{*258,391*}	CN(CC1CC1)c1nnnn1CC1CCC(F)(F)C1	35	17
603	**15**{*259*}	**11**{*391*}	**9**{*259,391*}	COCC(C)(C)Cn1nnnc1N(C)CC1CC1	10	5
604	**15**{*259*}	**11**{*337*}	**9**{*259,337*}	COCC(C)(C)Cn1nnnc1N(C)CC1CCOC1	37	18
605	**15**{*259*}	**11**{*300*}	**9**{*259,300*}	COCC(C)(C)Cn1nnnc1N1CCCOCC1	14	7
606	**15**{*260*}	**11**{*484*}	**9**{*260,484*}	CC1CCN(CC11CCCCC1)c1nnnn1[C@@H]1CCN(C1)C(C)=O	22	11
607	**15**{*260*}	**11**{*485*}	**9**{*260,485*}	CC(=O)N1CC[C@H](C1)n1nnnc1N1CCCC2(C	18	9

				CCCC2)CC1		
608	**15**{*261*}	**11**{*365*}	**9**{*261,365*}	CC1CC(CN1c1nnnn1C1CCN(C)C1=O)c1ccc(C)cc1	0	0
609	**15**{*261*}	**11**{*327*}	**9**{*261,327*}	CN1CCC(C1=O)n1nnnc1N1CCCC1c1ccsc1	0	0
610	**15**{*261*}	**11**{*302*}	**9**{*261,302*}	CN(CCOc1ccc(F)cc1)c1nnnn1C1CCN(C)C1=O	0	0
611	**15**{*262*}	**11**{*319*}	**9**{*262,319*}	CC(Cn1nnnc1N(C)CC1COCCO1)Sc1ccccc1	65	31
612	**15**{*263*}	**11**{*341*}	**9**{*263,341*}	CC(Cn1nnnc1N1CCCC1)Oc1ccccc1F	73	36
613	**15**{*264*}	**11**{*319*}	**9**{*264,319*}	CC(Cn1nnnc1N(C)CC1COCCO1)Oc1cccc(C)c1	0	0
614	**15**{*265*}	**11**{*319*}	**9**{*265,319*}	CC(Cn1nnnc1N(C)CC1COCCO1)Oc1ccccc1C	55	28
615	**15**{*266*}	**11**{*486*}	**9**{*266,486*}	CC(C)(C)OC(=O)N1C2CCC1CN(C2)c1nnnn1CCCC#C	8	4
616	**15**{*266*}	**11**{*487*}	**9**{*266,487*}	CC(C)(C)OC(=O)N1CC2CCC(C1)N2c1nnnn1CCCC#C	13	6
617	**15**{*266*}	**11**{*488*}	**9**{*266,488*}	CC(C)(C)OC(=O)[1C@]12COC[1C@H]1CN(C2)c1nnnn1CCCC#C	0	0
618	**15**{*266*}	**11**{*313*}	**9**{*266,313*}	CC(C)(C)OC(=O)N1C[C@H]2CN(C[C@H]2C1)c1nnnn1CCCC#C	40	17
619	**15**{*266*}	**11**{*489*}	**9**{*266,489*}	CC(C)(C)OC(=O)NCC12CC(C1)CN2c1nnnn1CCCC#C	0	0
620	**15**{*267*}	**11**{*490*}	**9**{*267,490*}	CC(O)C1CCN(CC1)c1nnnn1CC1(Cc2ccccc2)CC1	62	31
621	**15**{*268*}	**11**{*356*}	**9**{*268,356*}	CN(CC1CCC1)c1nnnn1Cc1ccc(CC(N)=O)cc1	30	16
622	**15**{*268*}	**11**{*333*}	**9**{*268,333*}	CC1(C)CN(CCS1)c1nnnn1Cc1ccc(CC(N)=O)cc1	25	12
623	**15**{*269*}	**11**{*319*}	**9**{*269,319*}	CSCc1ccc(Cn2nnnc2N(C)CC2COCCO2)cc1	45	18
624	**15**{*270*}	**11**{*485*}	**9**{*270,485*}	NC(=O)[C@H]1C[C@H](C1)n1nnnc1N1CCCC2(CCCCC2)CC1	35	17
625	**15**{*270*}	**11**{*365*}	**9**{*270,365*}	CC1CC(CN1c1nnnn1[C@@H]1C[C@@H](C1)C(N)=O)c1ccc(C)cc1	34	17

626	**15**{*270*}	**11**{*302*}	**9**{*270,302*}	CN(CCOc1ccc(F)cc1)c1nnnn1[C@@H]1C[C@@H](C1)C(N)=O	21	10
627	**15**{*270*}	**11**{*26*}	**9**{*270,26*}	NC(=O)[C@H]1C[C@H](C1)n1nnnc1N1CCc2cc(Cl)ccc2C1	10	4
628	**15**{*270*}	**11**{*484*}	**9**{*270,484*}	CC1CCN(CC11CCCCC1)c1nnnn1[C@@H]1C[C@@H](C1)C(N)=O	0	0
629	**15**{*271*}	**11**{*288*}	**9**{*271,288*}	CC(=O)N1CCCN(CC1)c1nnnn1CC1CC2CCC1CC2	30	16
630	**15**{*271*}	**11**{*395*}	**9**{*271,395*}	C(C1CC2CCC1CC2)n1nnnc1N1CCOC2(CCOC2)C1	0	0
631	**15**{*272*}	**11**{*319*}	**9**{*272,319*}	CCSc1ccc(Cn2nnnc2N(C)CC2COCCO2)cc1	66	33
632	**15**{*273*}	**11**{*356*}	**9**{*273,356*}	CN(CC1CCC1)c1nnnn1CCn1cc(Br)cn1	57	27
633	**15**{*274*}	**11**{*328*}	**9**{*274,328*}	Clc1ccc2n(CCn3nnnc3N3CCOCC3)ccc2c1	23	11
634	**15**{*275*}	**11**{*322*}	**9**{*275,322*}	CN(C1CC1)c1nnnn1Cc1ncc(Br)s1	0	0
635	**15**{*276*}	**11**{*288*}	**9**{*276,288*}	CC(=O)N1CCCN(CC1)c1nnnn1CC1CCC2(CC2)CC1	13	6
636	**15**{*277*}	**11**{*341*}	**9**{*277,341*}	FC(F)Oc1cccc(F)c1Cn1nnnc1N1CCCC1	36	18
637	**15**{*278*}	**11**{*349*}	**9**{*278,349*}	C#CCC1CCCN(C1)c1nnnn1Cc1nnnn1C1CC1	0	0
638	**15**{*278*}	**11**{*327*}	**9**{*278,327*}	C(c1nnnn1C1CC1)n1nnnc1N1CCCC1c1ccsc1	0	0
639	**15**{*279*}	**11**{*491*}	**9**{*279,491*}	CSC(C)Cn1nnnc1N1CCC(C1)N1CCCC1	0	0
640	**15**{*280*}	**11**{*322*}	**9**{*280,322*}	CN(C1CC1)c1nnnn1CCCn1cc(Br)cn1	39	20
641	**15**{*280*}	**11**{*391*}	**9**{*280,391*}	CN(CC1CC1)c1nnnn1CCCn1cc(Br)cn1	80	38
642	**15**{*281*}	**11**{*345*}	**9**{*281,345*}	C(c1nc2CCOCc2s1)n1nnnc1N1CCCCCCC1	27	13
643	**15**{*282*}	**11**{*350*}	**9**{*282,350*}	CN(CCC=C)c1nnnn1C1CC(C1)OCc1ccccc1	33	16
644	**15**{*283*}	**11**{*338*}	**9**{*283,338*}	CCC1CN(CC(CC)O1)c1nnnn1C1CCN(C1)C(=O)CC	38	18
645	**15**{*284*}	**11**{*355*}	**9**{*284,355*}	COCCC1(Cn2nnnc2N(C)Cc2cnn(C)c2)CCCC1	42	19

646	**15**{*285*}	**11**{*355*}	**9**{*285,355*}	CCOCCC1(Cn2nnnc2N(C)Cc2cnn(C)c2)CCCC1	33	16
647	**15**{*286*}	**11**{*288*}	**9**{*286,288*}	CCC1(Cn2nnnc2N2CCCN(CC2)C(C)=O)CCCC1	29	14
648	**15**{*287*}	**11**{*492*}	**9**{*287,492*}	CN(CC(C)(O)c1ccccc1)c1nnnn1CCc1ccnn1C	0	0
649	**15**{*287*}	**11**{*297*}	**9**{*287,297*}	Cn1nccc1CCn1nnnc1N1CCC(CC1)C1(C)OCCO1	20	9
650	**15**{*287*}	**11**{*492*}	**9**{*287,492*}	CN(CC(C)(O)c1ccccc1)c1nnnn1CCc1ccnn1C	20	11
651	**15**{*287*}	**11**{*298*}	**9**{*287,298*}	Cn1nccc1CCn1nnnc1N1CCCC(C1)C1(C)OCCO1	21	9
652	**15**{*288*}	**11**{*319*}	**9**{*288,319*}	CN(CC1COCCO1)c1nnnn1C1CCOC(C1)C(C)(C)C	38	17
653	**15**{*289*}	**11**{*338*}	**9**{*289,338*}	CCC1CN(CC(CC)O1)c1nnnn1C1CCOC(C1)C(C)C	26	13
654	**15**{*290*}	**11**{*338*}	**9**{*290,338*}	CCC1CN(CC(CC)O1)c1nnnn1CCCOC1CCOC1	29	15
655	**15**{*291*}	**11**{*328*}	**9**{*291,328*}	CC(C)c1csc(Cn2nnnc2N2CCOCC2)n1	0	0
656	**15**{*292*}	**11**{*288*}	**9**{*292,288*}	CC(=O)N1CCCN(CC1)c1nnnn1CCOCC1CCCC1	53	26
657	**15**{*293*}	**11**{*297*}	**9**{*293,297*}	CC1(OCCO1)C1CCN(CC1)c1nnnn1CCCc1ccco1	31	14
658	**15**{*293*}	**11**{*298*}	**9**{*293,298*}	CC1(OCCO1)C1CCCN(C1)c1nnnn1CCCc1ccco1	22	12
659	**15**{*294*}	**11**{*322*}	**9**{*294,322*}	CN(C1CC1)c1nnnn1Cc1cnn(CC(F)(F)F)c1	60	29
660	**15**{*294*}	**11**{*356*}	**9**{*294,356*}	CN(CC1CCC1)c1nnnn1Cc1cnn(CC(F)(F)F)c1	49	24
661	**15**{*295*}	**11**{*339*}	**9**{*295,339*}	CNC(=O)C(C)(C)Cn1nnnc1N(C)Cc1cccc(F)c1	0	0
662	**15**{*296*}	**11**{*339*}	**9**{*296,339*}	CCNC(=O)C(C)(C)Cn1nnnc1N(C)Cc1cccc(F)c1	30	15
663	**15**{*296*}	**11**{*338*}	**9**{*296,338*}	CCNC(=O)C(C)(C)Cn1nnnc1N1CC(CC)OC(CC)C1	0	0
664	**15**{*297*}	**11**{*338*}	**9**{*297,338*}	CCC1CN(CC(CC)O1)c1nnnn1CC(C)c1nccs1	0	0

665	**15**{*298*}	**11**{*303*}	**9**{*298,303*}	CCN(C)C(=O)Cn1nnnc1N1CCCC(C)C1C	46	21
666	**15**{*298*}	**11**{*417*}	**9**{*298,417*}	CCN(C)C(=O)Cn1nnnc1N1CCc2cccc(OC)c2C1	11	6
667	**15**{*299*}	**11**{*338*}	**9**{*299,338*}	CCC1CN(CC(CC)O1)c1nnnn1C1CC(OC)C1(C)C	26	13
668	**15**{*299*}	**11**{*327*}	**9**{*299,327*}	COC1CC(n2nnnc2N2CCCC2c2ccsc2)C1(C)C	56	28
669	**15**{*299*}	**11**{*349*}	**9**{*299,349*}	COC1CC(n2nnnc2N2CCCC(CC#C)C2)C1(C)C	0	0
670	**15**{*300*}	**11**{*493*}	**9**{*300,493*}	CC1CC2CCC(C1)N2c1nnnn1C1CN(C(=O)C1)C(C)(C)C	9	4
671	**15**{*301*}	**11**{*321*}	**9**{*301,321*}	CCSC1CCCC(C1)n1nnnc1N1CCC(CO)CC1	0	0
672	**15**{*302*}	**11**{*355*}	**9**{*302,355*}	CC(C)C1OCCCC1Cn1nnnc1N(C)Cc1cnn(C)c1	24	11
673	**15**{*303*}	**11**{*355*}	**9**{*303,355*}	CCOCCC1(Cn2nnnc2N(C)Cc2cnn(C)c2)CCC1	28	14
674	**15**{*304*}	**11**{*349*}	**9**{*304,349*}	COCCC1(Cn2nnnc2N2CCCC(CC#C)C2)CCC1	0	0
675	**15**{*304*}	**11**{*288*}	**9**{*304,288*}	COCCC1(Cn2nnnc2N2CCCN(CC2)C(C)=O)CCC1	52	26
676	**15**{*305*}	**11**{*288*}	**9**{*305,288*}	CC(C)CC1(Cn2nnnc2N2CCCN(CC2)C(C)=O)CC1	0	0
677	**15**{*306*}	**11**{*494*}	**9**{*306,494*}	COCC1CN(CCO1)c1nnnn1Cc1cscc1C	0	0
678	**15**{*306*}	**11**{*147*}	**9**{*306,147*}	Cc1cscc1Cn1nnnc1N1CCC(C1)n1cc(Cl)cn1	47	23
679	**15**{*306*}	**11**{*323*}	**9**{*306,323*}	Cc1cscc1Cn1nnnc1N1Cc2ccccc2NC(=O)C1	0	0
680	**15**{*306*}	**11**{*390*}	**9**{*306,390*}	Cc1cscc1Cn1nnnc1N1CCN(CC1)S(C)(=O)=O	0	0
681	**15**{*306*}	**11**{*495*}	**9**{*306,495*}	CC(=O)NCC1CN(CCO1)c1nnnn1Cc1cscc1C	28	15
682	**15**{*306*}	**11**{*176*}	**9**{*306,176*}	CN(Cc1cnc(C)s1)c1nnnn1Cc1cscc1C	0	0
683	**15**{*306*}	**11**{*496*}	**9**{*306,496*}	CC(C#C)N(C)c1nnnn1Cc1cscc1C	0	0
684	**15**{*306*}	**11**{*178*}	**9**{*306,178*}	CN(Cc1ccoc1)c1nnnn1Cc1cscc1C	19	10

685	**15**{*306*}	**11**{*108*}	**9**{*306,108*}	Cc1cscc1Cn1nnnc1N1CCC(CC1)N1CCCC1=O	0	0
686	**15**{*306*}	**11**{*177*}	**9**{*306,177*}	CC(C)C(=O)N1CCCN(CC1)c1nnnn1Cc1cscc1C	0	0
687	**15**{*306*}	**11**{*261*}	**9**{*306,261*}	Cc1cscc1Cn1nnnc1N1CCC(CC1)C1CCCO1	68	33
688	**15**{*306*}	**11**{*168*}	**9**{*306,168*}	Cc1cscc1Cn1nnnc1N1CCOC(C1)c1ccco1	31	16
689	**15**{*306*}	**11**{*497*}	**9**{*306,497*}	Cc1cscc1Cn1nnnc1N1CCN2C(C1)C(=O)NC2=O	0	0
690	**15**{*306*}	**11**{*19*}	**9**{*306,19*}	COC1(CCN(C1)c1nnnn1Cc1cscc1C)C(F)(F)F	0	0
691	**15**{*306*}	**11**{*375*}	**9**{*306,375*}	Cc1cscc1Cn1nnnc1N1CCN(CC1)c1ncccn1	38	18
692	**15**{*307*}	**11**{*288*}	**9**{*307,288*}	CCCC1(Cn2nnnc2N2CCCN(CC2)C(C)=O)CCC1	22	11
693	**15**{*308*}	**11**{*424*}	**9**{*308,424*}	CCC(OCCn1nnnc1N1CCCC(O)C1)c1ccccc1	0	0
694	**15**{*308*}	**11**{*423*}	**9**{*308,423*}	CCC(OCCn1nnnc1N1CCNC(=O)C1)c1ccccc1	0	0
695	**15**{*308*}	**11**{*321*}	**9**{*308,321*}	CCC(OCCn1nnnc1N1CCC(CO)CC1)c1ccccc1	21	9
696	**15**{*308*}	**11**{*328*}	**9**{*308,328*}	CCC(OCCn1nnnc1N1CCOCC1)c1ccccc1	28	14
697	**15**{*309*}	**11**{*338*}	**9**{*309,338*}	CCC1CN(CC(CC)O1)c1nnnn1CC1(CCOC)CC1	0	0
698	**15**{*310*}	**11**{*338*}	**9**{*310,338*}	CCOCCC1(Cn2nnnc2N2CC(CC)OC(CC)C2)CC1	45	23
699	**15**{*311*}	**11**{*355*}	**9**{*311,355*}	COC(Cn1nnnc1N(C)Cc1cnn(C)c1)C1CCCCC1	0	0
700	**15**{*312*}	**11**{*375*}	**9**{*312,375*}	COC1(Cn2nnnc2N2CCN(CC2)c2ncccn2)CCC1	25	12
701	**15**{*312*}	**11**{*338*}	**9**{*312,338*}	CCC1CN(CC(CC)O1)c1nnnn1CC1(CCC1)OC	27	13
702	**15**{*312*}	**11**{*287*}	**9**{*312,287*}	COC1(Cn2nnnc2N2CCN(CC2)C(=O)c2ccco2)CCC1	0	0
703	**15**{*312*}	**11**{*460*}	**9**{*312,460*}	COC1(Cn2nnnc2N2CCN(CC2)c2ccc(F)cc2)CCC1	28	14
704	**15**{*312*}	**11**{*498*}	**9**{*312,498*}	COC1(Cn2nnnc2N2CCN(CC2)c2ccccc2F)CCC1	0	0

705	**15**{*313*}	**11**{*338*}	**9**{*313,338*}	CCC1CN(CC(CC)O1)c1nnnn1CC(C)(C)C(C)(C)O	0	0
706	**15**{*314*}	**11**{*333*}	**9**{*314,333*}	CCc1nn(C)c(CC)c1Cn1nnnc1N1CCSC(C)(C)C1	0	0
707	**15**{*315*}	**11**{*337*}	**9**{*315,337*}	CSc1cccc(F)c1Cn1nnnc1N(C)CC1CCOC1	23	11
708	**15**{*316*}	**11**{*338*}	**9**{*316,338*}	CCC1CN(CC(CC)O1)c1nnnn1CCC1CC2CCC1O2	17	8
709	**15**{*317*}	**11**{*288*}	**9**{*317,288*}	CCCC1(Cn2nnnc2N2CCCN(CC2)C(C)=O)CC1	27	13
710	**15**{*317*}	**11**{*304*}	**9**{*317,304*}	CCCC1(Cn2nnnc2N2CCCC(CNC(=O)C(C)C)C2)CC1	30	14
711	**15**{*318*}	**11**{*304*}	**9**{*318,304*}	CC(C)C(=O)NCC1CCCN(C1)c1nnnn1C1CCC(C)C1	38	18
712	**15**{*319*}	**11**{*395*}	**9**{*319,395*}	CC(C)(Cn1nnnc1N1CCOC2(CCOC2)C1)C1CCCC1	16	7
713	**15**{*319*}	**11**{*288*}	**9**{*319,288*}	CC(=O)N1CCCN(CC1)c1nnnn1CC(C)(C)C1CCCC1	38	17
714	**15**{*320*}	**11**{*365*}	**9**{*320,365*}	CO[C@H]1C[C@@H](C1)n1nnnc1N1CC(CC1C)c1ccc(C)cc1	60	28
715	**15**{*320*}	**11**{*327*}	**9**{*320,327*}	CO[C@H]1C[C@@H](C1)n1nnnc1N1CCCC1c1ccsc1	189	89
716	**15**{*320*}	**11**{*302*}	**9**{*320,302*}	CO[C@H]1C[C@@H](C1)n1nnnc1N(C)CCOc1ccc(F)cc1	0	0
717	**15**{*321*}	**11**{*349*}	**9**{*321,349*}	CCC1(Cn2nnnc2N2CCCC(CC#C)C2)CCOCC1	10	5
718	**15**{*321*}	**11**{*288*}	**9**{*321,288*}	CCC1(Cn2nnnc2N2CCCN(CC2)C(C)=O)CCOCC1	0	0
719	**15**{*322*}	**11**{*302*}	**9**{*322,302*}	CN(CCOc1ccc(F)cc1)c1nnnn1C1CC(C1)C(N)=O	30	15
720	**15**{*323*}	**11**{*349*}	**9**{*323,349*}	COCC1CC(C1)n1nnnc1N1CCCC(CC#C)C1	15	7
721	**15**{*323*}	**11**{*327*}	**9**{*323,327*}	COCC1CC(C1)n1nnnc1N1CCCC1c1ccsc1	68	34
722	**15**{*323*}	**11**{*302*}	**9**{*323,302*}	COCC1CC(C1)n1nnnc1N(C)CCOc1ccc(F)cc1	16	8
723	**15**{*324*}	**11**{*349*}	**9**{*324,349*}	CS(=O)(=O)C1(Cn2nnnc2N2CCCC(CC#C)C2)CC1	13	6

724	**15**{*324*}	**11**{*350*}	**9**{*324,350*}	CN(CCC=C)c1nnnn1CC1(CC1)S(C)(=O)=O	22	11
725	**15**{*325*}	**11**{*338*}	**9**{*325,338*}	CCC1CN(CC(CC)O1)c1nnnn1CC1CCOC(C)C1	18	9
726	**15**{*326*}	**11**{*179*}	**9**{*326,179*}	CC1(Cn2nnnc2N2C[C@H]3[C@H](CO)[C@H]3C2)CCCc2ccccc12	24	12
727	**15**{*327*}	**11**{*304*}	**9**{*327,304*}	CC(C)C(=O)NCC1CCCN(C1)c1nnnn1C1CC2(CCC2)C1	30	15
728	**15**{*327*}	**11**{*472*}	**9**{*327,472*}	CC(C)(C)OC(=O)N[C@@H]1CCN(C1)c1nnnn1C1CC2(CCC2)C1	34	18
729	**15**{*328*}	**11**{*302*}	**9**{*328,302*}	CCO[C@H]1C[C@H](C1)n1nnnc1N(C)CCOc1ccc(F)cc1	0	0
730	**15**{*328*}	**11**{*327*}	**9**{*328,327*}	CCO[C@H]1C[C@H](C1)n1nnnc1N1CCCC1c1ccsc1	34	16
731	**15**{*328*}	**11**{*349*}	**9**{*328,349*}	CCO[C@H]1C[C@H](C1)n1nnnc1N1CCCC(CC#C)C1	29	15
732	**15**{*329*}	**11**{*302*}	**9**{*329,302*}	CCO[C@H]1C[C@@H](C1)n1nnnc1N(C)CCOc1ccc(F)cc1	18	9
733	**15**{*329*}	**11**{*327*}	**9**{*329,327*}	CCO[C@H]1C[C@@H](C1)n1nnnc1N1CCCC1c1ccsc1	62	33
734	**15**{*329*}	**11**{*349*}	**9**{*329,349*}	CCO[C@H]1C[C@@H](C1)n1nnnc1N1CCCC(CC#C)C1	33	15
735	**15**{*330*}	**11**{*499*}	**9**{*330,499*}	O=S1(=O)CCCCC1Cn1nnnc1N1CCCC2(CC2)CC1	25	13
736	**15**{*330*}	**11**{*493*}	**9**{*330,493*}	CC1CC2CCC(C1)N2c1nnnn1CC1CCCCS1(=O)=O	8	4
737	**15**{*331*}	**11**{*300*}	**9**{*331,300*}	FC(F)(F)c1cc(Cn2nnnc2N2CCCOCC2)cs1	55	27
738	**15**{*331*}	**11**{*337*}	**9**{*331,337*}	CN(CC1CCOC1)c1nnnn1Cc1csc(c1)C(F)(F)F	25	13
739	**15**{*332*}	**11**{*500*}	**9**{*332,500*}	CON1CCC(CC1)n1nnnc1N1CCCC(C1)c1cc2ccccc2[nH]1	0	0
740	**15**{*333*}	**11**{*501*}	**9**{*333,501*}	CCN(CC(C)=C)c1nnnn1C1COC2(CCC2)C1	35	18
741	**15**{*333*}	**11**{*302*}	**9**{*333,302*}	CN(CCOc1ccc(F)cc1)c1nnnn1C1COC2(CCC2)C1	47	24

742	**15**{*334*}	**11**{*391*}	**9**{*334,391*}	CCS(=O)(=O)c1ccc(Cn2nnnc2N(C)CC2CC2)cc1	6	3
743	**15**{*335*}	**11**{*430*}	**9**{*335,430*}	CCOC(=O)[1C@@H]1[1C@@H]2CCN(C[1C@H]12)c1nnnn1[C@@H]1CCO[C@@H]1C	31	15
744	**15**{*335*}	**11**{*436*}	**9**{*335,436*}	COC(=O)[1C@]12CCC[1C@H]1N(CC2)c1nnnn1[C@@H]1CCO[C@@H]1C	0	0
745	**15**{*335*}	**11**{*359*}	**9**{*335,359*}	C[C@H]1OCC[C@H]1n1nnnc1N1C[C@@H]2C[C@H](C1)c1cccc(=O)n1C2	12	6
746	**15**{*335*}	**11**{*419*}	**9**{*335,419*}	C[C@H]1OCC[C@H]1n1nnnc1N1C2CCC1CC1(CC1(F)F)C2	0	0
747	**15**{*335*}	**11**{*502*}	**9**{*335,502*}	C[C@H]1OCC[C@H]1n1nnnc1N1CCC2(C1)Oc1ccccc1O2	0	0
748	**15**{*335*}	**11**{*371*}	**9**{*335,371*}	C[C@H]1OCC[C@H]1n1nnnc1N1CCOC2(CCc3ccccc23)C1	0	0
749	**15**{*335*}	**11**{*408*}	**9**{*335,408*}	C[C@H]1OCC[C@H]1n1nnnc1N1CCCC2(CCCC2)C1	21	10
750	**15**{*335*}	**11**{*404*}	**9**{*335,404*}	COC(=O)[1C@]12CN(C[1C@H]1CCCC2)c1nnnn1[C@@H]1CCO[C@@H]1C	13	6
751	**15**{*335*}	**11**{*406*}	**9**{*335,406*}	C[C@H]1OCC[C@H]1n1nnnc1N1CCC(C)C2(CCC2)C1	18	9
752	**15**{*335*}	**11**{*413*}	**9**{*335,413*}	C[C@H]1OCC[C@H]1n1nnnc1N1CC(C)OC2(CCCC2)C1	23	11
753	**15**{*335*}	**11**{*407*}	**9**{*335,407*}	C[C@H]1OCC[C@H]1n1nnnc1N1CCC2(C1)CCCCC2	40	19
754	**15**{*335*}	**11**{*457*}	**9**{*335,457*}	CCc1ncc2C3CCC(Cc2n1)N3c1nnnn1[C@@H]1CCO[C@@H]1C	0	0
755	**15**{*335*}	**11**{*503*}	**9**{*335,503*}	C[C@H]1OCC[C@H]1n1nnnc1N1CCCN2C(Cc3ccccc23)C1	0	0
756	**15**{*335*}	**11**{*421*}	**9**{*335,421*}	C[C@H]1OCC[C@H]1n1nnnc1N1CCC2(C1)OCc1ccccc21	7	3
757	**15**{*335*}	**11**{*467*}	**9**{*335,467*}	C[C@H]1OCC[C@H]1n1nnnc1N1C2CCC1CC(CC(F)(F)F)C2	0	0
758	**15**{*335*}	**11**{*402*}	**9**{*335,402*}	C[C@H]1OCC[C@H]1n1nnnc1N1CC(C)OC2(CCCCC2)C1	0	0
759	**15**{*335*}	**11**{*104*}	**9**{*335,104*}	C[C@H]1OCC[C@H]1n1nnnc1N1CCOCC2(CC	0	0

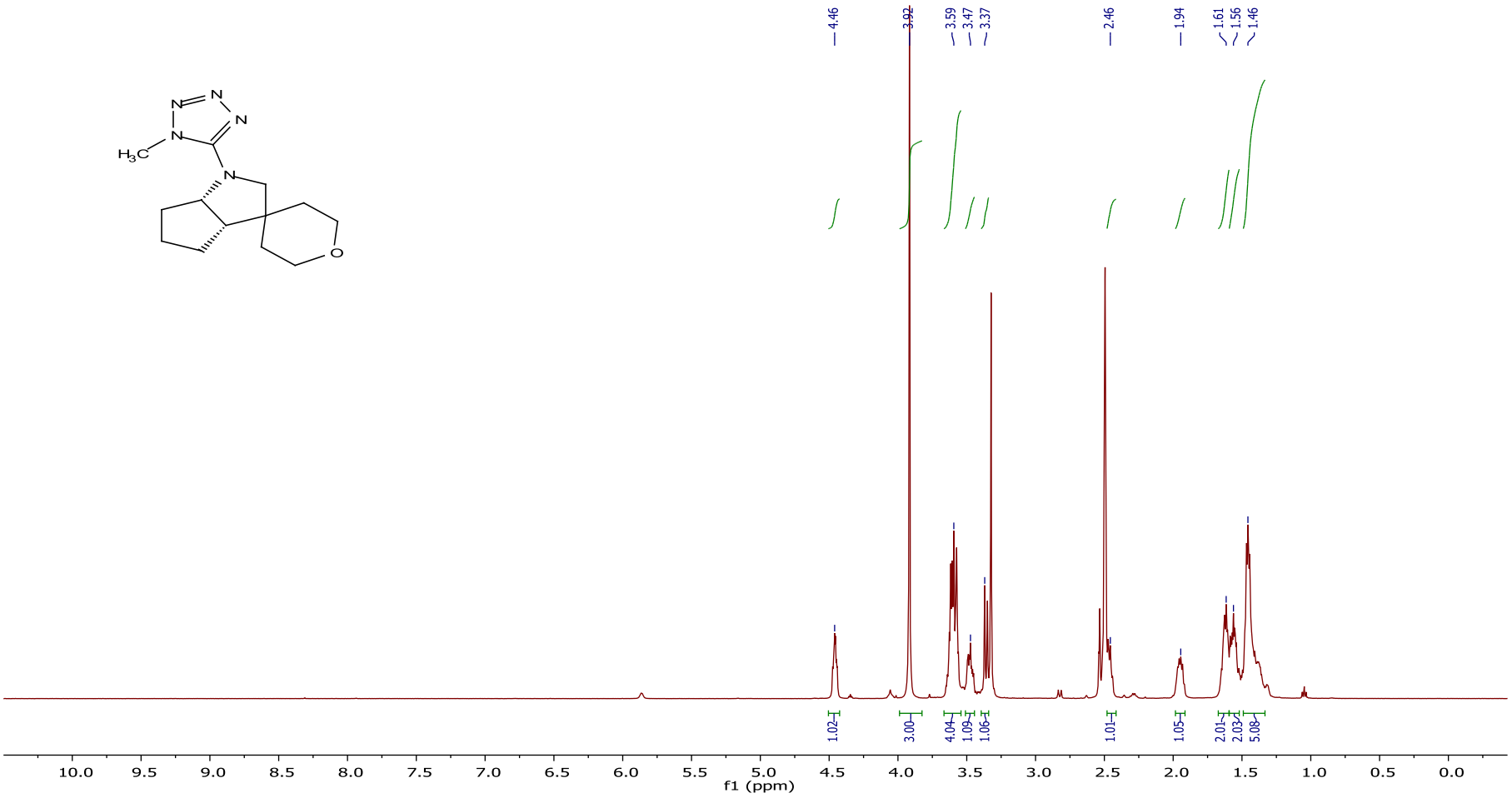
				CC2)C1		
760	**15**{*335*}	**11**{*409*}	**9**{*335,409*}	C[C@H]1OCC[C@H]1n1nnnc1N1CCSC2(CCCCC2)C1	0	0
761	**15**{*335*}	**11**{*412*}	**9**{*335,412*}	CON(CC1CC2CCC1C2)c1nnnn1[C@@H]1CCO[C@@H]1C	0	0
762	**15**{*335*}	**11**{*282*}	**9**{*335,282*}	C[C@H]1OCC[C@H]1n1nnnc1N1CCN(C(C)=O)C2(CCCCC2)C1	17	8
763	**15**{*336*}	**11**{*288*}	**9**{*336,288*}	CCC[1C@@H]1C[1C@H]1n1nnnc1N1CCCN(CC1)C(C)=O	33	16
764	**15**{*336*}	**11**{*304*}	**9**{*336,304*}	CCC[1C@@H]1C[1C@H]1n1nnnc1N1CCCC(CNC(=O)C(C)C)C1	17	8
765	**15**{*337*}	**11**{*322*}	**9**{*337,322*}	CN(C1CC1)c1nnnn1C1CCOC(C1)c1ccnn1C	25	12
766	**15**{*337*}	**11**{*356*}	**9**{*337,356*}	CN(CC1CCC1)c1nnnn1C1CCOC(C1)c1ccnn1C	30	16
767	**15**{*338*}	**11**{*322*}	**9**{*338,322*}	CN(C1CC1)c1nnnn1C[C@@H]1CCCN(C)[C@H]1c1ccnn1C	0	0
768	**15**{*338*}	**11**{*391*}	**9**{*338,391*}	CN(CC1CC1)c1nnnn1C[C@@H]1CCCN(C)[C@H]1c1ccnn1C	33	16
769	**15**{*339*}	**11**{*288*}	**9**{*339,288*}	CC(=O)N1CCCN(CC1)c1nnnn1CC(C1CCC1)C1CCC1	21	10
770	**15**{*339*}	**11**{*395*}	**9**{*339,395*}	C(C(C1CCC1)C1CCC1)n1nnnc1N1CCOC2(CCOC2)C1	32	15
771	**15**{*340*}	**11**{*504*}	**9**{*340,504*}	O=C1CN(CCN1C1CC1)c1nnnn1CCC1CCC2(CCC2)O1	11	6
772	**15**{*340*}	**11**{*319*}	**9**{*340,319*}	CN(CC1COCCO1)c1nnnn1CCC1CCC2(CCC2)O1	53	25
773	**15**{*341*}	**11**{*346*}	**9**{*341,346*}	CCN(C)c1nnnn1Cc1nc(n2CCCCc12)C(F)(F)F	70	34
774	**15**{*342*}	**11**{*288*}	**9**{*342,288*}	CC(=O)N1CCCN(CC1)c1nnnn1CC(C)(C)C1CCC1	0	0
775	**15**{*343*}	**11**{*288*}	**9**{*343,288*}	CC(=O)N1CCCN(CC1)c1nnnn1CC1(C)CC1(Cl)Cl	0	0
776	**15**{*344*}	**11**{*304*}	**9**{*344,304*}	CC(C)[1C@@H]1C[1C@H]1n1nnnc1N1CCCC(CNC(=O)C(C)C)C1	36	17

777	**15**{*345*}	**11**{*304*}	**9**{*345,304*}	CC(C)C[1C@@H]1C[1C@H]1n1nnnc1N1CCCC(CNC(=O)C(C)C)C1	34	17
778	**15**{*346*}	**11**{*391*}	**9**{*346,391*}	CN(CC1CC1)c1nnnn1C[1C@@H]1CCO[1C@H]1c1c(C)nn(C)c1C	32	17
779	**15**{*347*}	**11**{*327*}	**9**{*347,327*}	CC(C)(C)O[C@H]1C[C@H](C1)n1nnnc1N1CCCC1c1ccsc1	0	0
780	**15**{*347*}	**11**{*349*}	**9**{*347,349*}	CC(C)(C)O[C@H]1C[C@H](C1)n1nnnc1N1CCCC(CC#C)C1	0	0
781	**15**{*348*}	**11**{*349*}	**9**{*348,349*}	COC(=O)CC1CC(C1)n1nnnc1N1CCCC(CC#C)C1	14	7
782	**15**{*348*}	**11**{*327*}	**9**{*348,327*}	COC(=O)CC1CC(C1)n1nnnc1N1CCCC1c1ccsc1	31	16
783	**15**{*349*}	**11**{*302*}	**9**{*349,302*}	CCN1CCC(C1=O)n1nnnc1N(C)CCOc1ccc(F)cc1	0	0
784	**15**{*350*}	**11**{*302*}	**9**{*350,302*}	CN(CCOc1ccc(F)cc1)c1nnnn1[C@H]1C[C@@H](C1)C(N)=O	13	6
785	**15**{*351*}	**11**{*338*}	**9**{*351,338*}	CCC1CN(CC(CC)O1)c1nnnn1CCC1(COC)CC1	33	16
786	**15**{*352*}	**11**{*338*}	**9**{*352,338*}	CCC1CN(CC(CC)O1)c1nnnn1CCCC1(O)CCC1	38	20
787	**15**{*353*}	**11**{*501*}	**9**{*353,501*}	CCN(CC(C)=C)c1nnnn1CCN1CC2CCCCN2C1=O	0	0
788	**15**{*354*}	**11**{*327*}	**9**{*354,327*}	C(C1SCCS1)n1nnnc1N1CCCC1c1ccsc1	8	4
789	**15**{*354*}	**11**{*349*}	**9**{*354,349*}	C#CCC1CCCN(C1)c1nnnn1CC1SCCS1	0	0
790	**15**{*355*}	**11**{*297*}	**9**{*355,297*}	CC1(OCCO1)C1CCN(CC1)c1nnnn1C1COC(C1)C1CC1	37	17
791	**15**{*355*}	**11**{*298*}	**9**{*355,298*}	CC1(OCCO1)C1CCCN(C1)c1nnnn1C1COC(C1)C1CC1	8	4
792	**15**{*356*}	**11**{*350*}	**9**{*356,350*}	CN(CCC=C)c1nnnn1C1CCN(C2CCCCC2)C1=O	0	0
793	**15**{*357*}	**11**{*349*}	**9**{*357,349*}	CO[C@@H]1C[C@H](Cn2nnnc2N2CCCC(CC#C)C2)C1	60	28
794	**15**{*357*}	**11**{*327*}	**9**{*357,327*}	CO[C@@H]1C[C@H](Cn2nnnc2N2CCCC2c2ccsc2)C1	44	22
795	**15**{*358*}	**11**{*349*}	**9**{*358,349*}	O=C1C(CCN1C1CCC1)n1nnnc1N1CCCC(CC#	0	0

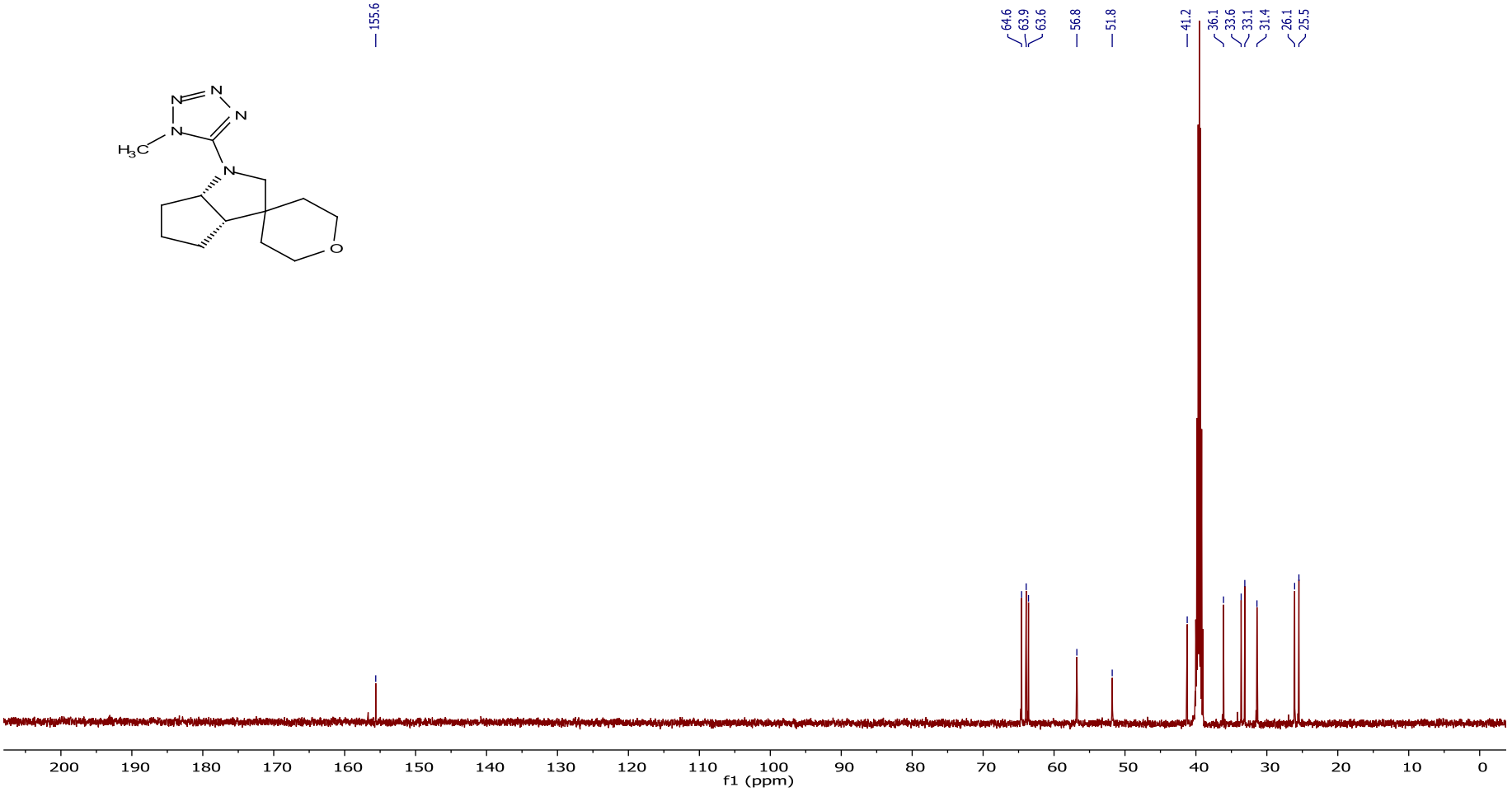
				C)C1		
796	**15**{*358*}	**11**{*350*}	**9**{*358,350*}	CN(CCC=C)c1nnnn1C1CCN(C2CCC2)C1=O	0	0
797	**15**{*359*}	**11**{*505*}	**9**{*359,505*}	CC1CC2(CCC(Cn3nnnc3N3CC(C)CC(C)C3)O2)CO1	34	16
798	**15**{*359*}	**11**{*465*}	**9**{*359,465*}	CC1CC2(CCC(Cn3nnnc3N3CCC(C)C(C)C3)O2)CO1	22	11
799	**15**{*359*}	**11**{*501*}	**9**{*359,501*}	CCN(CC(C)=C)c1nnnn1CC1CCC2(COC(C)C2)O1	21	10
800	**15**{*359*}	**11**{*340*}	**9**{*359,340*}	CC1CC2(CCC(Cn3nnnc3N3CCCCCC3)O2)CO1	73	34
801	**15**{*359*}	**11**{*480*}	**9**{*359,480*}	CC1CC2(CCC(Cn3nnnc3N3CCC(C)CC3)O2)CO1	17	8
802	**15**{*359*}	**11**{*479*}	**9**{*359,479*}	CC1CC2(CCC(Cn3nnnc3N3CCCC(C)C3)O2)CO1	26	13
803	**15**{*360*}	**11**{*506*}	**9**{*360,506*}	CN(CC=C)c1nnnn1CC1(C)CCOC2(CCC2)C1	27	14
804	**15**{*360*}	**11**{*473*}	**9**{*360,473*}	CCO[C@H]1CCN(C1)c1nnnn1CC1(C)CCOC2(CCC2)C1	56	26
805	**15**{*361*}	**11**{*350*}	**9**{*361,350*}	CN(CCC=C)c1nnnn1C[1C@@H]1CCO[1C@H]1c1ccccc1	22	11
806	**15**{*362*}	**11**{*501*}	**9**{*362,501*}	CCN(CC(C)=C)c1nnnn1CC12COCCN1C(=O)COC2	9	5
807	**15**{*363*}	**11**{*501*}	**9**{*363,501*}	CCN(CC(C)=C)c1nnnn1CC1CC2(CO1)CCOCC2	16	8
808	**15**{*364*}	**11**{*501*}	**9**{*364,501*}	CCN(CC(C)=C)c1nnnn1CC1CC2CCC(C1)S2(=O)=O	43	21
809	**15**{*365*}	**11**{*501*}	**9**{*365,501*}	CCN(CC(C)=C)c1nnnn1CC1CCC2(CCOCC2)CO1	24	12
810	**15**{*366*}	**11**{*501*}	**9**{*366,501*}	CCN(CC(C)=C)c1nnnn1CCC1CCC2(CCOCC2)CO1	37	18
811	**15**{*367*}	**11**{*288*}	**9**{*367,288*}	CC(=O)N1CCCN(CC1)c1nnnn1CCC1CCCC1(F)F	0	0
812	**15**{*368*}	**11**{*504*}	**9**{*368,504*}	O=C1CN(CCN1C1CC1)c1nnnn1CC1CCC2(CCC2)CO1	0	0

813	**15**{*369*}	**11**{*349*}	**9**{*369,349*}	NC(=O)CC1CC(C1)n1nnnc1N1CCCC(CC#C)C1	26	13
814	**15**{*369*}	**11**{*327*}	**9**{*369,327*}	NC(=O)CC1CC(C1)n1nnnc1N1CCCC1c1ccsc1	38	20
815	**15**{*370*}	**11**{*504*}	**9**{*370,504*}	O=C1CN(CCN1C1CC1)c1nnnn1CC1CC2CCC(C1)S2	0	0
816	**15**{*370*}	**11**{*507*}	**9**{*370,507*}	OC1(CCN(C1)c1nnnn1CC1CC2CCC(C1)S2)C(F)F	24	11
817	**15**{*371*}	**11**{*350*}	**9**{*371,350*}	COC1(Cn2nnnc2N(C)CCC=C)CCS(=O)(=O)C1	9	4
818	**15**{*372*}	**11**{*325*}	**9**{*372,325*}	O=c1[nH]ncn1C1CCN(CC1)c1nnnn1CC12CC1CCCC2	32	15
819	**15**{*373*}	**11**{*349*}	**9**{*373,349*}	FC(F)(F)C1CCC(Cn2nnnc2N2CCCC(CC#C)C2)O1	5	2
820	**15**{*373*}	**11**{*350*}	**9**{*373,350*}	CN(CCC=C)c1nnnn1CC1CCC(O1)C(F)(F)F	15	7
821	**15**{*374*}	**11**{*508*}	**9**{*374,508*}	FC1(F)[1C@@H](Cn2nnnc2N2CCC3(COC3)C2)[1C@@H]1c1ccccc1	0	0
822	**15**{*374*}	**11**{*509*}	**9**{*374,509*}	FC1(F)[1C@@H](Cn2nnnc2N2C3CCC2CC3)[1C@@H]1c1ccccc1	0	0
823	**15**{*374*}	**11**{*179*}	**9**{*374,179*}	OC[C@H]1[C@@H]2CN(C[C@H]12)c1nnnn1C[1C@@H]1[1C@@H](c2ccccc2)C1(F)F	0	0
824	**15**{*374*}	**11**{*510*}	**9**{*374,510*}	FC1(F)[1C@@H](Cn2nnnc2N2CC3CC3C2)[1C@@H]1c1ccccc1	0	0
825	**15**{*375*}	**11**{*511*}	**9**{*375,511*}	CN(C)C(=O)C1CCN(C1)c1nnnn1[1C@@H]1[1C@H]2Cc3ccccc3[1C@@H]12	71	36
826	**15**{*375*}	**11**{*504*}	**9**{*375,504*}	O=C1CN(CCN1C1CC1)c1nnnn1[1C@@H]1[1C@H]2Cc3ccccc3[1C@@H]12	0	0
827	**15**{*376*}	**11**{*504*}	**9**{*376,504*}	O=C1CN(CCN1C1CC1)c1nnnn1CC1CCCC2(CCC2)O1	0	0
828	**15**{*377*}	**11**{*501*}	**9**{*377,501*}	CCN(CC(C)=C)c1nnnn1CC1CCC2(CCOCC2)O1	17	8
829	**15**{*378*}	**11**{*511*}	**9**{*378,511*}	CN(C)C(=O)C1CCN(C1)c1nnnn1C[1C@]12C[1C@H]1CCC2	26	13
830	**15**{*378*}	**11**{*472*}	**9**{*378,472*}	CC(C)(C)OC(=O)N[C@@H]1CCN(C1)c1nnnn1C[1C@]12C[1C@H]1CCC2	21	11

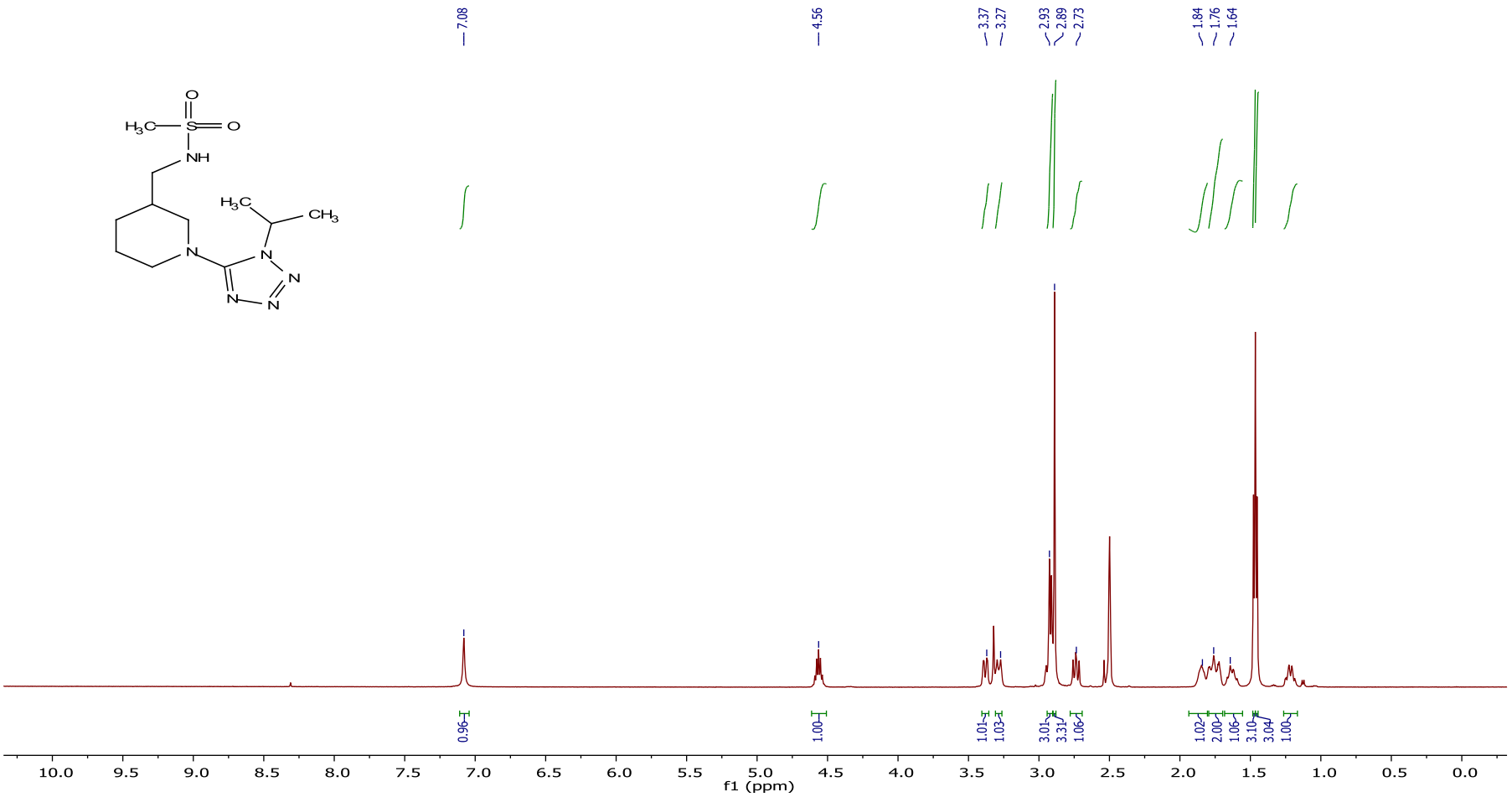
^{1}H NMR spectrum of the compound **8**{*2,8*}.



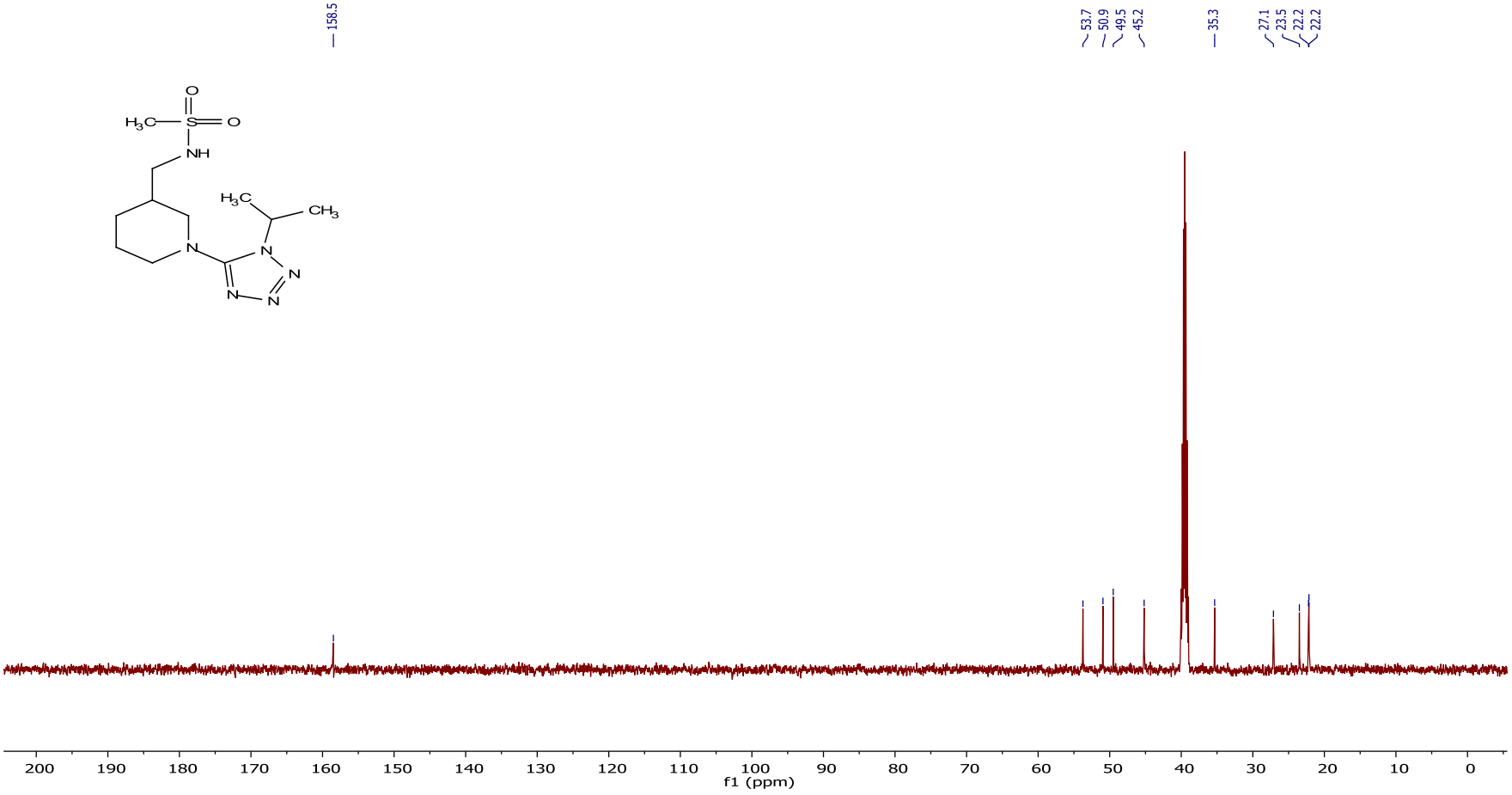
^{13}C NMR spectrum of the compound **8**{*2,8*}.



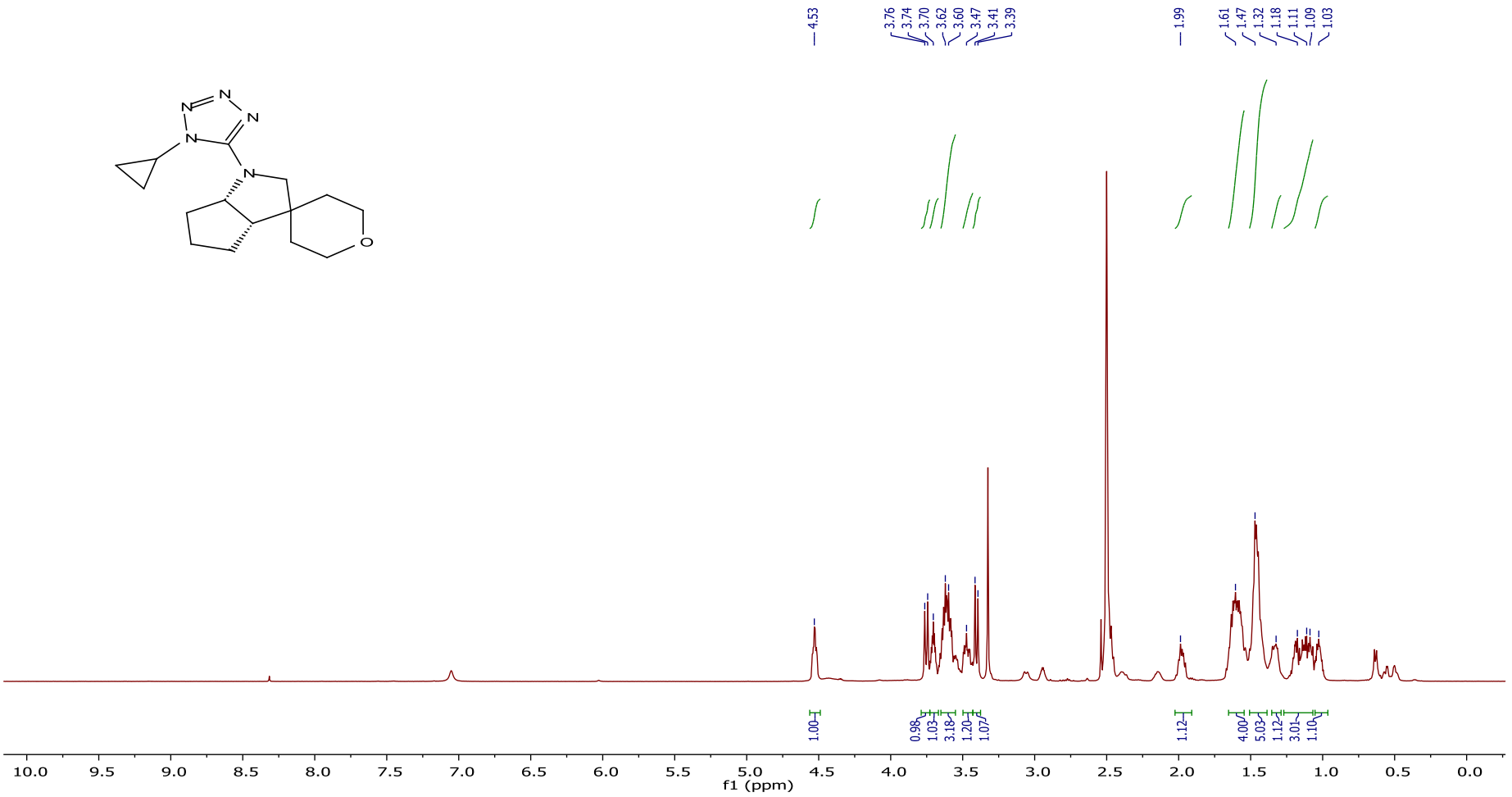
^{1}H NMR spectrum of the compound **8**{*10,50*}.



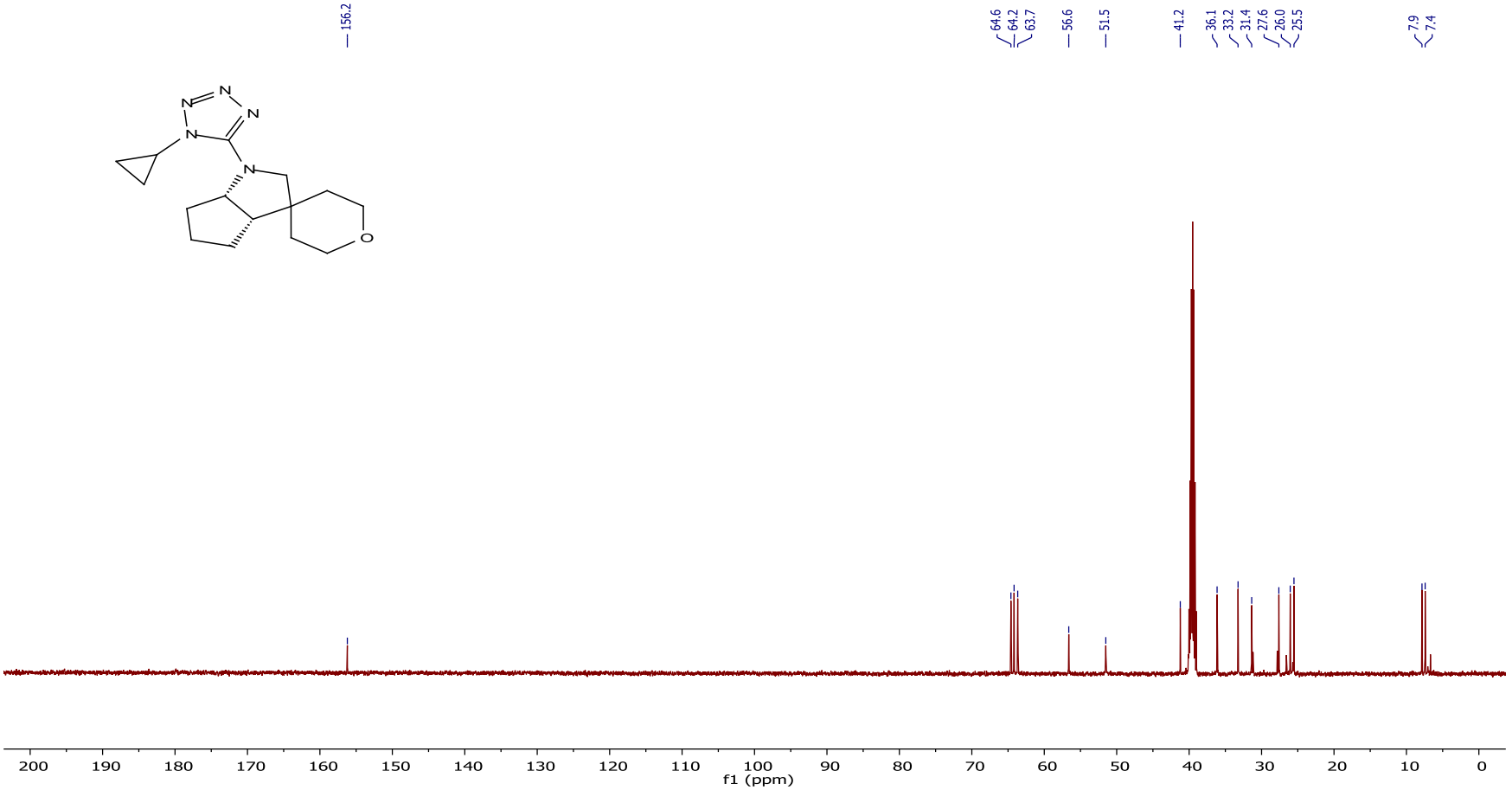
^{13}C NMR spectrum of the compound **8**{*10,50*}.



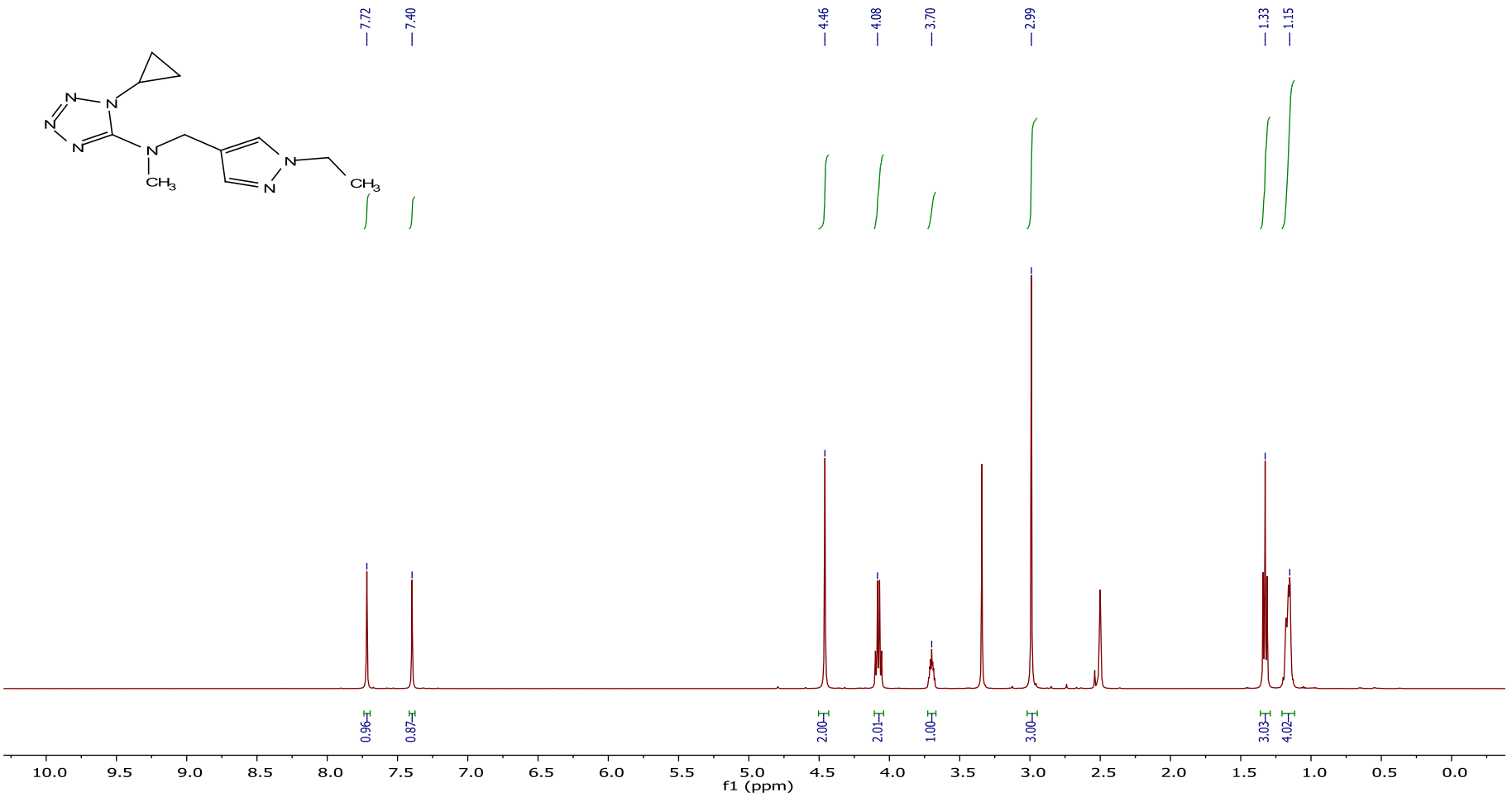
^{1}H NMR spectrum of the compound **8**{*15,8)*}.



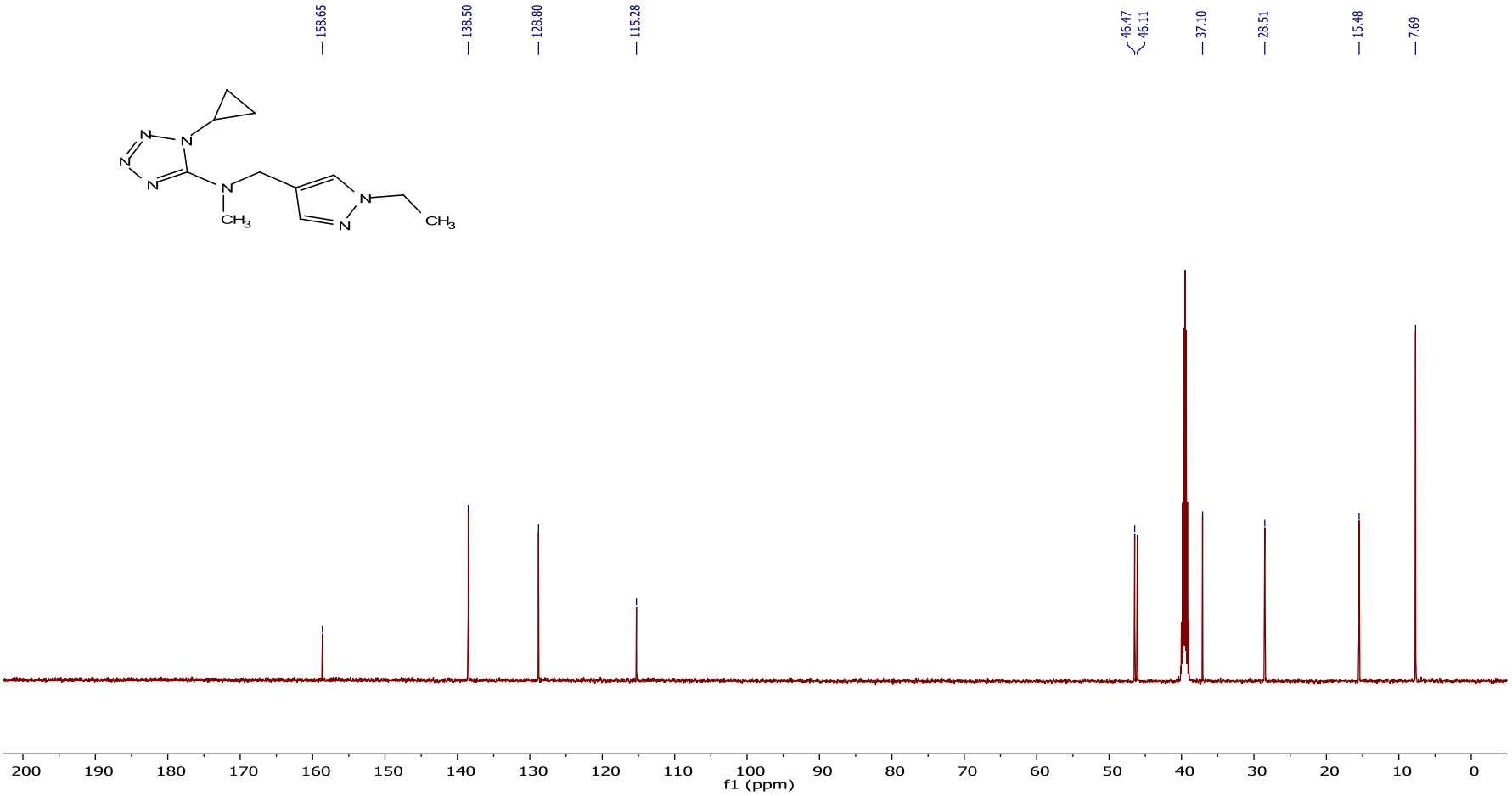
^{13}C NMR spectrum of the compound **8**{*15,8)*}.



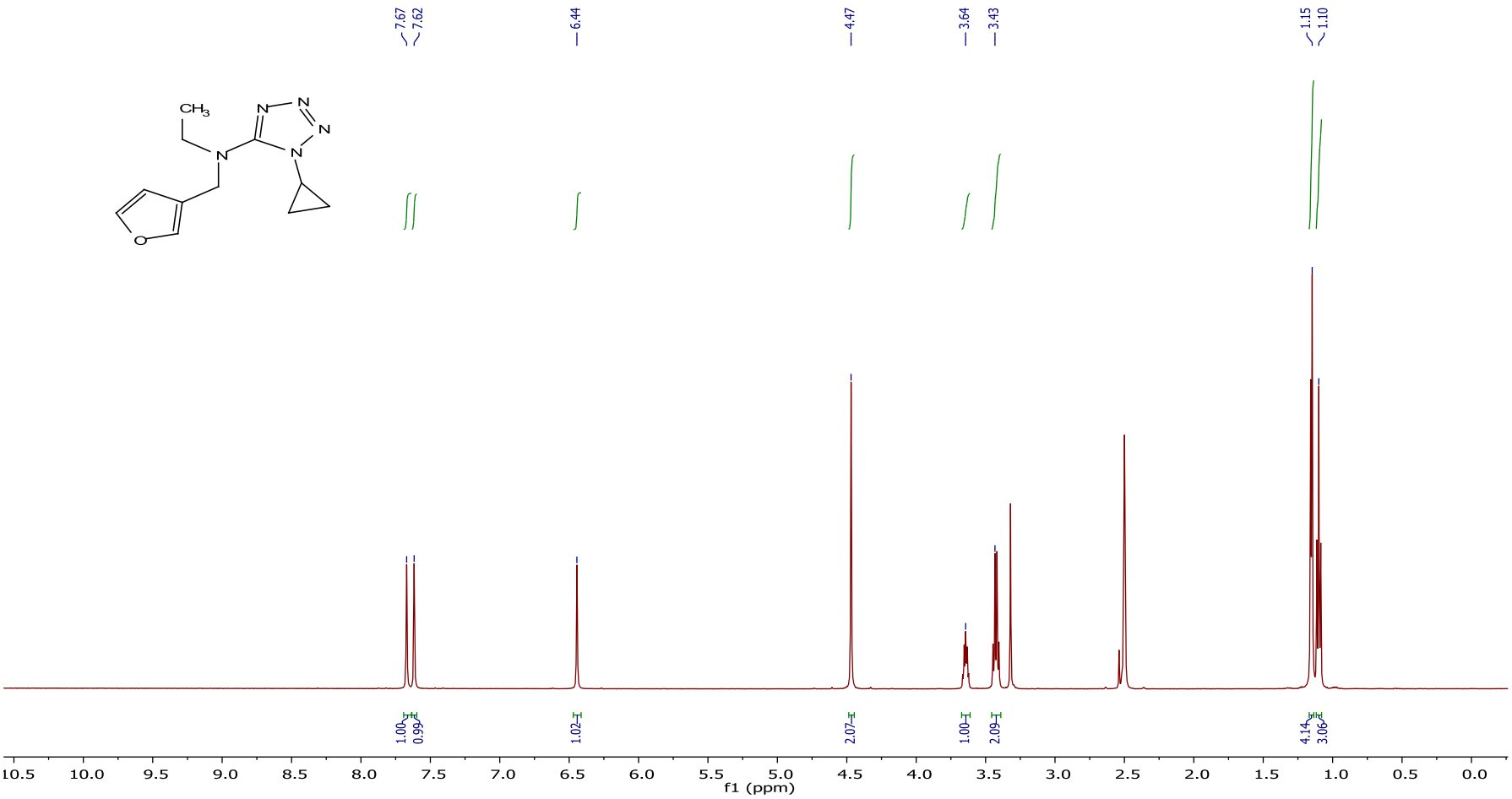
^{1}H NMR spectrum of the compound **8**{*15,71*}.



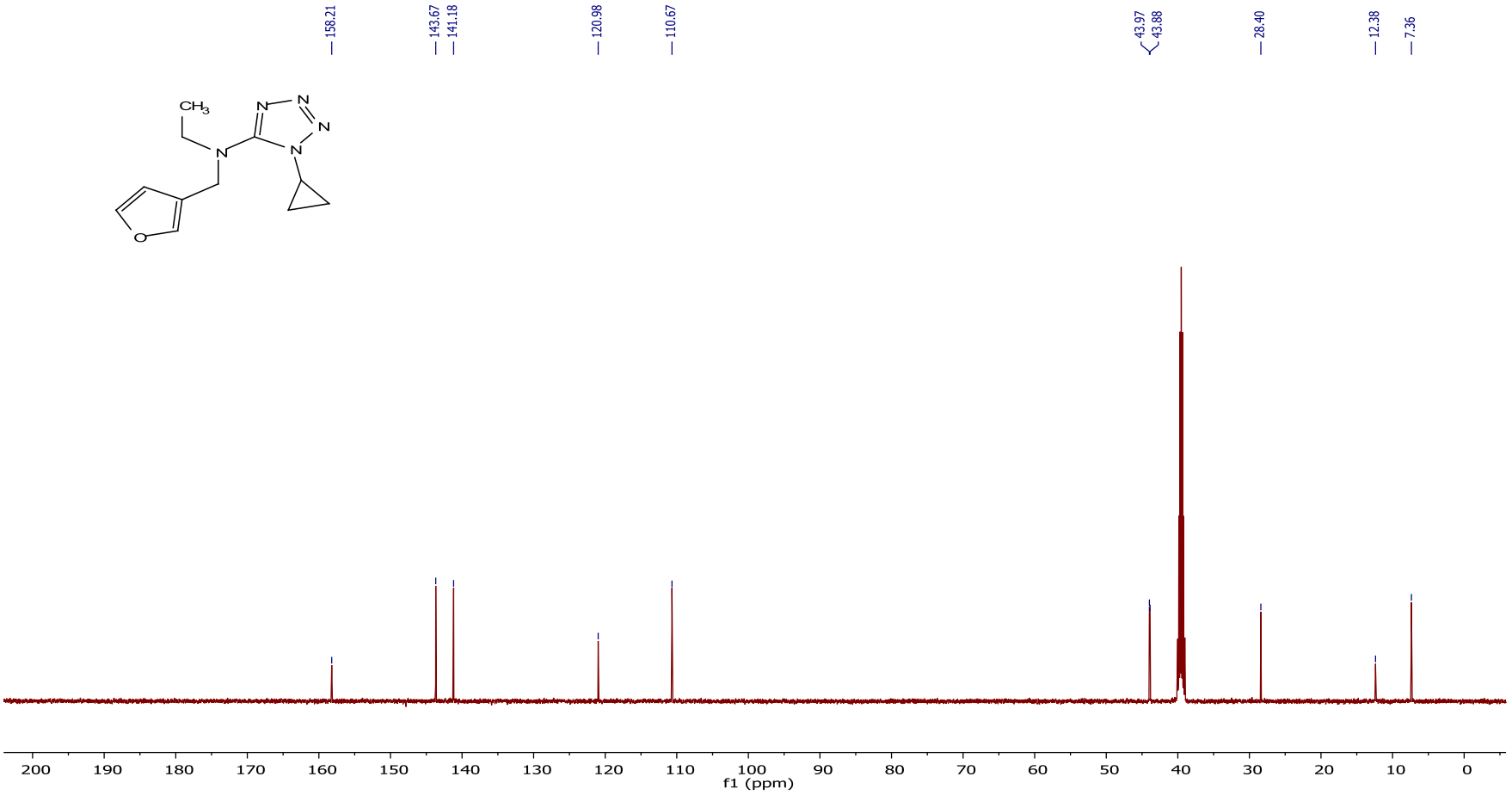
^{13}C NMR spectrum of the compound **8**{*15,71*}.



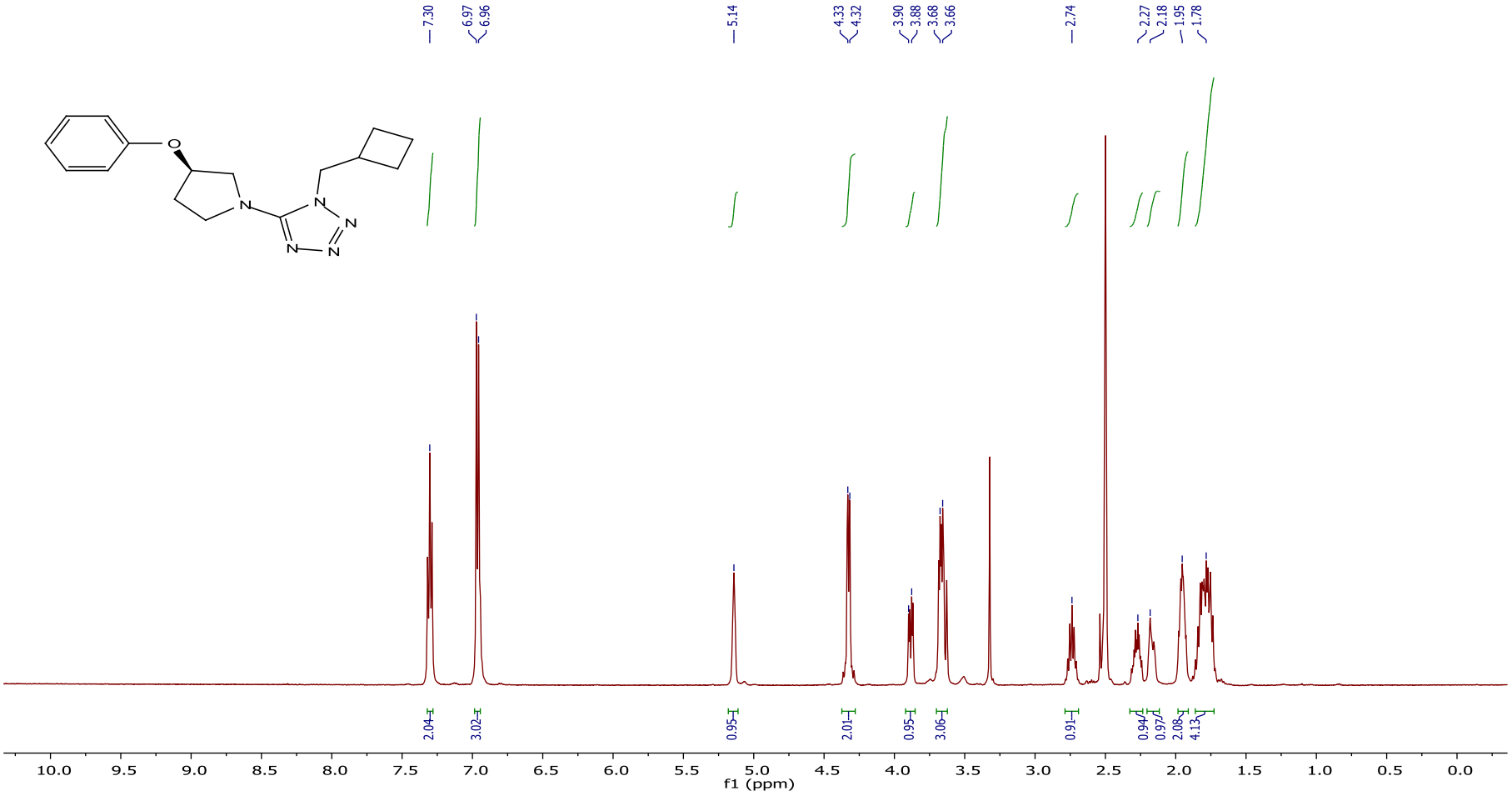
^{1}H NMR spectrum of the compound **8**{*15,72)*}.



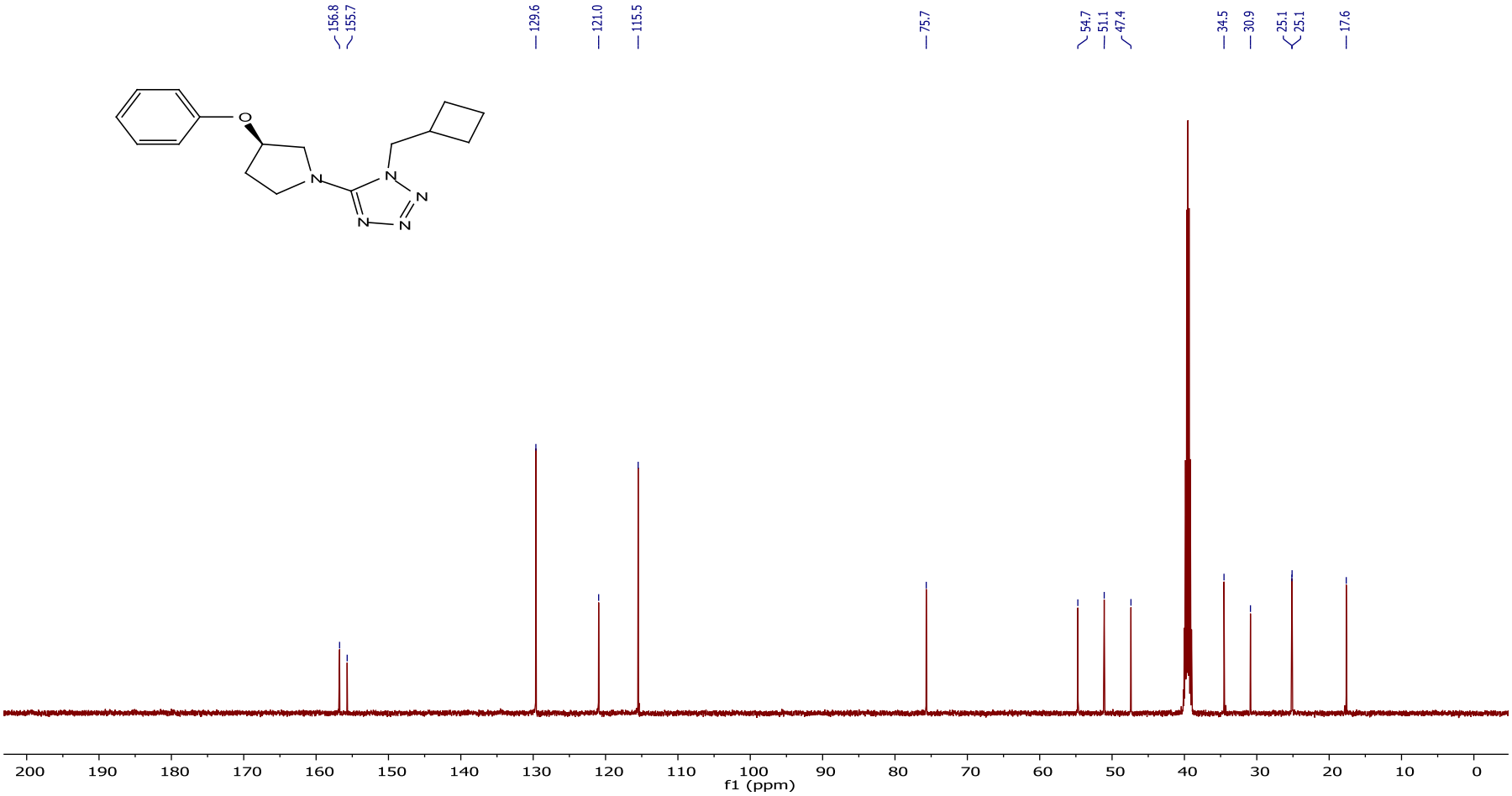
^{13}C NMR spectrum of the compound **8**{*15,72)*}.



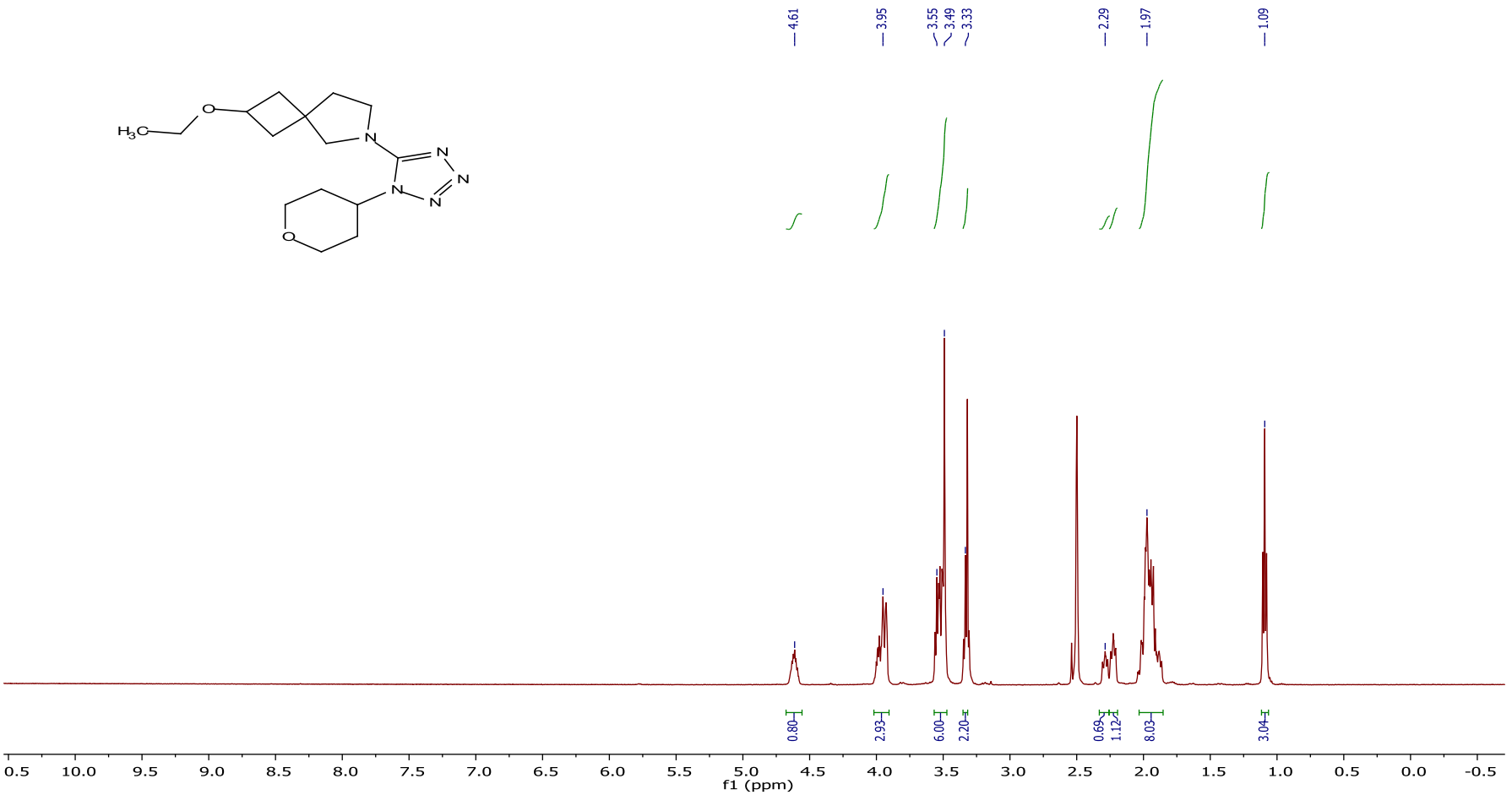
^{1}H NMR spectrum of the compound **8**{*36,164*}.



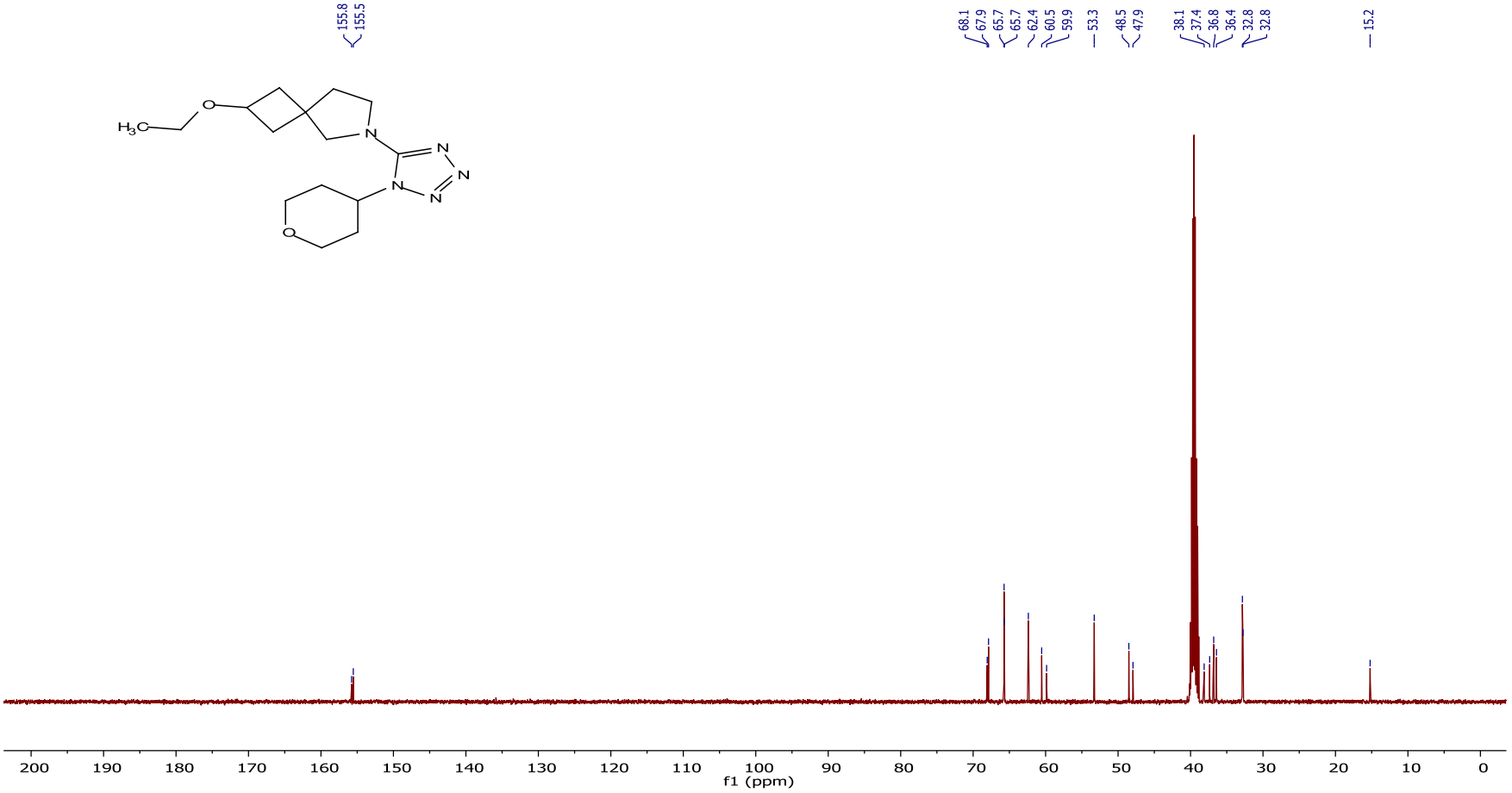
^{13}C NMR spectrum of the compound **8**{*36,164*}.



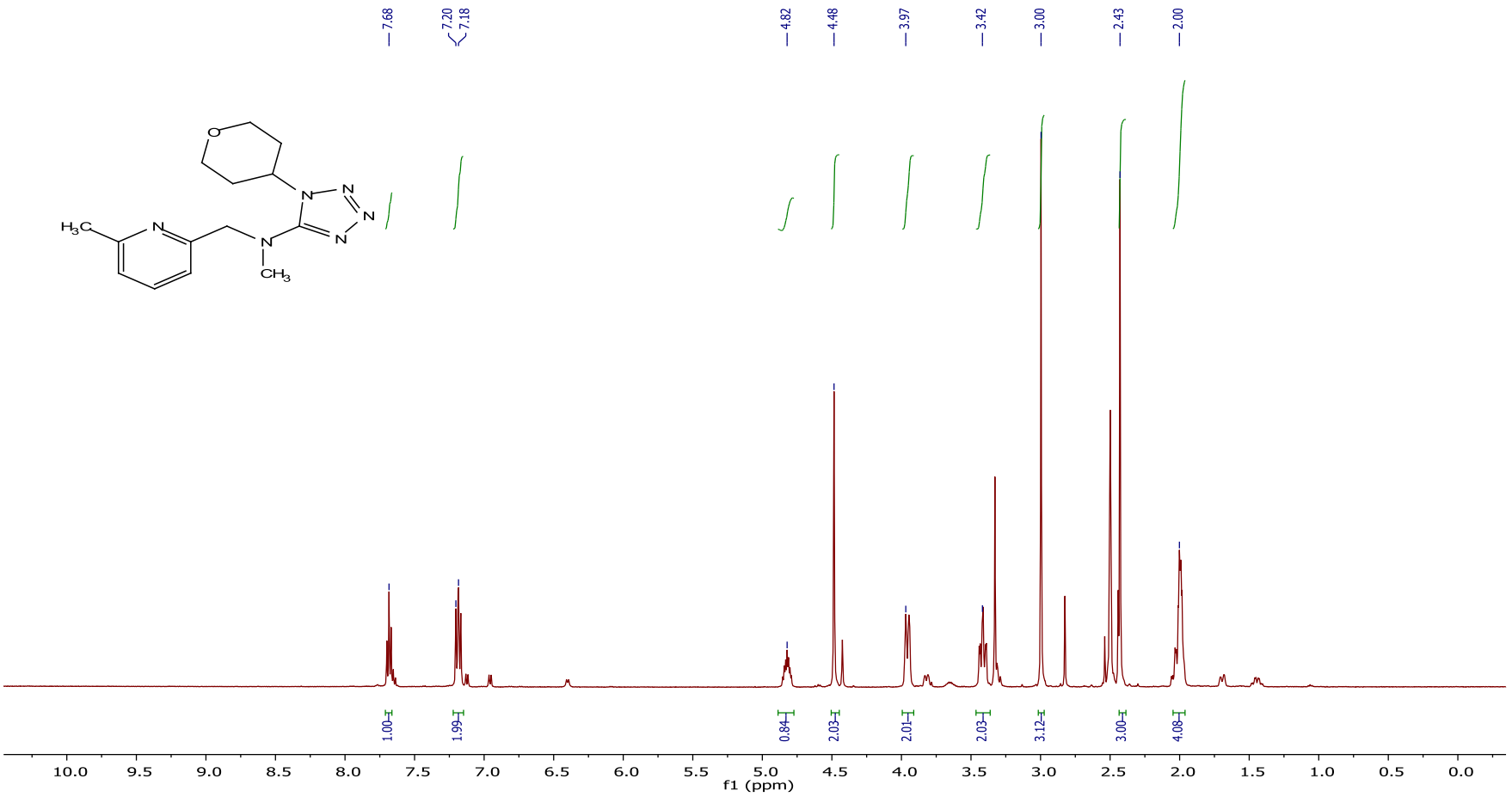
^{1}H NMR spectrum of the compound **8**{*40,188*}.



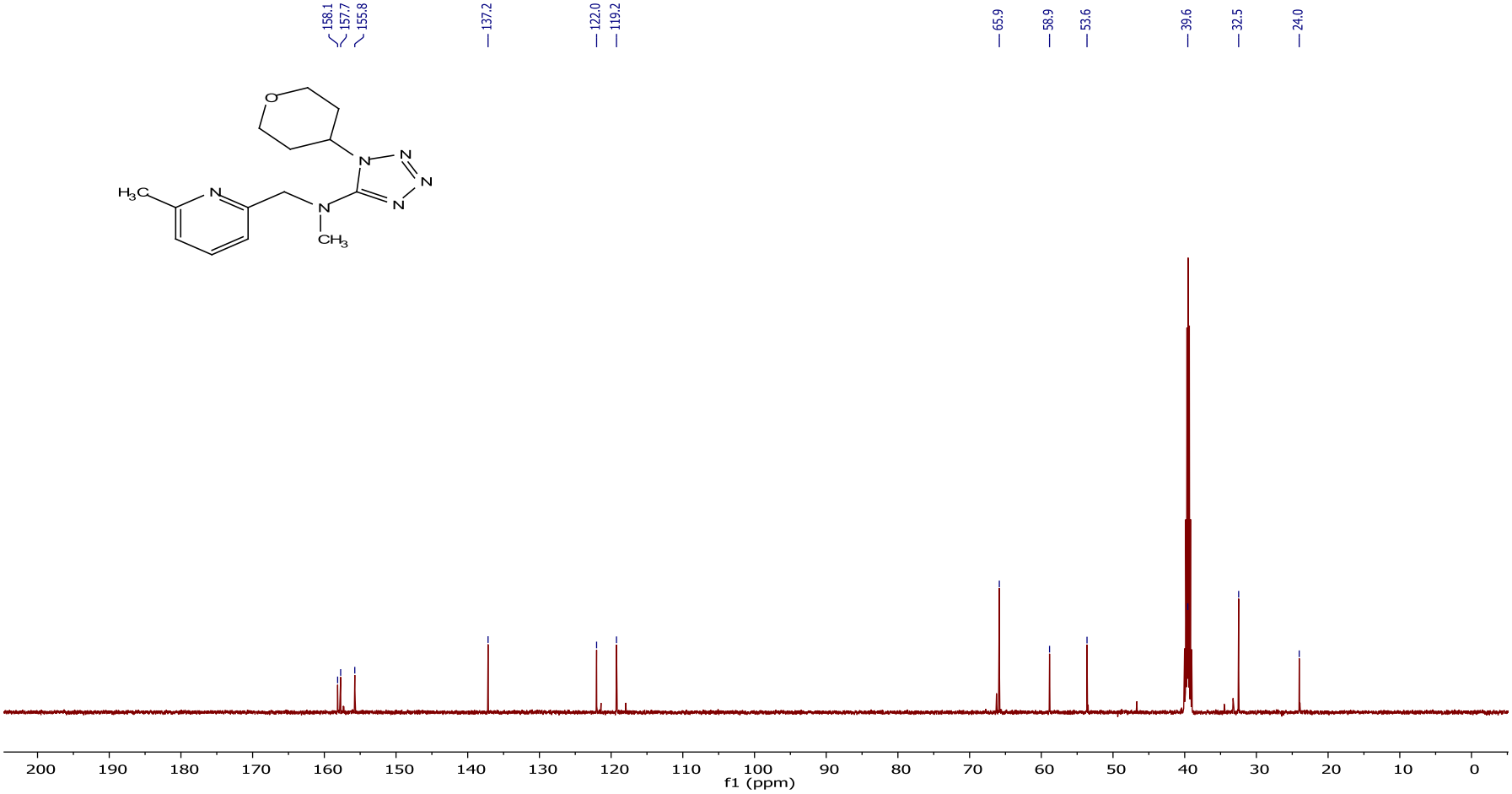
^{13}C NMR spectrum of the compound **8**{*40,188*}.



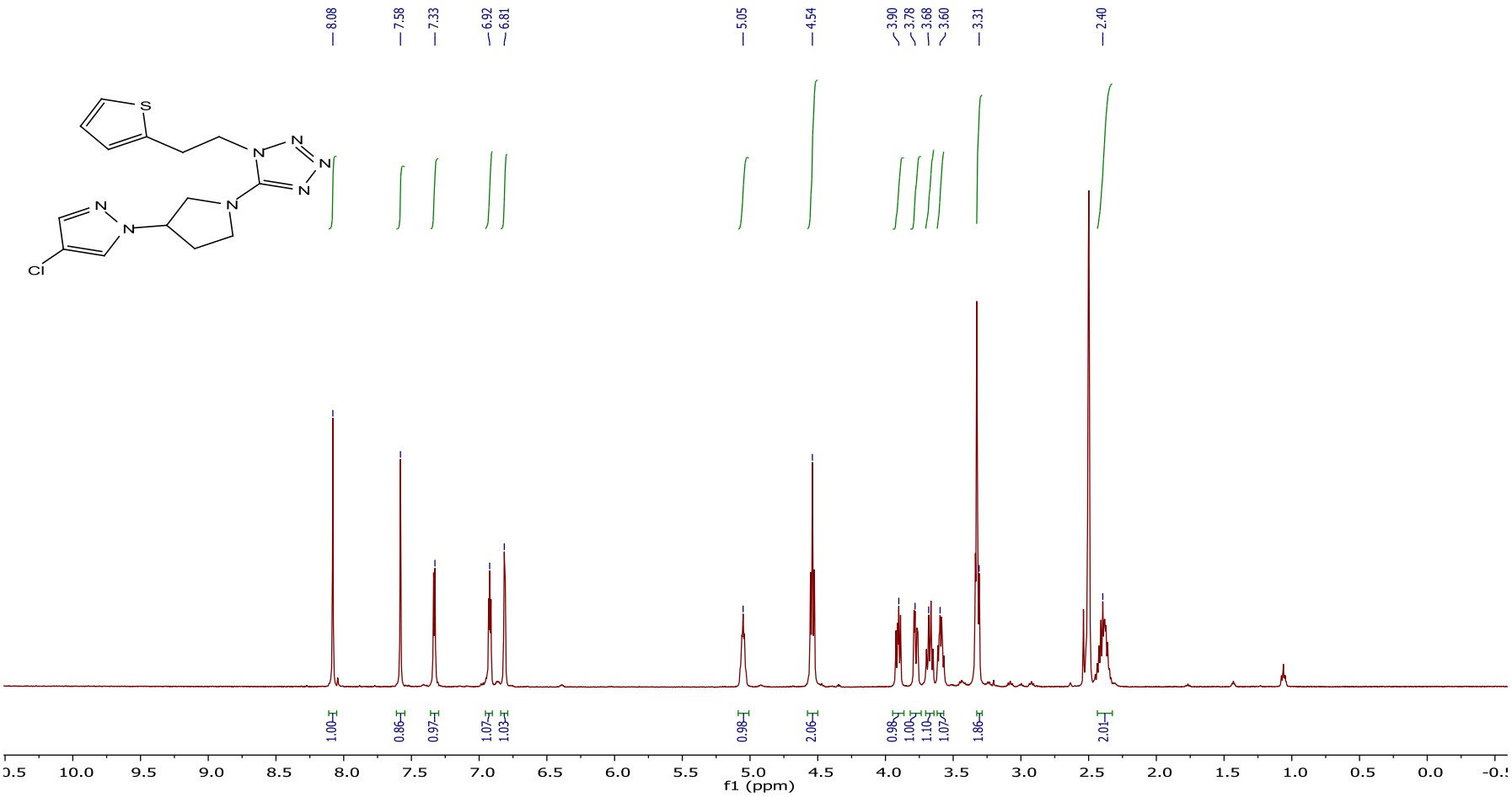
^{1}H NMR spectrum of the compound **8**{*40,192*}.



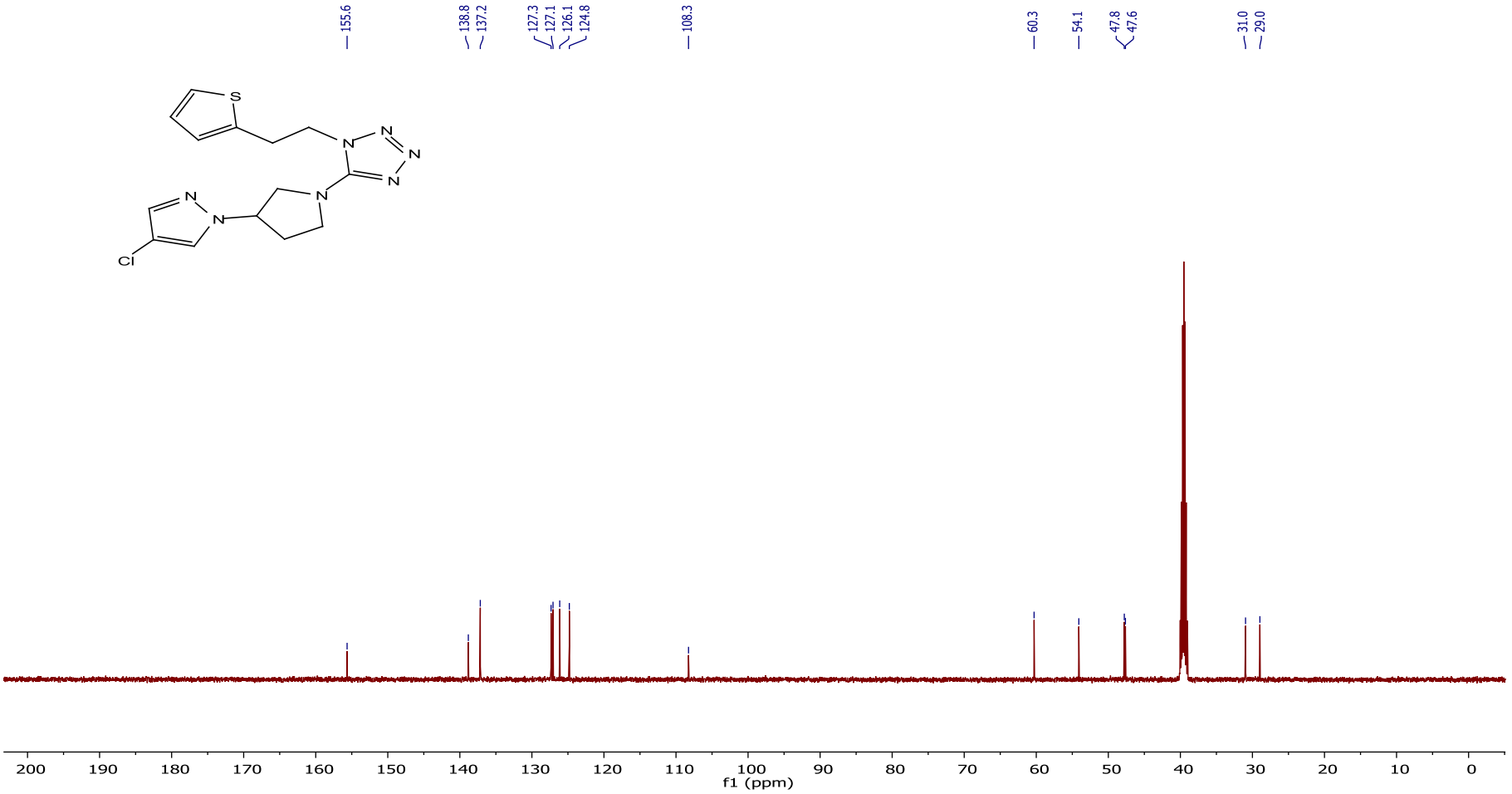
^{13}C NMR spectrum of the compound **8**{*40,192*}.



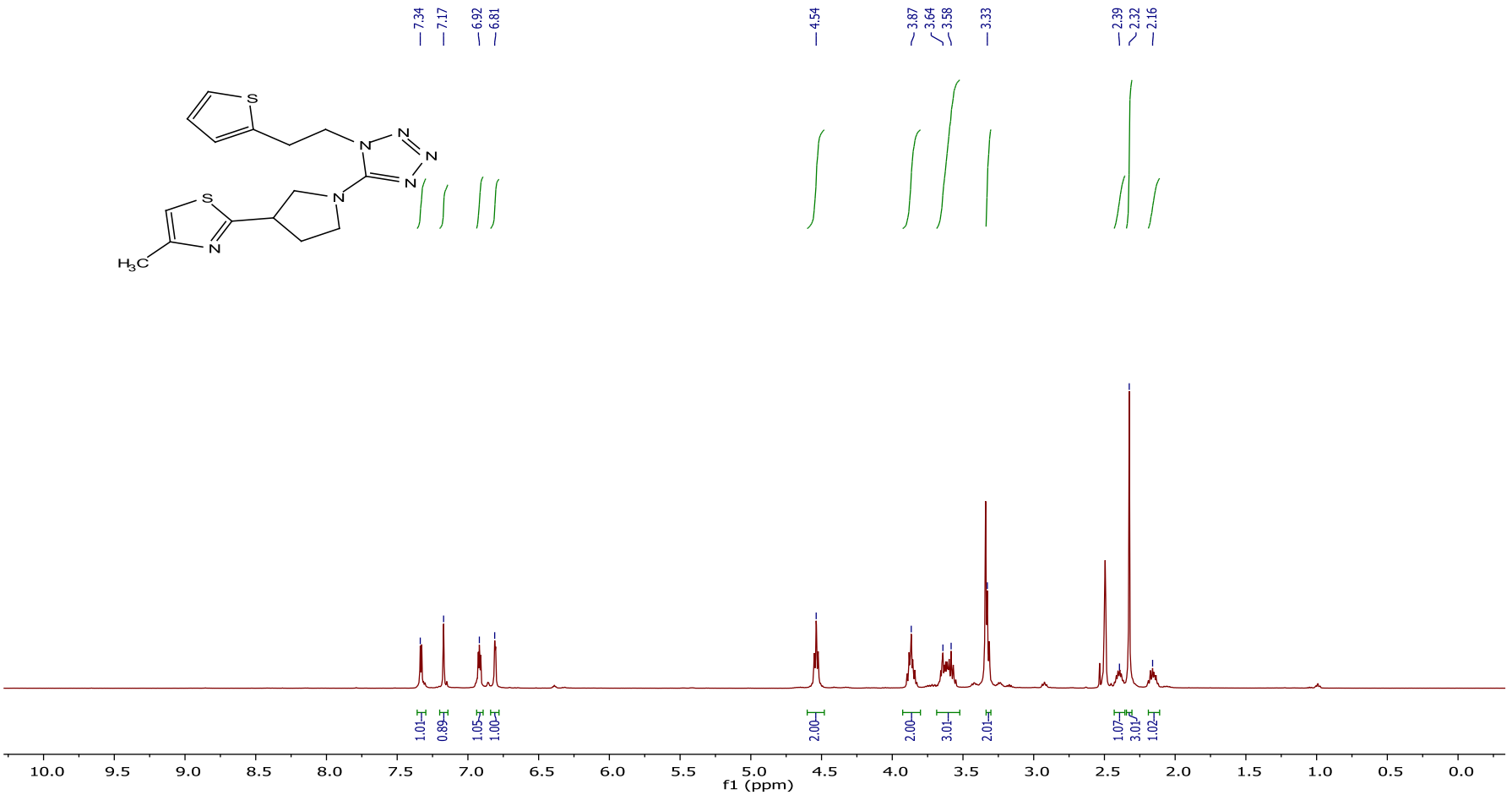
^{1}H NMR spectrum of the compound **8**{*41,147*}.



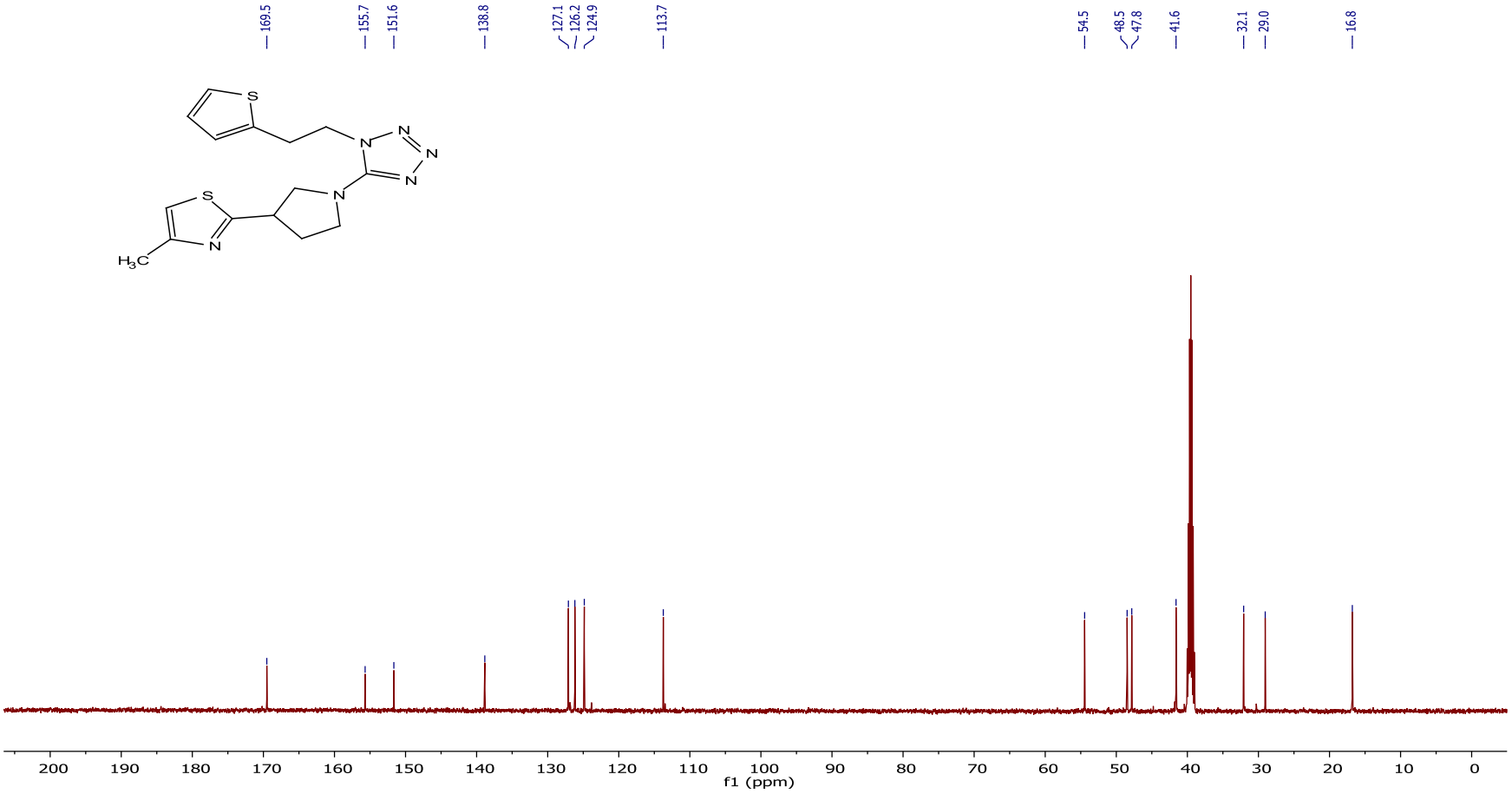
^{13}C NMR spectrum of the compound **8**{*41,147*}.



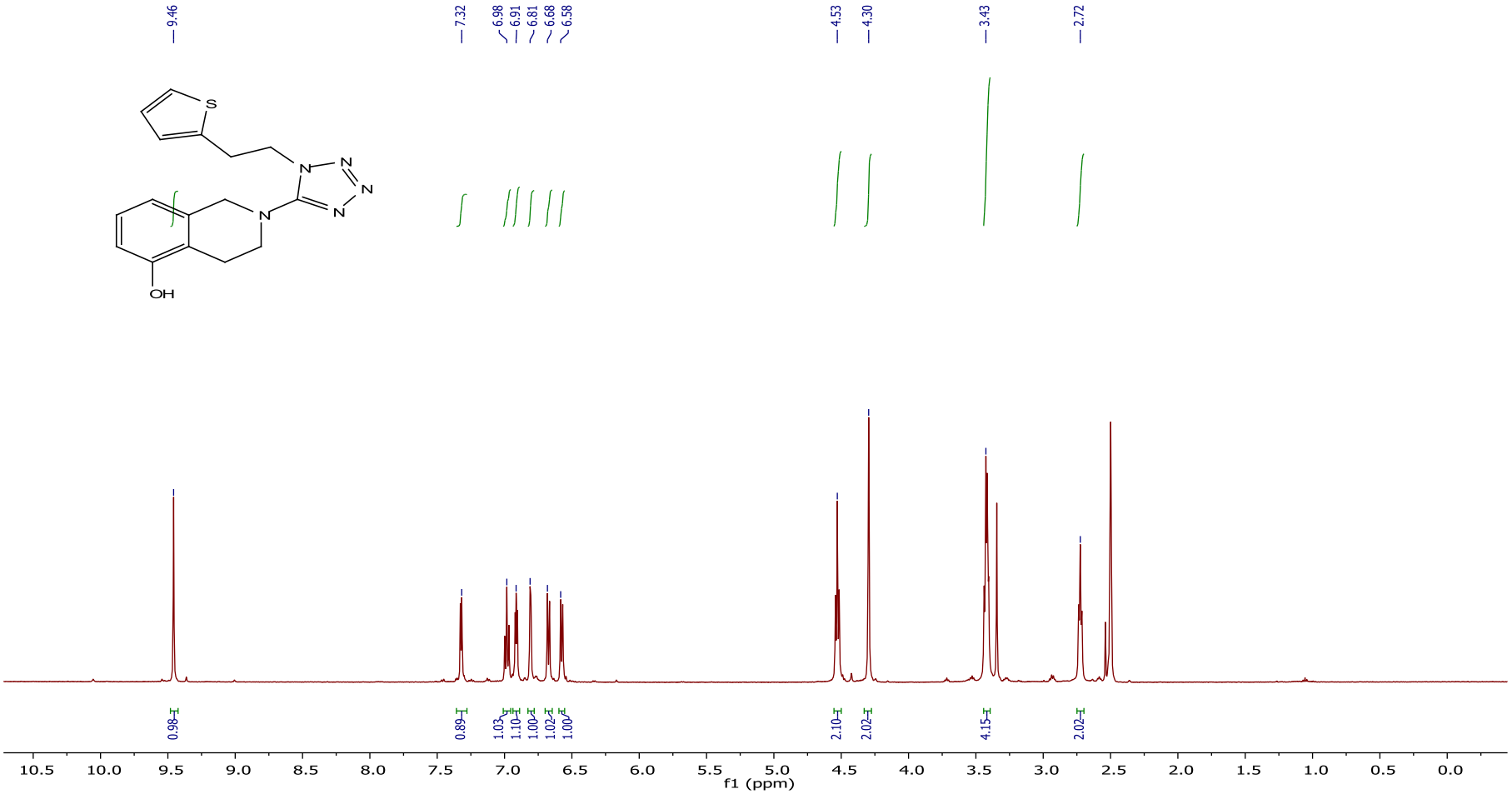
^{1}H NMR spectrum of the compound **8**{*41,148*}.



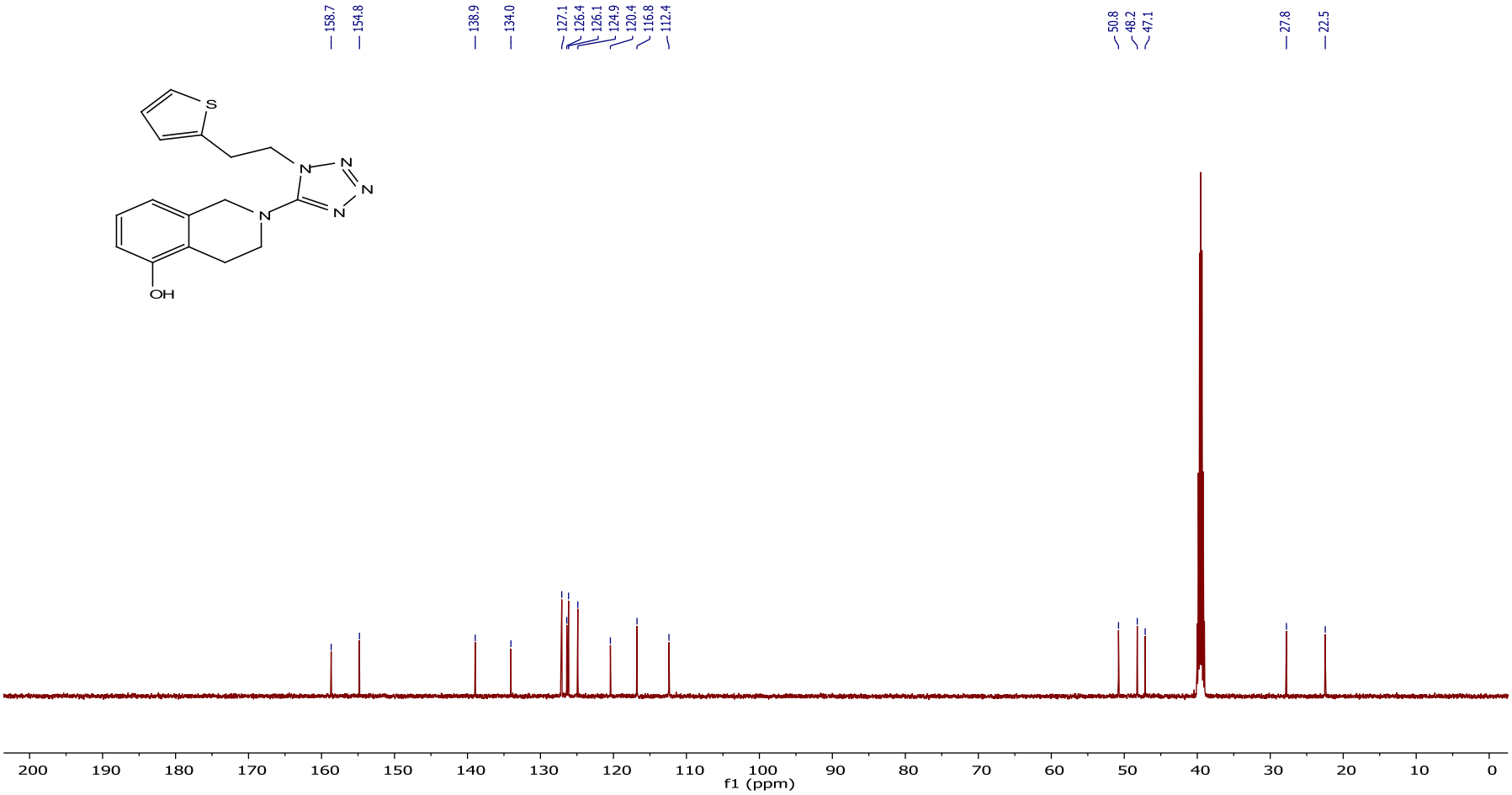
^{13}C NMR spectrum of the compound **8**{*41,148*}.



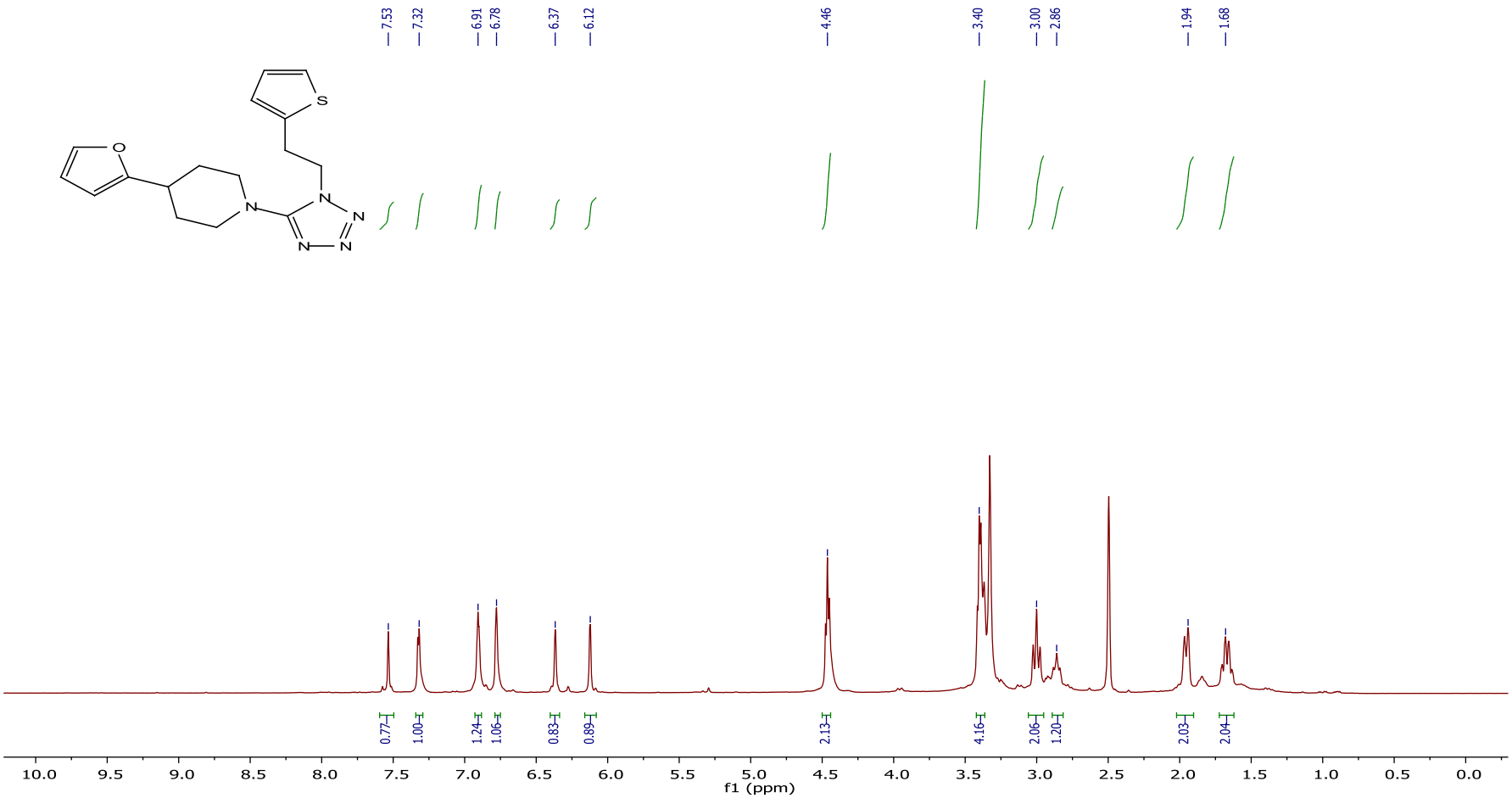
^{1}H NMR spectrum of the compound **8**{*41,210*}.



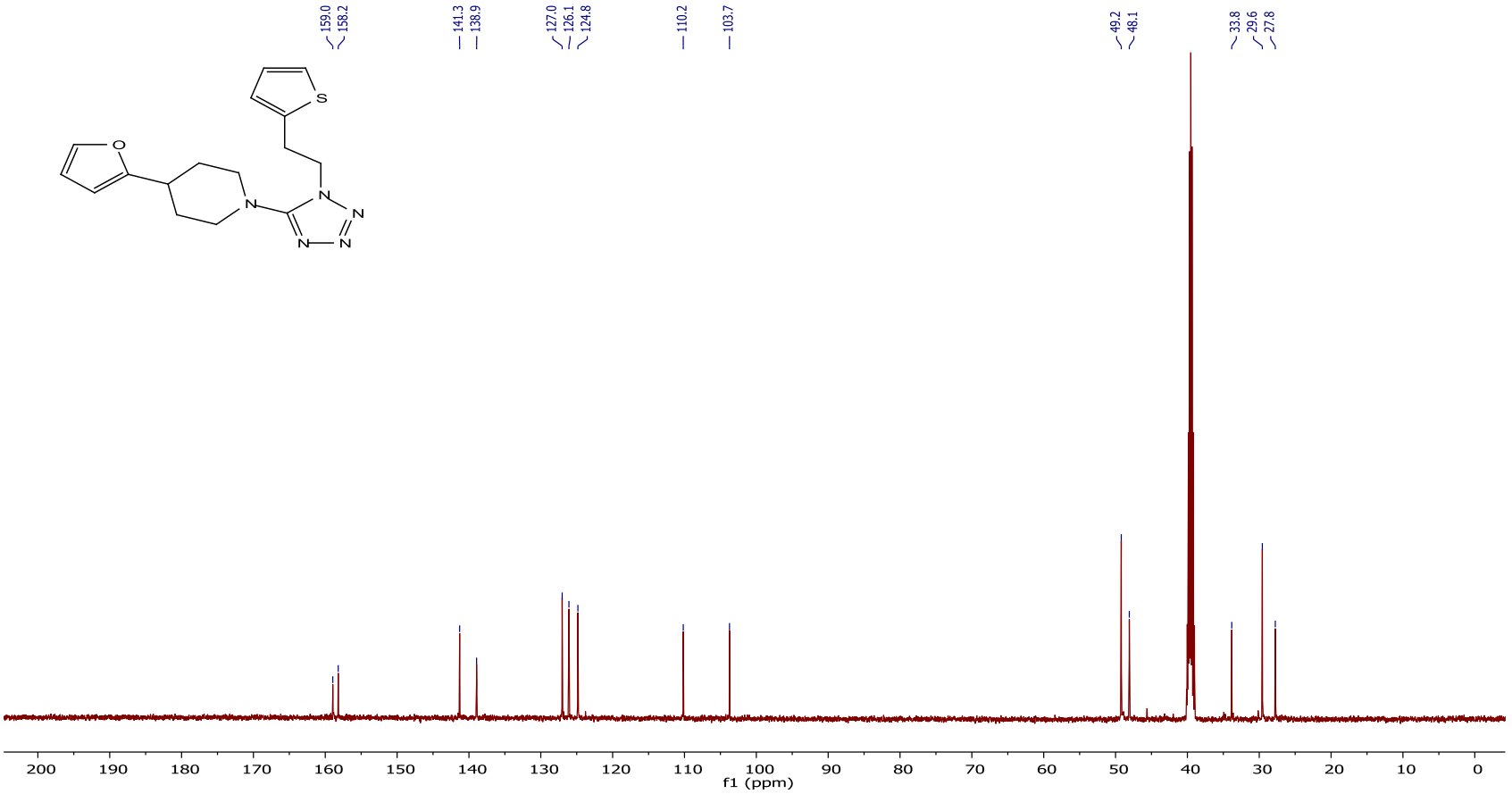
^{13}C NMR spectrum of the compound **8**{*41,210*}.



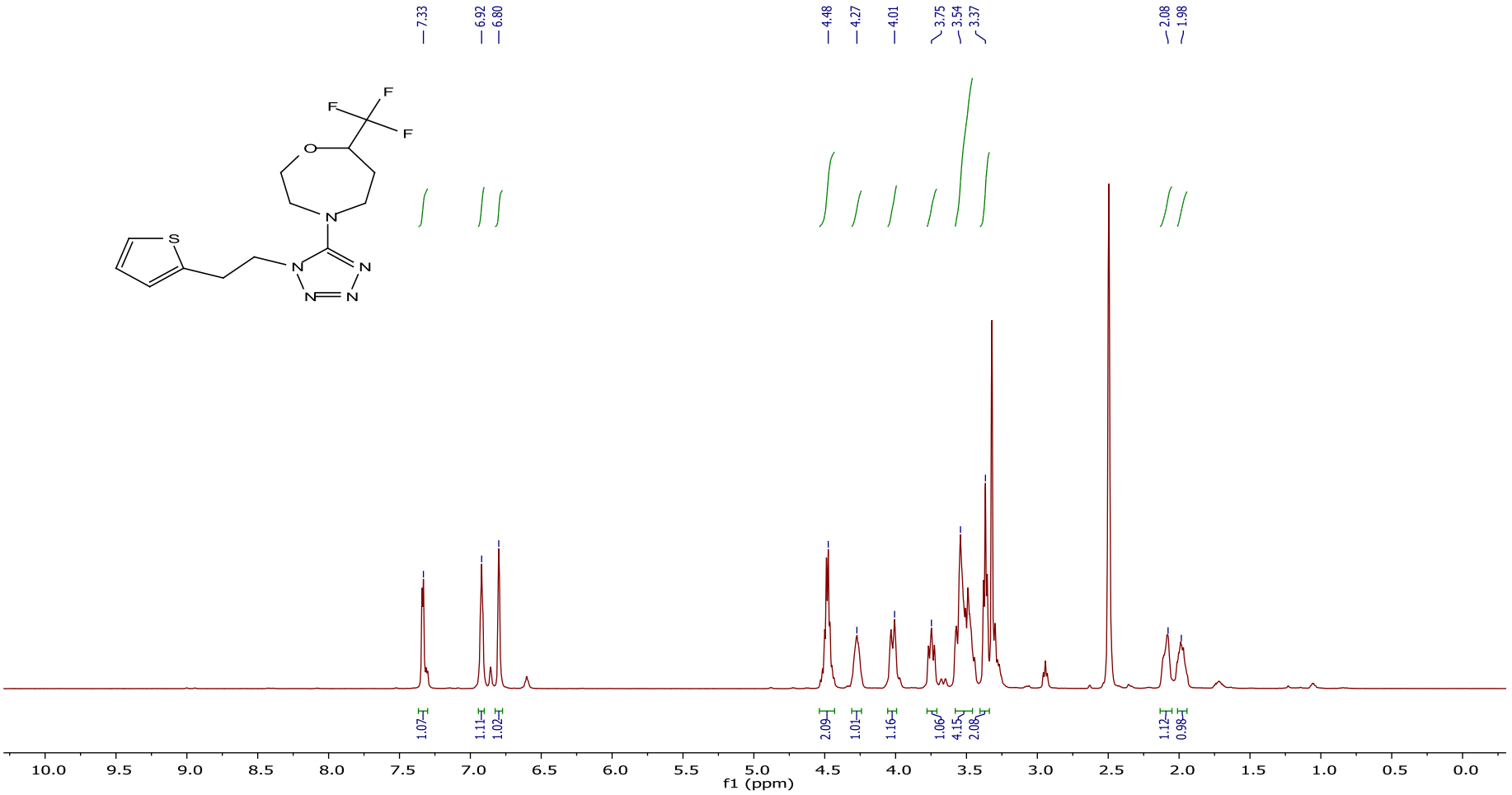
^{1}H NMR spectrum of the compound **8**{*41,211*}.



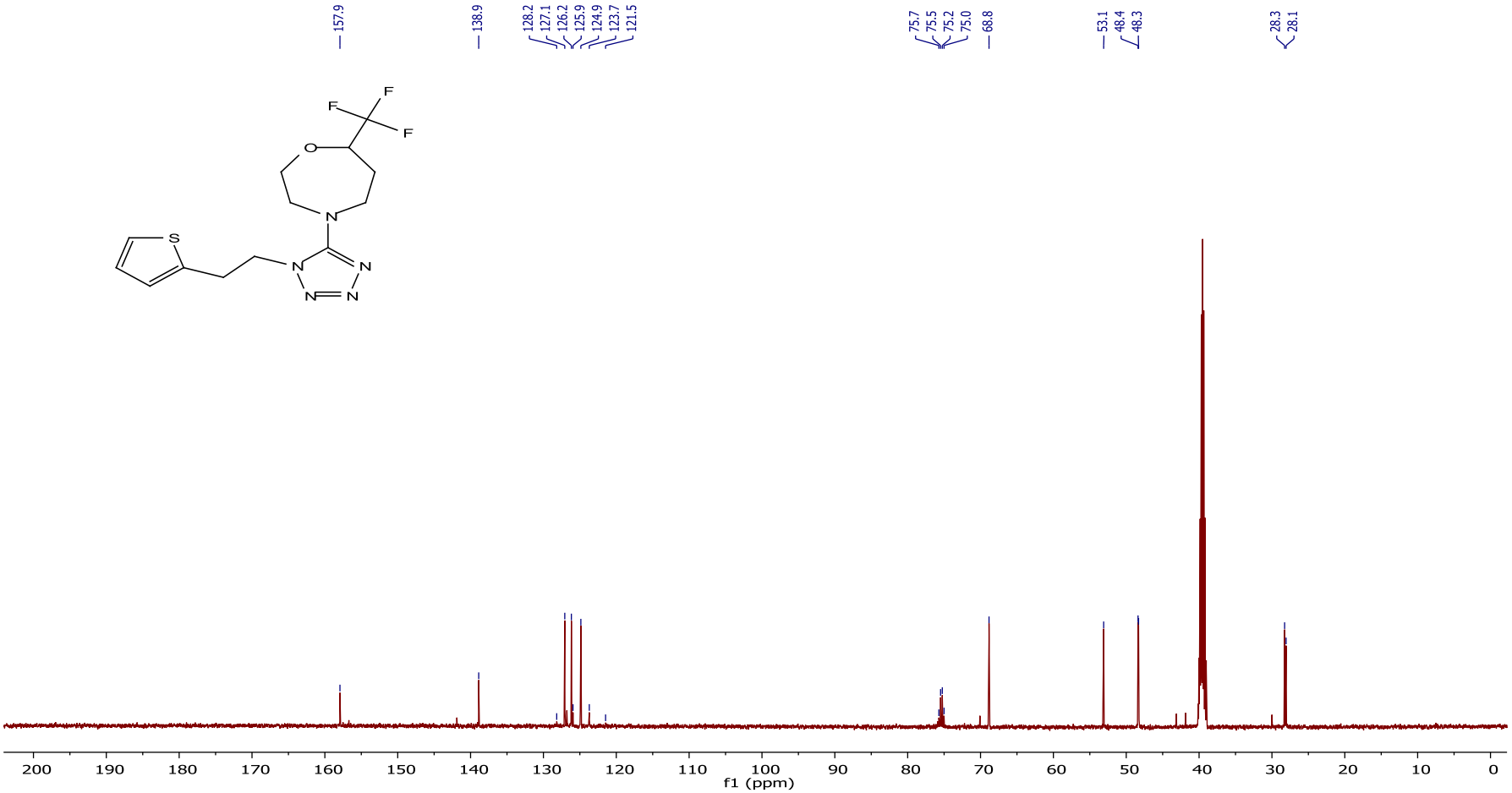
^{13}C NMR spectrum of the compound **8**{*41*,*211*}.



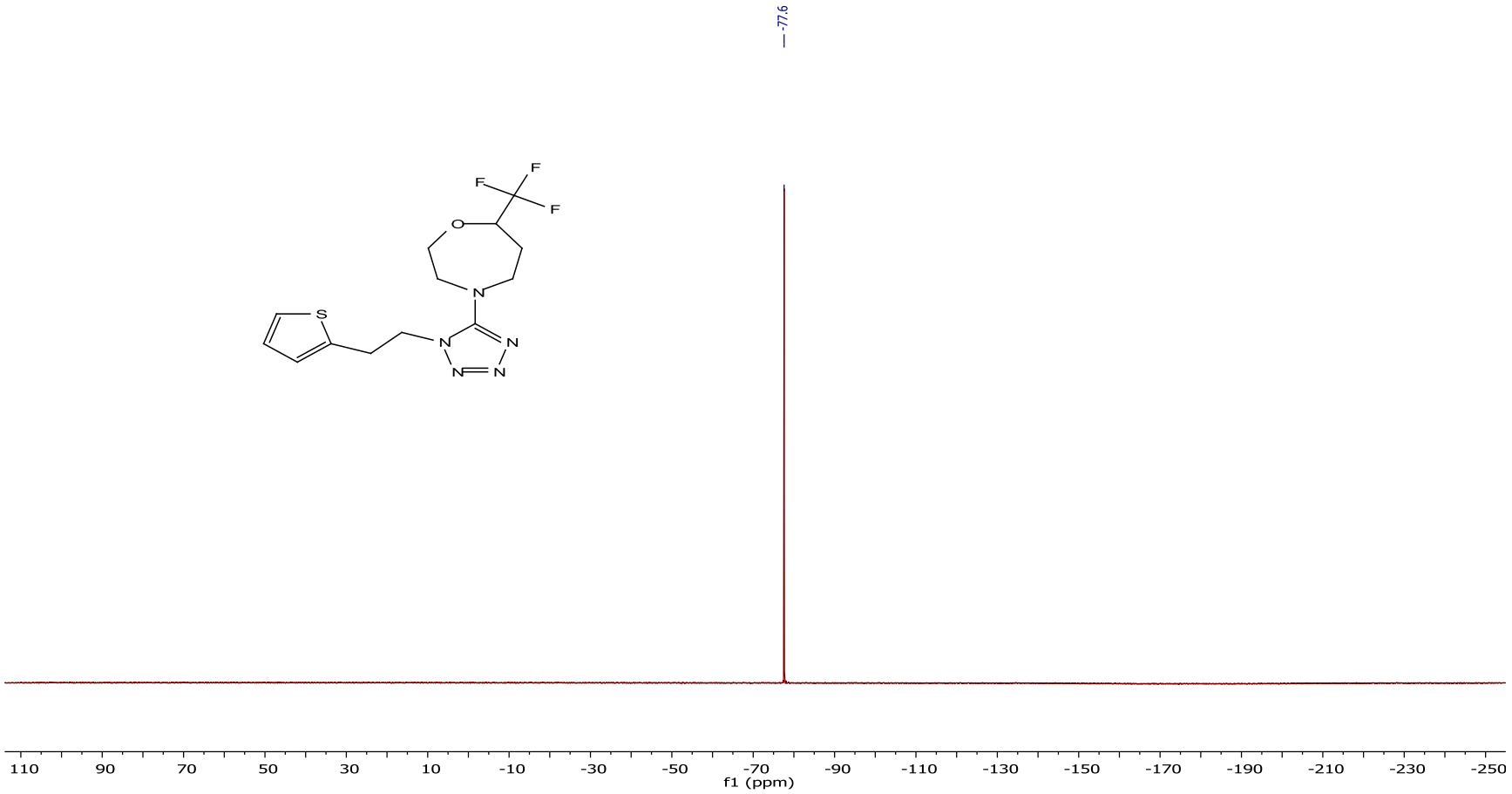
^{1}H NMR spectrum of the compound **8**{*41,212*}.



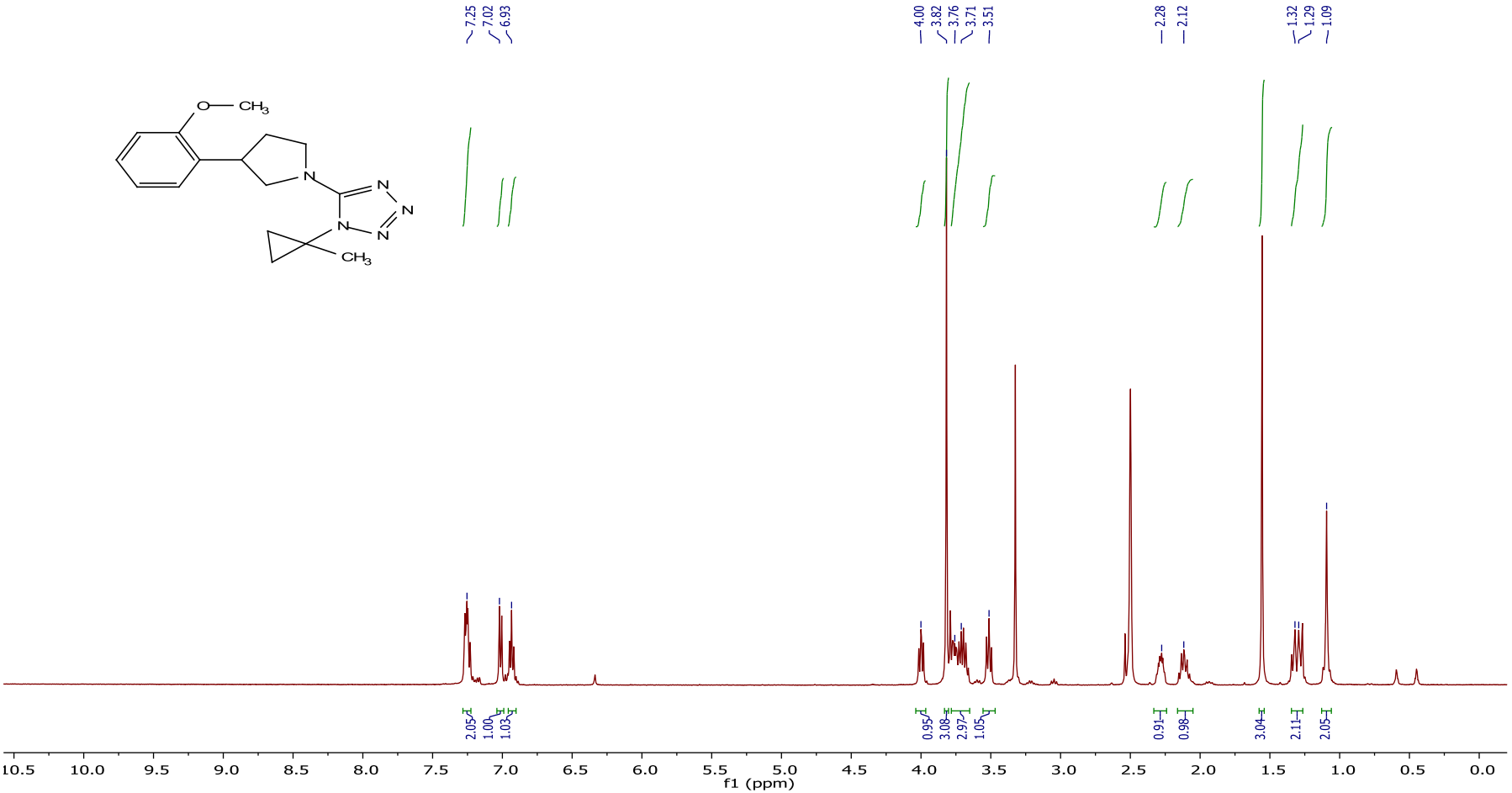
^{13}C NMR spectrum of the compound **8**{*41*,*212*}.



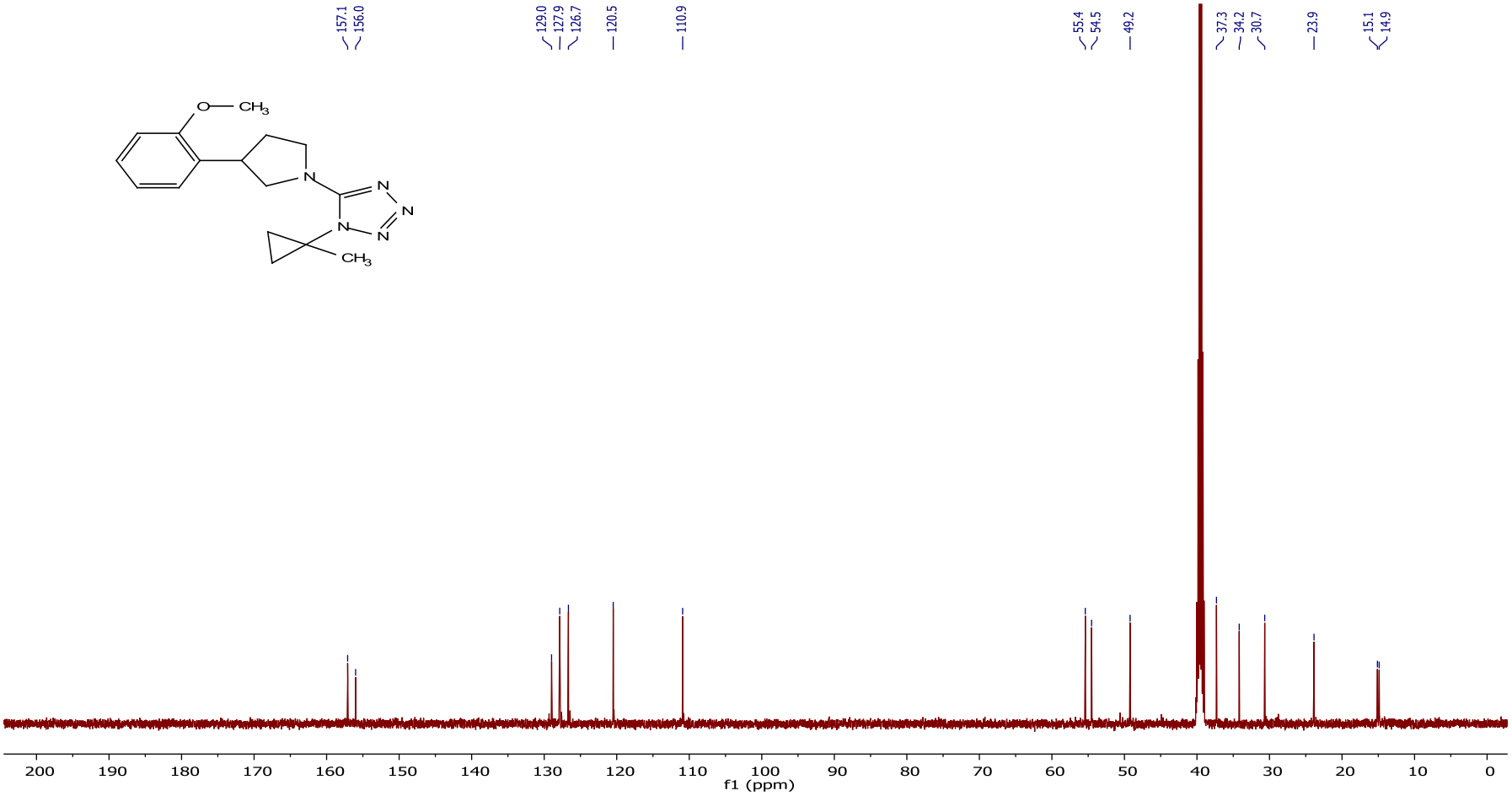
^{19}F NMR spectrum of the compound **8**{*41*,*212*}.



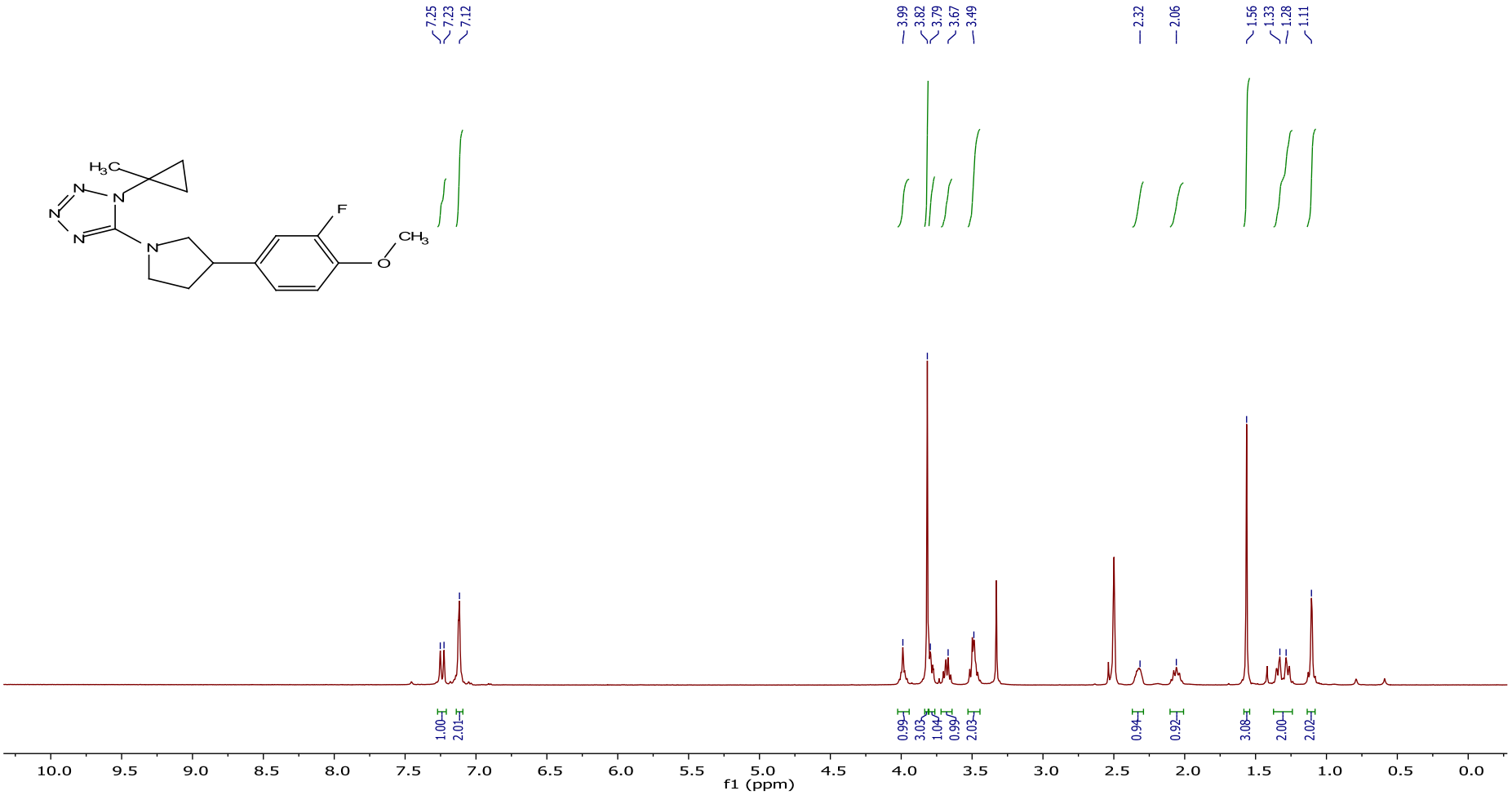
^{1}H NMR spectrum of the compound **8**{*42,193*}.



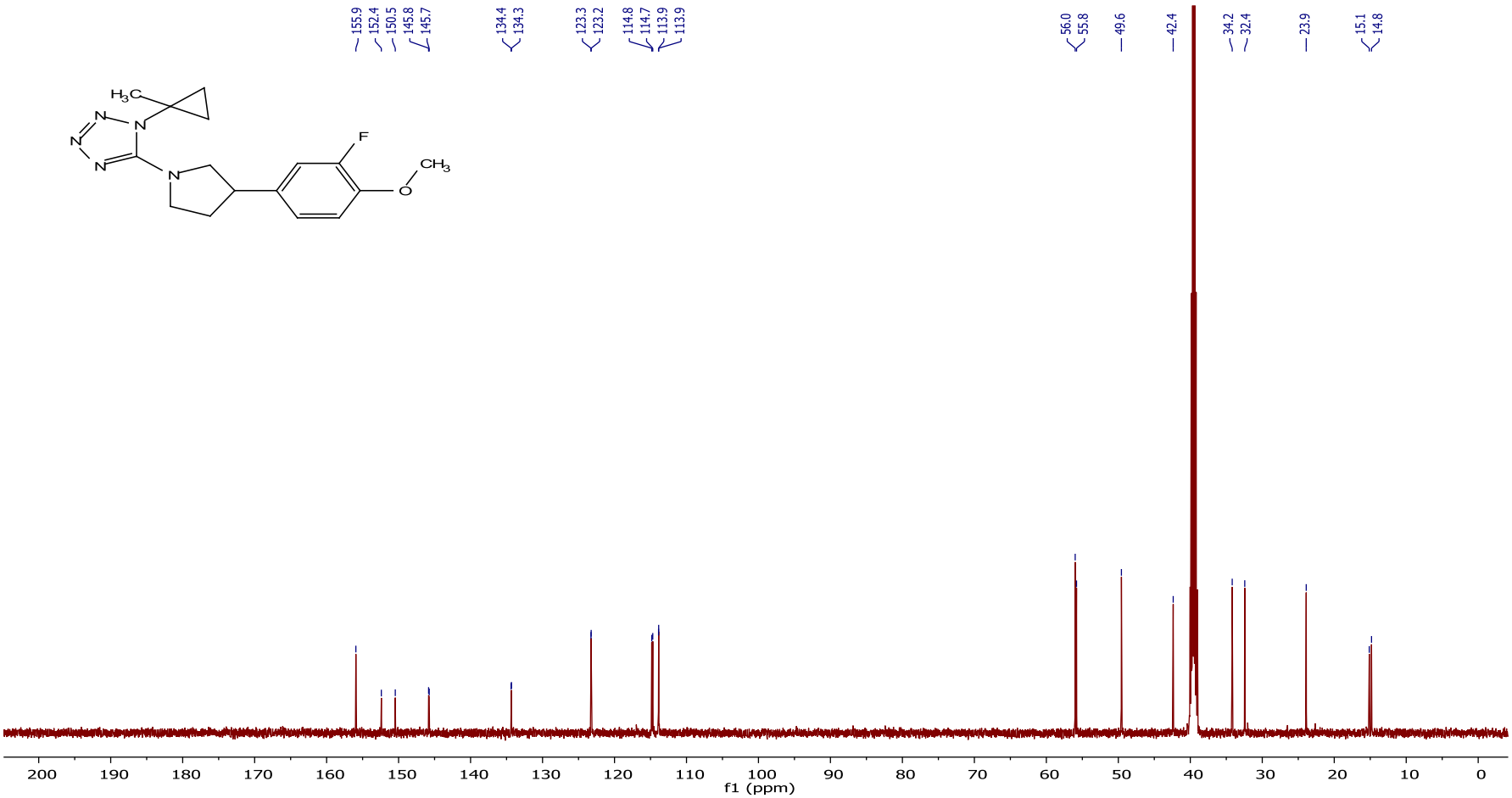
^{13}C NMR spectrum of the compound **8**{*42,193*}.



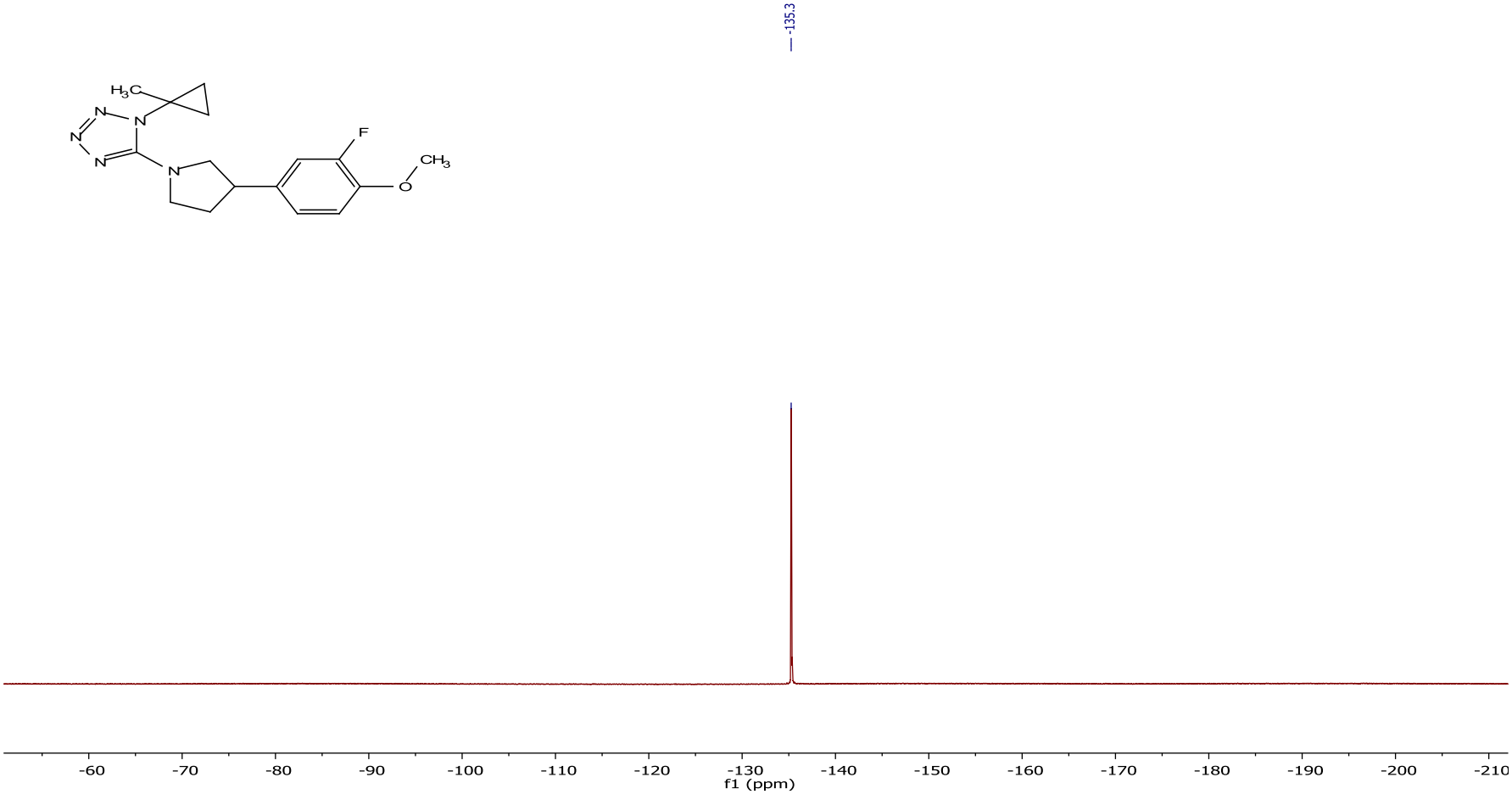
^{1}H NMR spectrum of the compound **8**{*42,227*}.



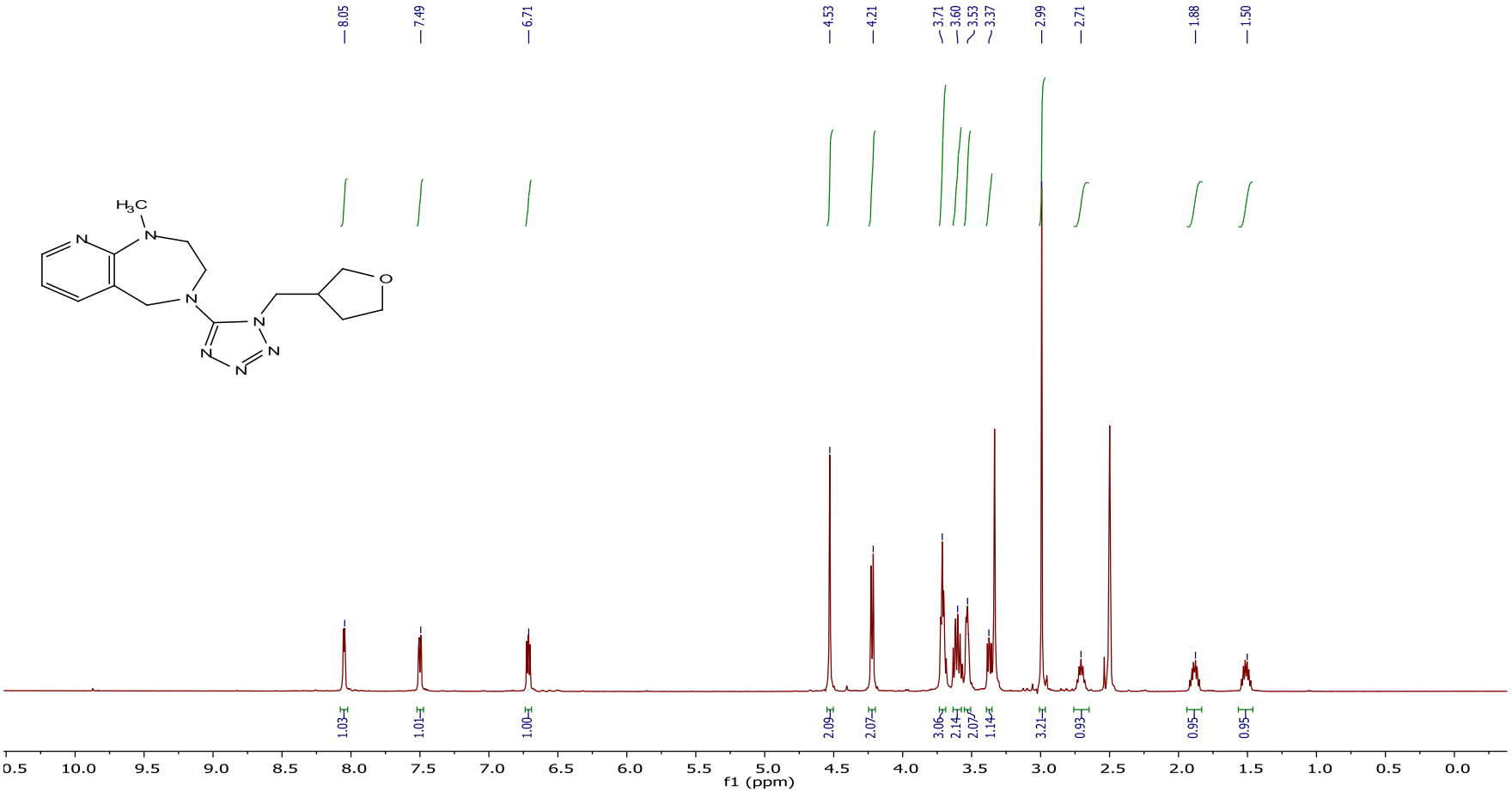
^{13}C NMR spectrum of the compound **8**{*42,227*}.



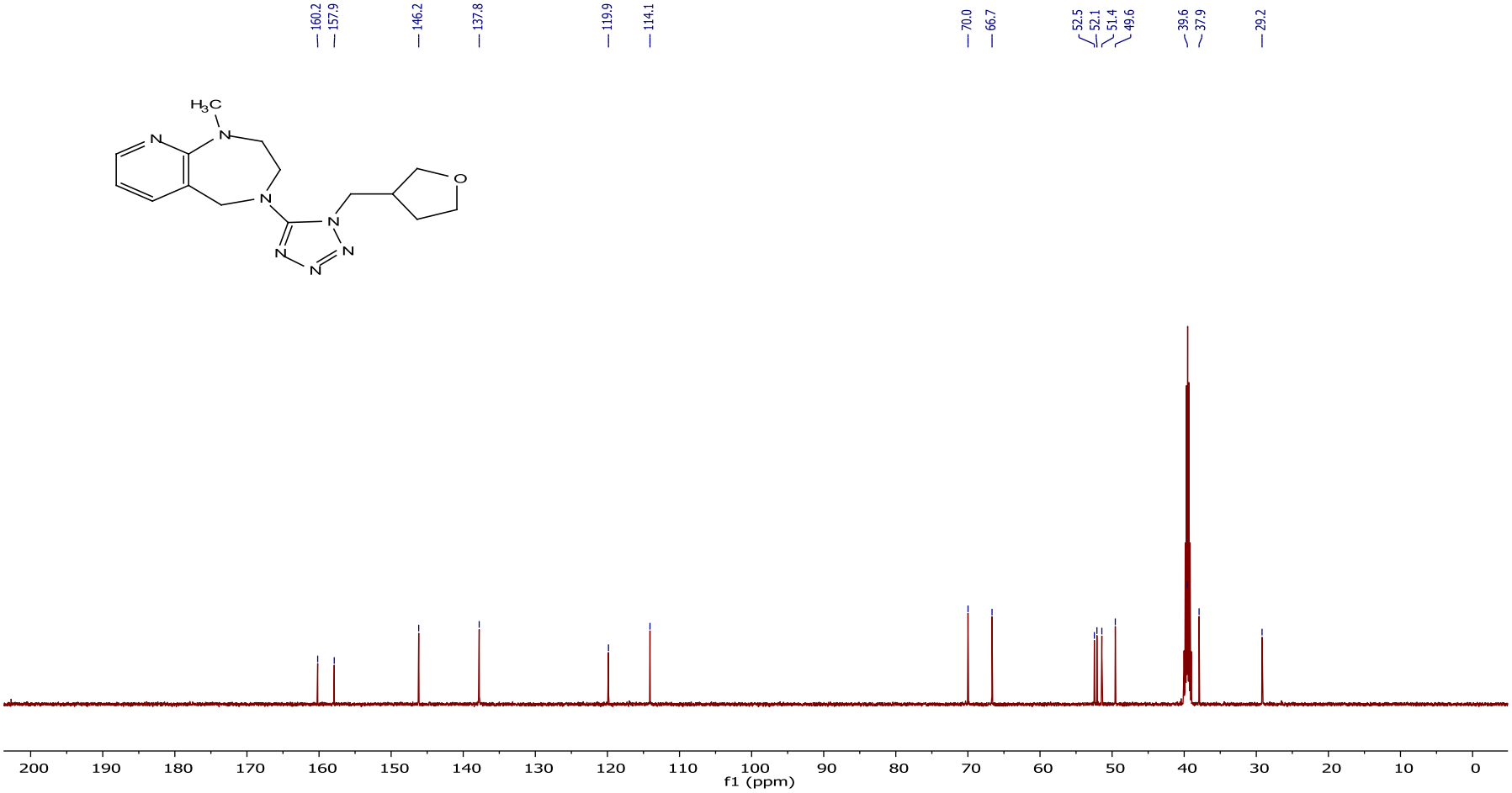
^{19}F NMR spectrum of the compound **8**{*42,227*}.



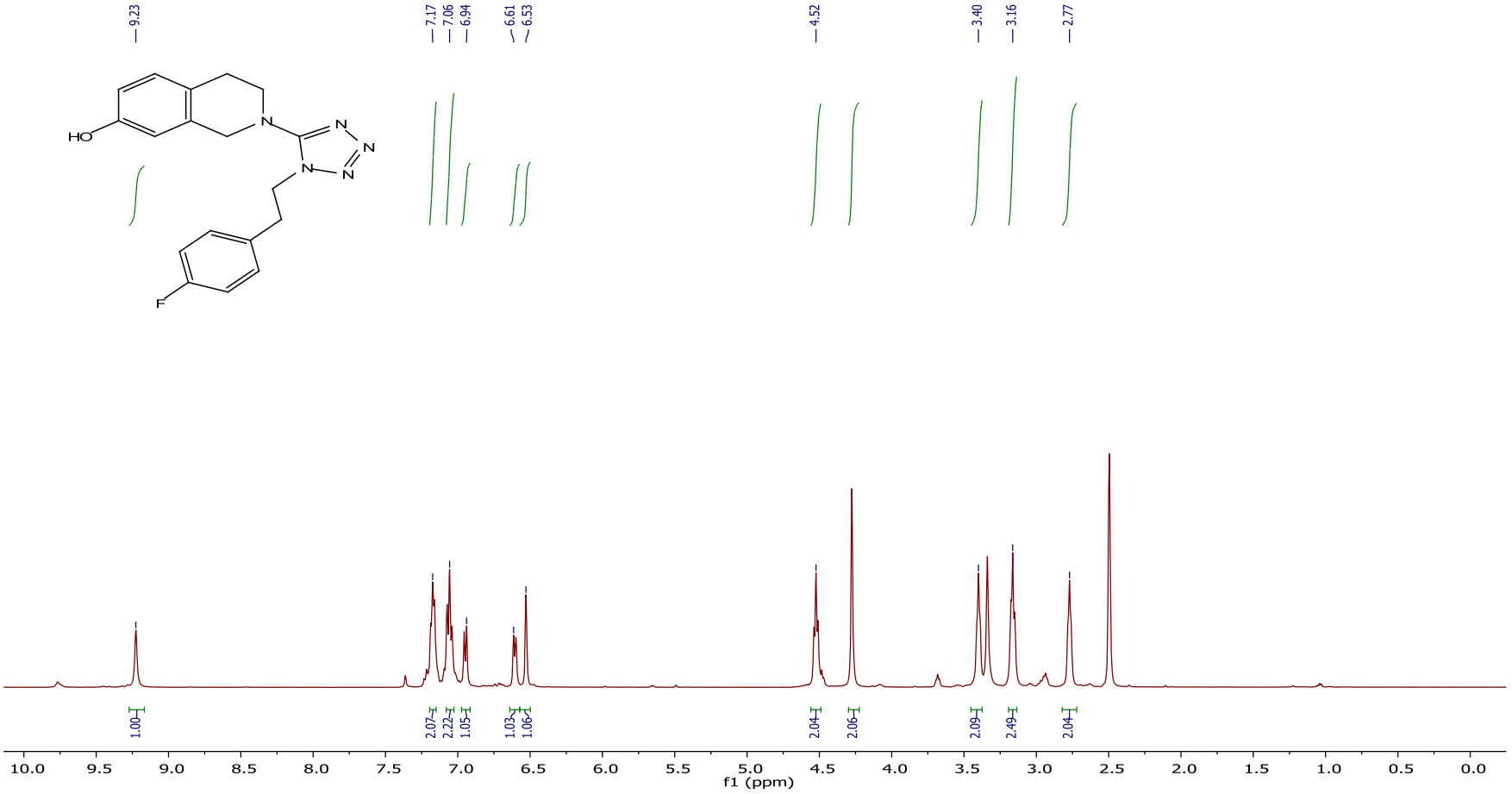
^{1}H NMR spectrum of the compound **8**{*51,251*}.



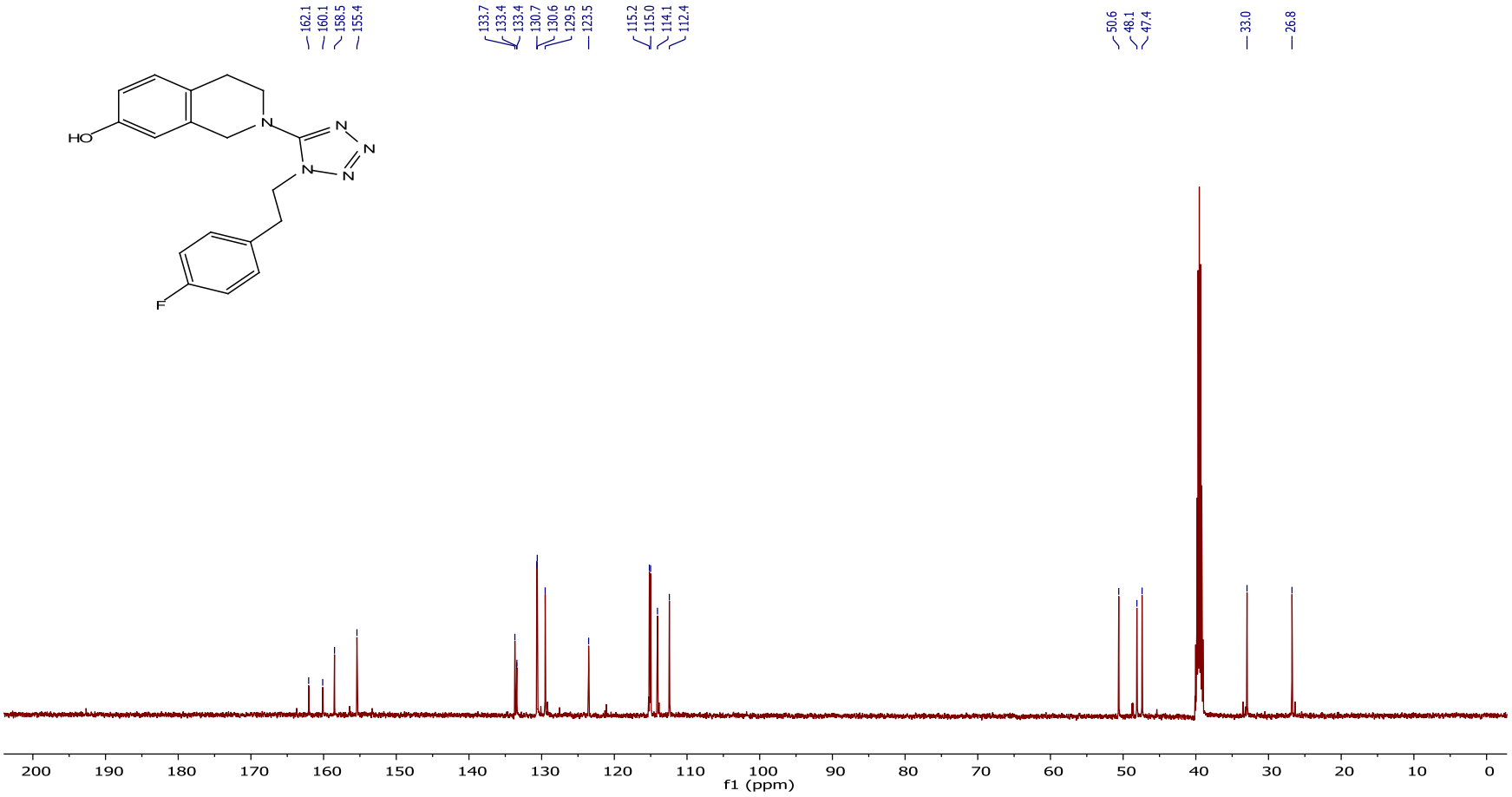
^{13}C NMR spectrum of the compound **8**{*51,251*}.



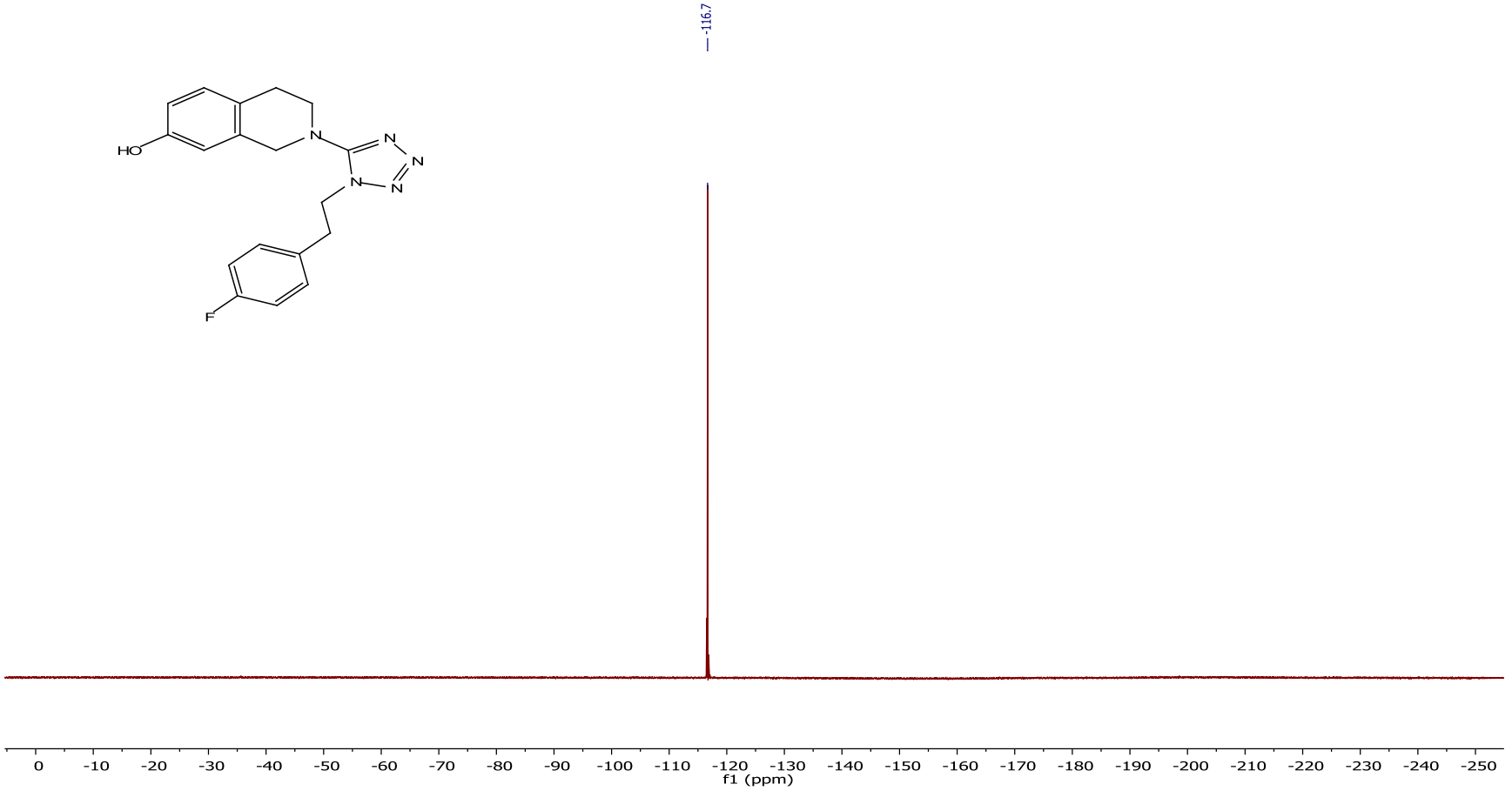
^{1}H NMR spectrum of the compound **8**{*53,236*}.



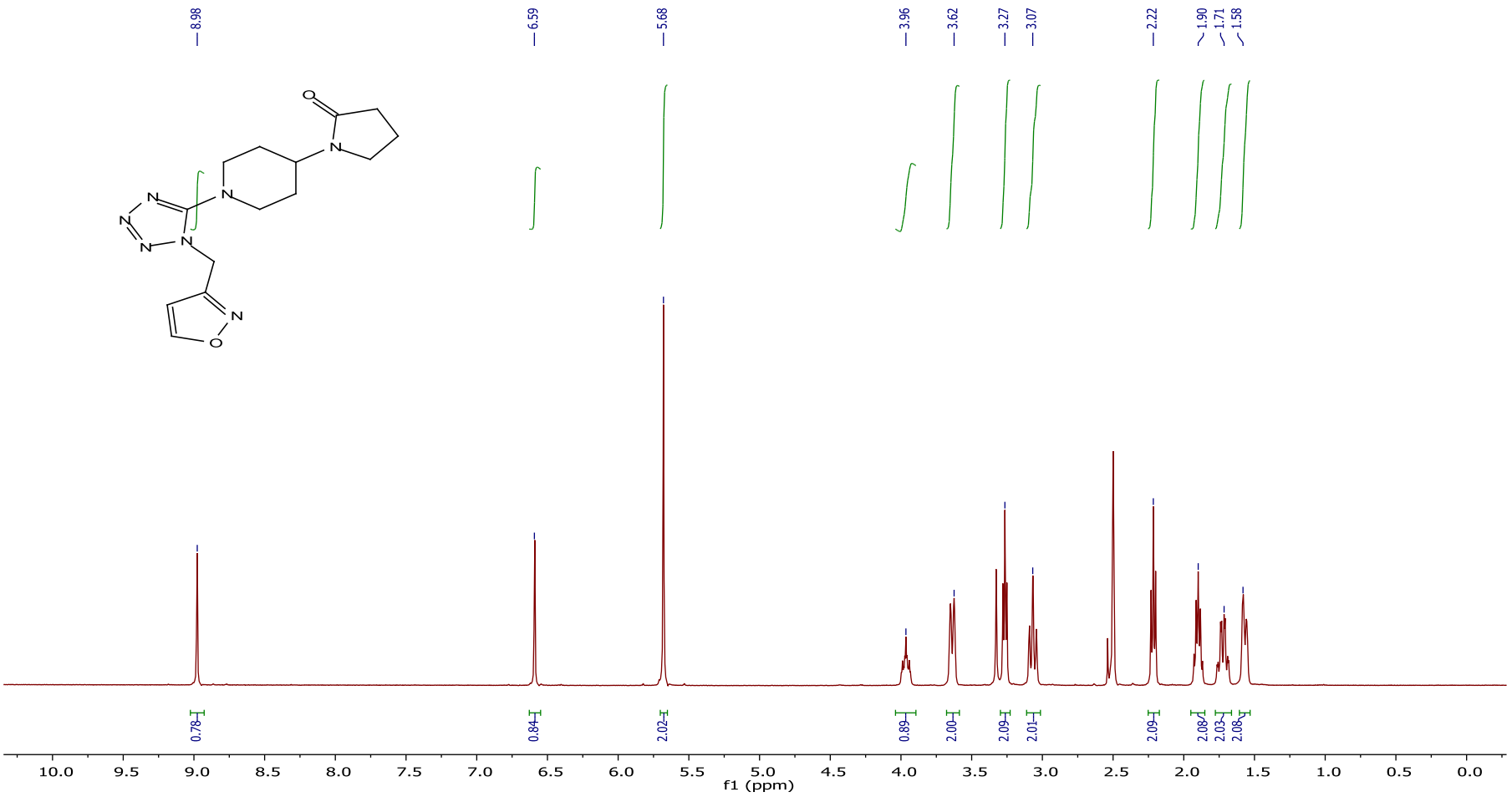
^{13}C NMR spectrum of the compound **8**{*53,236*}.



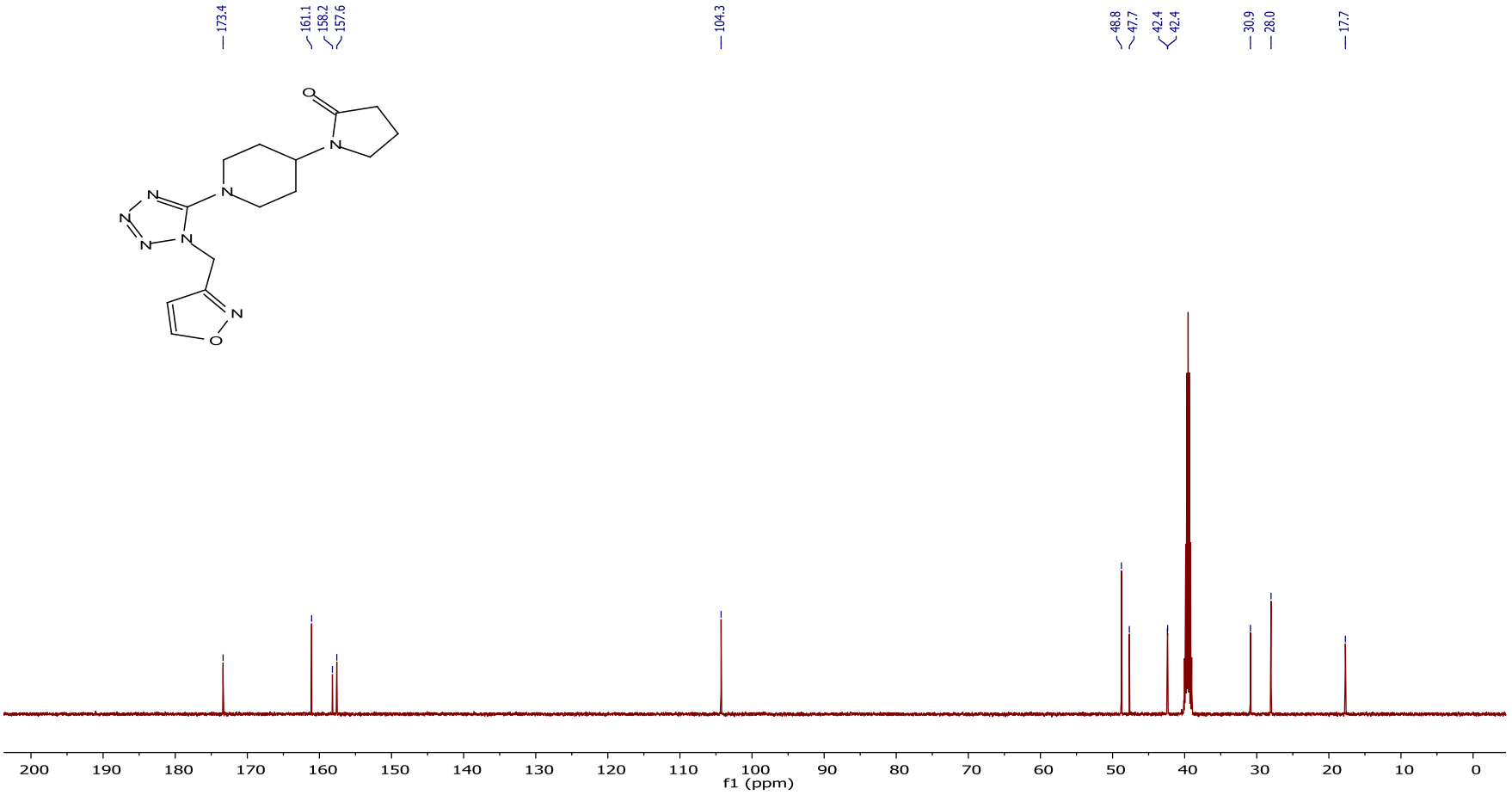
^{19}F NMR spectrum of the compound **8**{*53*,*236*}.



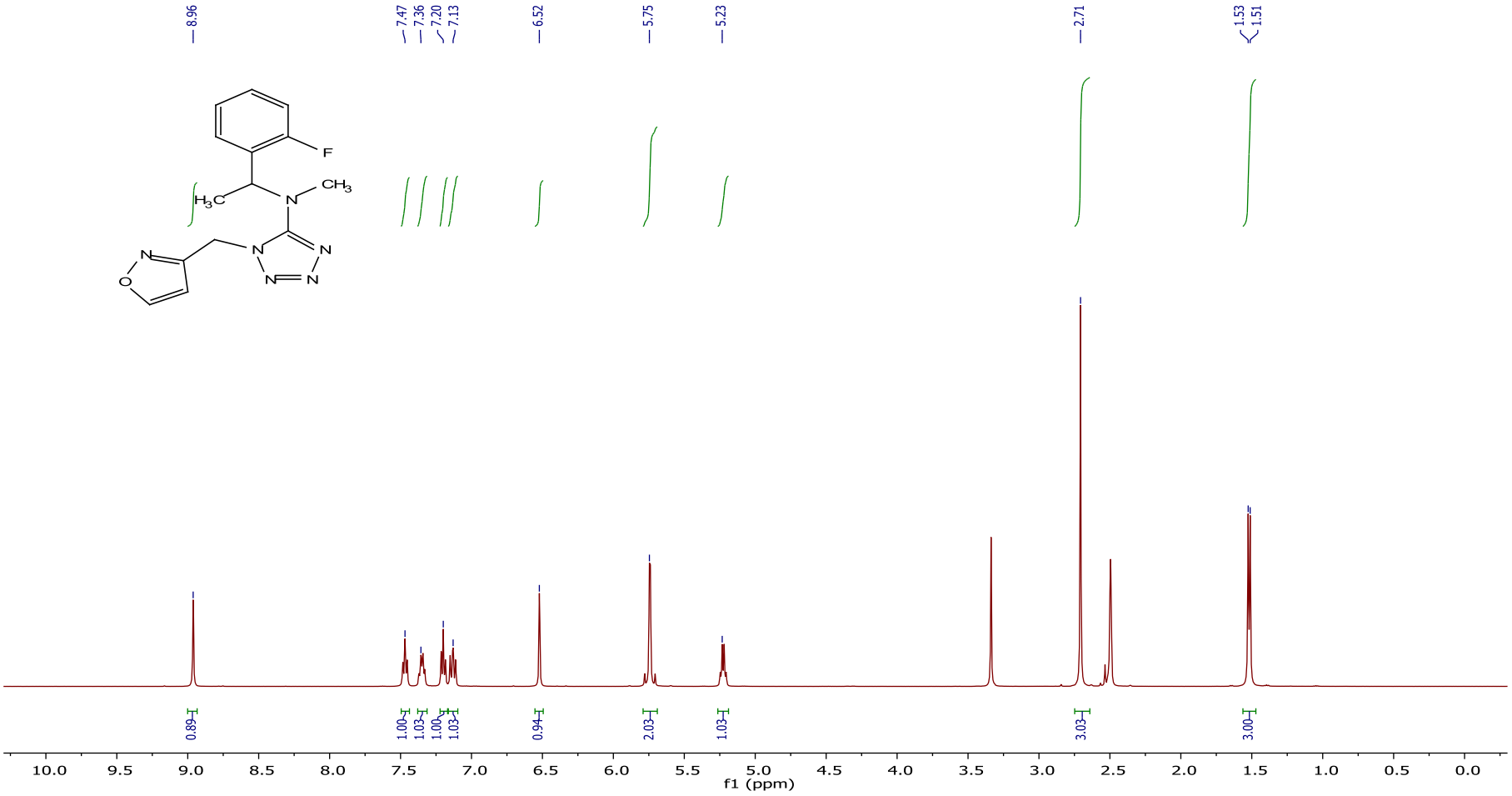
^{1}H NMR spectrum of the compound **8**{*56,108*}.



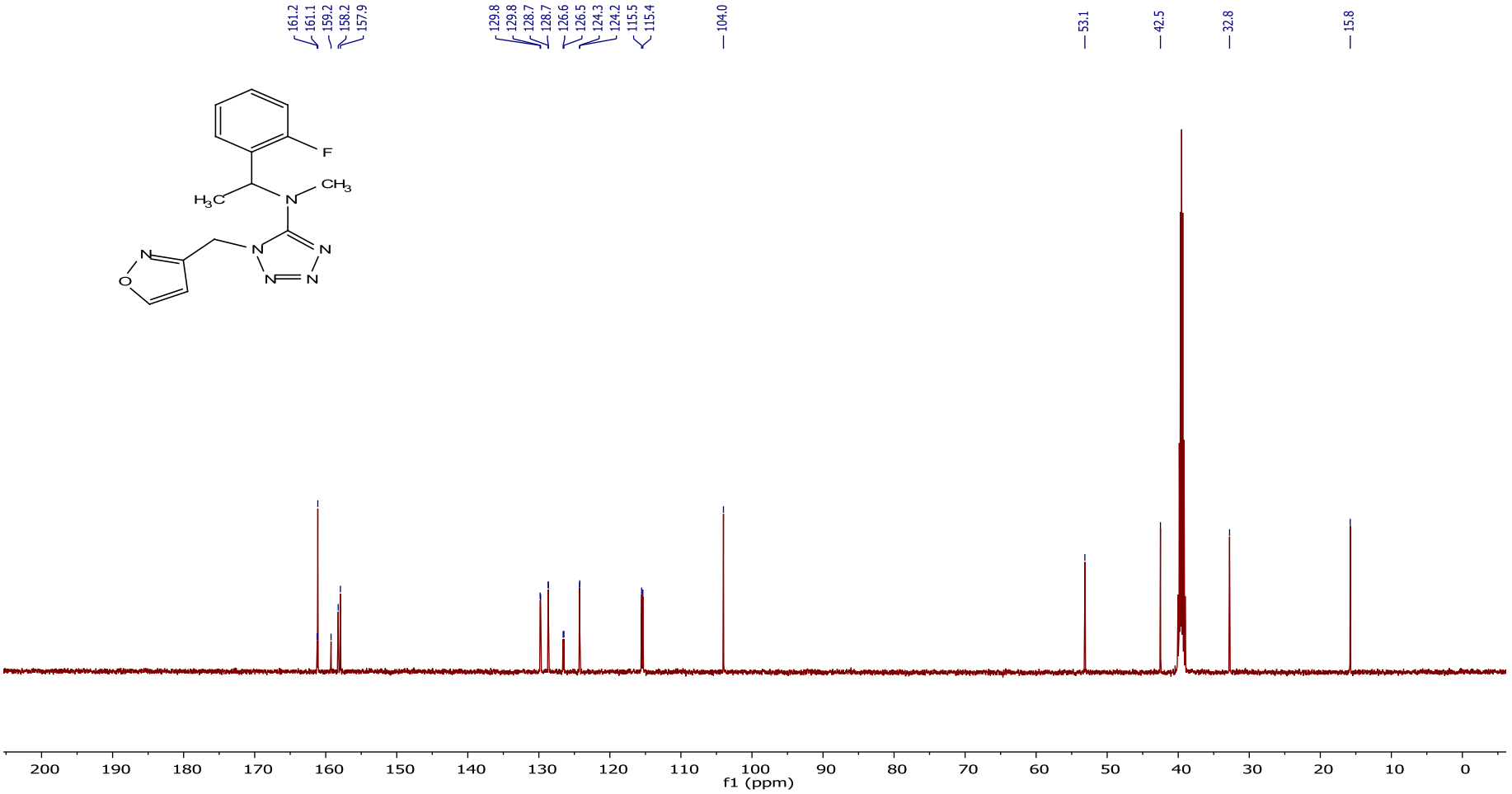
^{13}C NMR spectrum of the compound **8**{*56,108*}.



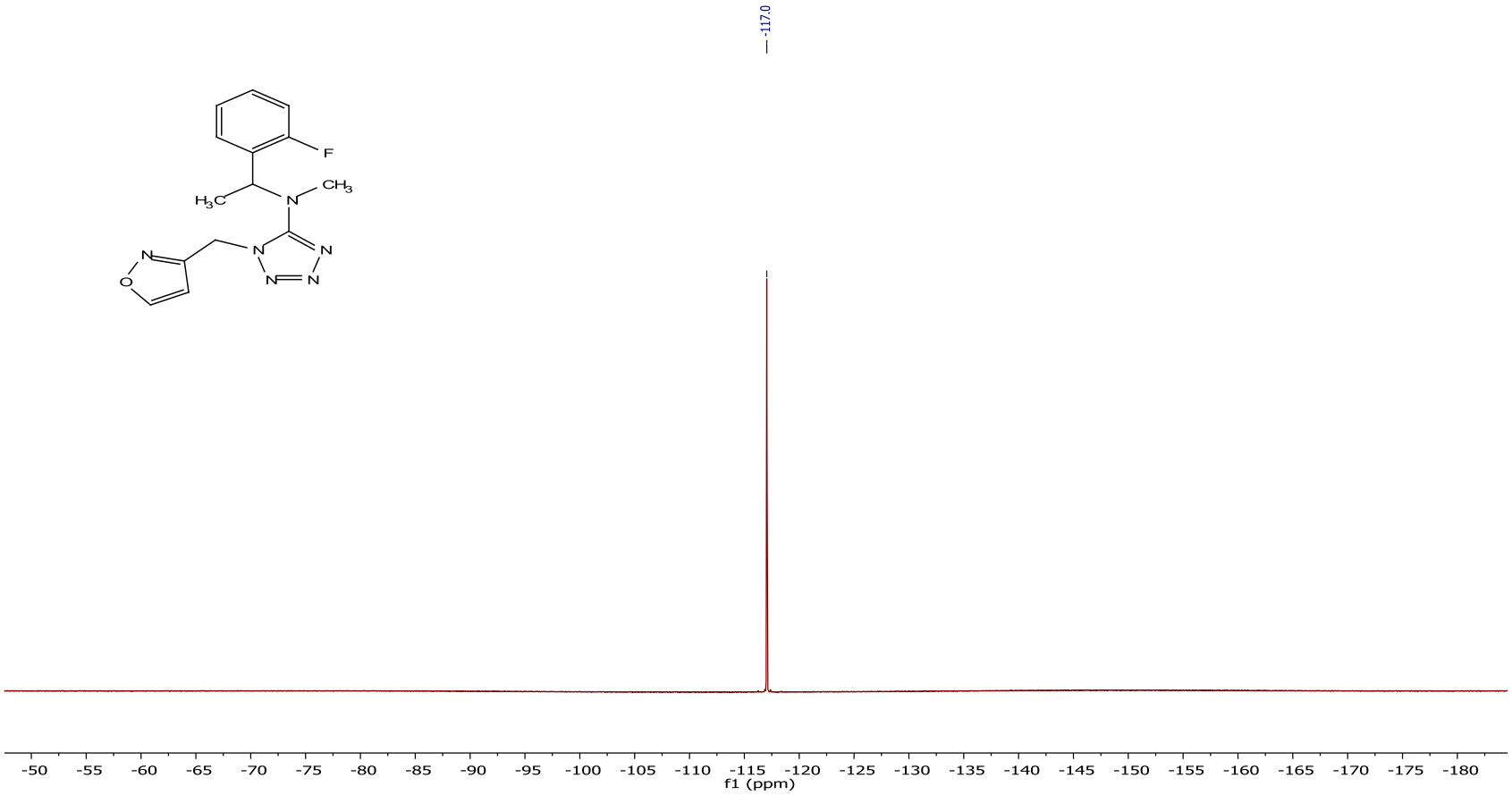
^{1}H NMR spectrum of the compound **8**{*56,271*}.



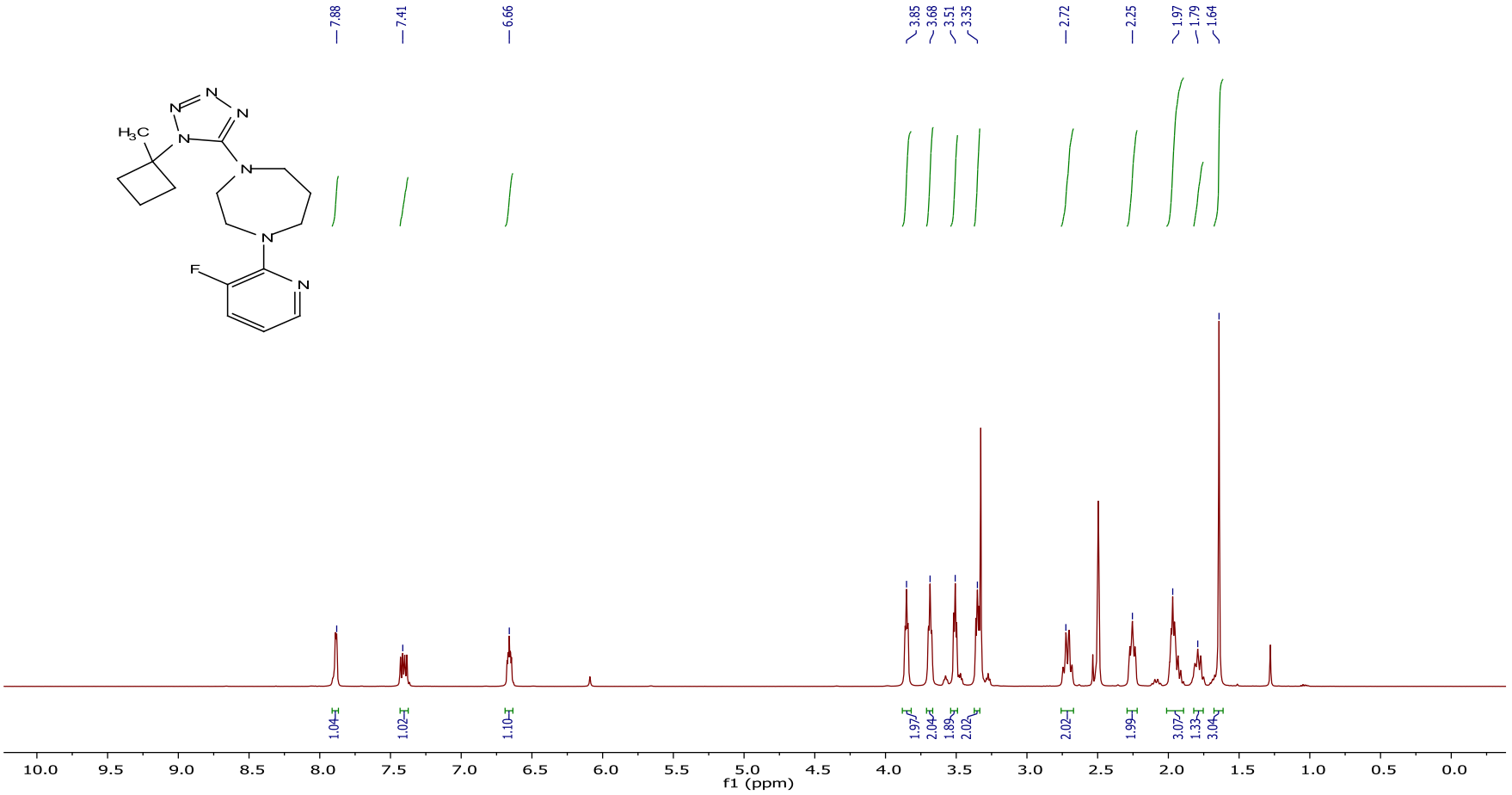
^{13}C NMR spectrum of the compound **8**{*56,271*}.



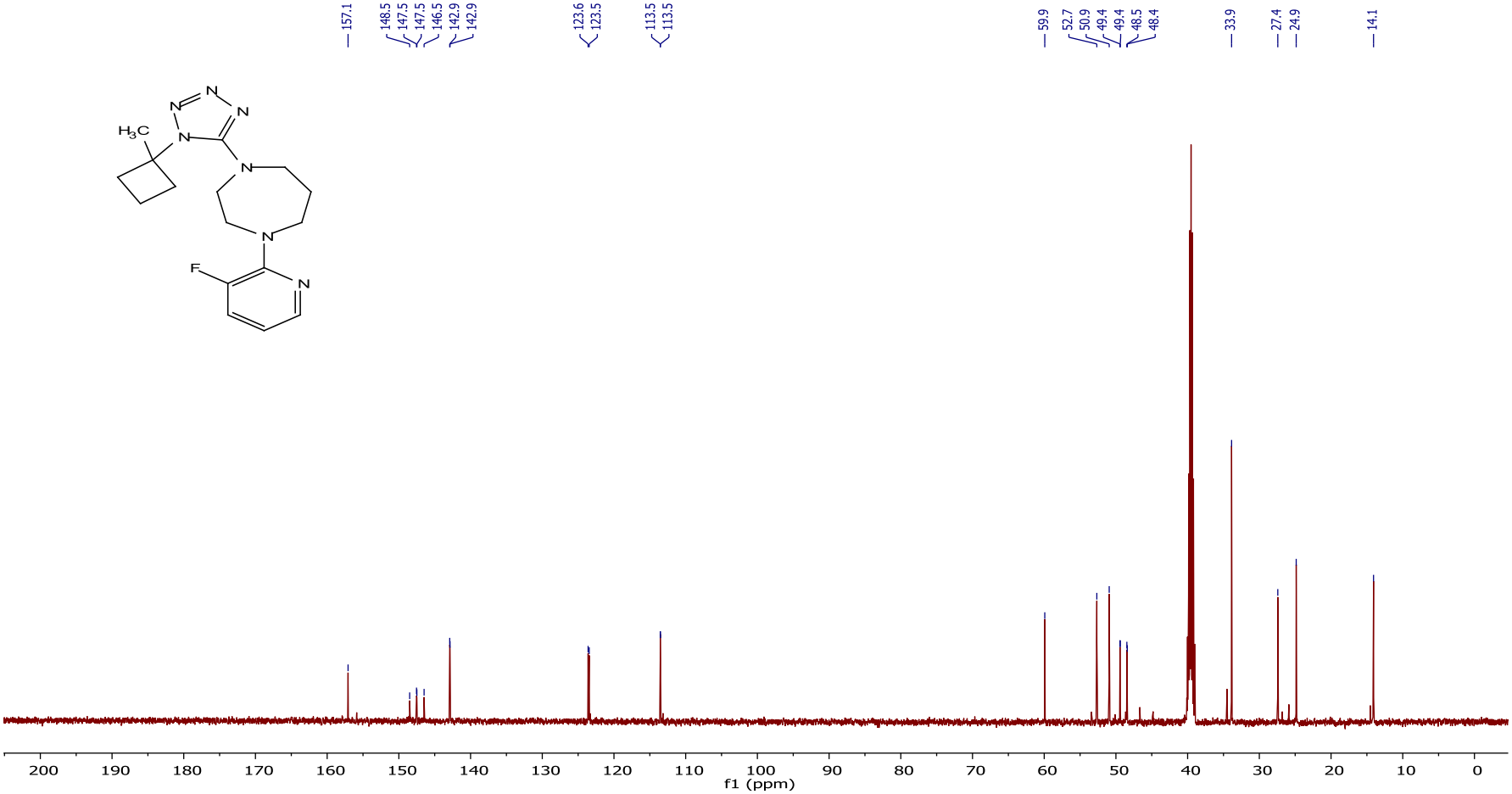
^{19}F NMR spectrum of the compound **8**{*56,271*}.



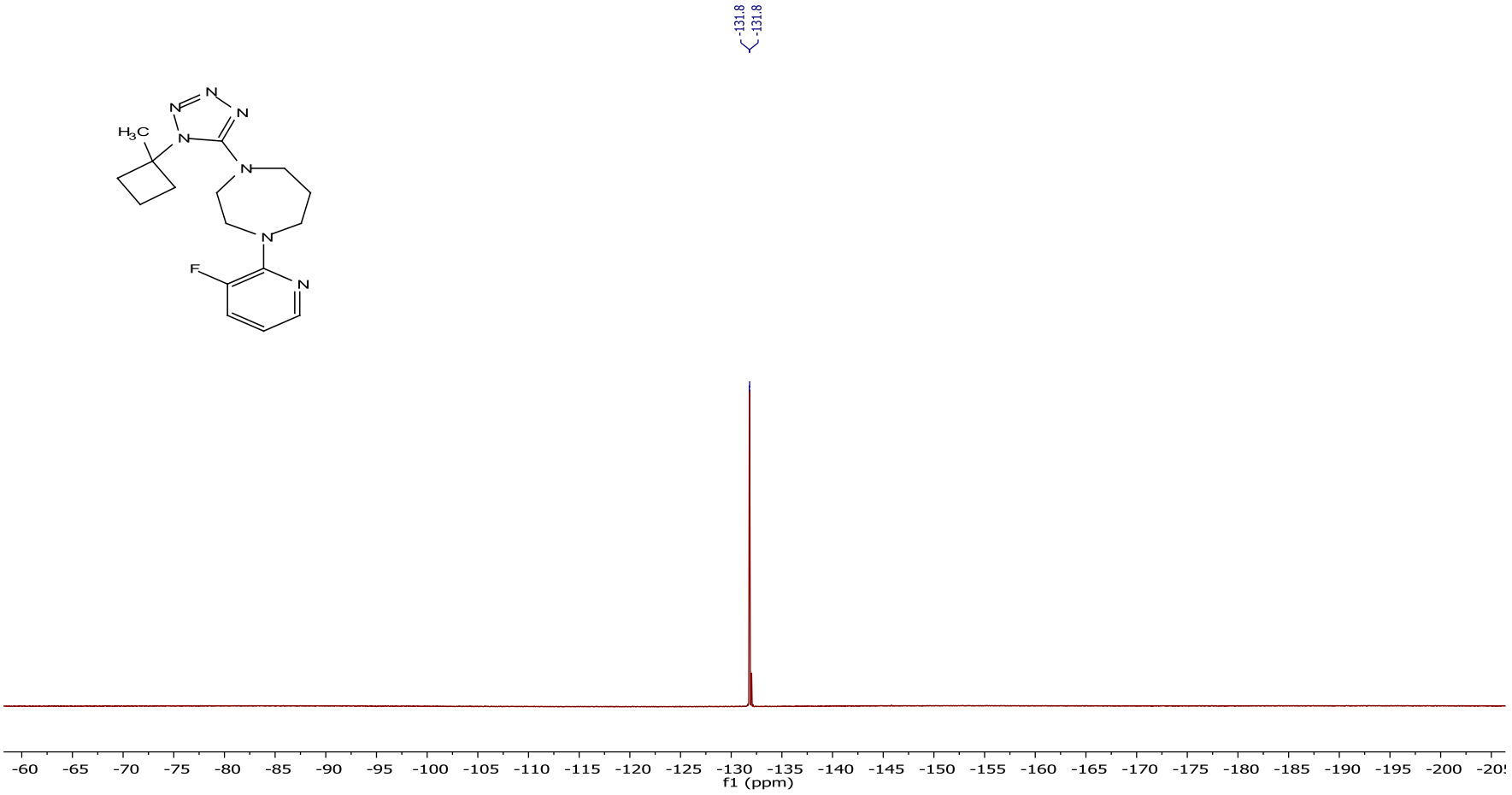
^{1}H NMR spectrum of the compound **8**{*58,280*}.



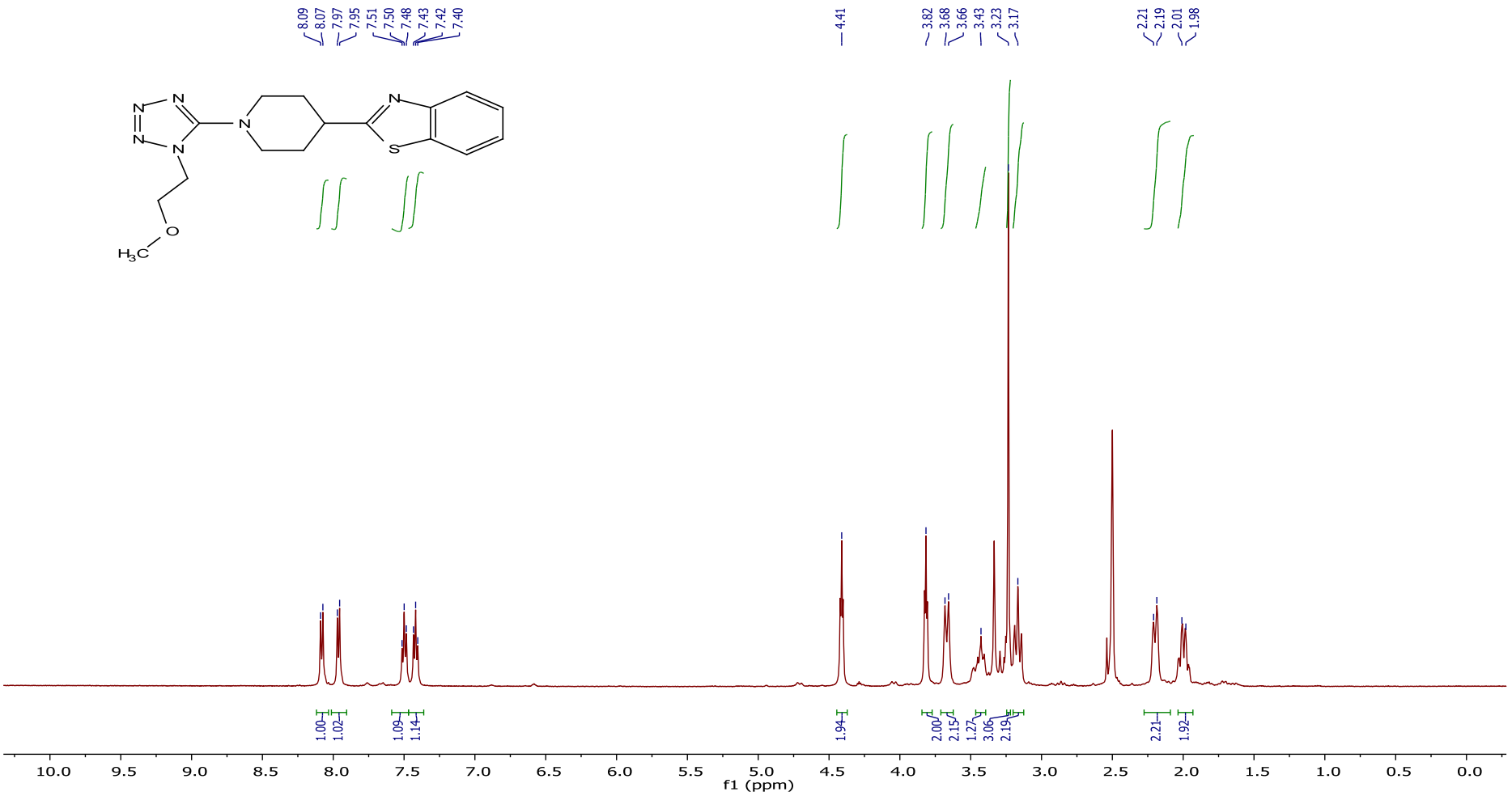
^{13}C NMR spectrum of the compound **8**{*58,280*}.



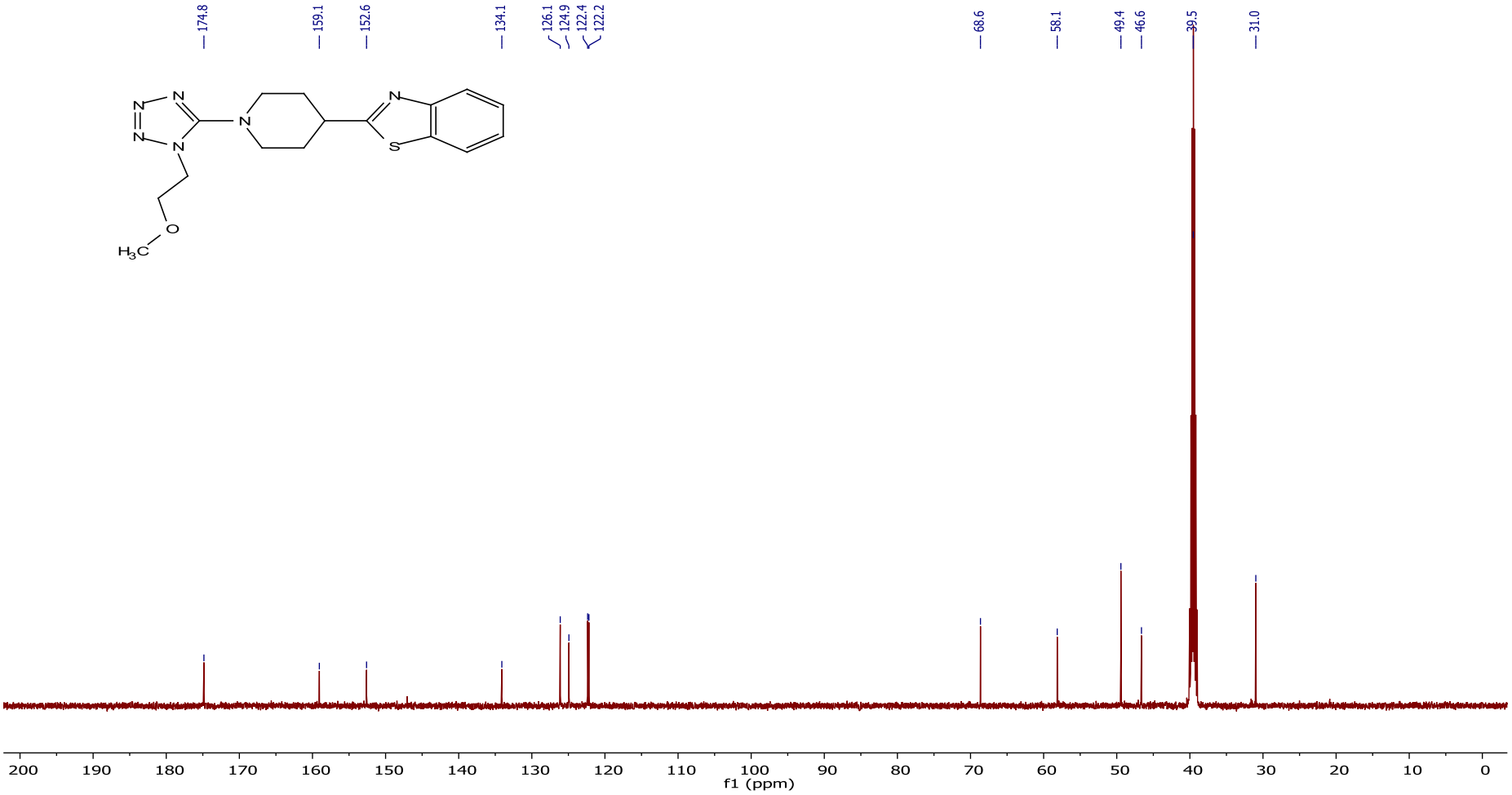
^{19}F NMR spectrum of the compound **8**{*58,280*}.



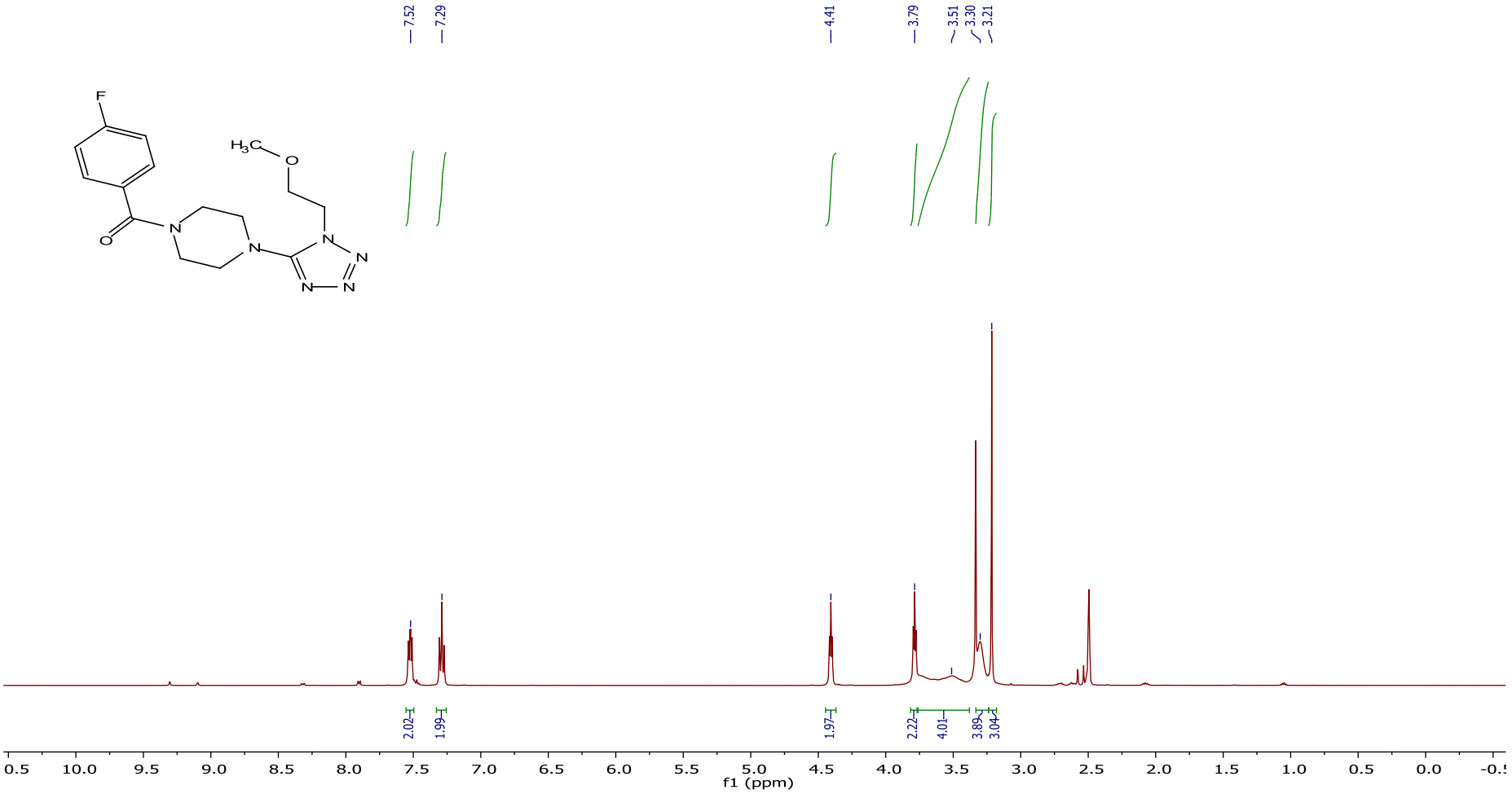
^{1}H NMR spectrum of the compound **9**{*4,289*}.



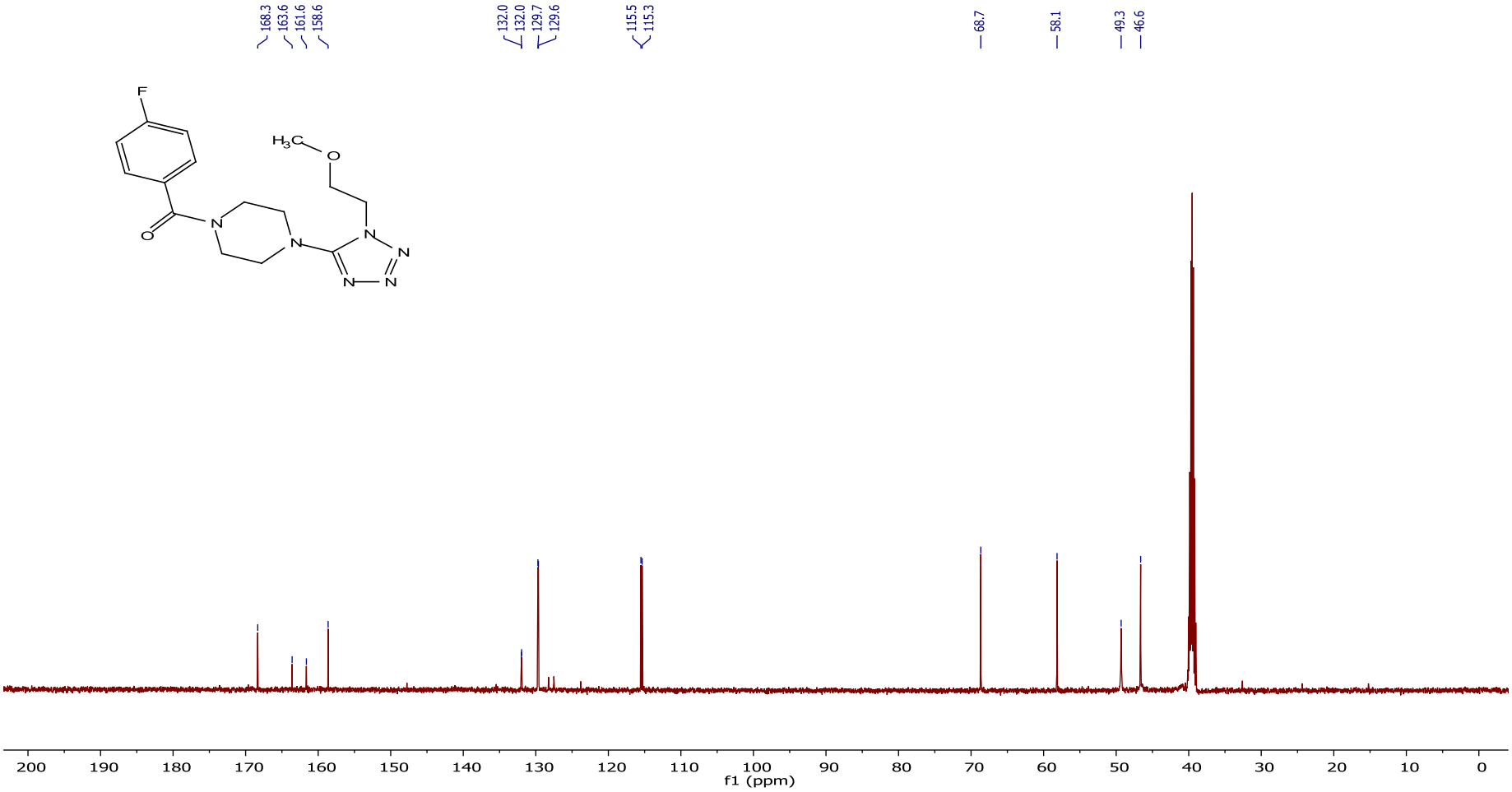
^{13}C NMR spectrum of the compound **9**{*4,289*}.



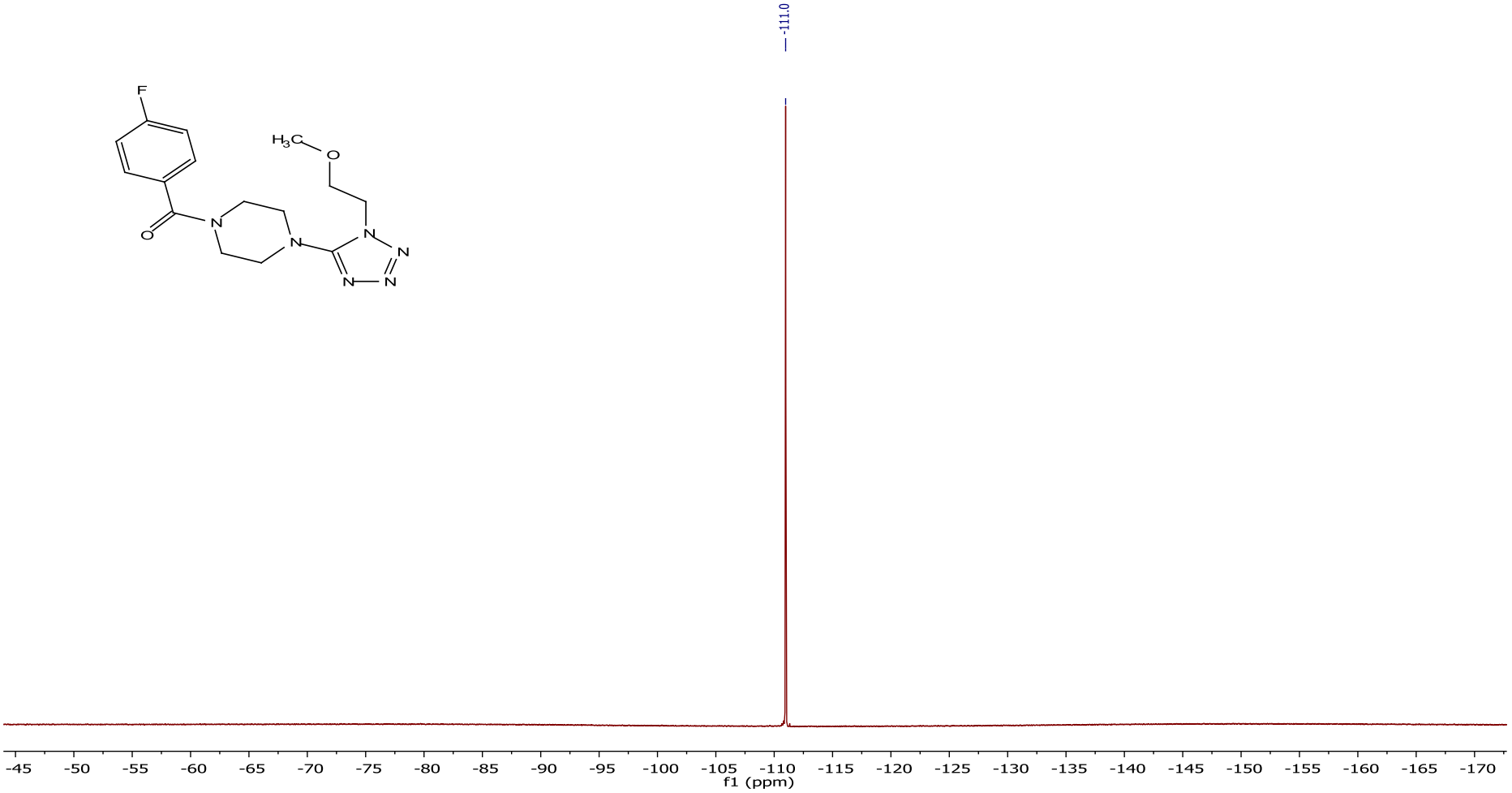
^{1}H NMR spectrum of the compound **9**{*4,291*}.



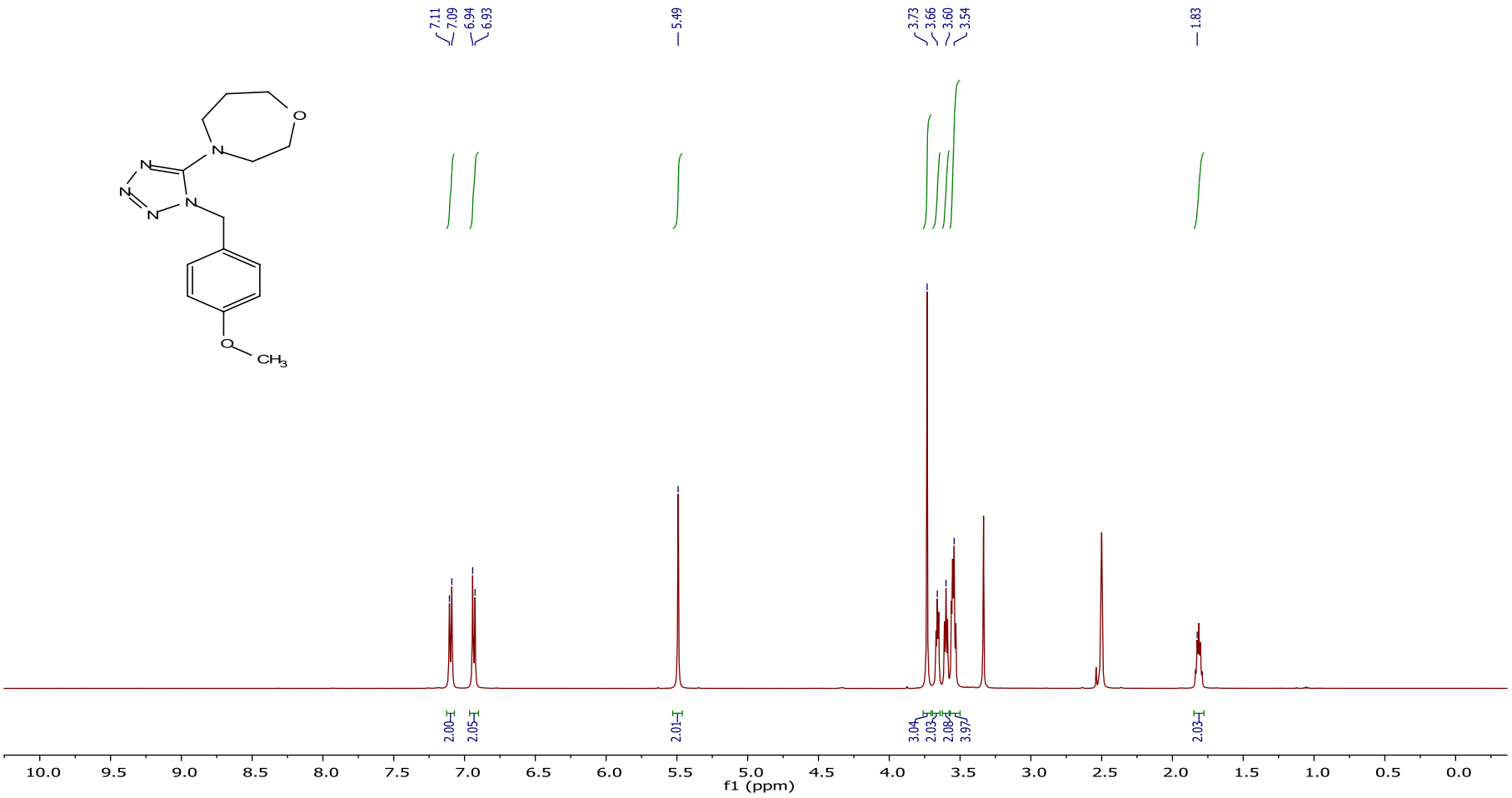
^{13}C NMR spectrum of the compound **9**{*4,291*}.



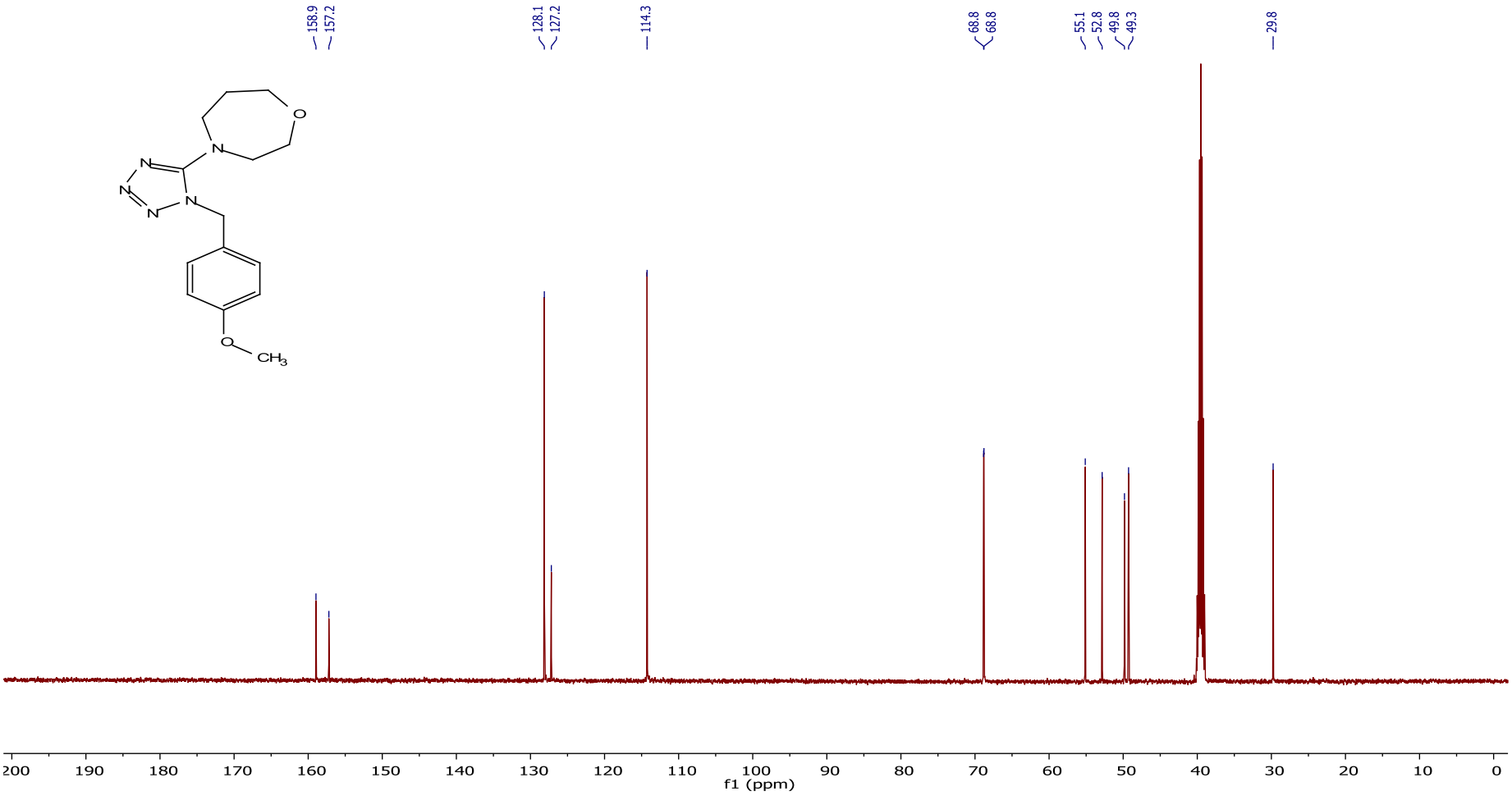
^{19}F NMR spectrum of the compound **9**{*4,291*}.



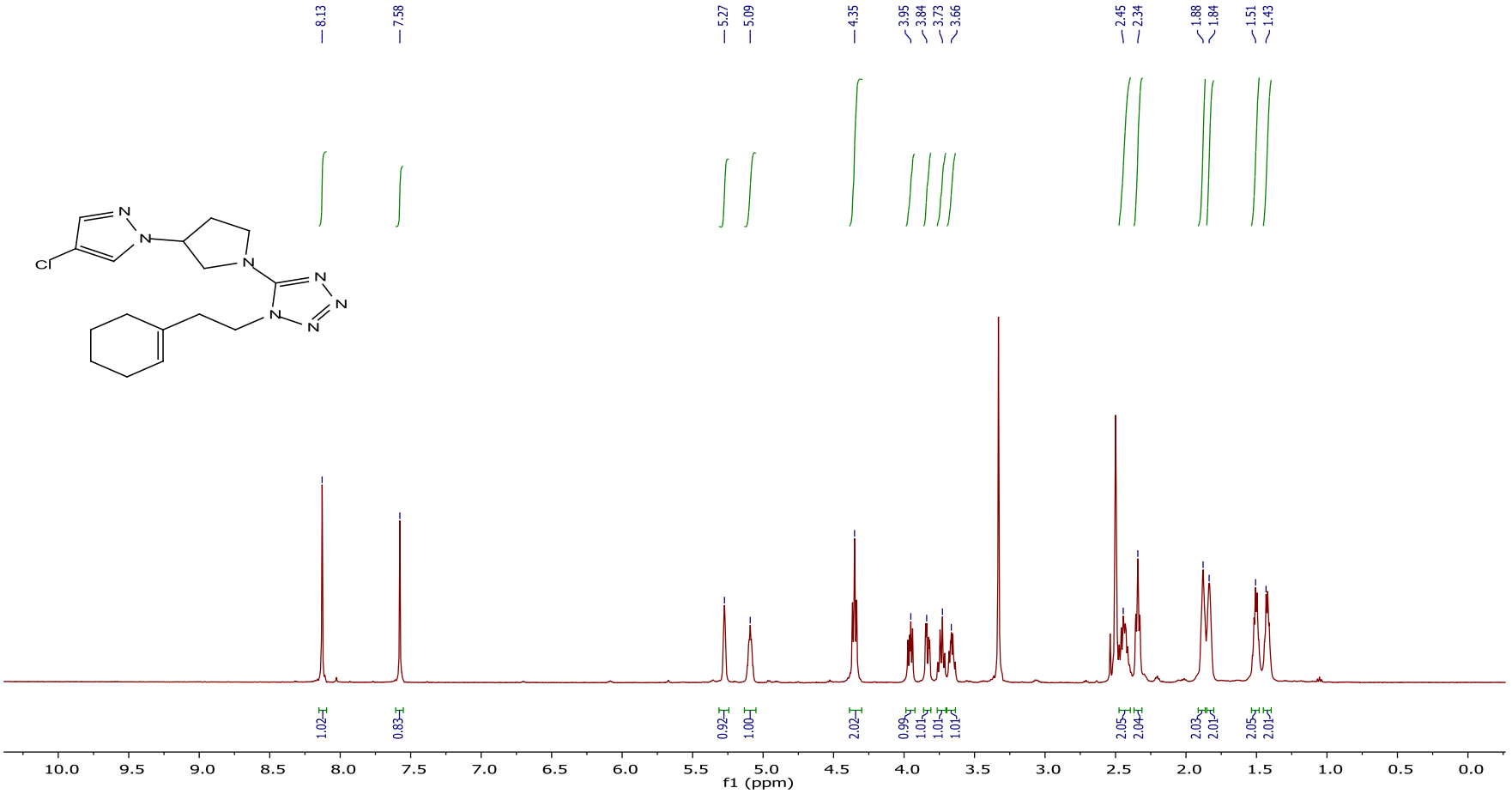
^{1}H NMR spectrum of the compound **9**{*18,300*}.



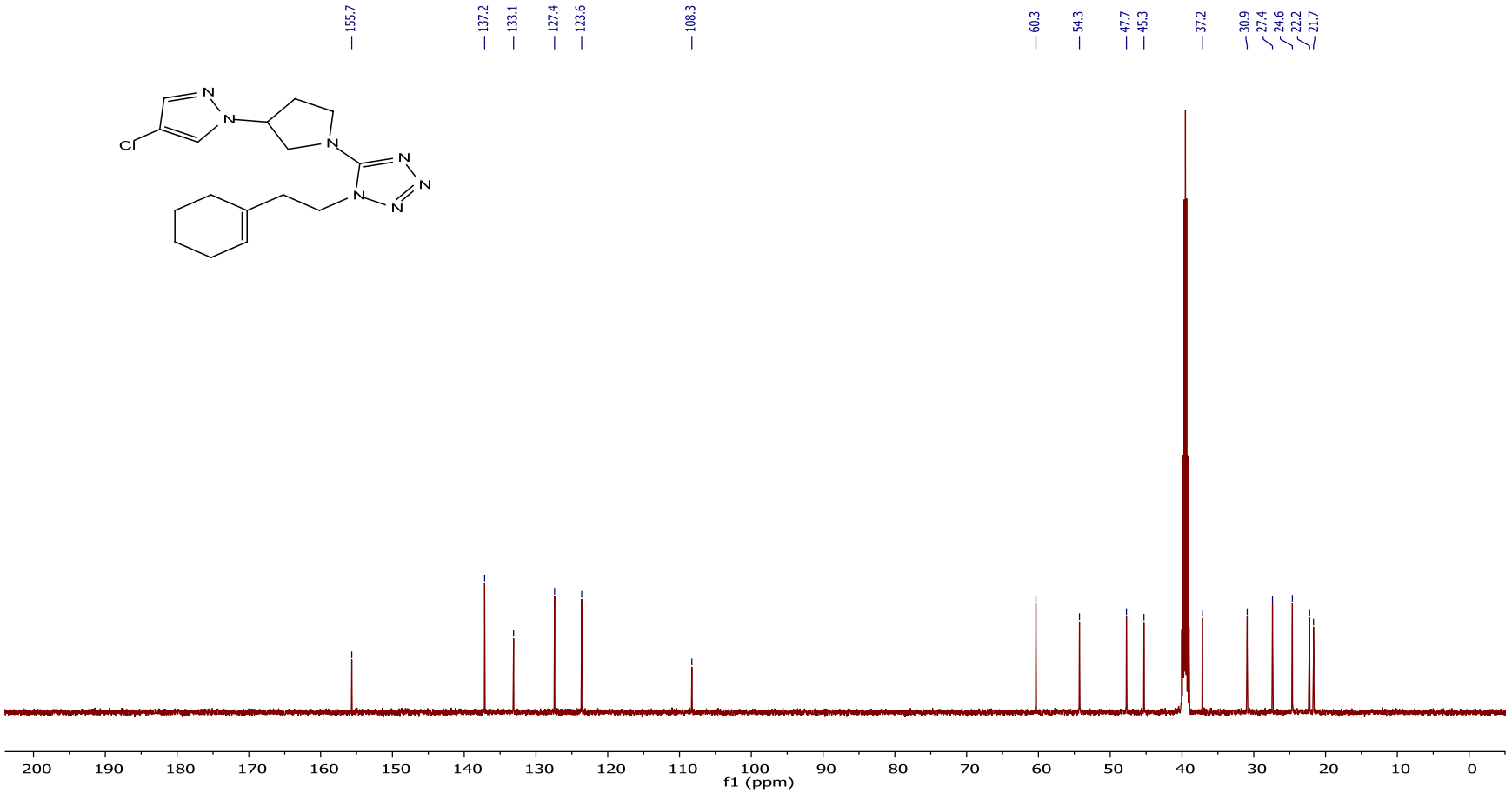
^{13}C NMR spectrum of the compound **9**{*18,300*}.



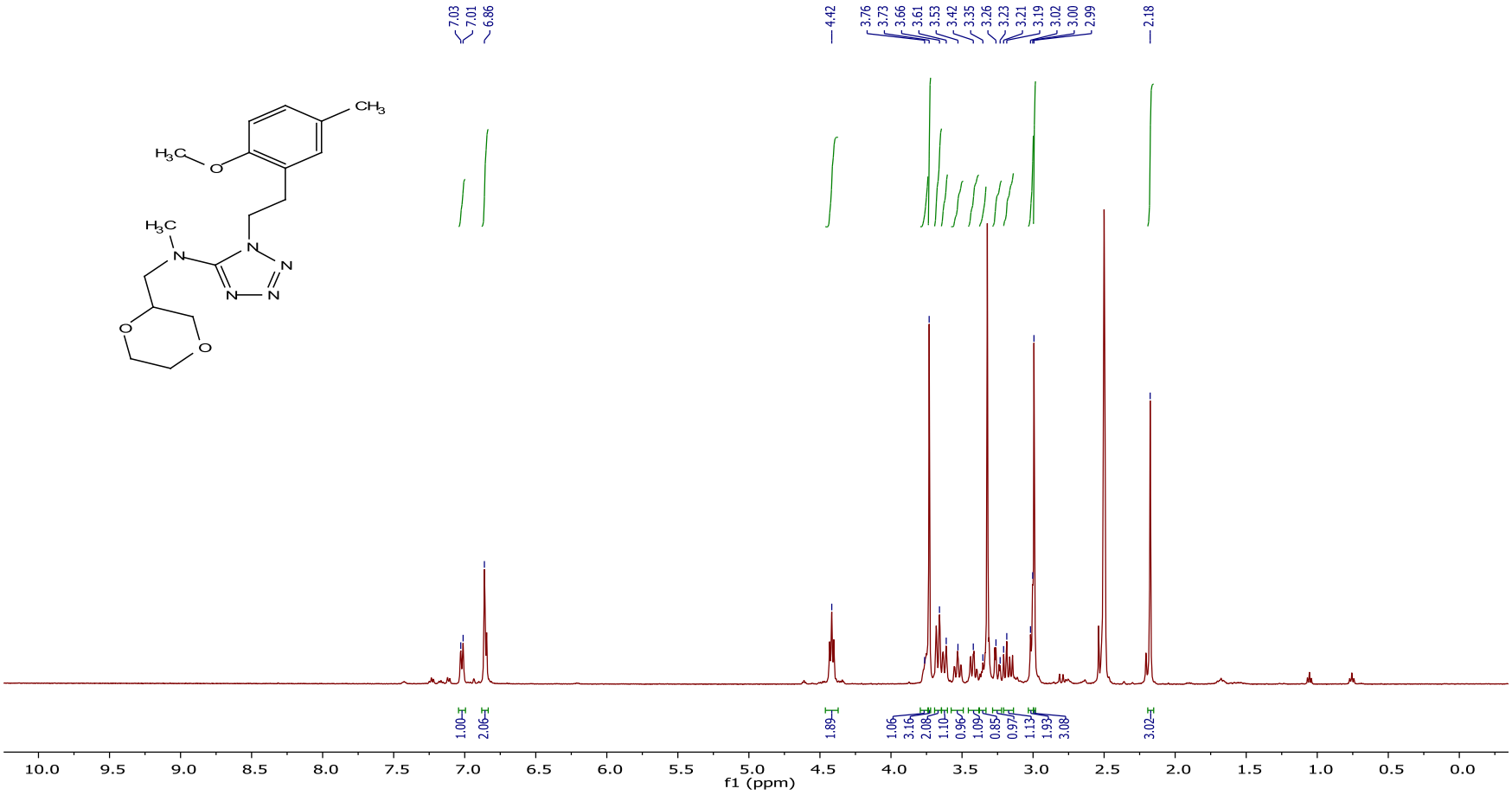
^{1}H NMR spectrum of the compound **9**{*25*,*147*}.



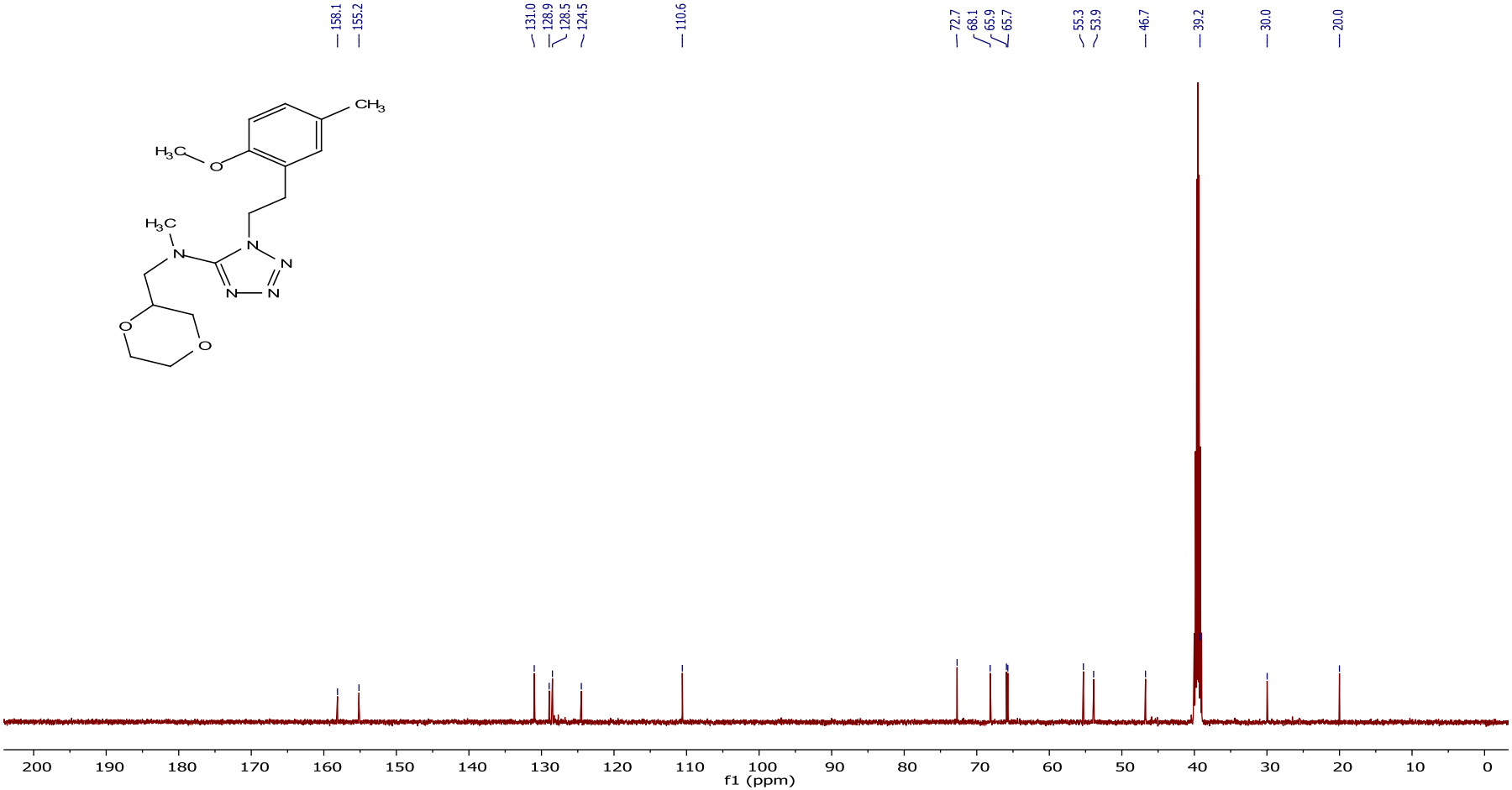
^{13}C NMR spectrum of the compound **9**{*25*,*147*}.



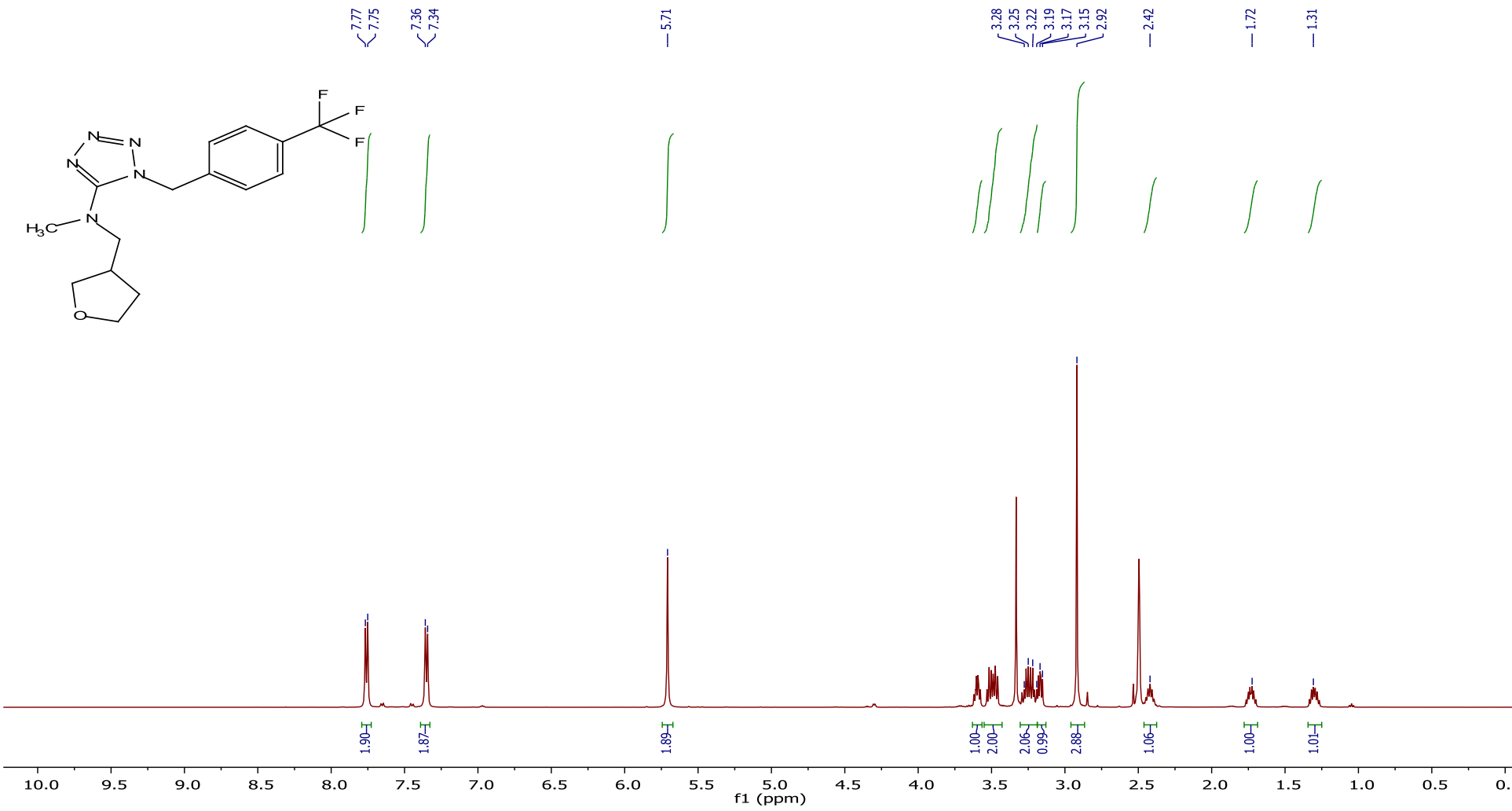
^{1}H NMR spectrum of the compound **9**{*52*,*319*}.



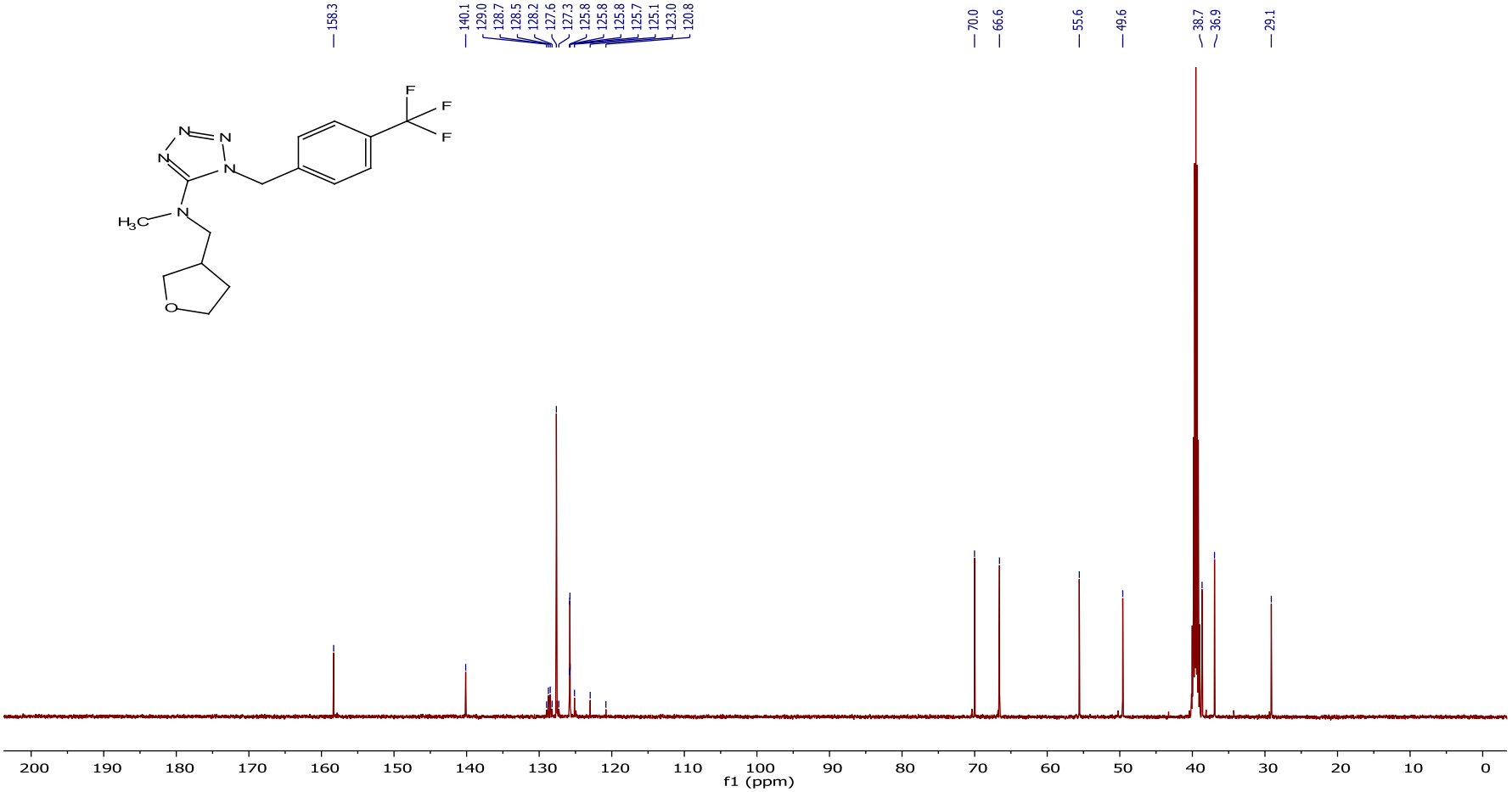
^{13}C NMR spectrum of the compound **9**{*52,319*}.



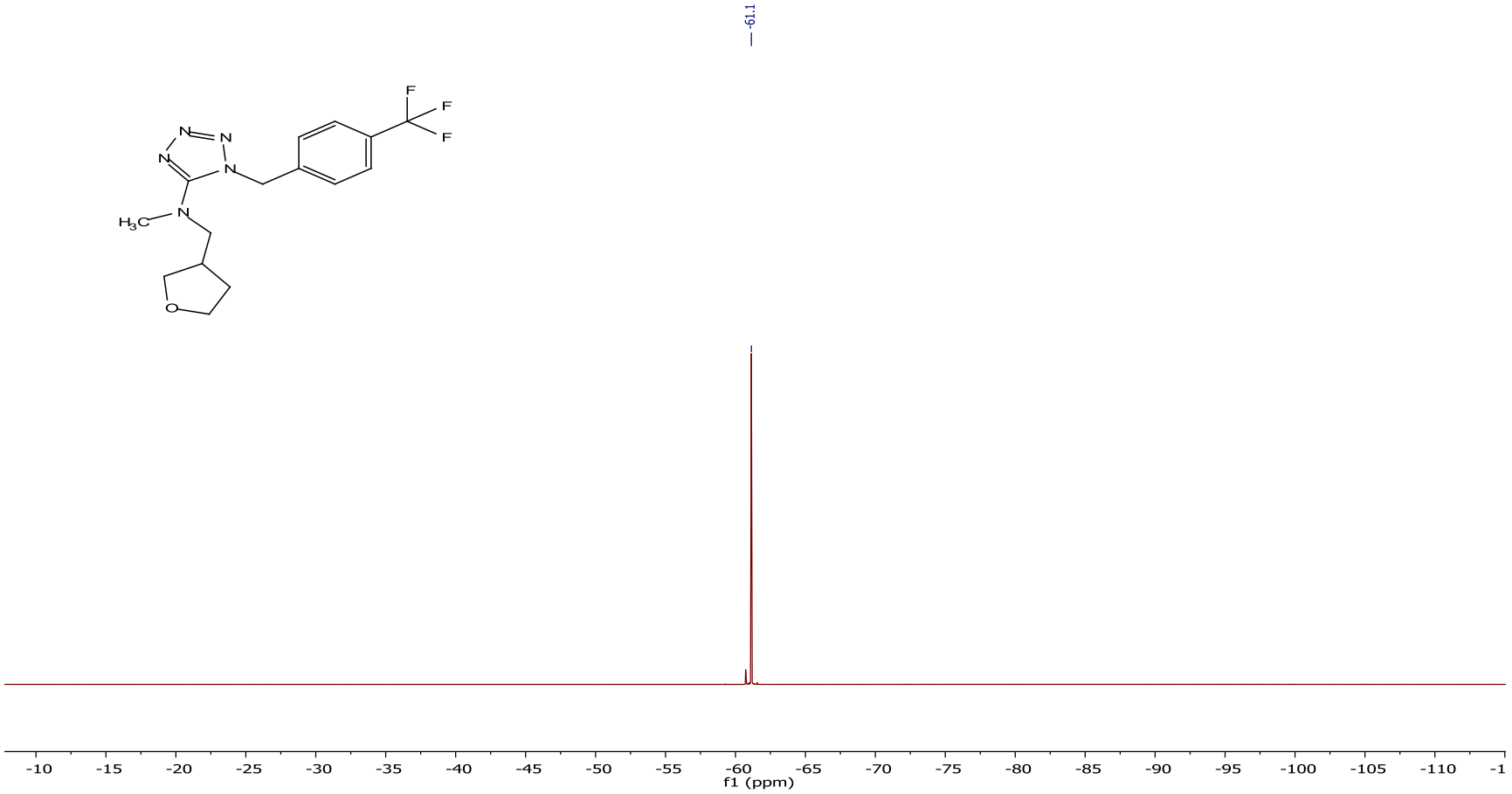
^{1}H NMR spectrum of the compound **9**{*55*,*337*}.



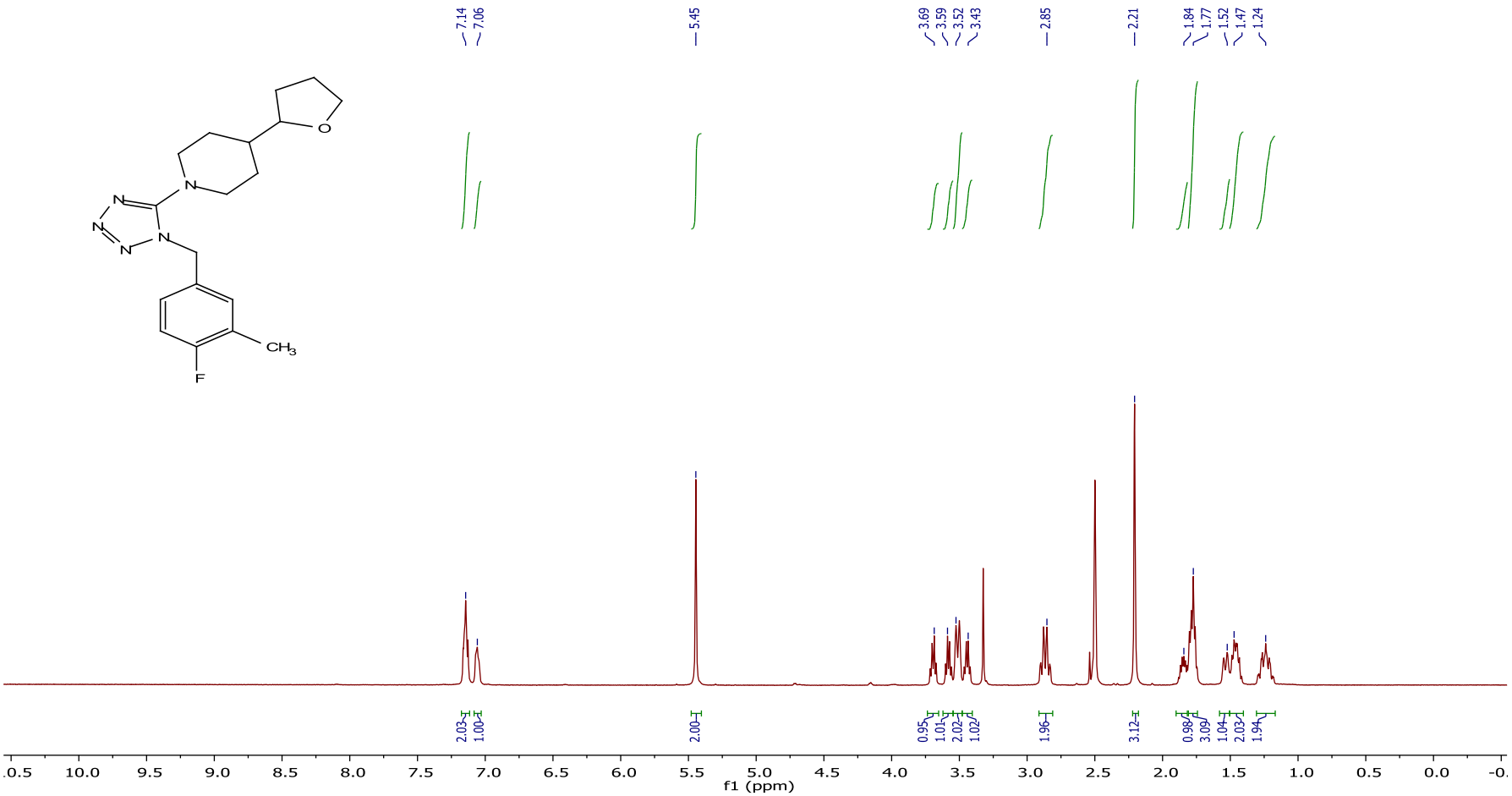
^{13}C NMR spectrum of the compound **9**{*55,337*}.



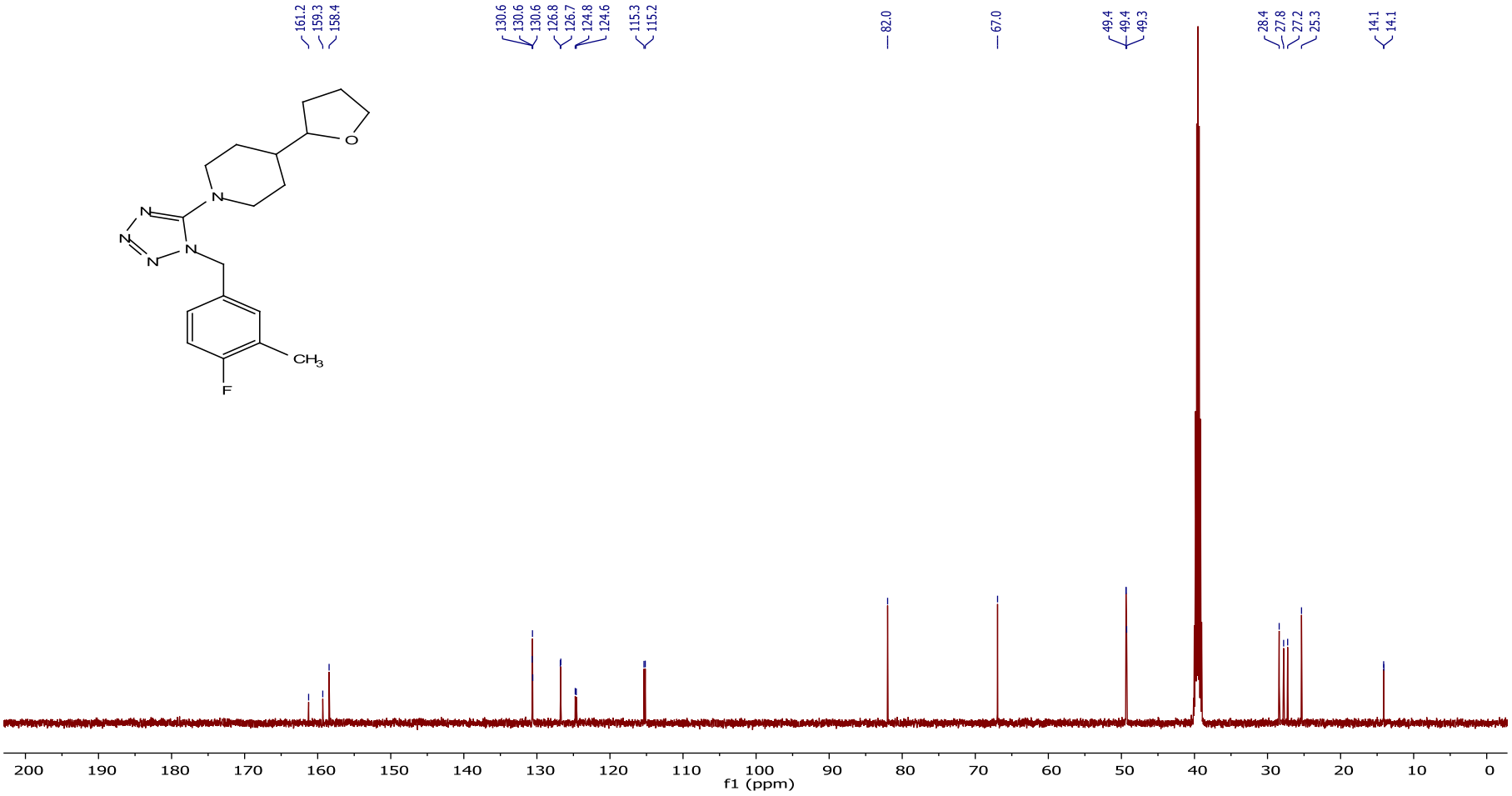
^{19}F NMR spectrum of the compound **9**{*55,337*}.



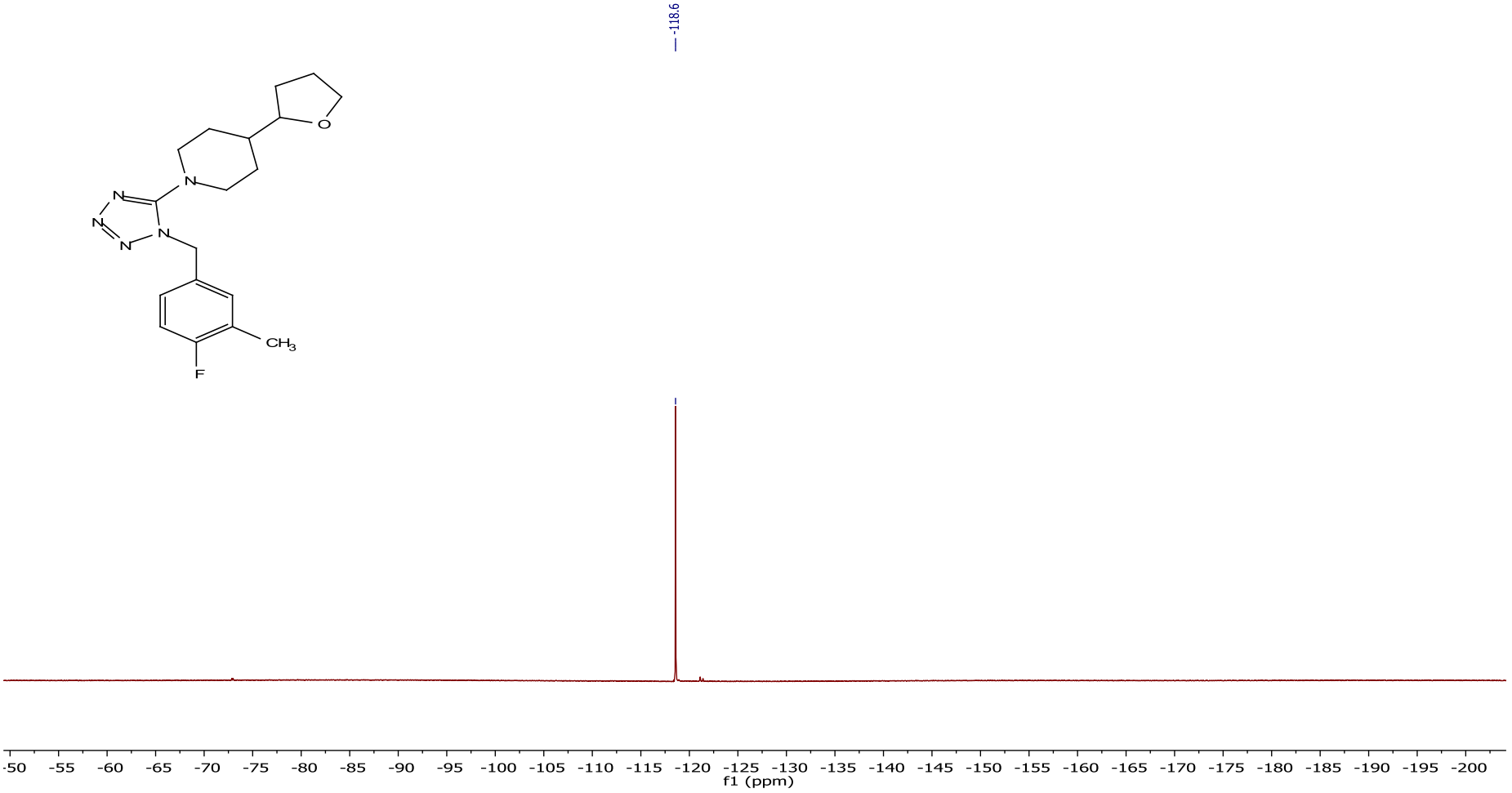
^{1}H NMR spectrum of the compound **9**{*57,261*}.



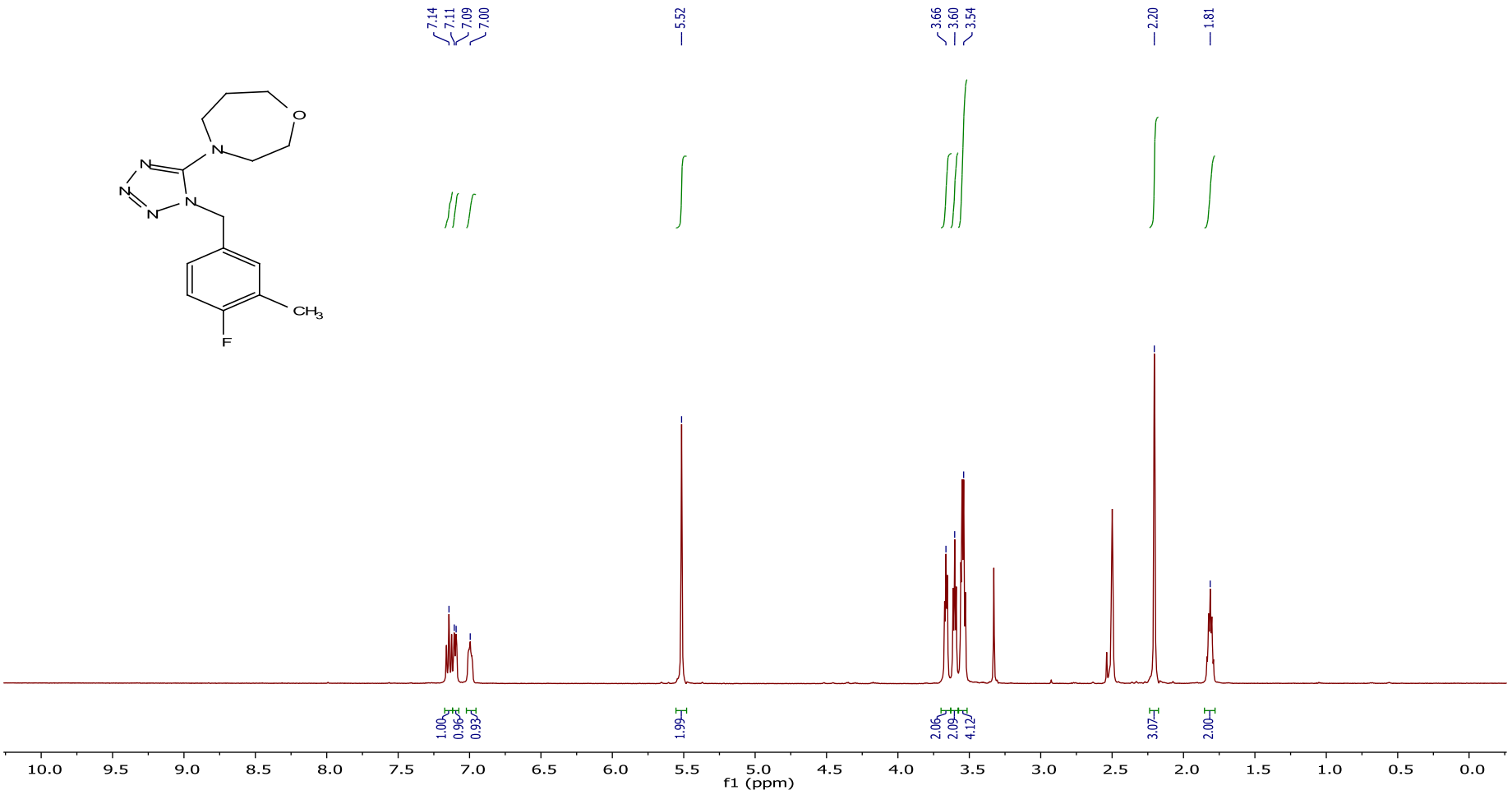
^{13}C NMR spectrum of the compound **9**{*57,261*}.



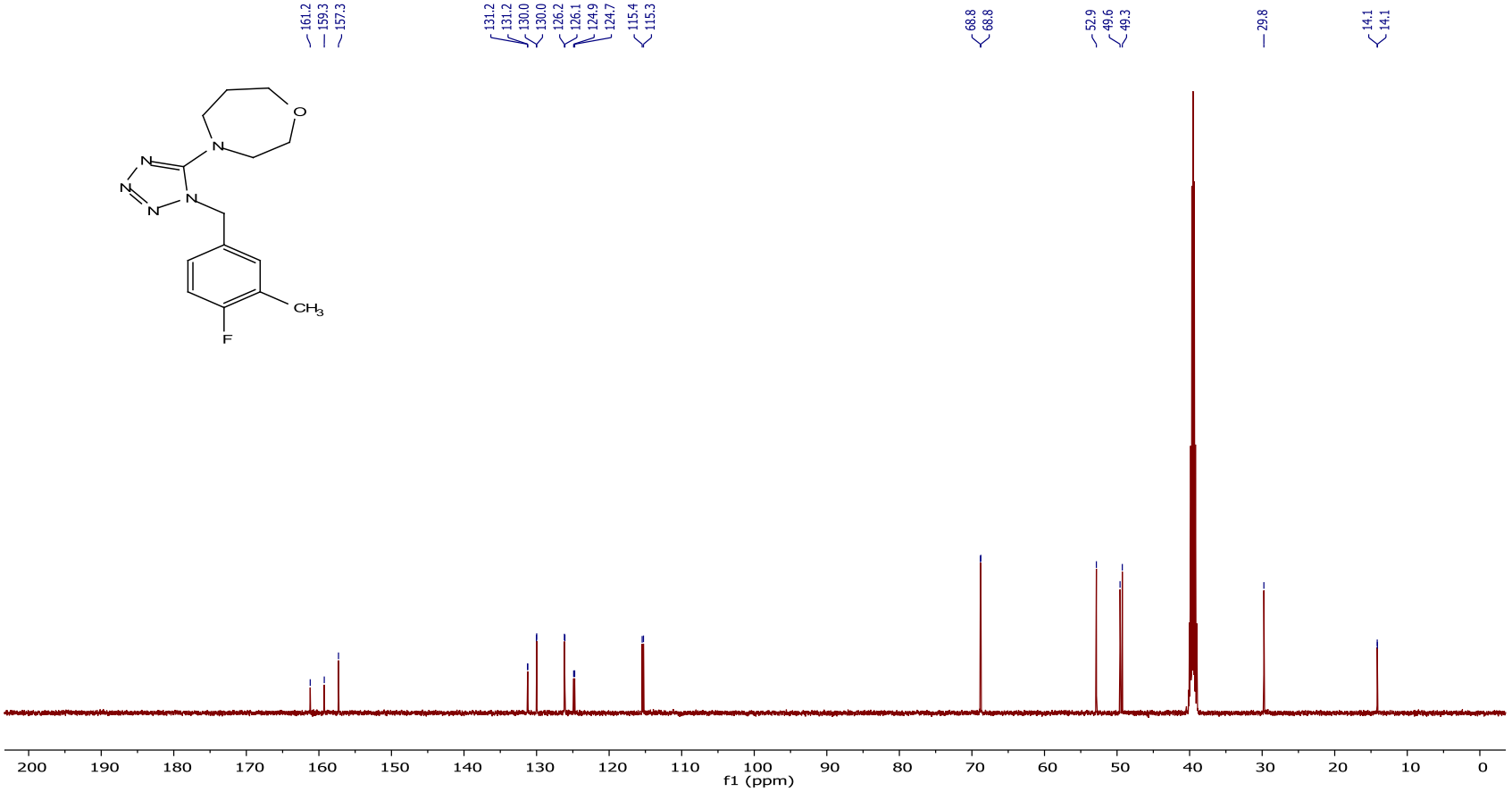
^{19}F NMR spectrum of the compound **9**{*57,261*}.



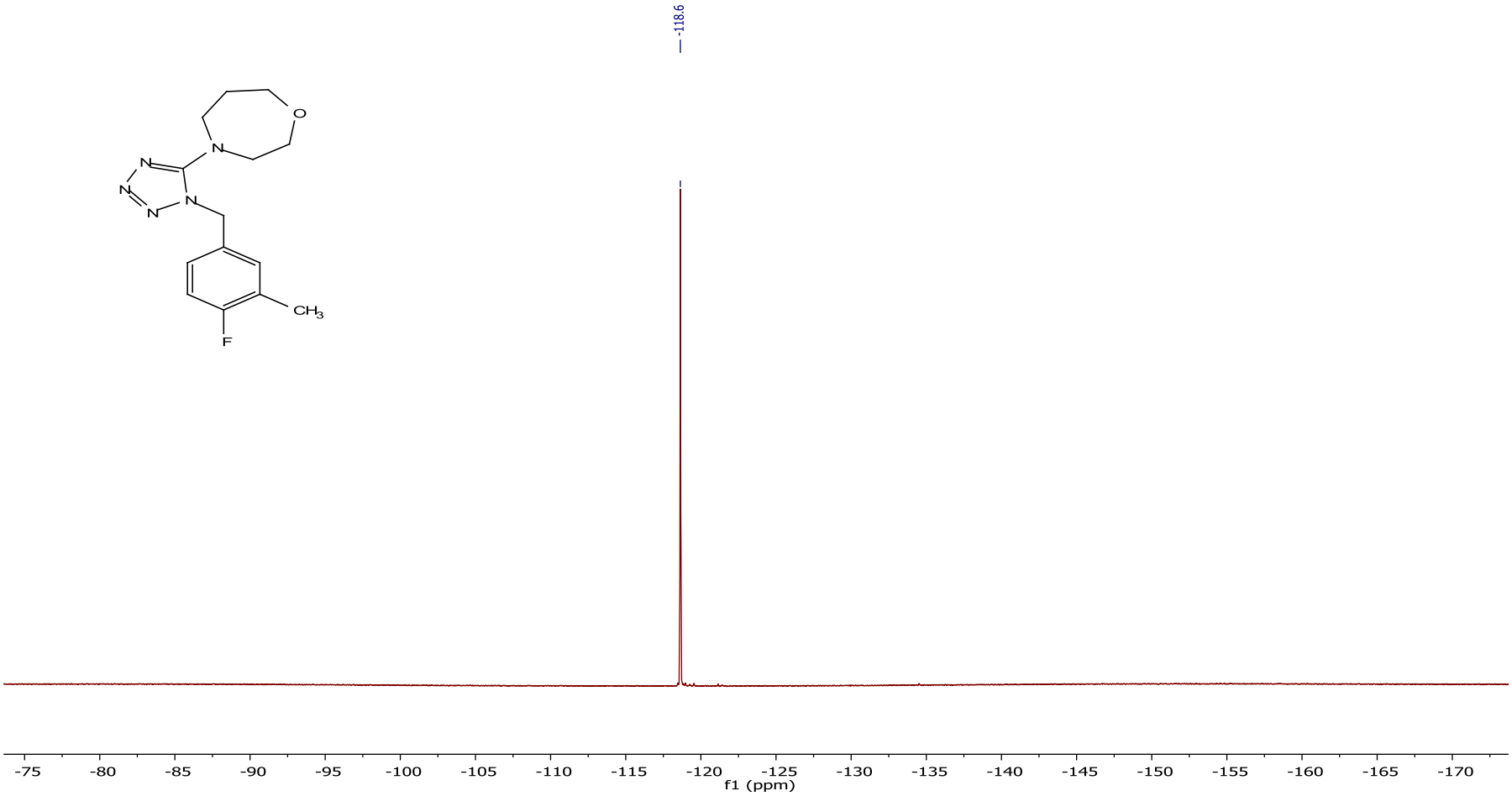
^{1}H NMR spectrum of the compound **9**{*57,300*}.



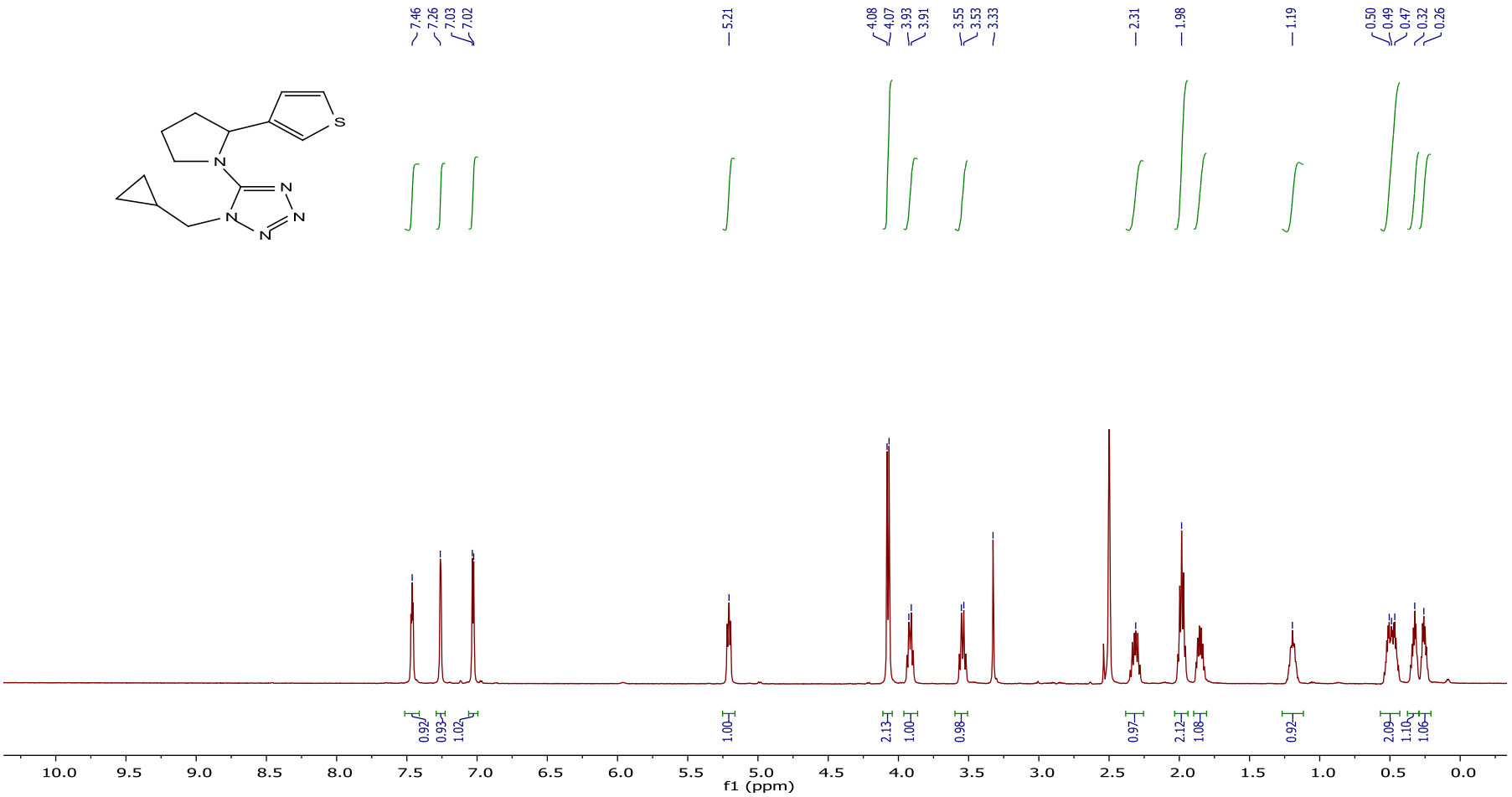
^{13}C NMR spectrum of the compound **9**{*57,300*}.



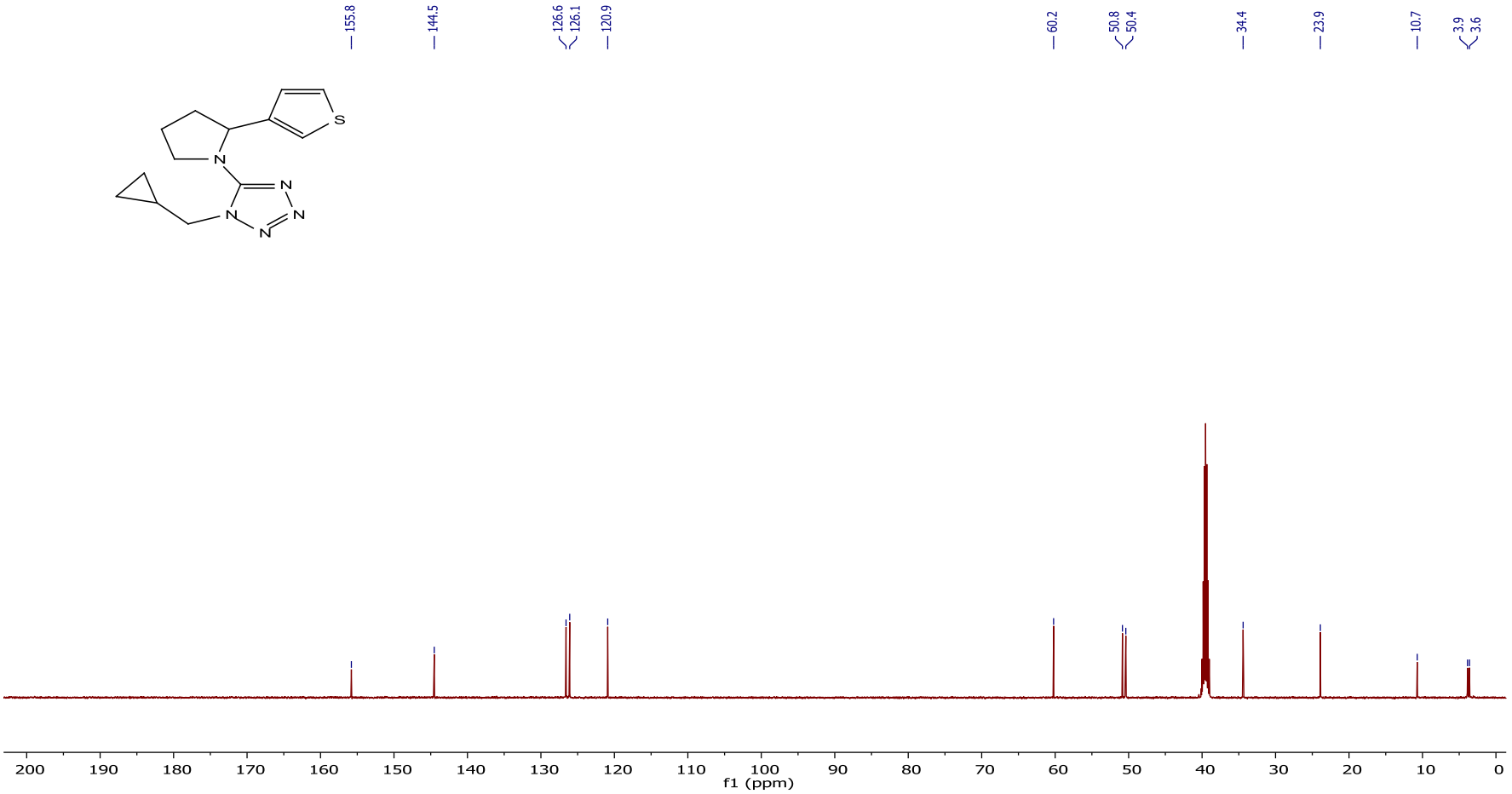
^{19}F NMR spectrum of the compound **9**{*57,300*}.



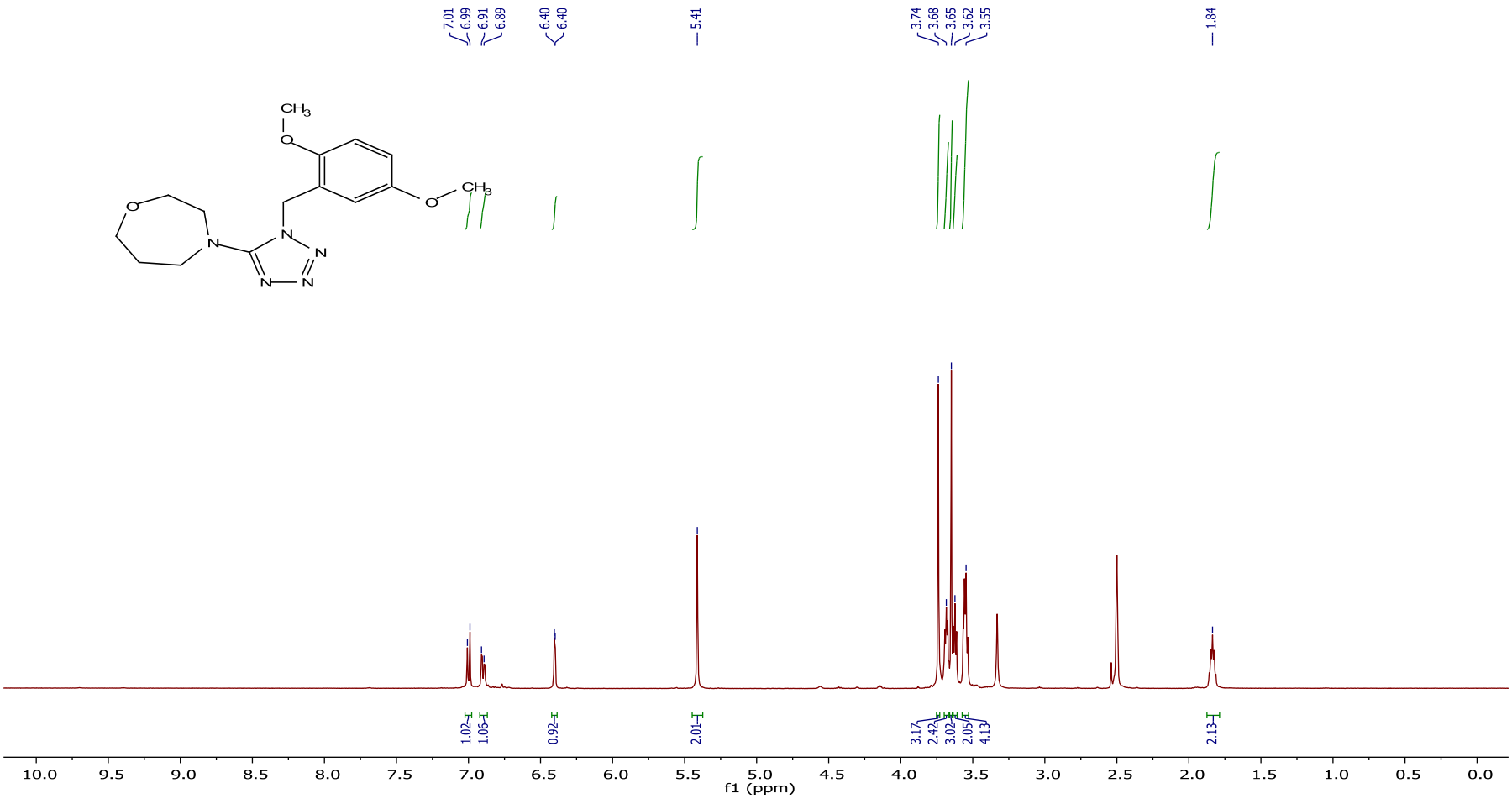
^{1}H NMR spectrum of the compound **9**{*63,327*}.



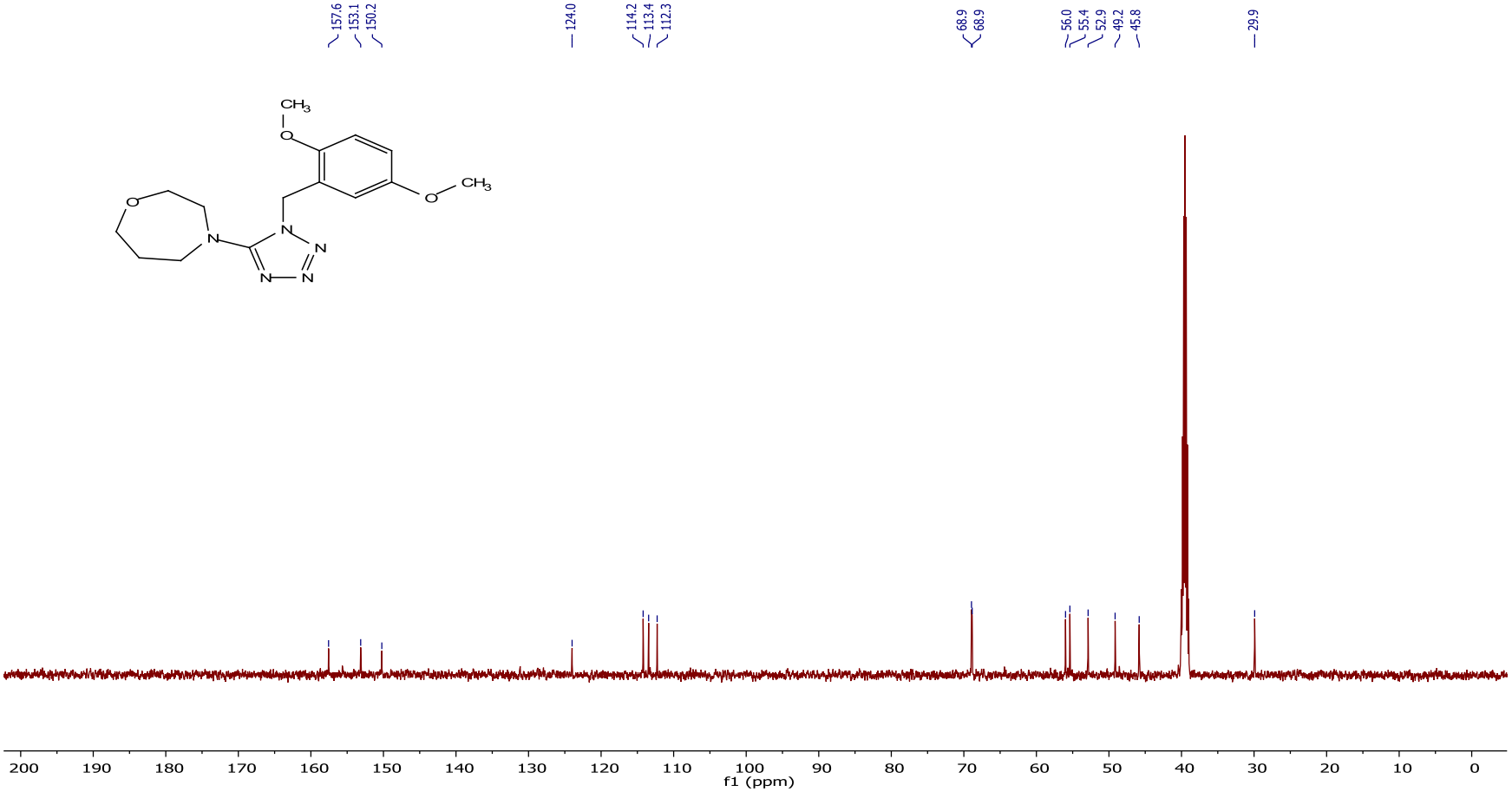
^{13}C NMR spectrum of the compound **9**{*63,327*}.



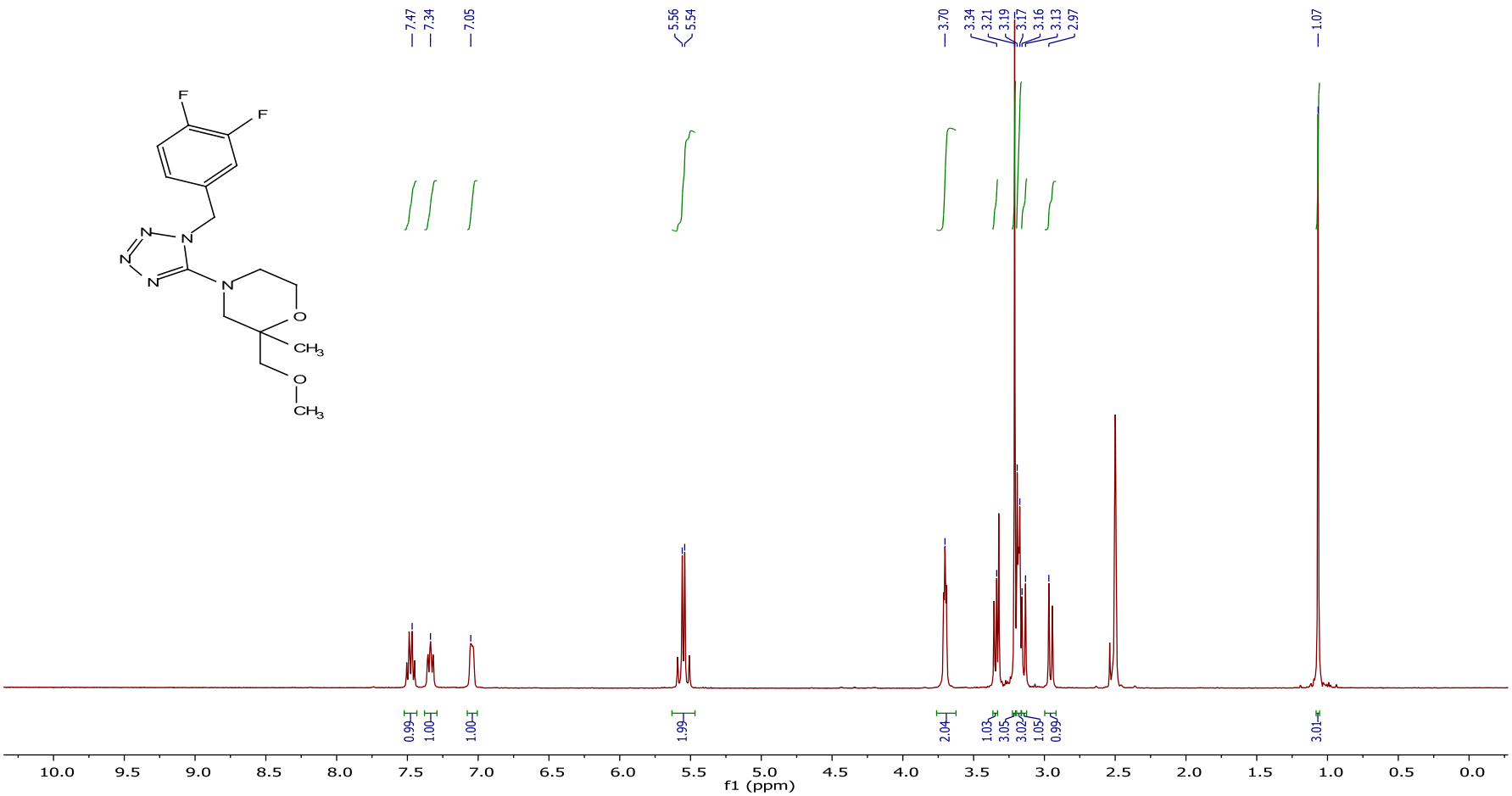
^{1}H NMR spectrum of the compound **9**{*68,300*}.



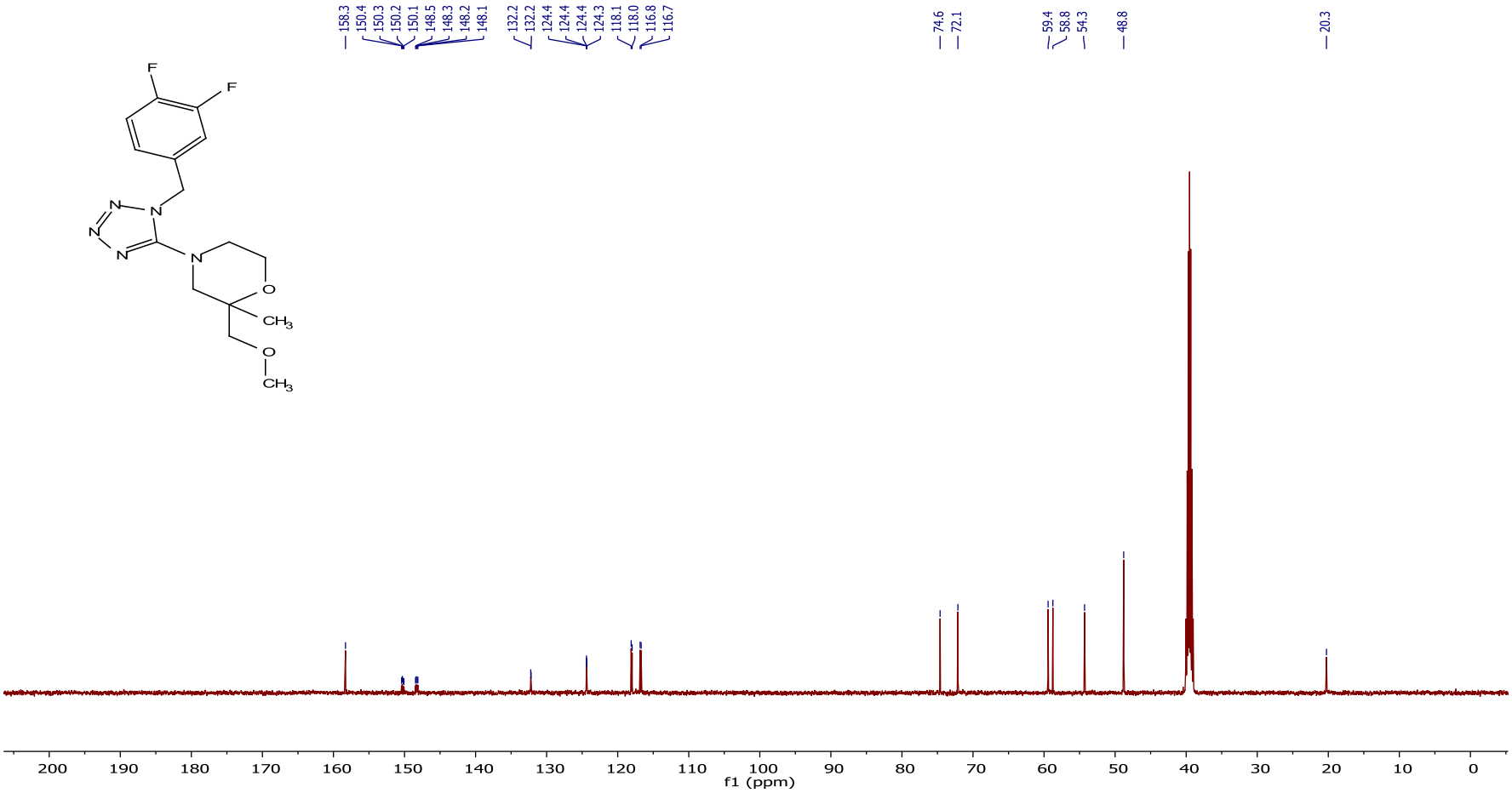
^{13}C NMR spectrum of the compound **9**{*68,300*}.



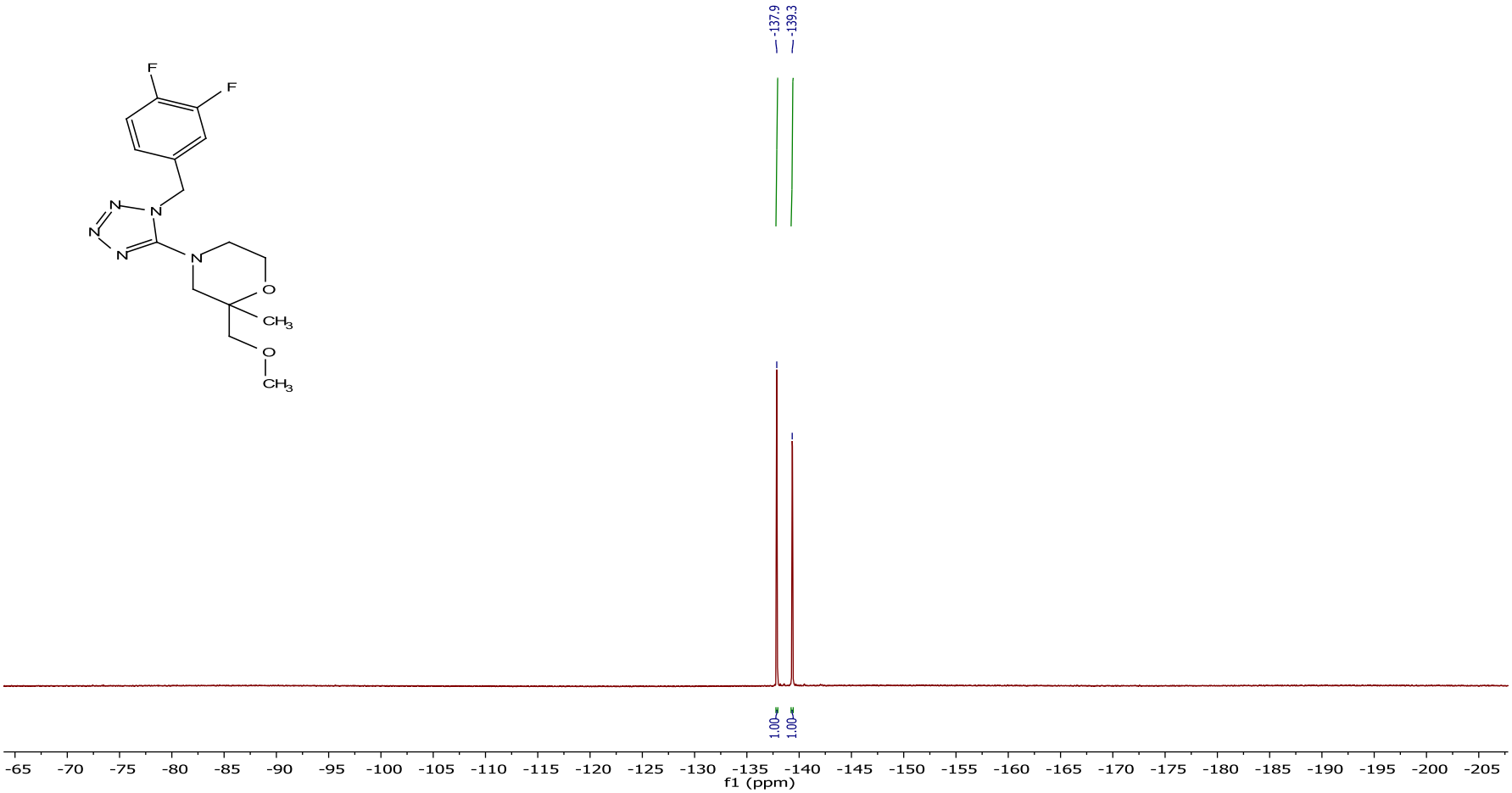
^{1}H NMR spectrum of the compound **9**{*77,363*}.



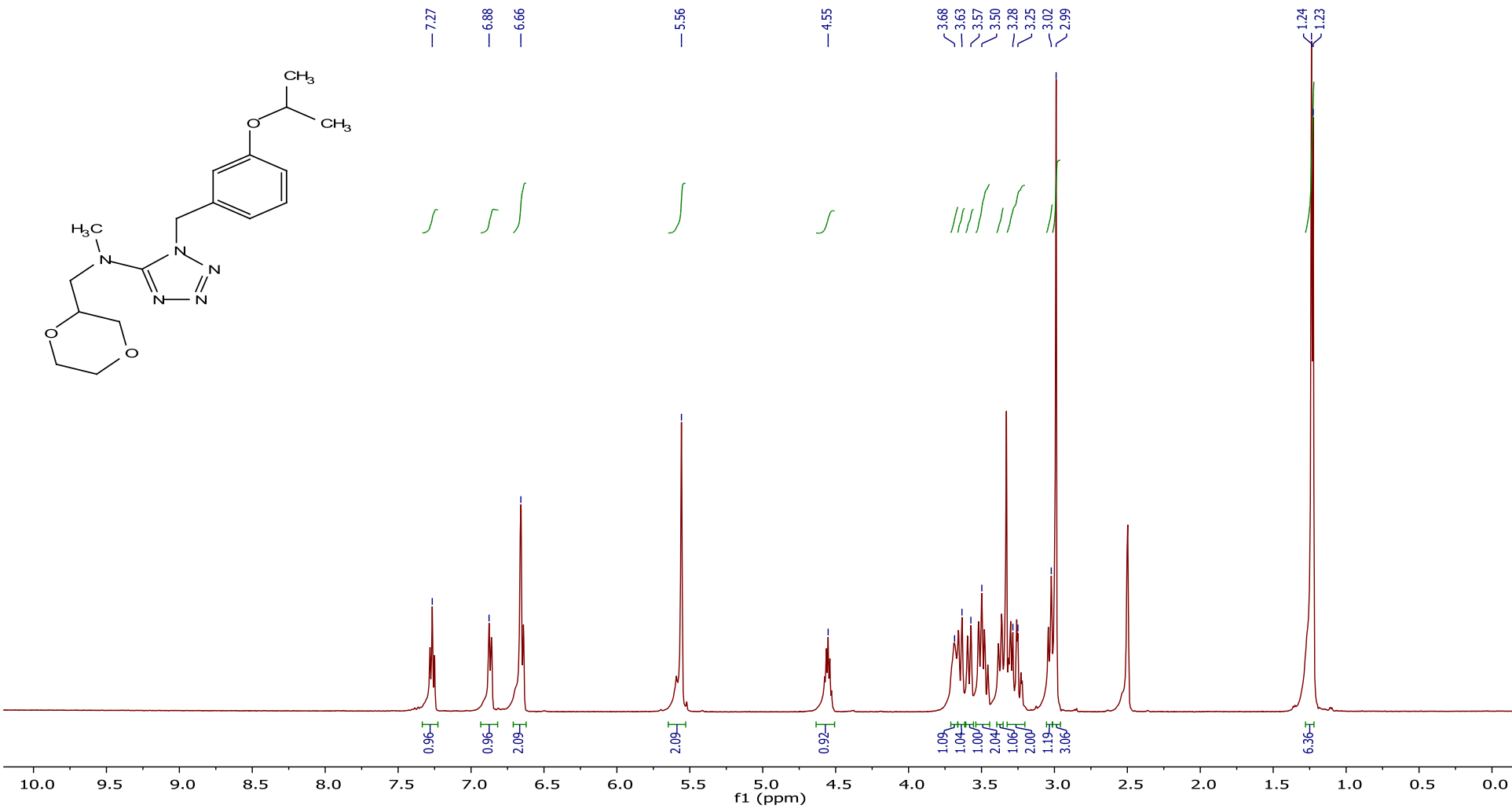
^{13}C NMR spectrum of the compound **9**{*77,363*}.



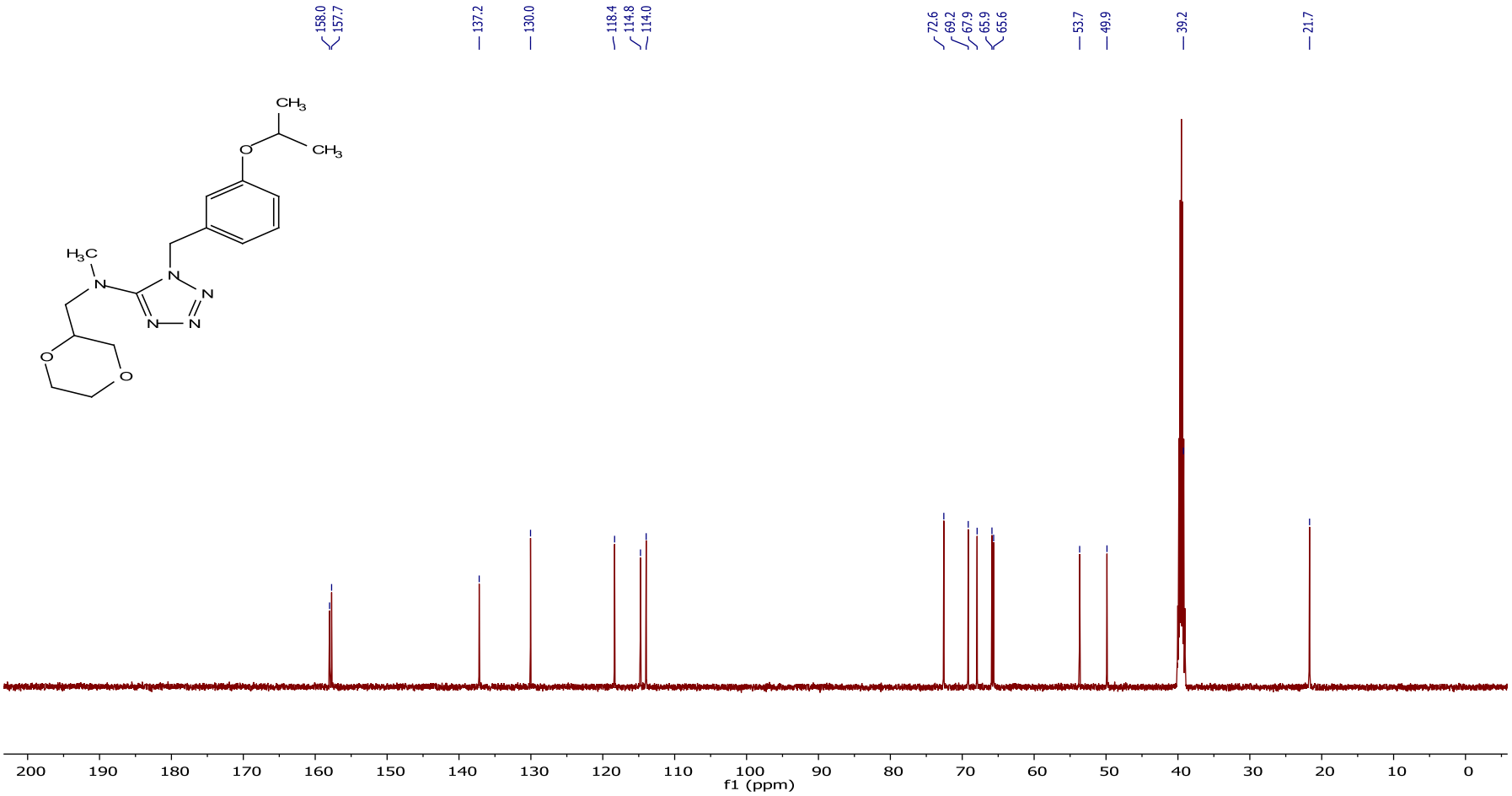
^{19}F NMR spectrum of the compound **9**{*77,363*}.



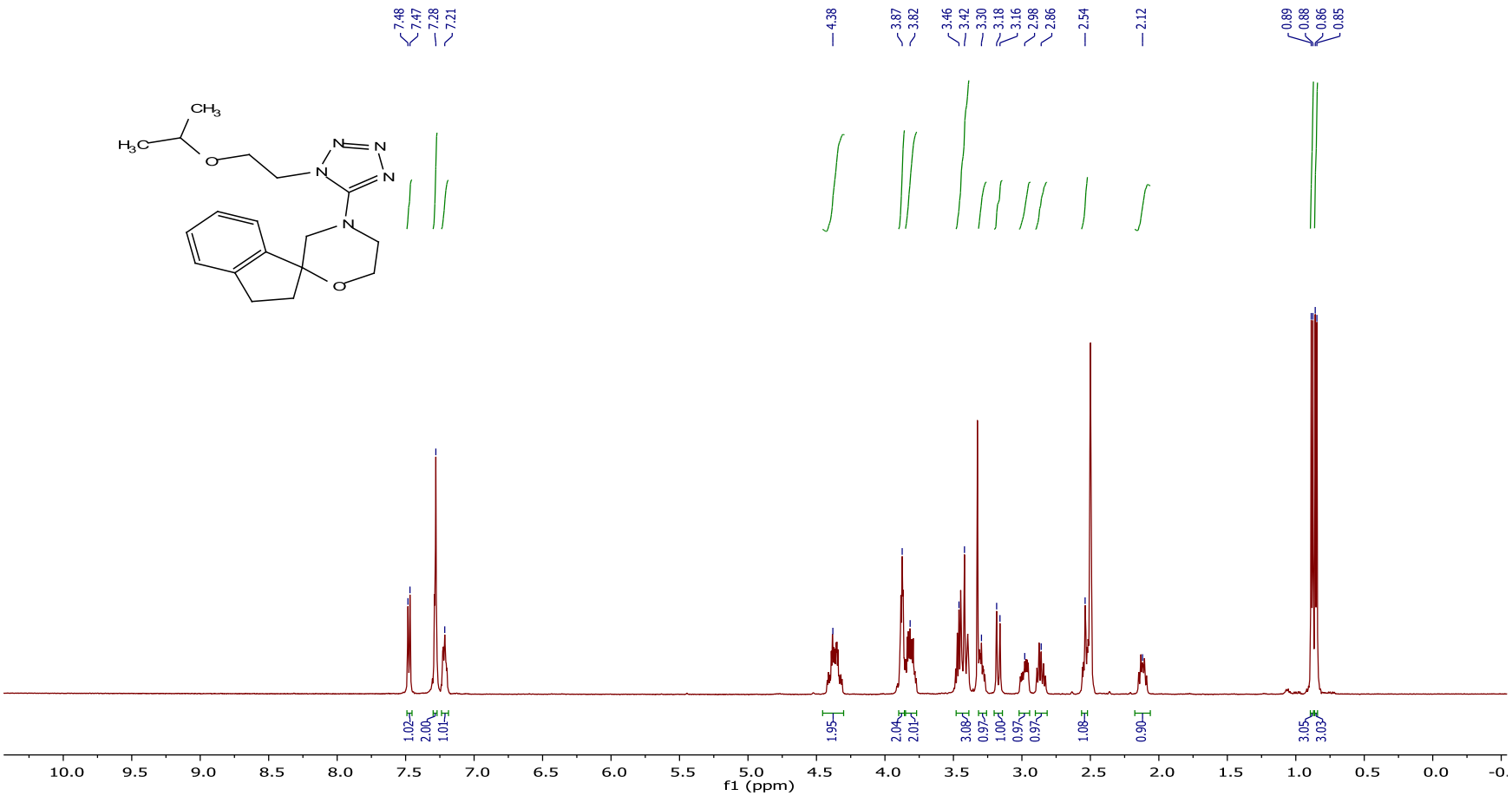
^{1}H NMR spectrum of the compound **9**{*84,319*}.



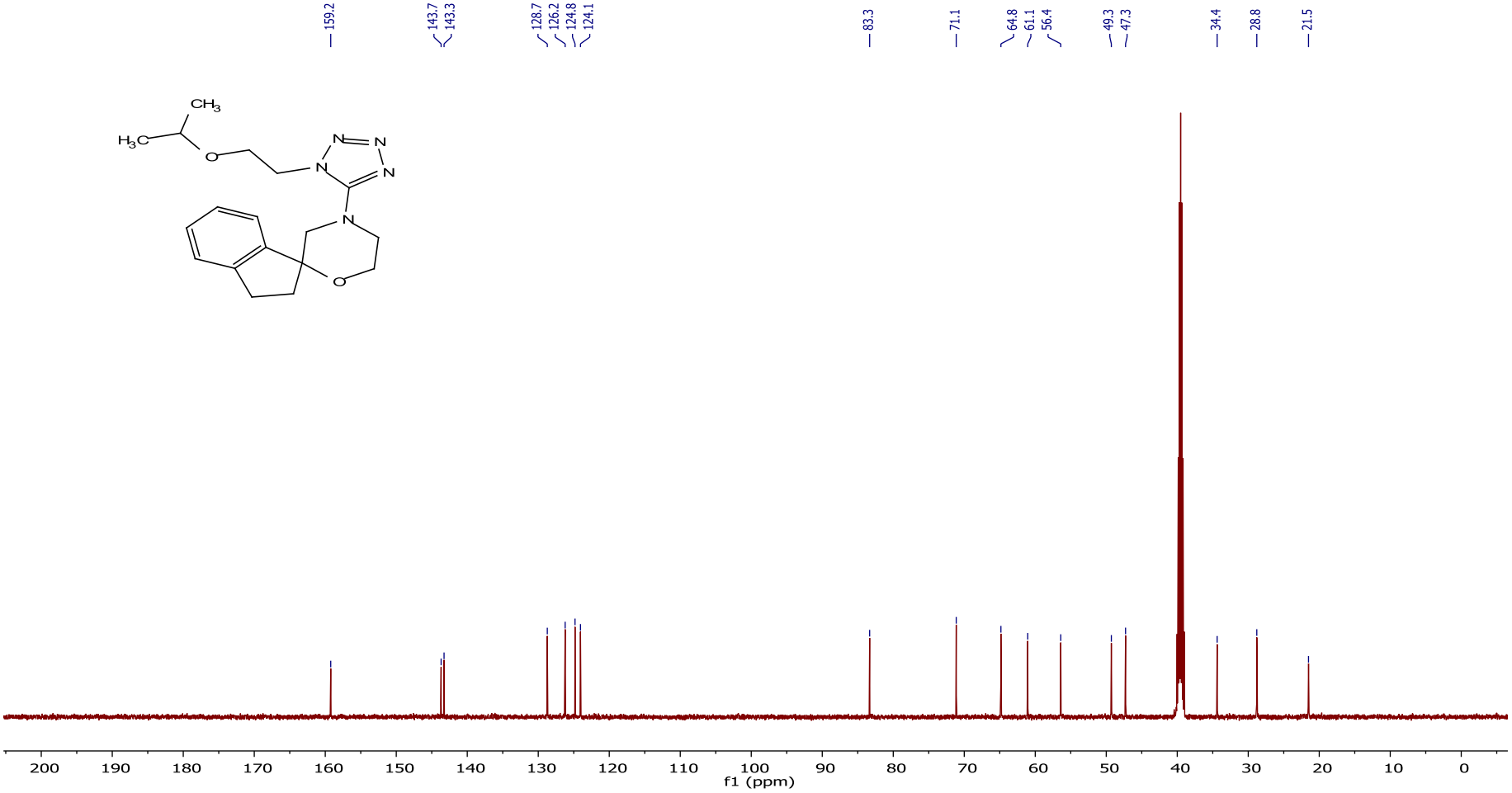
^{13}C NMR spectrum of the compound **9**{*84,319*}.



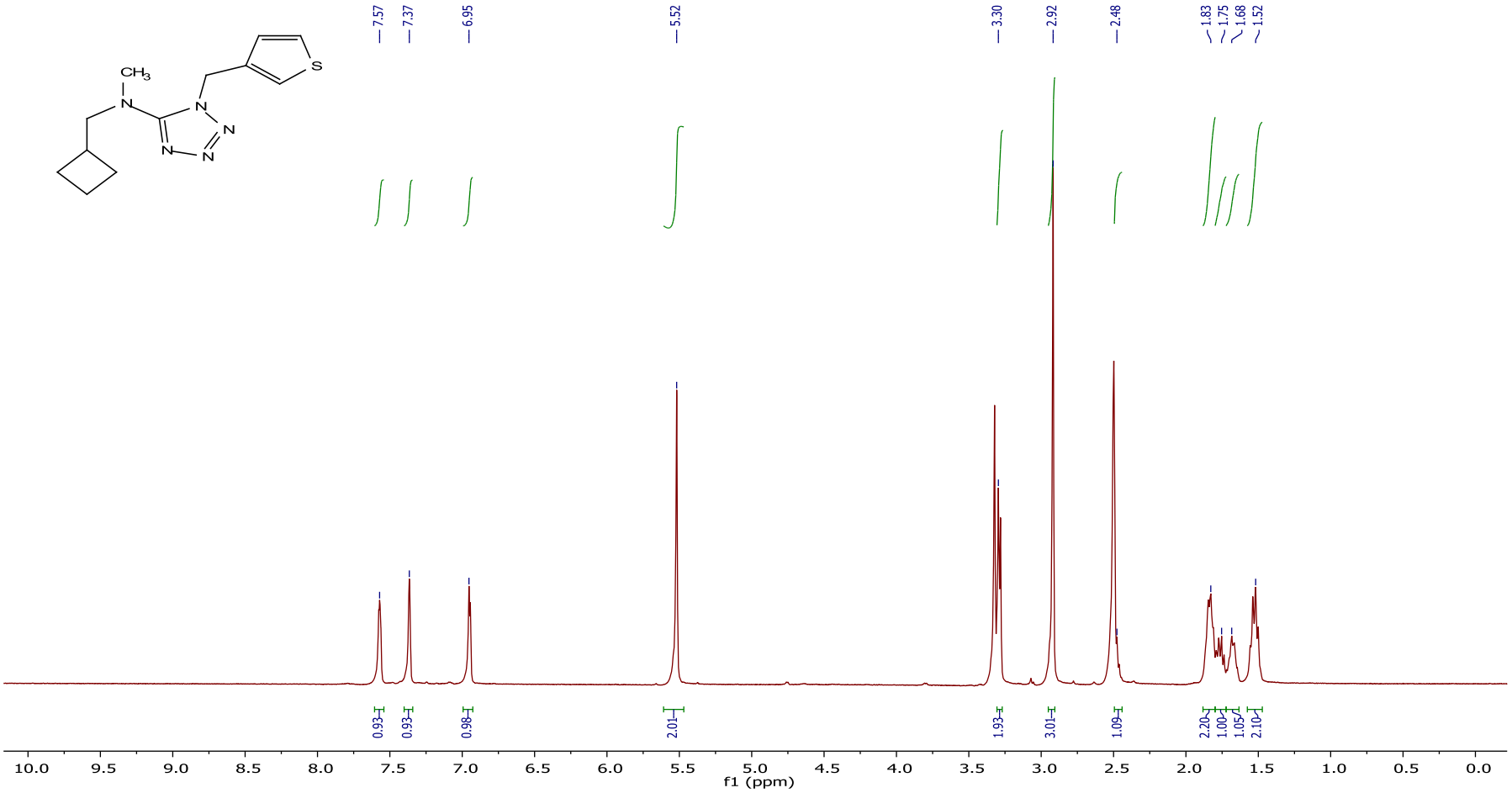
^{1}H NMR spectrum of the compound **9**{*90,371*}.



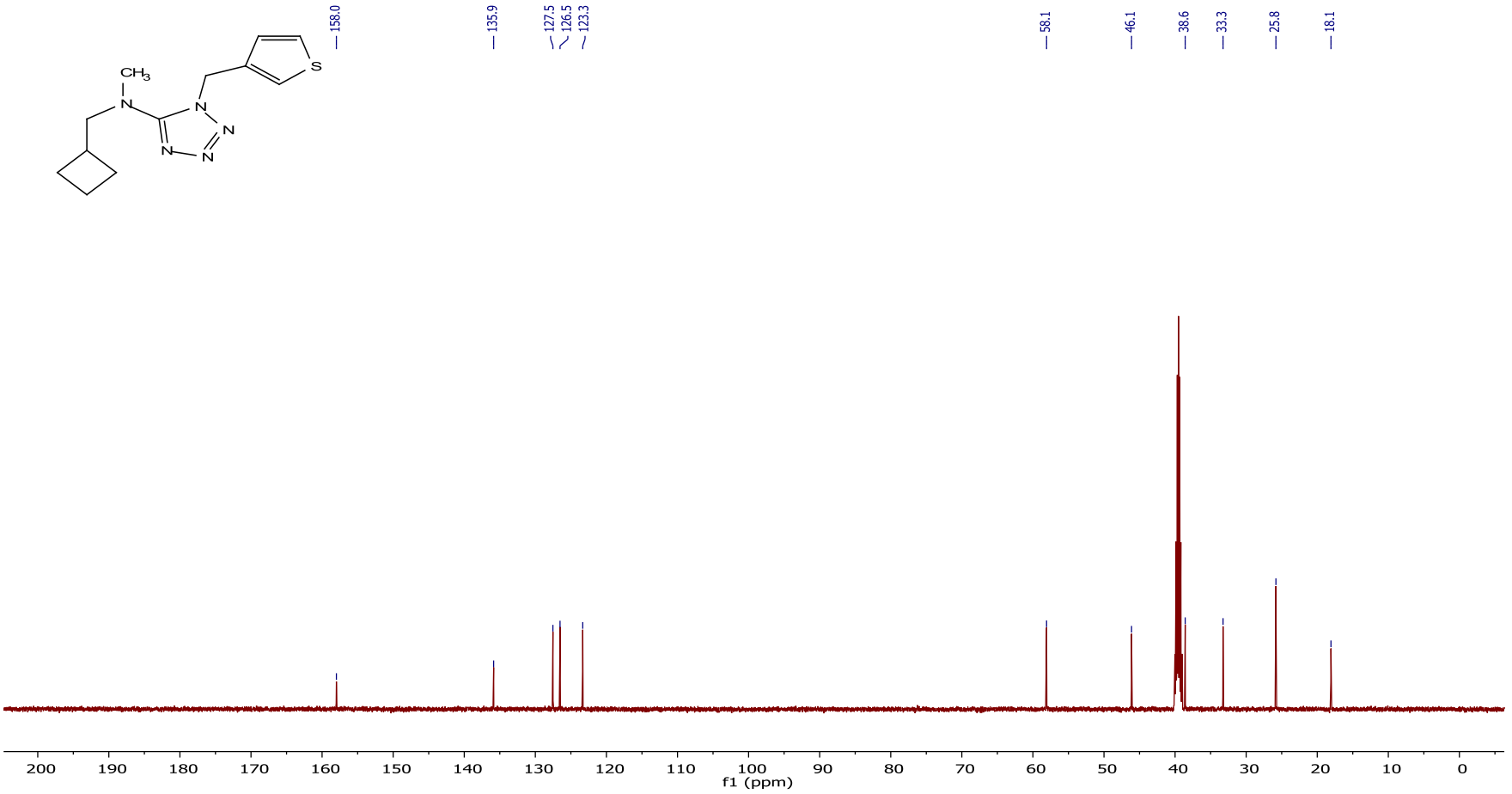
^{13}C NMR spectrum of the compound **9**{*90,371*}.



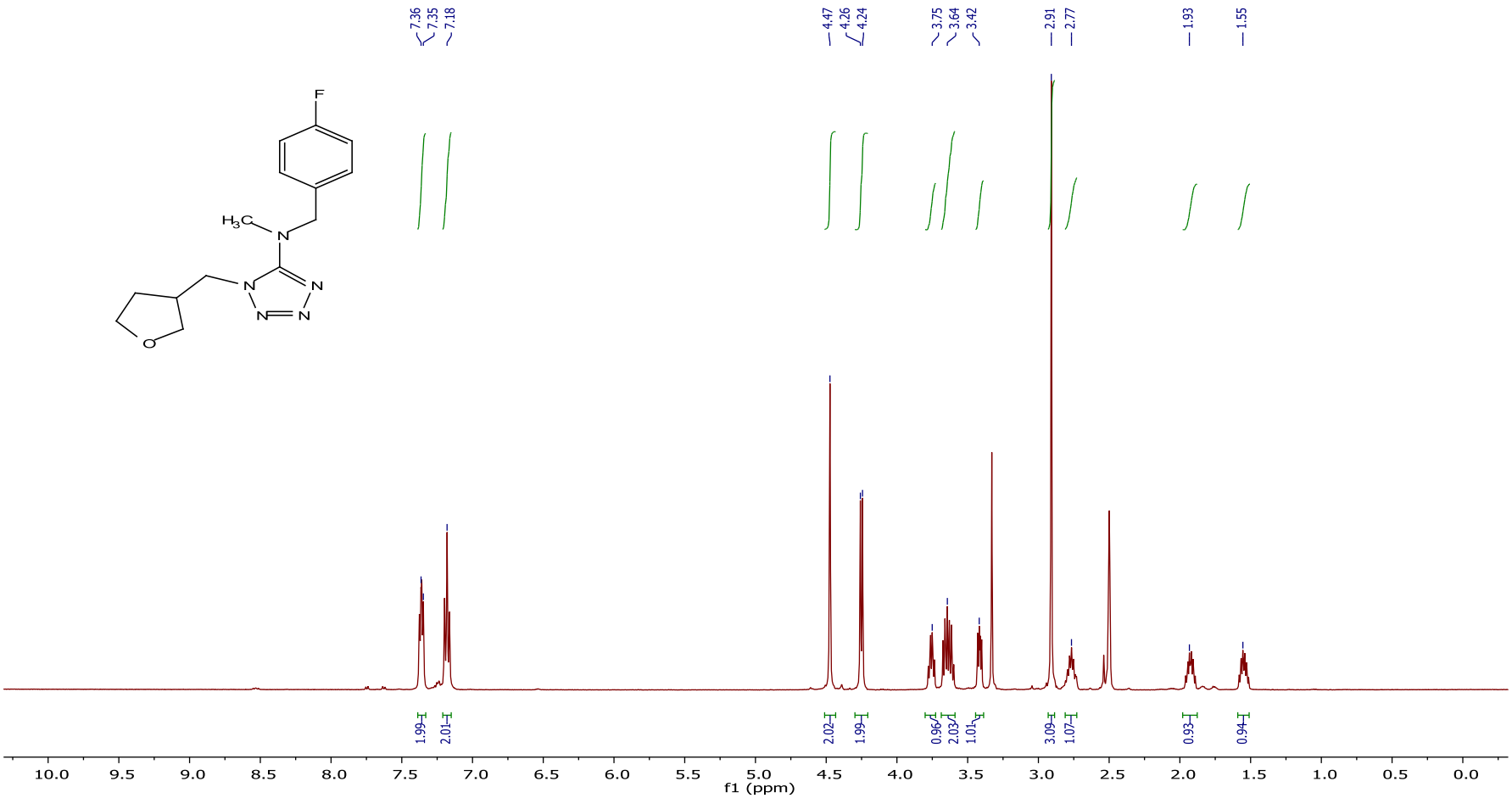
^{1}H NMR spectrum of the compound **9**{*102,356*}.



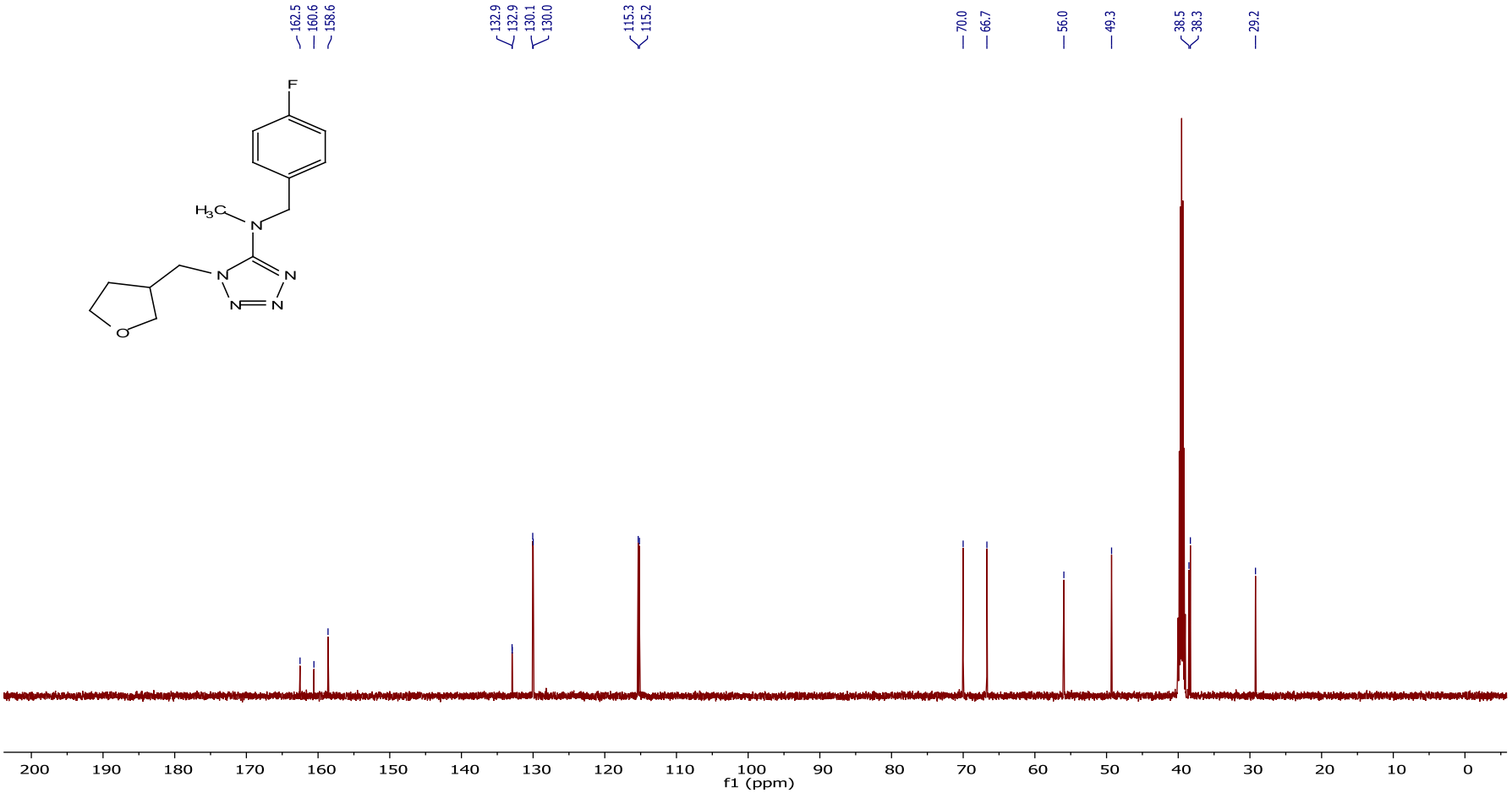
^{13}C NMR spectrum of the compound **9**{*102,356*}.



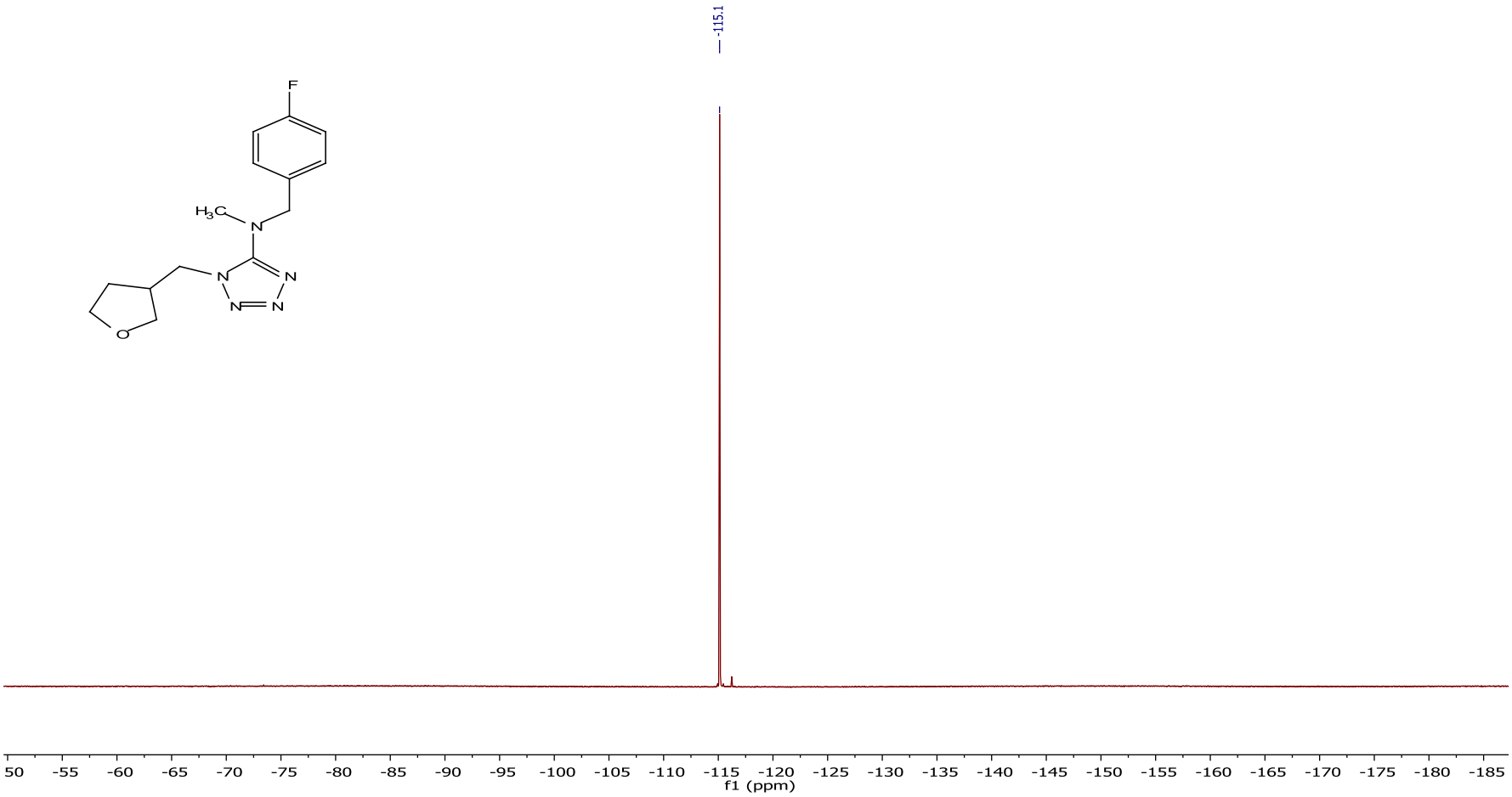
^{1}H NMR spectrum of the compound **9**{*103,386*}.



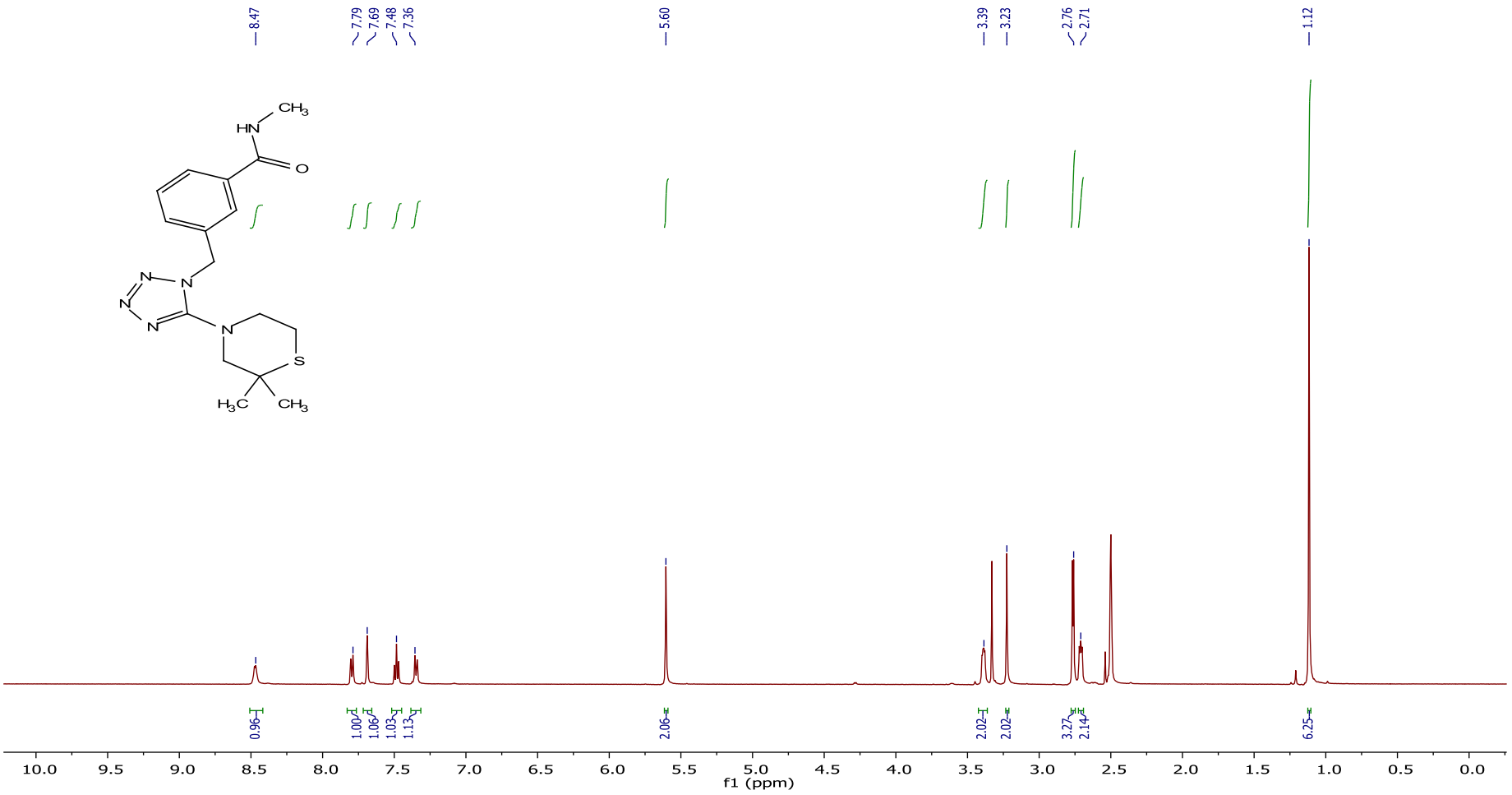
^{13}C NMR spectrum of the compound **9**{*103,386*}.



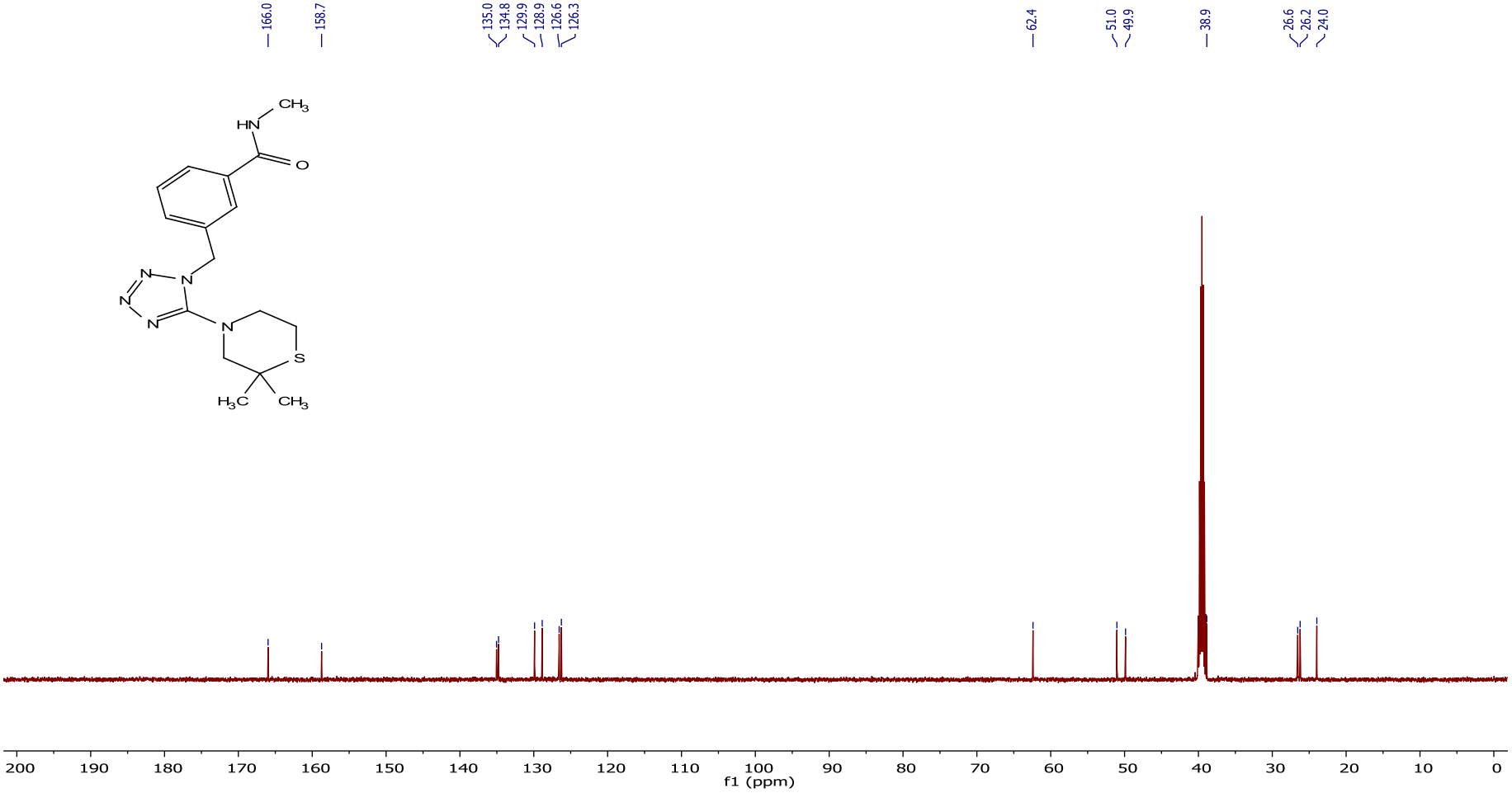
^{19}F NMR spectrum of the compound **9**{*103,386*}.



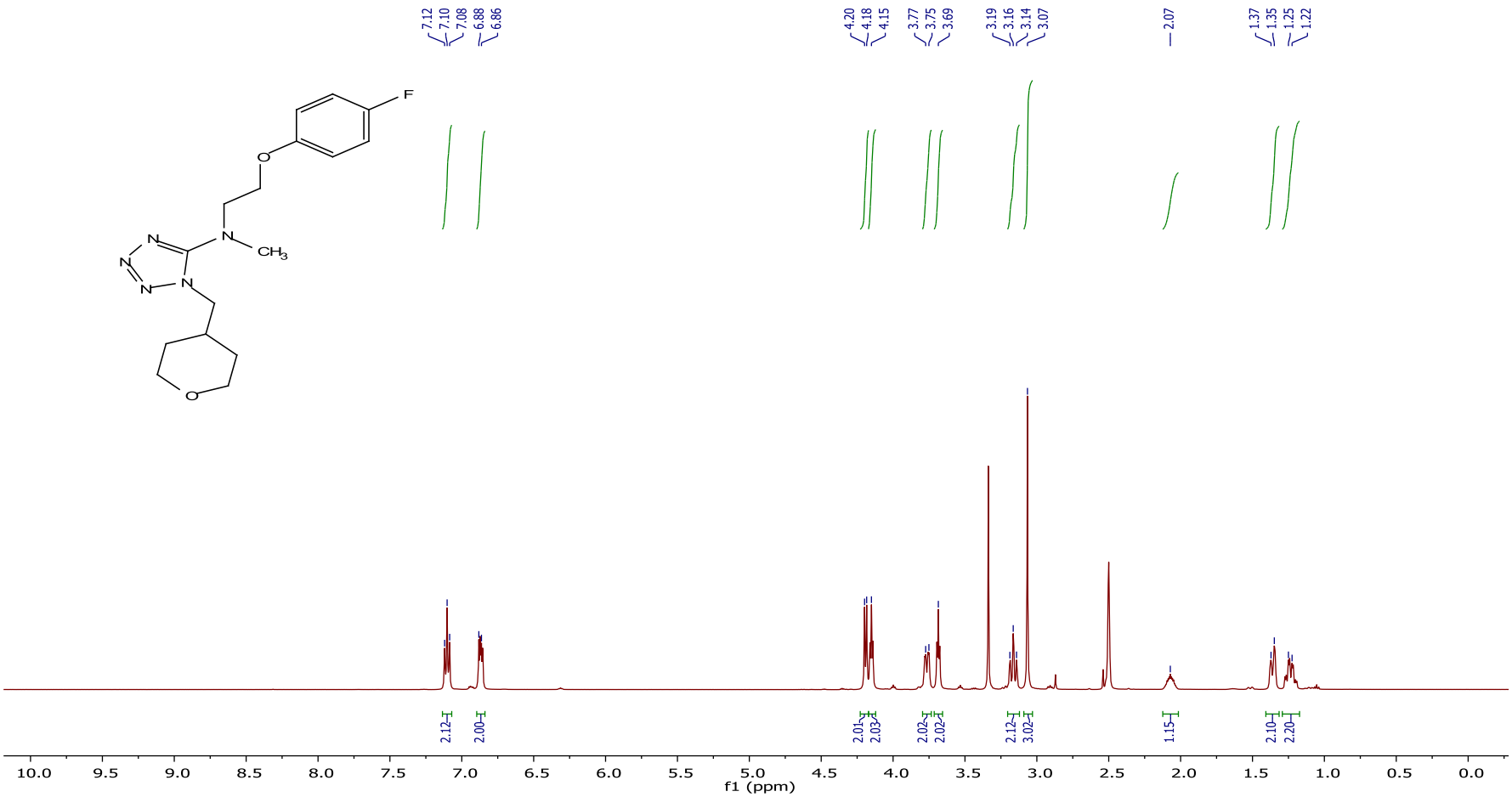
^{1}H NMR spectrum of the compound **9**{*110,333*}.



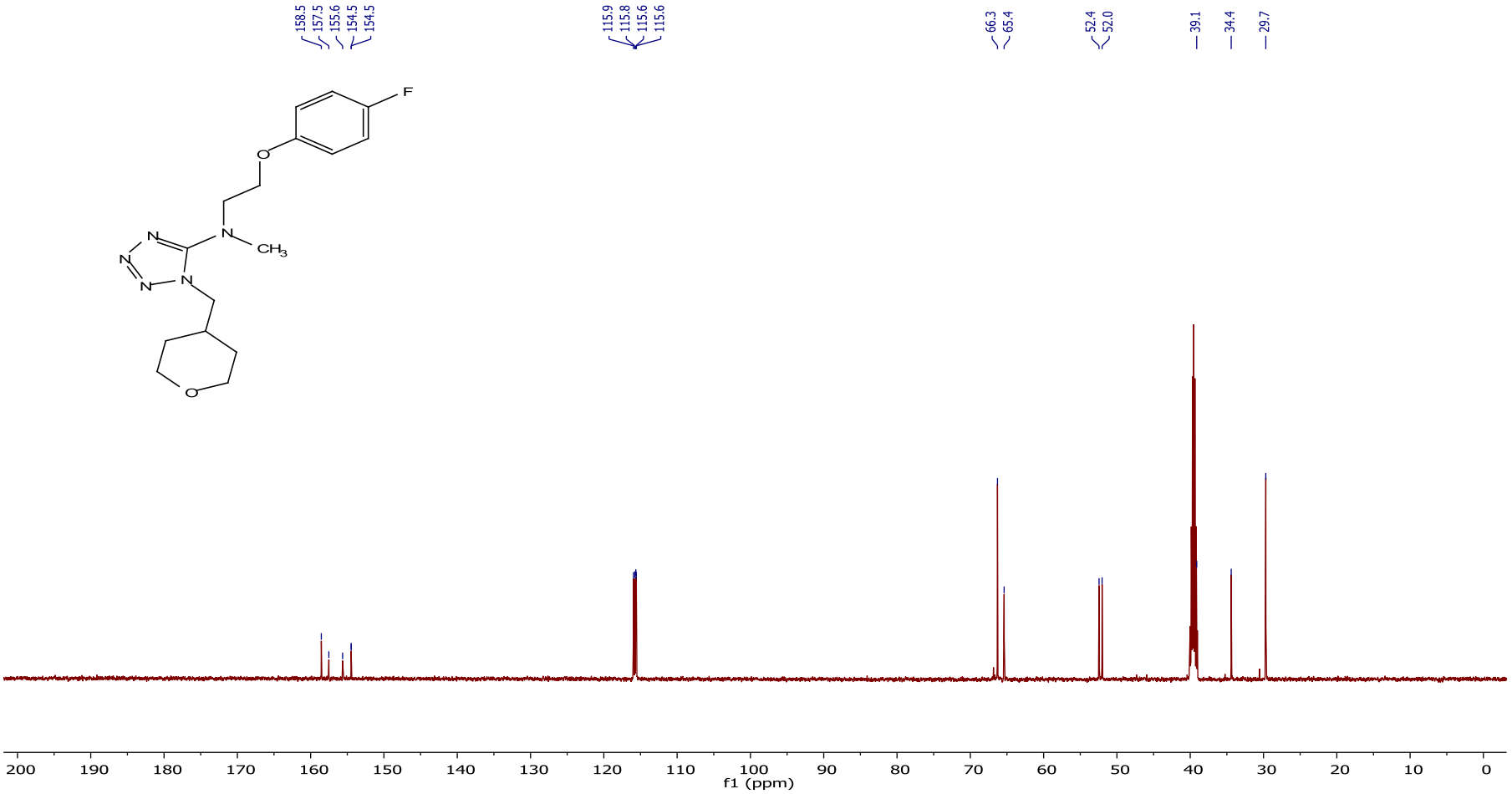
^{13}C NMR spectrum of the compound **9**{*110,333*}.



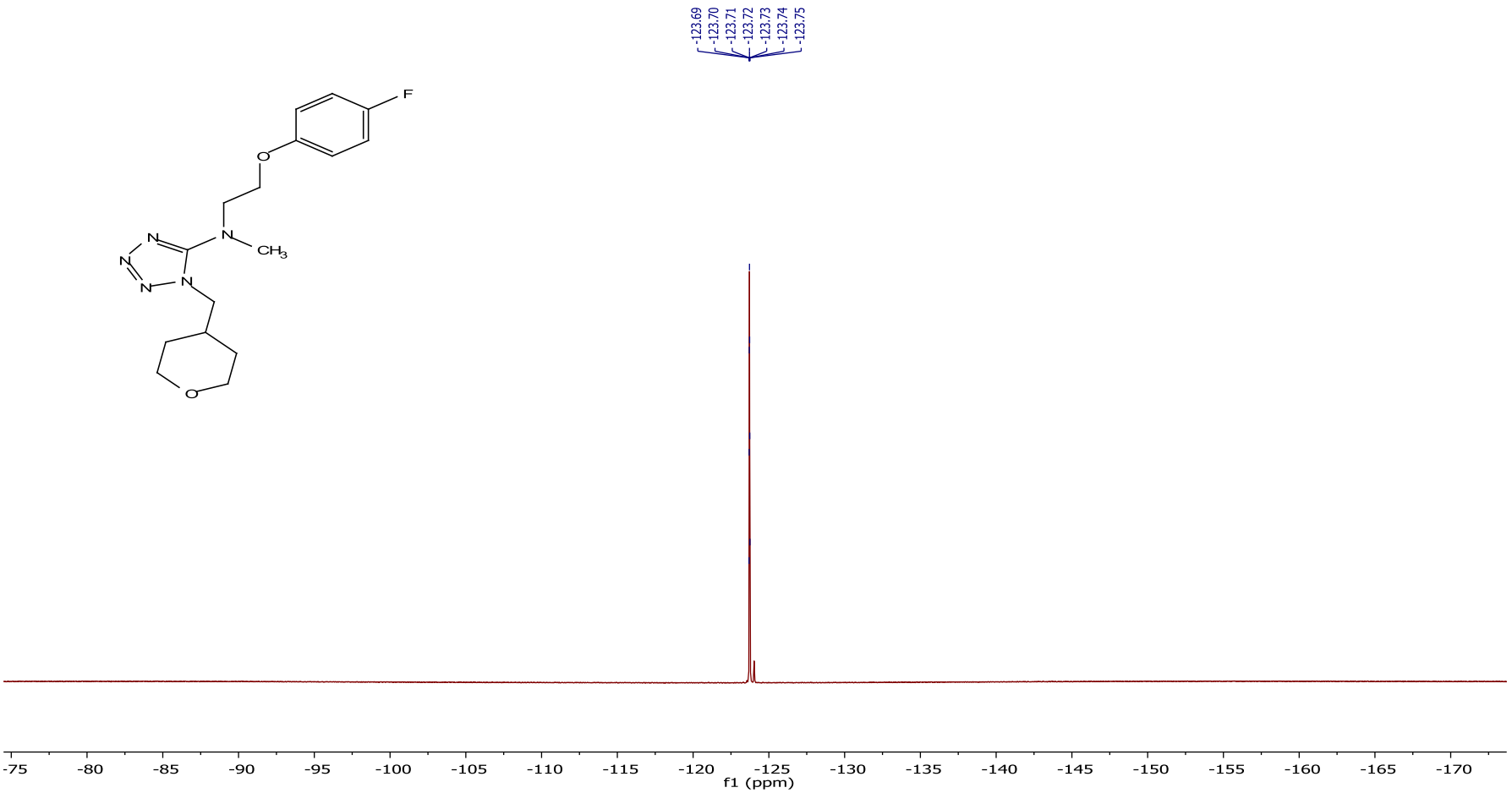
^{1}H NMR spectrum of the compound **9**{*121,302*}.



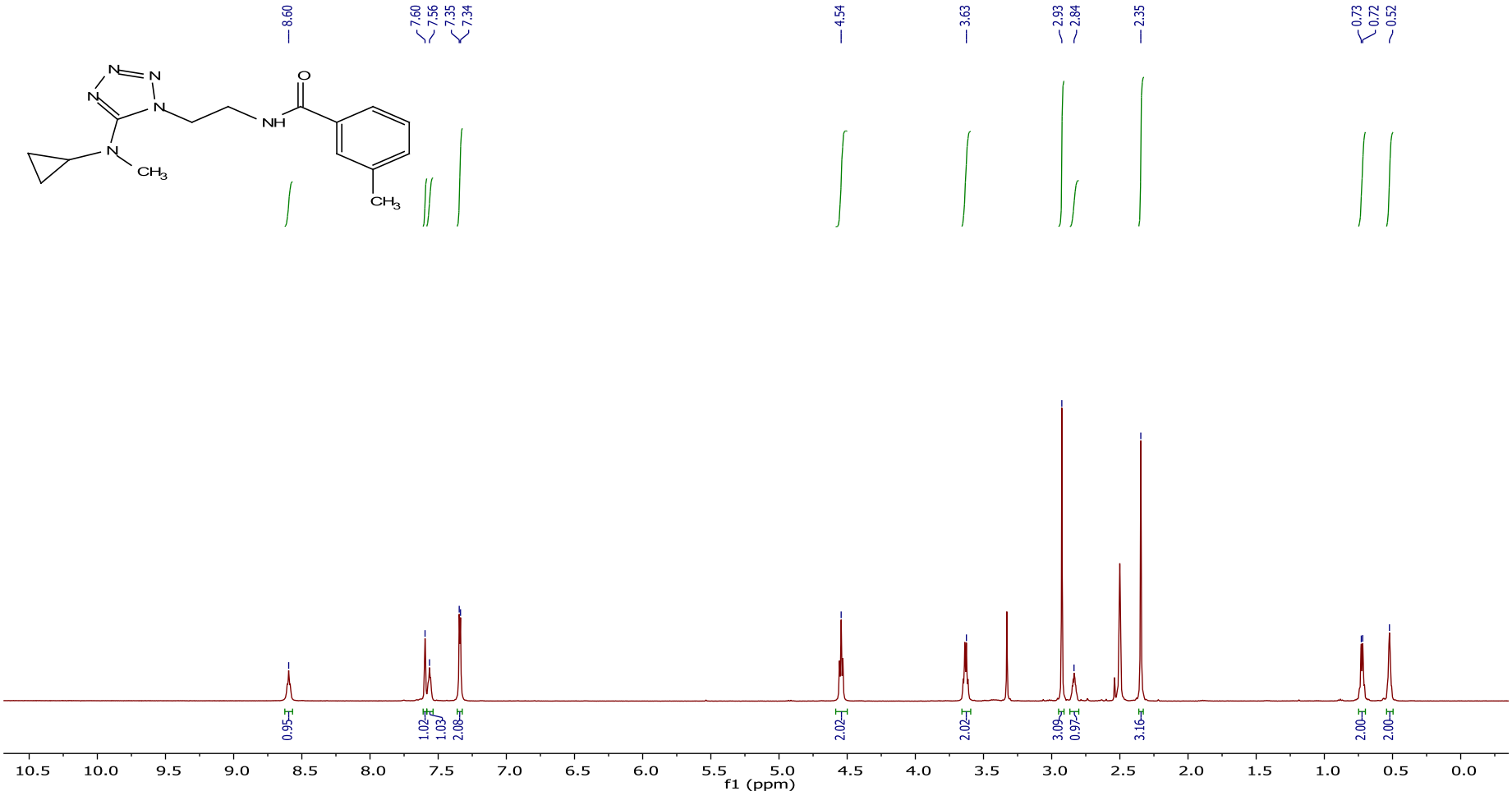
^{13}C NMR spectrum of the compound **9**{*121,302*}.



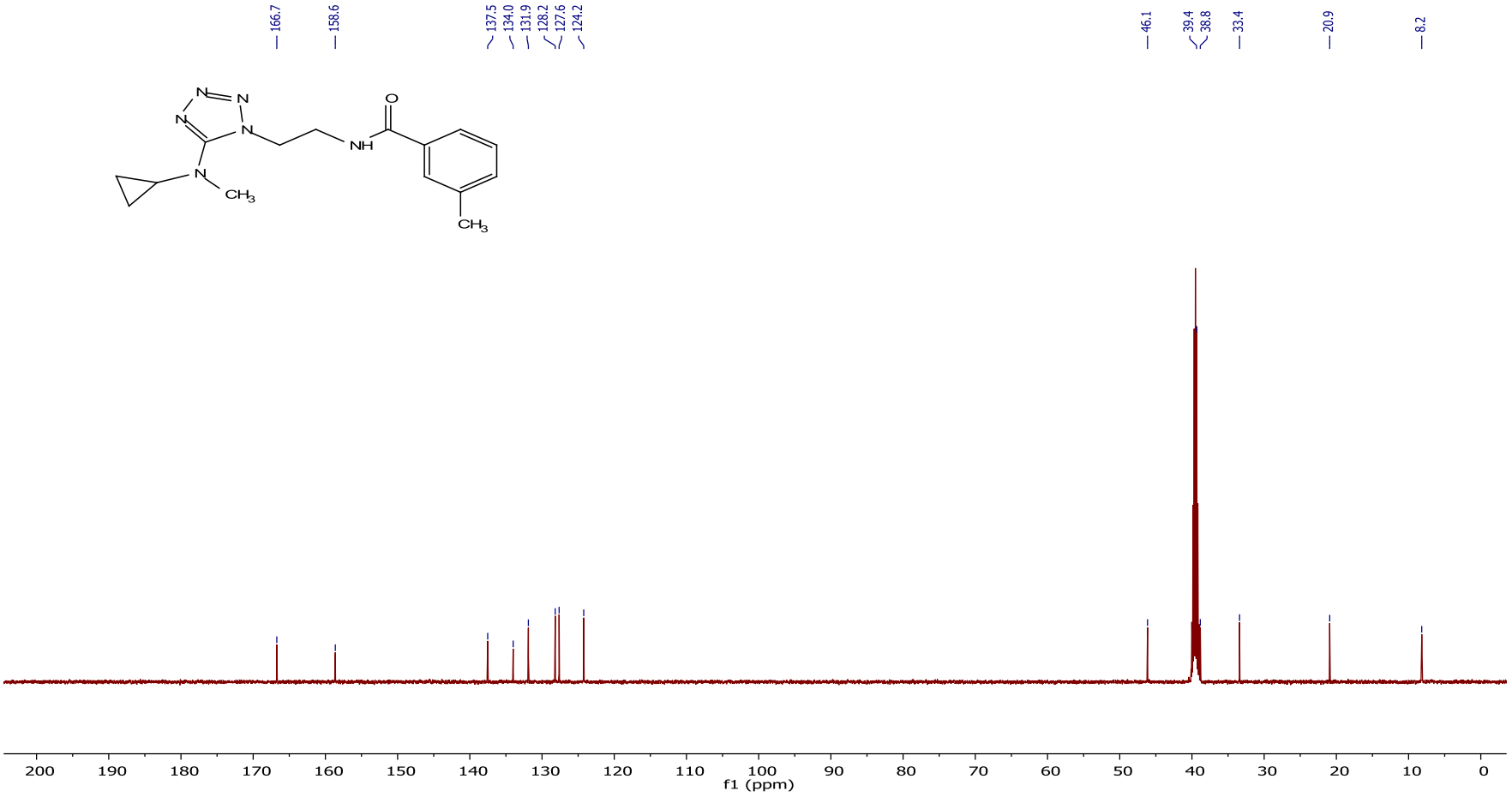
^{19}F NMR spectrum of the compound **9**{*121,302*}.



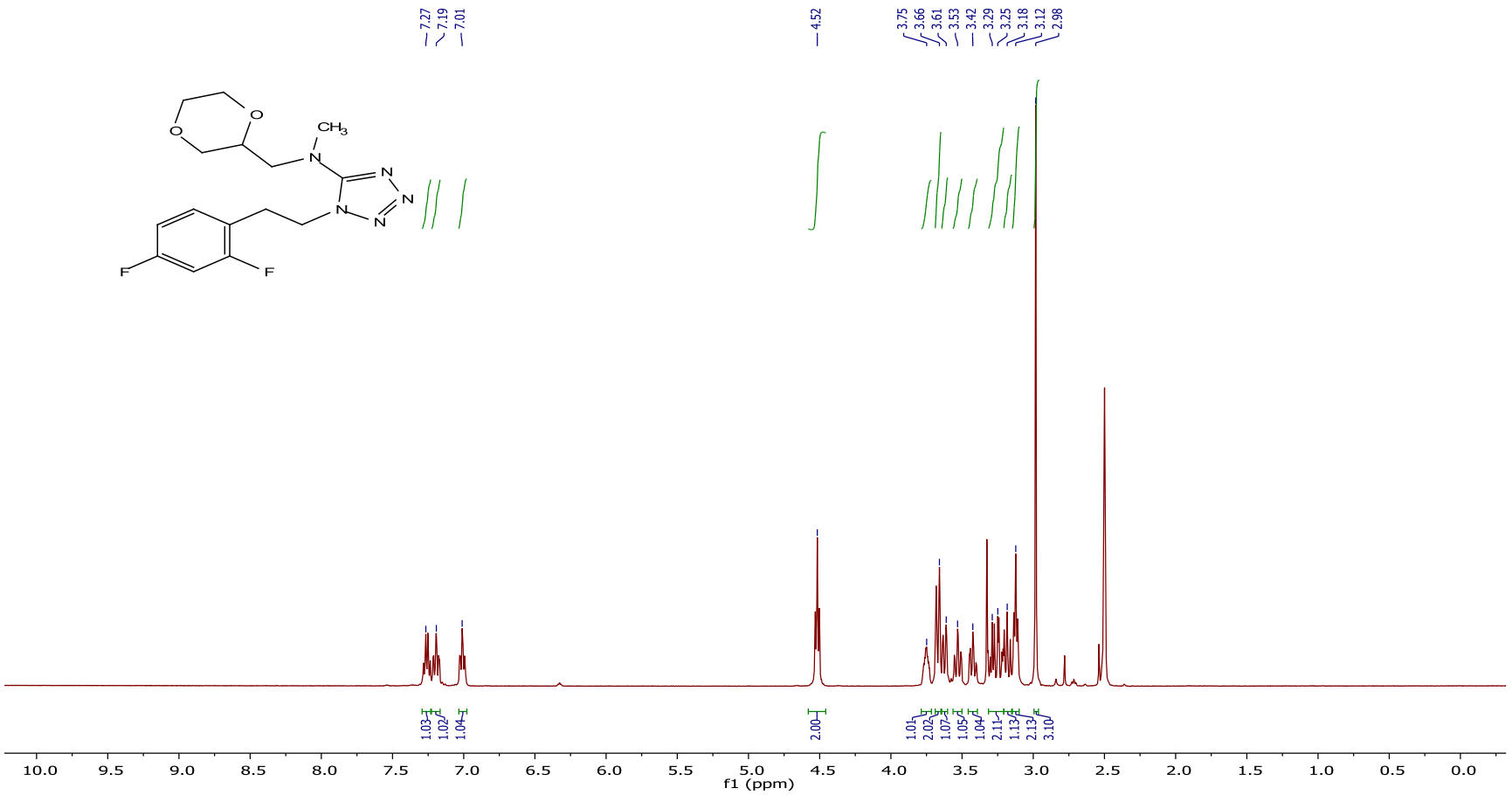
^{1}H NMR spectrum of the compound **9**{*(146,322}*.



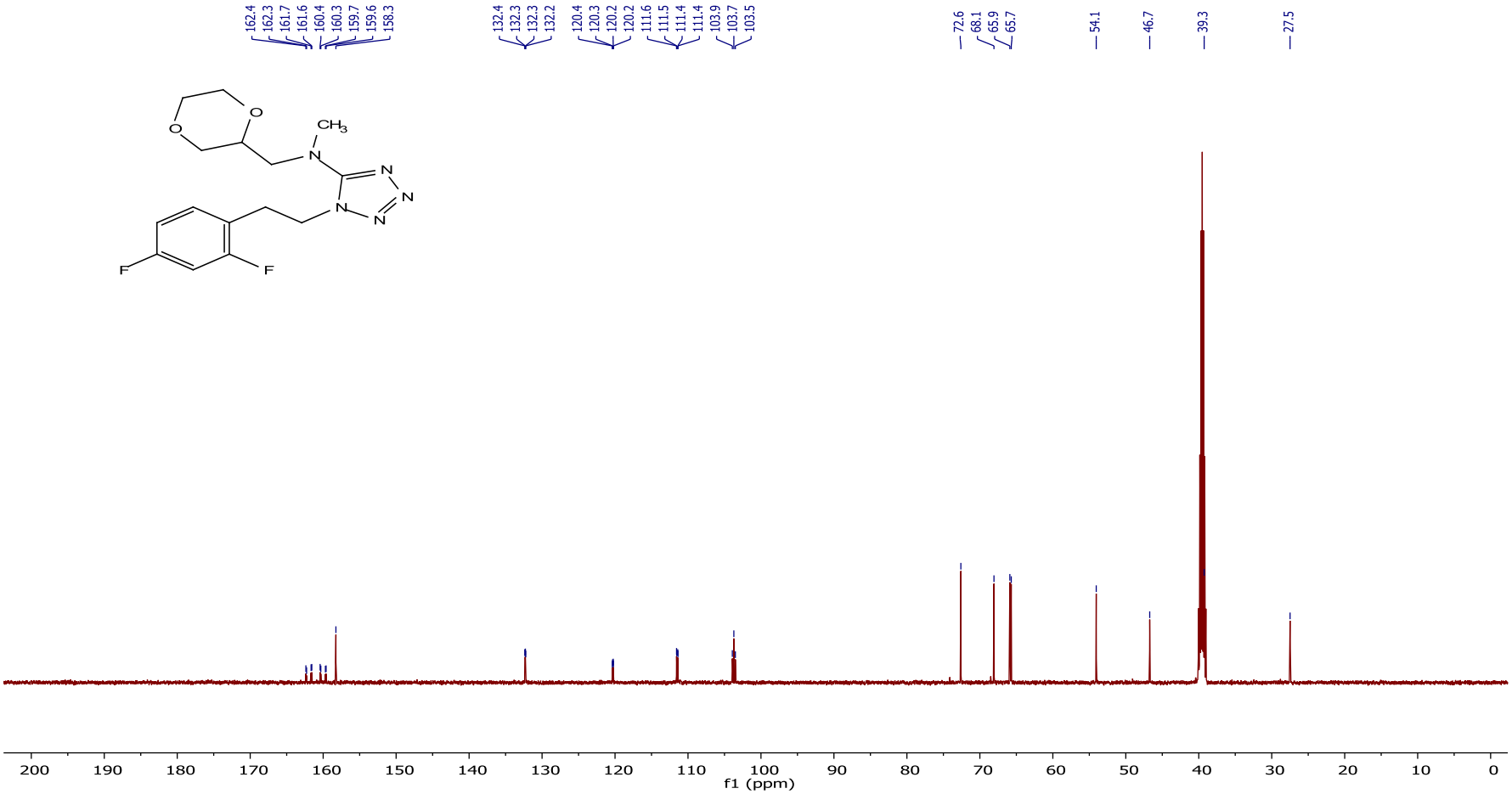
^{13}C NMR spectrum of the compound **9**{*(146,322}*.



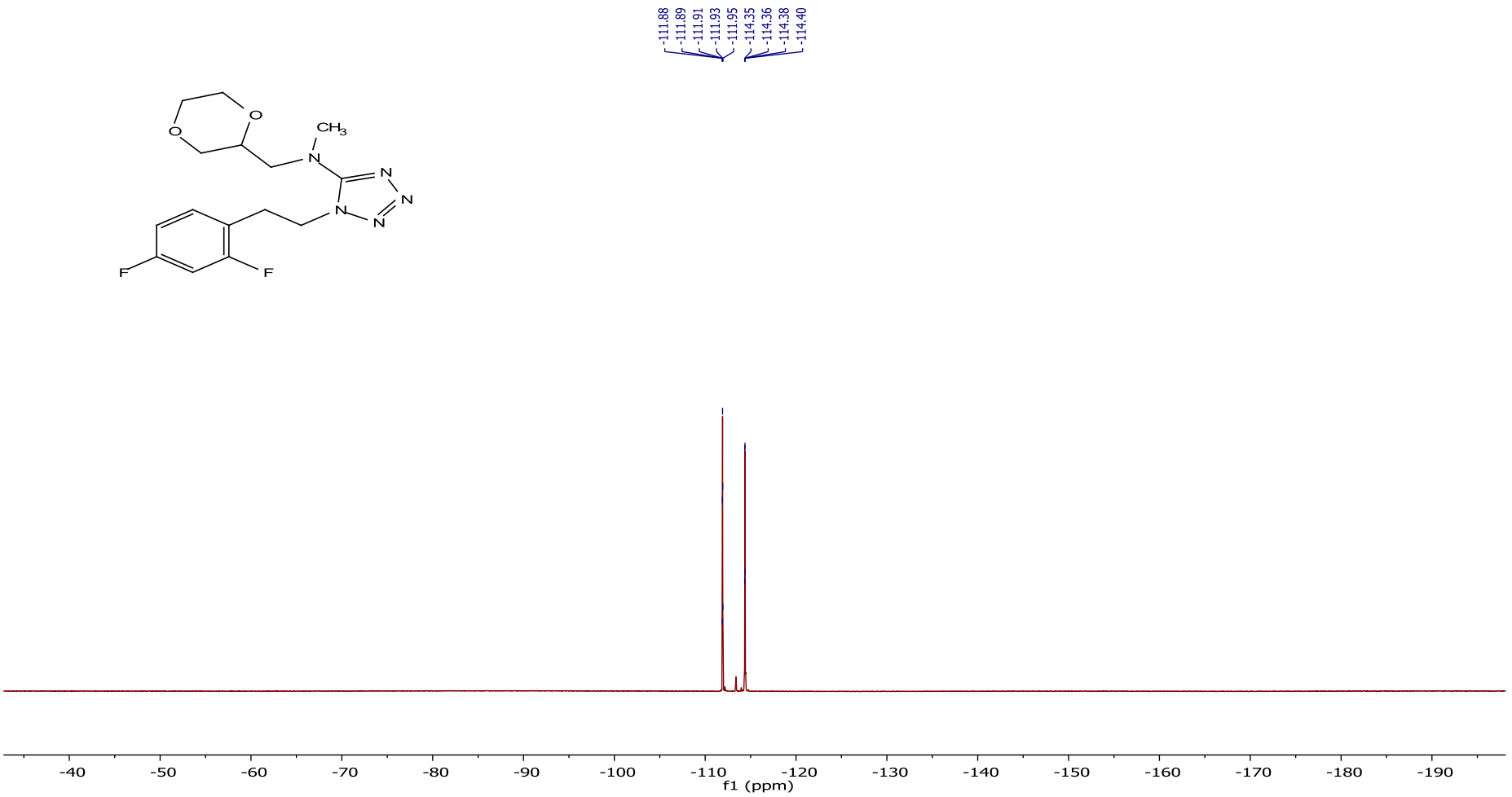
^{1}H NMR spectrum of the compound **9**{*175,299*}.



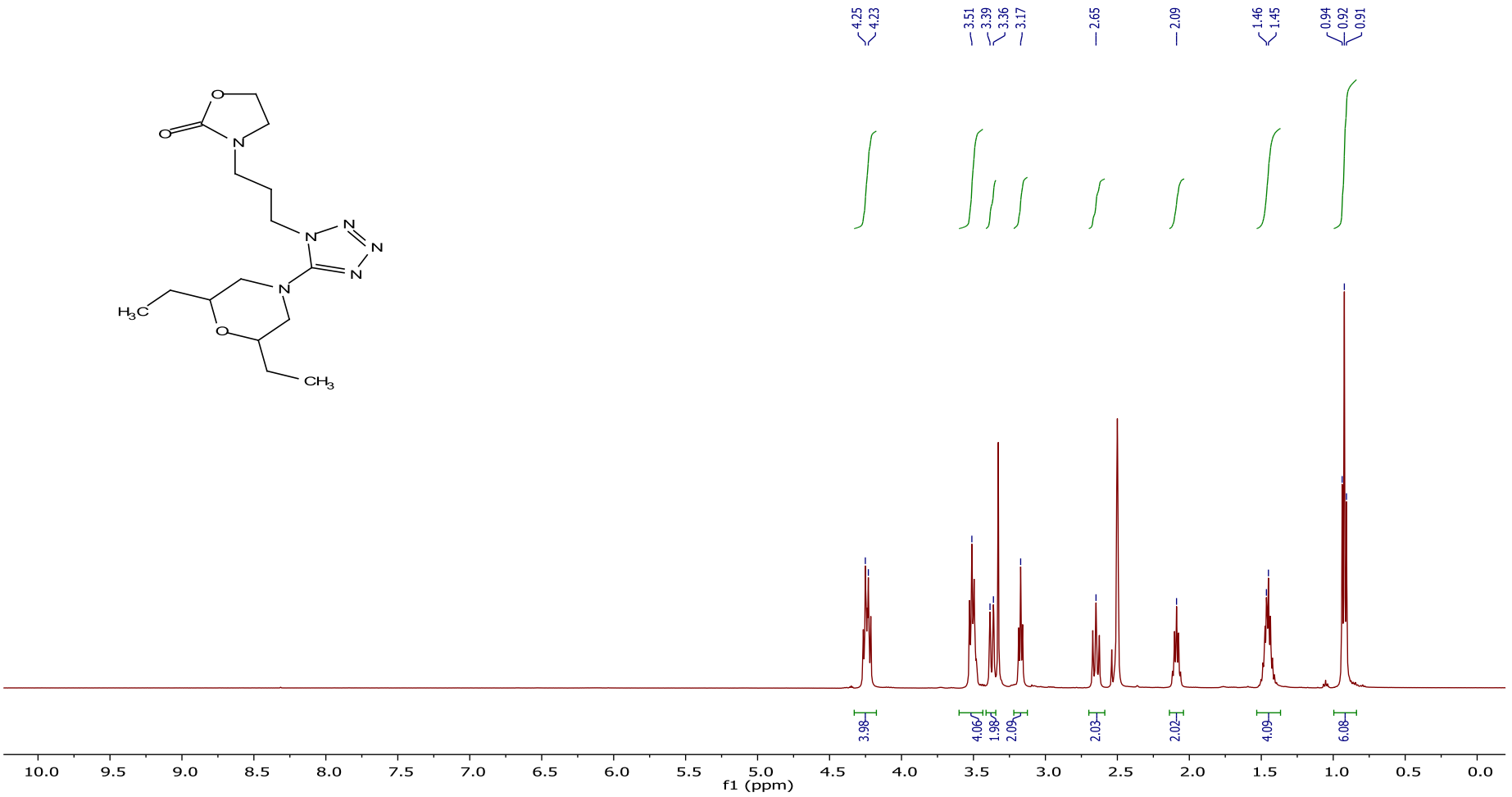
^{13}C NMR spectrum of the compound **9**{*175,299*}.



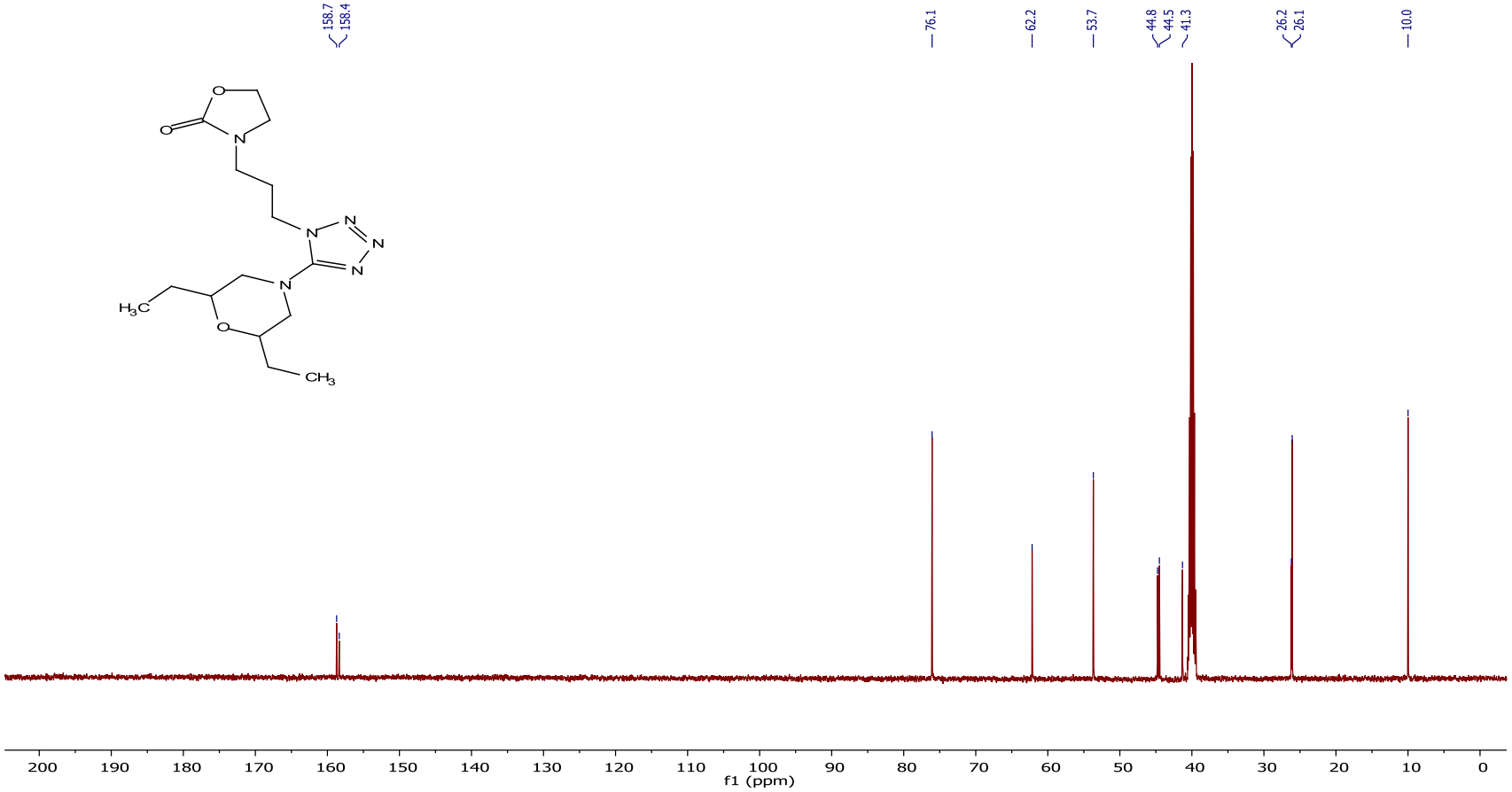
^{19}F NMR spectrum of the compound **9**{*175*,*299*}.



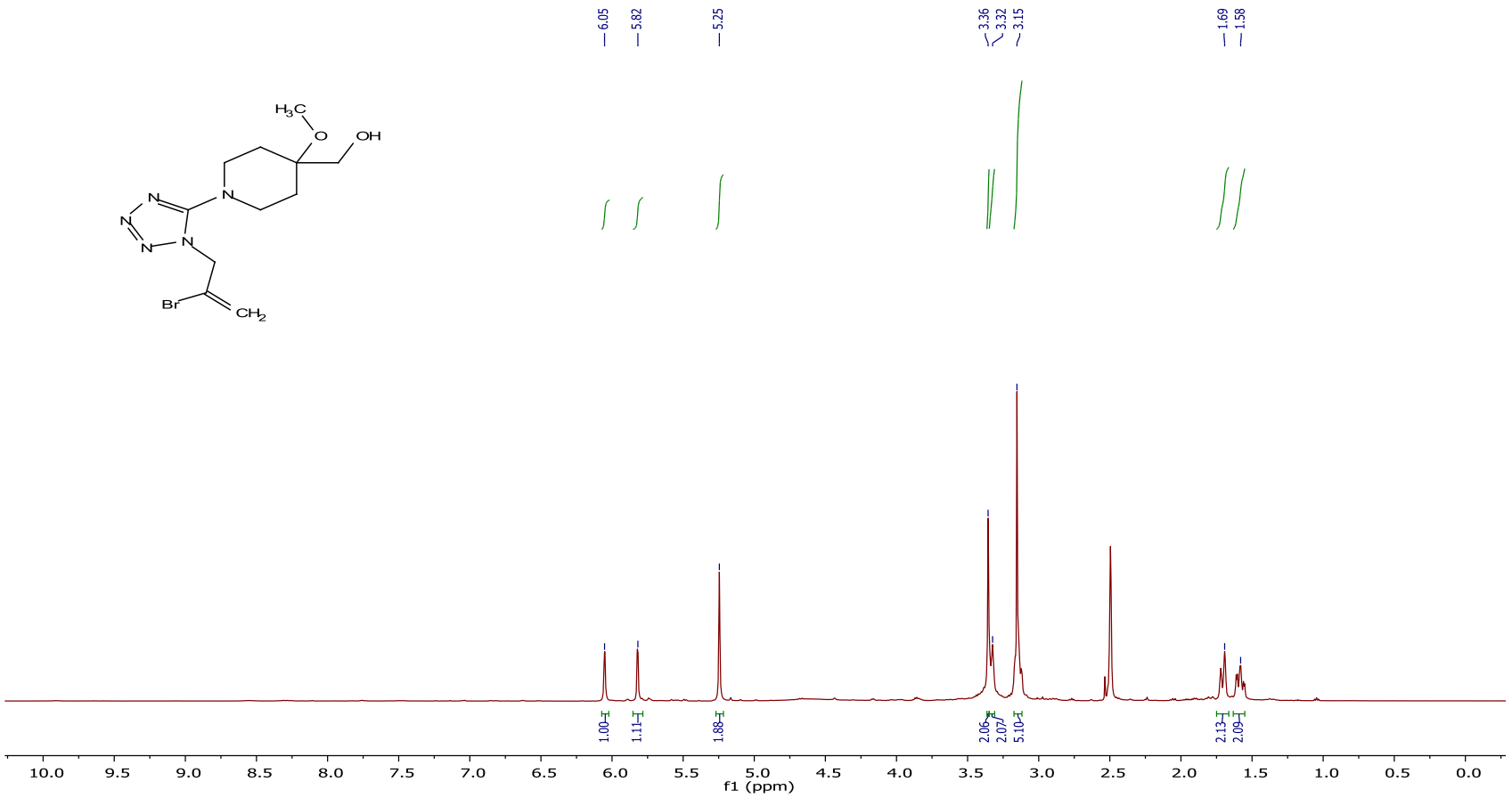
^{1}H NMR spectrum of the compound **9**{*151,319*}.



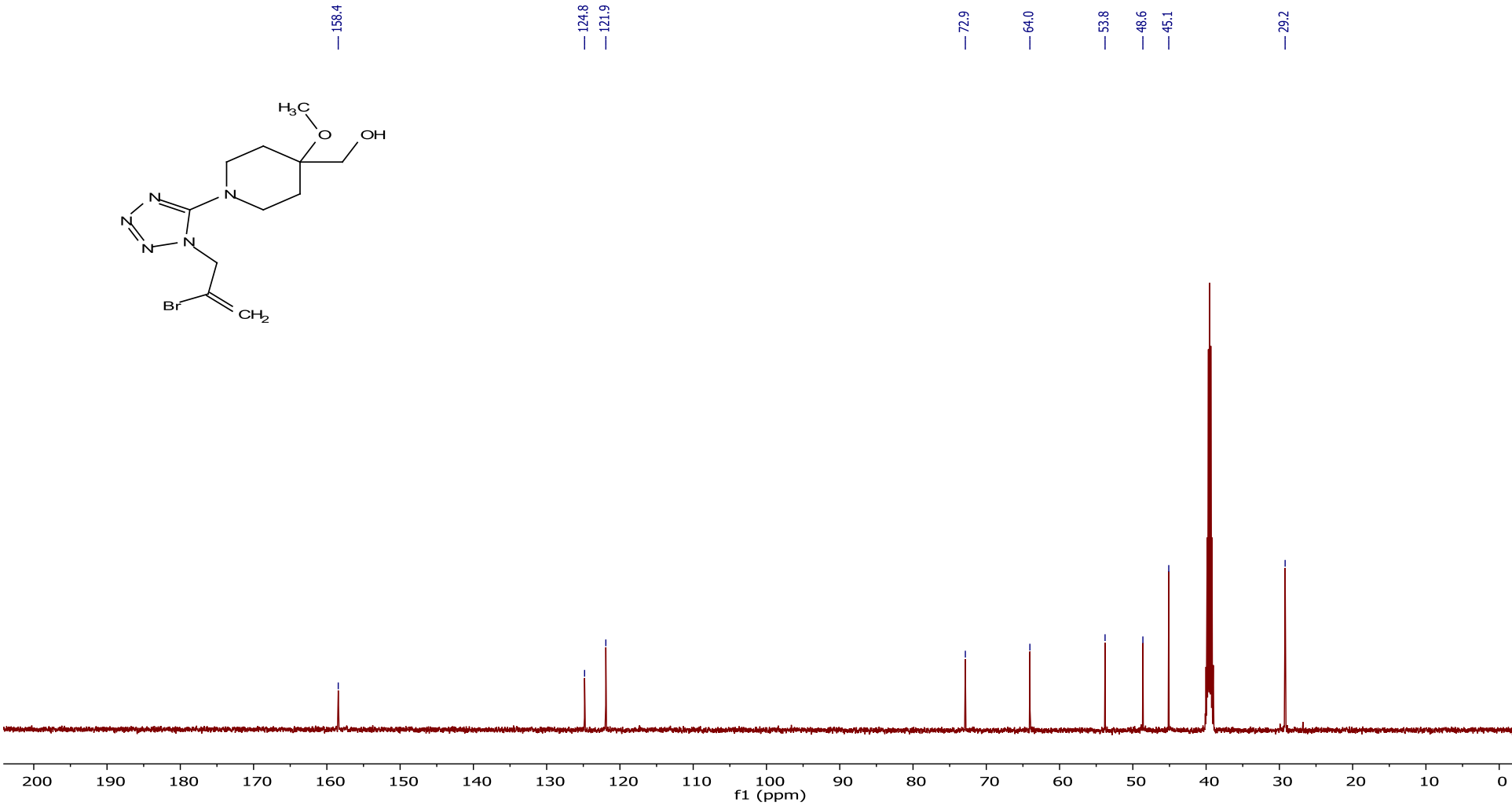
^{13}C NMR spectrum of the compound **9**{*151,319*}.



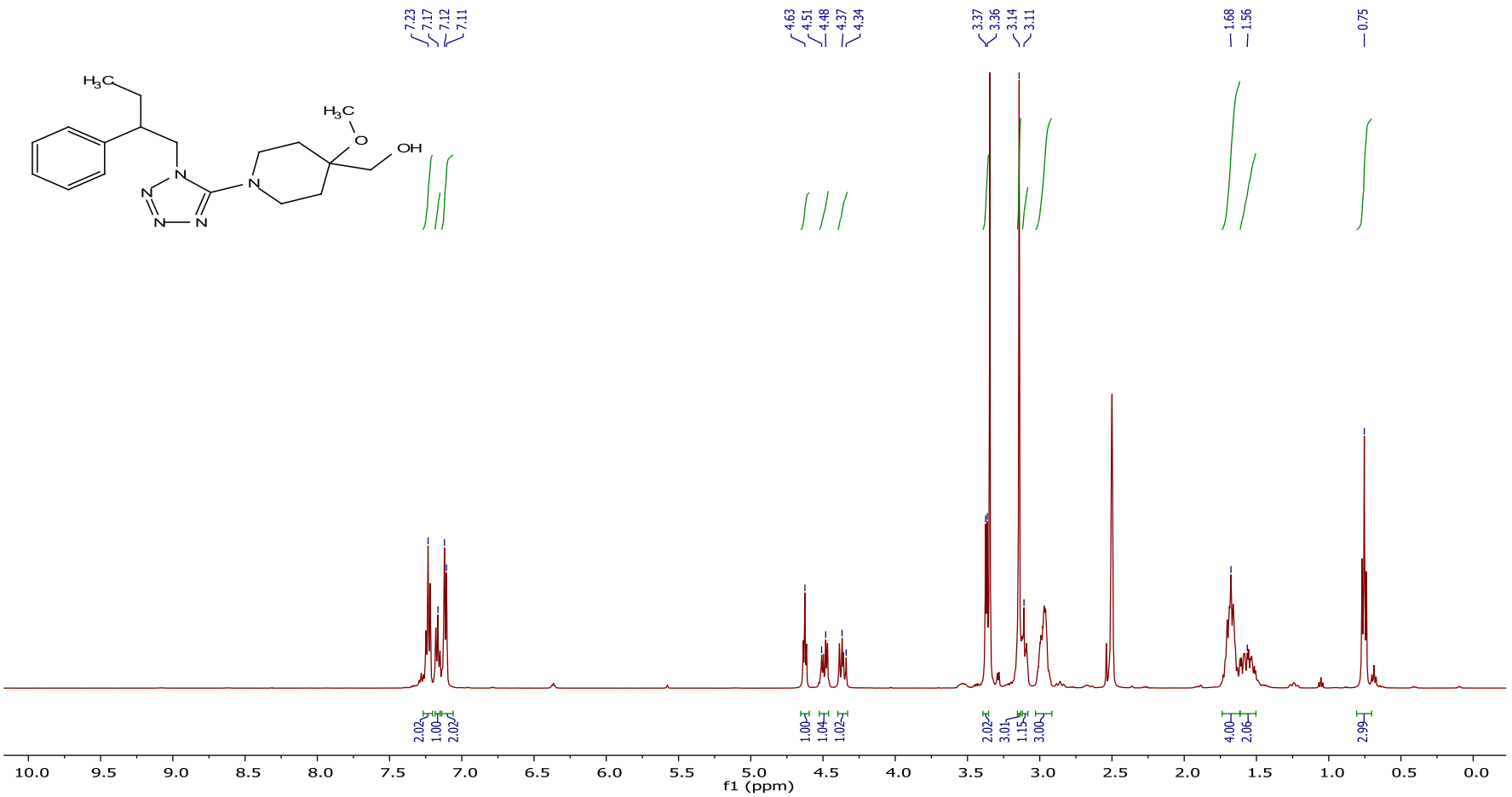
^{1}H NMR spectrum of the compound **9**{*165,299*}.



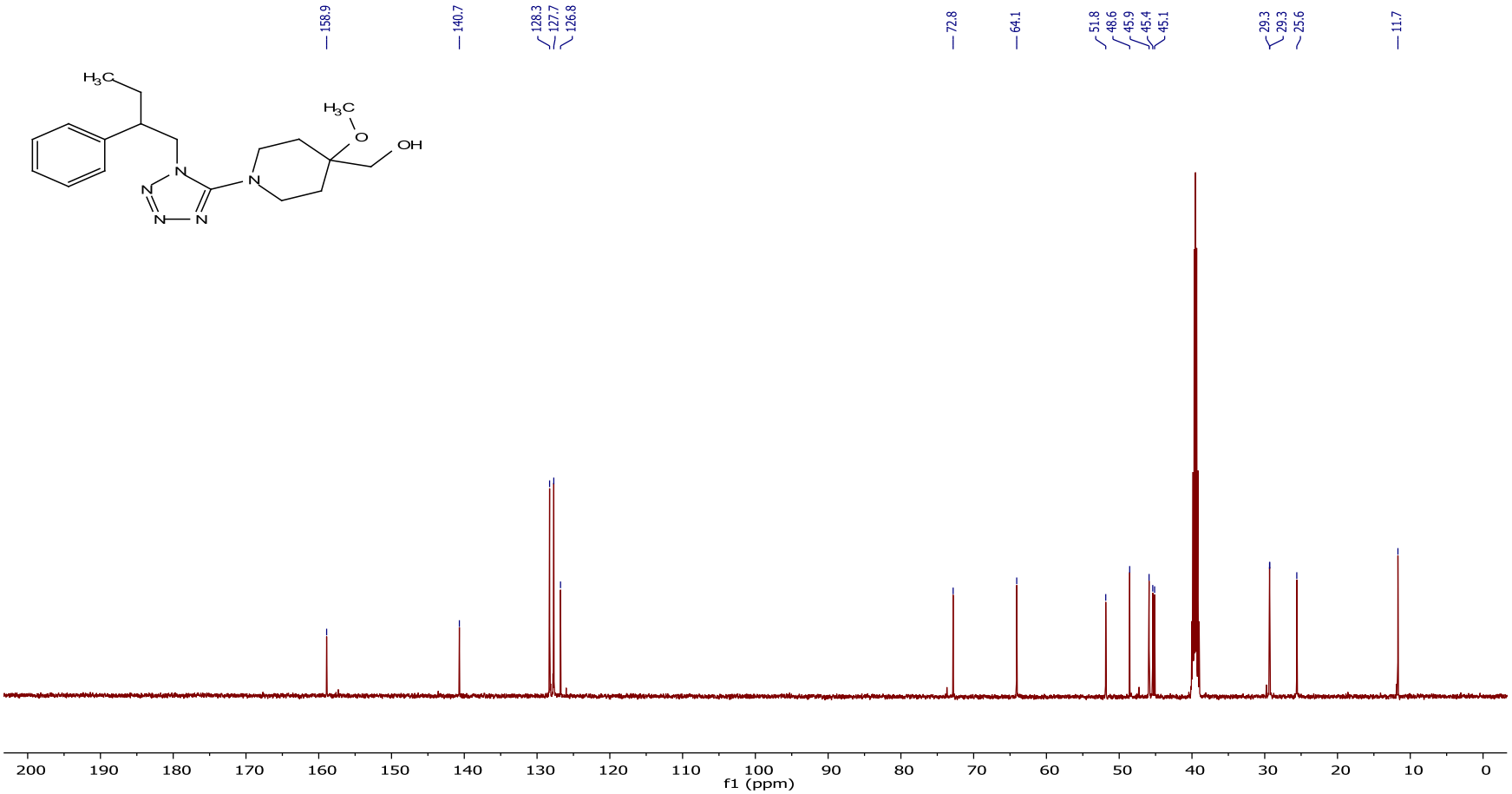
^{13}C NMR spectrum of the compound **9**{*165,299*}.



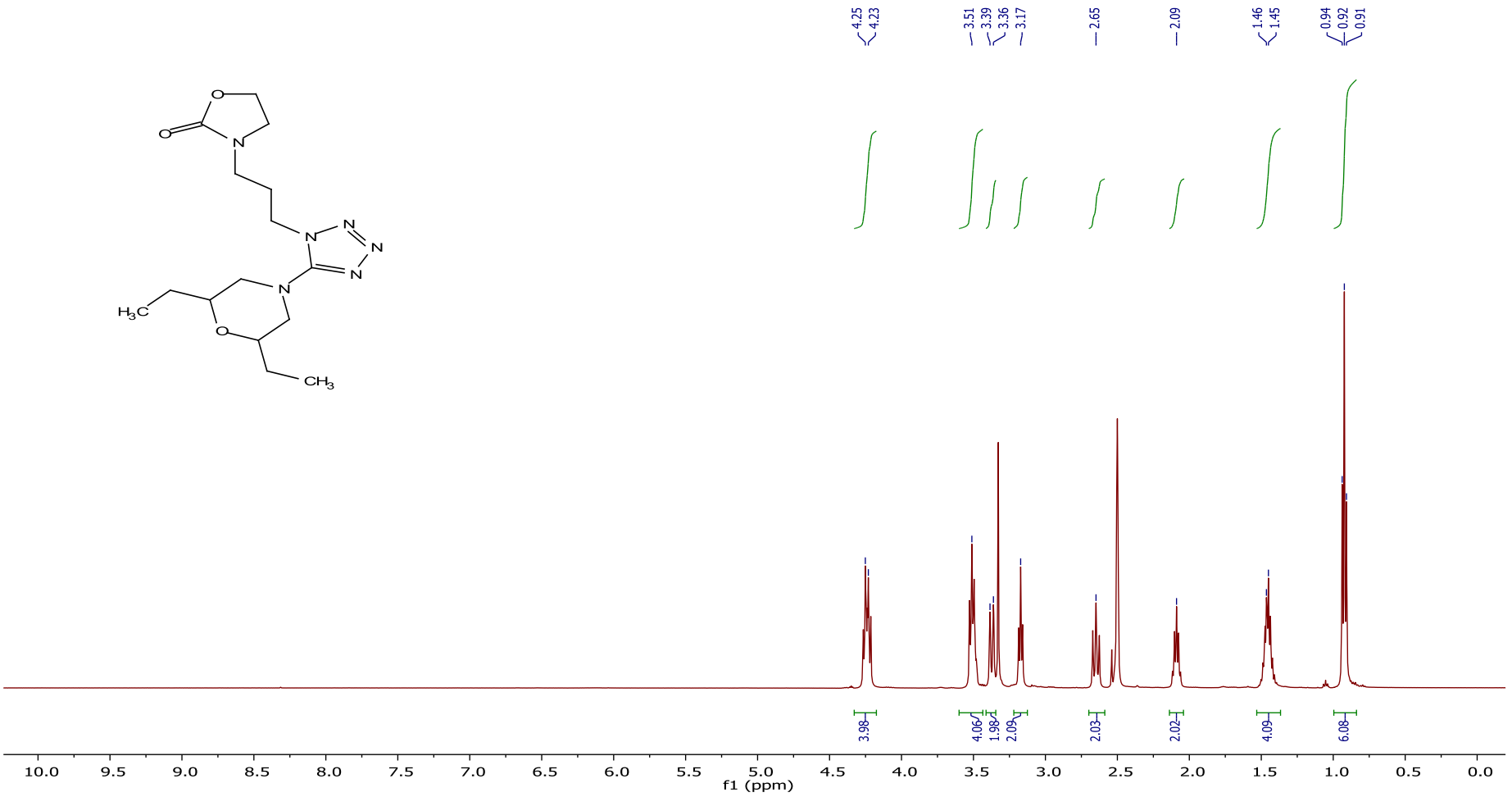
^{1}H NMR spectrum of the compound **9**{*175,299*}.



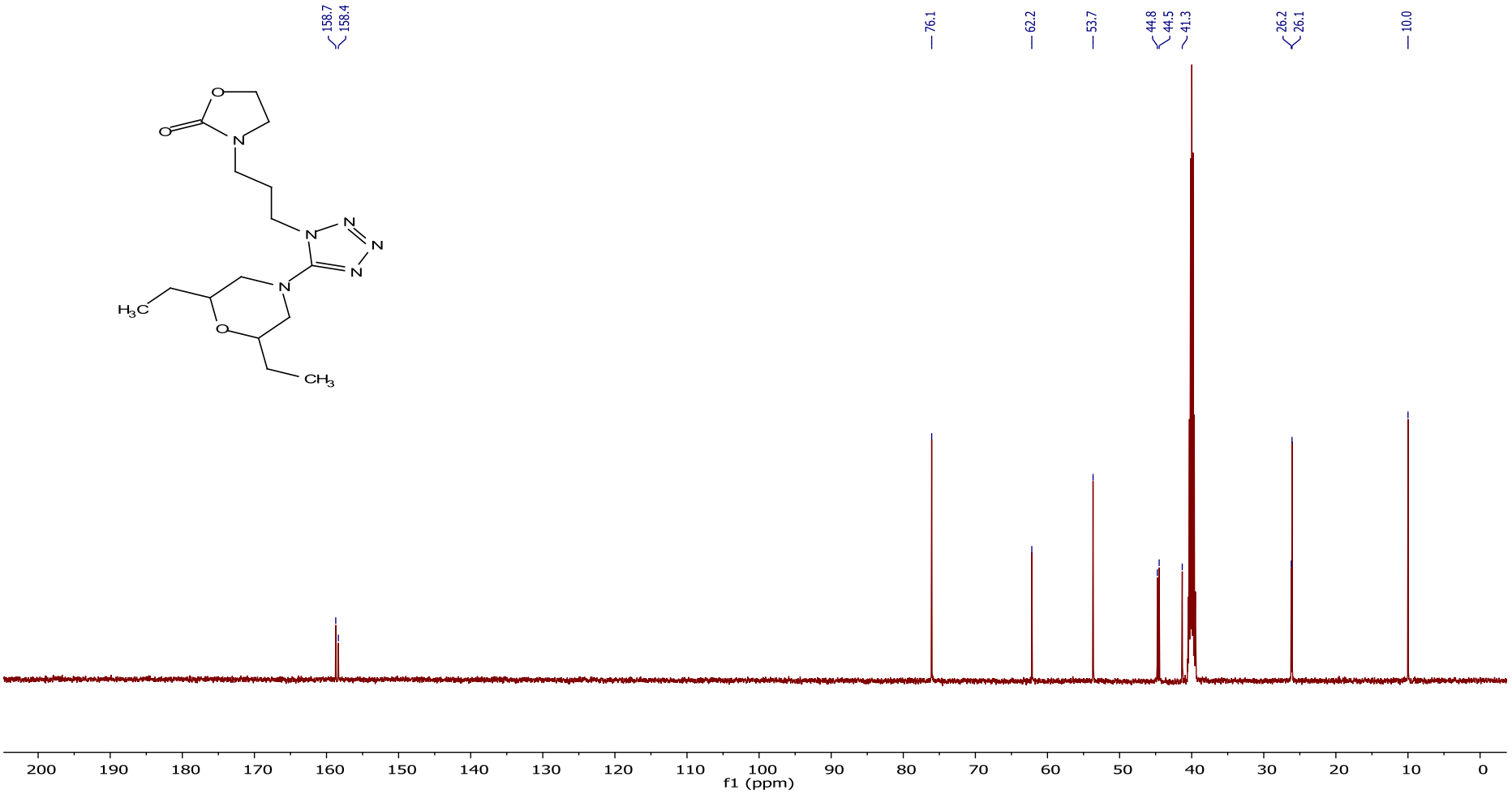
^{13}C NMR spectrum of the compound **9**{*175,299*}.



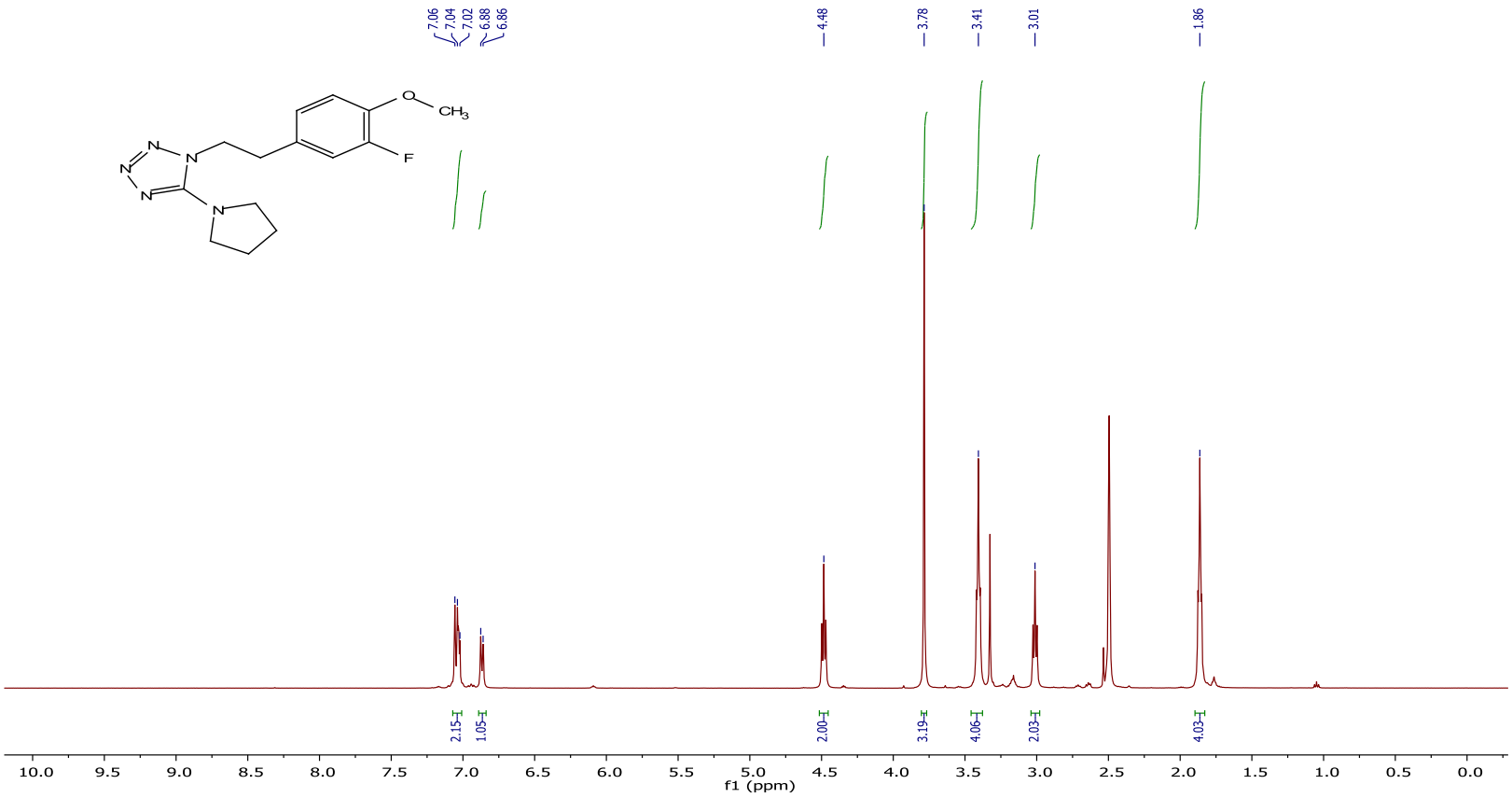
^{1}H NMR spectrum of the compound **9**{*188,338*}.



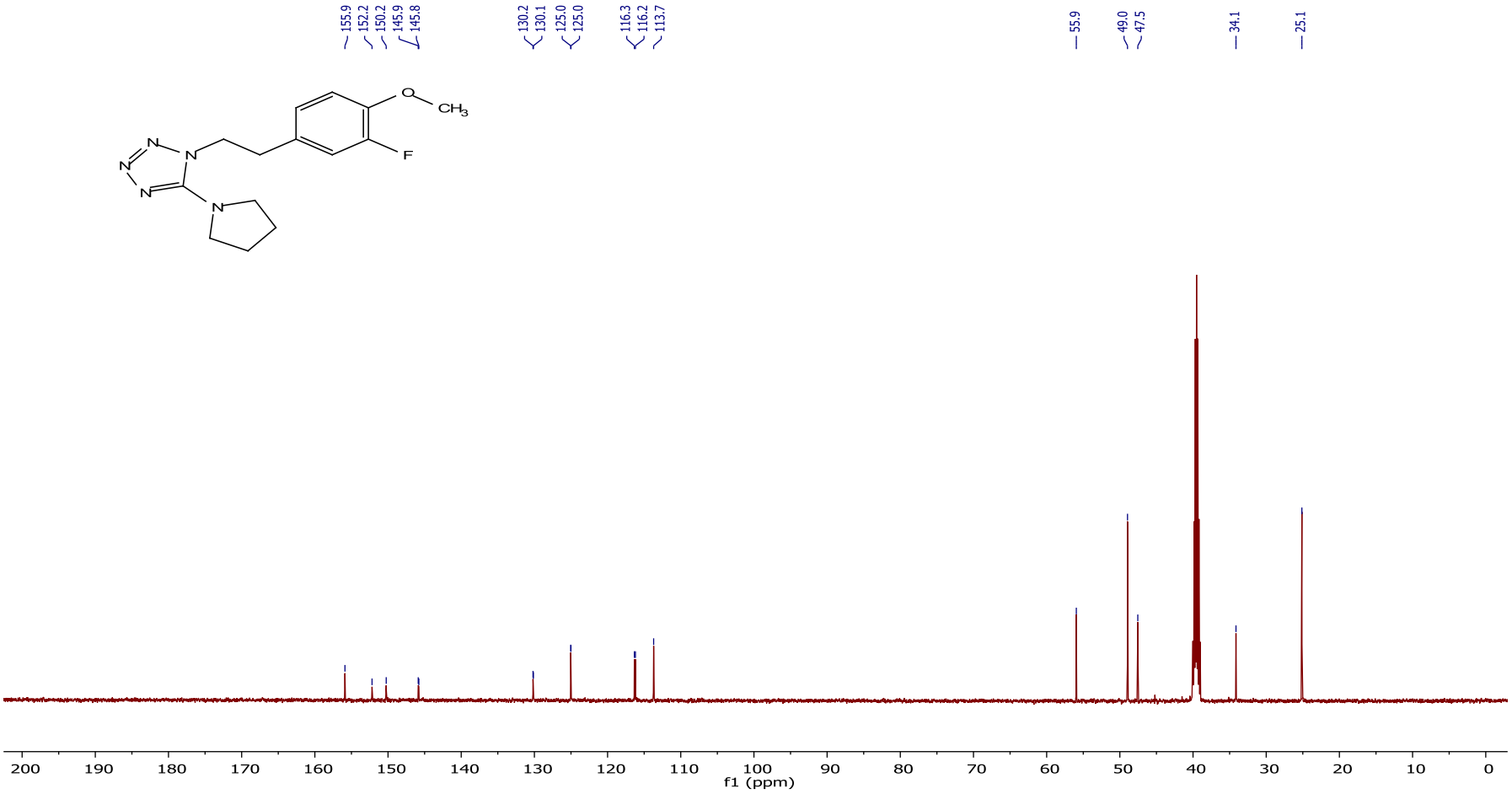
^{13}C NMR spectrum of the compound **9**{*188,338*}.



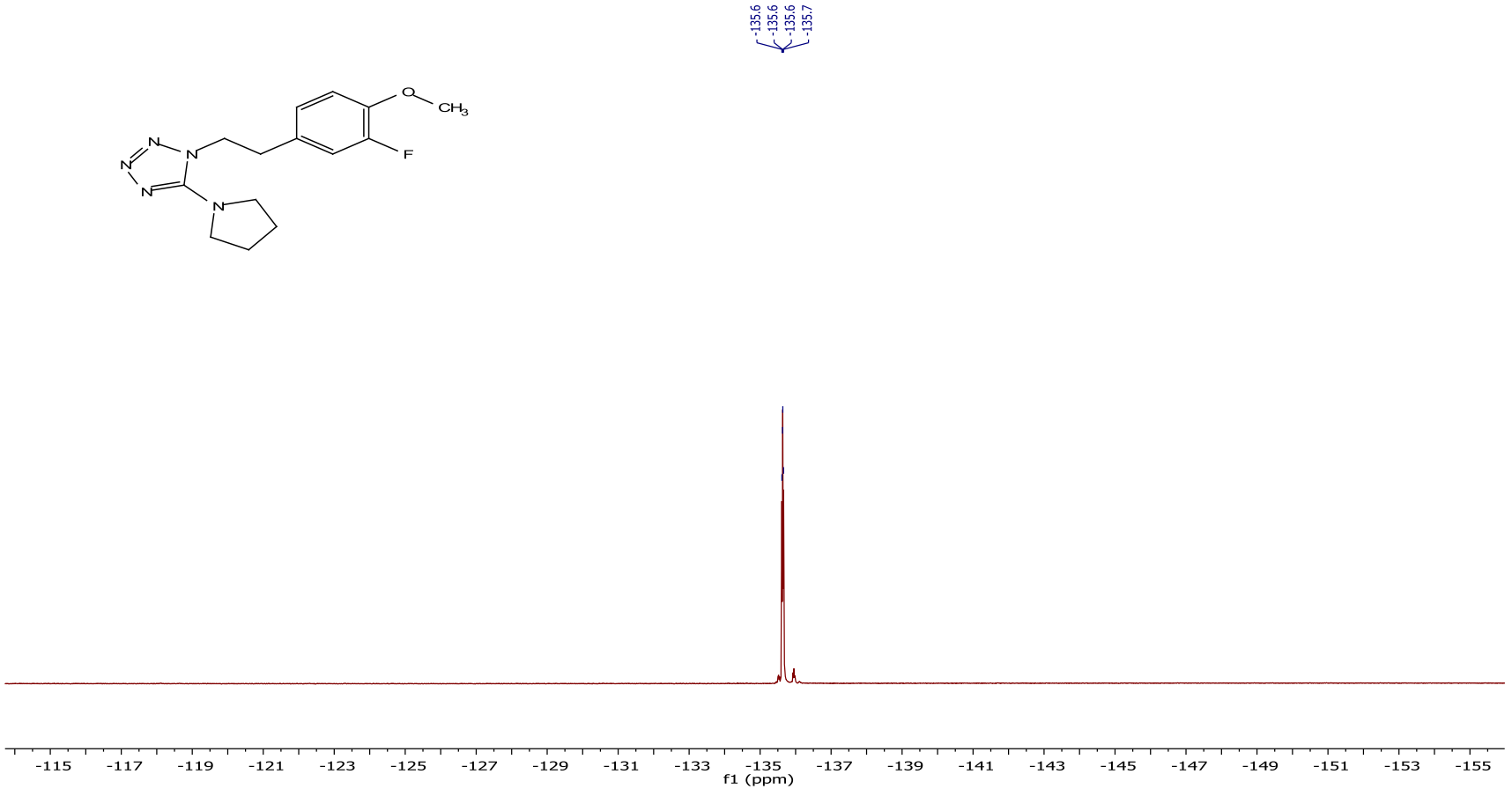
^{1}H NMR spectrum of the compound **9**{*190,341*}.



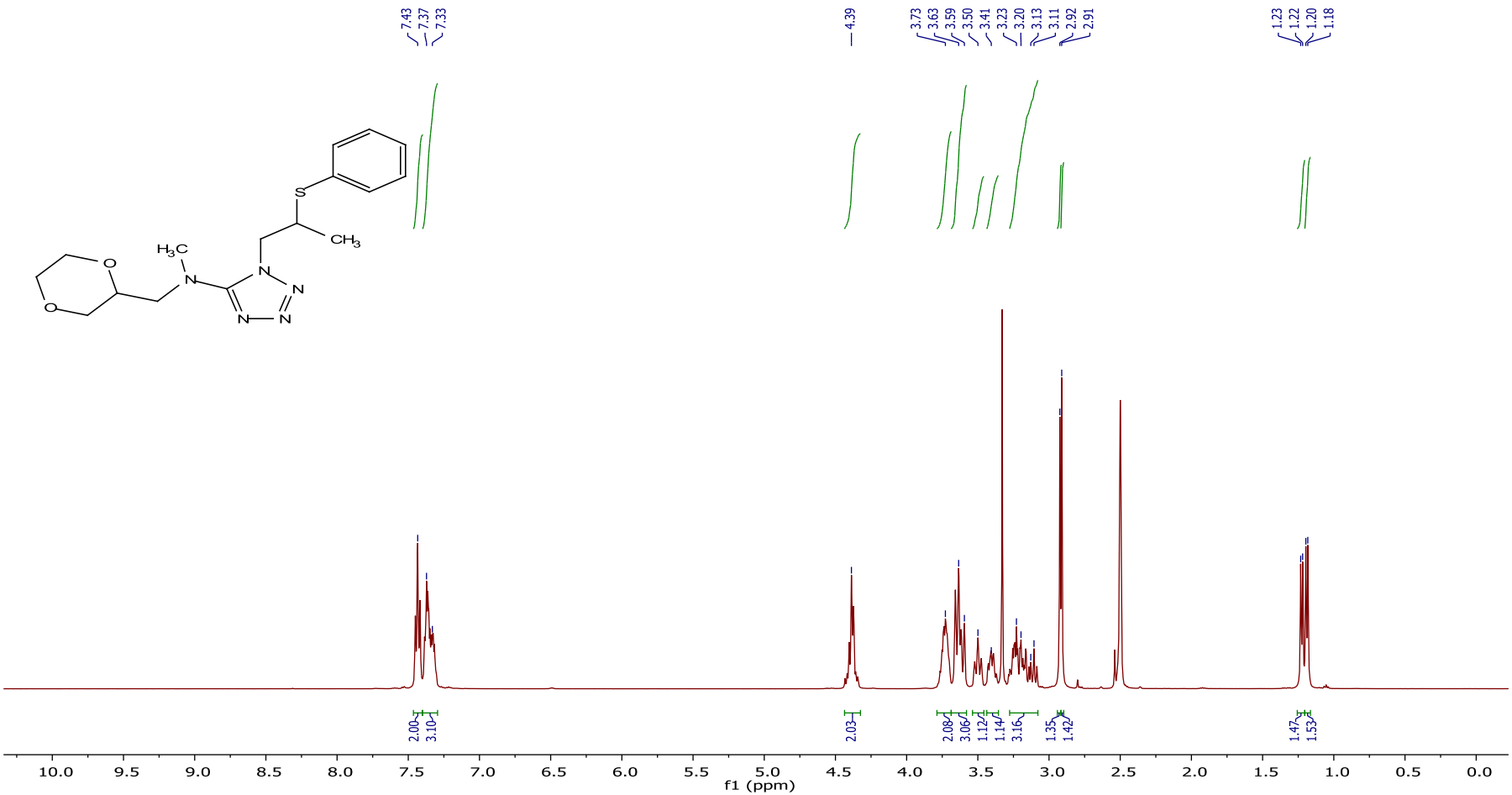
^{13}C NMR spectrum of the compound **9**{*190,341*}.



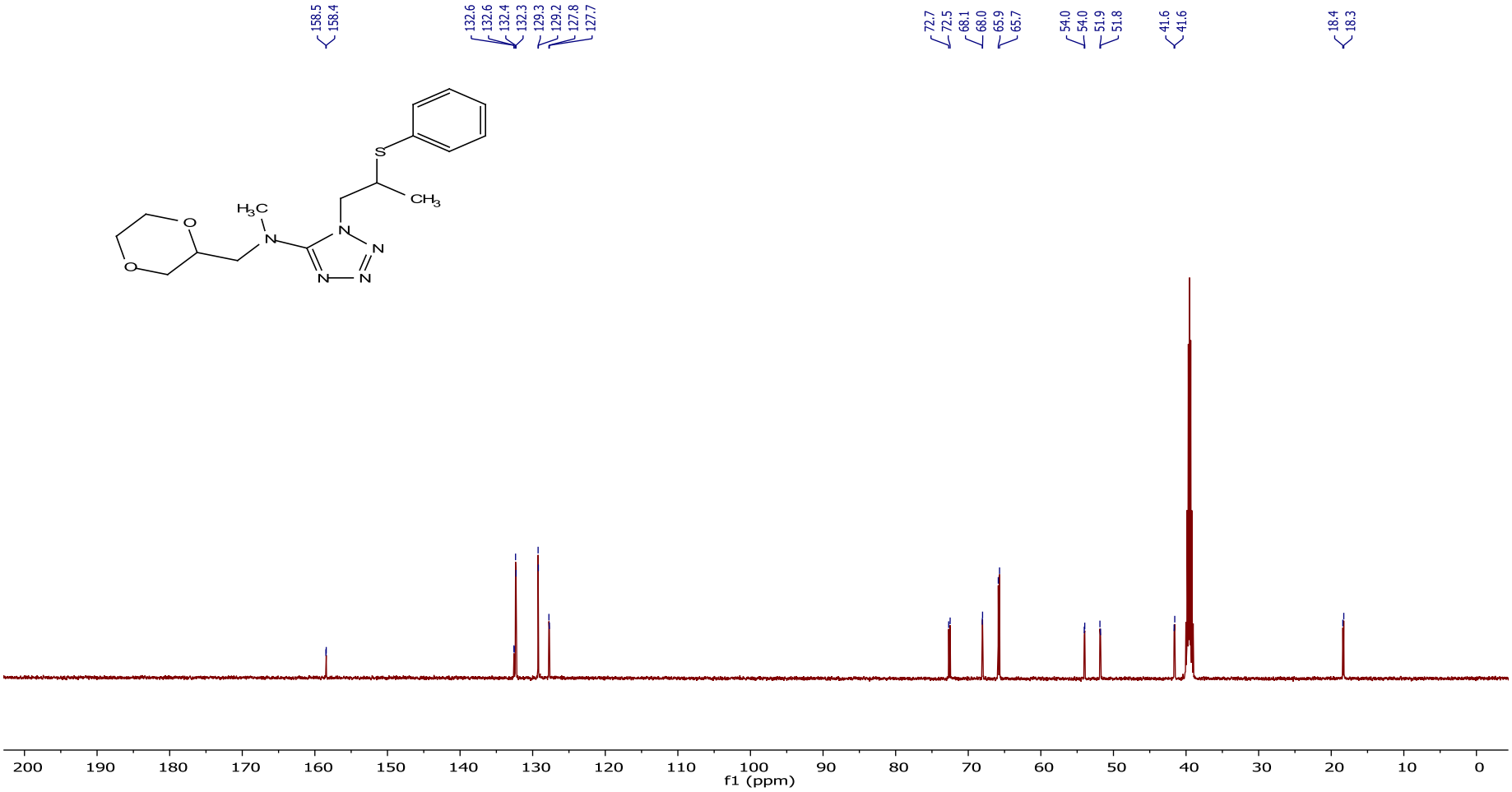
^{19}F NMR spectrum of the compound **9**{*190,341*}.



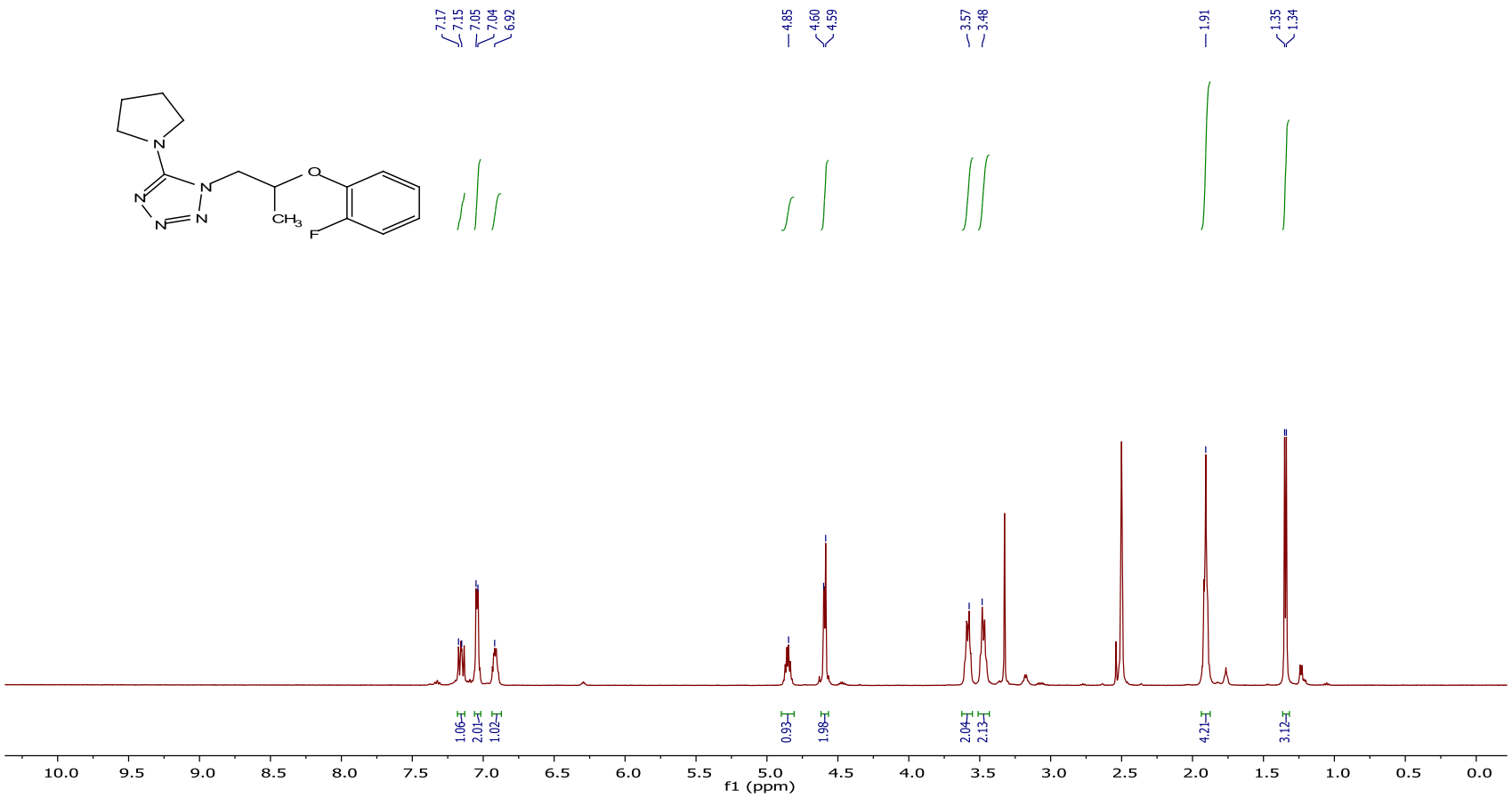
^{1}H NMR spectrum of the compound **9**{*262,319*}.



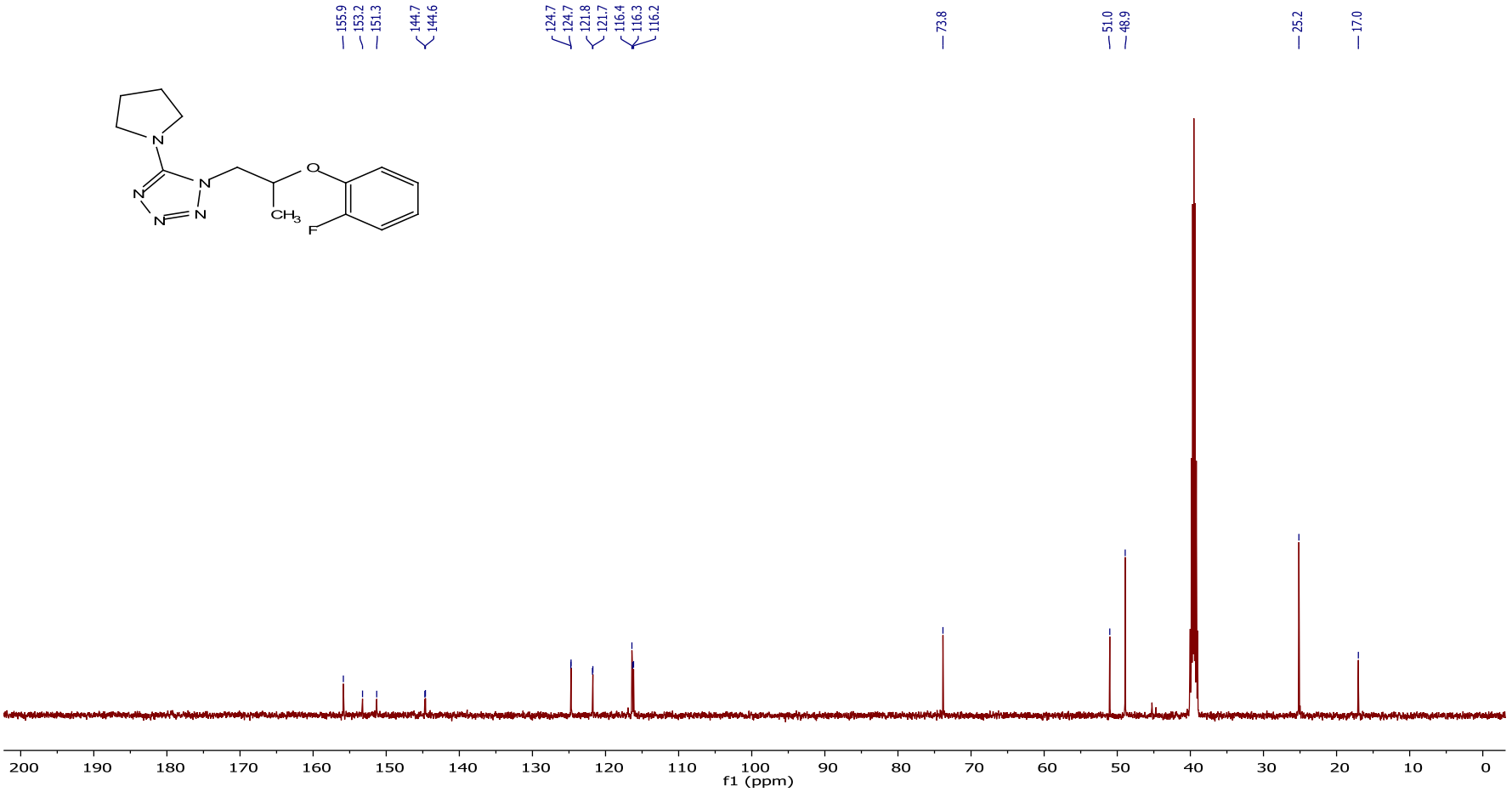
^{13}C NMR spectrum of the compound **9**{*262,319*}.



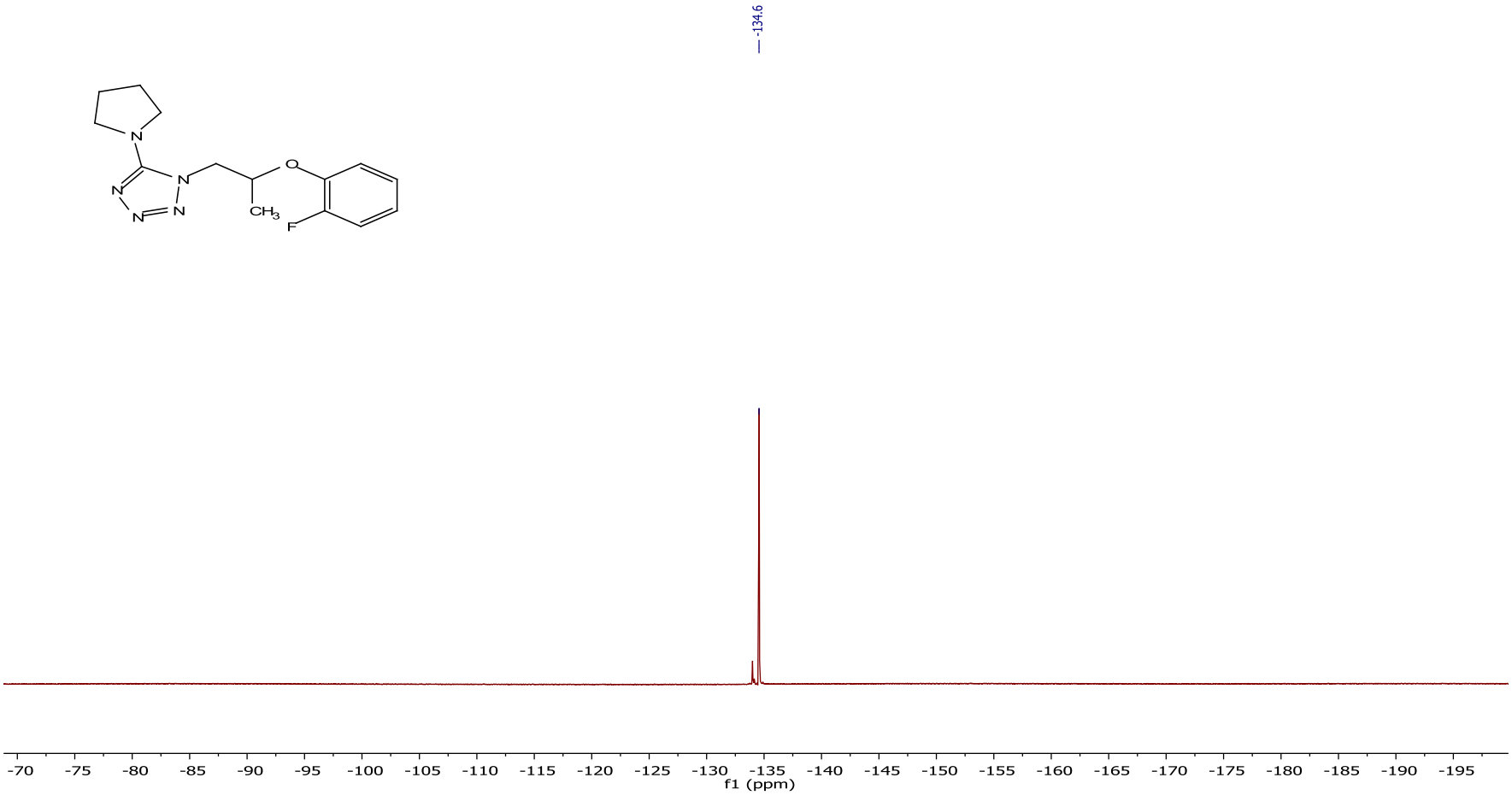
^{1}H NMR spectrum of the compound **9**{*263,341*}.



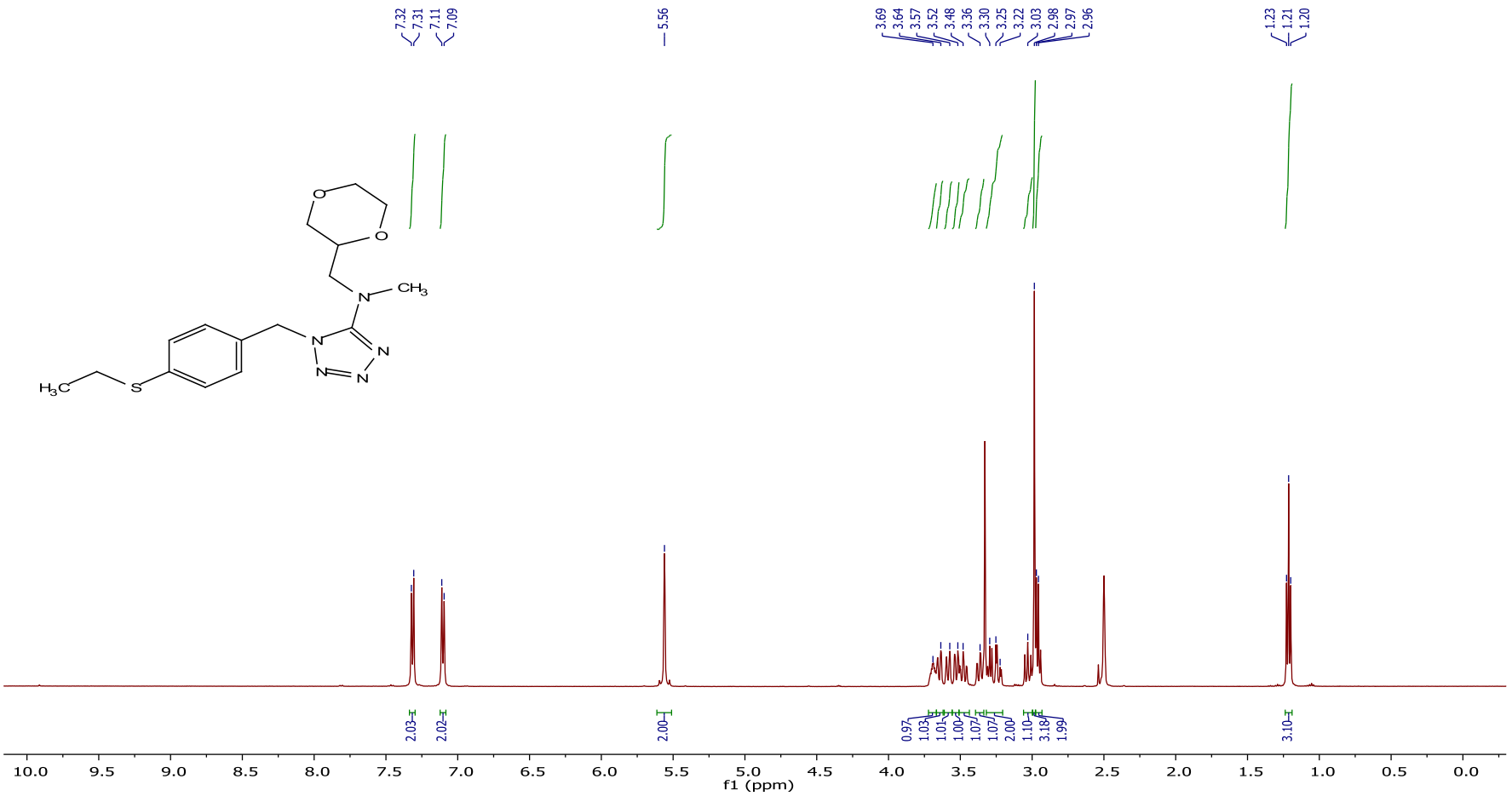
^{13}C NMR spectrum of the compound **9**{*263,341*}.



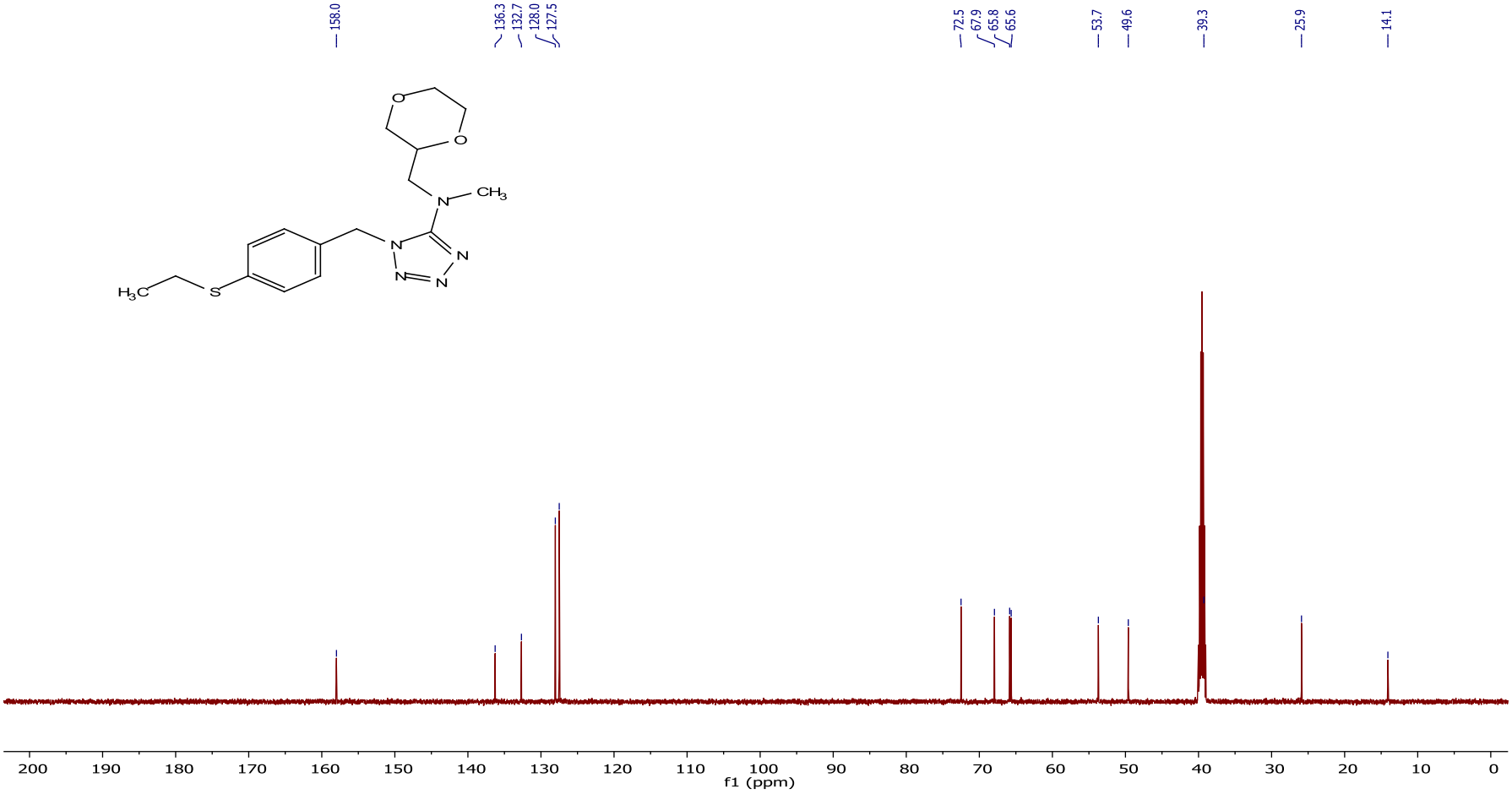
^{19}F NMR spectrum of the compound **9**{*263,341*}.



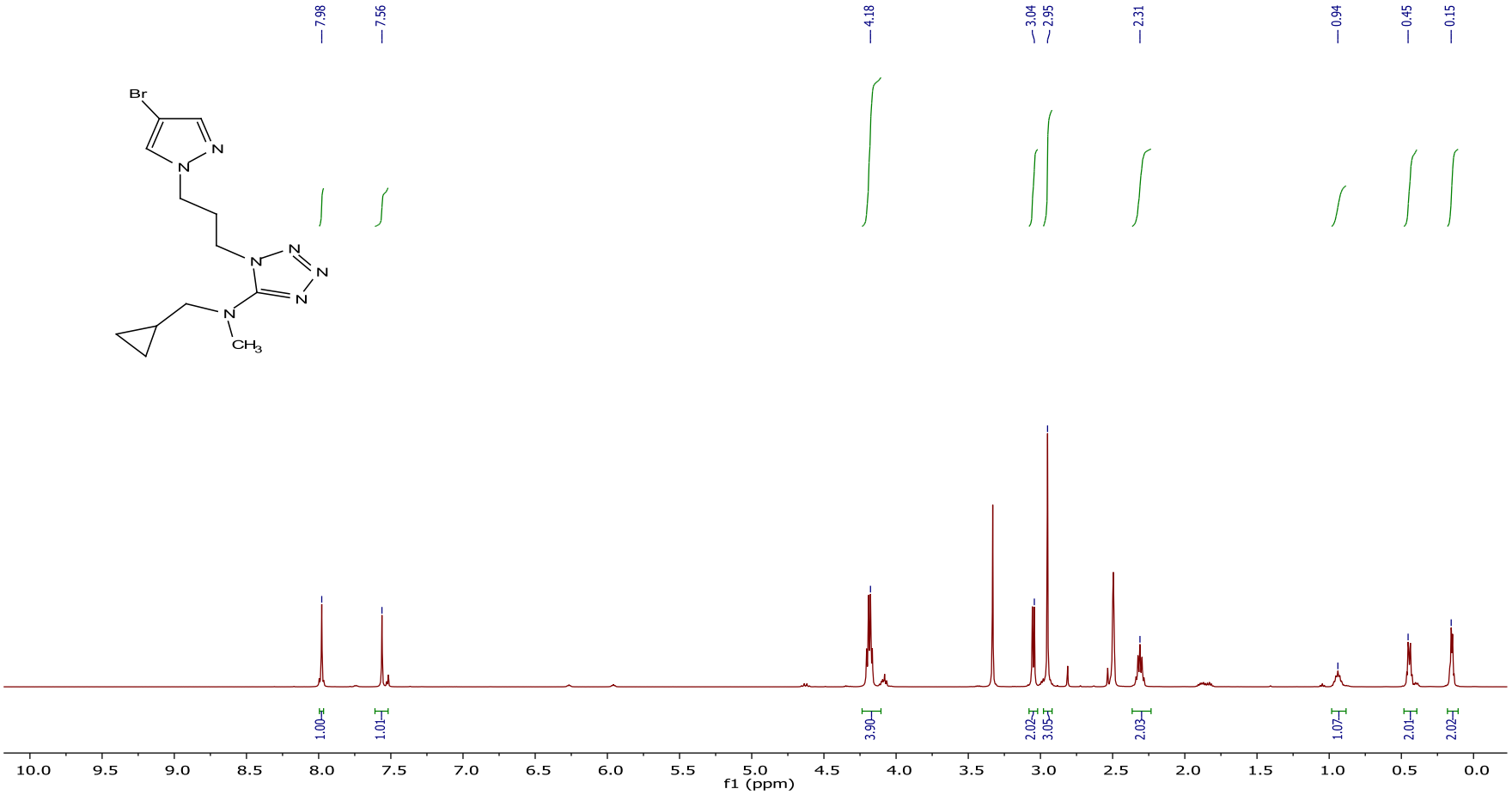
^{1}H NMR spectrum of the compound **9**{*272,319*}.



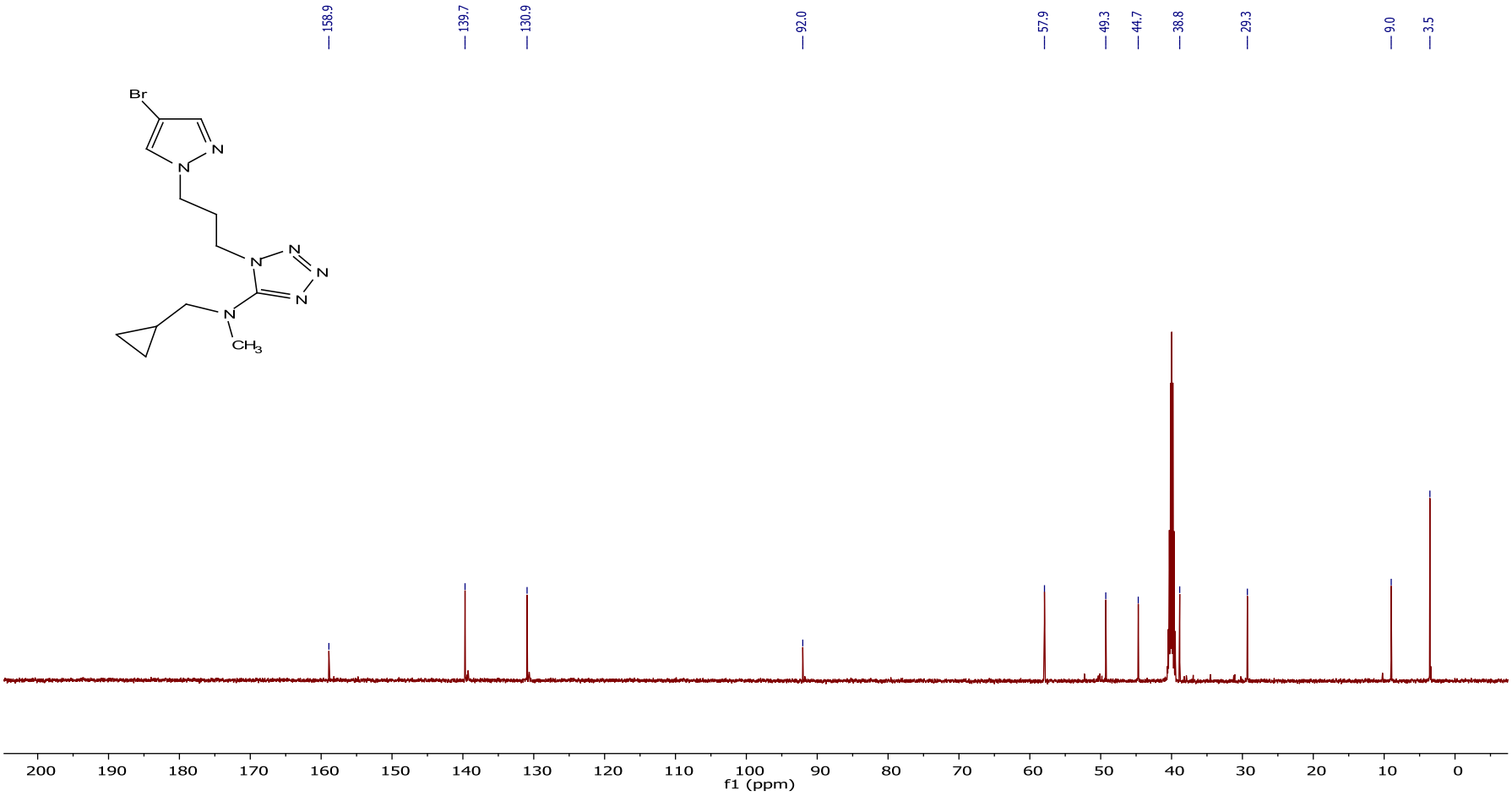
^{13}C NMR spectrum of the compound **9**{*272,319*}.



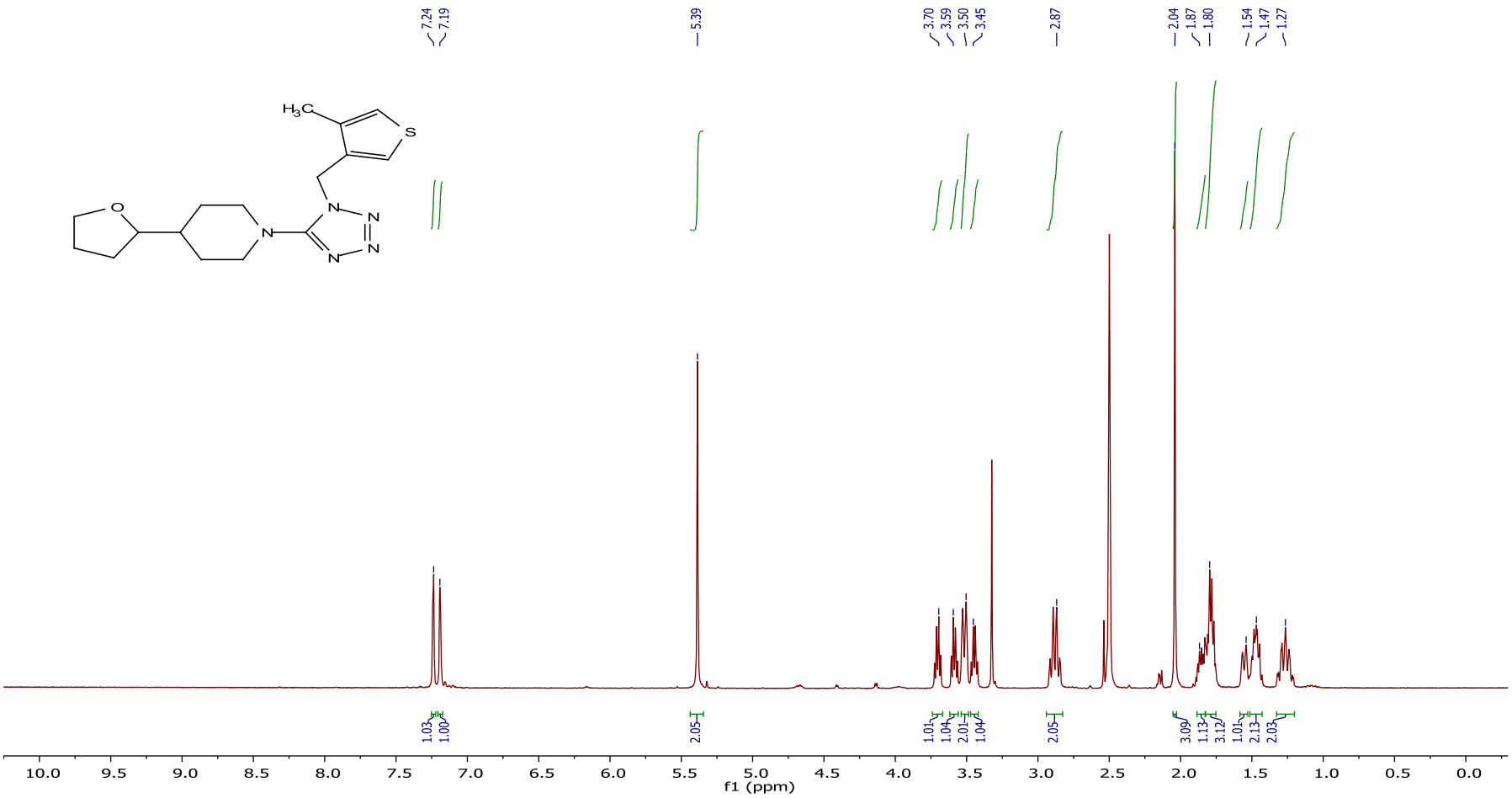
^{1}H NMR spectrum of the compound **9**{*280,391*}.



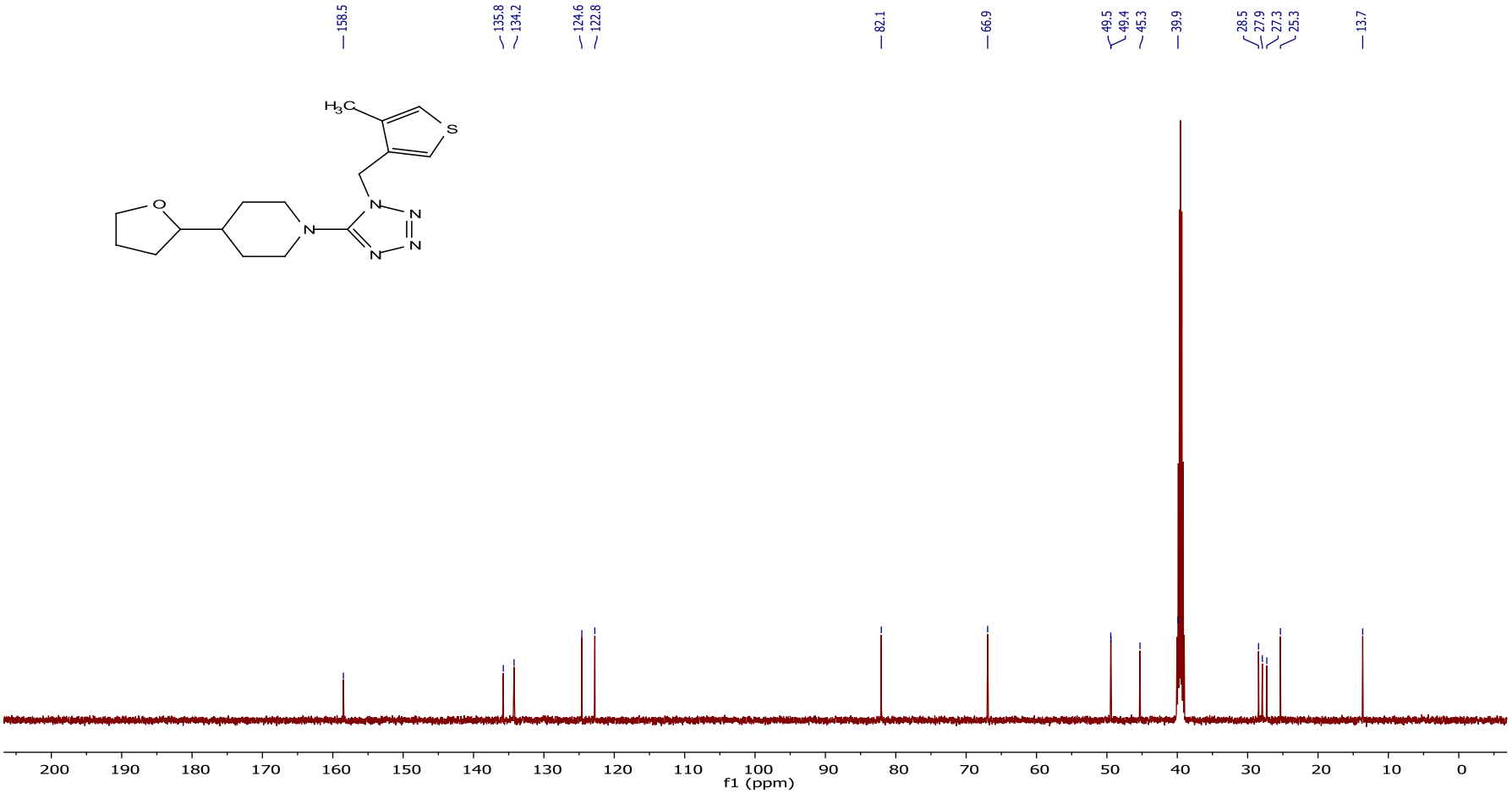
^{13}C NMR spectrum of the compound **9**{*280,391*}.



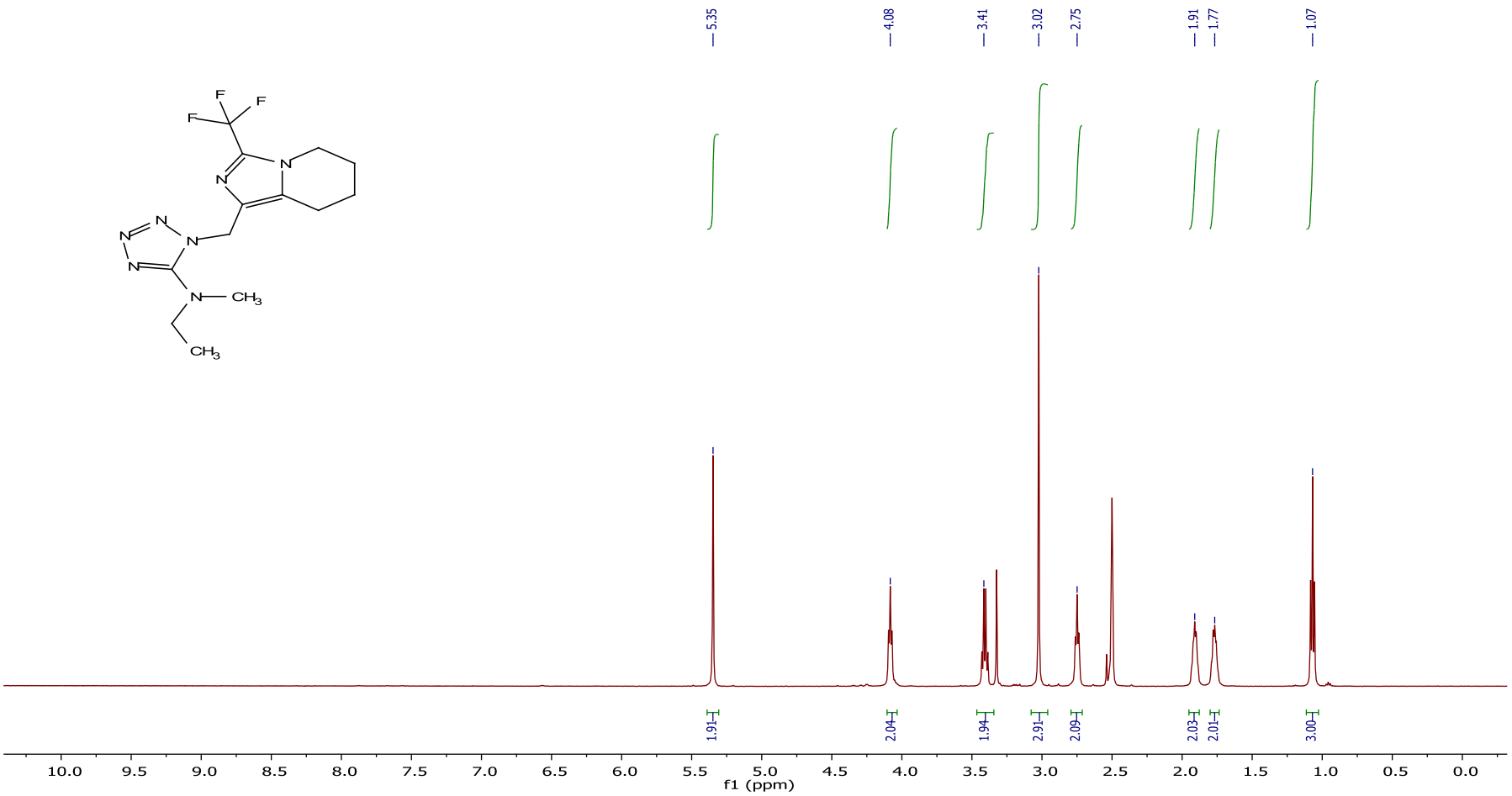
^{1}H NMR spectrum of the compound **9**{*306,261*}.



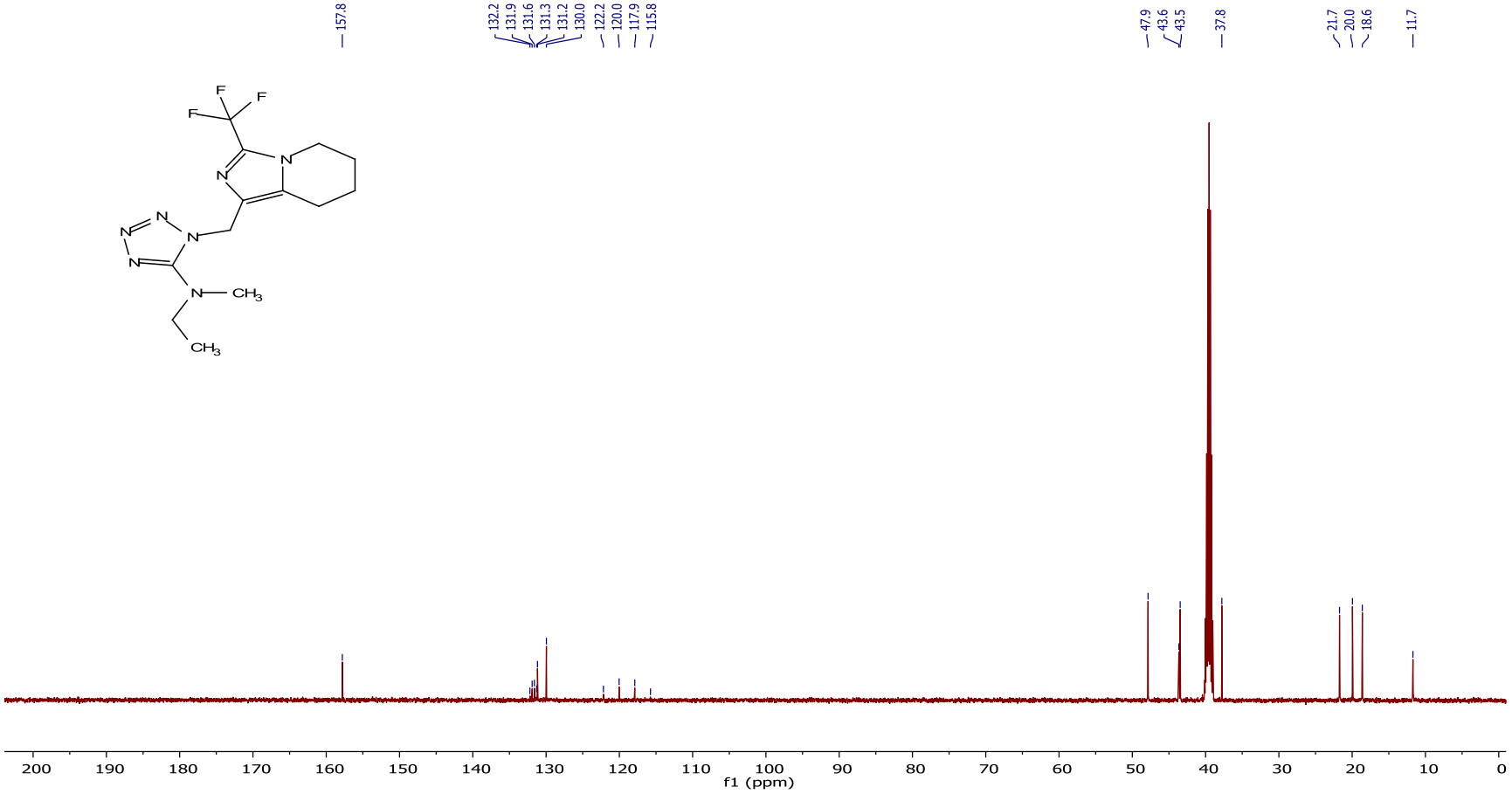
^{13}C NMR spectrum of the compound **9**{*306,261*}.



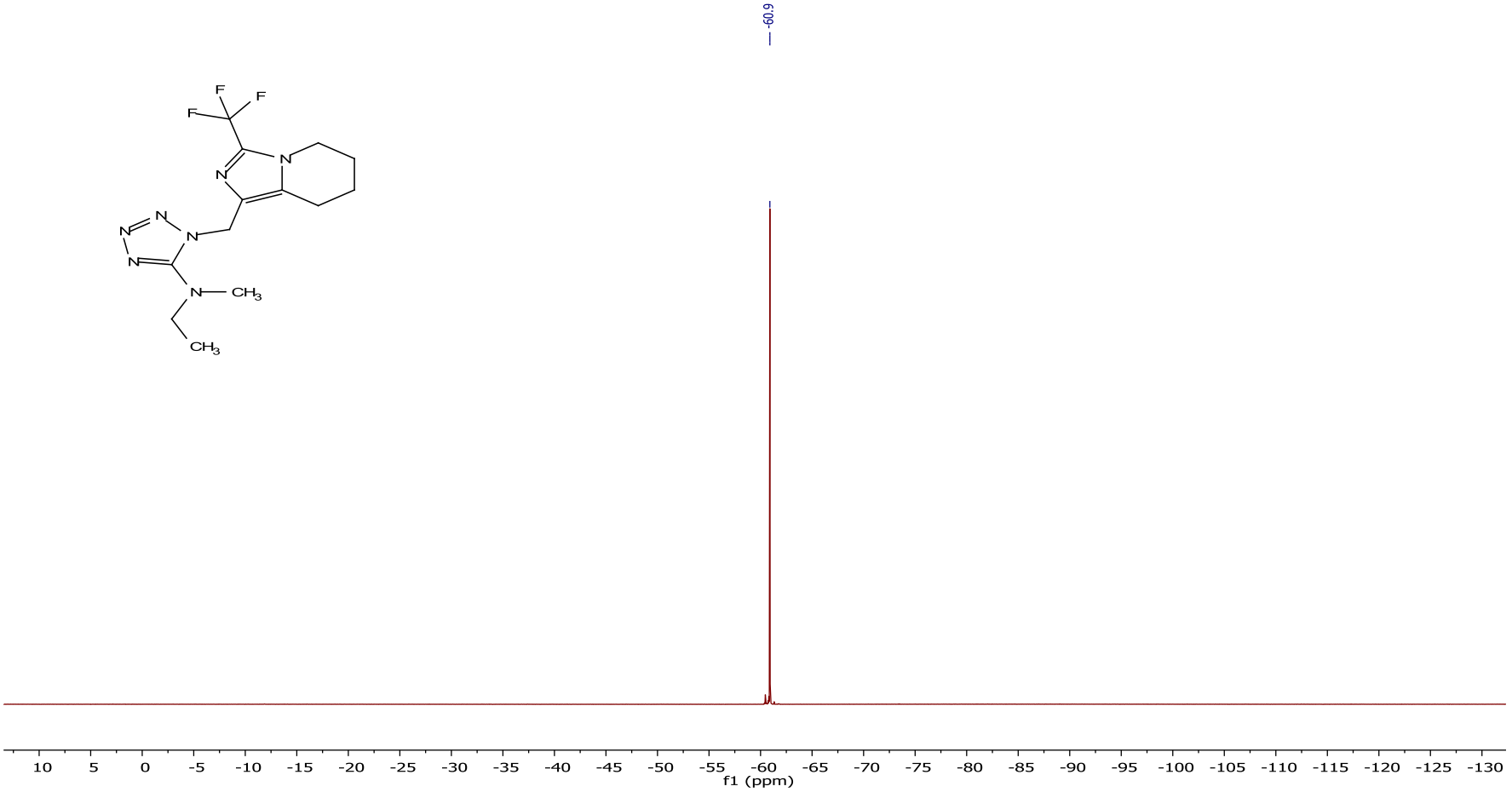
^{1}H NMR spectrum of the compound **9**{*341,346*}.



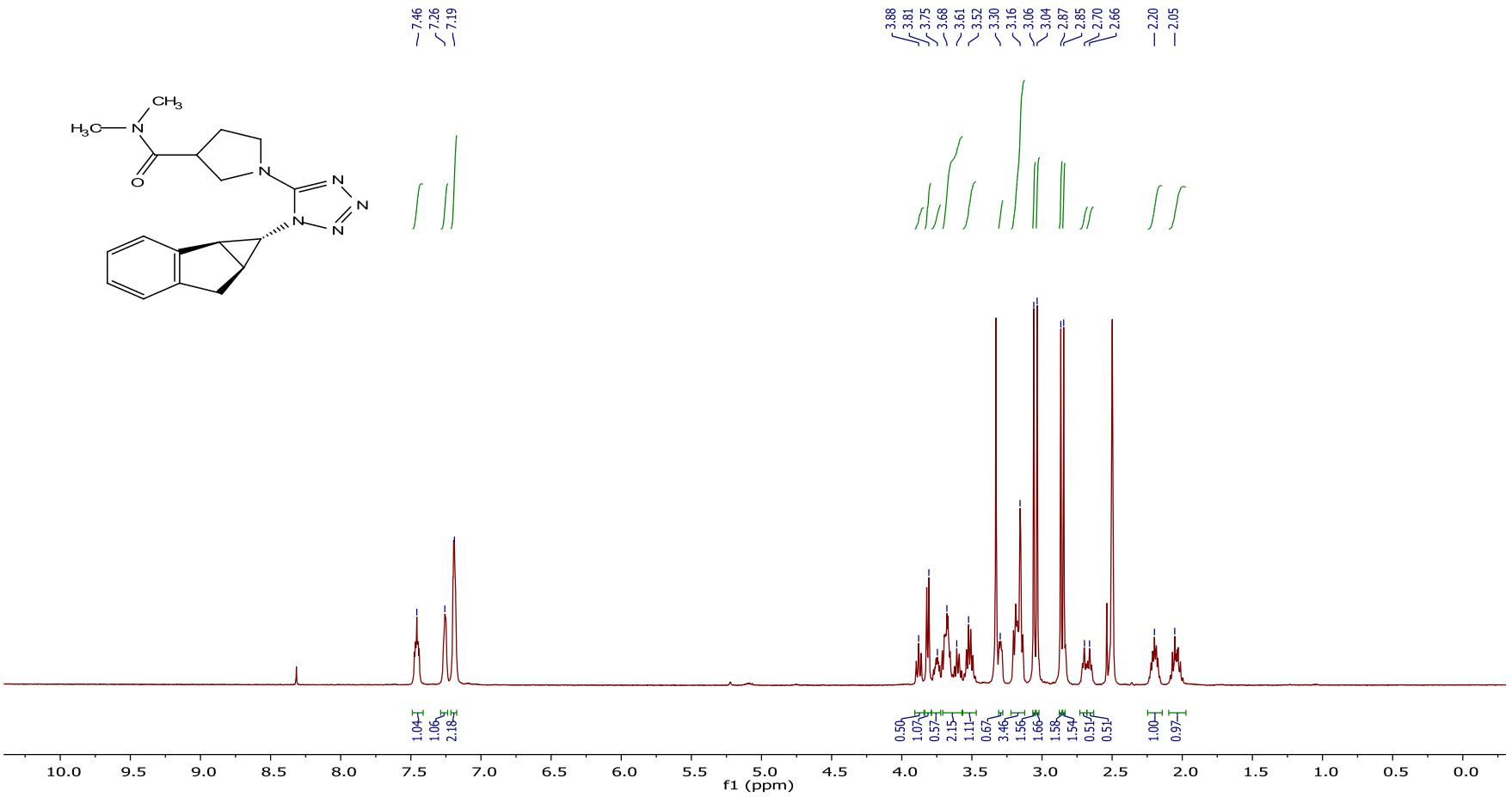
^{13}C NMR spectrum of the compound **9**{*341,346*}.



^{19}F NMR spectrum of the compound **9**{*341*,*346*}.



^{1}H NMR spectrum of the compound **9**{*375,511*}.



^{13}C NMR spectrum of the compound **9**{*375,511*}.