Discovery of novel pimprinine and streptochlorin derivatives as potential antifungal agents

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1. Compound Data

Intermediate：

*1-(1H-indol-3-yl)ethan-1-one (**2**)*: Yellow crystal; Yield: 71%. m.p.: 188.6-191.8℃. ^{1}H NMR (400 MHz, Acetone-*d6*) δ 10.99 (s, 1H), 8.40-8.31 (m, 1H), 8.23 (d, *J* = 3.2 Hz, 1H), 7.54-7.49 (m, 1H), 7.29-7.17 (m, 2H), 2.49 (s, 3H).

target compounds:

*1.1 5-(1H-indol-3-yl)oxazole (**3a**)*: Yellow powder; Yield: 51%. m.p.:174.7-176.5 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.62 (s, 1H), 8.36 (d, *J* = 2.0 Hz, 1H), 7.90 (s, 1H), 7.83 (d, *J* = 2.8 Hz, 1H), 7.54 – 7.47 (m, 2H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.20 – 7.14 (m, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 149.7, 147.8, 136.5, 123.7, 123.6, 122.3, 120.3, 119.5, 118.8, 112.2, 103.7. HRMS (MALDI): m/z calcd for $C_{11}H_8N_2O$ ($[M + H]^+$) 185.0709, Found 185.0709.

*1.2 5-(1H-indol-3-yl)-2-methyloxazole (**3b**)*: Light yellow powder; Yield: 53%. m.p.: 202.7-204.8 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.50 (s, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.71 (d, *J* = 2.8 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.27 (s, 1H), 7.22 – 7.10 (m, 2H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 158.5, 147.8, 136.8, 124.2, 122.4, 122.3, 120.2, 119.6, 119.6, 111.9, 105.0, 12.9. HRMS (MALDI): m/z calcd for $C_{12}H_{10}N_2O$ ($[M + H]^+$) 199.0866, Found 199.0862.

*1.3 2-ethyl-5-(1H-indol-3-yl)oxazole (**3c**)*: Light yellow powder; Yield: 42%. m.p.: 157.4-158.6 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.53 (s, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 2.8 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.29 (s, 1H), 7.16 (dt, *J* = 25.2, 7.2 Hz, 2H), 2.82 (q, *J* = 7.6 Hz, 2H), 1.30 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 162.9, 147.7, 136.8, 124.2, 122.5, 122.3, 120.2, 119.7, 119.4, 111.9, 105.1, 21.2, 10.8. HRMS (MALDI): m/z calcd for $C_{13}H_{12}N_2O$ ($[M + H]^+$) 213.1022, Found 213.1087.

*1.4 5-(1H-indol-3-yl)-2-isobutyloxazole (**3d**)*: Yellow powder; Yield: 43%. m.p.: 137.9-139.6 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.52 (s, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.71 (d, *J* = 2.8 Hz, 1H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.28 (s, 1H), 7.22 – 7.09 (m, 2H), 2.67 (d, *J* = 7.2 Hz, 2H), 2.24 – 2.04 (m, 1H), 0.97 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 161.4, 147.7, 136.8, 124.2, 122.5, 122.3, 120.2, 119.7, 119.4, 111.9, 105.1, 36.6, 27.4, 21.8. HRMS (MALDI): m/z calcd for $C_{15}H_{16}N_2O$ ($[M + H]^+$) 241.1335, Found 241.1331.

*1.5 2-cyclohexyl-5-(1H-indol-3-yl)oxazole (**3e**)*: Light pink powder; Yield: 53%. m.p.: 177.6-179.3 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 10.67 (s, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.74 (d, *J* = 2.4 Hz, 1H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.27 – 7.22 (m, 1H), 7.22 – 7.14 (m, 2H), 2.87 (dq, *J* = 11.2, 4.0 Hz, 1H), 2.17 – 2.09 (m, 2H), 1.91 – 1.79 (m, 2H), 1.78 – 1.67 (m, 2H), 1.66 – 1.47 (m, 2H), 1.45 – 1.32 (m, 2H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 165.1, 147.4, 136.8, 124.2, 122.4, 122.3, 120.2, 119.7, 119.3, 111.9, 105.2, 37.2, 30.6, 25.7, 25.4. HRMS (MALDI): m/z calcd for $C_{17}H_{18}N_2O$ ($[M + H]^+$) 267.1492, Found 267.1487.

*1.6 5-(1H-indol-3-yl)-2-phenyloxazole (**3f**)*: Yellow solid; Yield: 47%. m.p.: 225.6-227.8 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 10.80 (s, 1H), 8.19 – 8.12 (m, 2H), 8.04 – 7.99 (m, 1H), 7.95 (d, *J* = 2.4 Hz, 1H), 7.59 – 7.48 (m, 5H), 7.24 (qd, *J* = 7.2, 3.6 Hz, 2H). ^{13}C NMR (100 MHz,

Acetone-d_6) δ 158.8, 148.6, 136.9, 129.8, 128.9, 128.0, 125.7, 124.2, 123.3, 122.5, 121.1, 120.5, 119.7, 112.0, 104.8. HRMS (MALDI): m/z calcd for $C_{17}H_{12}N_2O$ ([M + H]$^+$) 261.1022, Found 261.1023.

*1.7 5-(1H-indol-3-yl)-2-(2-(methylthio)ethyl)oxazole (**3g**)*: Yellow powder; Yield: 40%. m.p.: 141.2-143.2 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.53 (s, 1H), 7.83 (d, J = 8.0 Hz, 1H), 7.73 (d, J = 2.4 Hz, 1H), 7.44 (d, J = 8.0 Hz, 1H), 7.30 (s, 1H), 7.15 (dt, J = 14.8, 7.2 Hz, 2H), 3.09 (t, J = 7.2 Hz, 2H), 2.90 (t, J = 7.2 Hz, 2H), 2.08 (s, 3H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 160.4, 148.0, 136.8, 124.2, 122.6, 122.4, 120.3, 119.7, 119.5, 111.9, 105.0, 30.9, 28.3, 14.4. HRMS (MALDI): m/z calcd for $C_{14}H_{14}N_2SO$ ([M + H]$^+$) 259.0900, Found 259.0900.

*1.8 4-chloro-5-(1H-indol-3-yl)oxazole (**4a**)*: White powder; Yield: 58%. m.p.:164.1-165.8 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.80 (s, 1H), 8.50 (s, 1H), 7.94 – 7.87 (m, 2H), 7.51 (s, 1H), 7.27 – 7.20 (m, 1H), 7.20 – 7.14 (m, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 149.5 (d, J = 3.3 Hz), 142.8, 136.0, 124.8, 124.1, 122.6, 120.5, 120.1, 119.9, 112.3, 101.5. HRMS (MALDI): m/z calcd for $C_{11}H_7ClN_2O$ ([M + H]$^+$) 219.0320, Found 219.0320.

*1.9 4-chloro-5-(1H-indol-3-yl)-2-methyloxazole (**4b**)*: White powder; Yield: 65%. m.p.: 183-185.5 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.72 (s, 1H), 7.91 (d, J = 8.0 Hz, 1H), 7.84 (d, J = 2.8 Hz, 1H), 7.49 (d, J = 8.0 Hz, 1H), 7.18 (dt, J = 27.2, 7.2 Hz, 2H), 2.52 (s, 3H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 158.2, 142.6, 136.3, 124.6, 123.7, 122.6, 120.7, 120.4, 111.9, 111.8, 102.9, 13.2. HRMS (MALDI): m/z calcd for $C_{12}H_9ClN_2O$ ([M + H]$^+$) 233.0476, Found 233.0478.

*1.10 4-chloro-2-ethyl-5-(1H-indol-3-yl)oxazole (**4c**)*: Yellow powder; Yield: 57%. m.p.: 135.4-138.1 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 10.83 (s, 1H), 8.02 (d, J = 8.0 Hz, 1H), 7.90 (s, 1H), 7.53 (d, J = 8.0 Hz, 1H), 7.28 – 7.15 (m, 2H), 2.89 (q, J = 7.6 Hz, 2H), 1.39 (t, J = 5.6 Hz, 3H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 162.4, 142.5, 136.2, 124.6, 123.6, 122.6, 120.7, 120.4, 120.4, 111.9, 102.9, 21.4, 10.4. HRMS (MALDI): m/z calcd for $C_{13}H_{11}ClN_2O$ ([M + H]$^+$) 247.0633, Found 247.0634.

*1.11 4-chloro-5-(1H-indol-3-yl)-2-isobutyloxazole (**4d**)*: Light yellow powder; Yield: 80%. m.p.: 106-107.7 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 10.82 (s, 1H), 8.02 (d, J = 8.0 Hz, 1H), 8.02 (d, J = 8.0 Hz, 1H), 7.91 (s, 1H), 7.21 (dt, J = 24.0, 7.2 Hz, 2H), 2.75 (d, J = 7.2 Hz, 2H), 2.30 – 2.16 (m, 1H), 1.05 (d, J = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 160.8, 142.6, 136.3, 124.6, 123.8, 122.6, 120.7, 120.5, 120.3, 111.9, 103.0, 36.7, 27.4, 21.7. HRMS (MALDI): m/z calcd for $C_{15}H_{15}ClN_2O$ ([M + H]$^+$) 275.0946, Found 275.0945.

*1.12 4-chloro-2-cyclohexyl-5-(1H-indol-3-yl)oxazole (**4e**)*: Yellow powder; Yield: 62%. m.p.: 189.8-192.1 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 10.82 (s, 1H), 8.03 (d, J = 8.0 Hz, 1H), 7.91 (d, J = 2.8 Hz, 1H), 7.54 (d, J = 8.0 Hz, 1H), 7.31 – 7.15 (m, 2H), 2.94 (tt, J = 11.2, 3.6 Hz, 1H), 2.17 (dd, J = 13.2, 3.2 Hz, 2H), 2.06 (dt, J = 4.4, 2.4 Hz, 2H), 1.90 – 1.81 (m, 2H), 1.74 – 1.66 (m, 2H), 1.54 – 1.42 (m, 2H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 164.4, 142.2, 136.3, 124.6, 123.7, 122.6, 120.5, 120.4, 111.9, 103.0, 100.0, 37.3, 30.3, 25.6, 25.2. HRMS (MALDI): m/z calcd for $C_{17}H_{17}ClN_2O$ ([M + H]$^+$) 301.1102, Found 301.1104.

*1.13 4-chloro-5-(1H-indol-3-yl)-2-phenyloxazole (**4f**)*: Light yellow powder; Yield: 57%. m.p.: 191.9-194 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 10.94 (s, 1H), 8.15 (d, J = 7.6 Hz, 2H), 8.05 (s, 1H), 7.68 – 7.43 (m, 5H), 7.33 – 7.23 (m, 2H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 157.5, 143.5, 136.2, 130.5, 129.1, 127.0, 125.9, 125.7, 124.3, 122.8, 122.4, 120.8, 120.4, 112.0, 102.8. HRMS (MALDI): m/z calcd for $C_{17}H_{11}ClN_2O$ ([M + H]$^+$) 295.0633, Found 295.0640.

*1.14 4-bromo-5-(1H-indol-3-yl)oxazole (**5a**)*: Brown powder; Yield: 62%. m.p.: 153.8-155.2 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.81 (s, 1H), 8.52 (s, 1H), 8.00 (d, J = 2.8 Hz, 1H), 7.94 (d, J = 8.0 Hz, 1H), 7.54 (d, J = 8.0 Hz, 1H), 7.27 – 7.23 (m, 1H), 7.21 – 7.16 (m, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 150.5, 145.2, 136.0, 124.9, 124.3, 122.6, 120.6, 120.0, 112.4, 107.2, 101.7. HRMS (MALDI): m/z calcd for $C_{11}H_7BrN_2O$ ([M + H]$^+$) 262.9815, Found 262.9815.

*1.15 4-bromo-5-(1H-indol-3-yl)-2-methyloxazole (**5b**)*: Yellow powder; Yield: 76%. m.p.: 202.7-204.8 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.71 (s, 1H), 7.91 (t, J = 5.6 Hz, 2H), 7.50 (d, J = 8.0 Hz, 1H), 7.22 (t, J = 7.6 Hz, 1H), 7.15 (t, J = 7.6 Hz, 1H), 2.54 (s, 3H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 158.5, 147.8, 136.8, 124.1, 122.4, 122.3, 120.2, 119.6, 119.6, 111.9, 105.0, 12.9. HRMS (MALDI): m/z calcd for $C_{12}H_9BrN_2O$ ([M + H]$^+$) 276.9971, Found 276.9968.

*1.16 4-bromo-2-ethyl-5-(1H-indol-3-yl)oxazole (**5c**)*: Yellow powder; Yield: 60%. m.p.: 137.7-139.4 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 10.82 (s, 1H), 8.03 (d, J = 8.0 Hz, 1H), 8.00 (d, J = 2.8 Hz, 1H), 7.53 (d, J = 8.0 Hz, 1H), 7.27 – 7.15 (m, 2H), 2.94 – 2.87 (q, 2H), 1.38 (t, J = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 163.3, 145.0, 136.3, 124.8, 124.0, 122.9, 122.6, 120.5, 111.9, 107.4, 103.1, 21.4, 10.5. HRMS (MALDI): m/z calcd for $C_{13}H_{11}BrN_2O$ ([M + H]$^+$) 291.0128, Found 291.0132.

*1.17 4-bromo-5-(1H-indol-3-yl)-2-isobutyloxazole (**5d**)*: Yellow powder; Yield: 74%. m.p.: 105.2-106.6 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 10.84 (s, 1H), 8.03 (d, J = 8.0 Hz, 1H), 7.91 (s, 1H), 7.54 (d, J = 8.0 Hz, 1H), 7.27 – 7.15 (m, 2H), 2.76 (d, J = 7.2 Hz, 2H), 2.30 – 2.17 (m, 1H), 1.06 (d, J = 4.4 Hz, 6H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 160.8, 142.6, 136.3, 124.6, 123.8, 123.6, 122.6, 120.5, 120.3, 111.9, 103.0, 36.7, 27.4, 21.7. HRMS (MALDI): m/z calcd for $C_{15}H_{15}BrN_2O$ ([M + H]$^+$) 319.0441, Found 319.0448.

*1.18 4-bromo-2-cyclohexyl-5-(1H-indol-3-yl)oxazole (**5e**)*: Yellow powder; Yield: 76%. m.p.: 173.8-176.6 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 10.80 (s, 1H), 8.03 (d, J = 8.0 Hz, 1H), 8.00 (s, 1H), 7.53 (d, J = 8.0 Hz, 1H), 7.21 (dt, J = 14.8, 7.2 Hz, 2H), 3.03 – 2.89 (m, 1H), 2.16 (d, J = 11.2 Hz, 2H), 1.92 – 1.79 (m, 2H), 1.70 (dd, J = 18.8, 10.0 Hz, 2H), 1.66 – 1.49 (m, 2H), 1.36 (m, J = 27.2, 14.4, 6.4 Hz, 2H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 165.3, 144.6, 136.2, 124.8, 123.9, 123.8, 122.6, 120.5, 111.9, 107.4, 103.2, 37.2, 30.3, 25.6, 25.3. HRMS (MALDI): m/z calcd for $C_{17}H_{17}BrN_2O$ ([M + H]$^+$) 345.0597, Found 345.0602.

*1.19 4-bromo-5-(1H-indol-3-yl)-2-phenyloxazole (**5f**)*: Yellow powder; Yield: 70%. m.p.: 166.0-169.9 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 8.22 (dd, J = 6.0, 2.4 Hz, 1H), 8.16 (d, J = 1.6 Hz, 1H), 8.15 (d, J = 3.2 Hz, 2H), 7.83 – 7.35 (m, 5H), 7.28 – 7.26 (m, 1H). ^{13}C NMR (100 MHz,

Acetone-d_6) δ 158.6, 145.9, 136.2, 130.5, 129.1, 126.9, 125.7, 124.7, 124.5, 122.8, 120.8, 120.5, 112.0, 109.1, 102.9. HRMS (MALDI): m/z calcd for $C_{17}H_{11}BrN_2O$ ([M + H]$^+$) 339.0128, Found 339.0139.

*1.20 4-bromo-5-(1H-indol-3-yl)-2-(2-(methylthio)ethyl)oxazole (**5g**)*: Light yellow powder; Yield: 53%. m.p.: 135.8-137.7 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 10.84 (s, 1H), 8.06 (d, J = 8.0 Hz, 1H), 8.02 (s, 1H), 7.53 (t, J = 12.8 Hz, 1H), 7.22 (dt, J = 15.2, 7.2 Hz, 2H), 3.22 (t, J = 7.2 Hz, 2H), 3.02 (t, J = 7.2 Hz, 2H), 2.18 (s, 3H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 160.9, 145.3, 136.2, 124.8, 124.1, 124.0, 122.6, 120.5, 111.9, 107.4, 103.0, 30.6, 28.3, 14.3. HRMS (MALDI): m/z calcd for $C_{14}H_{13}BrN_2SO$ ([M + H]$^+$) 337.0005, Found 337.0002.

*1.21 5-(5-fluoro-1H-indol-3-yl)-2-methyloxazole (**8a**)*: Brown solid; Yield: 35%. m.p.: 218.2 – 219.2 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 10.73 (s, 1H), 7.87 (dd, J = 8.8, 5.2 Hz, 1H), 7.73 (d, J = 2.4 Hz, 1H), 7.26 (dd, J = 10.0, 2.4 Hz, 1H), 7.23 (s, 1H), 7.00 (td, J = 9.2, 2.4 Hz, 1H), 2.48 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 159.6 (d, J = 235.7 Hz), 158.9, 147.4, 136.8 (d, J = 12.9 Hz), 123.9 (d, J = 3.3 Hz), 121.0 (d, J = 9.9 Hz), 120.9, 120.0, 108.9 (d, J = 24.2 Hz), 104.6, 98.5 (d, J = 25.8 Hz), 14.0. HRMS (ESI): m/z calcd for $C_{12}H_9FN_2O$ ([M + H]$^+$) 217.0772, Found 217.0772.

*1.22 5-(5-chloro-1H-indol-3-yl)-2-methyloxazole (**8b**)*: Yellow solid; Yield: 50%. m.p.: 213.1 – 214.0 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 10.81 (s, 1H), 7.88 (d, J = 8.8 Hz, 1H), 7.76 (d, J = 2.8 Hz, 1H), 7.57 (d, J = 2.0 Hz, 1H), 7.24 (s, 1H), 7.18 (dd, J = 8.4, 2.0 Hz, 1H), 2.48 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 159.0, 147.2, 137.2, 127.3, 124.4, 122.8, 121.3, 120.7, 120.1, 112.1, 104.7, 14.0. HRMS (ESI): m/z calcd for $C_{12}H_9ClN_2O$ ([M + H]$^+$) 233.0476, Found 233.0472.

*1.23 5-(5-bromo-1H-indol-3-yl)-2-methyloxazole (**8c**)*: Yellow solid; Yield: 43%. m.p.: 219.3 – 220.1 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 10.84 (s, 1H), 8.03 (d, J = 2.0 Hz, 1H), 7.77 (d, J = 2.8 Hz, 1H), 7.48 (d, J = 8.8 Hz, 1H), 7.33 (dd, J = 8.8, 2.0 Hz, 1H), 7.25 (s, 1H), 2.48 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.6, 146.7, 135.2, 125.3, 124.6 (d, J = 25.6 Hz), 121.6, 119.8, 114.1, 112.8, 103.8, 30.7, 13.6. HRMS (ESI): m/z calcd for $C_{12}H_9BrN_2O$ ([M + H]$^+$) 276.9971, Found 276.9971.

*1.24 2-methyl-5-(4-methyl-1H-indol-3-yl)oxazole (**8d**)*: Yellow solid; Yield: 32%. m.p.: 166.1 – 167.2 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 10.75 (s, 1H), 7.53 (d, J = 2.8 Hz, 1H), 7.37 (d, J = 8.4 Hz, 1H), 7.11 (t, J = 7.6 Hz, 1H), 7.00 (s, 1H), 6.90 (d, J = 7.2 Hz, 1H), 2.49 (s, 3H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 160.2, 147.4, 136.9, 130.0, 125.9, 125.3, 123.9, 122.3, 121.5, 109.7, 104.0, 19.5, 13.1. HRMS (ESI): m/z calcd for $C_{13}H_{12}N_2O$ ([M + H]$^+$) 213.1022, Found 213.1024.

*1.25 5-(6-fluoro-1H-indol-3-yl)-2-methyloxazole (**8e**)*: Yellow solid; Yield: 61%. m.p.: 234.6–235.3 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.59 (s, 1H), 7.83 (dd, J = 8.8, 5.6 Hz, 1H), 7.73 (d, J = 2.8 Hz, 1H), 7.32 (s, 1H), 7.25 (dd, J = 10.0, 2.4 Hz, 1H), 7.03–6.96 (m, 1H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 159.3 (d, J = 235.7 Hz), 158.6, 147.1, 136.4 (d, J = 12.7 Hz), 123.6 (d, J = 2.9 Hz), 120.7 (d, J = 10.1 Hz), 120.5, 119.6, 108.6 (d, J = 24.4 Hz), 104.2, 98.2

(d, *J* = 25.6 Hz), 13.7. HRMS (ESI): m/z calcd for $C_{12}H_9FN_2O$ ([M + H]$^+$) 217.0772, Found 217.0770.

*1.26 5-(6-chloro-1H-indol-3-yl)-2-methyloxazole (**8f**)*: Yellow solid; Yield: 66%. m.p.: 206.7 – 208.1 °C. ^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 11.65 (s, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.77 (d, *J* = 2.8 Hz, 1H), 7.51 (d, *J* = 2.0 Hz, 1H), 7.31 (s, 1H), 7.19 – 7.11 (m, 1H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, DMSO-*d*$_6$) δ 158.6, 146.9, 136.9, 126.9, 124.1, 122.4, 121.0, 120.4, 119.8, 111.8, 104.3, 13.7. HRMS (ESI): m/z calcd for $C_{12}H_9ClN_2O$ ([M + H]$^+$) 233.0476, Found 233.0475.

*1.27 2-methyl-5-(5-methyl-1H-indol-3-yl) oxazole (**8g**)*: Yellow solid; Yield: 39%. m.p.: 167.5–168.2 °C. ^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 11.42 (s, 1H), 7.68 (d, *J* = 2.8 Hz, 1H), 7.63 (s, 1H), 7.36 (d, *J* = 8.4 Hz, 1H), 7.29 (s, 1H), 7.02 (dd, *J* = 8.4, 1.2 Hz, 1H), 2.48 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, DMSO-*d*$_6$) δ 158.2, 147.6, 134.8, 128.8, 123.9, 123.8, 123.0, 119.2, 119.2, 111.8, 103.5, 21.4, 13.7. HRMS (ESI): m/z calcd for $C_{13}H_{12}N_2O$ ([M + H]$^+$) 213.1022, Found 213.1015.

*1.28 5-(6-fluoro-1H-indol-3-yl)-2-ethyloxazole (**8h**)*: Yellow solid; Yield: 59%. m.p.: 232.8–234.1 °C. ^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 11.60 (s, 1H), 7.83 (dt, *J* = 8.4, 4.0 Hz, 1H), 7.74 (d, *J* = 2.8 Hz, 1H), 7.32 (s, 1H), 7.25 (dd, *J* = 10.0, 2.4 Hz, 1H), 7.00 (ddd, *J* = 9.6, 8.8, 2.4 Hz, 1H), 2.82 (q, *J* = 7.6 Hz, 2H), 1.30 (t, *J* = 8.8, 6.4 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-*d*$_6$) δ 162.8, 159.3 (d, *J* = 235.7 Hz), 146.9, 136.5 (d, *J* = 12.8 Hz), 123.7 (d, *J* = 3.5 Hz), 120.7 (d, *J* = 10.2 Hz), 120.5, 119.5, 108.6 (d, *J* = 24.5 Hz), 104.3, 98.2 (d, *J* = 25.7 Hz), 21.1, 11.3. HRMS (ESI): m/z calcd for $C_{13}H_{11}FN_2O$ ([M + H]$^+$) 231.0928, Found 231.0926.

*1.29 5-(6-chloro-1H-indol-3-yl)-2-ethyloxazole (**8i**)*: Yellow solid; Yield: 58%. m.p.: 190.1–191.2 °C. ^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 11.65 (s, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.78 (d, *J* = 2.8 Hz, 1H), 7.50 (dd, *J* = 2.8, 1.2 Hz, 1H), 7.31 (s, 1H), 7.17 – 7.10 (m, 1H), 2.82 (q, *J* = 7.6 Hz, 2H), 1.32 – 1.28 (t, 3H). ^{13}C NMR (100 MHz, DMSO-*d*$_6$) δ 162.8, 146.7, 136.8, 126.9, 124.1, 122.4, 121.0, 120.4, 119.6, 111.8, 104.3, 21.1, 11.3. HRMS (ESI): m/z calcd for $C_{13}H_{11}ClN_2O$ ([M + H]$^+$) 247.0633, Found 247.0632.

*1.30 5-(6-bromo-1H-indol-3-yl)-2-ethyloxazole (**8j**)*: Yellow solid; Yield: 36%. m.p.: 191.2–192.8 °C. ^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 11.66 (s, 1H), 7.78 (dd, *J* = 10.8, 5.6 Hz, 2H), 7.65 (d, *J* = 1.6 Hz, 1H), 7.31 (s, 1H), 7.26 (dd, *J* = 8.4, 2.0 Hz, 1H), 2.82 (q, *J* = 7.6 Hz, 2H), 1.30 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-*d*$_6$) δ 162.9, 146.7, 137.3, 124.0, 123.0, 122.7, 121.3, 119.6, 114.9, 114.7, 104.3, 21.1, 11.3. HRMS (ESI): m/z calcd for $C_{13}H_{11}BrN_2O$ ([M + H]$^+$) 291.0128, Found 291.0119.

*1.31 2-ethyl-5-(5-methyl-1H-indol-3-yl)oxazole (**8k**)*: Yellow solid; Yield: 45%. m.p.: 168.4 – 169.9 °C. ^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 11.40 (s, 1H), 7.66 (d, *J* = 2.8 Hz, 1H), 7.60 (dd, *J* = 1.6, 0.8 Hz, 1H), 7.36 – 7.30 (m, 1H), 7.25 (d, *J* = 9.6 Hz, 1H), 7.05 – 6.98 (m, 1H), 2.81 (q, *J* = 7.6 Hz, 2H), 2.43 (s, 3H), 1.30 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-*d*$_6$) δ 162.5, 147.5, 134.8, 128.8, 123.9, 123.8, 123.0, 119.2, 119.0, 111.8, 103.6, 21.4, 21.1, 11.3. HRMS (ESI): m/z calcd for $C_{14}H_{14}N_2O$ ([M + H]$^+$) 227.1179, Found 227.1173.

*1.32 4-chloro-5-(5-fluoro-1H-indol-3-yl)-2-methyloxazole (**9a**)*: White solid; Yield: 30%. m.p.: 193.3 – 194.1 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 10.89 (s, 1H), 8.00 (dd, J = 8.8, 5.6 Hz, 1H), 7.94 – 7.86 (m, 1H), 7.28 (dd, J = 10.0, 2.4 Hz, 1H), 7.01 (ddd, J = 9.6, 8.8, 2.4 Hz, 1H), 2.54 (s, 3H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 160.1 (d, J = 236.8 Hz), 158.3, 142.2, 136.3 (d, J = 12.8 Hz), 124.2 (d, J = 3.3 Hz), 121.5 (d, J = 10.2 Hz), 121.3, 121.0, 108.9 (d, J = 24.7 Hz), 103.1, 97.9 (d, J = 26.2 Hz), 13.1. HRMS (ESI): m/z calcd for $C_{12}H_8ClFN_2O$ ([M + H]$^+$) 251.0382, Found 251.0388.

*1.33 4-chloro-5-(5-chloro-1H-indol-3-yl)-2-methyloxazole (**9b**)*: White solid; Yield: 35%. m.p.: 178.6-179.7 – 194.1 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 10.95 (s, 1H), 7.99 (d, J = 8.8 Hz, 1H), 7.92 (d, J = 2.8 Hz, 1H), 7.63 – 7.54 (m, 1H), 7.23 – 7.15 (m, 1H), 2.54 (s, 3H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 158.4, 142.0, 136.7, 128.0, 124.6, 124.4, 123.2, 121.6, 120.8, 111.7, 103.2, 13.2. HRMS (ESI): m/z calcd for $C_{12}H_8Cl_2N_2O$ ([M + H]$^+$) 267.0086, Found 267.0086.

*1.34 5-(5-bromo-1H-indol-3-yl)-4-chloro-2-methyloxazole (**9c**)*: White solid; Yield: 42%. m.p.: 221.2 – 222.6 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 11.02 (s, 1H), 8.16 (d, J = 2.0 Hz, 1H), 7.95 (d, J = 2.8 Hz, 1H), 7.52 (d, J = 8.8 Hz, 1H), 7.37 (dd, J = 8.8, 2.0 Hz, 1H), 2.56 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 159.0, 141.9, 135.1, 126.1, 125.9, 125.4, 122.4, 120.7, 114.7, 113.3, 101.8, 14.3. HRMS (ESI): m/z calcd for $C_{12}H_8BrClN_2O$ ([M + H]$^+$) 310.9581, Found 310.9592.

*1.35 4-chloro-5-(6-fluoro-1H-indol-3-yl)-2-methyloxazole (**9d**)*: White solid; Yield: 39%. m.p.: 203.1 – 204.9 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.79 (s, 1H), 7.89 (dd, *J* = 19.6, 11.6 Hz, 2H), 7.29 (d, *J* = 9.6 Hz, 1H), 7.03 (t, *J* = 8.8 Hz, 1H), 2.52 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.3, 158.5, 158.4, 141.9, 136.0 (d, *J* = 12.8 Hz), 124.8 (d, *J* = 3.4 Hz), 121.2 (d, *J* = 10.4 Hz), 120.6 (d, *J* = 83.7 Hz), 108.9 (d, *J* = 24.6 Hz), 101.9, 98.2 (d, *J* = 25.9 Hz), 13.9. HRMS (ESI): m/z calcd for $C_{12}H_8ClFN_2O$ ([M + H]$^+$) 251.0382, Found 251.0377.

*1.36 4-chloro-2-ethyl-5-(6-fluoro-1H-indol-3-yl)oxazole (**9e**)*: White solid; Yield: 52%. m.p.: 189.2 – 191.2 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.85 (s, 1H), 7.91 – 7.88 (m, 2H), 7.55 (dd, *J* = 2.0, 0.4 Hz, 1H), 7.18 (dd, *J* = 8.8, 2.0 Hz, 1H), 2.90 – 2.84 (q, 2H), 1.33 – 1.28 (t, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.5, 141.6, 136.4, 127.2, 125.2, 122.9, 121.4, 120.7, 120.4, 111.9, 102.1, 21.2, 10.8. HRMS (ESI): m/z calcd for $C_{13}H_{10}ClFN_2O$ ([M + H]$^+$) 265.0538, Found 265.0534.

*1.37 4-chloro-5-(6-chloro-1H-indol-3-yl)-2-methyloxazole (**9f**)*: White solid; Yield: 33%. m.p.: 185.9 – 186.7 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.86 (s, 1H), 7.90 (d, *J* = 8.4 Hz, 2H), 7.56 (s, 1H), 7.18 (d, *J* = 8.0 Hz, 1H), 2.53 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.6, 141.7, 136.4, 127.2, 125.2, 122.8, 121.4, 120.7, 120.4, 111.9, 102.0, 13.9. HRMS (ESI): m/z calcd for $C_{12}H_8Cl_2N_2O$ ([M + H]$^+$) 267.0086, Found 267.0081.

*1.38 4-chloro-5-(6-chloro-1H-indol-3-yl)-2-ethyloxazole (**9g**)*: White solid; Yield: 74%. m.p.: 195.5 – 196.9 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.85 (s, 1H), 7.92 – 7.86 (m, 2H), 7.55 (dd, *J* = 2.0, 0.4 Hz, 1H), 7.23 – 7.15 (m, 1H), 2.87 (q, *J* = 7.6 Hz, 2H), 1.33 – 1.28 (t, 3H). ^{13}C NMR

(100 MHz, DMSO-d_6) δ 162.5, 141.6, 136.4, 127.2, 125.2, 122.9, 121.4, 120.7, 120.4, 111.9, 102.1, 21.2, 10.8. HRMS (ESI): m/z calcd for $C_{13}H_{10}Cl_2N_2O$ ($[M + H]^+$) 281.0243, Found 281.0244.

*1.39 5-(6-bromo-1H-indol-3-yl)-4-chloro-2-ethyloxazole (**9h**)*: White solid; Yield: 60%. m.p.: 203.4–204.7 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.86 (s, 1H), 7.89 (d, J = 1.6 Hz, 1H), 7.84 (d, J = 8.8 Hz, 1H), 7.69 (d, J = 1.6 Hz, 1H), 7.29 (d, J = 8.4 Hz, 1H), 2.87 (q, J = 14.0, 7.2 Hz, 2H), 1.30 (t, J = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.6, 141.5, 136.8, 125.1, 123.3, 123.1, 121.7, 120.4, 115.2, 114.9, 102.1, 21.2, 10.8. HRMS (ESI): m/z calcd for $C_{13}H_{10}BrClN_2O$ ($[M + H]^+$) 324.9738, Found 324.9736.

*1.40 4-chloro-2-ethyl-5-(5-methyl-1H-indol-3-yl) oxazole (**9i**)*: White solid; Yield: 41%. m.p.: 191.5 – 192.9 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.61 (s, 1H), 7.78 (d, J = 2.8 Hz, 1H), 7.67 (d, J = 0.8 Hz, 1H), 7.38 (d, J = 8.4 Hz, 1H), 7.04 (dd, J = 8.4, 1.6 Hz, 1H), 2.87 (q, J = 7.6 Hz, 2H), 2.42 (s, 3H), 1.31 (t, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.2, 142.3, 134.3, 129.0, 124.4, 124.2, 124.1, 119.8, 119.5, 111.9, 101.3, 21.5, 21.2, 10.9. HRMS (ESI): m/z calcd for $C_{14}H_{13}ClN_2O$ ($[M + H]^+$) 261.0789, Found 261.0787.

*1.41 4-bromo-5-(5-fluoro-1H-indol-3-yl)-2-methyloxazole (**10a**)*: White solid; Yield: 41%. m.p.: 178.6 – 179.8 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 10.89 (s, 1H), 8.04 – 7.98 (m, 2H), 7.29 (dd, J = 9.6, 2.4 Hz, 1H), 7.01 (td, J = 9.2, 2.4 Hz, 1H), 2.55 (s, 3H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 160.1 (d, J = 236.8 Hz), 159.2, 144.6, 136.3 (d, J = 12.8 Hz), 124.5 (d, J = 3.3 Hz), 121.6 (d, J = 10.1 Hz), 121.5, 108.9 (d, J = 24.6 Hz), 107.7, 103.3, 97.9 (d, J = 26.2 Hz), 13.1. HRMS (ESI): m/z calcd for $C_{12}H_8BrFN_2O$ ($[M + H]^+$) 294.9877, Found 294.9880.

*1.42 4-bromo-5-(5-chloro-1H-indol-3-yl)-2-methyloxazole (**10b**)*: White solid; Yield: 43%. m.p.: 178.6 – 179.7 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 10.94 (s, 1H), 8.04 – 7.98 (m, 2H), 7.59 (d, J = 2.0 Hz, 1H), 7.19 (dd, J = 8.4, 2.0 Hz, 1H), 2.55 (s, 3H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 159.4, 144.5, 136.5, 128.0, 124.9, 124.7, 121.7, 120.8, 111.7, 107.8, 103.3, 13.1. HRMS (ESI): m/z calcd for $C_{12}H_8BrClN_2O$ ($[M + H]^+$) 310.9581, Found 310.9586.

*1.43 4-bromo-5-(5-bromo-1H-indol-3-yl)-2-methyloxazole (**10c**)*: Yellow solid; Yield: 56%. m.p.: 183.5 – 185.2 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 11.02 (s, 1H), 8.16 (d, J = 2.0 Hz, 1H), 8.05 (d, J = 2.8 Hz, 1H), 7.52 (d, J = 8.8 Hz, 1H), 7.37 (dd, J = 8.8, 2.0 Hz, 1H), 2.58 (s, 3H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 160.1, 145.2, 137.3 (d, J = 15.6 Hz), 128.7, 125.5 (d, J = 16.4 Hz), 124.1, 122.4, 121.5, 112.4 (d, J = 5.2 Hz), 108.5, 104.0 (d, J = 4.8 Hz), 13.8. HRMS (ESI): m/z calcd for $C_{12}H_8Br_2N_2O$ ($[M + H]^+$) 354.9076, Found 354.9079.

*1.44 4-bromo-2-methyl-5-(4-methyl-1H-indol-3-yl)oxazole (**10d**)*: White solid; Yield: 49%. m.p.: 151.0–151.9 °C. ^{1}H NMR (400 MHz, Acetone-d_6) δ 10.81 (s, 1H), 7.64 (d, J = 2.8 Hz, 1H), 7.38 (d, J = 8.4 Hz, 1H), 7.11 (t, J = 7.6 Hz, 1H), 6.91 (d, J = 7.2 Hz, 1H), 2.51 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, Acetone-d_6) δ 160.5, 144.2, 136.6, 129.7, 127.3, 125.6, 122.5, 121.6, 113.5, 109.8, 101.3, 18.9, 13.3. HRMS (ESI): m/z calcd for $C_{13}H_{11}BrN_2O$ ($[M + H]^+$) 291.0128, Found 291.0123.

*1.45 4-bromo-5-(6-fluoro-1H-indol-3-yl)-2-methyloxazole (**10e**)*: White solid; Yield: 66%. m.p.: 198.8–199.4 °C. ^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 11.77 (s, 1H), 7.93 – 7.87 (m, 2H), 7.29 (dd, *J* = 10.0, 2.4 Hz, 1H), 7.06 – 6.99 (m, 1H), 2.53 (s, 3H). ^{13}C NMR (100 MHz, DMSO-*d*$_6$) δ 159.4, 159.4 (d, *J* = 236.2 Hz), 144.3, 136.0 (d, *J* = 12.9 Hz), 124.9 (d, *J* = 3.4 Hz), 121.3 (d, *J* = 10.3 Hz), 121.1, 108.9 (d, *J* = 24.5 Hz), 107.4, 102.2, 98.2 (d, *J* = 25.8 Hz), 13.8. HRMS (ESI): m/z calcd for $C_{12}H_8BrFN_2O$ ([M + H]$^+$) 294.9877, Found 294.9877.

*1.46 4-bromo-2-ethyl-5-(6-fluoro-1H-indol-3-yl) oxazole (**10f**)*: White solid; Yield: 37%. m.p.: 163.1–163.9 °C. ^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 11.84 (s, 1H), 7.95 (d, *J* = 2.8 Hz, 1H), 7.89 (d, *J* = 8.8 Hz, 1H), 7.55 (d, *J* = 1.6 Hz, 1H), 7.18 (dd, *J* = 8.8, 2.0 Hz, 1H), 2.88 (q, *J* = 7.6 Hz, 2H), 1.30 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-*d*$_6$) δ 163.3, 159.4 (d, *J* = 236.1 Hz), 144.2, 136.0 (d, *J* = 12.8 Hz), 124.9 (d, *J* = 3.4 Hz), 121.3 (d, *J* = 10.3 Hz), 121.1, 109.0 (d, *J* = 24.6 Hz), 107.4, 102.2, 98.3 (d, *J* = 25.7 Hz), 21.2, 10.9. HRMS (ESI): m/z calcd for $C_{13}H_{10}BrFN_2O$ ([M + H]$^+$) 309.0033, Found 309.0027.

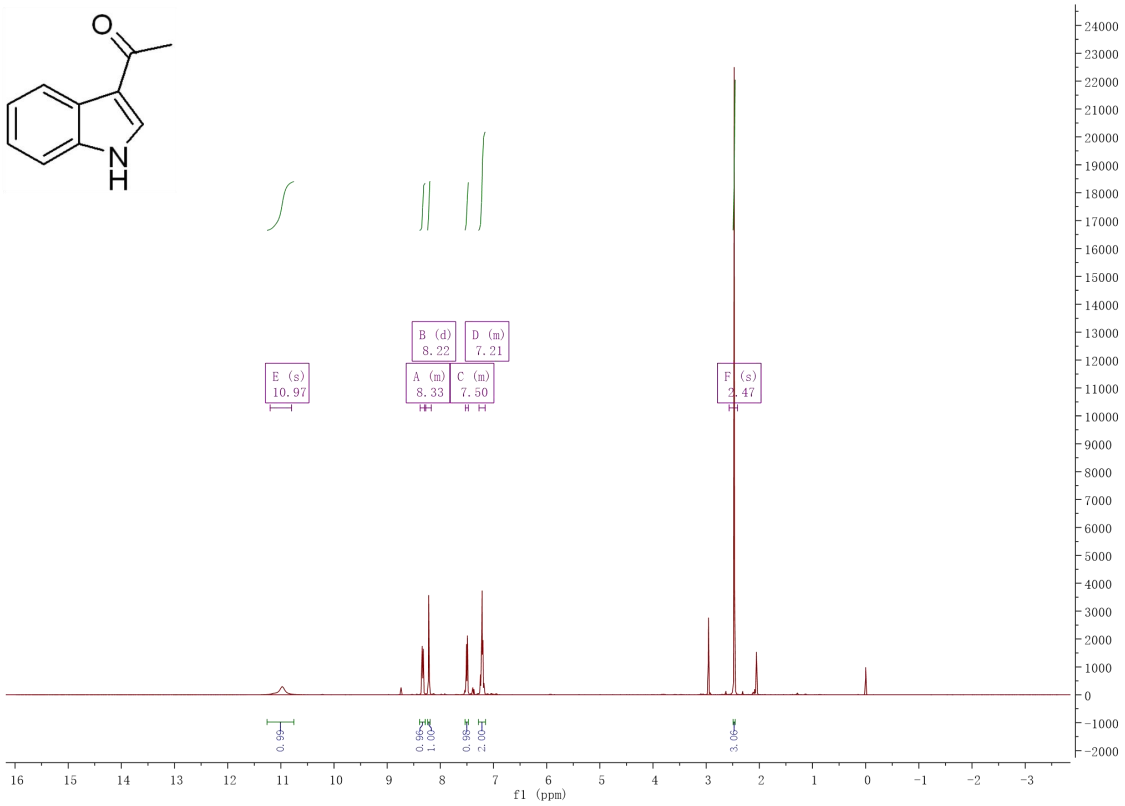
*1.47 4-bromo-5-(6-chloro-1H-indol-3-yl)-2-methyloxazole (**10g**)*: White solid; Yield: 68%. m.p.: 186.1–187.5 °C. ^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 11.84 (s, 1H), 7.93 (dd, *J* = 24.4, 6.0 Hz, 2H), 7.55 (d, *J* = 2.4 Hz, 1H), 7.18 (dd, *J* = 8.8, 2.4 Hz, 1H), 2.53 (s, 3H). ^{13}C NMR (100 MHz, DMSO-*d*$_6$) δ 159.5, 144.1, 136.4, 127.2, 125.3, 123.0, 121.5, 120.7, 111.9, 107.6, 102.3, 13.8. HRMS (ESI): m/z calcd for $C_{12}H_8BrClN_2O$ ([M + H]$^+$) 310.9581, Found 310.9579.

*1.48 4-bromo-5-(6-chloro-1H-indol-3-yl)-2-ethyloxazole (**10h**)*: White solid; Yield: 54%. m.p.: 176.2 – 177.4 °C. ^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 11.84 (s, 1H), 7.96 (d, *J* = 2.8 Hz, 1H), 7.89 (d, *J* = 8.8 Hz, 1H), 7.55 (d, *J* = 1.6 Hz, 1H), 7.18 (dd, *J* = 8.8, 2.0 Hz, 1H), 2.88 (q, *J* = 7.6 Hz, 2H), 1.31 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-*d*$_6$) δ 163.5, 144.0, 136.4, 127.2, 125.3, 123.0, 121.5, 120.7, 111.9, 107.6, 102.3, 21.2, 10.9. HRMS (ESI): m/z calcd for $C_{13}H_{10}BrClN_2O$ ([M + H]$^+$) 324.9738, Found 324.9740.

*1.49 4-bromo-5-(6-bromo-1H-indol-3-yl)-2-ethyloxazole (**10i**)*: White solid; Yield: 70%. m.p.: 172.5 – 174.4 °C. ^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 11.85 (s, 1H), 7.96 (d, *J* = 3.2 Hz, 1H), 7.85 (d, *J* = 9.2 Hz, 1H), 7.71 (d, *J* = 2.0 Hz, 1H), 7.30 (dd, *J* = 10.4, 2.0 Hz, 1H), 2.88 (q, *J* = 16.8, 8.0 Hz, 2H), 1.31 (t, *J* = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-*d*$_6$) δ 163.4, 144.0, 136.8, 125.2, 123.3, 123.3, 121.8, 115.2, 114.9, 107.6, 102.3, 21.2, 10.9. HRMS (ESI): m/z calcd for $C_{13}H_{10}Br_2N_2O$ ([M + H]$^+$) 368.9233, Found 368.9234.

2. ^{1}H-NMR

Compound 2



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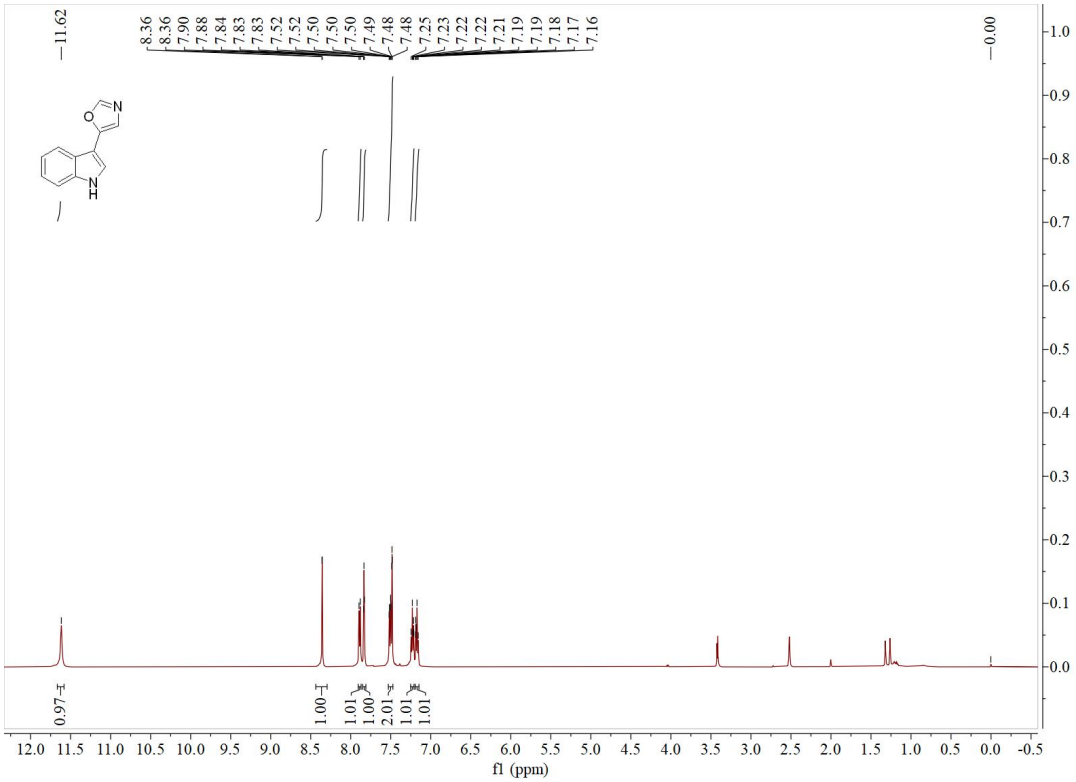
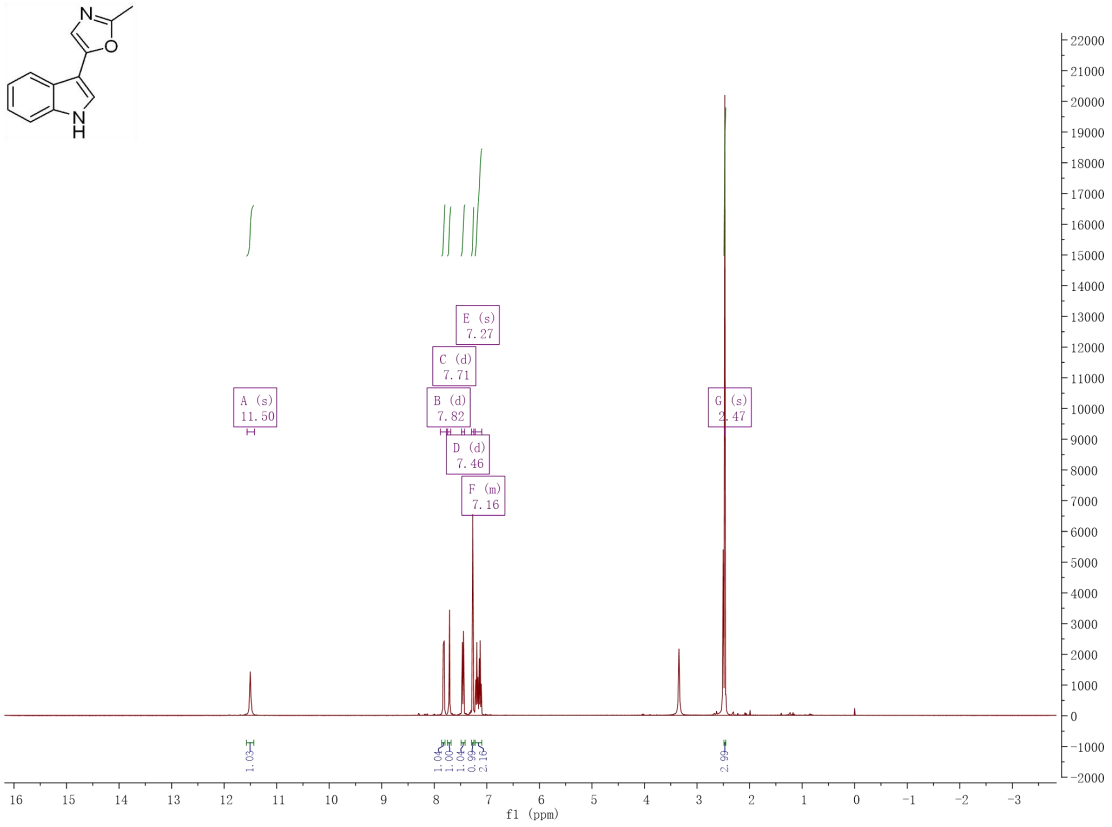
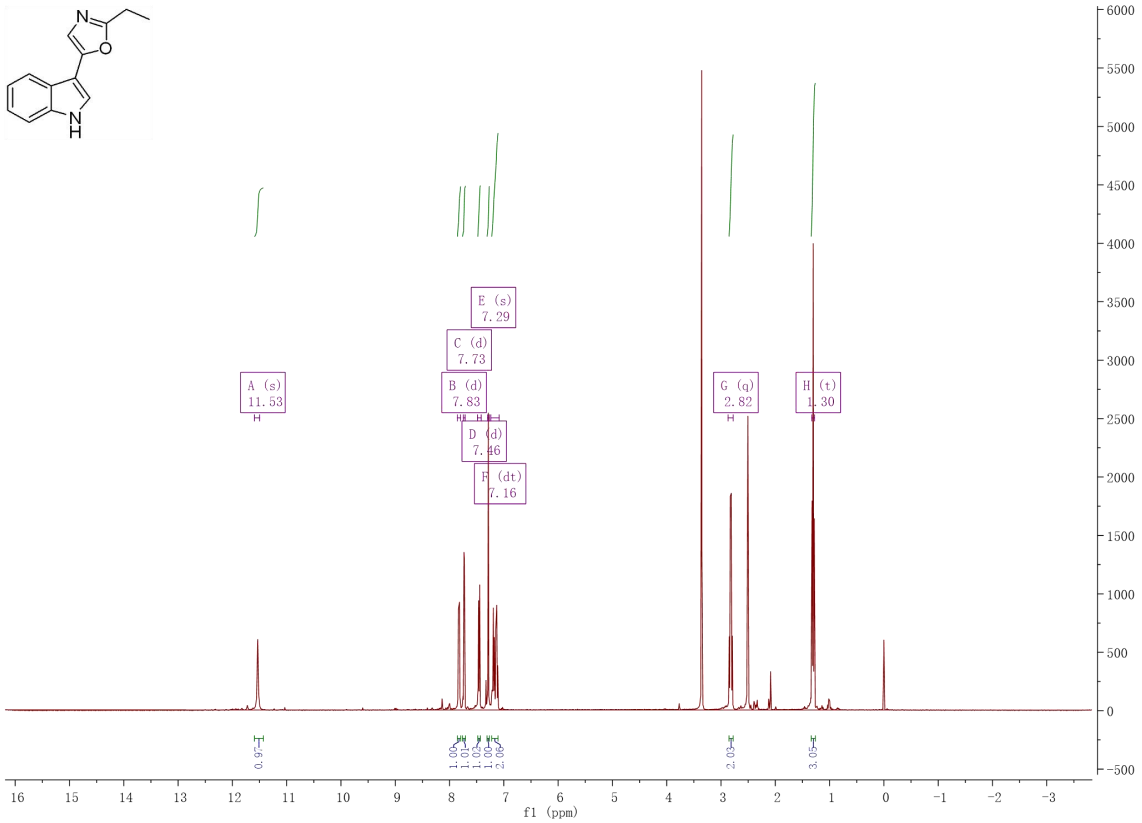


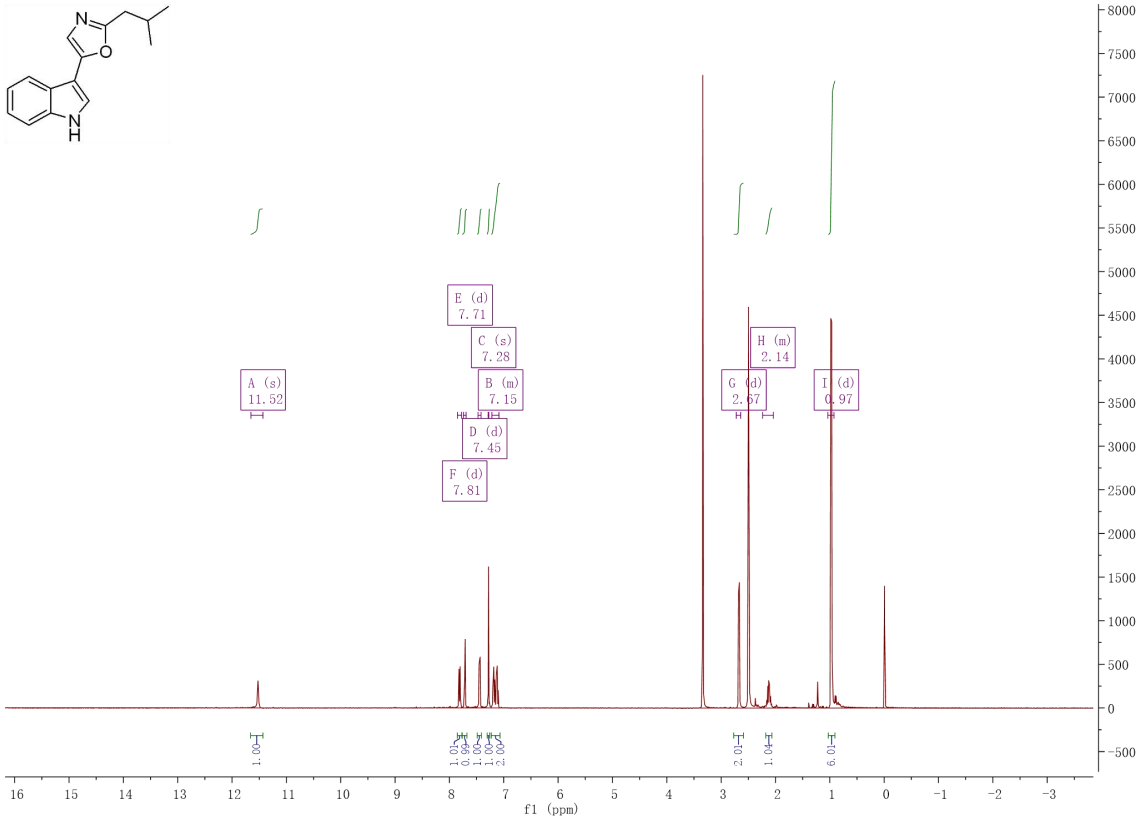
Compound 3b



Compound 3c



Compound 3d



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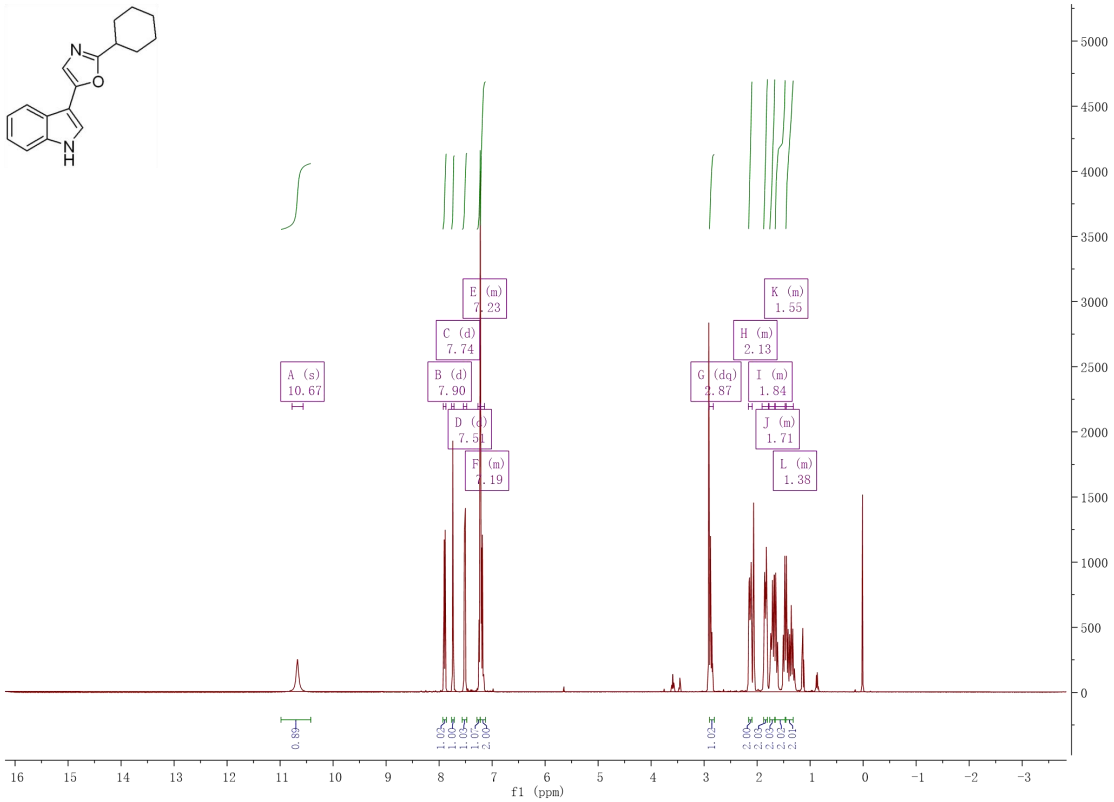
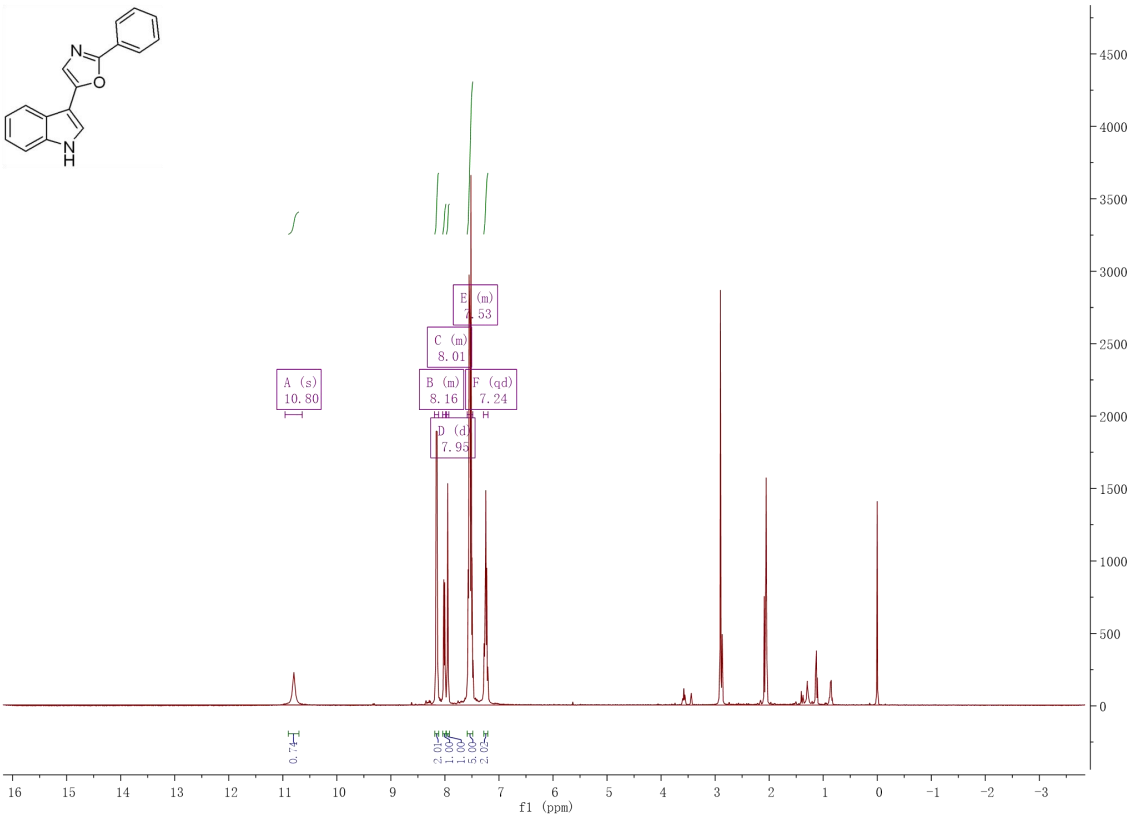
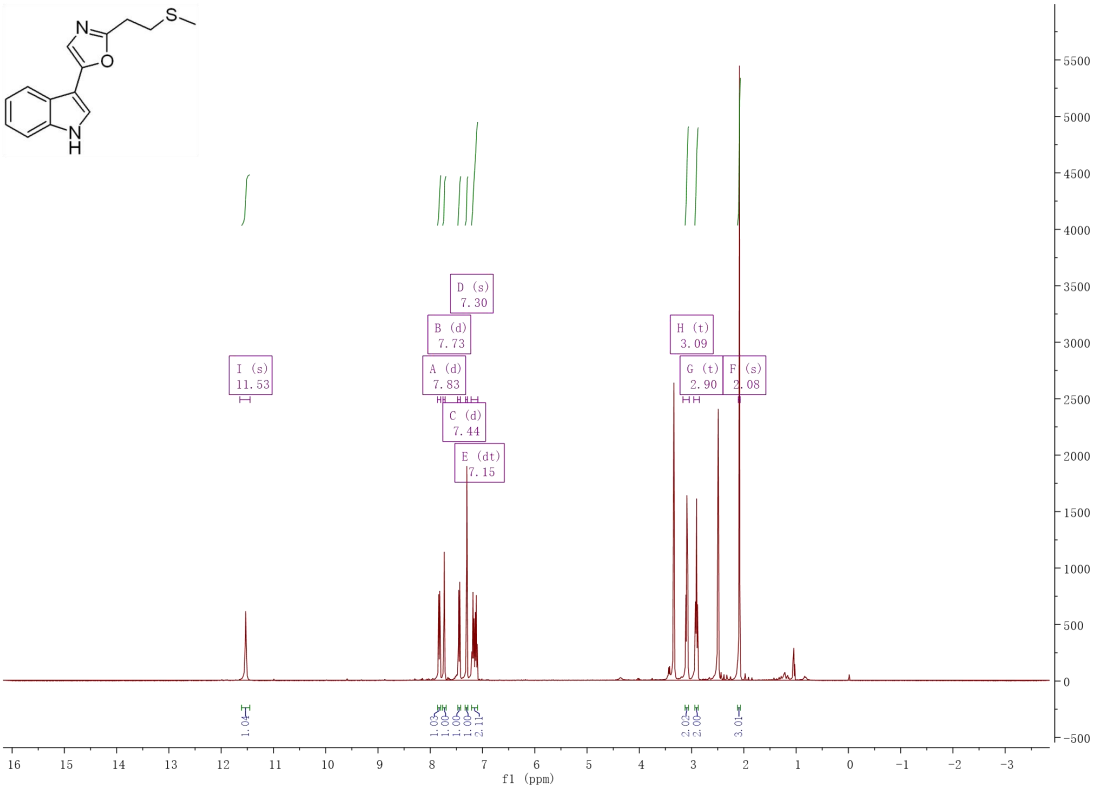


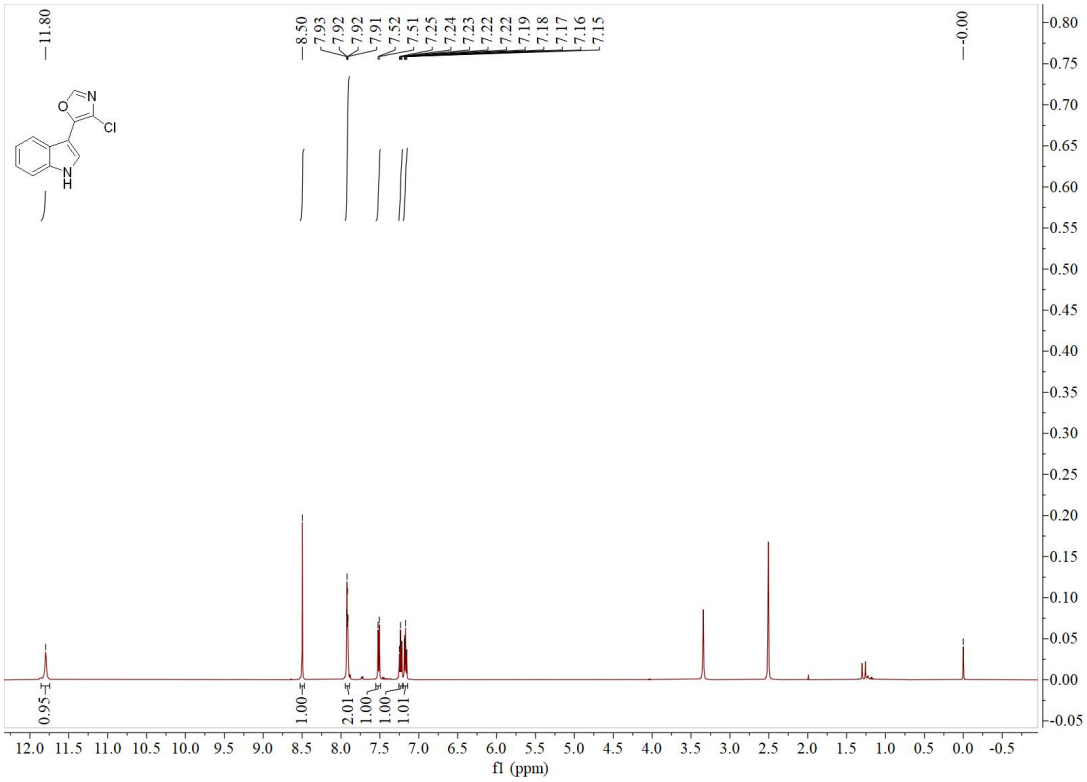
Compound 3f



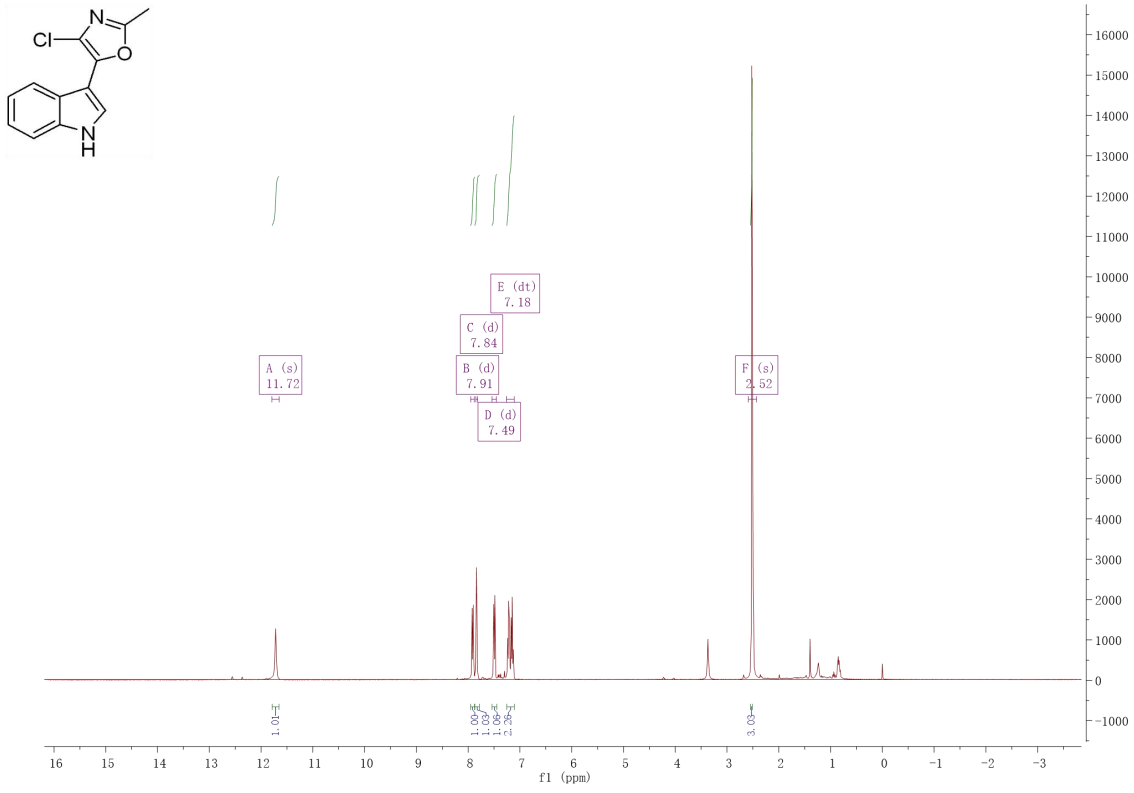
Compound 3g



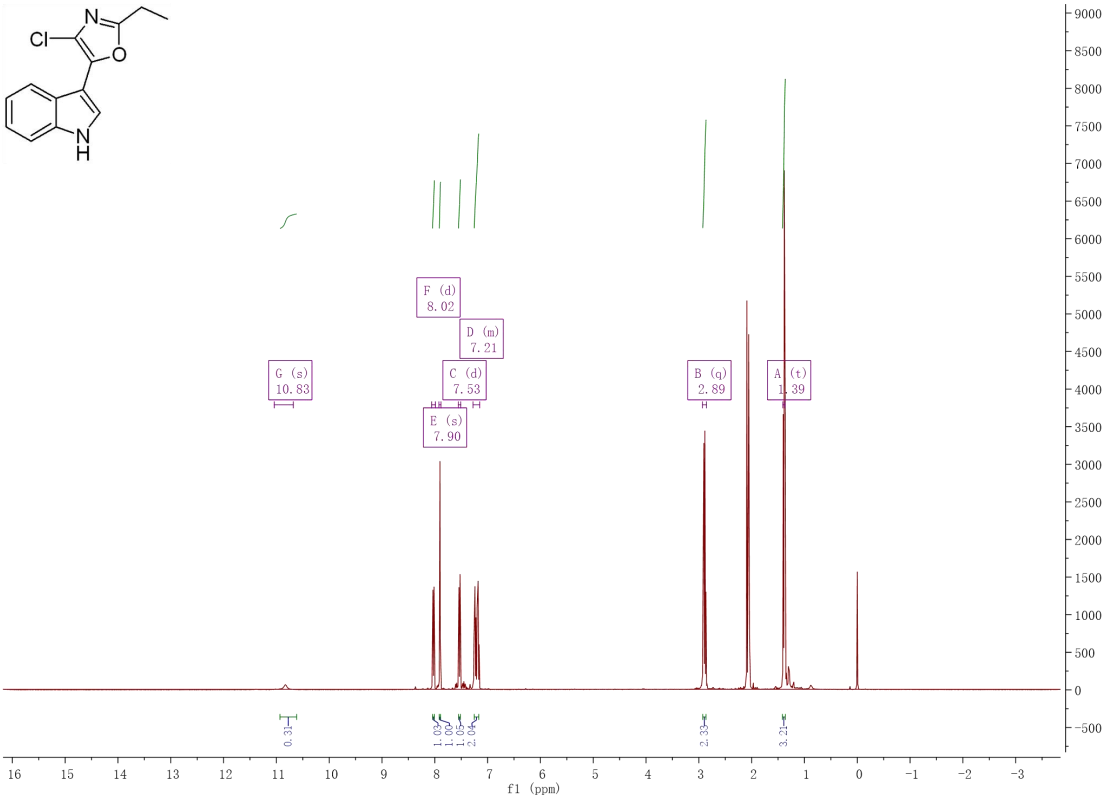
Compound 4a



Compound 4b



Compound 4c



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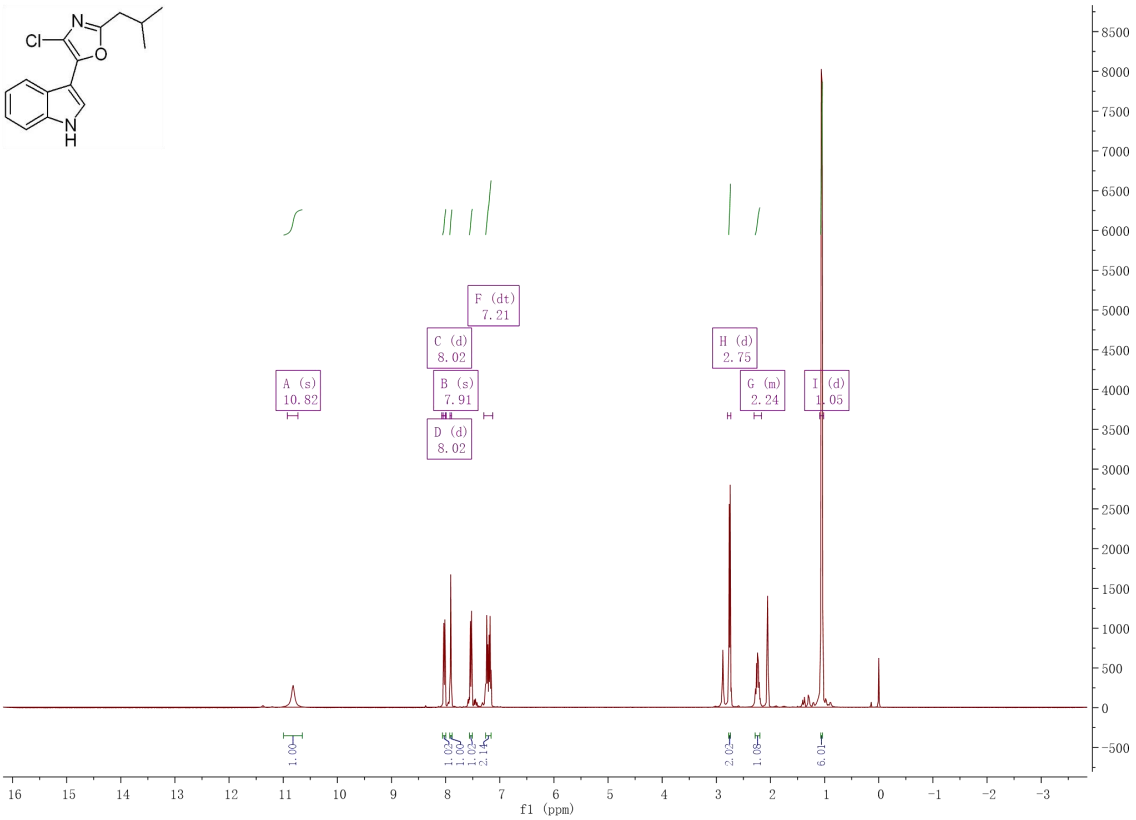

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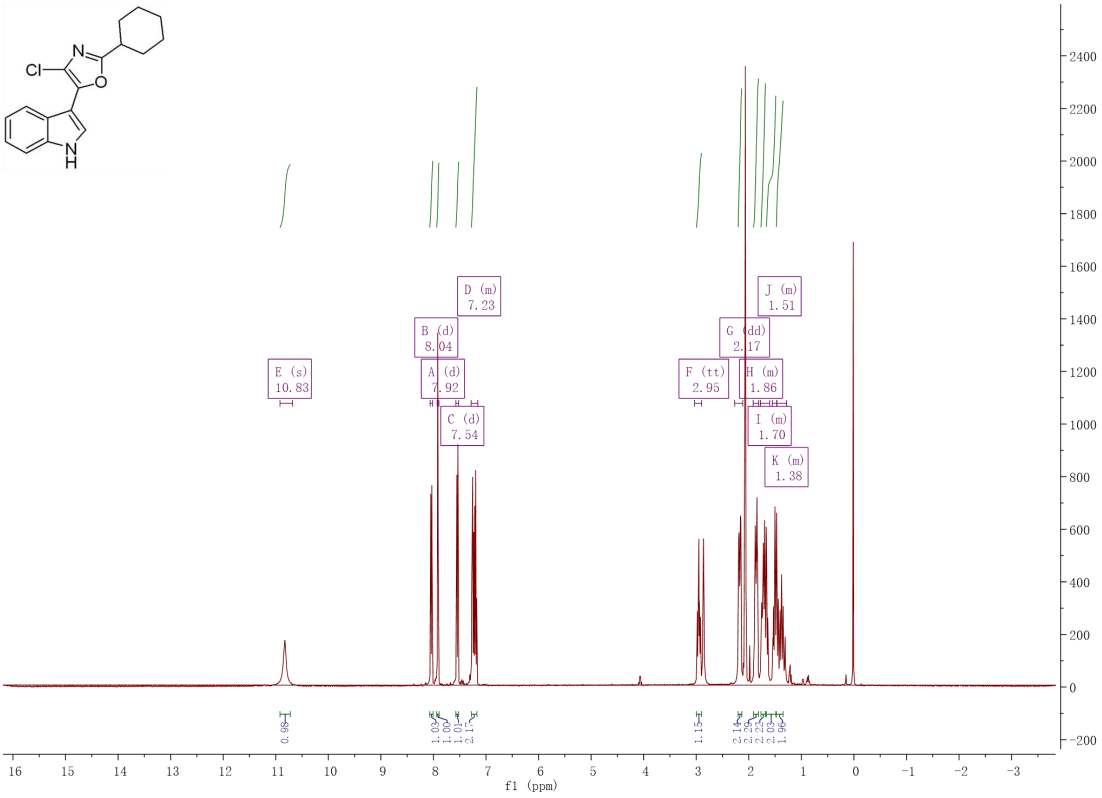

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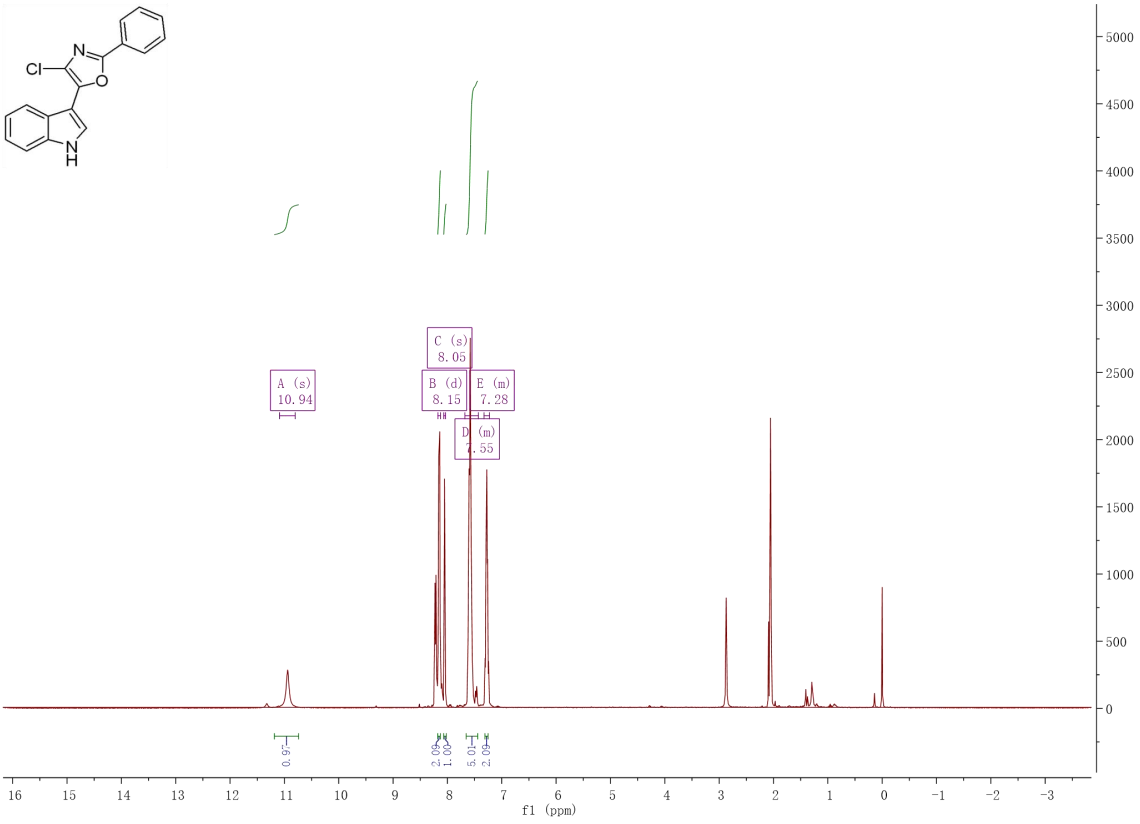
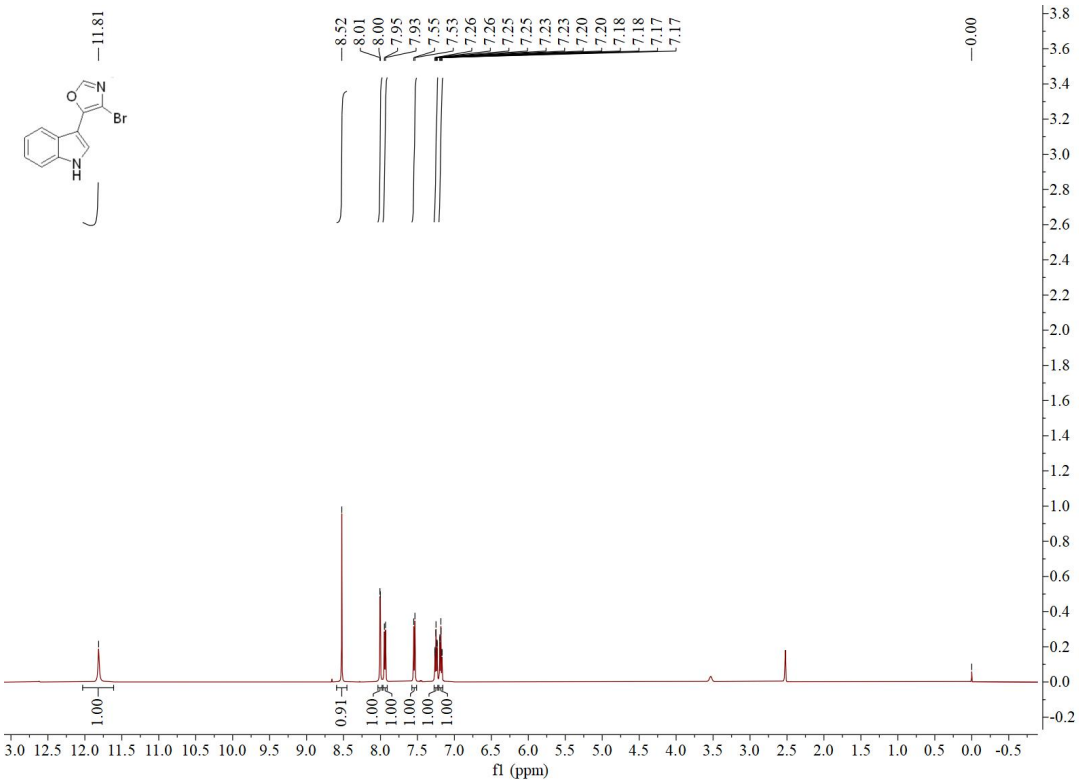


Compound 5a



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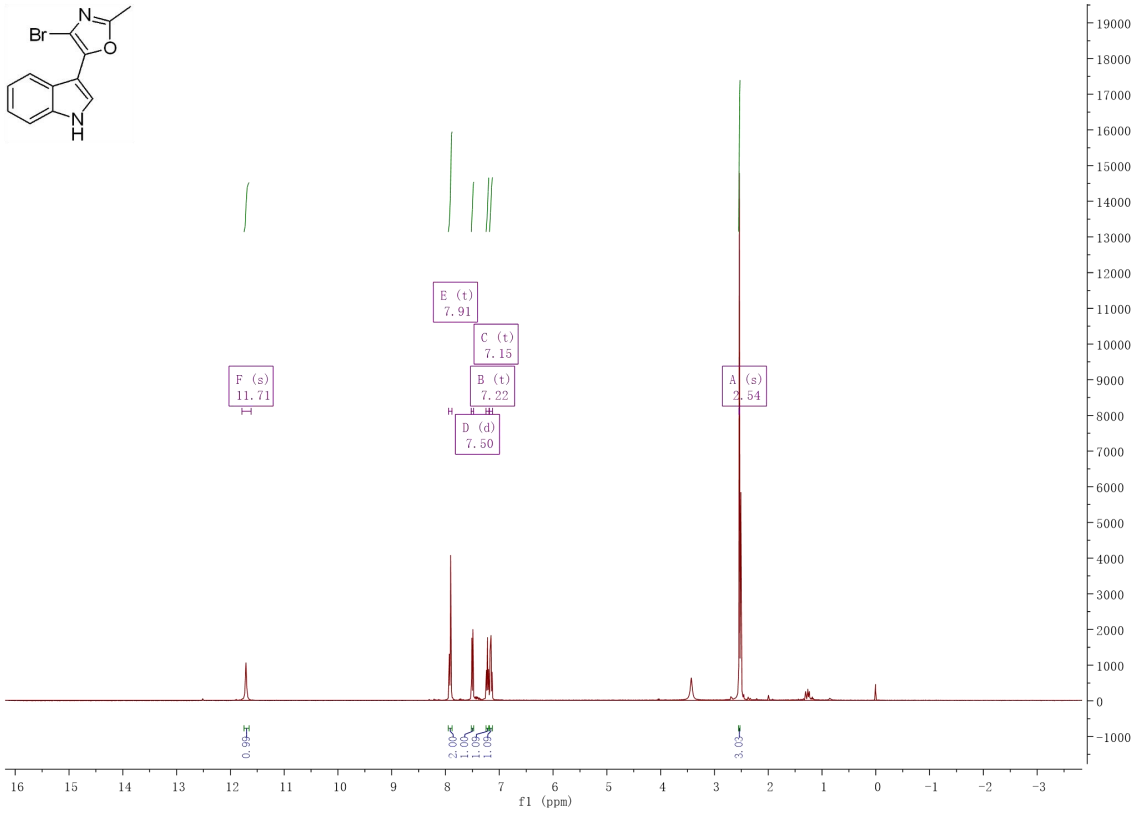

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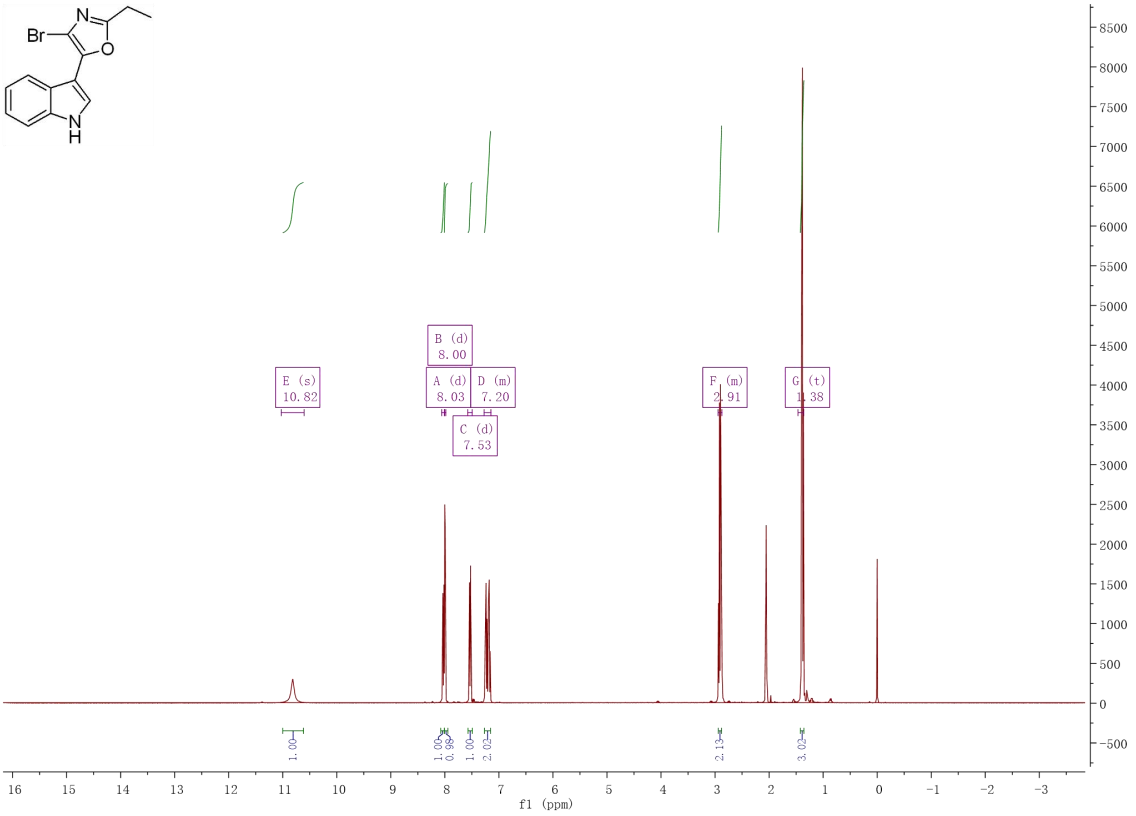

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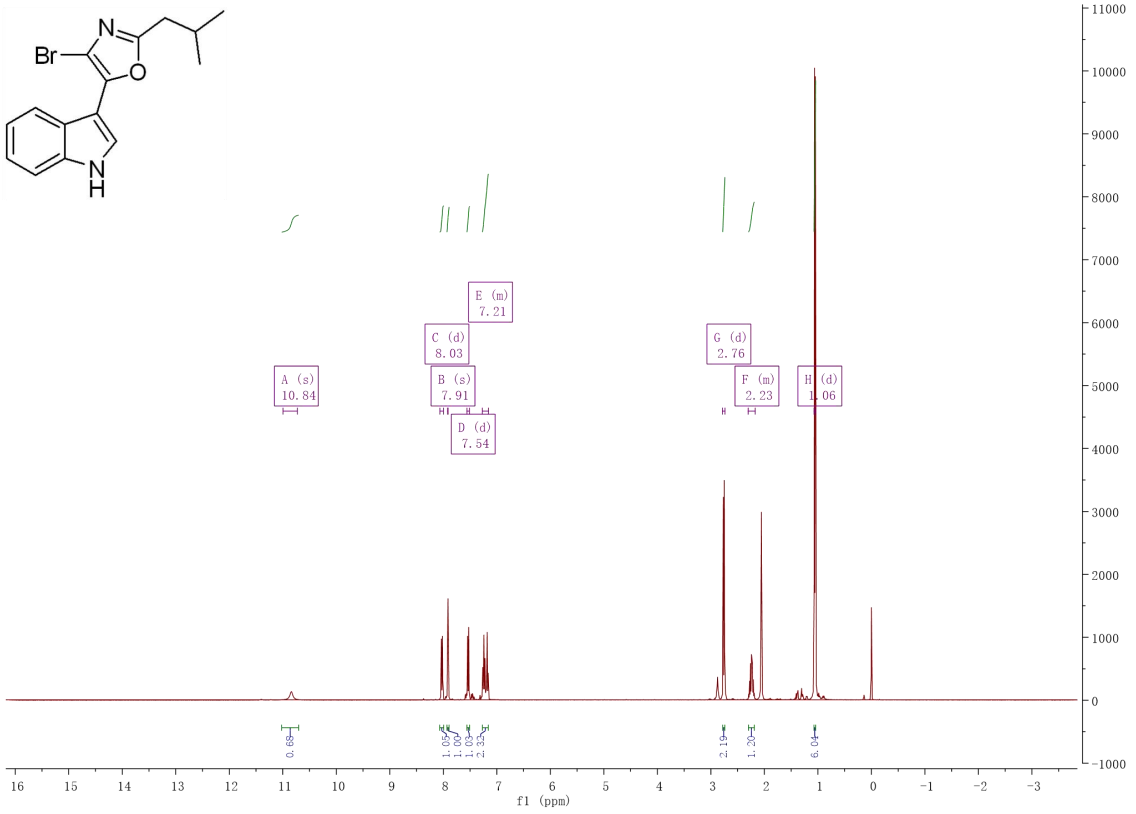

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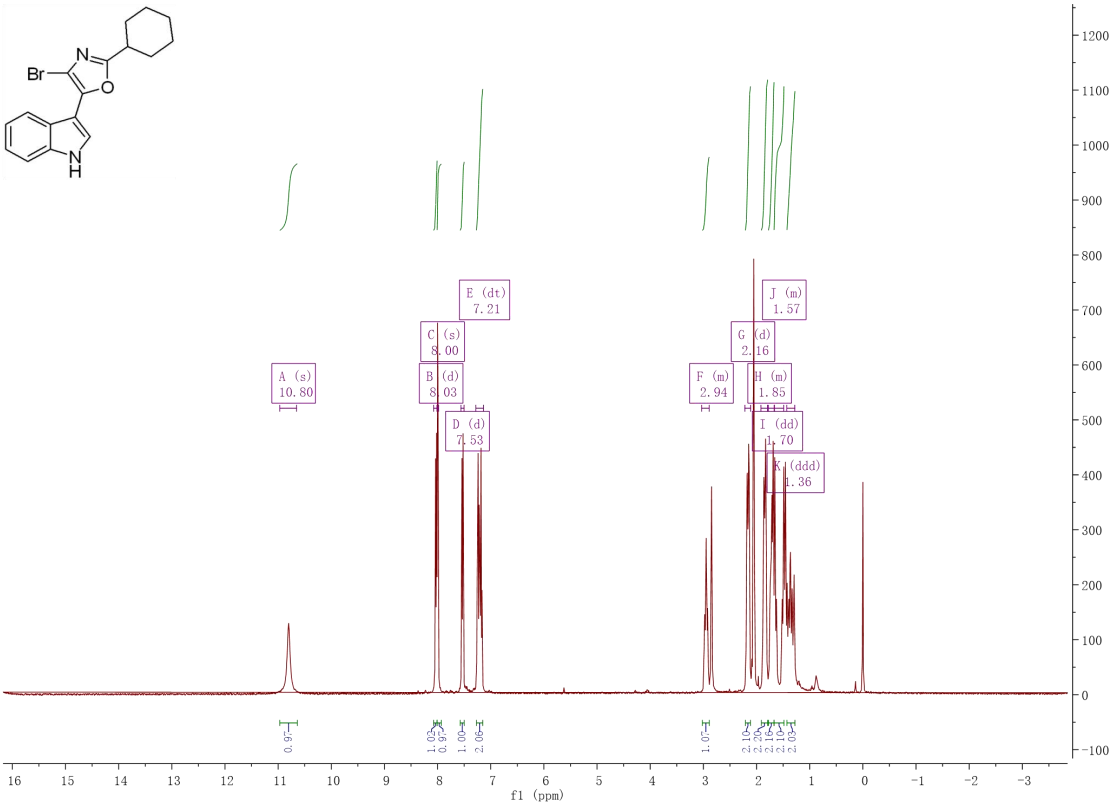

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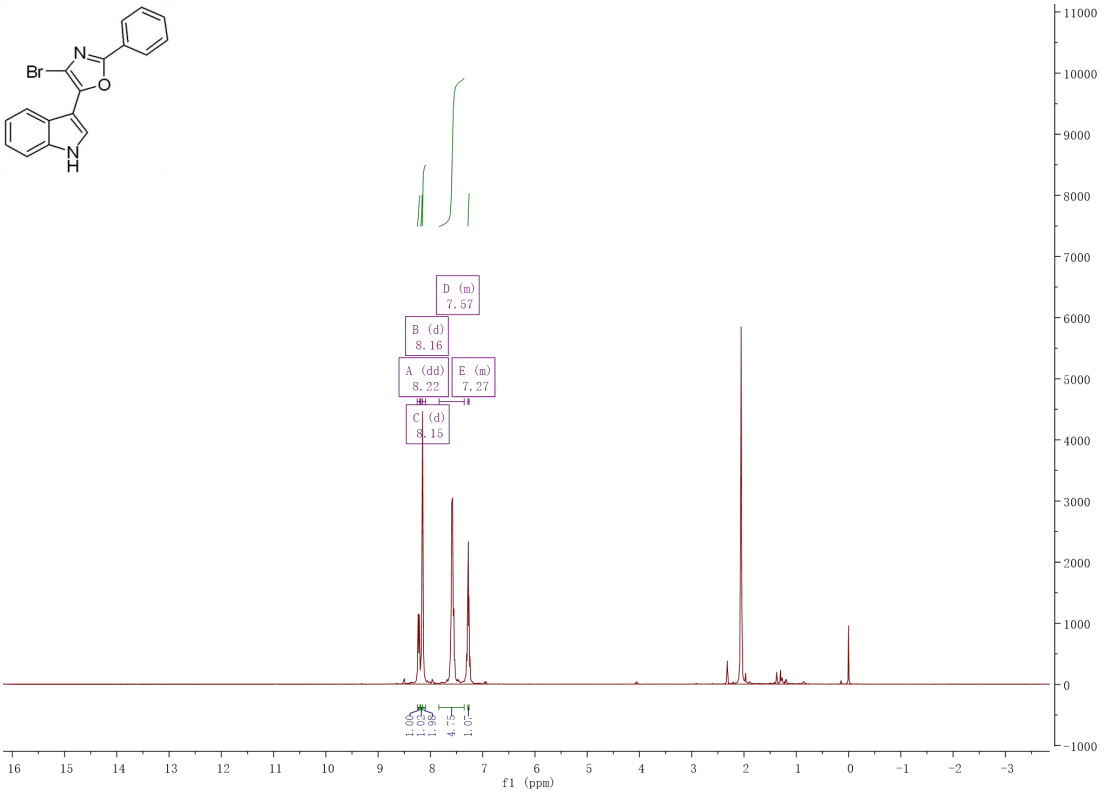
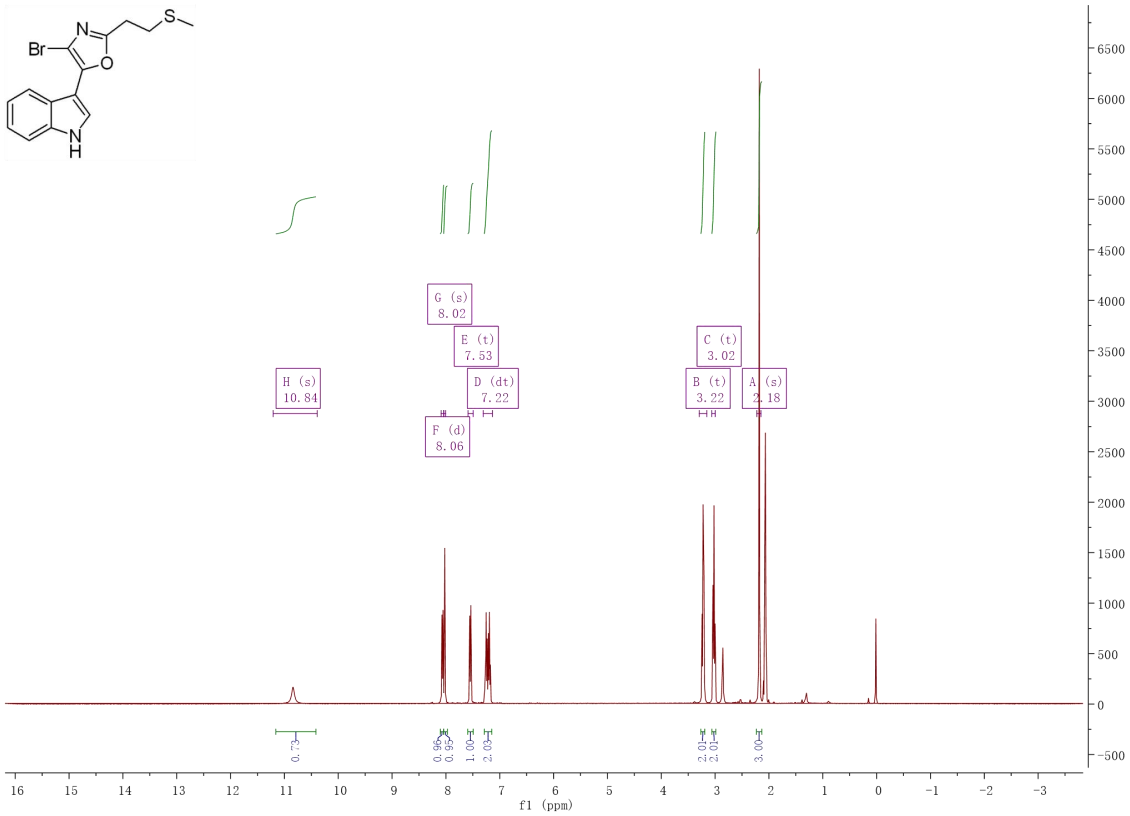
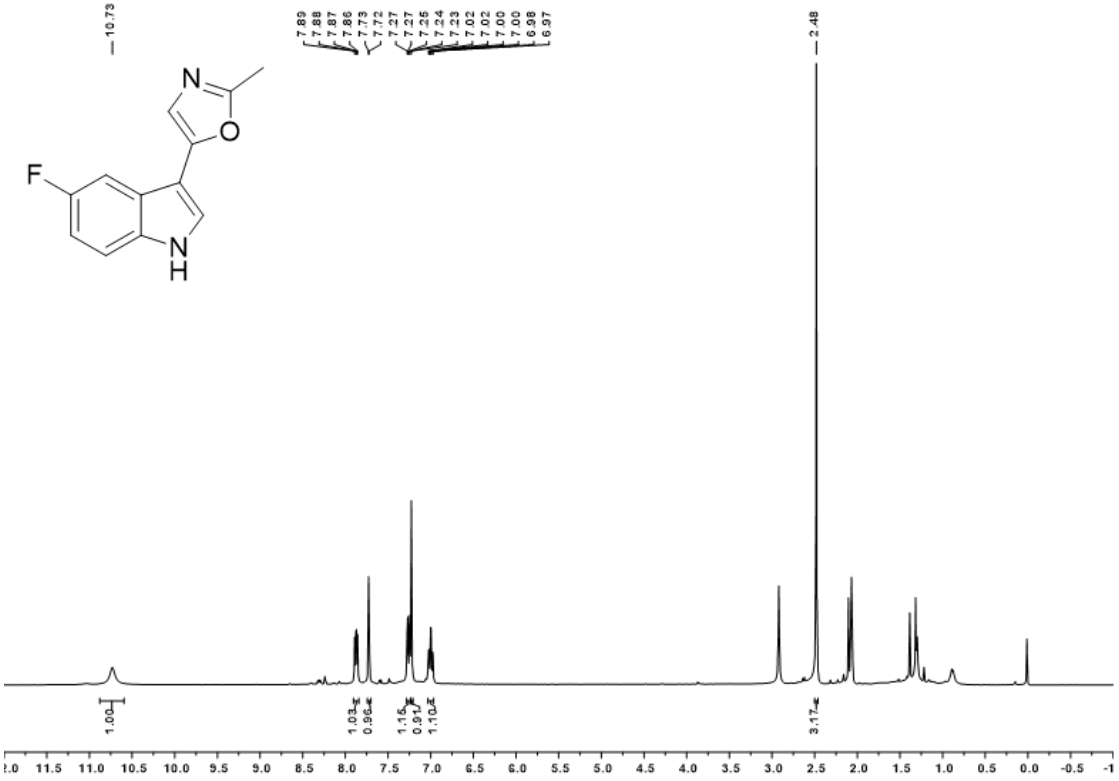


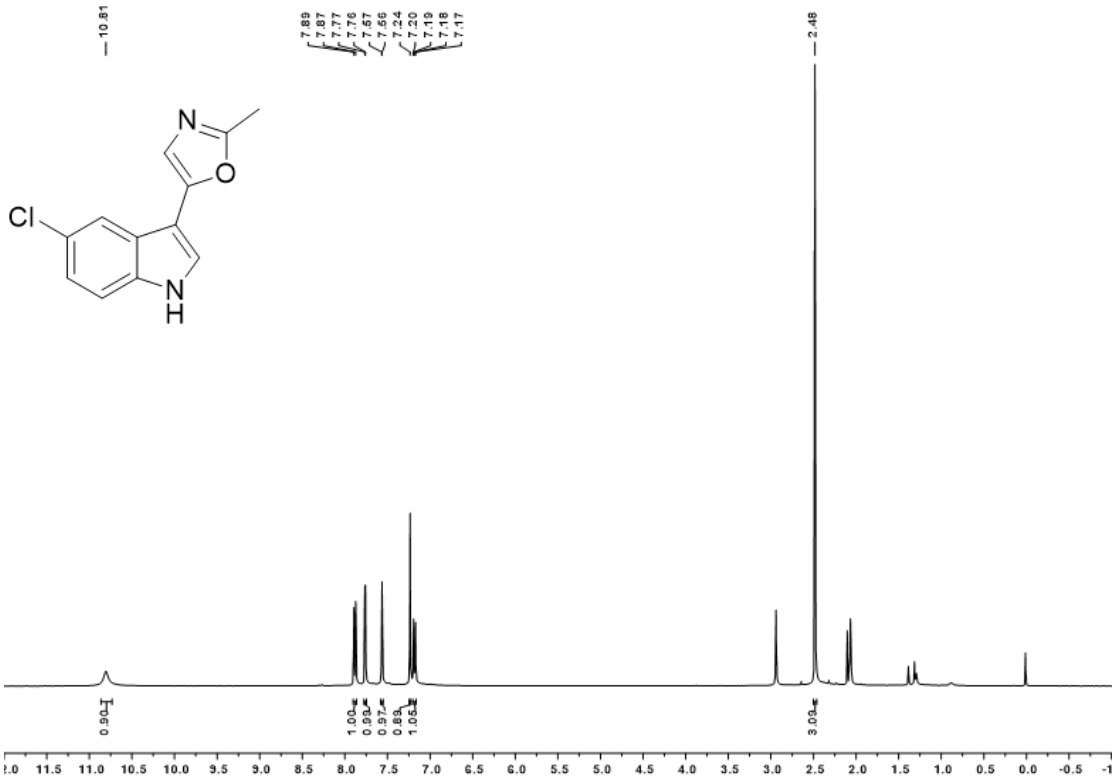
Compound 5g



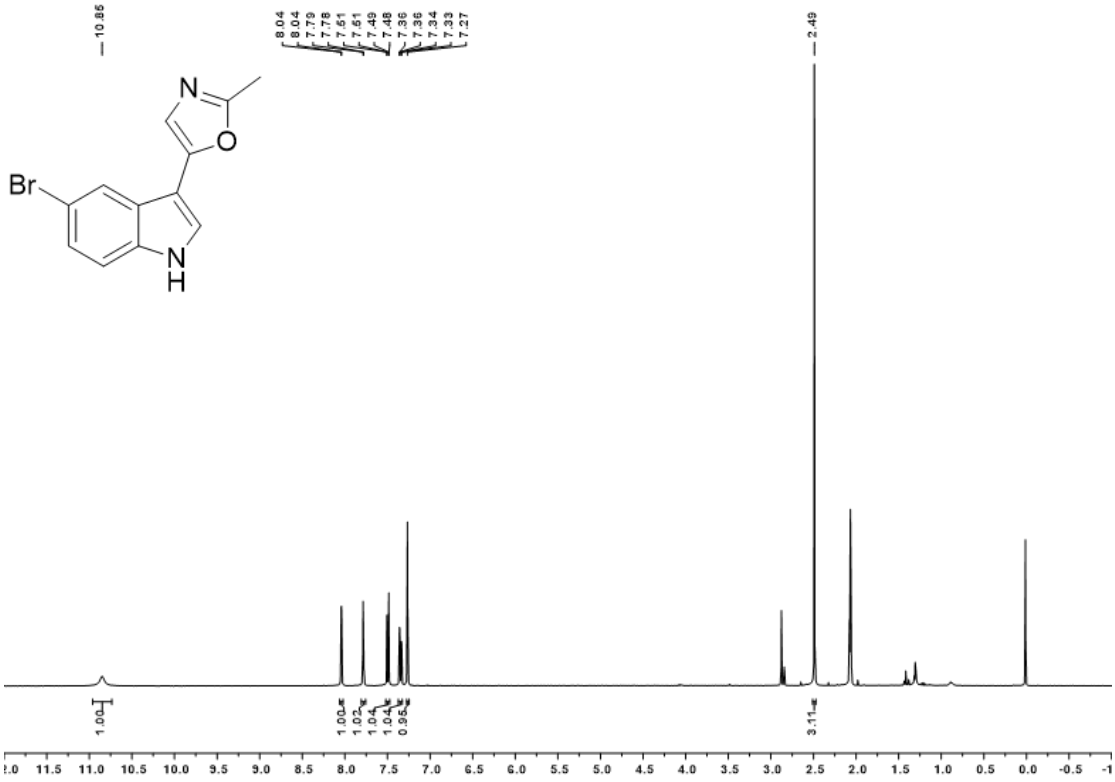
Compound 8a



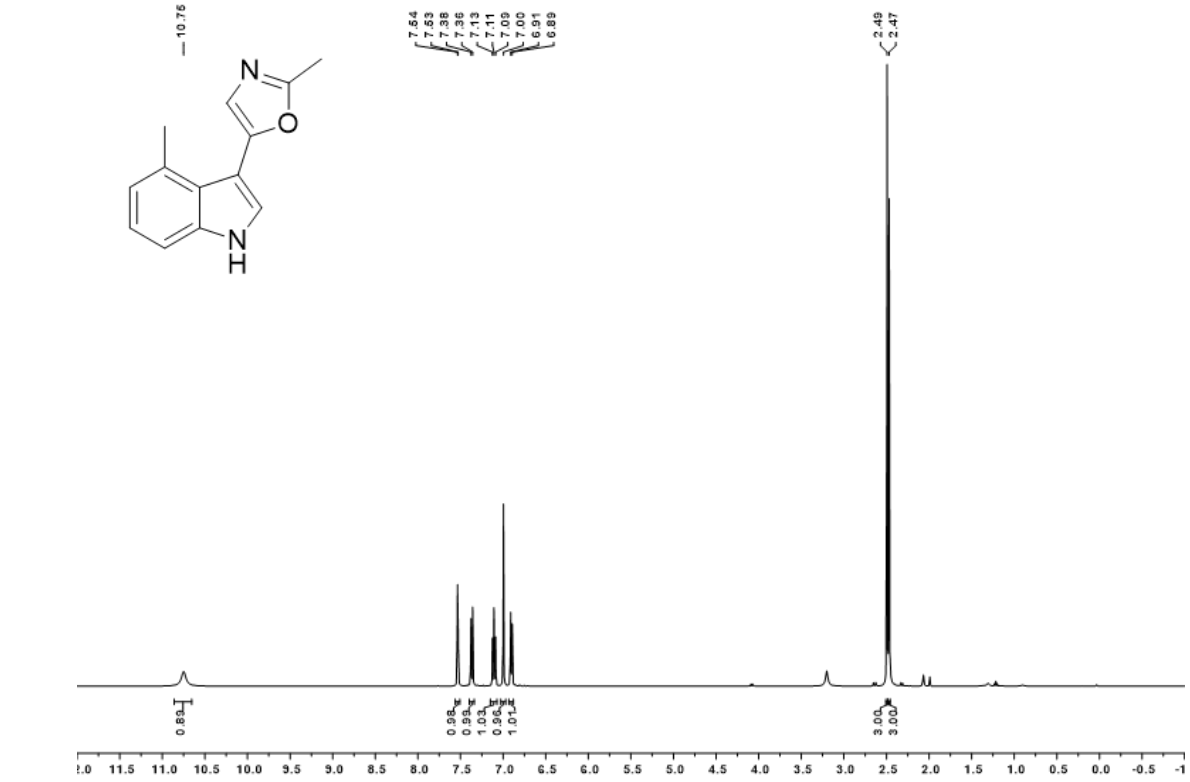
Compound 8b



Compound 8c



Compound 8d



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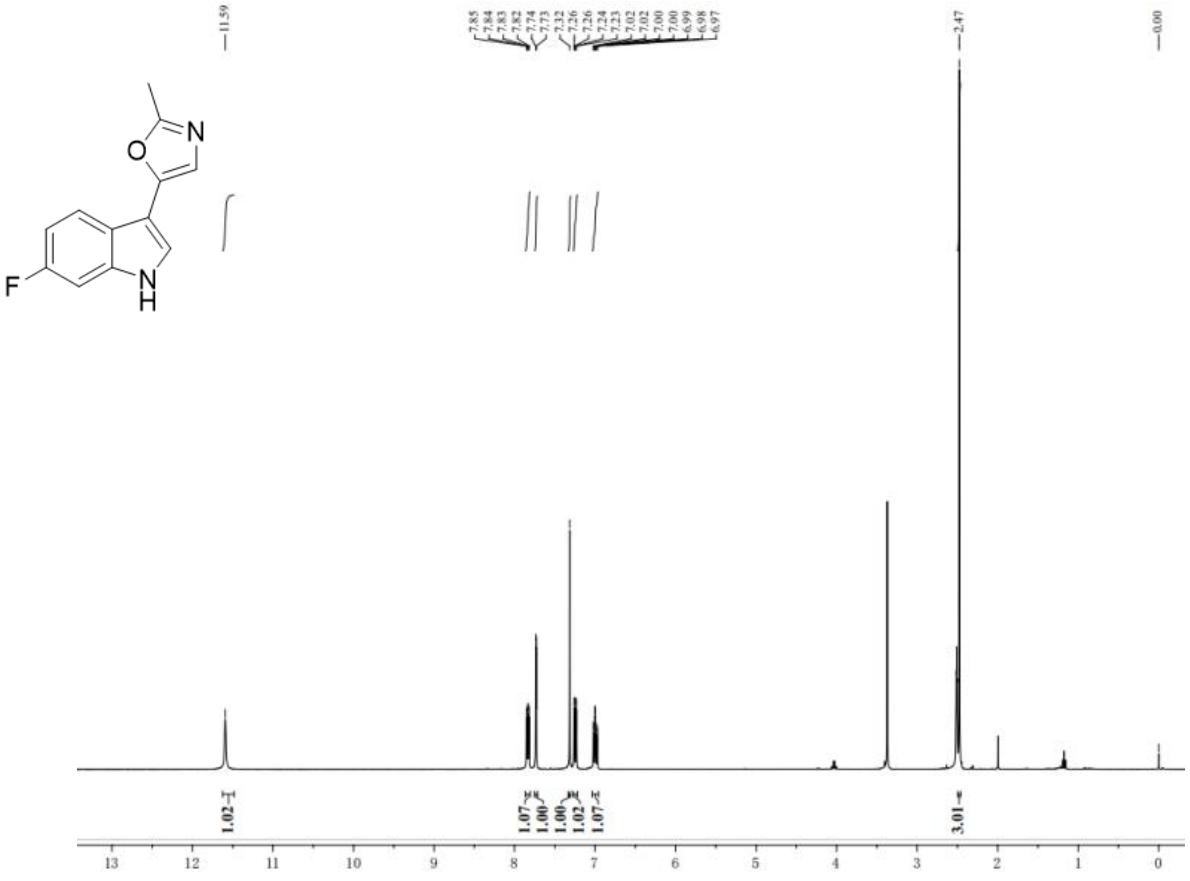

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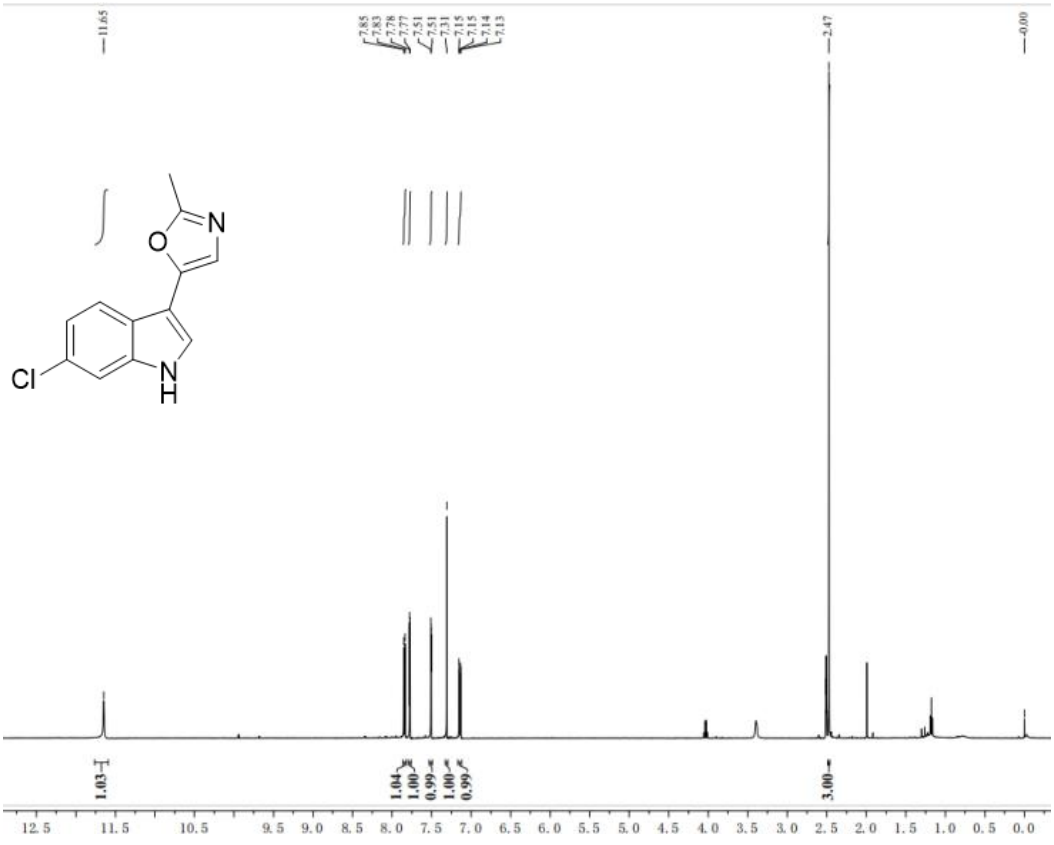
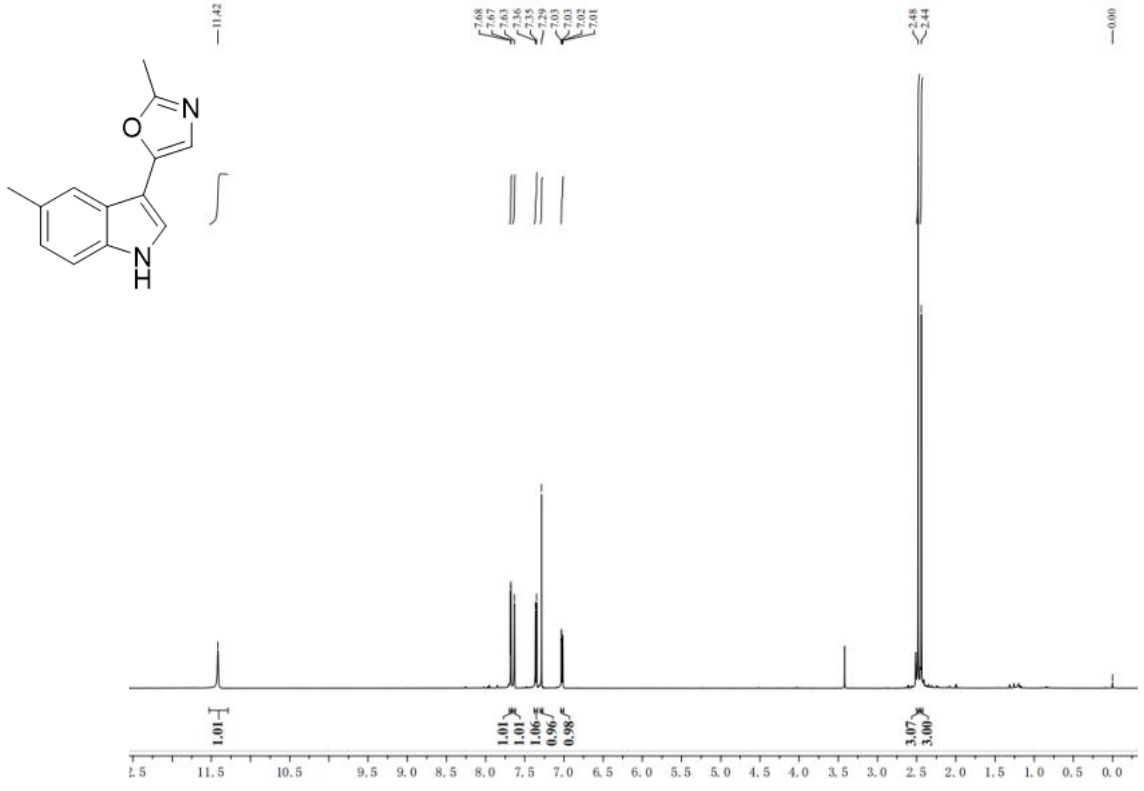
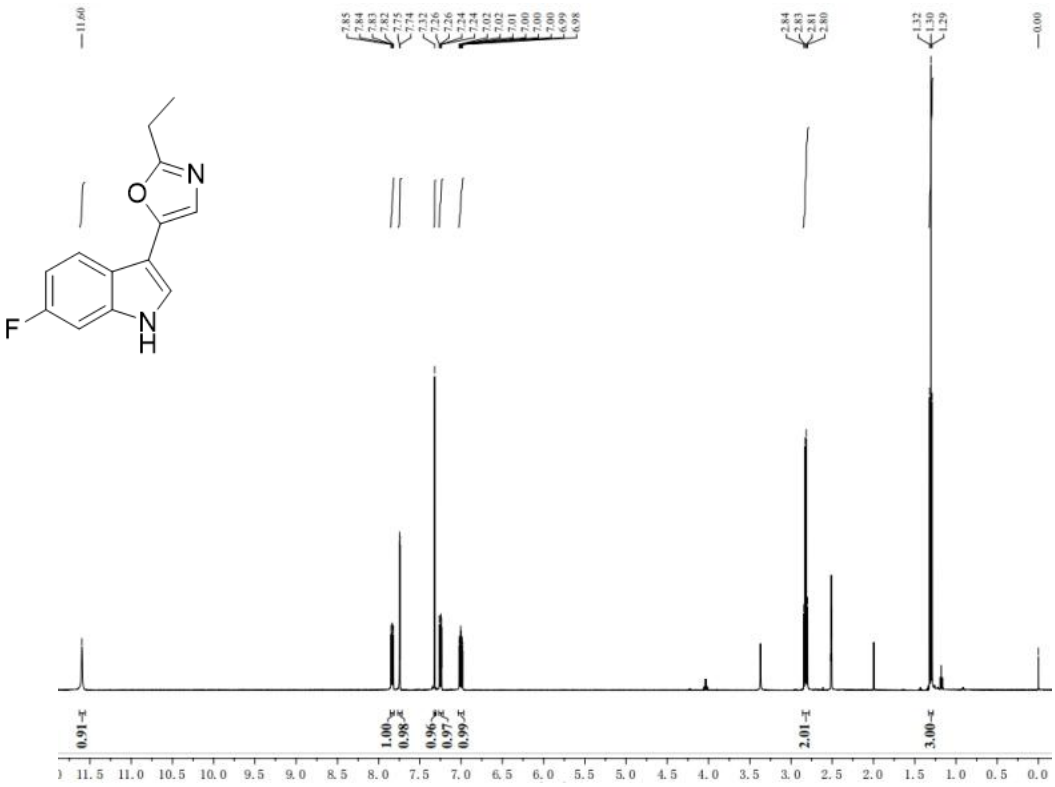


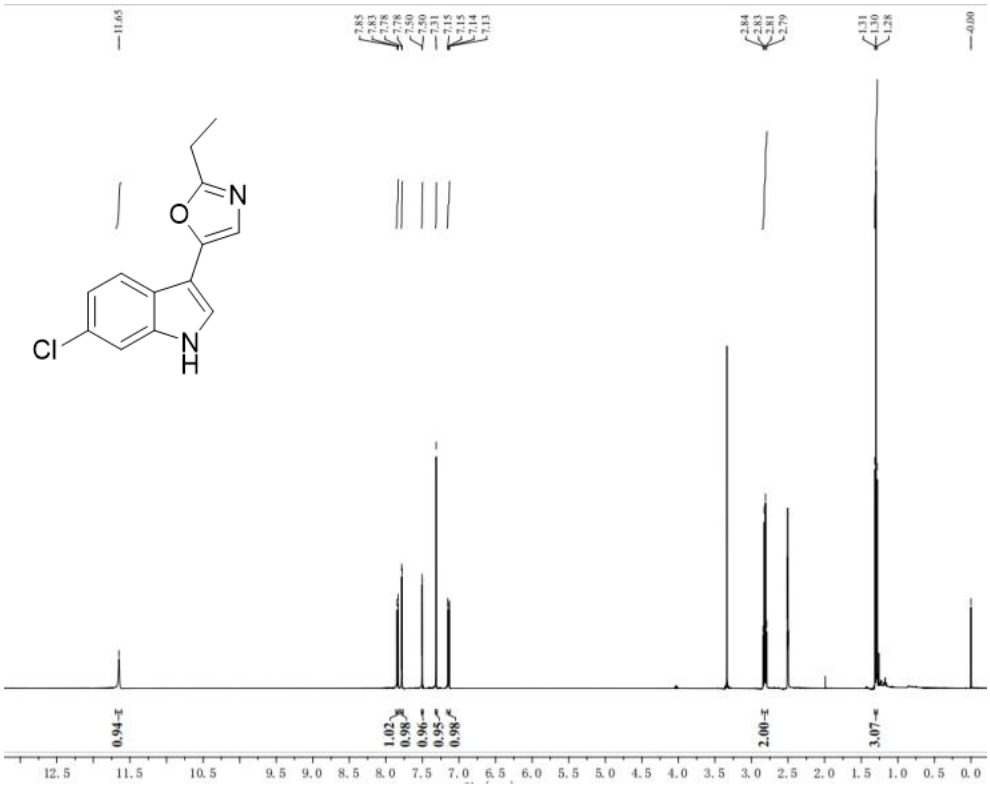
Compound 8g



Compound 8h



Compound 8i



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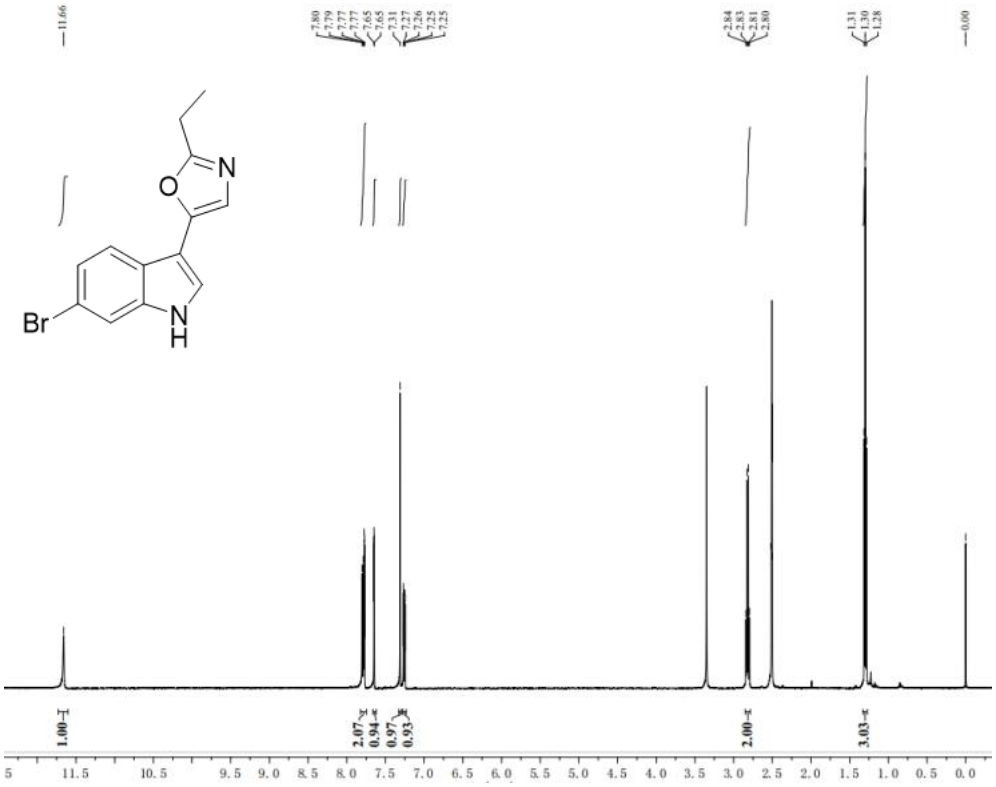
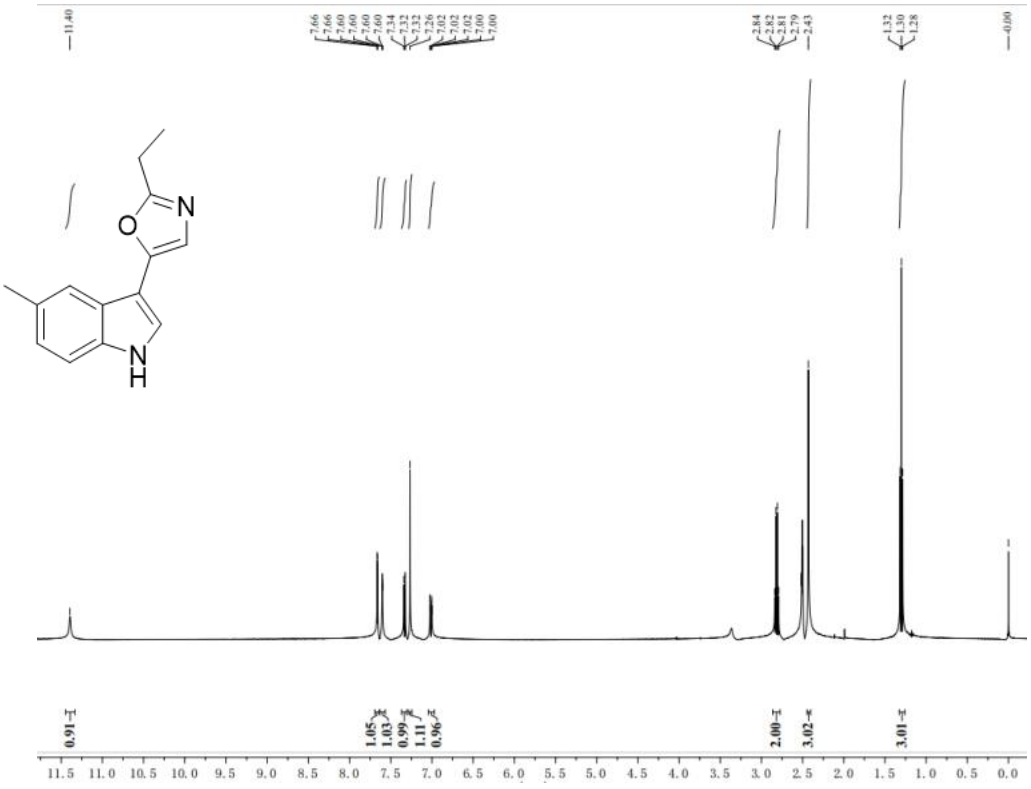
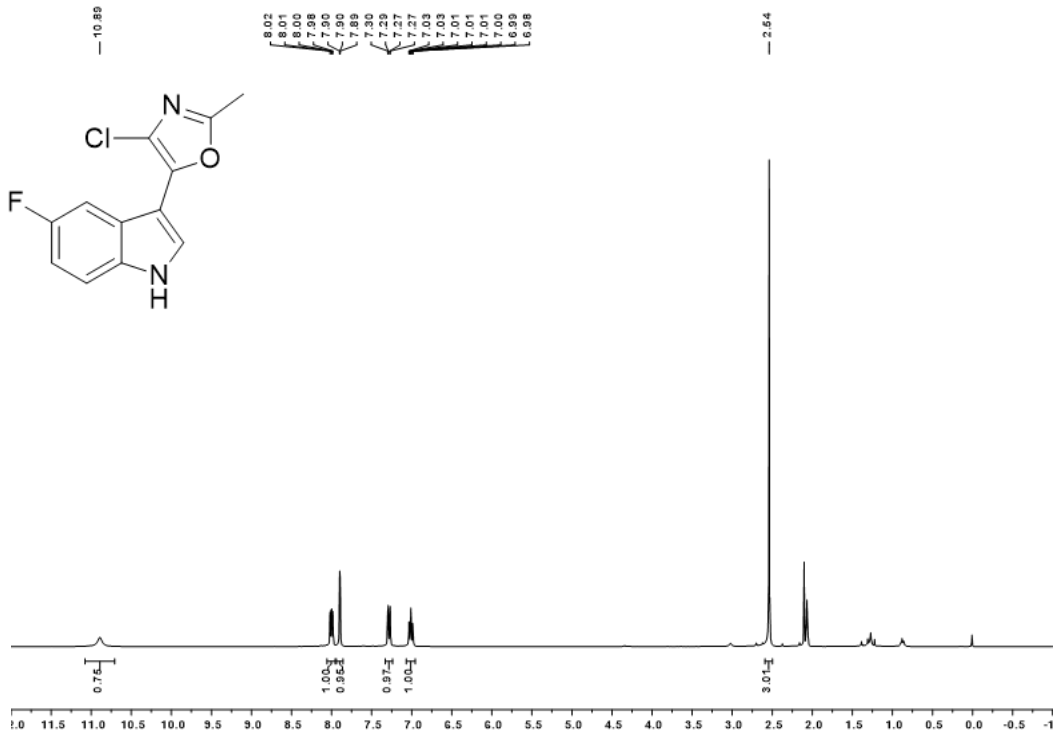


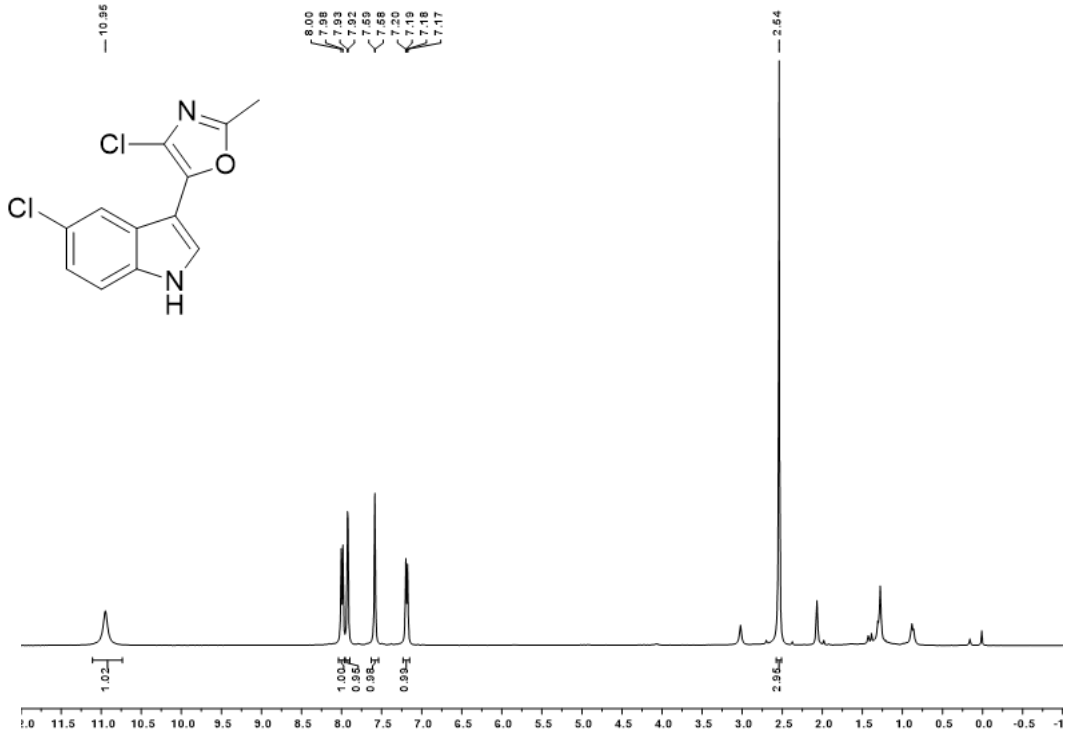
Compound 8k



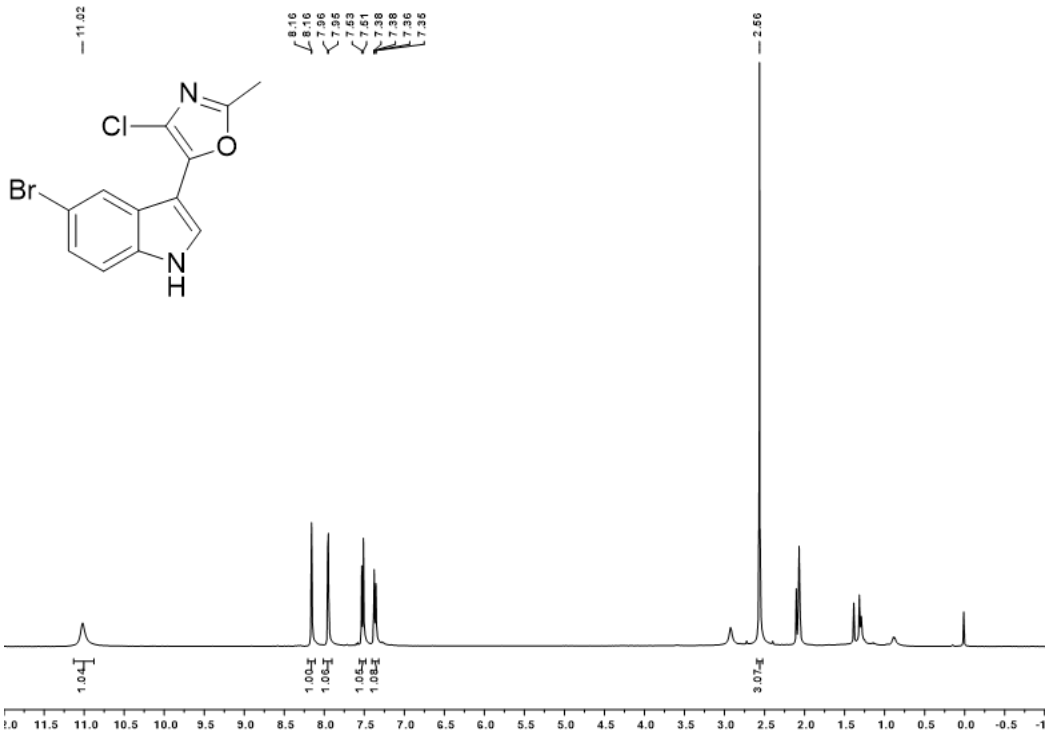
Compound 9a



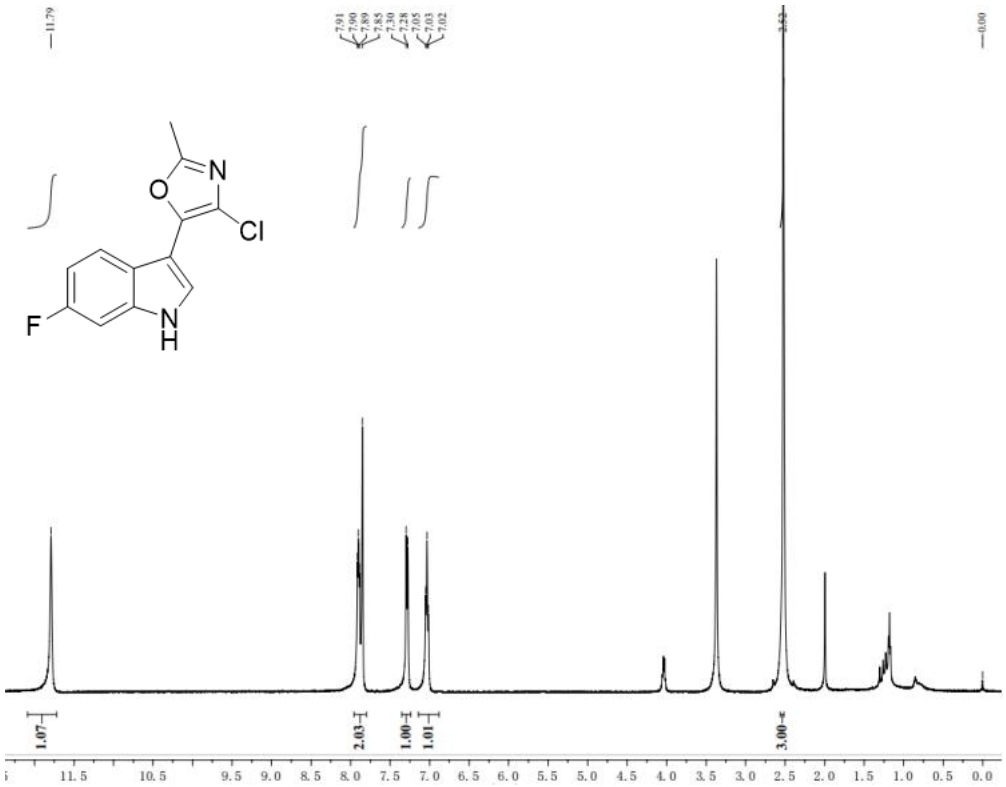
Compound 9b



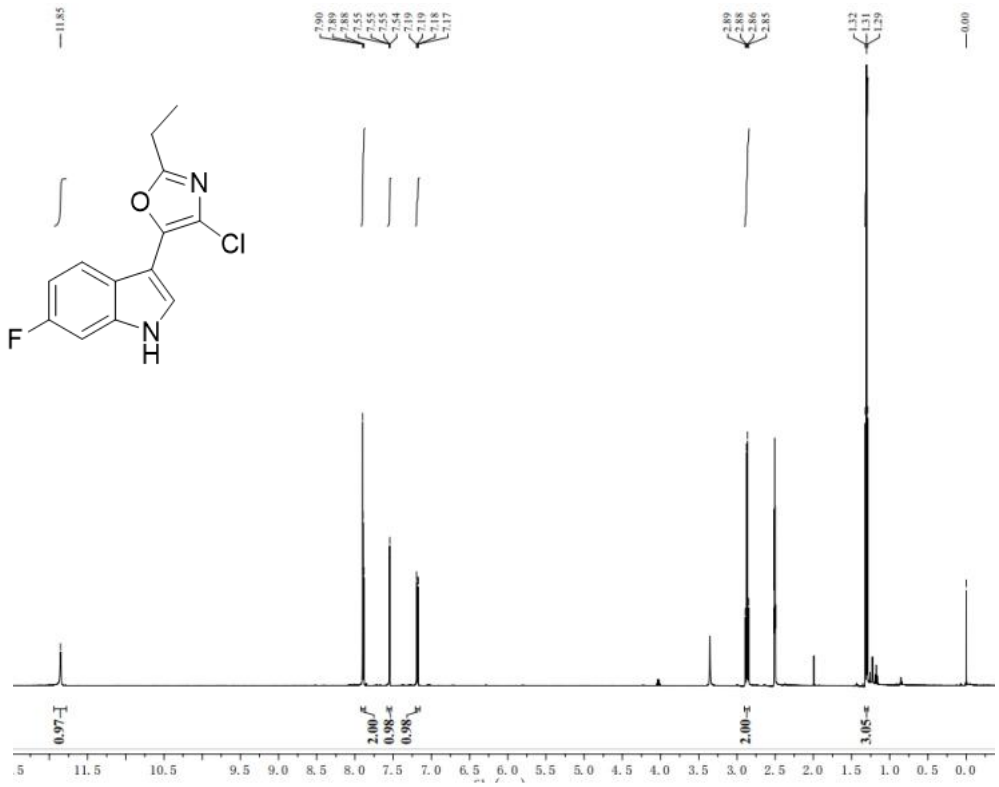
Compound 9c



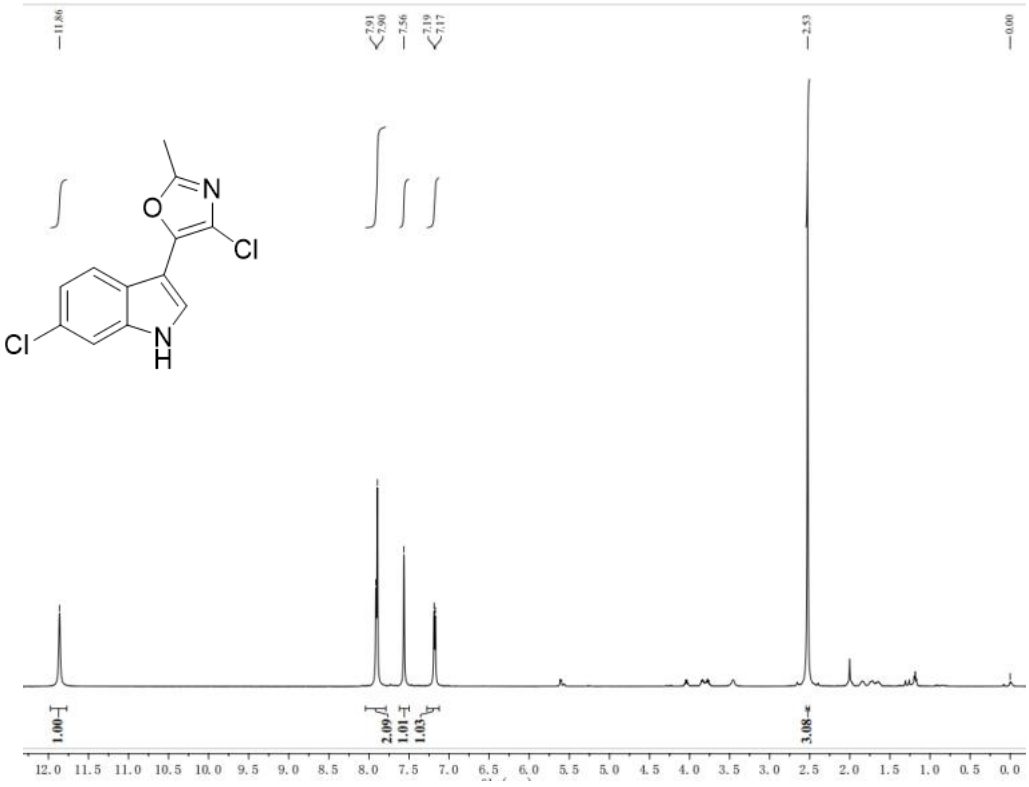
Compound 9d



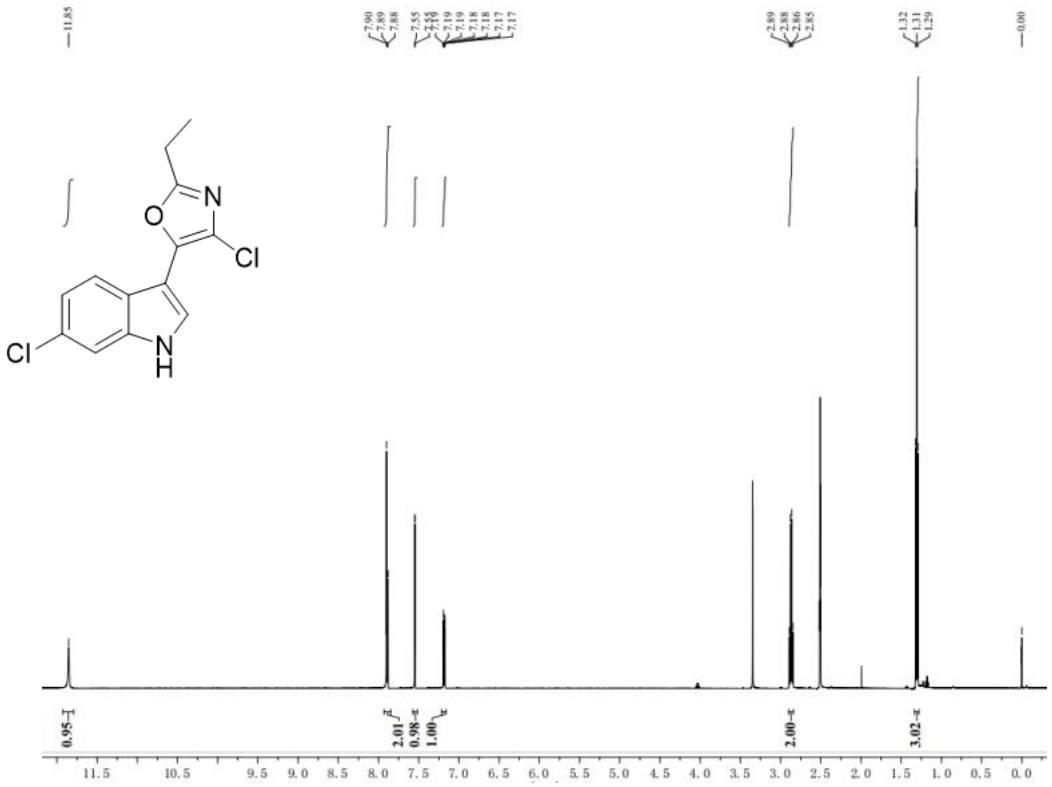
Compound 9e



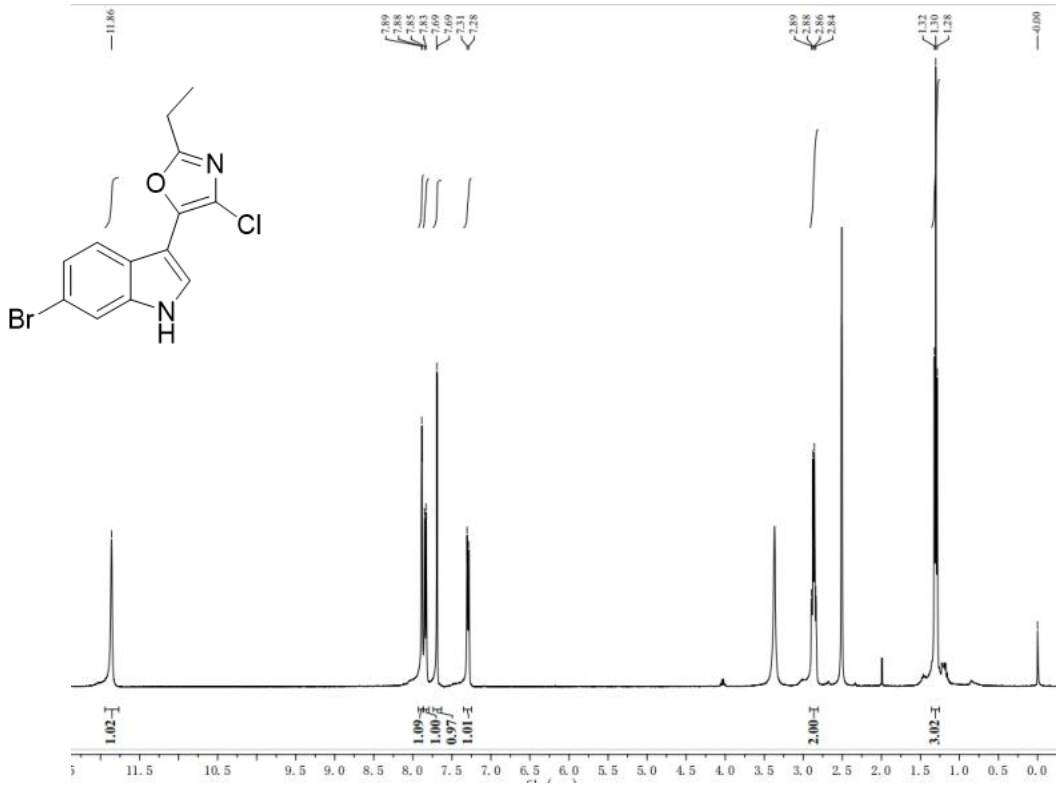
Compound 9f



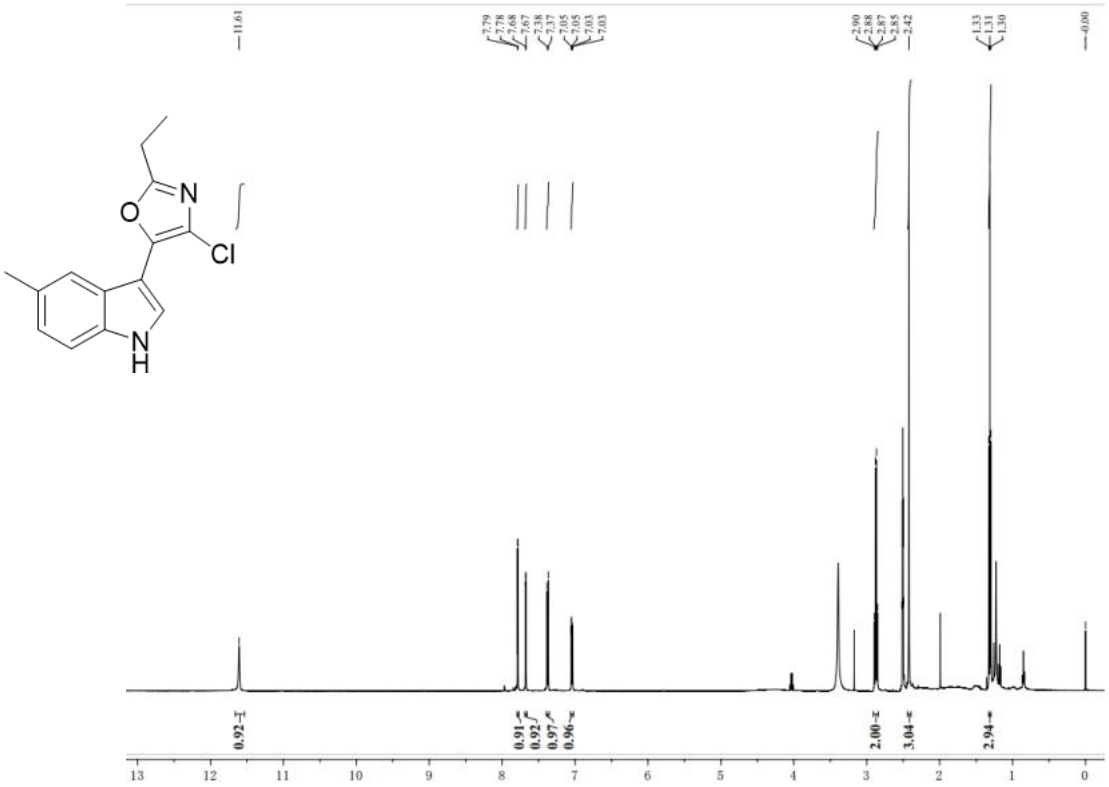
Compound 9g



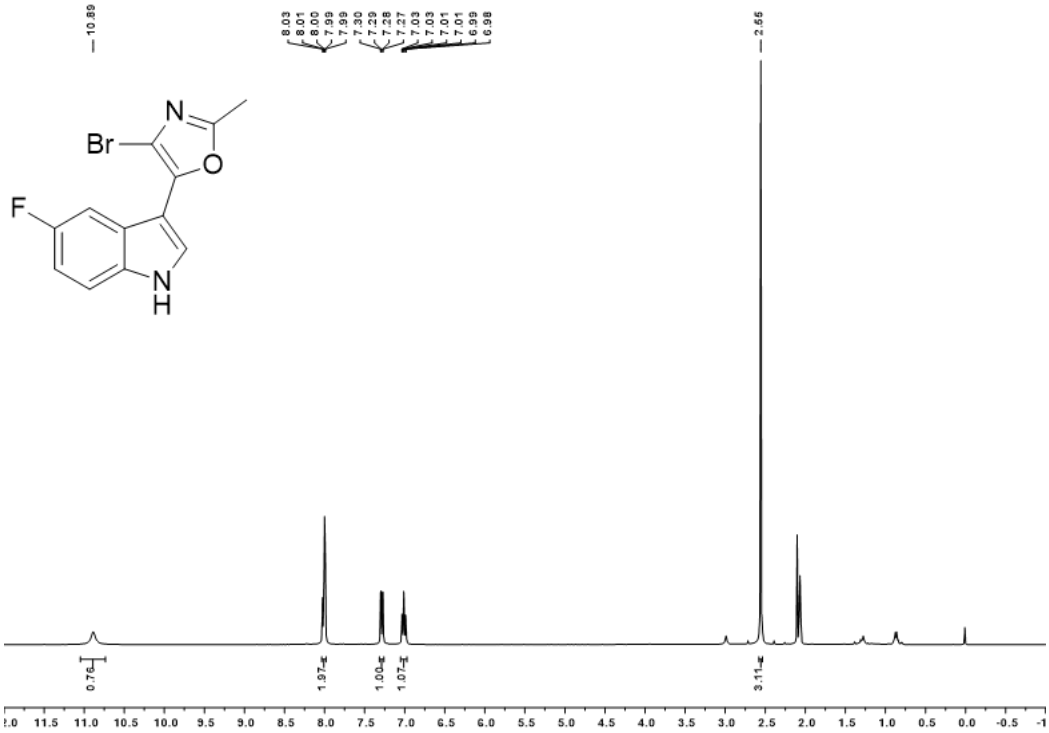
Compound 9h



Compound 9i



Compound 10a



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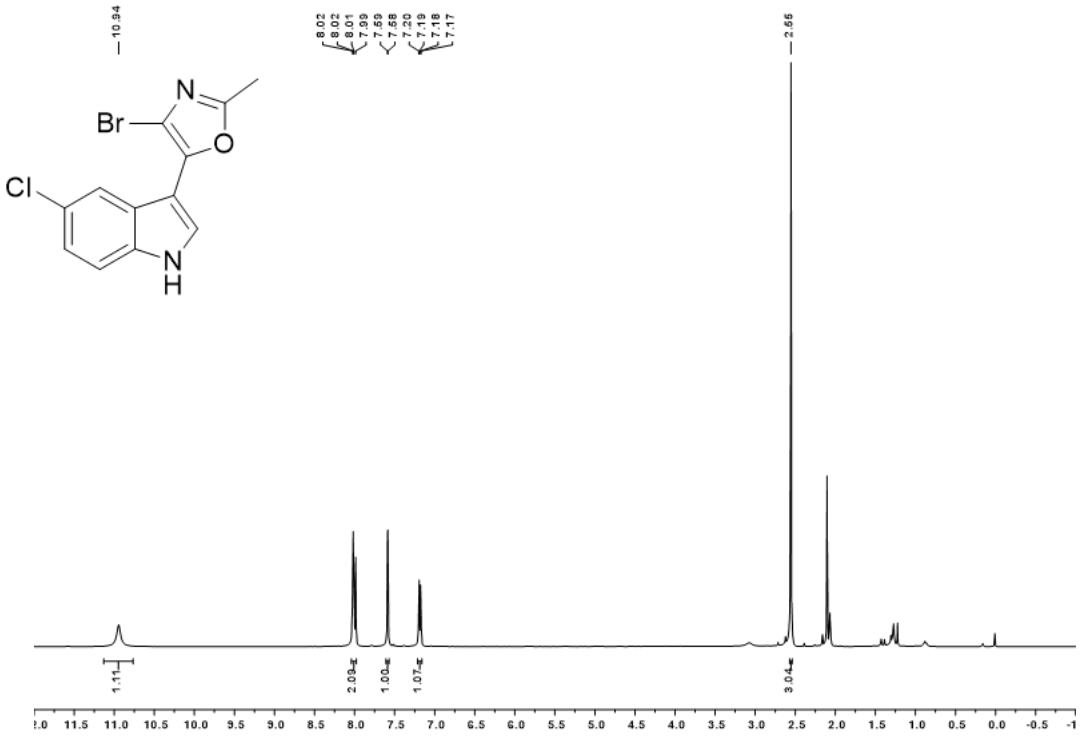
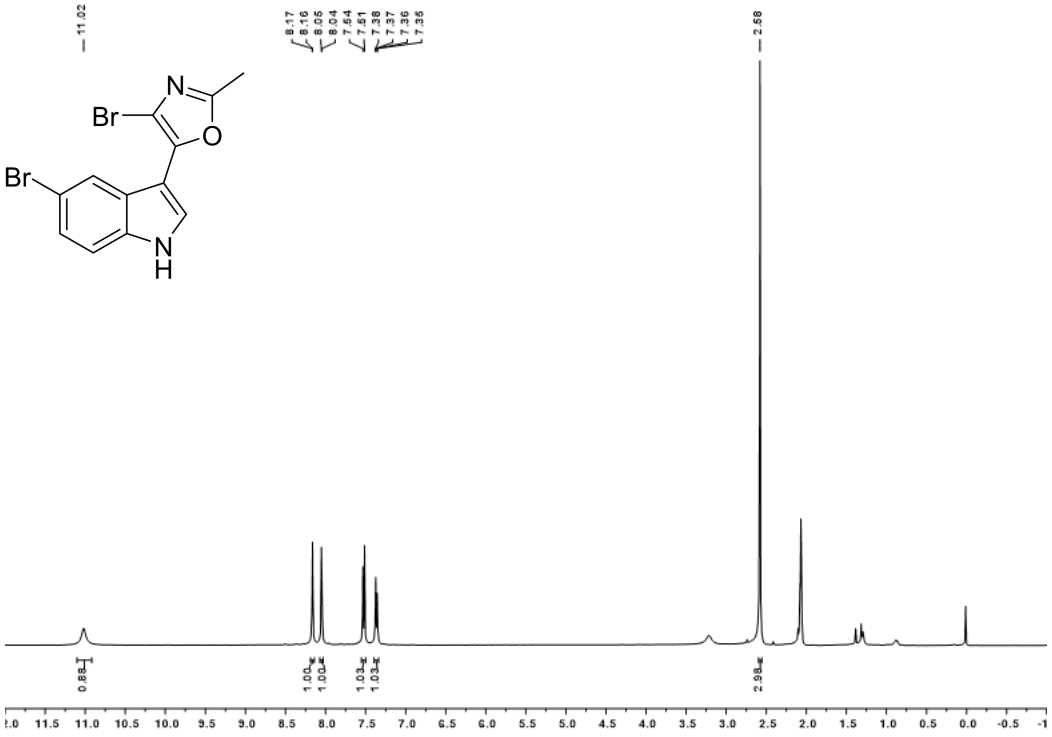
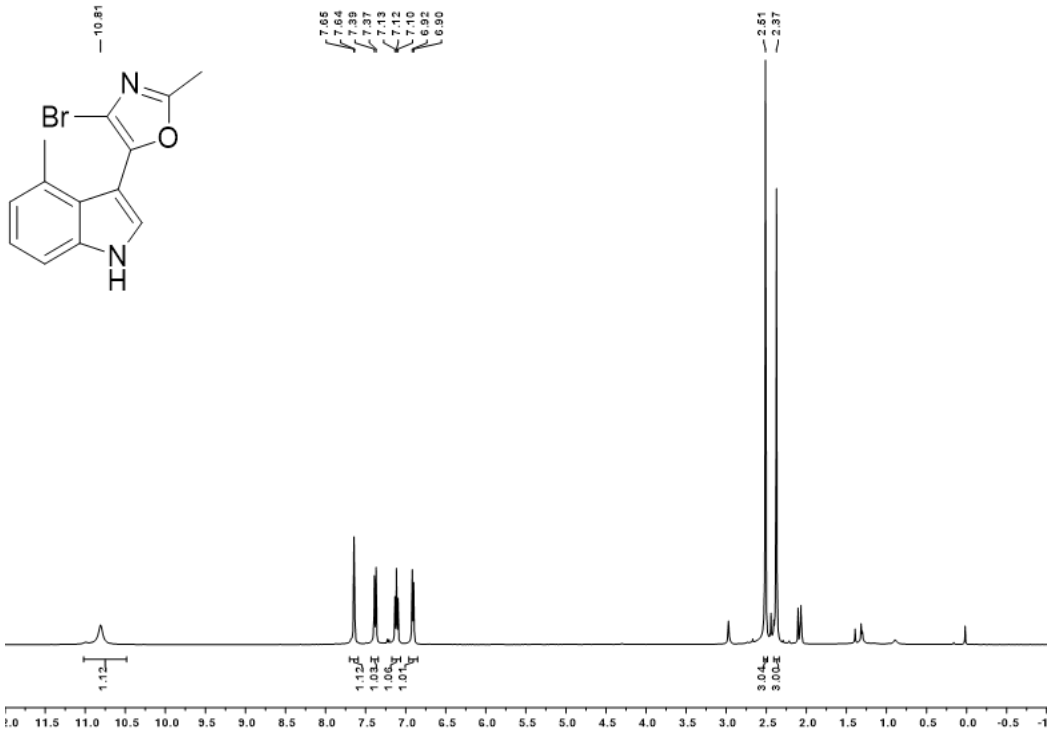


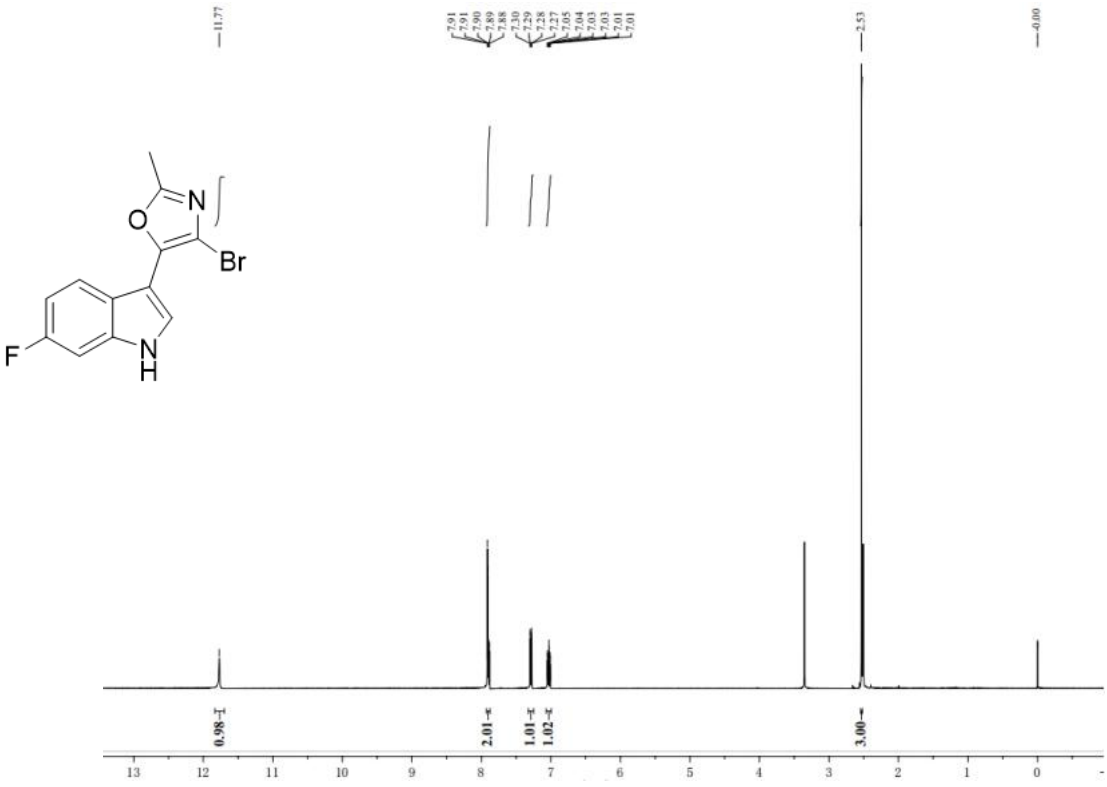
Compound 10c



Compound 10d



Compound 10e



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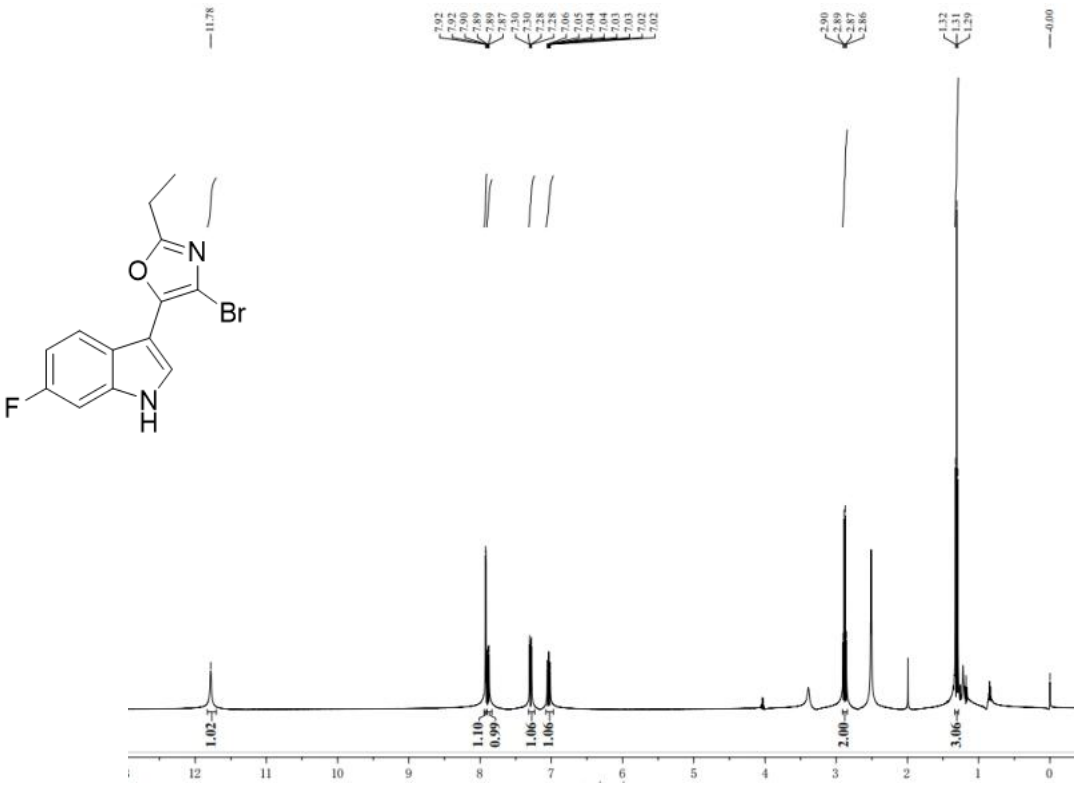
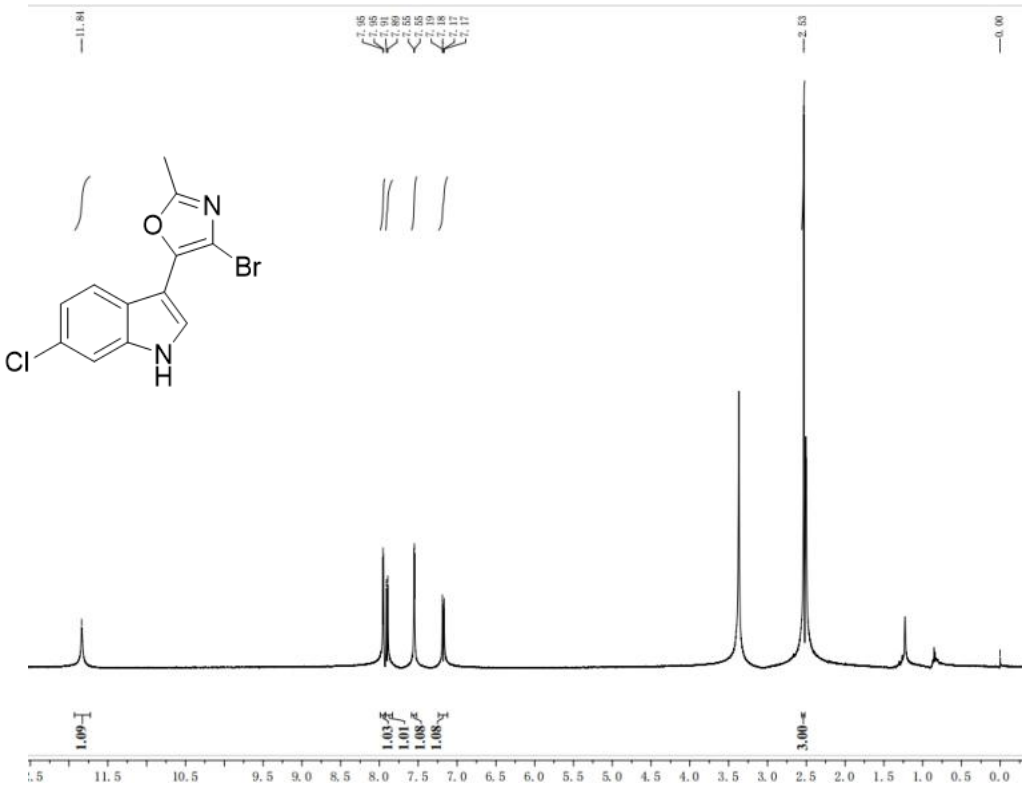


Compound 10g



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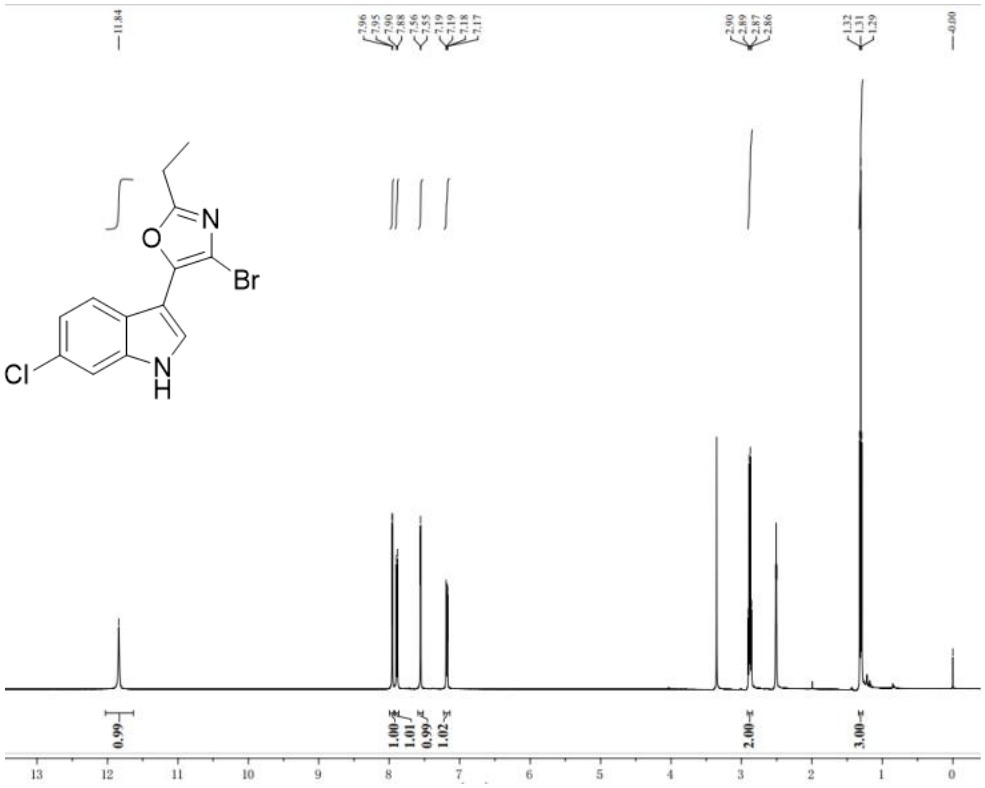

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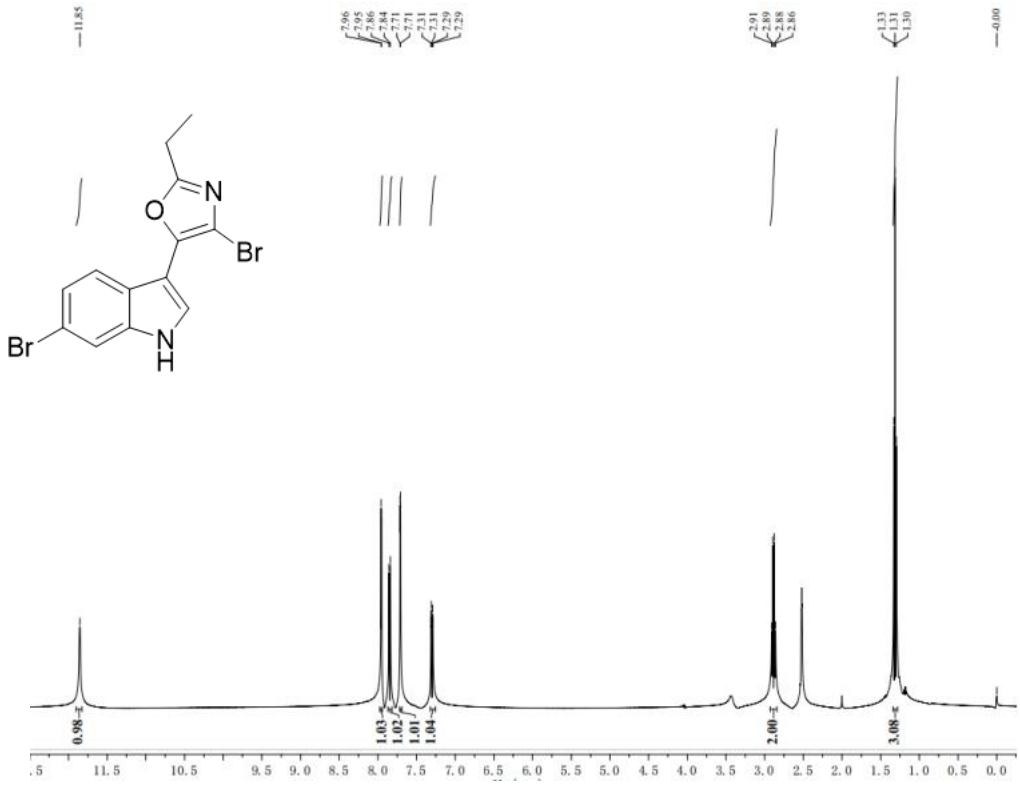
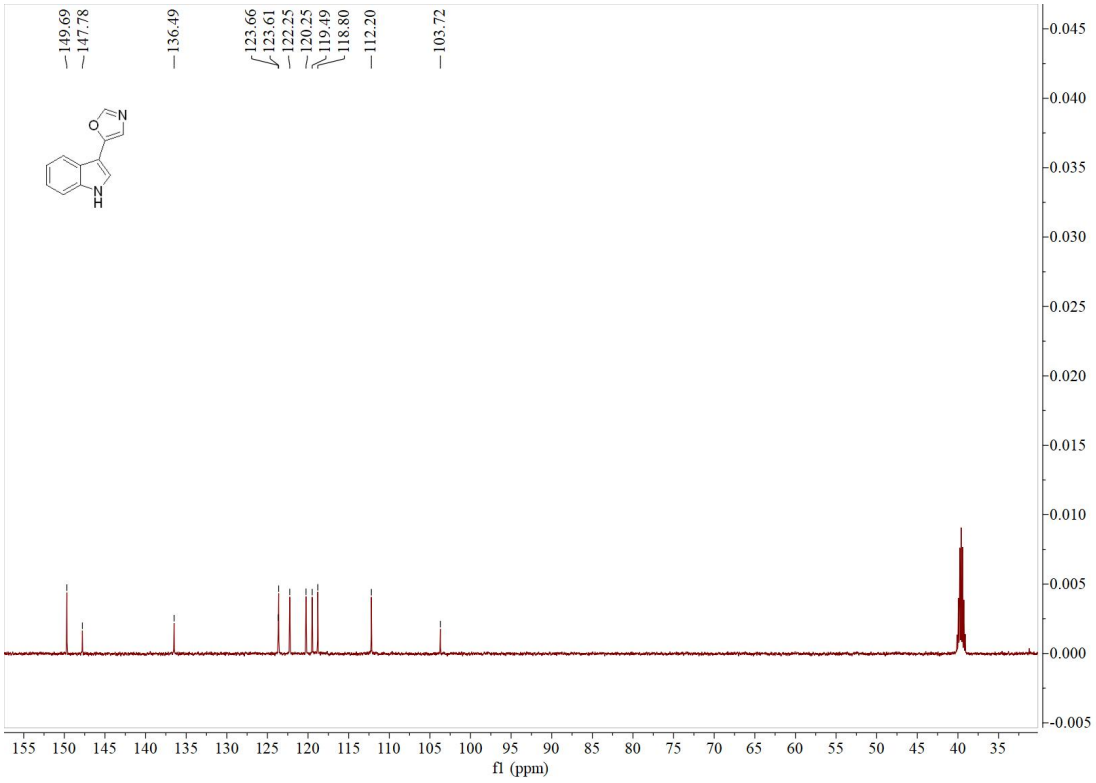
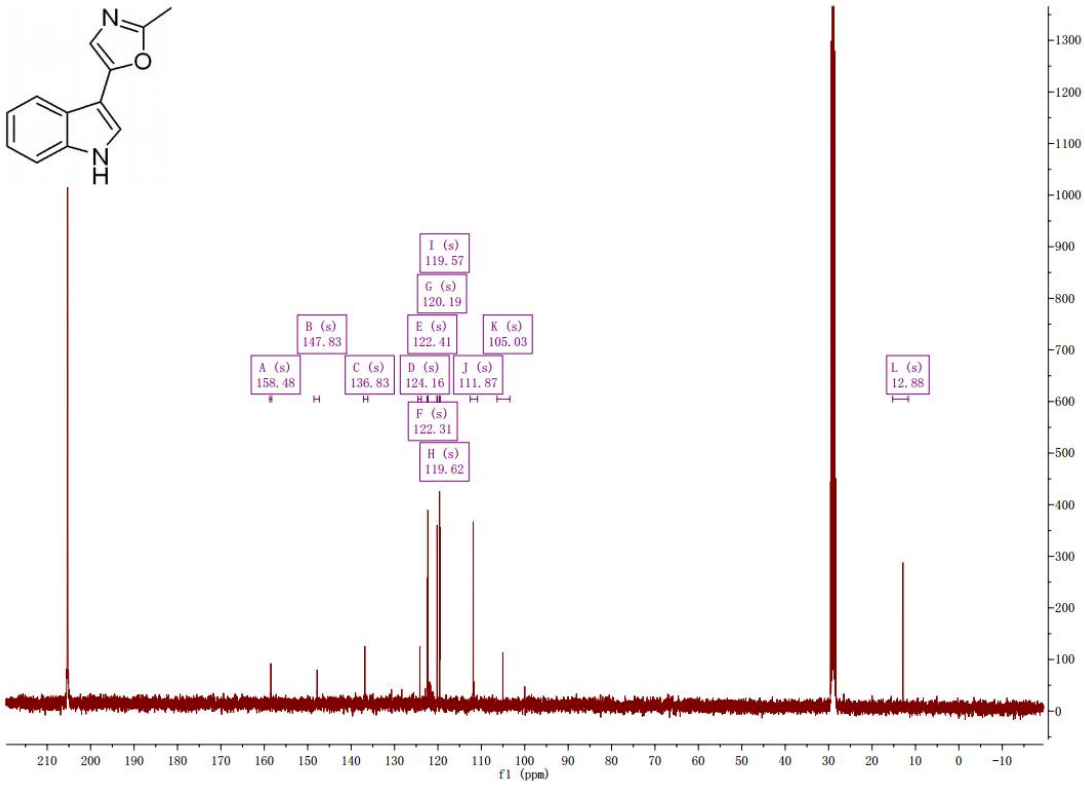


3. ^{13}C NMR

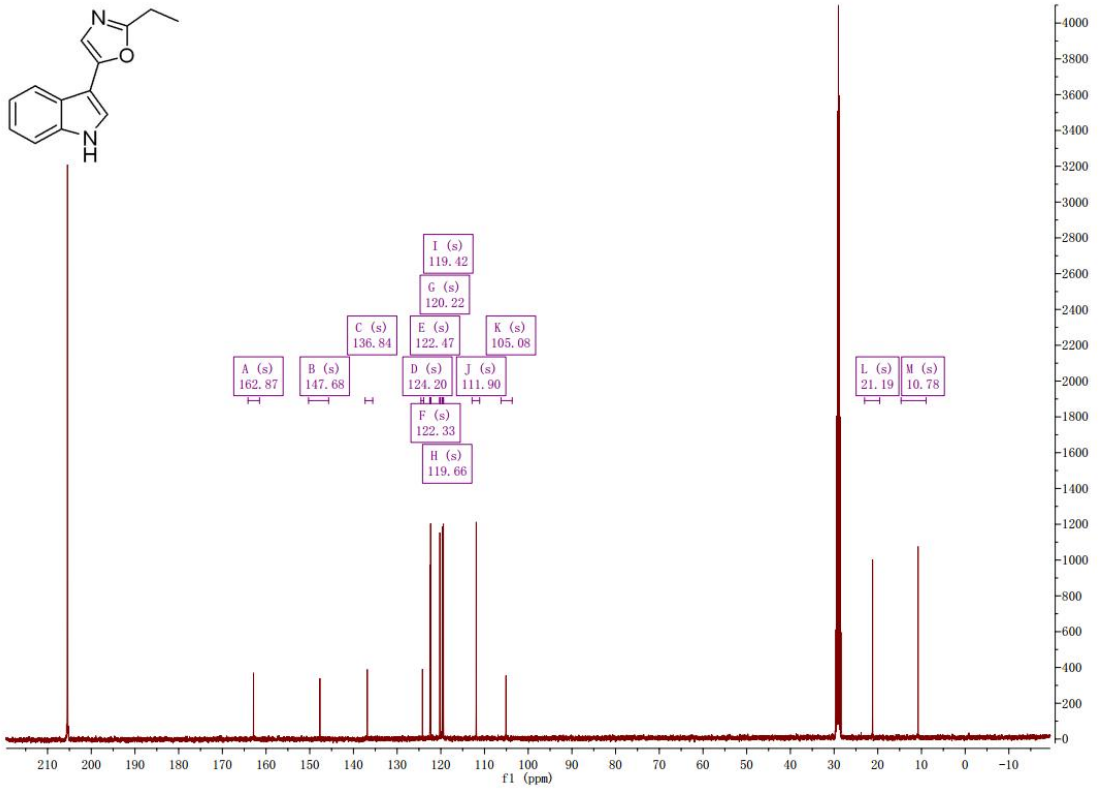
Compound 3a



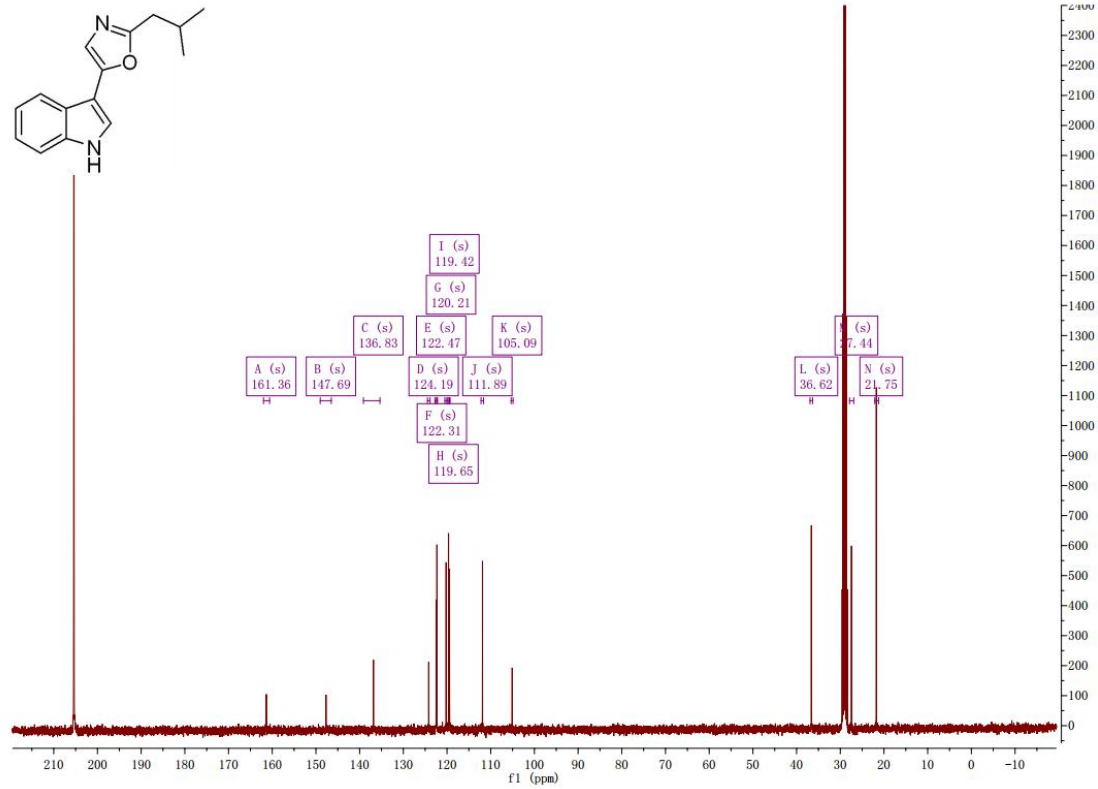
Compound 3b



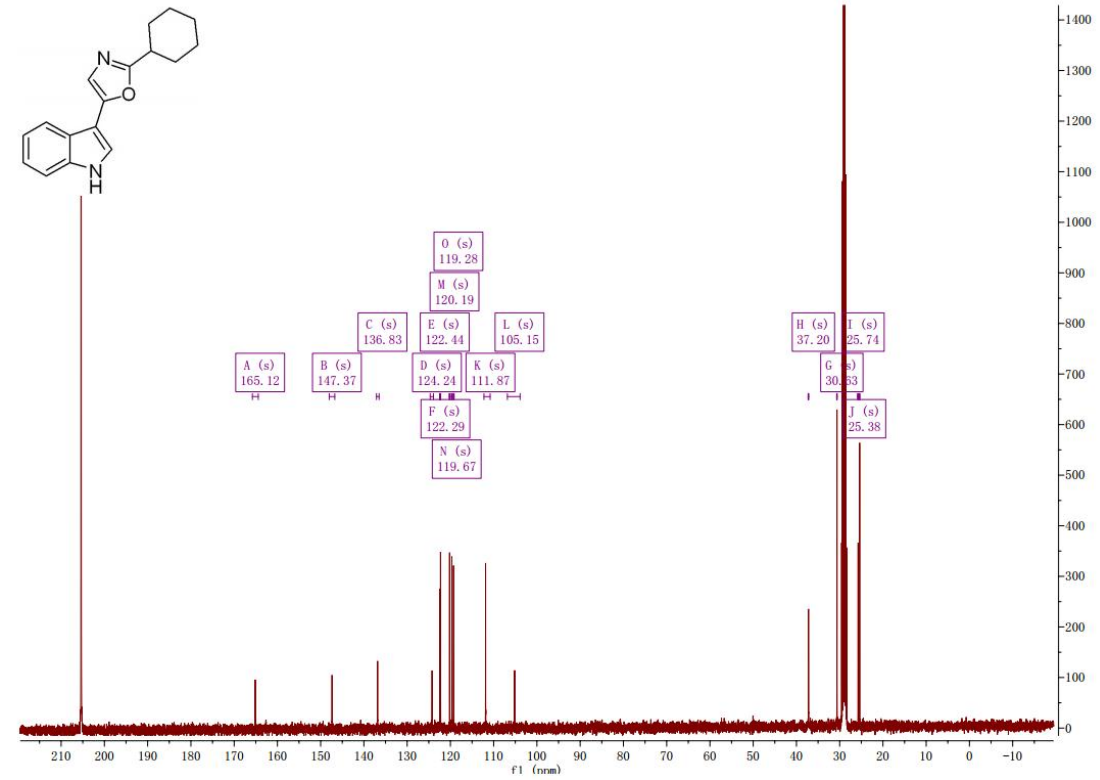
Compound 3c



Compound 3d



Compound 3e



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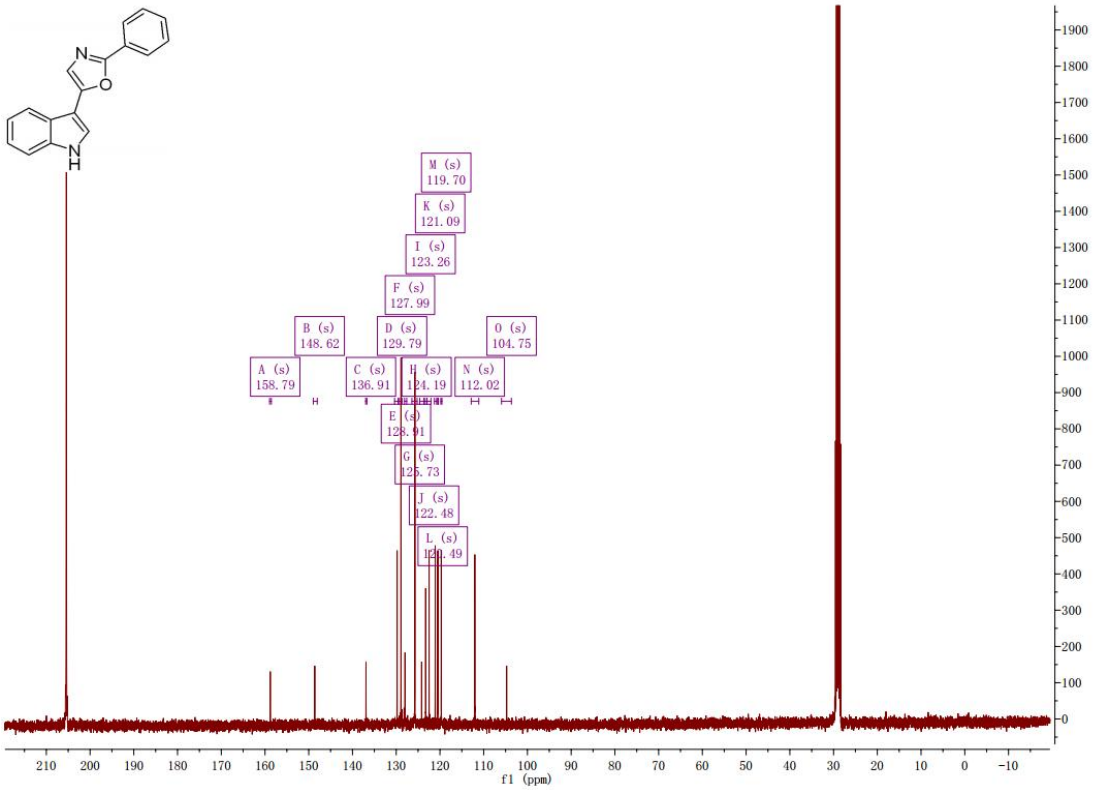
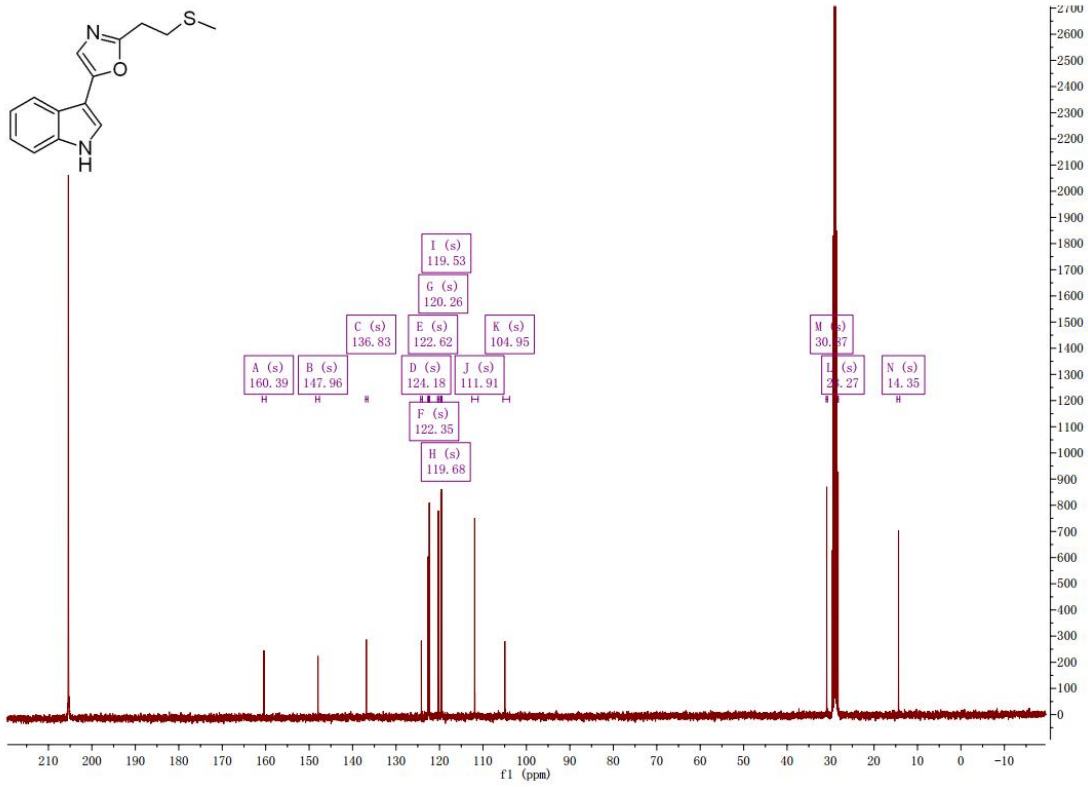
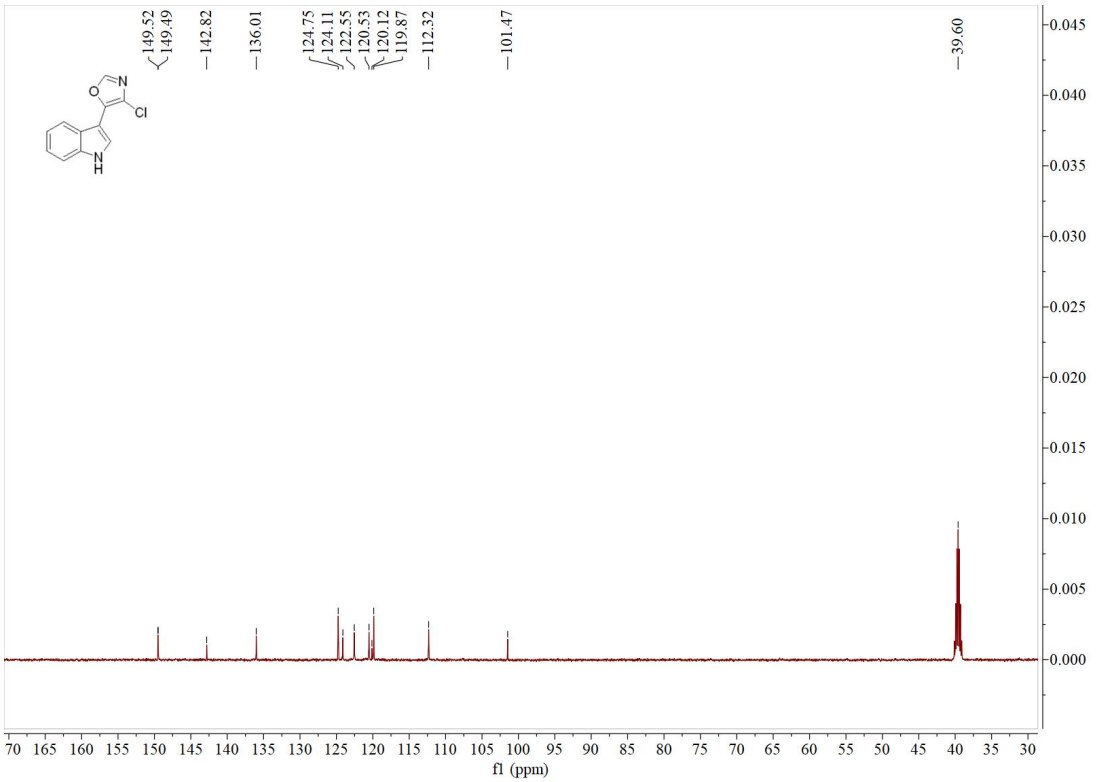


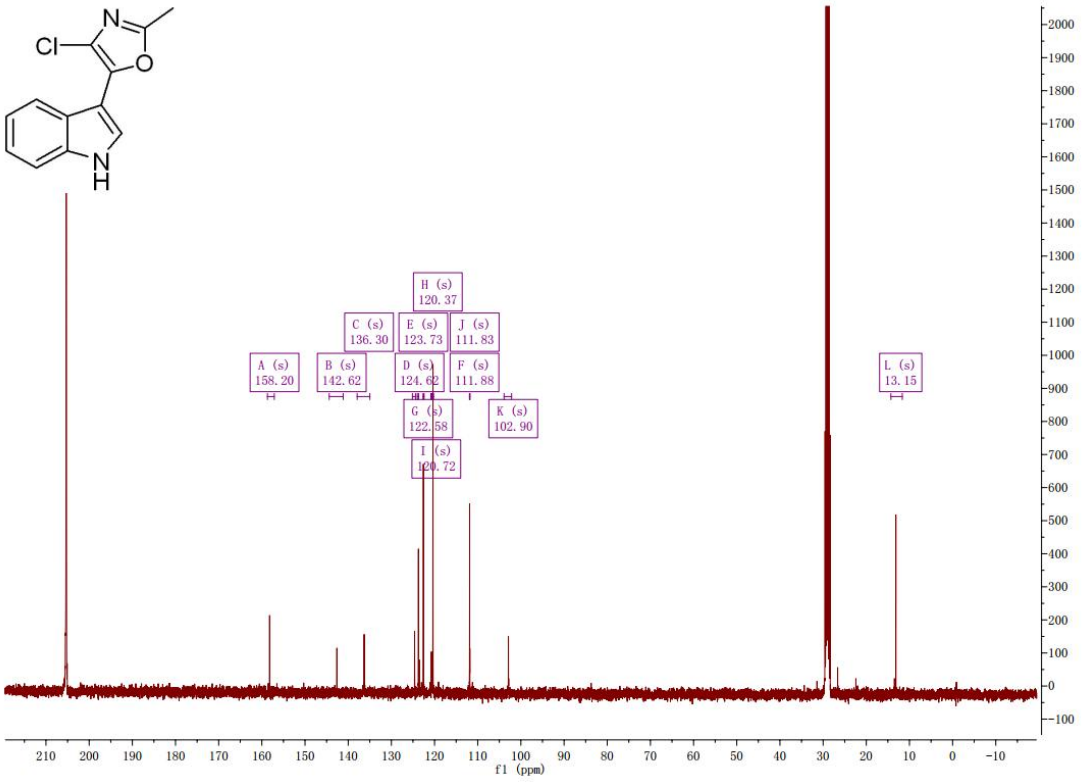
Compound 3g



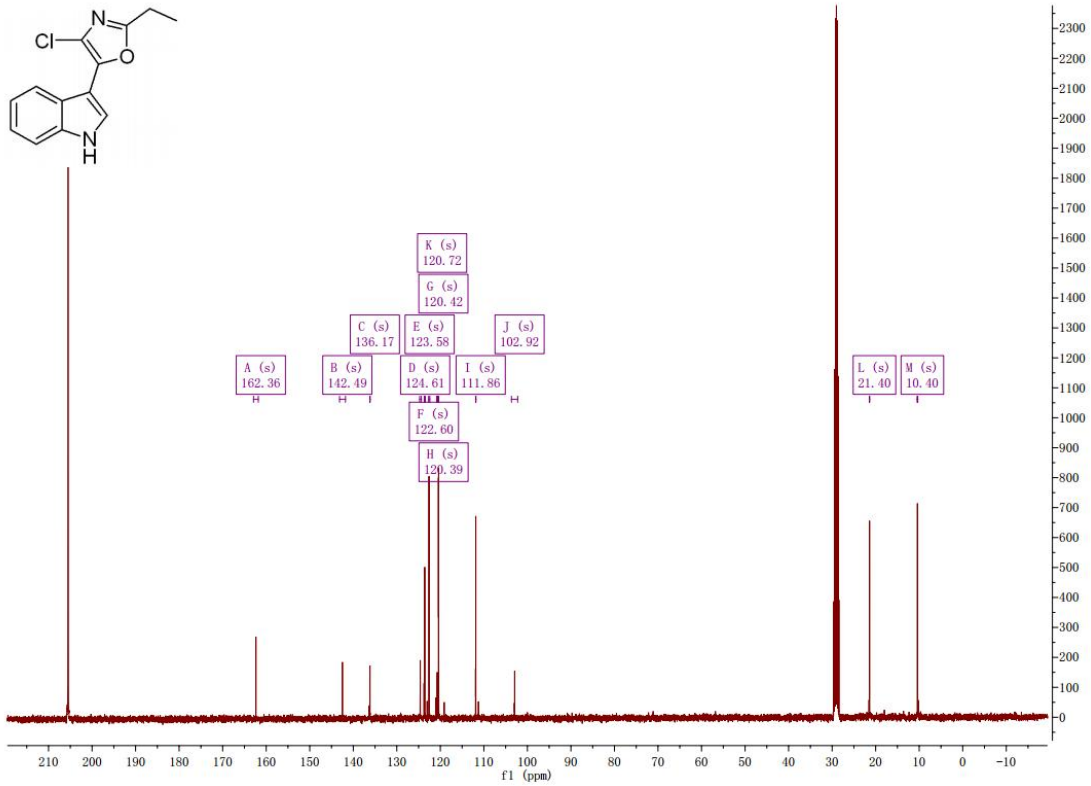
Compound 4a



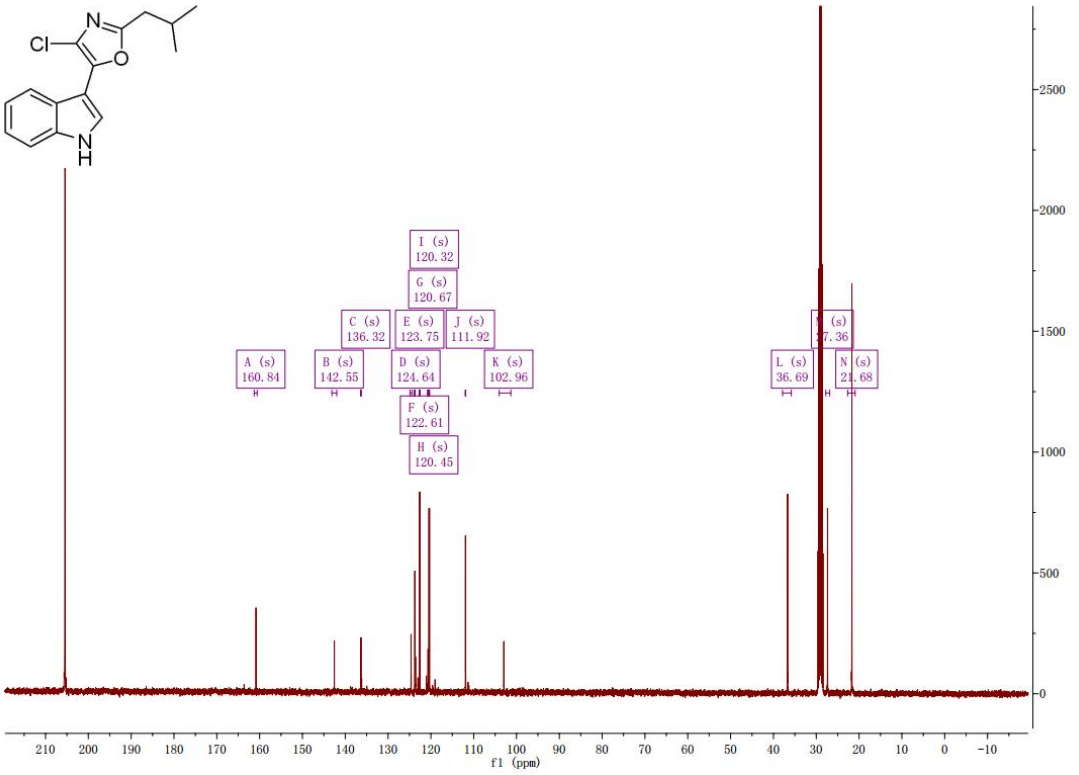
Compound 4b



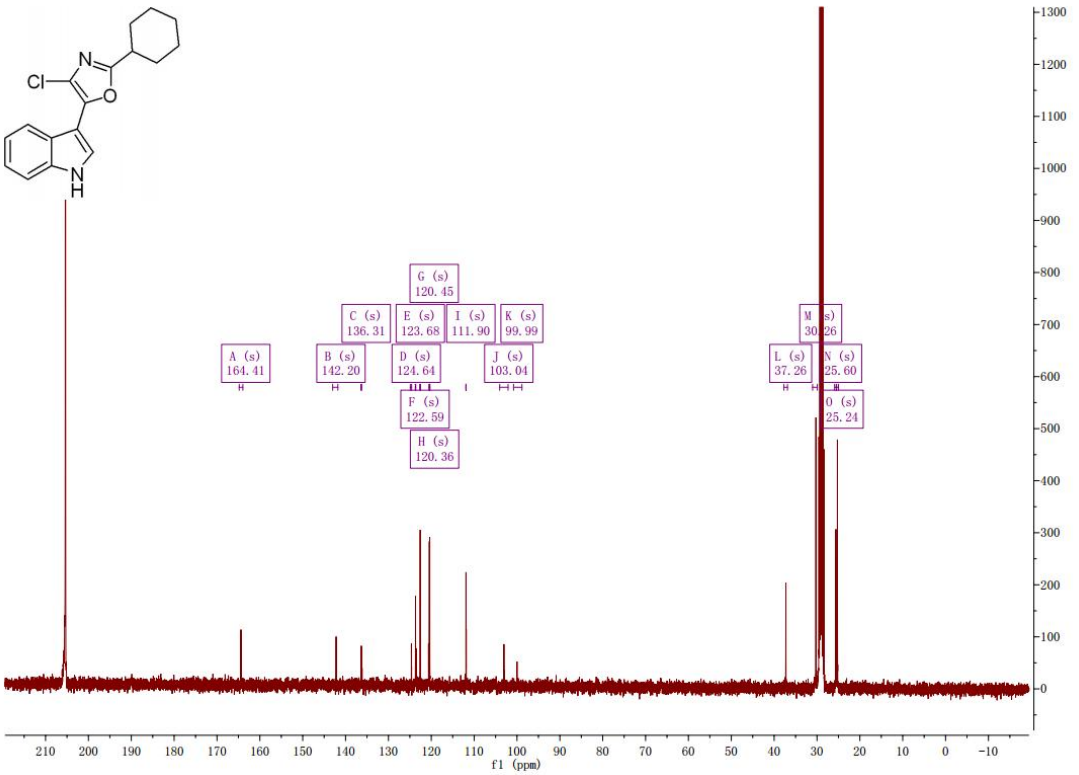
Compound 4c



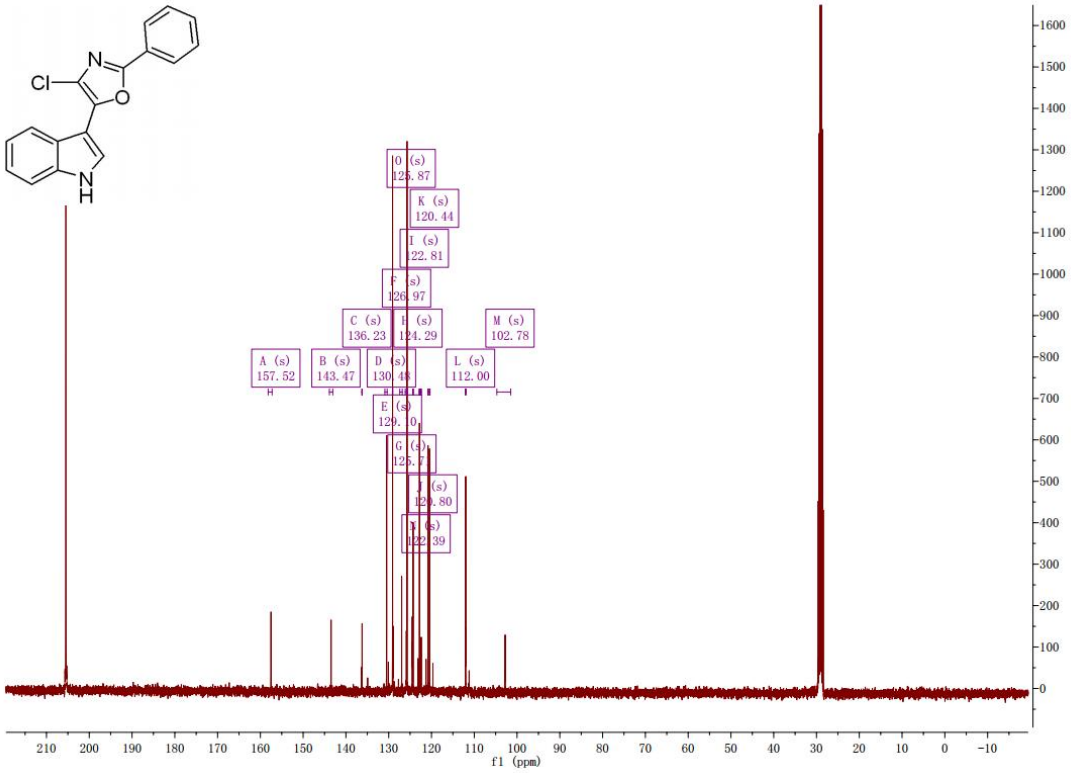
Compound 4d



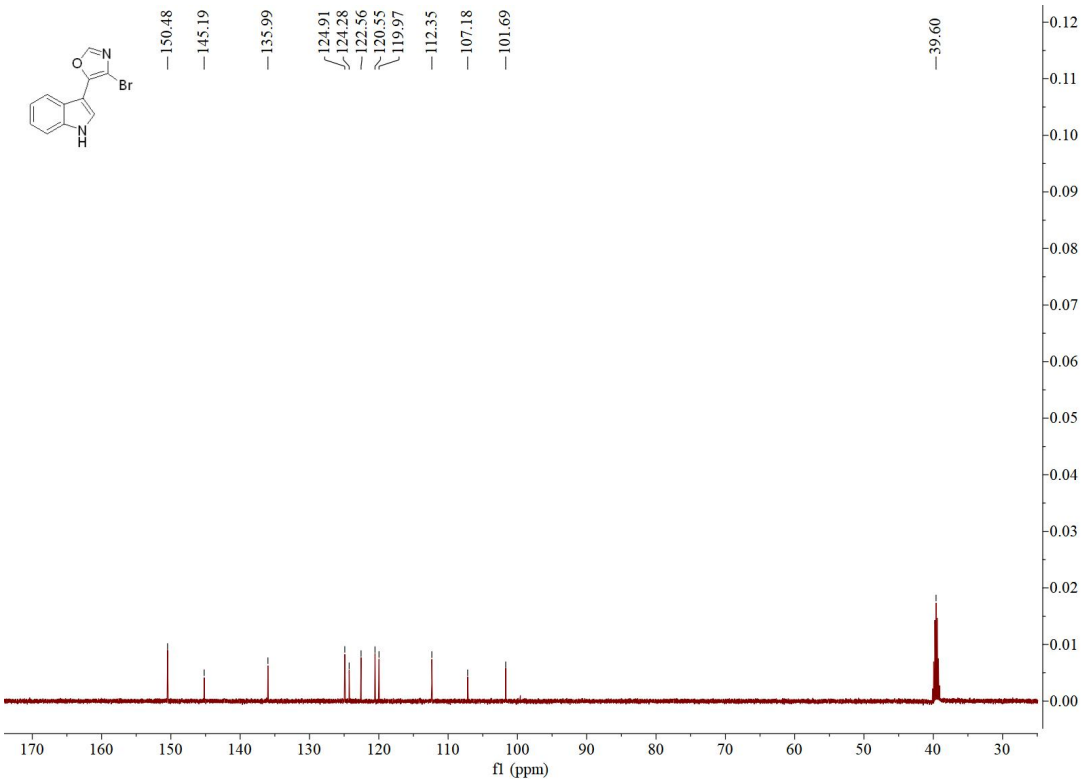
Compound 4e



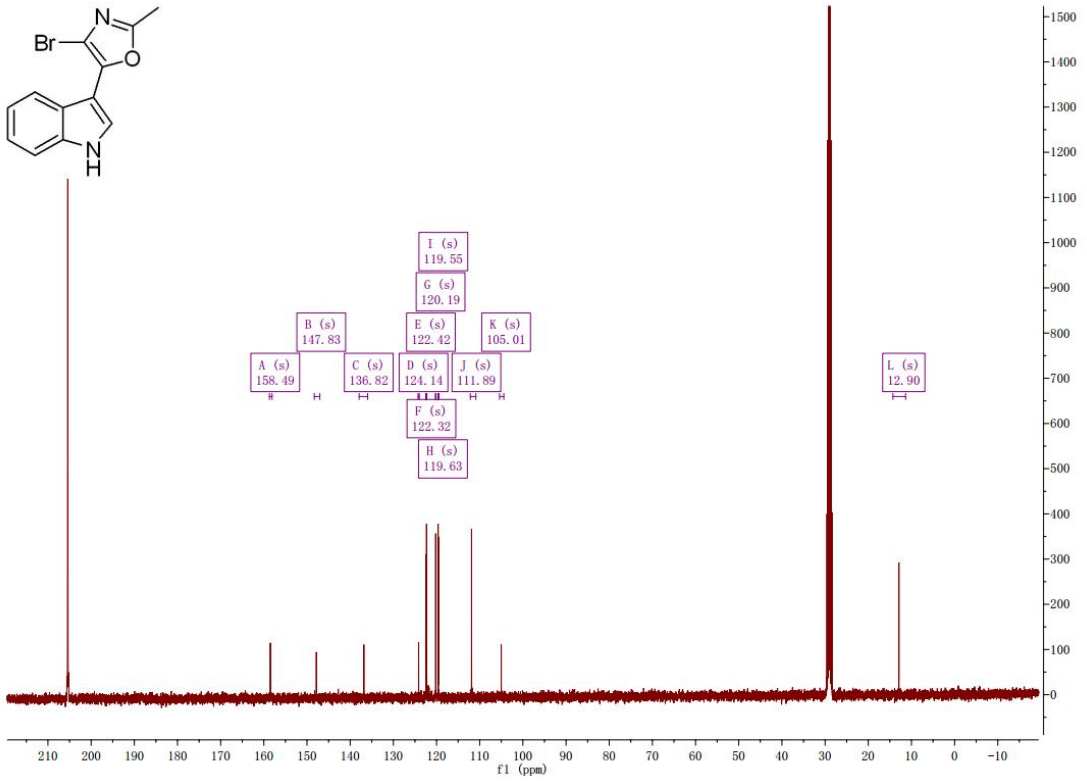
Compound 4f



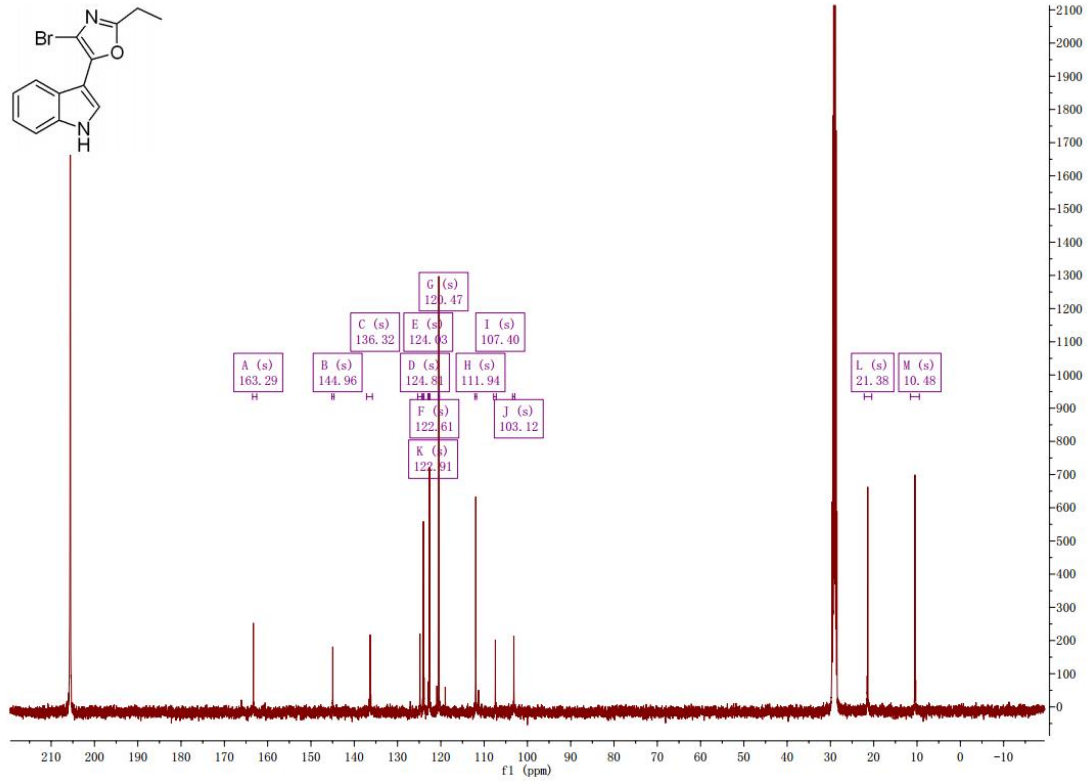
Compound 5a



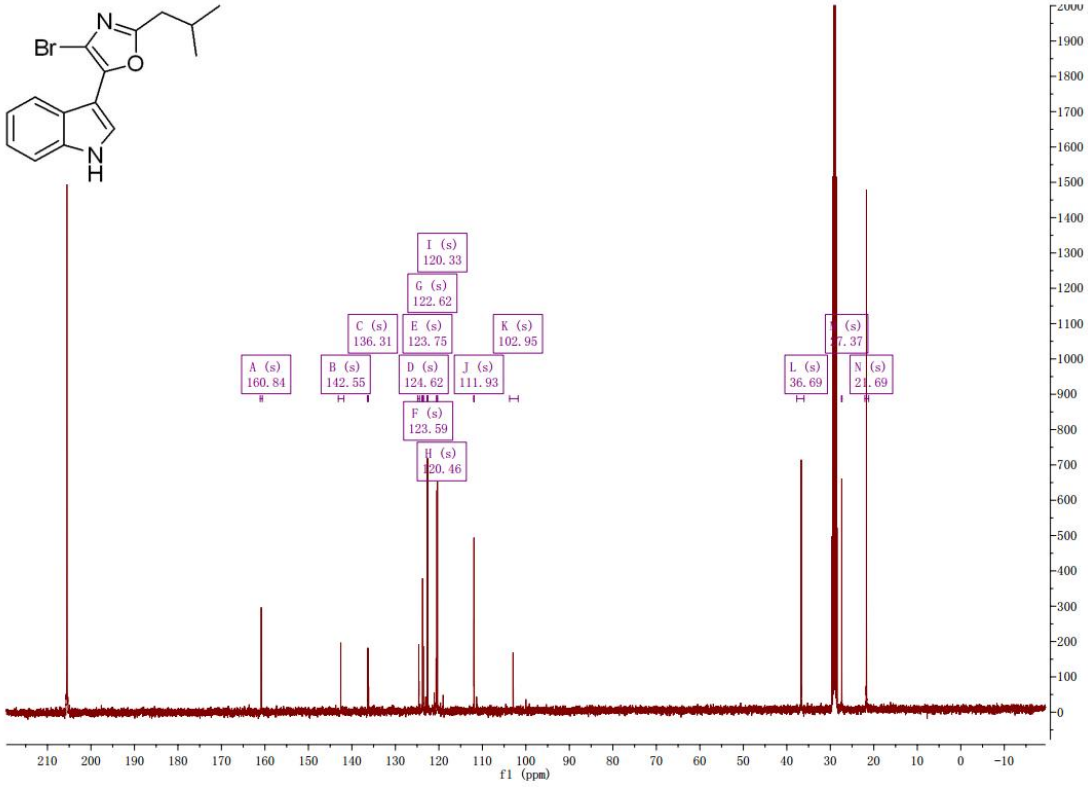
Compound 5b



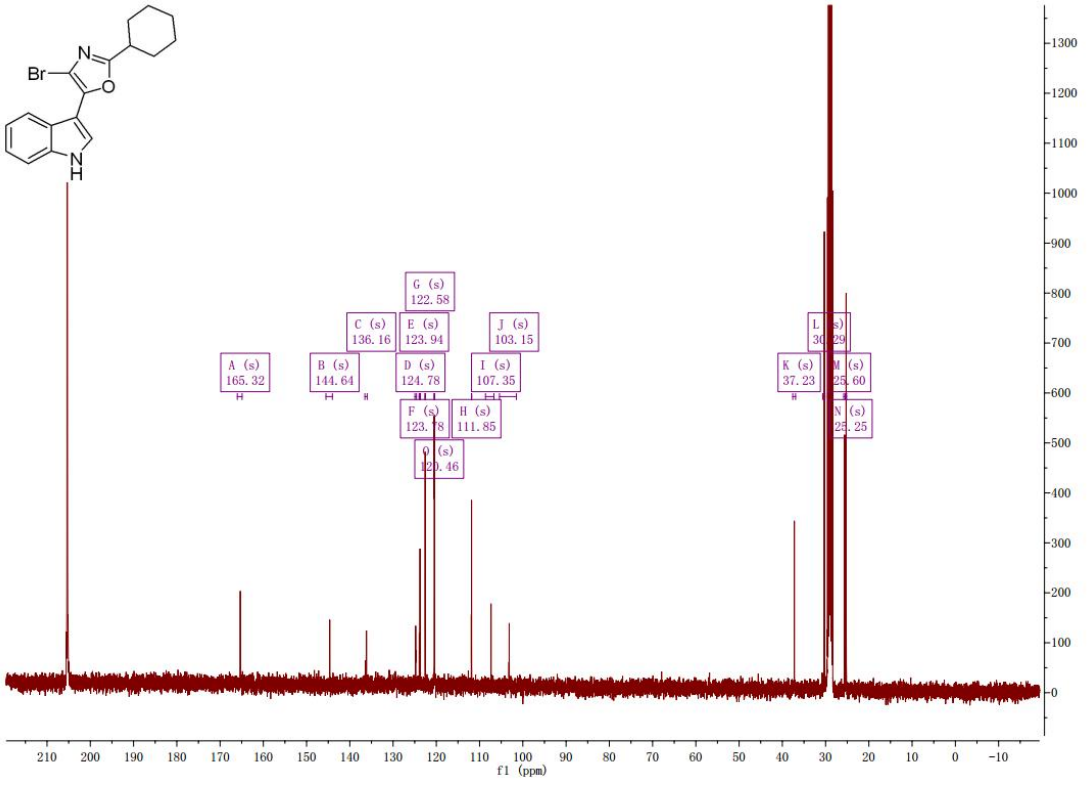
Compound 5c



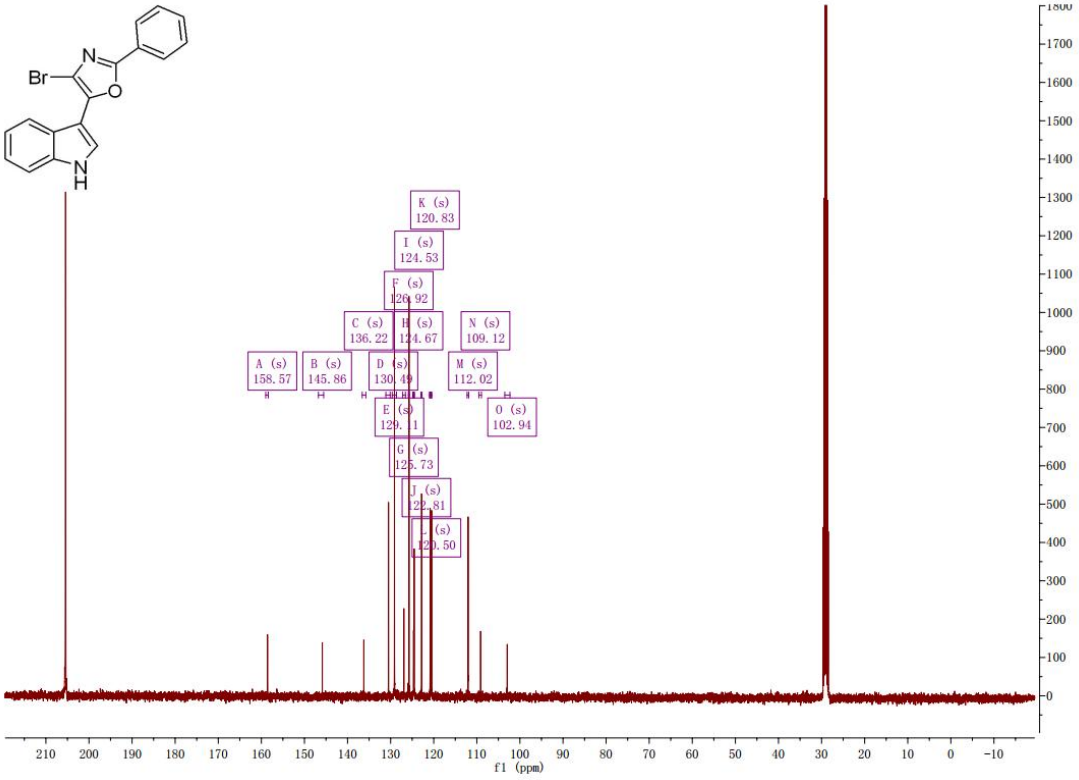
Compound 5d



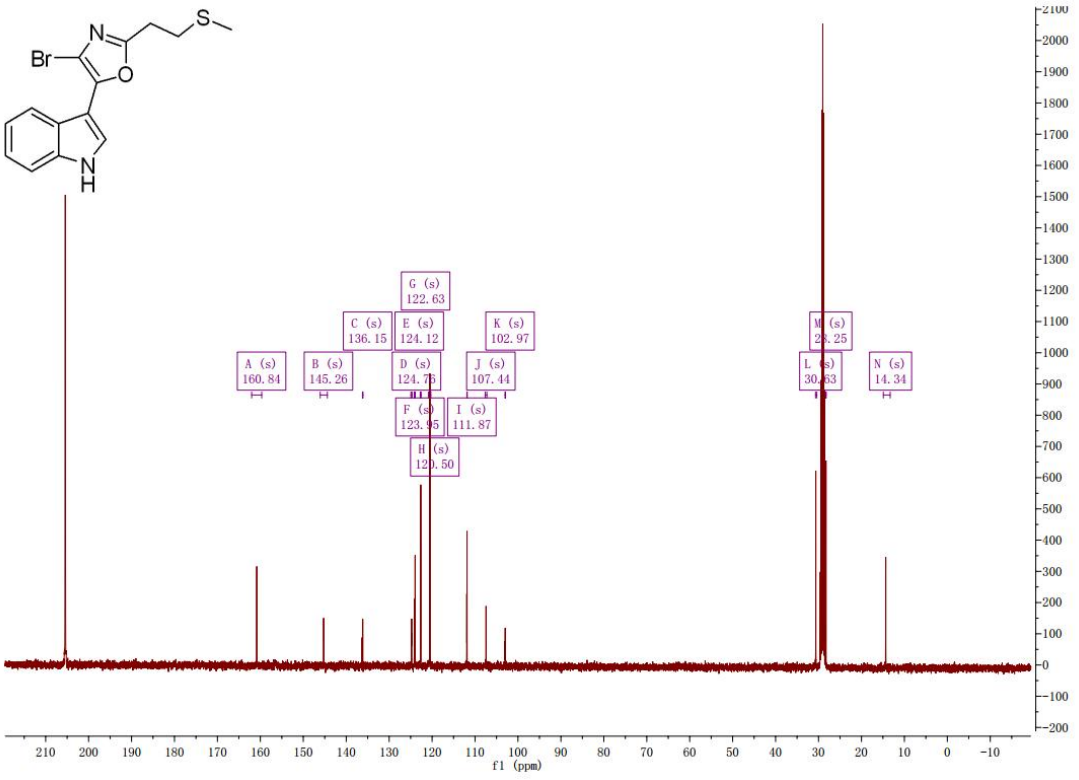
Compound 5e



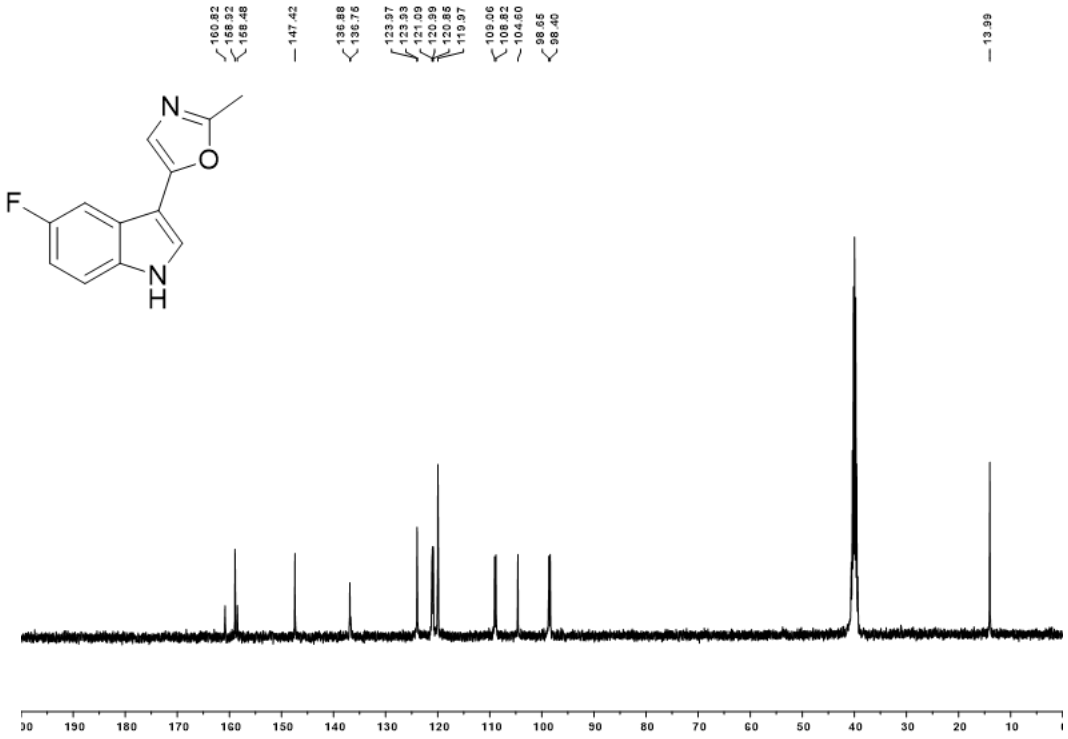
Compound 5f



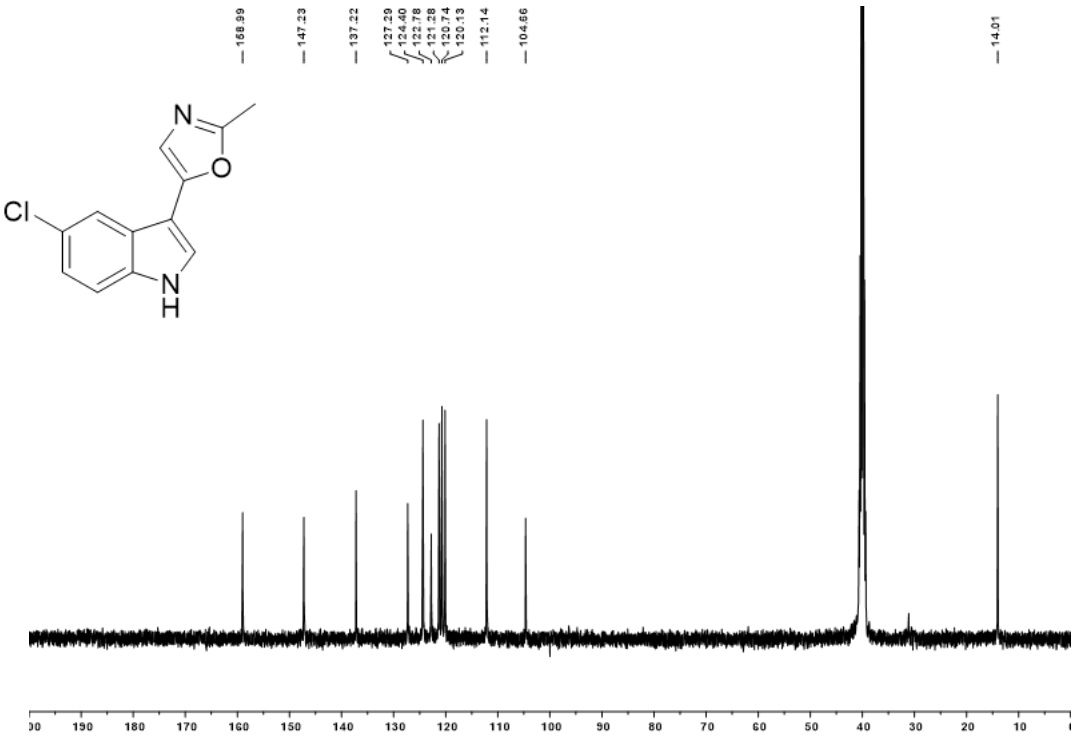
Compound 5g



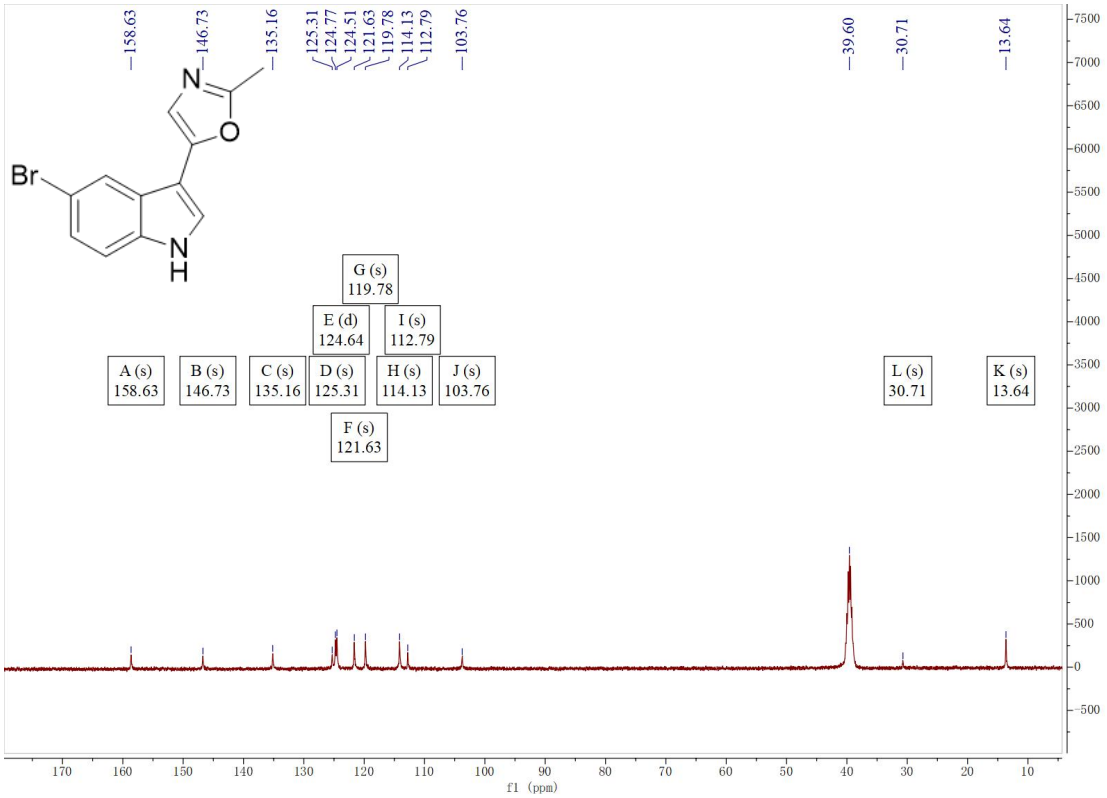
Compound 8a



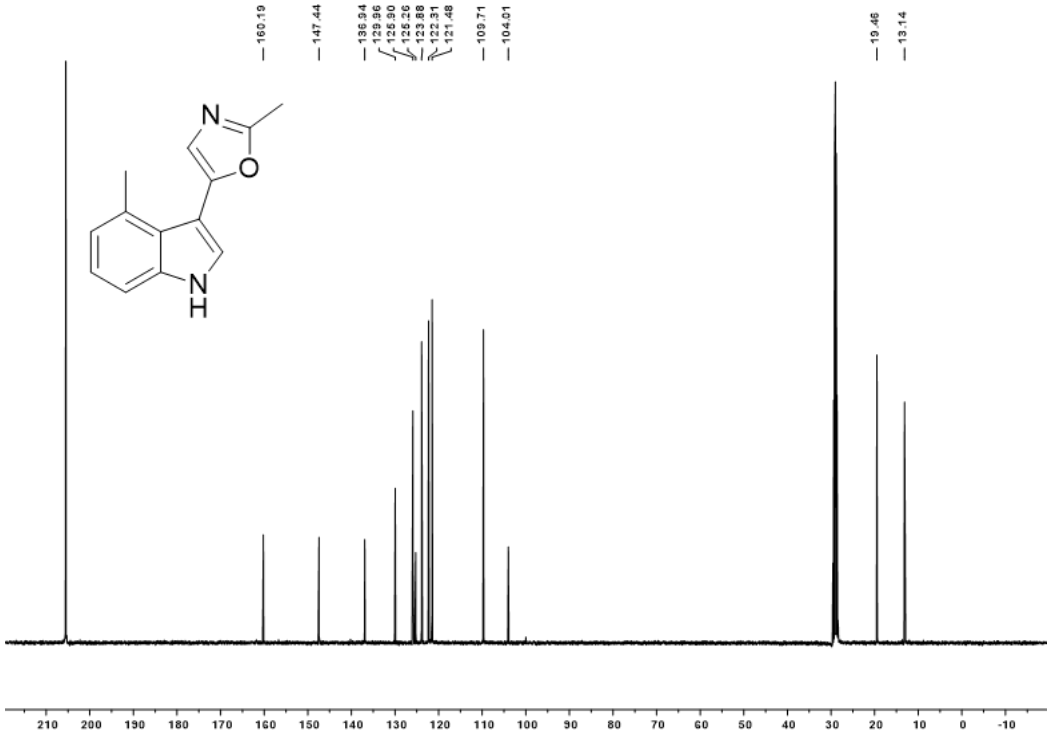
Compound 8b



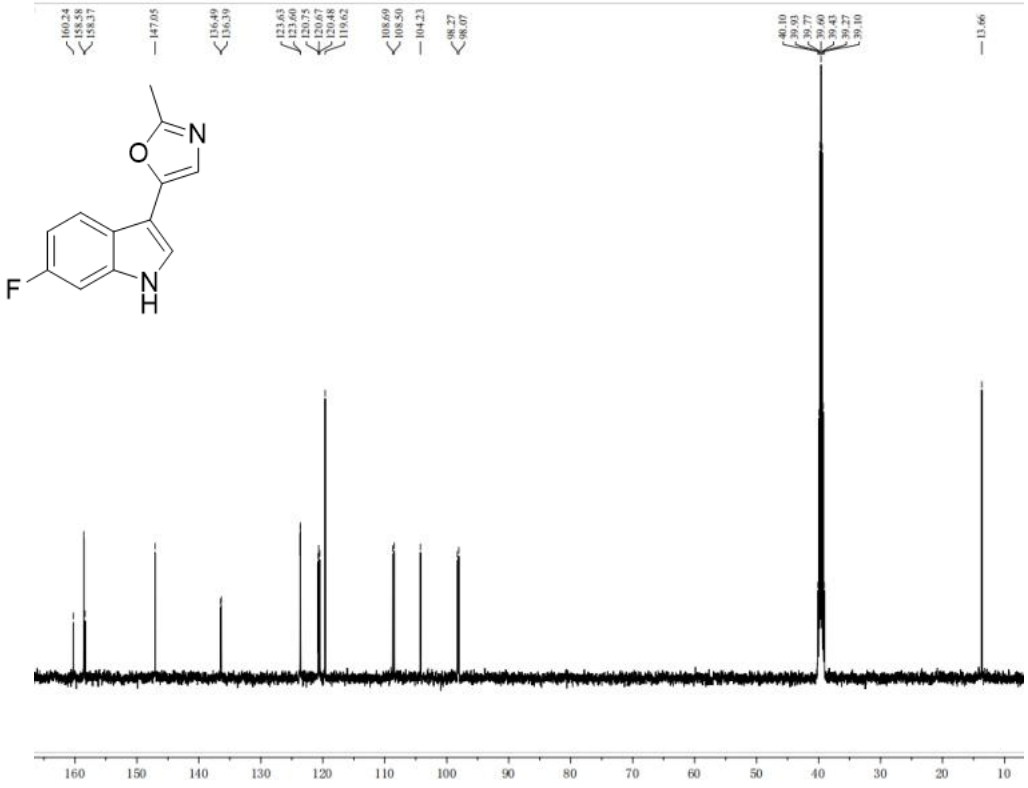
Compound 8c



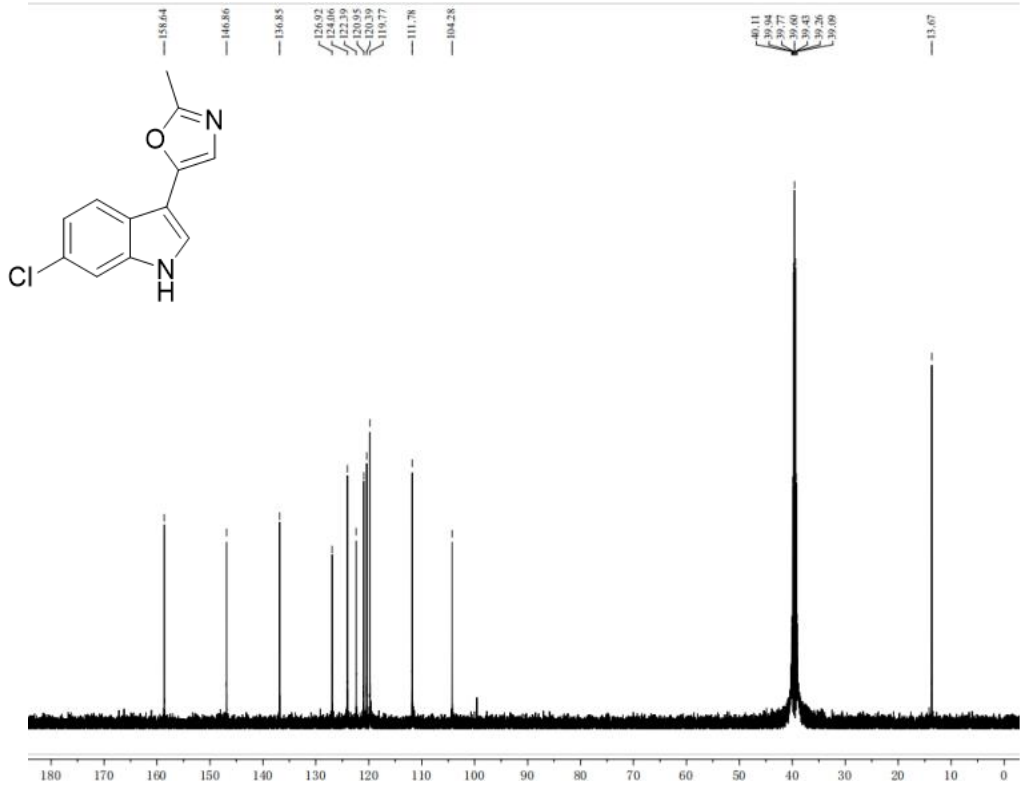
Compound 8d



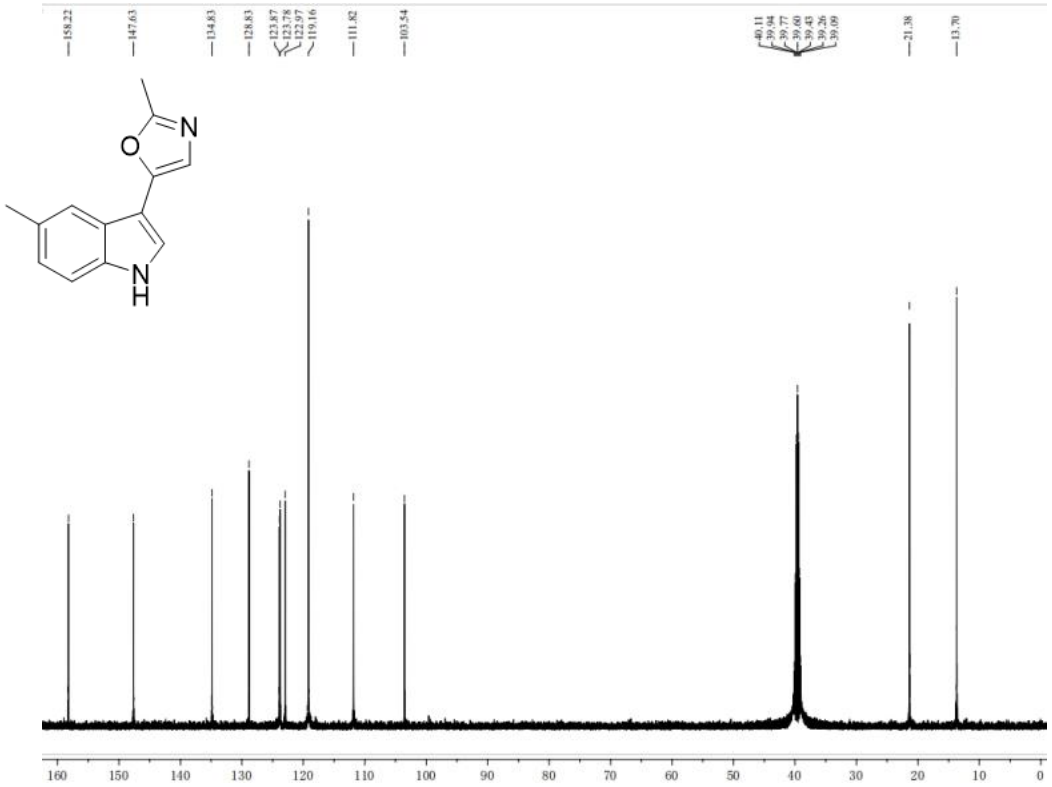
Compound 8e



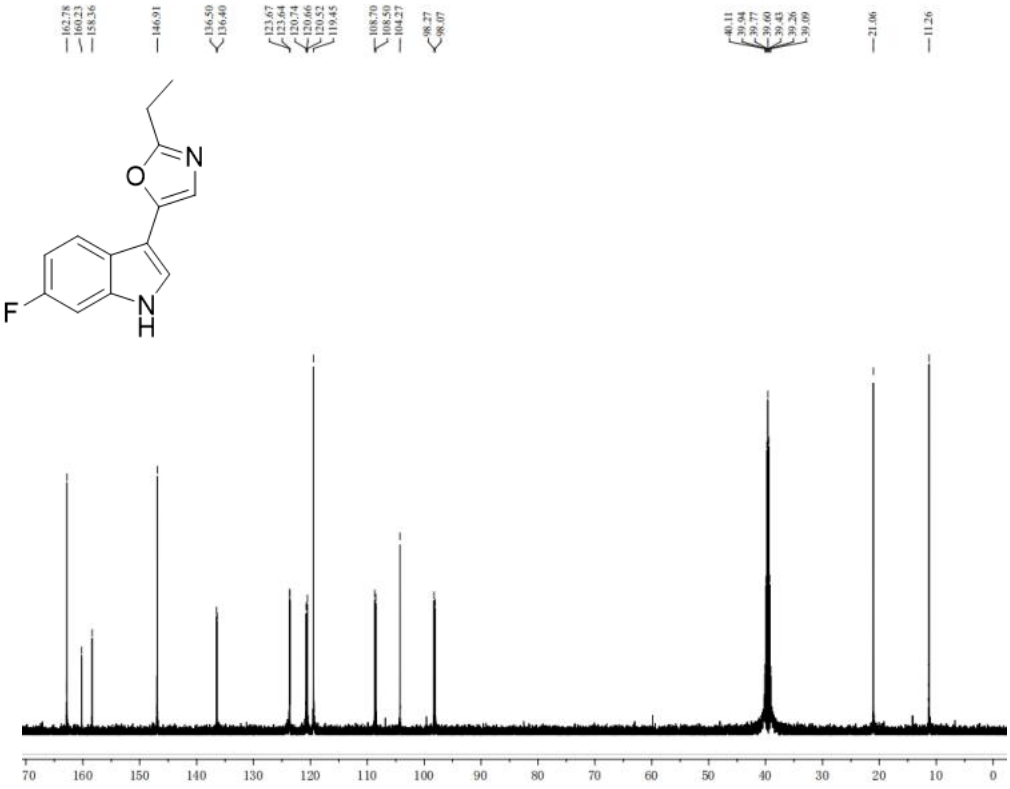
Compound 8f



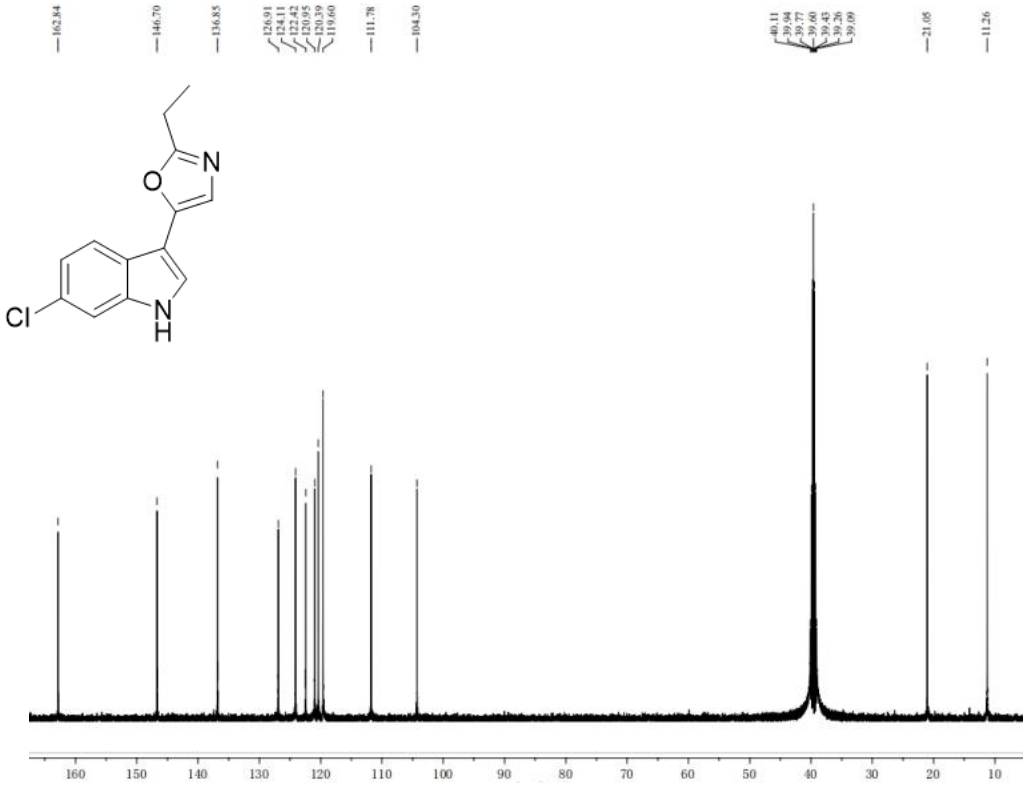
Compound 8g



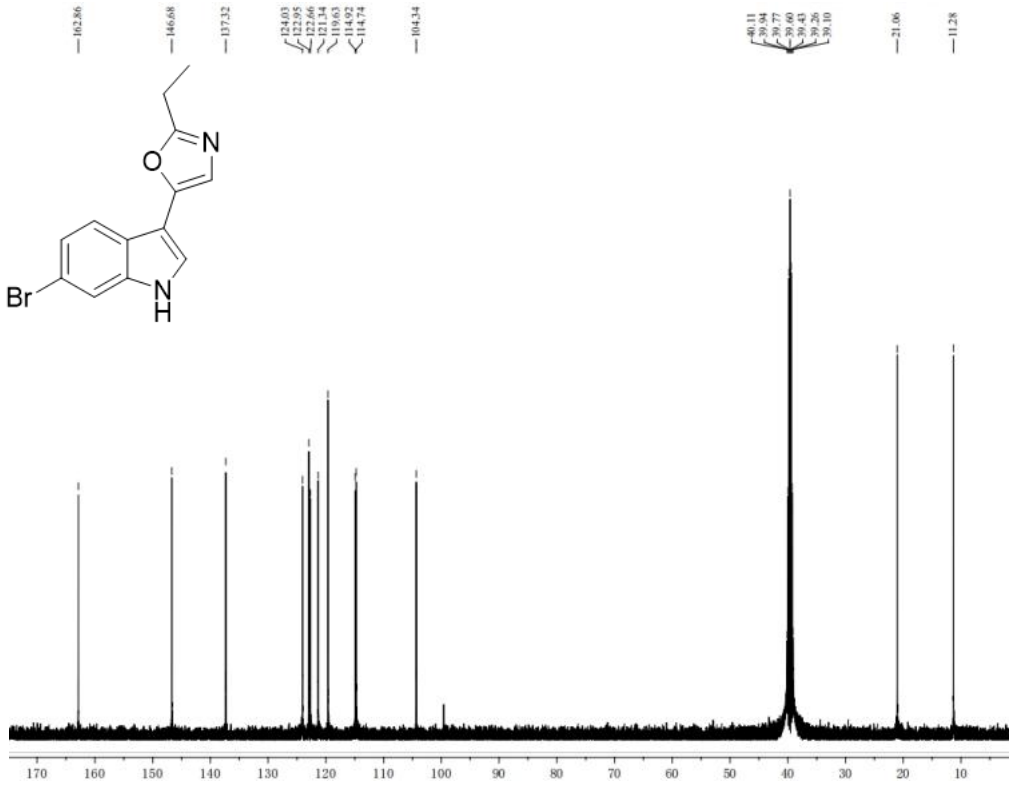
Compound 8h



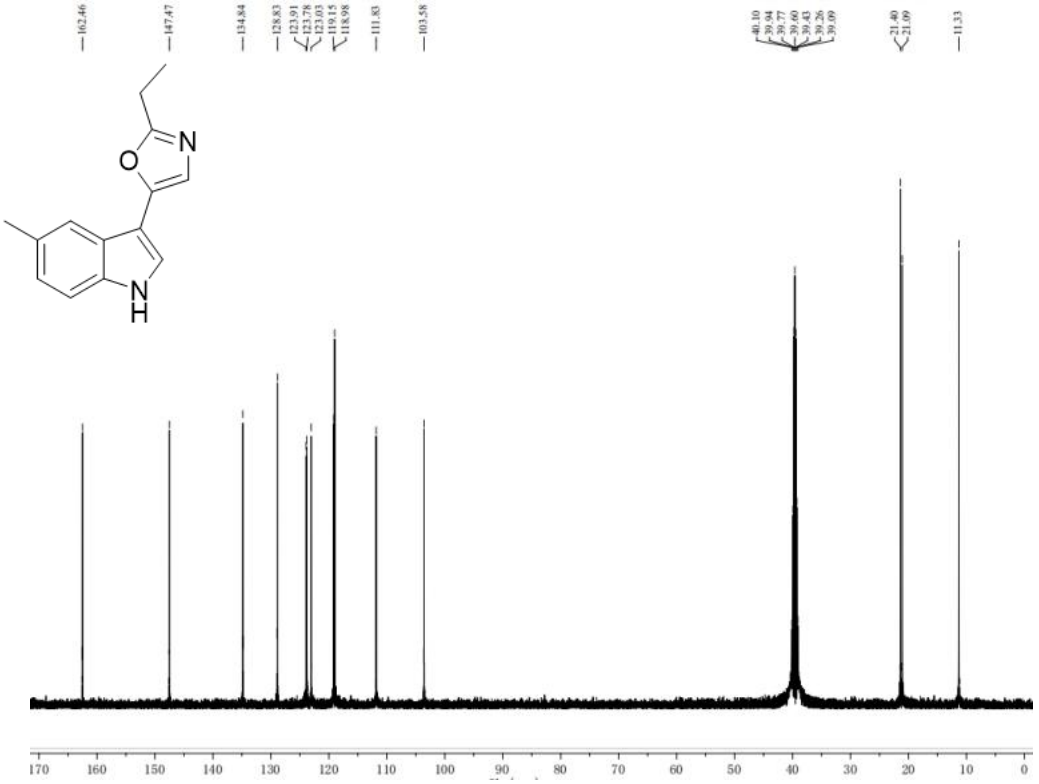
Compound 8i



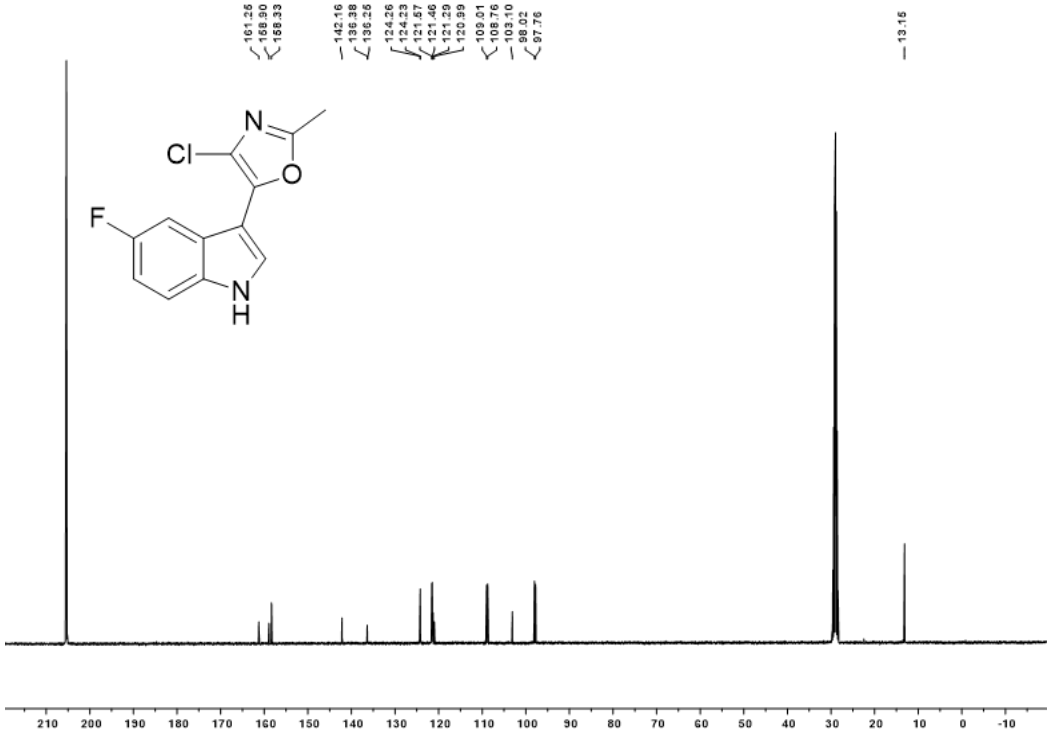
Compound 8j



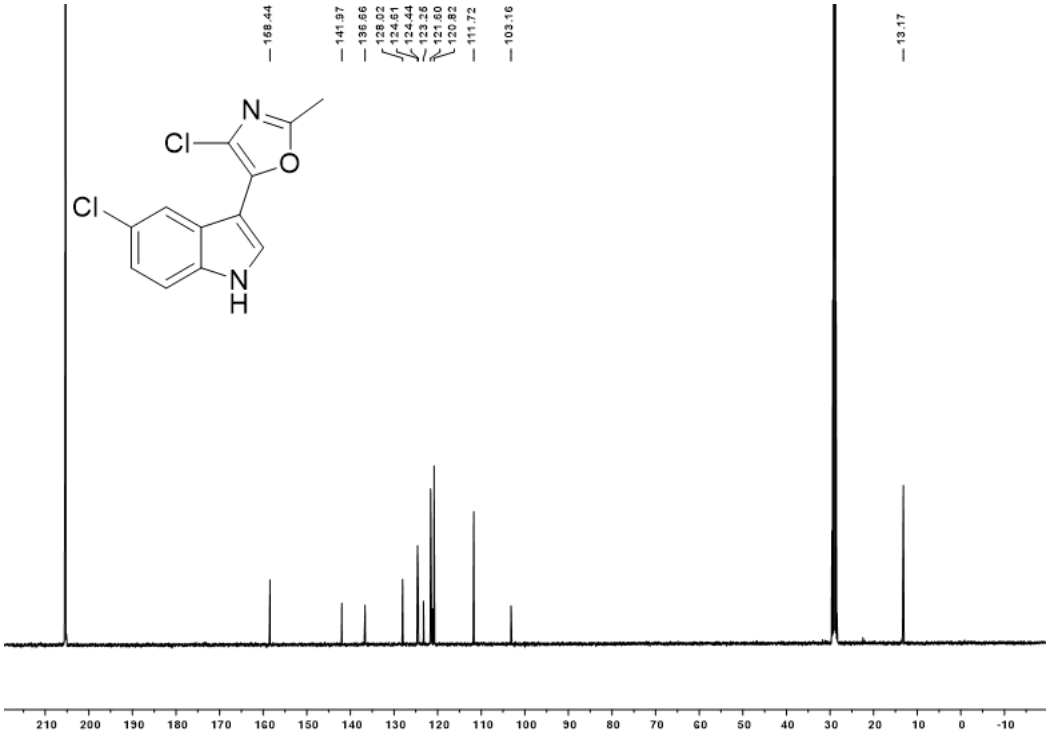
Compound 8k



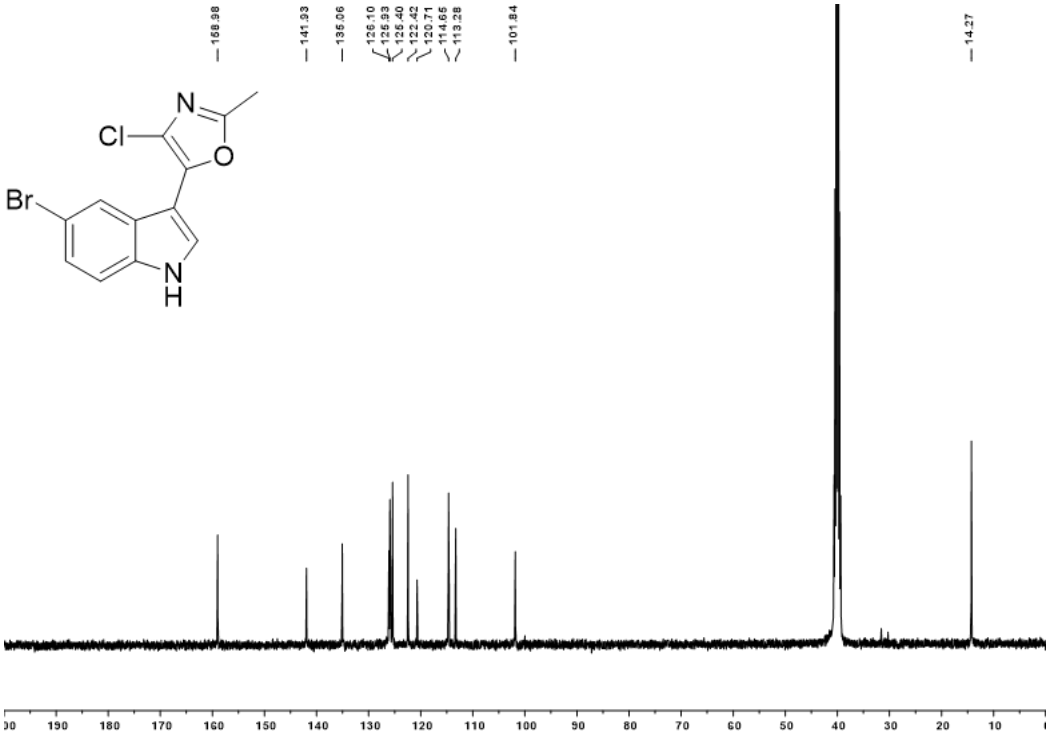
Compound 9a



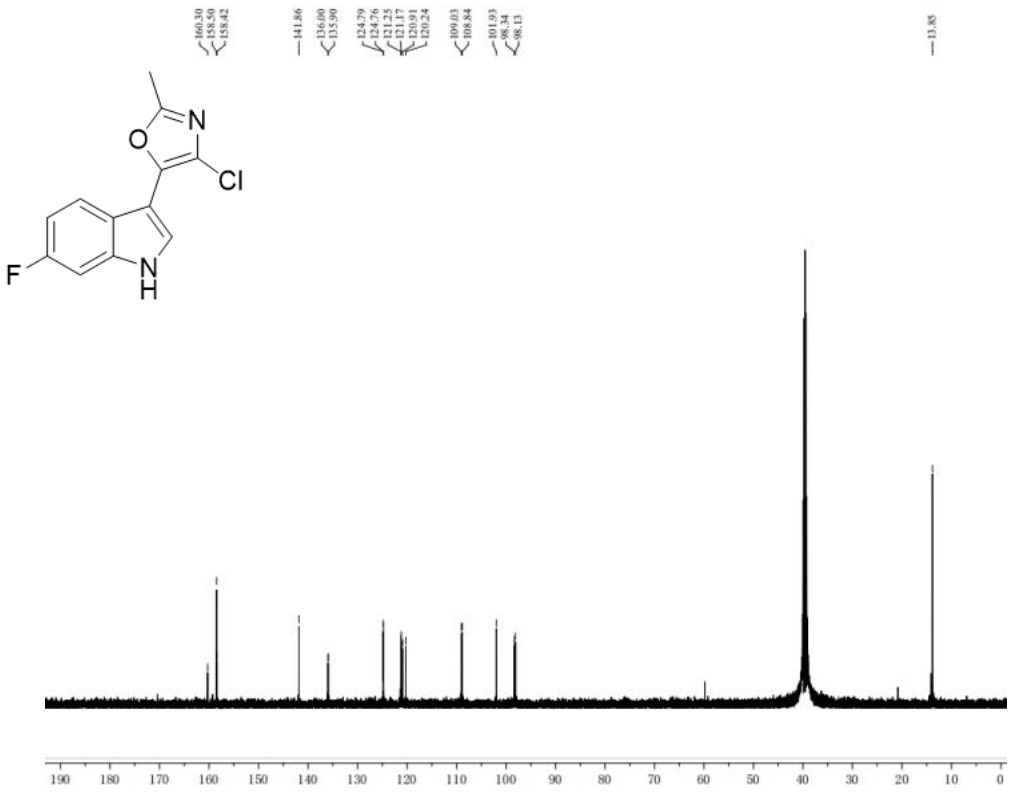
Compound 9b



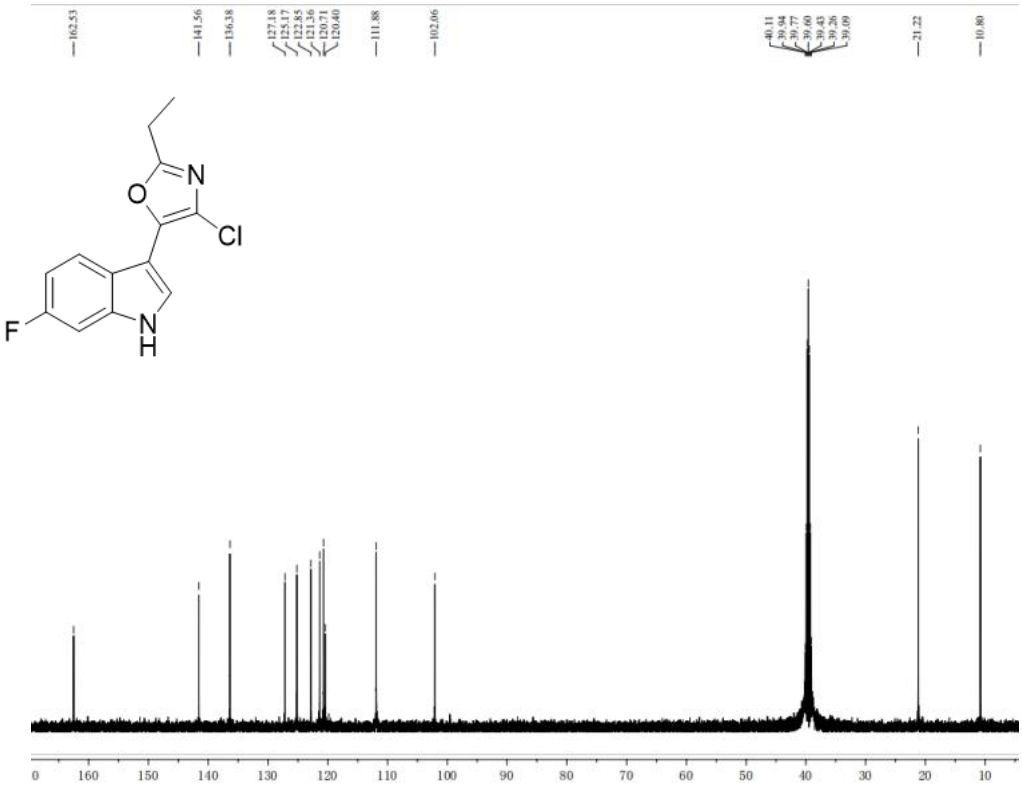
Compound 9c



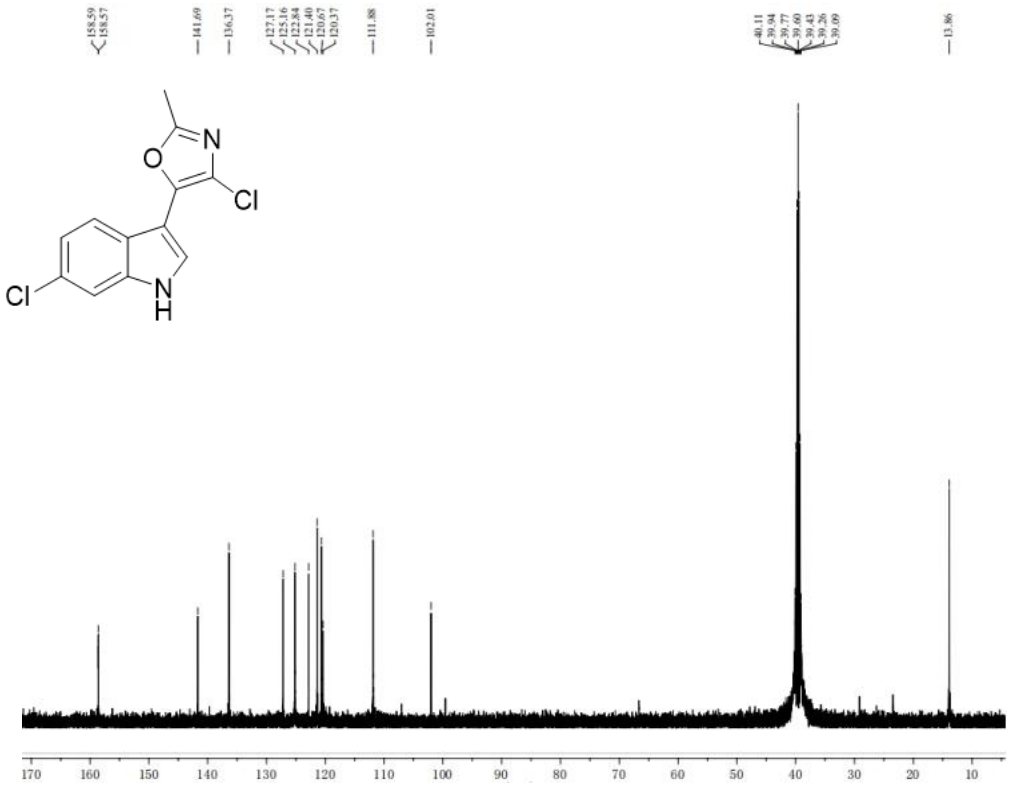
Compound 9d



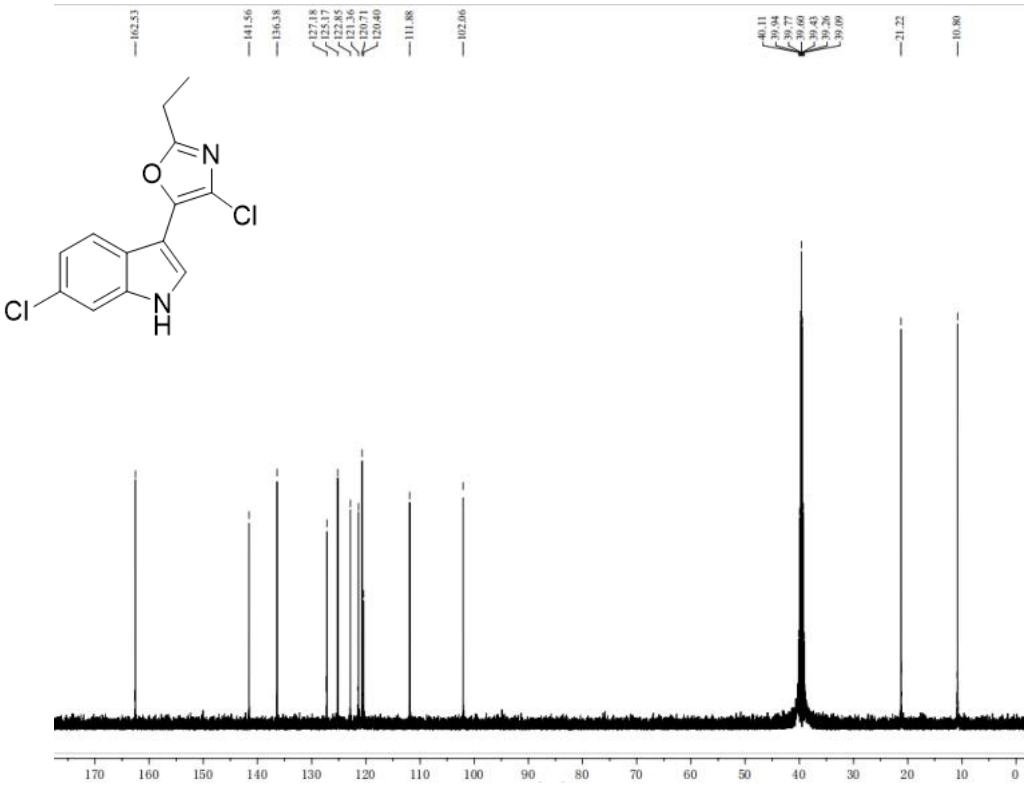
Compound 9e



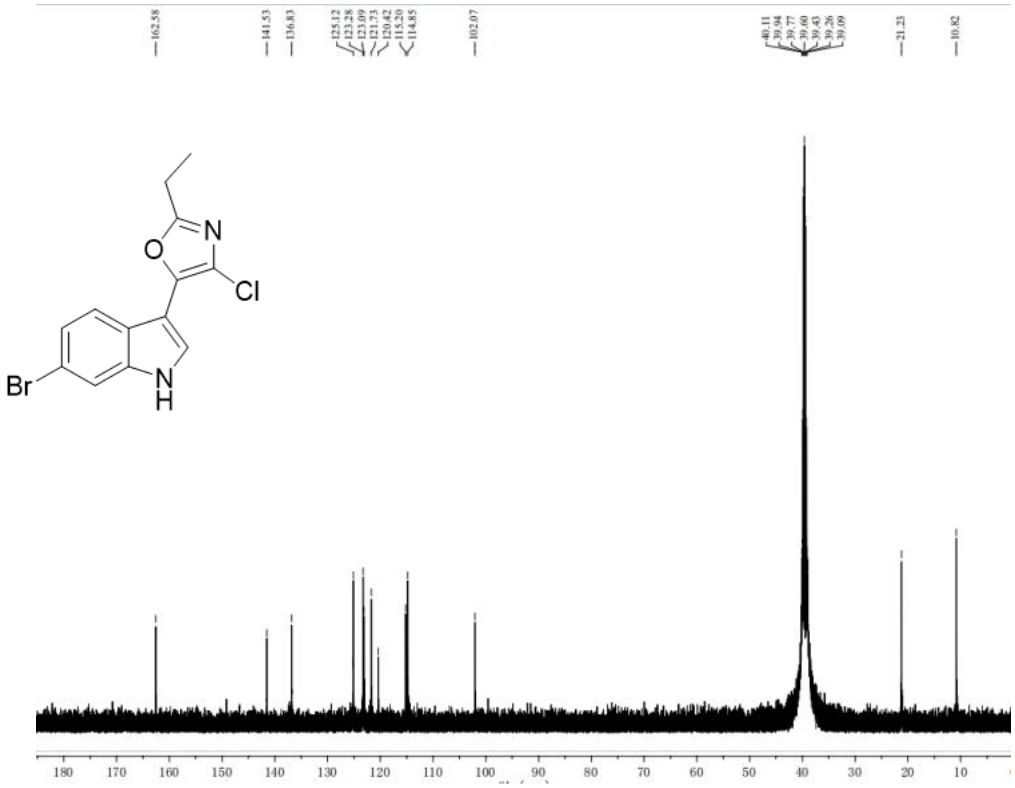
Compound 9f



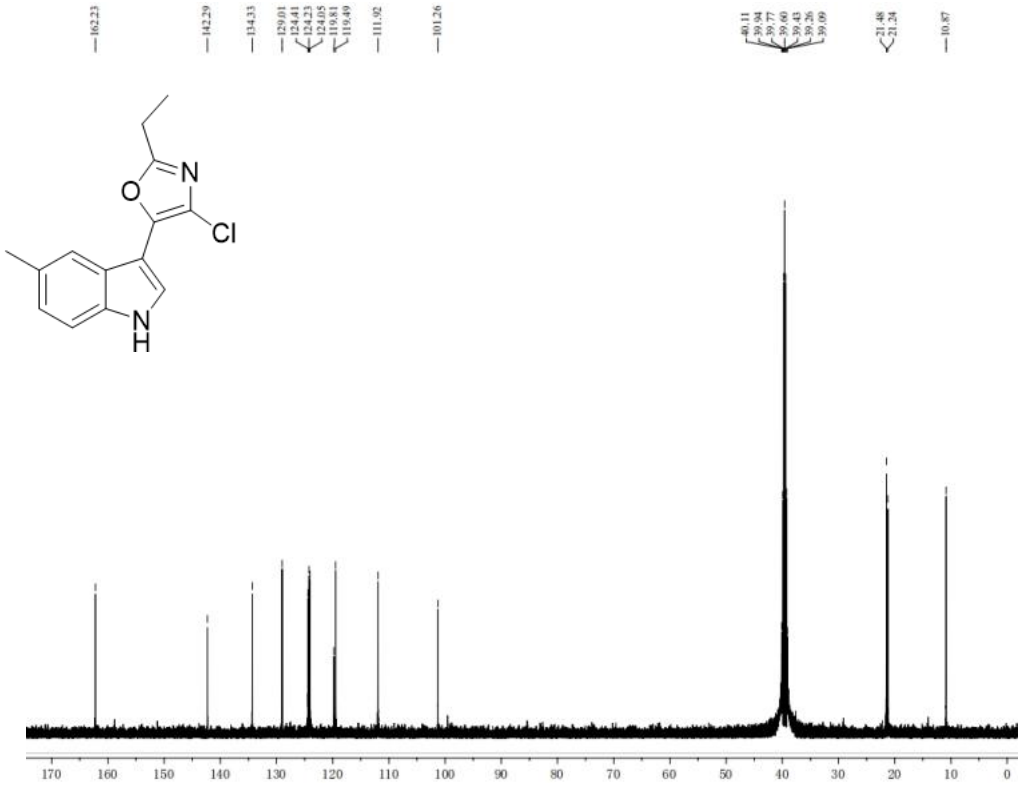
Compound 9g



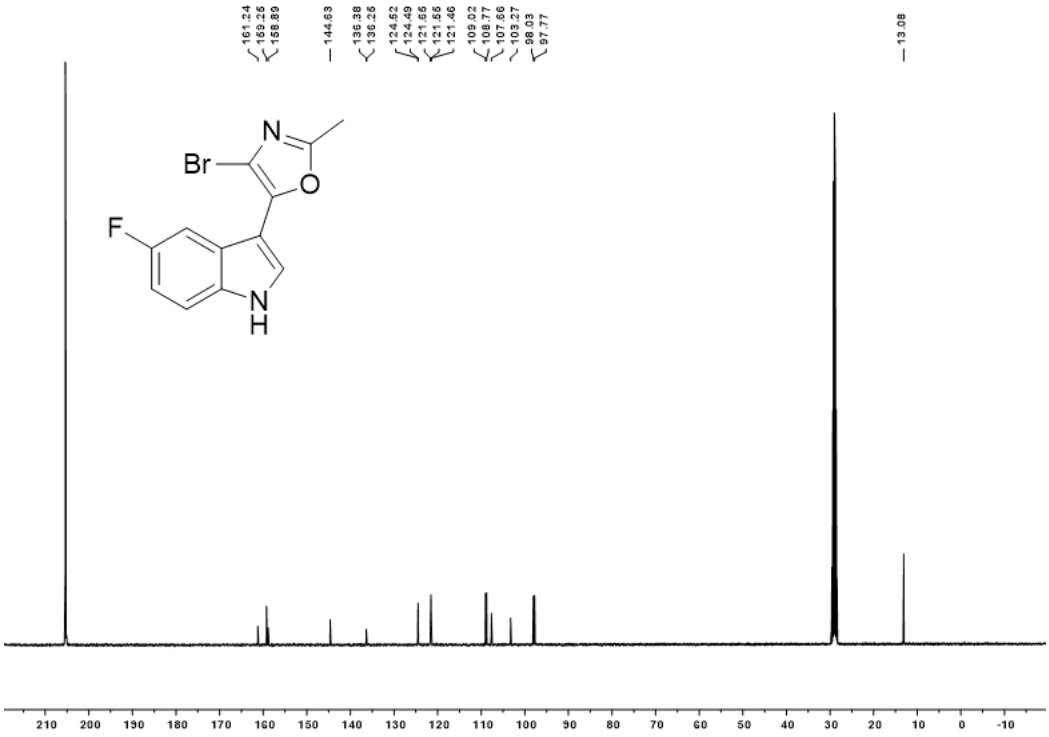
Compound 9h



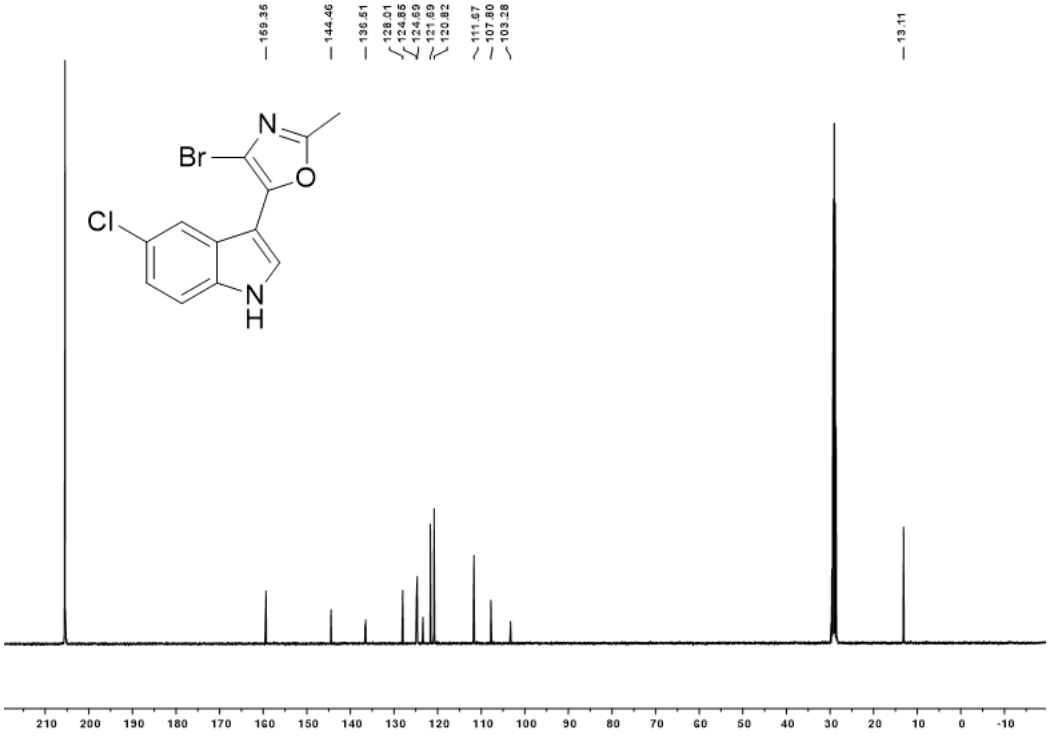
Compound 9i



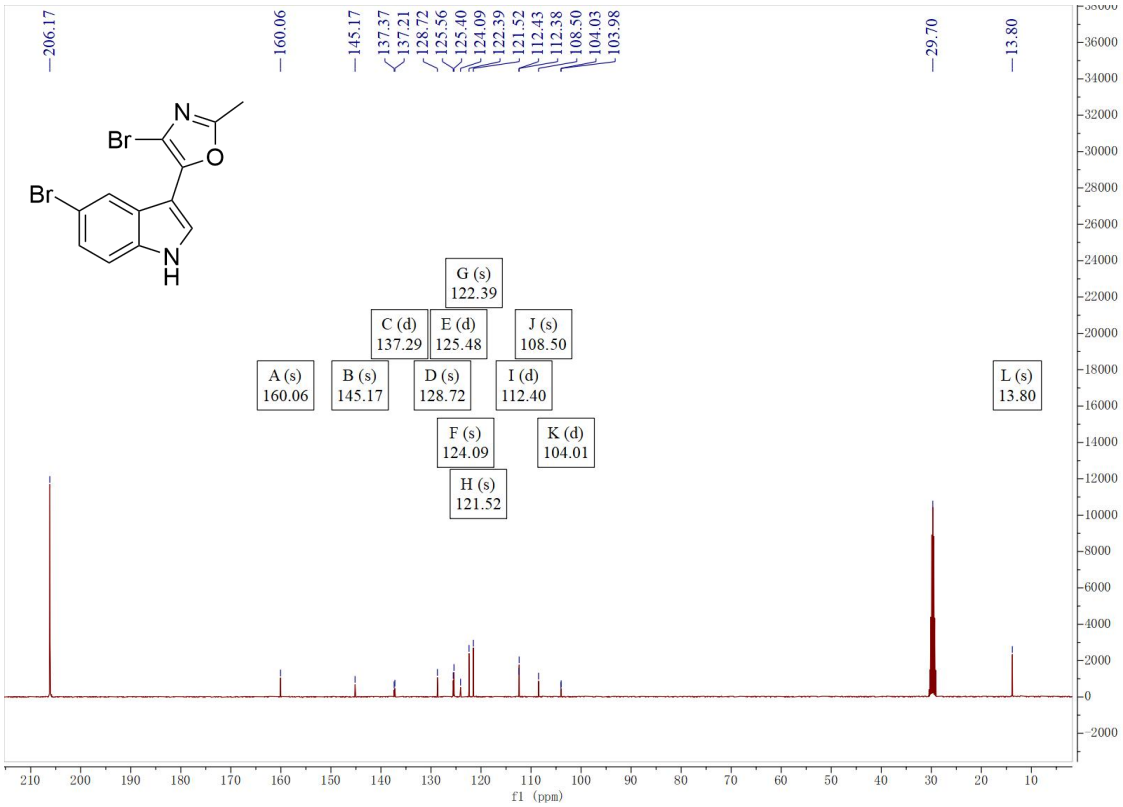
Compound 10a



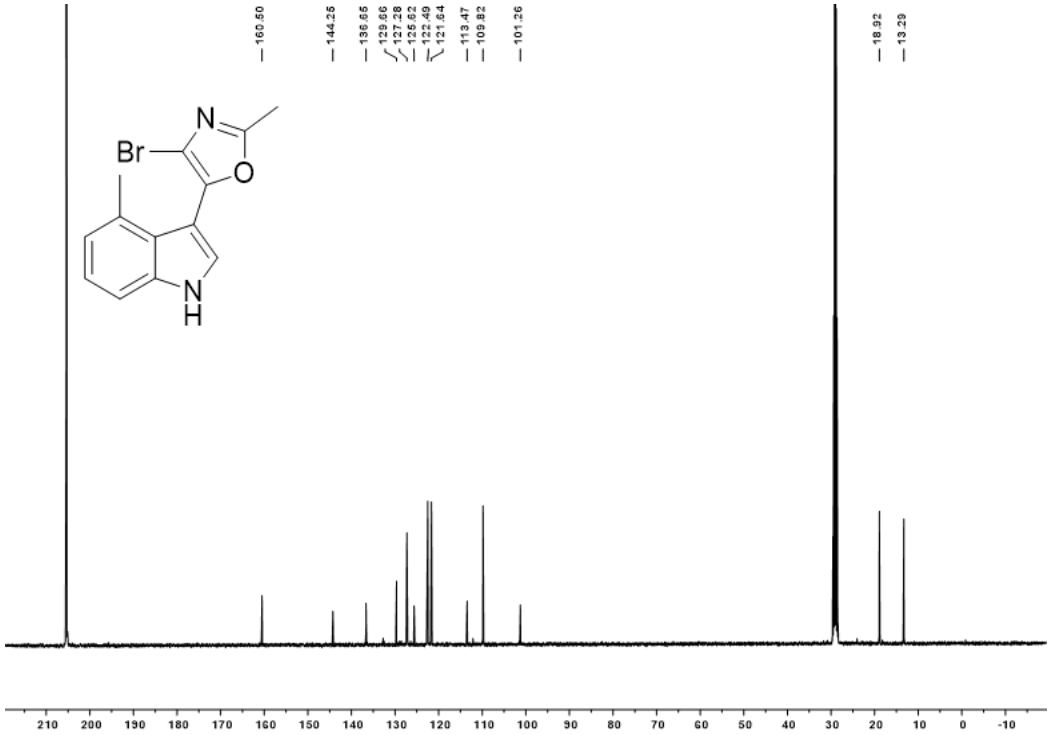
Compound 10b



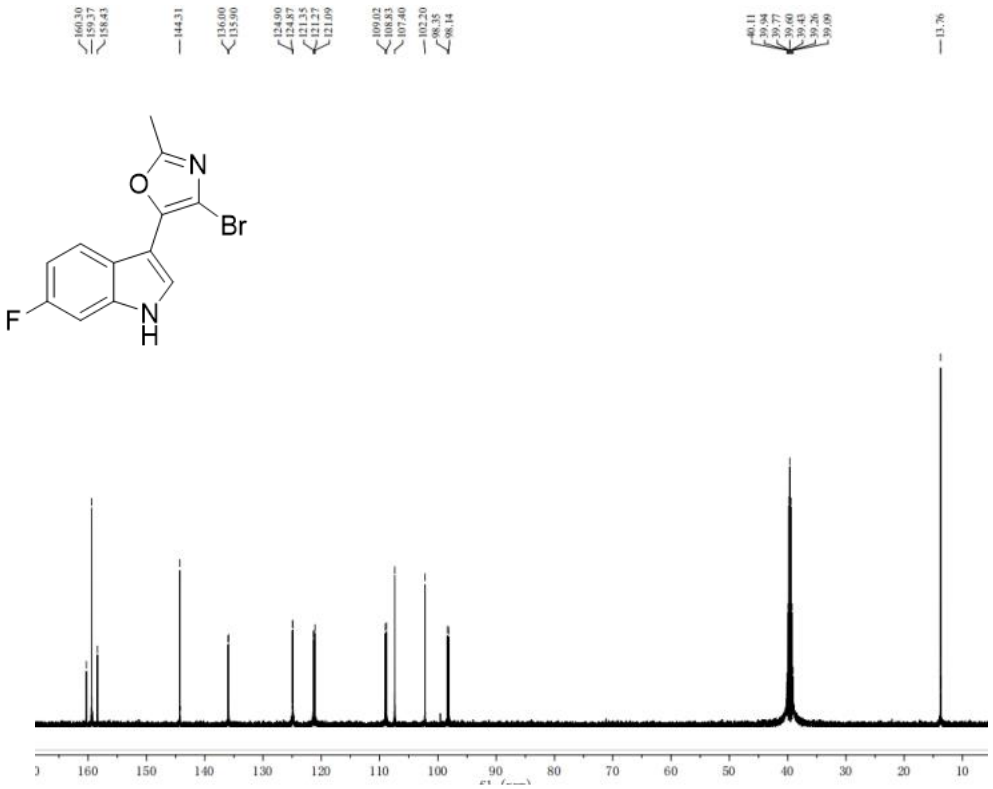
Compound 10c



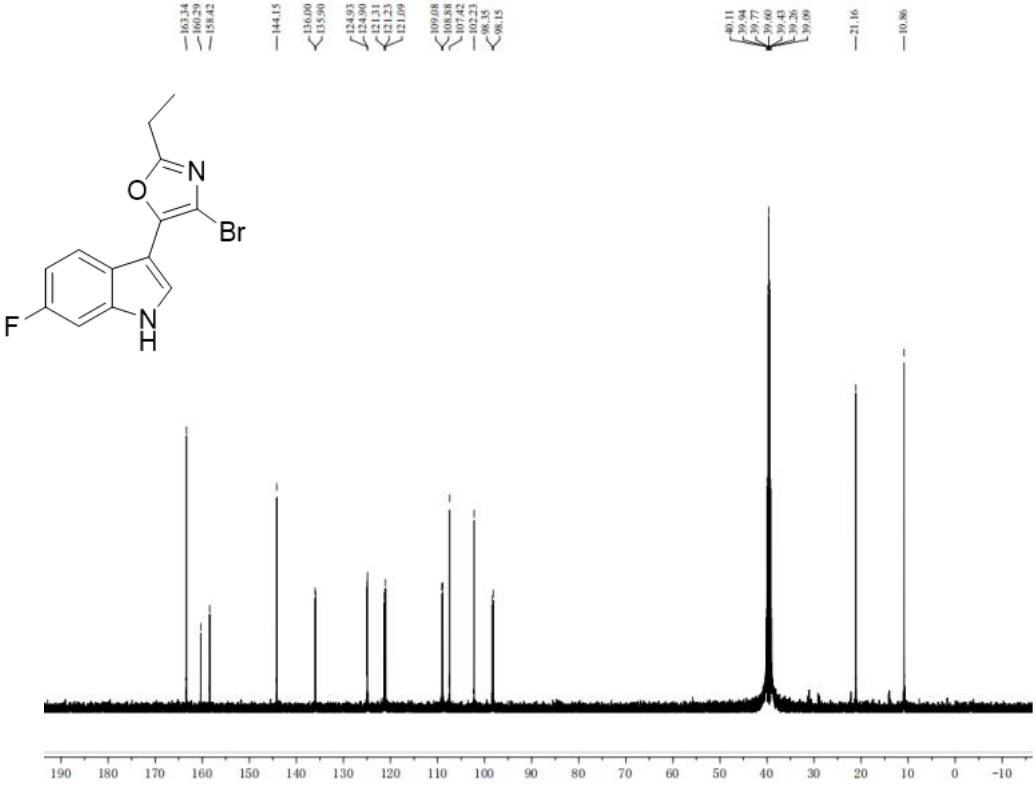
Compound 10d



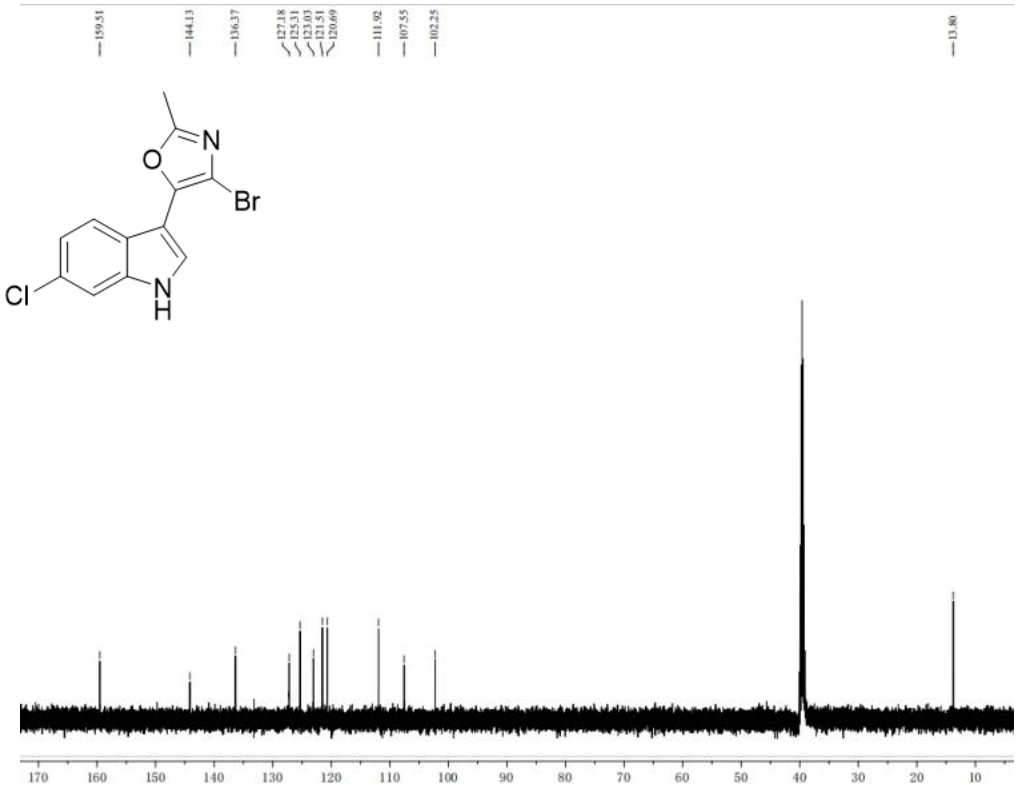
Compound 10e



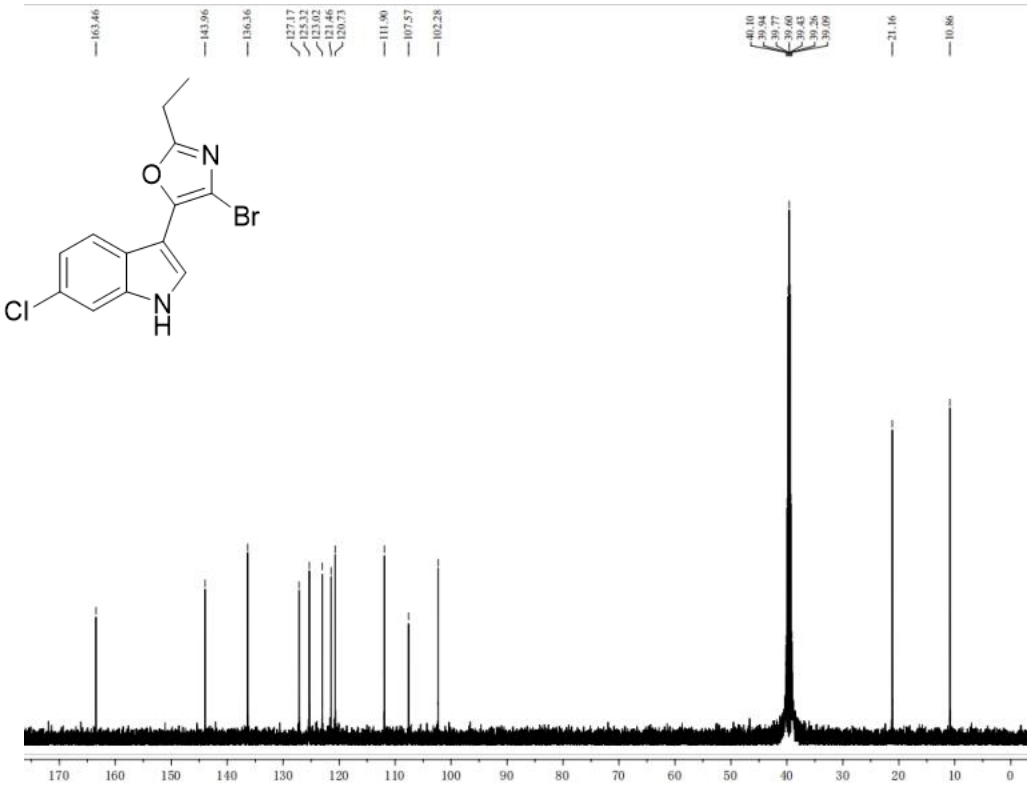
Compound 10f



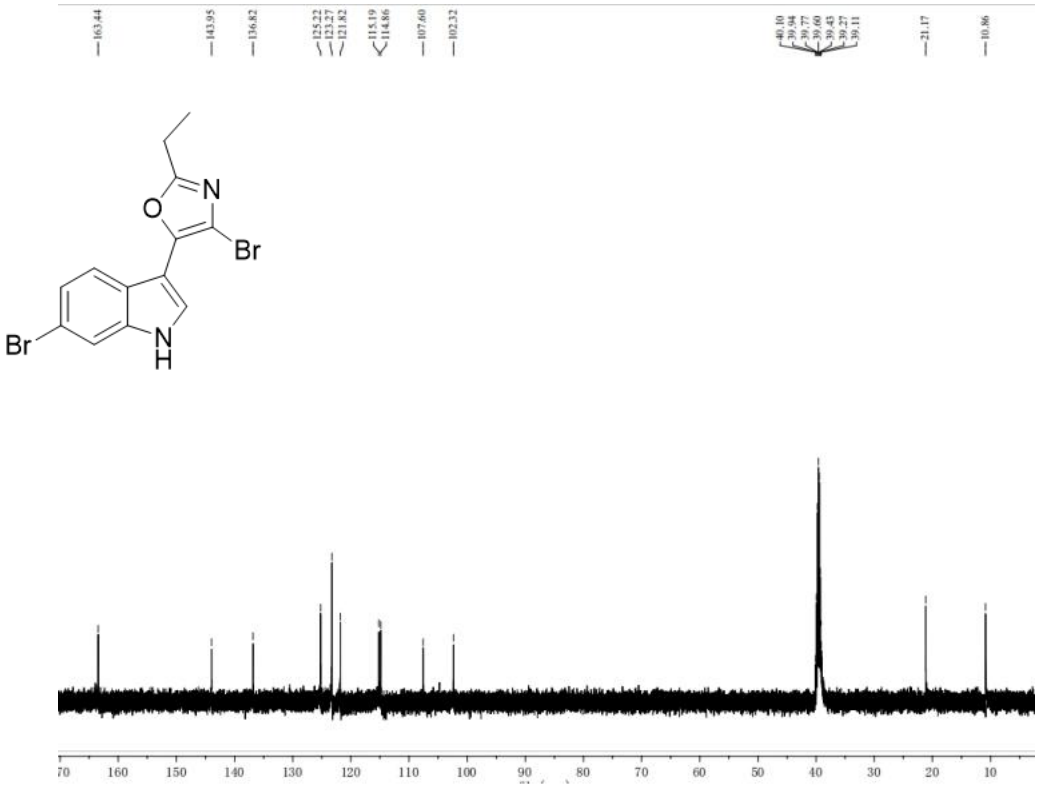
Compound 10g



Compound 10h



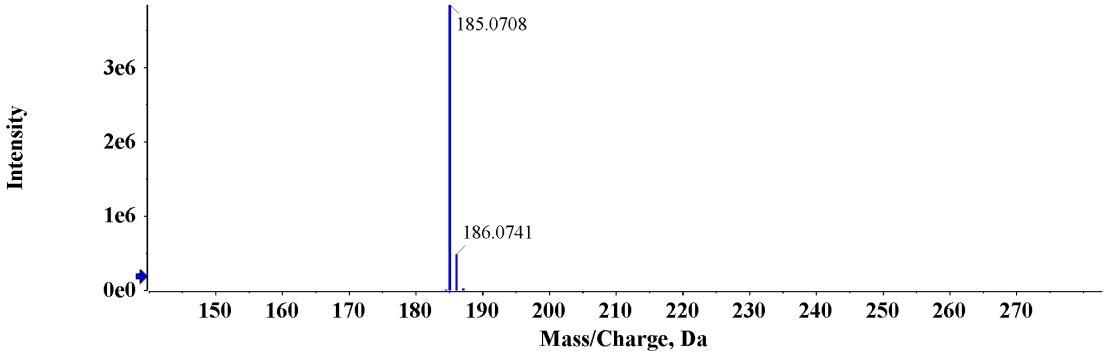
Compound 10i



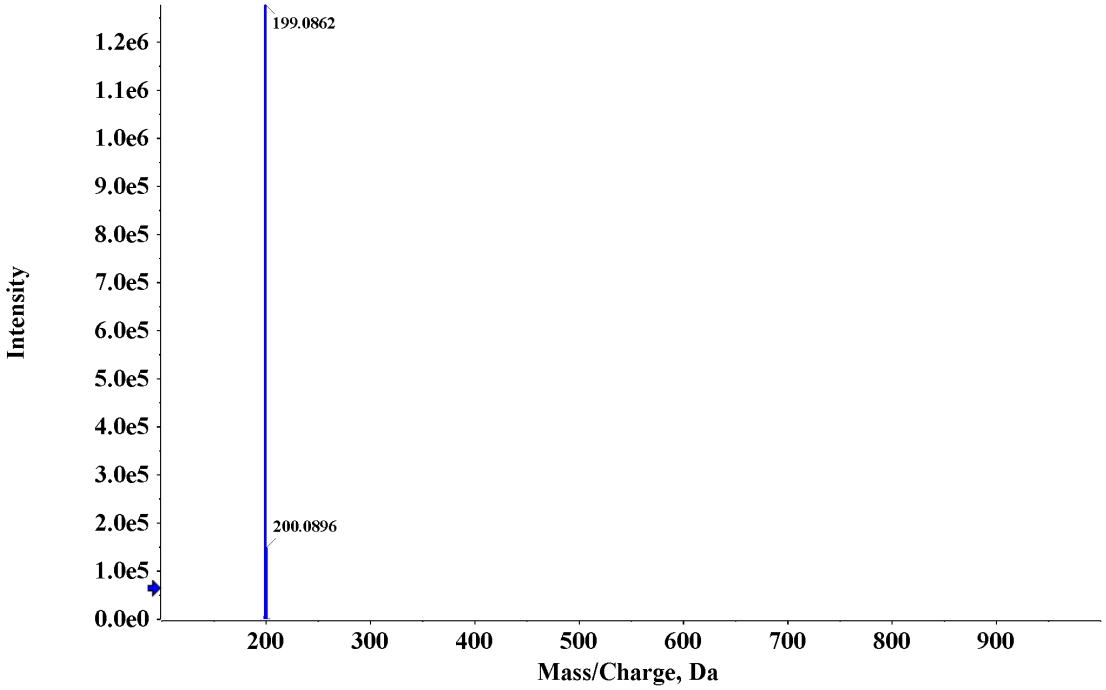
4. HR-MS

Compound 3a

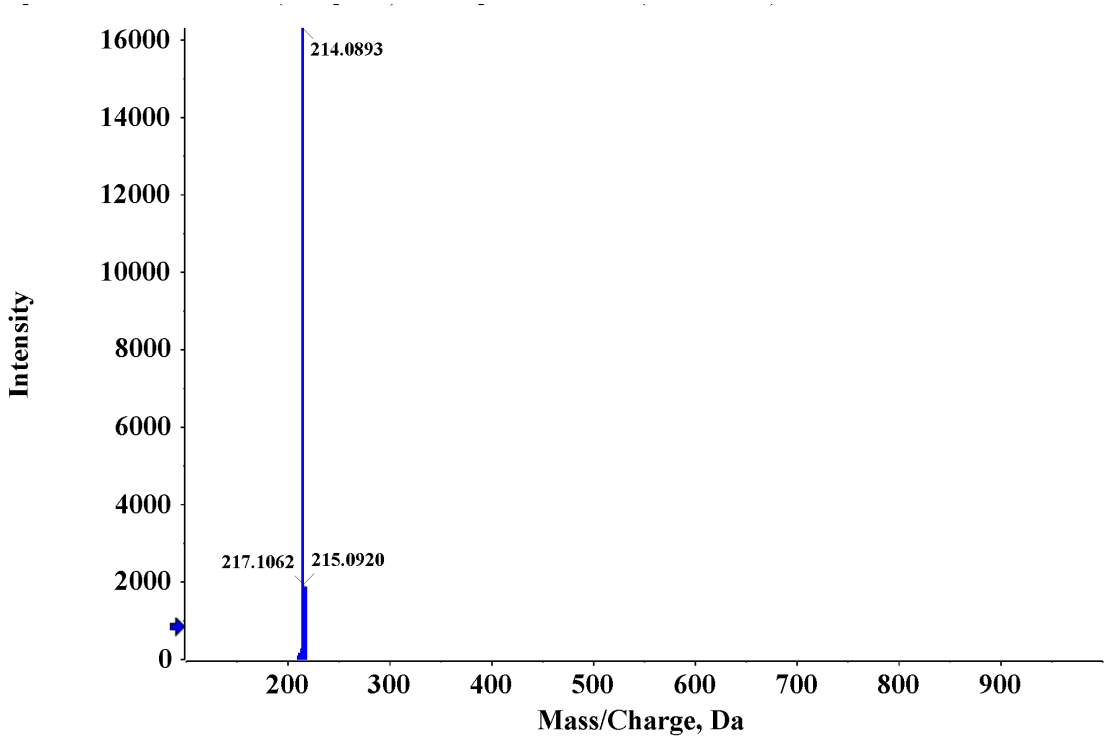
Spectrum from 3.wiff (sample 1) - Sample004, +TOF MS (90 - 1000) from 2.084 to 2.091 min



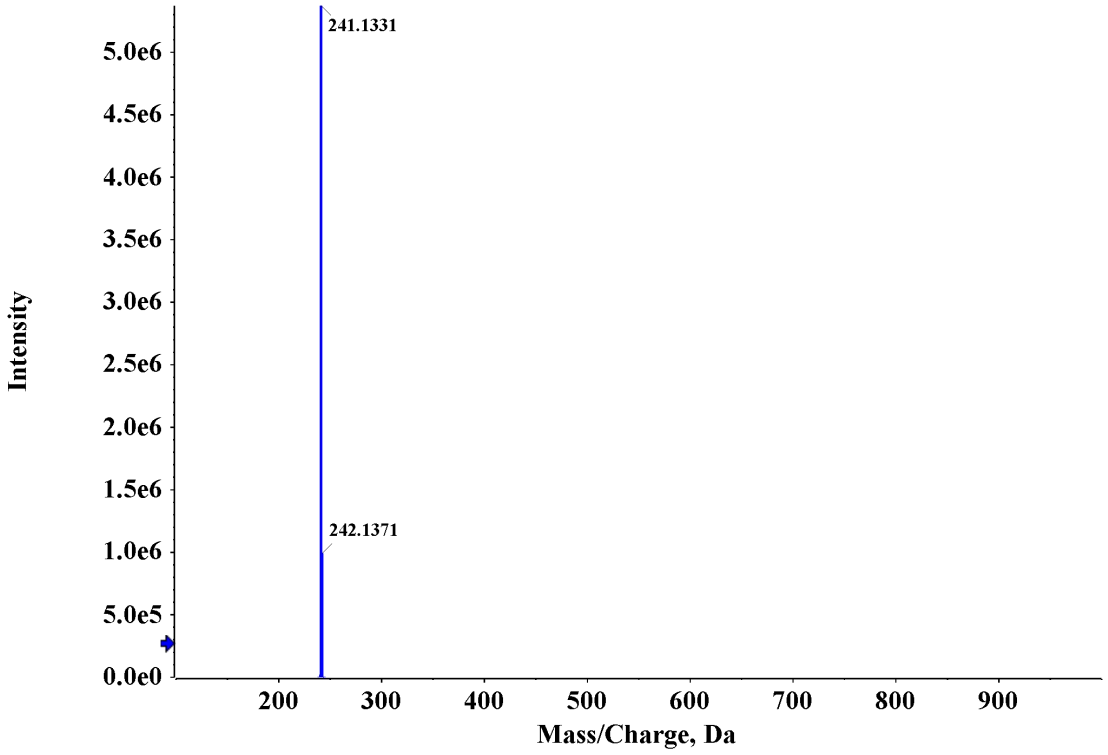
Compound 3b



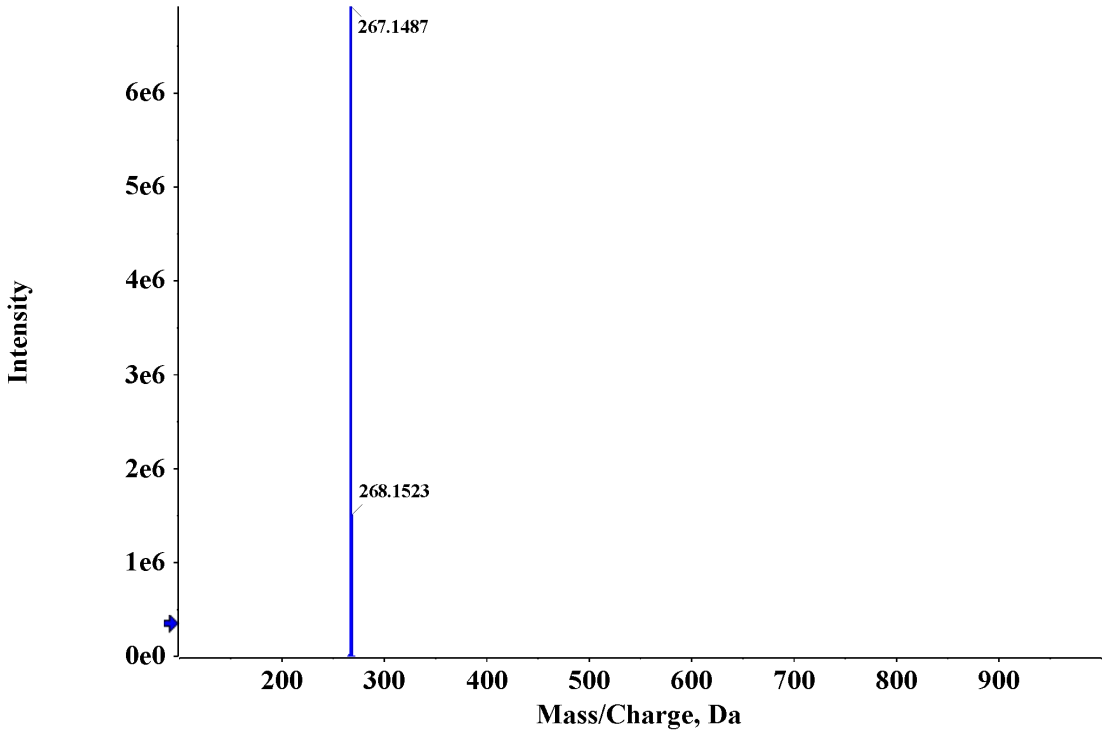
Compound 3c



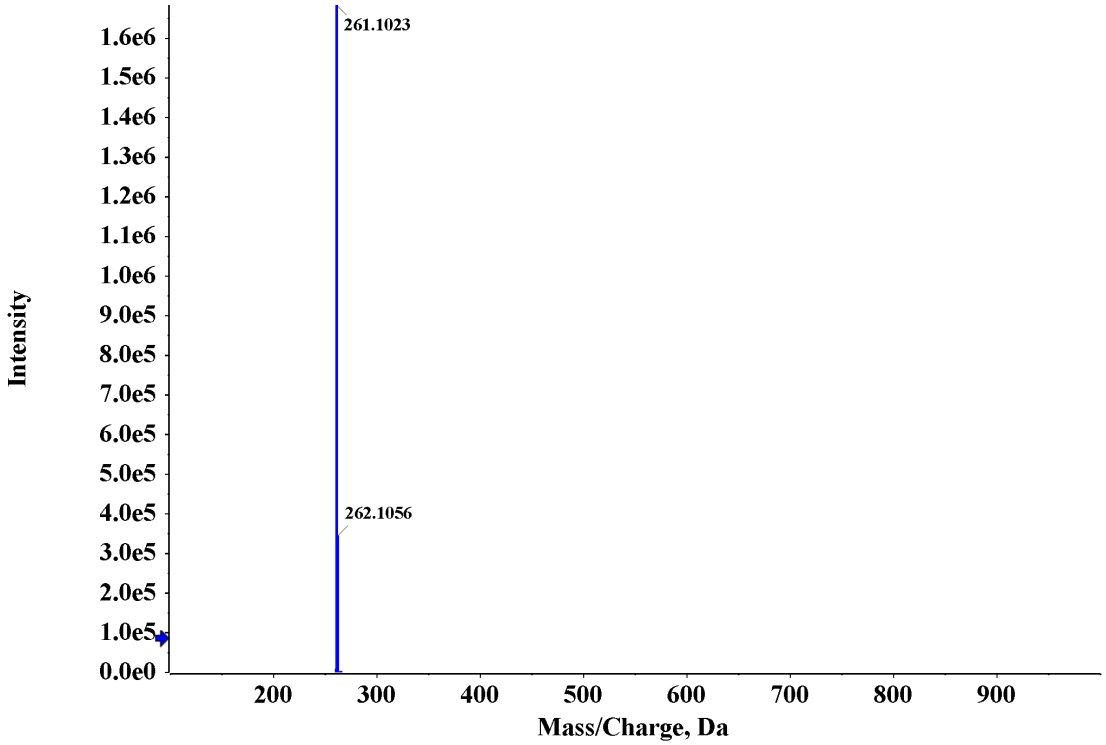
Compound 3d



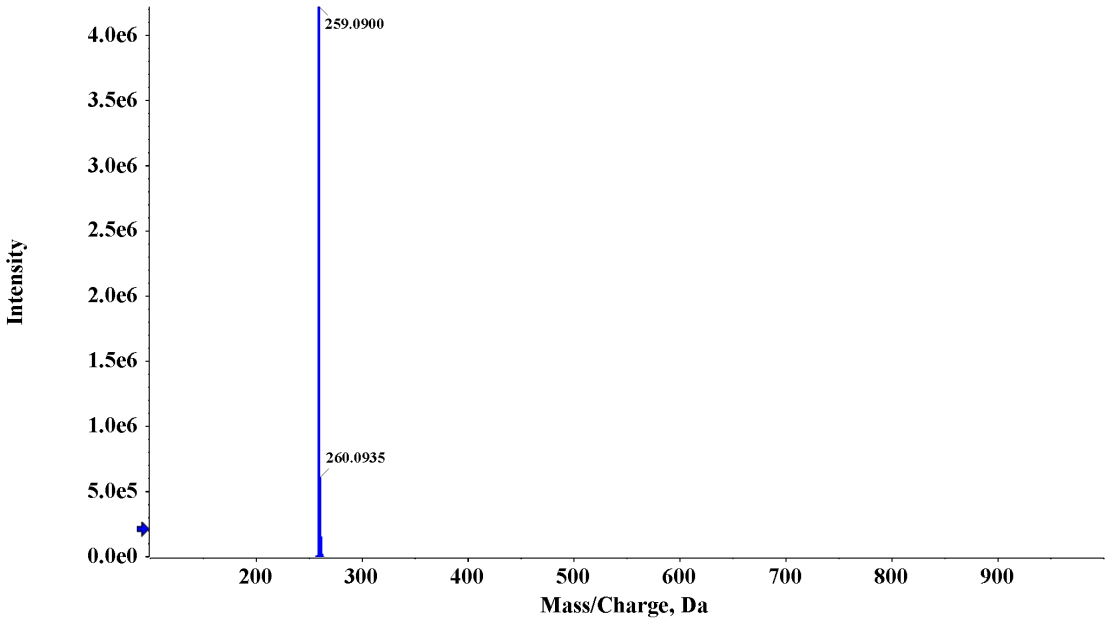
Compound 3e



Compound 3f

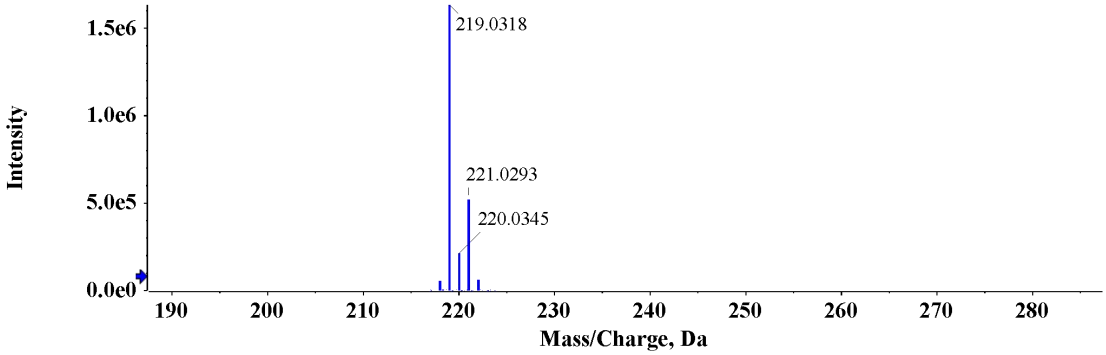


Compound 3g

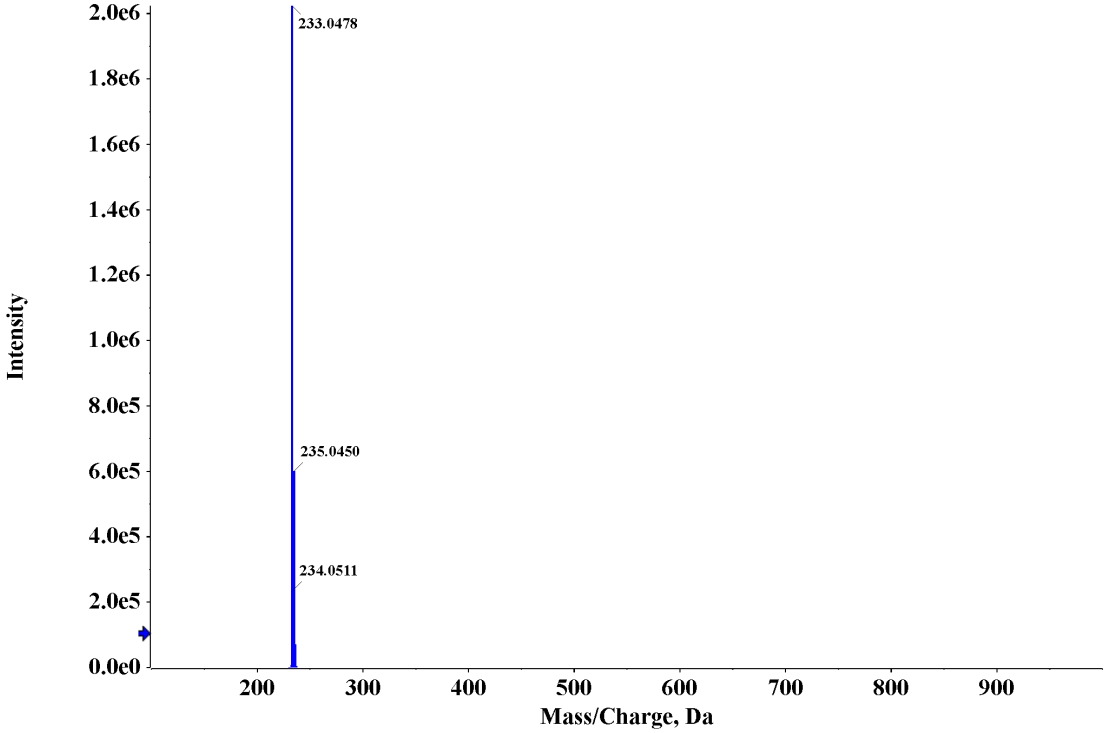


Compound 4a

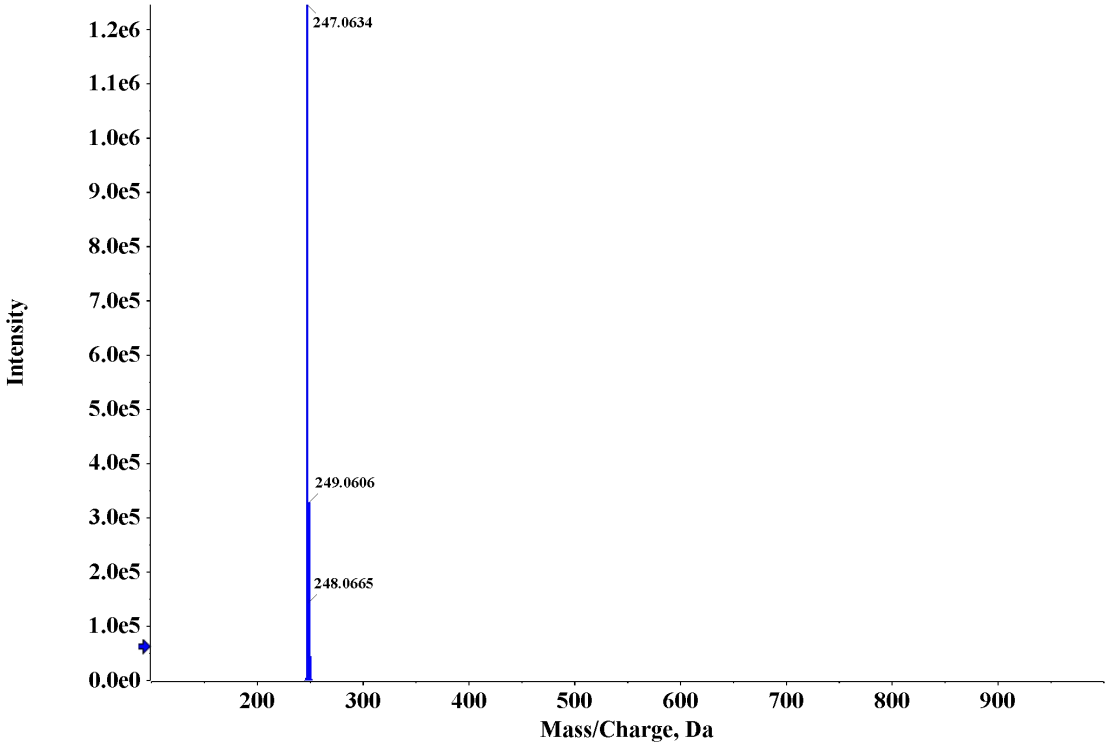
Spectrum from 1.wiff (sample 1) - Sample002, +TOF MS (90 - 1000) from 2.118 to 2.126 min



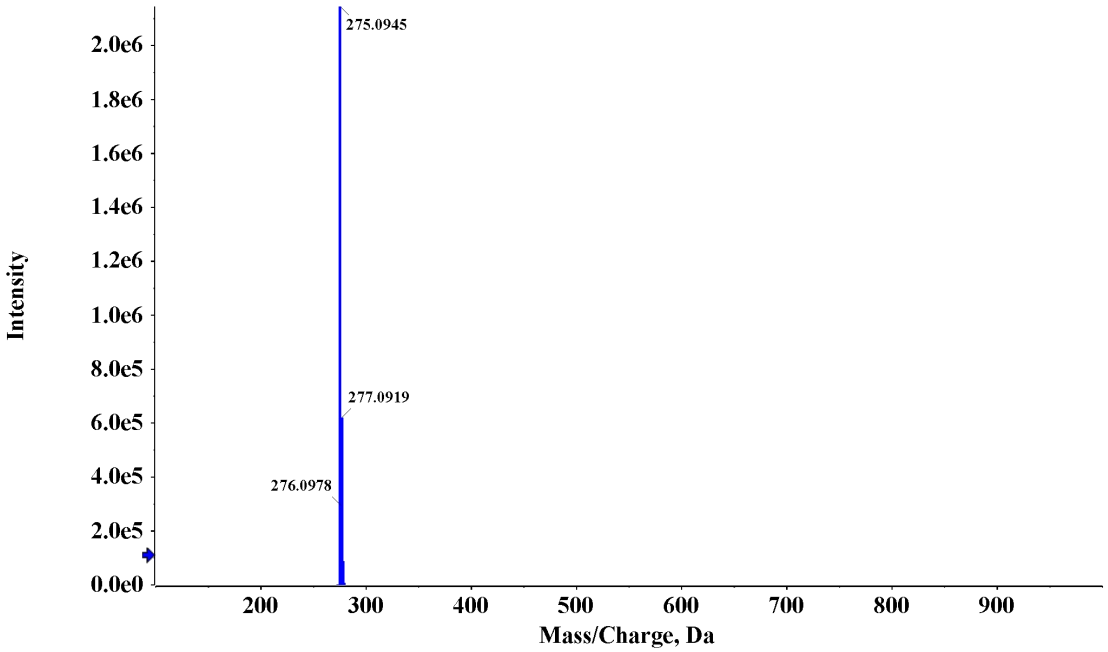
Compound 4b



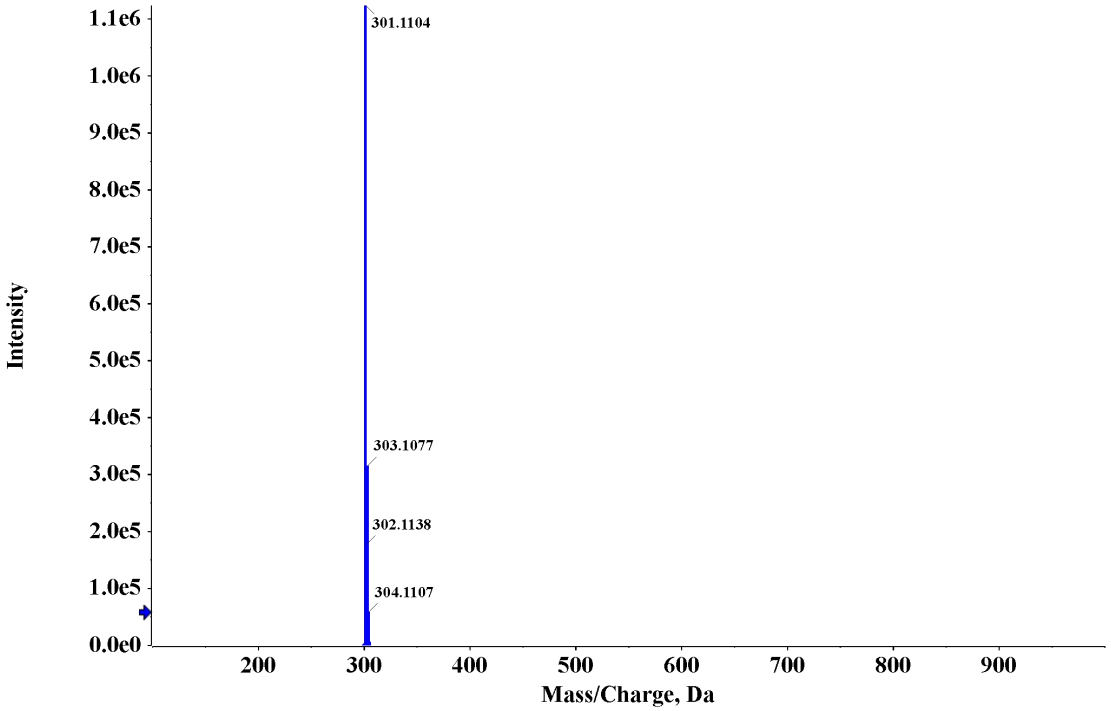
Compound 4c



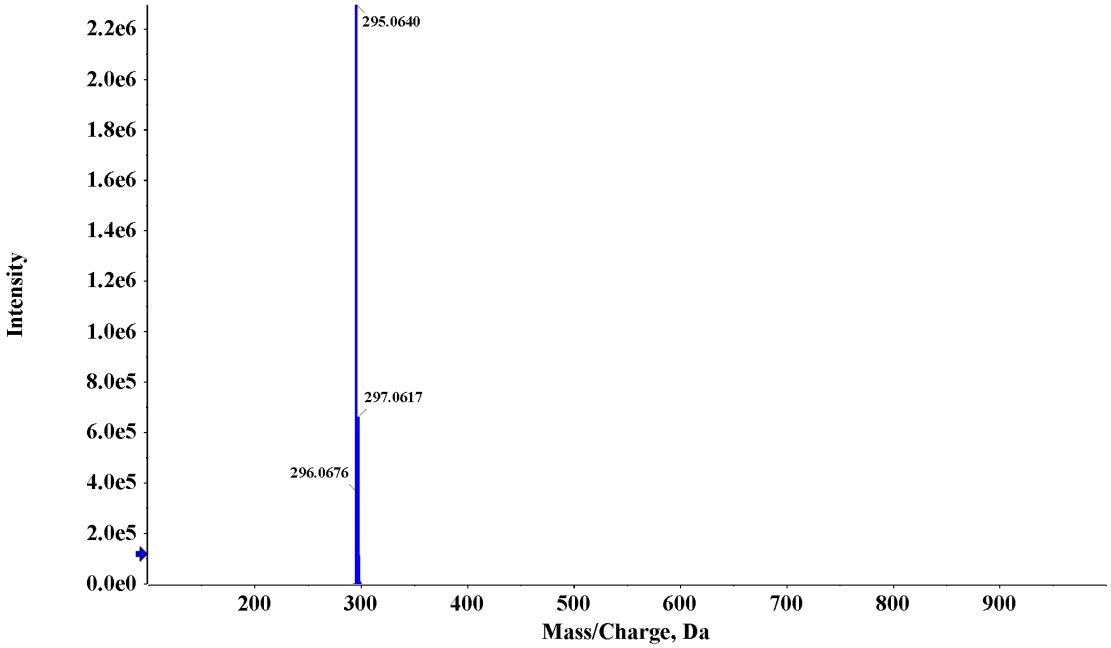
Compound 4d



Compound 4e

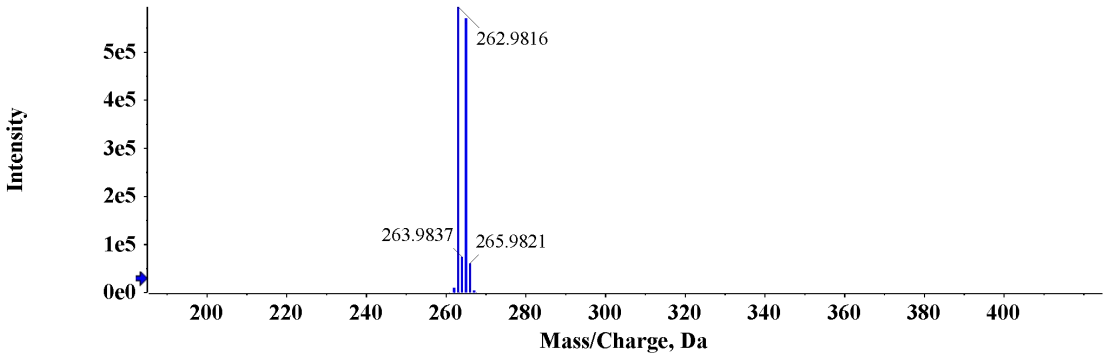


Compound 4f

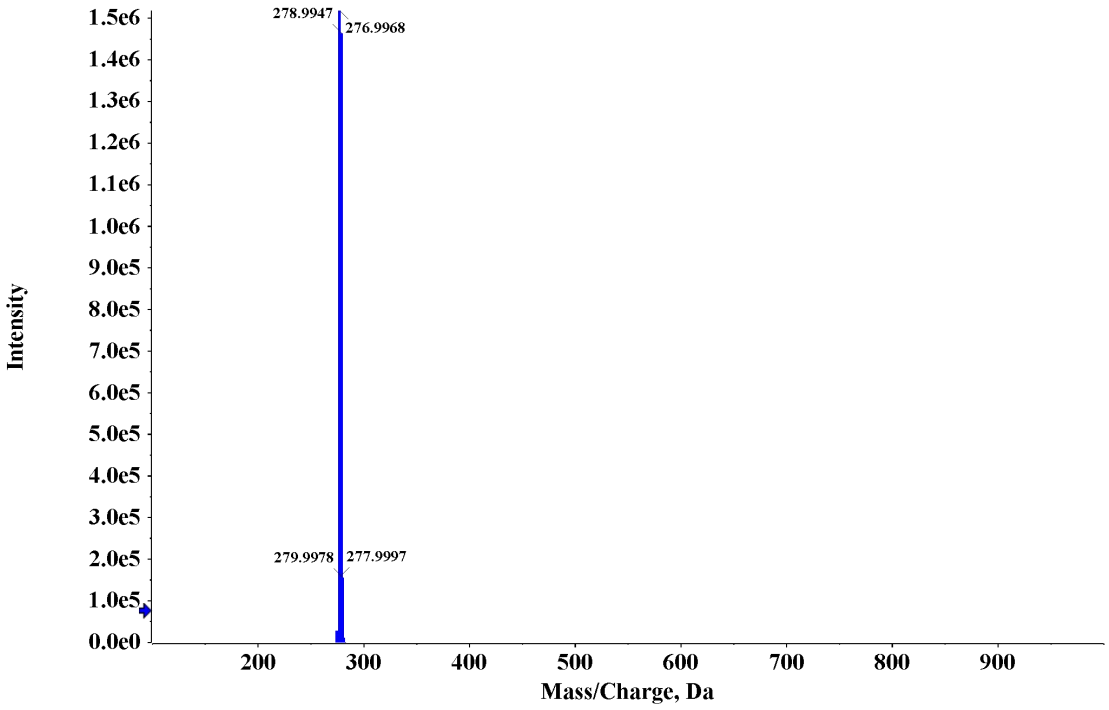


Compound 5a

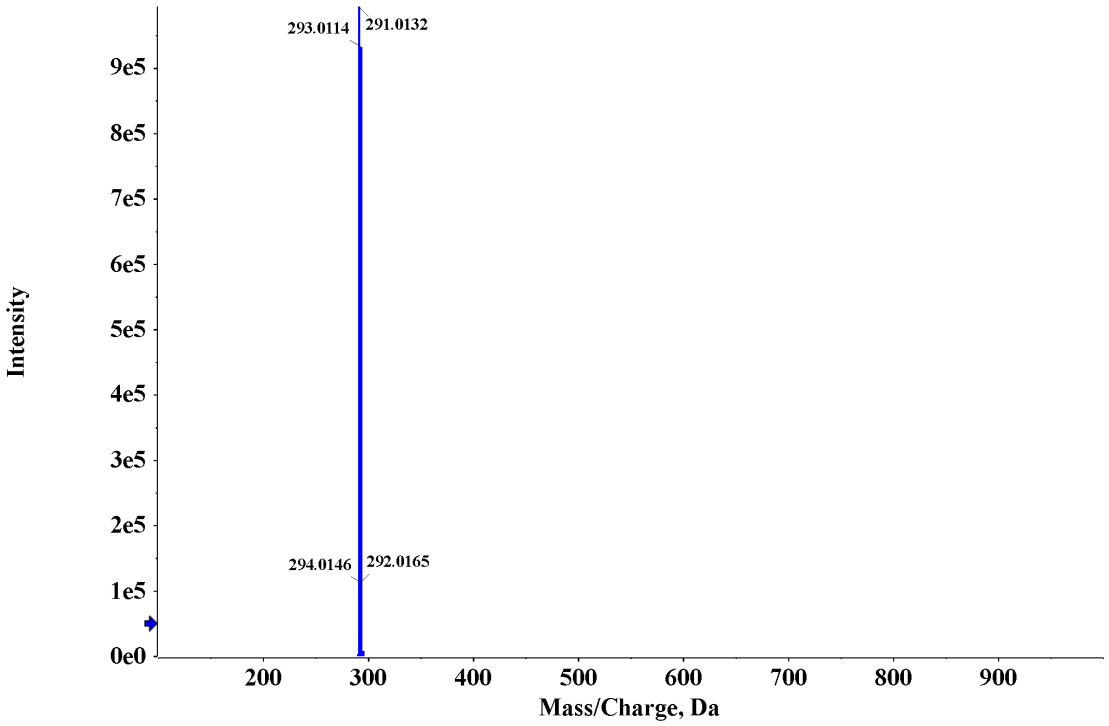
Spectrum from 2.wiff (sample 1) - Sample003, +TOF MS (90 - 1000) from 2.194 to 2.202 min



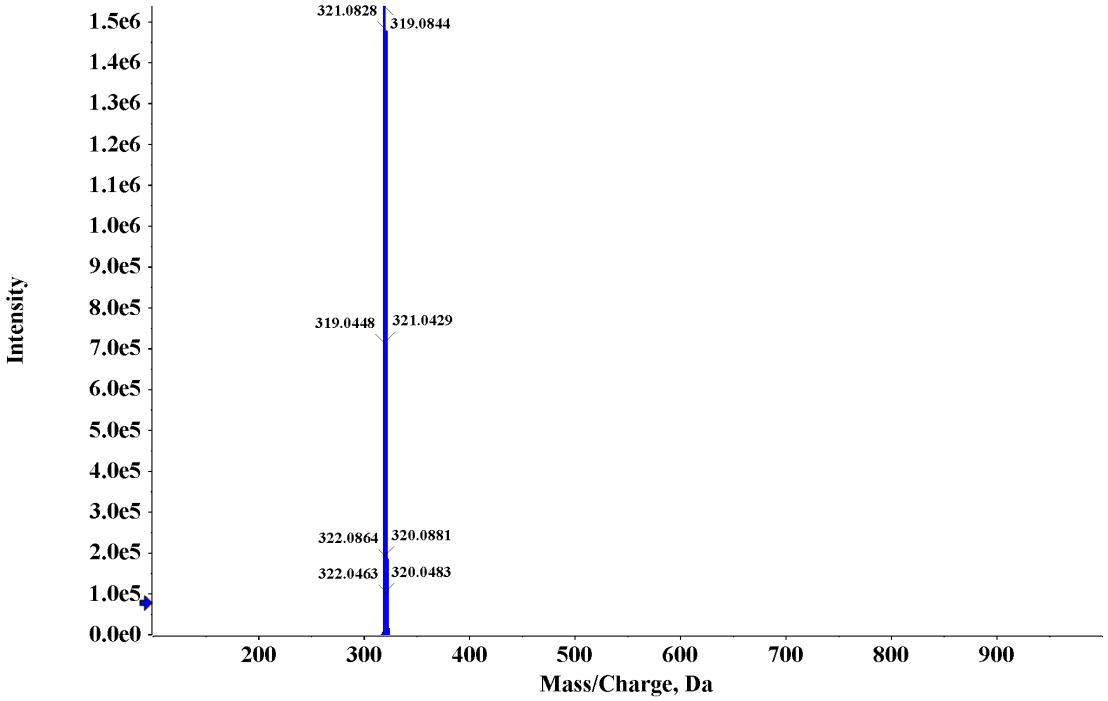
Compound 5b



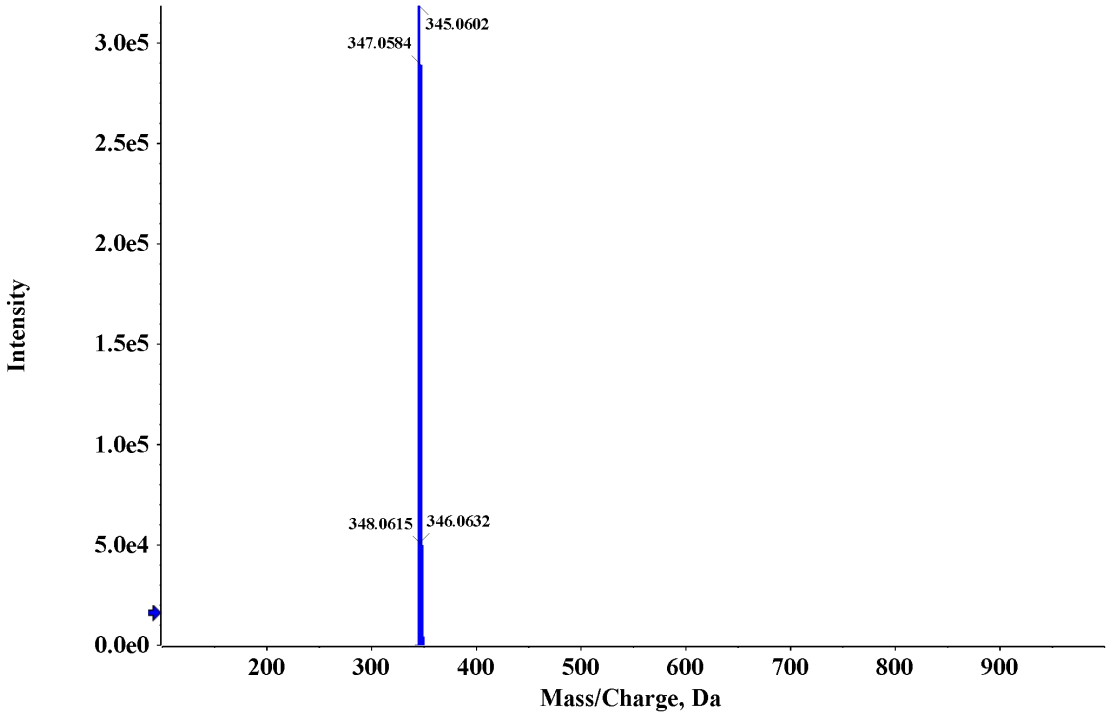
Compound 5c



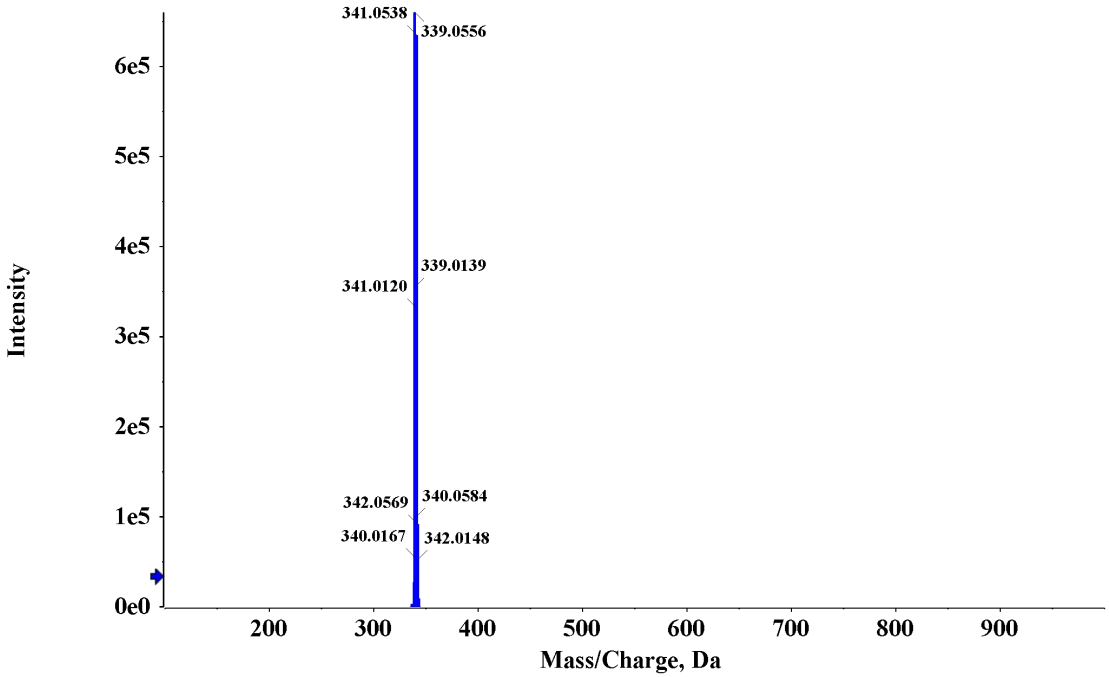
Compound 5d



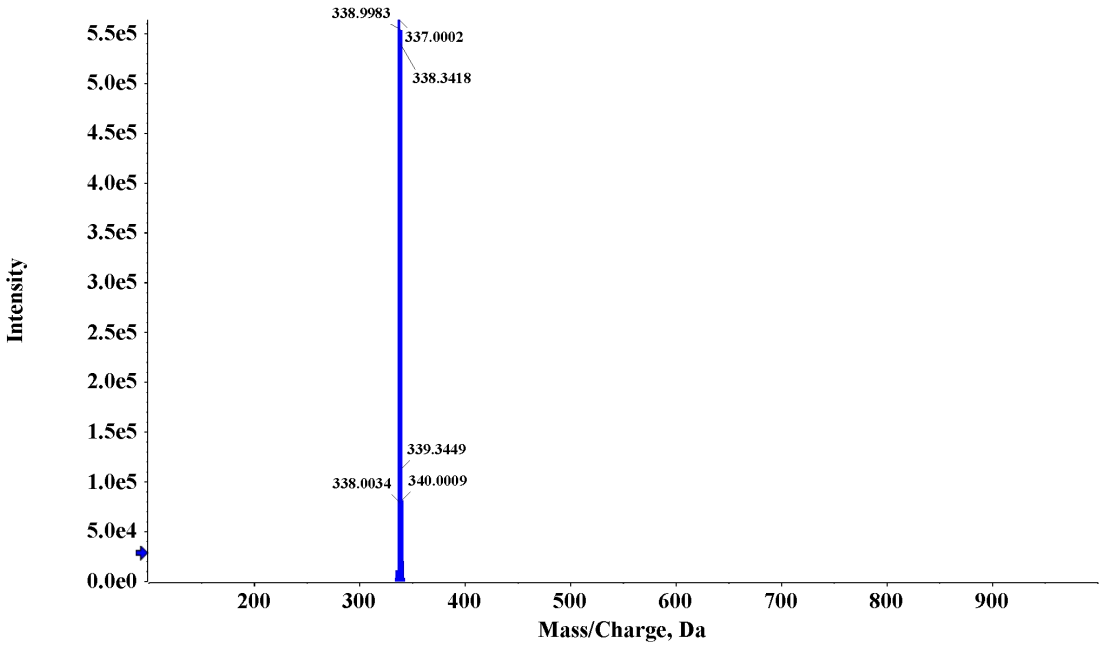
Compound 5e



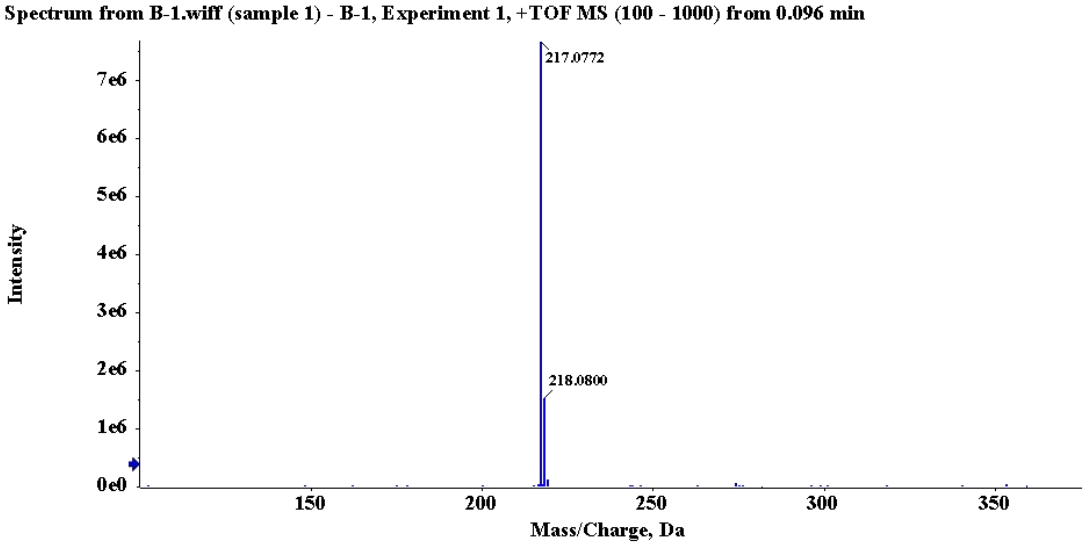
Compound 5f



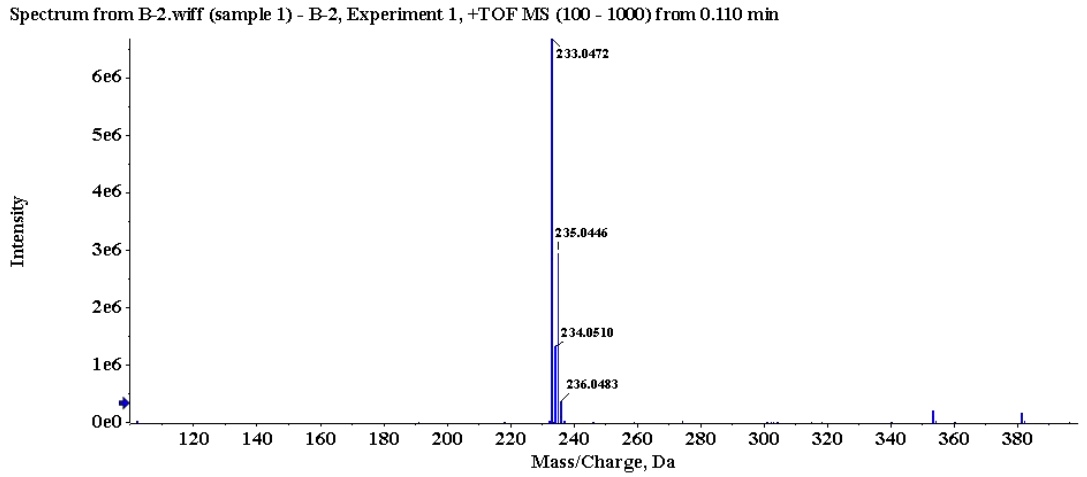
Compound 5g



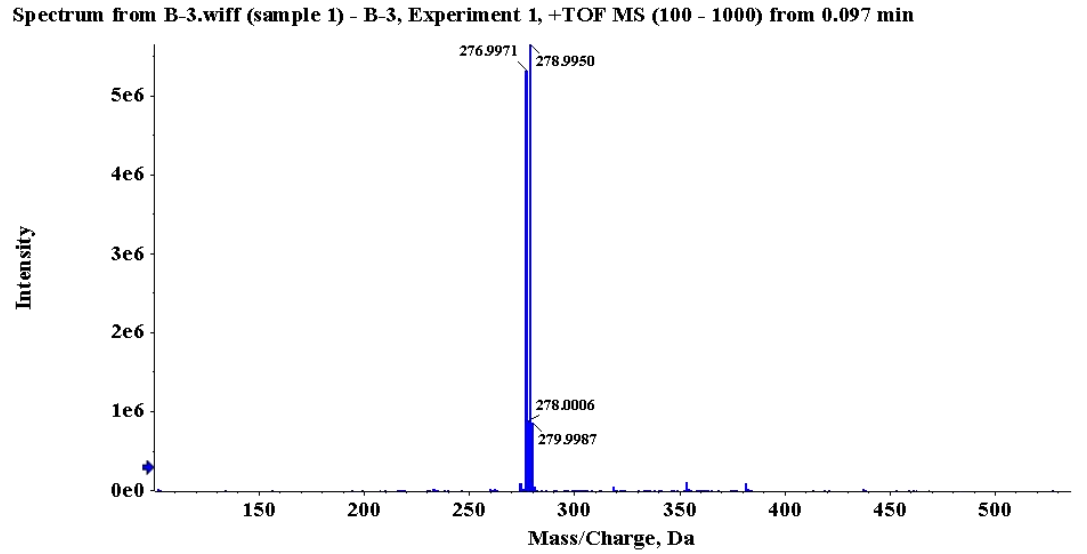
Compound 8a



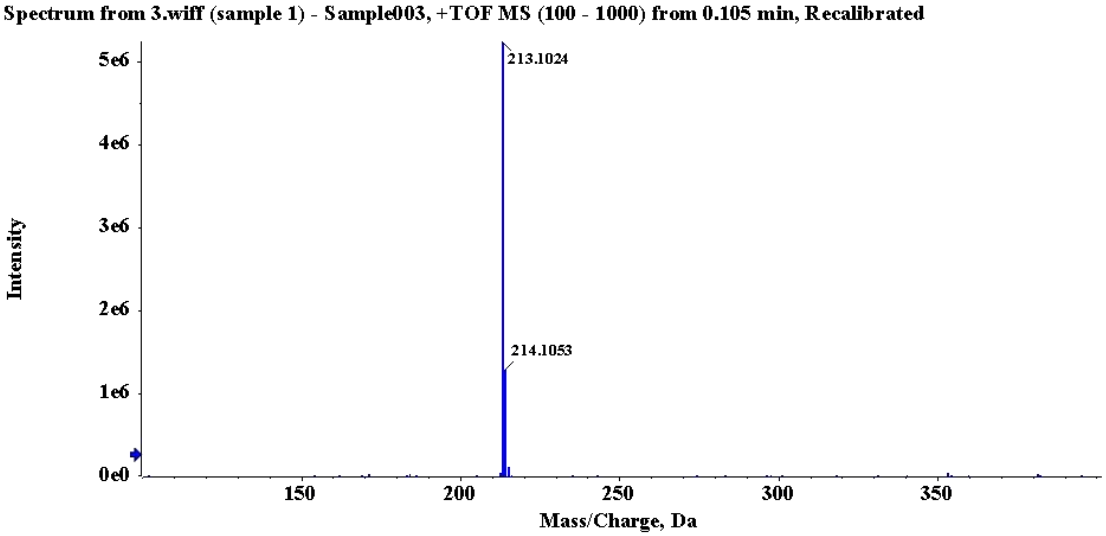
Compound 8b



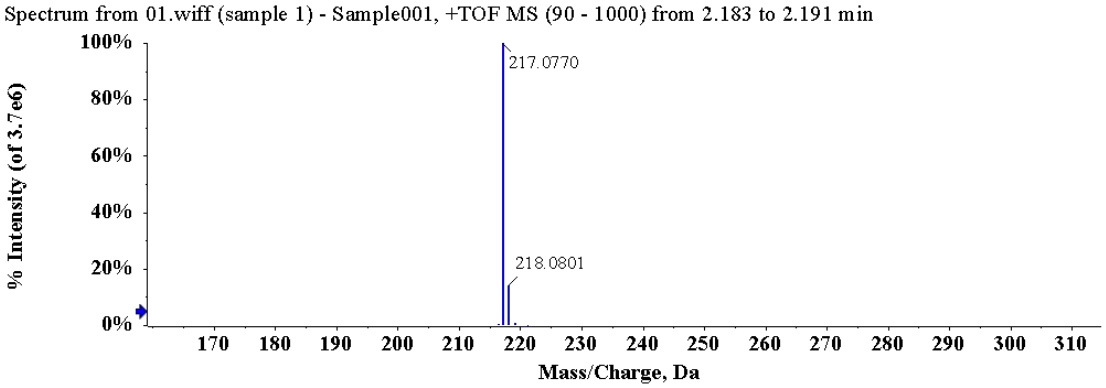
Compound 8c



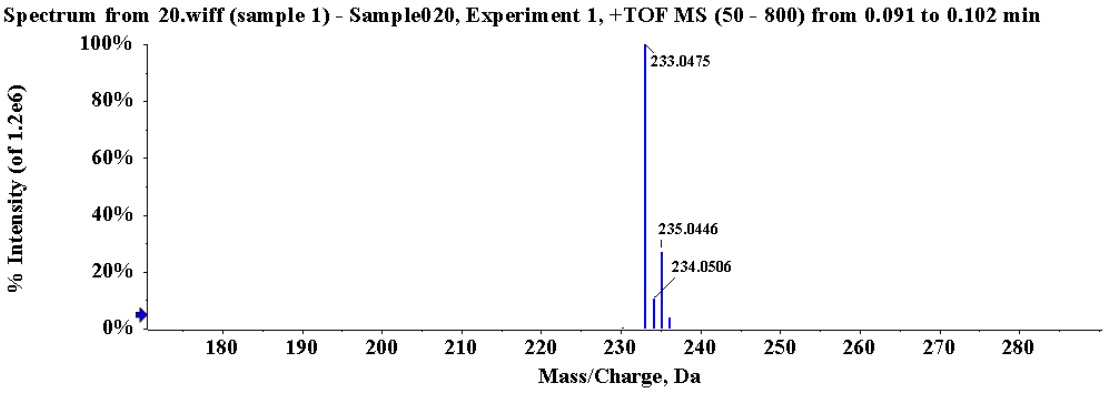
Compound 8d



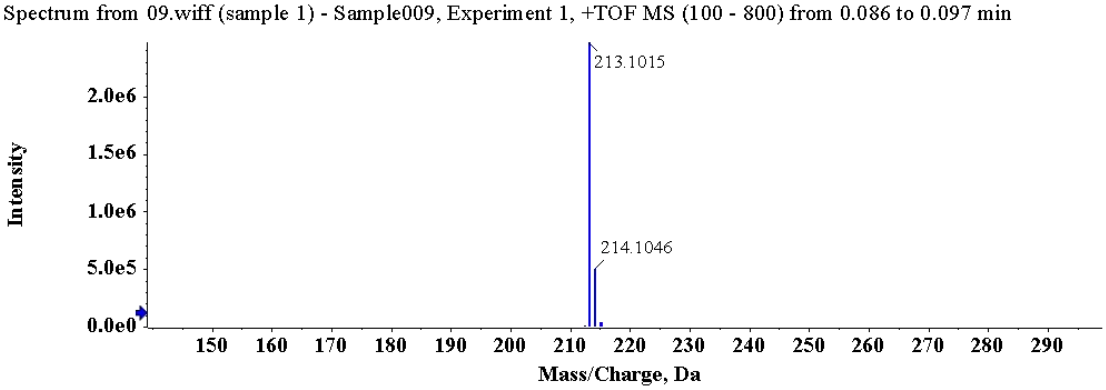
Compound 8e



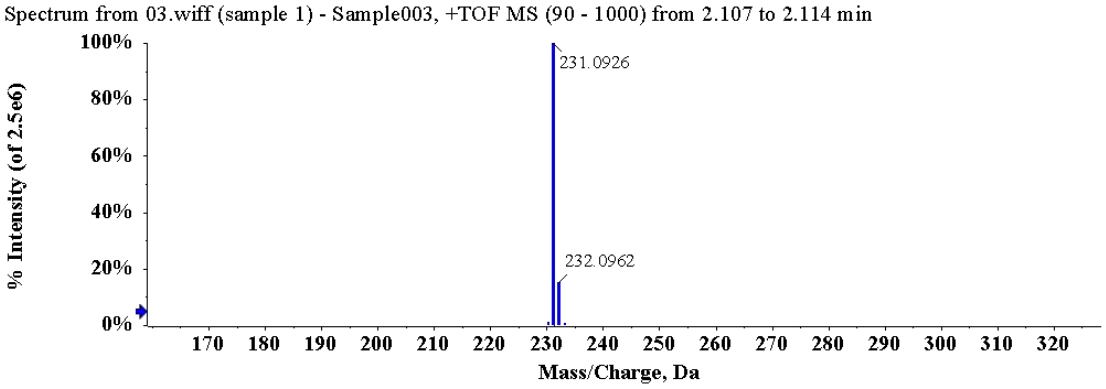
Compound 8f



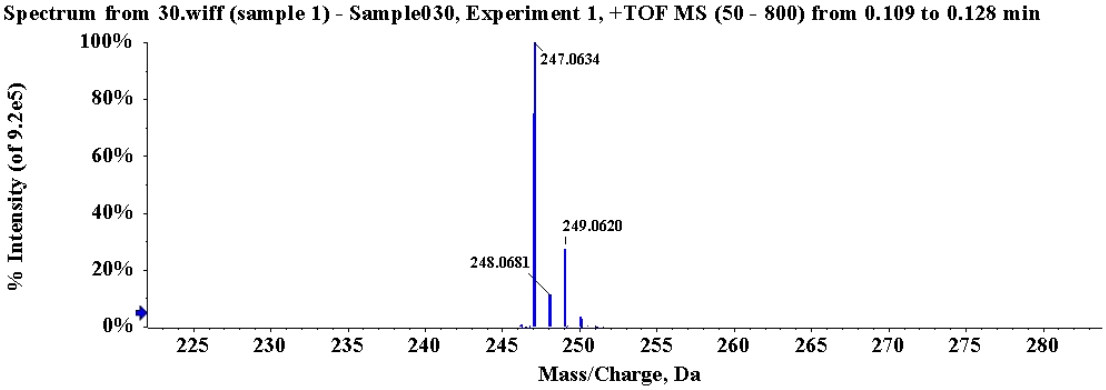
Compound 8g



Compound 8h

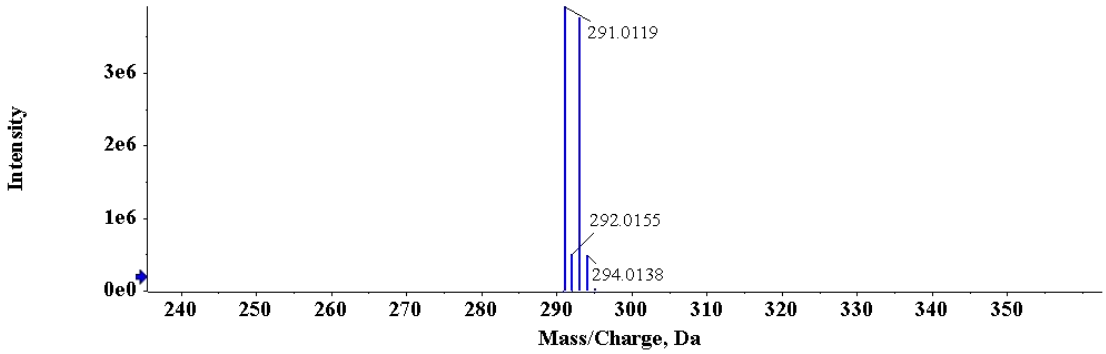


Compound 8i



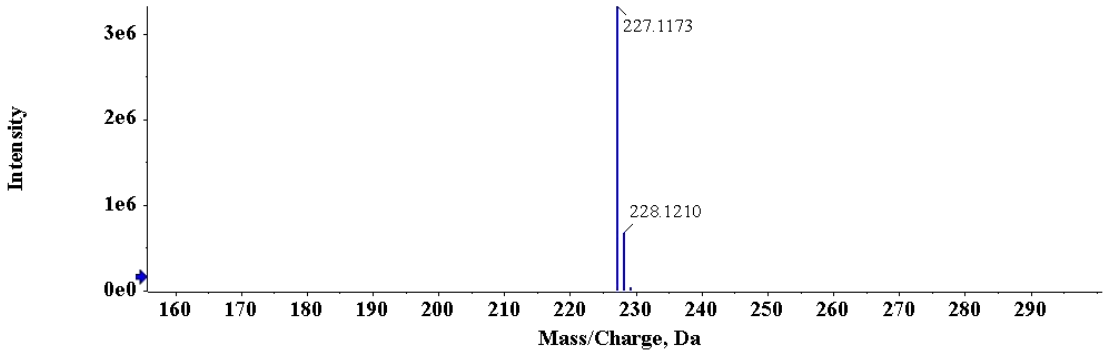
Compound 8j

Spectrum from 06.wiff (sample 1) - Sample006, Experiment 1, +TOF MS (100 - 800) from 0.096 to 0.107 min



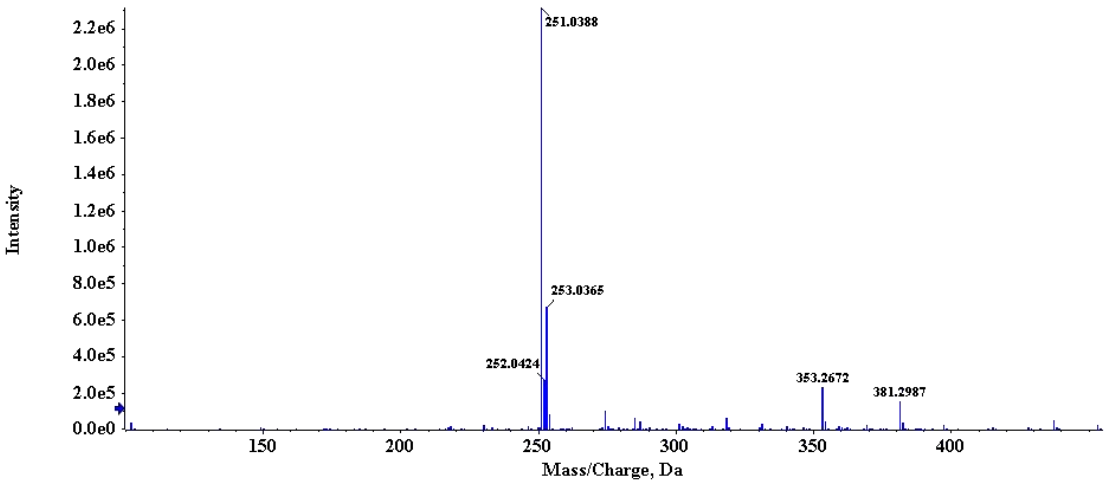
Compound 8k

Spectrum from 10.wiff (sample 1) - Sample010, Experiment 1, +TOF MS (100 - 800) from 0.101 to 0.112 min

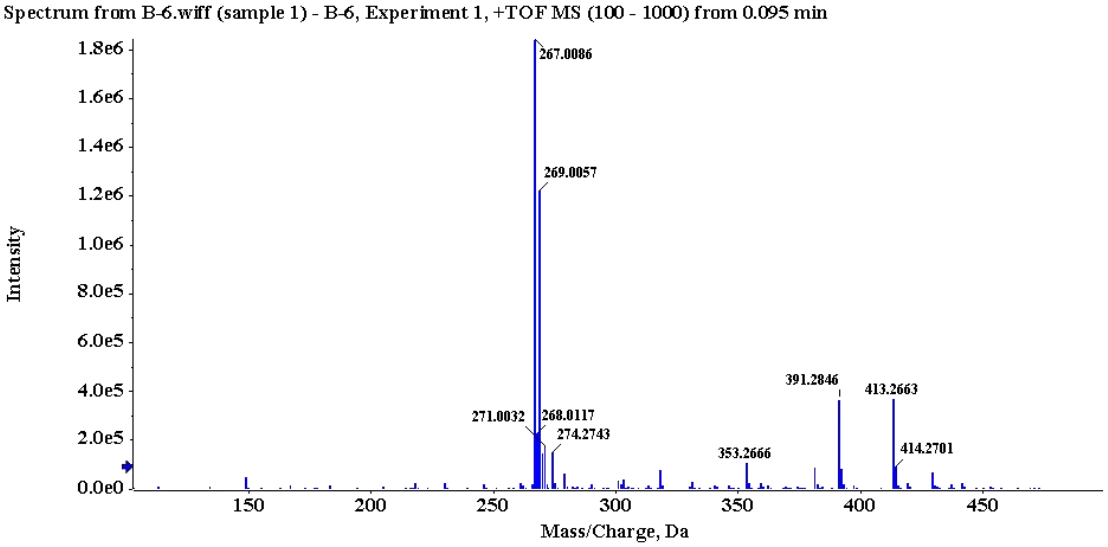


Compound 9a

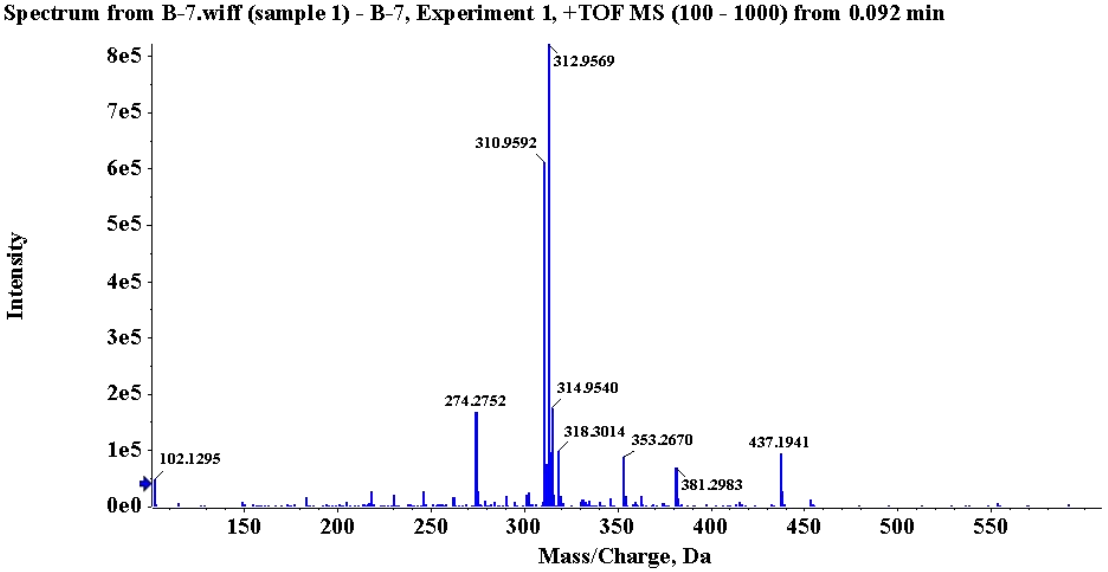
Spectrum from B-5.wiff (sample 1) - B-5, Experiment 1, +TOF MS (100 - 1000) from 0.096 min



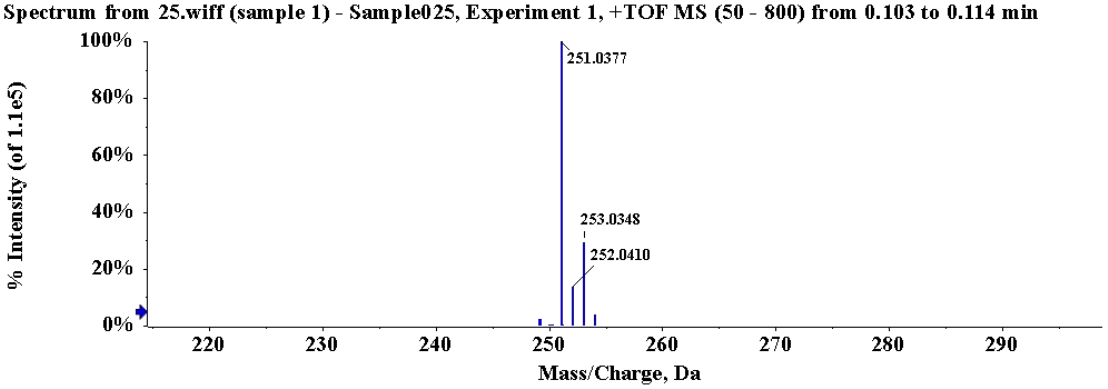
Compound 9b



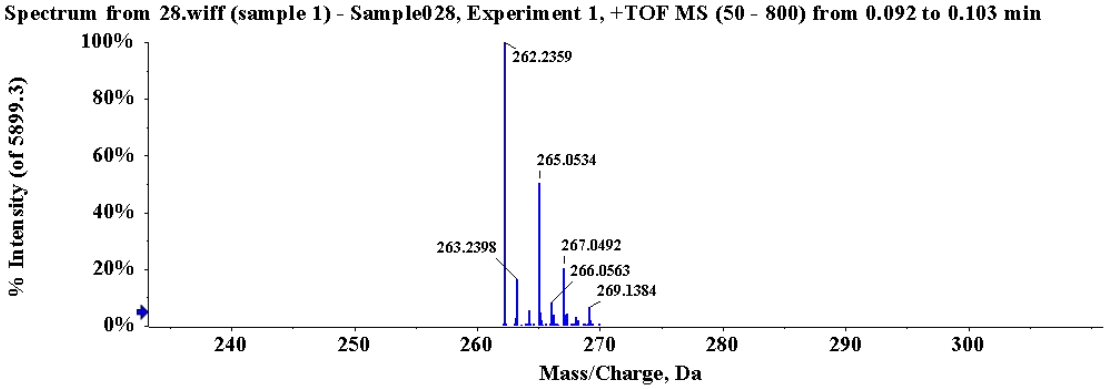
Compound 9c



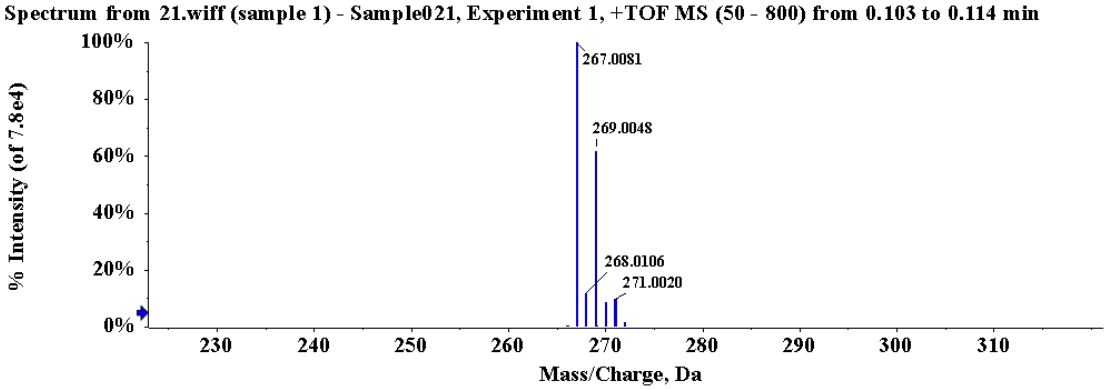
Compound 9d



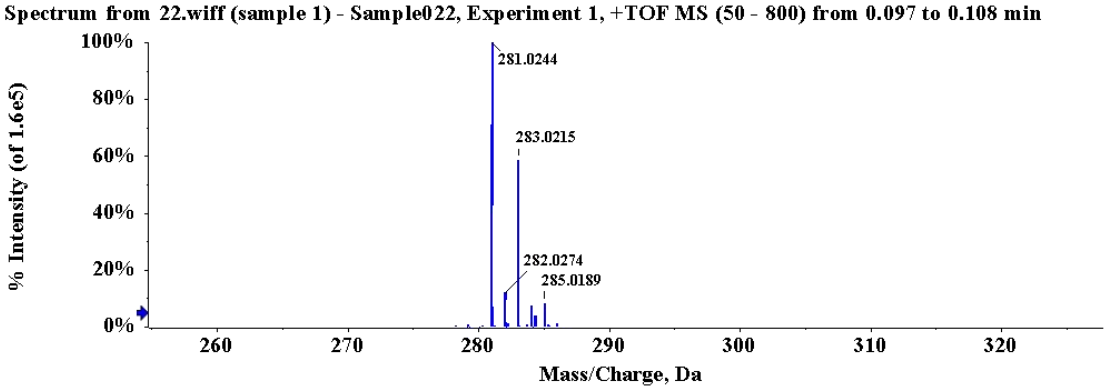
Compound 9e



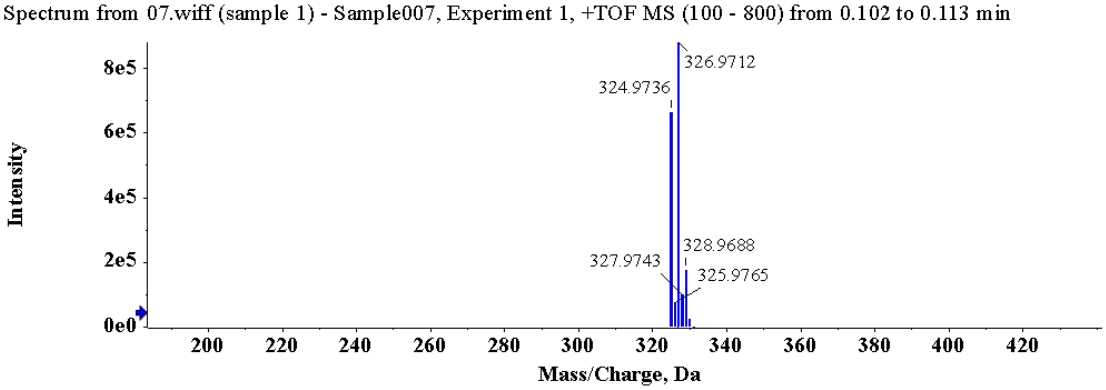
Compound 9f



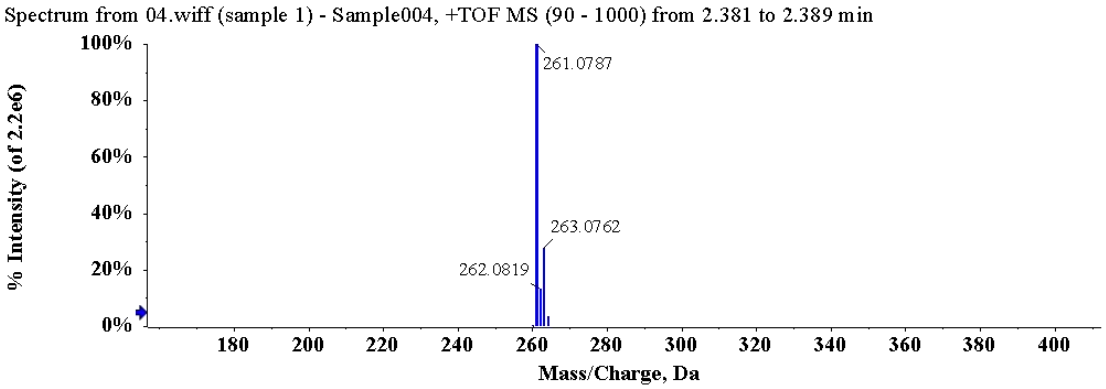
Compound 9g



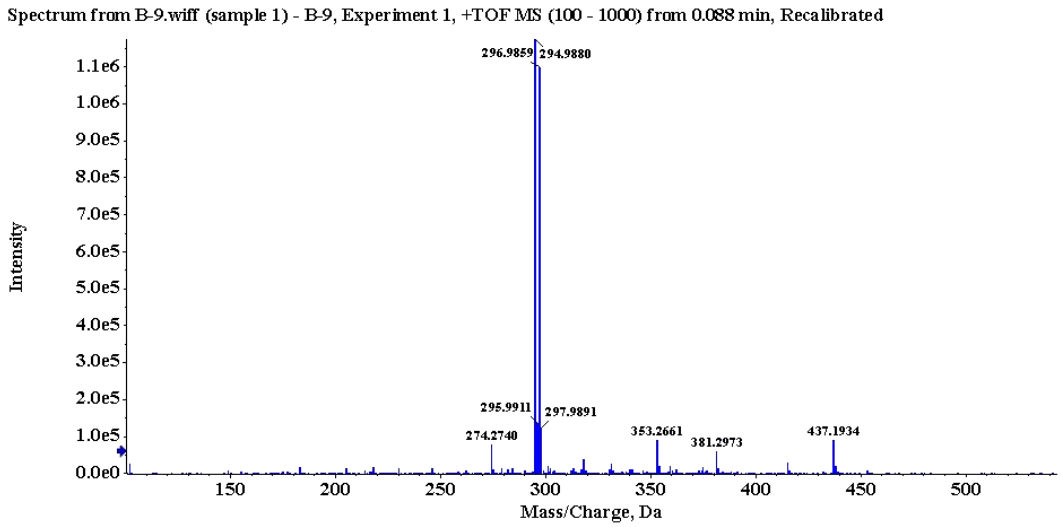
Compound 9h



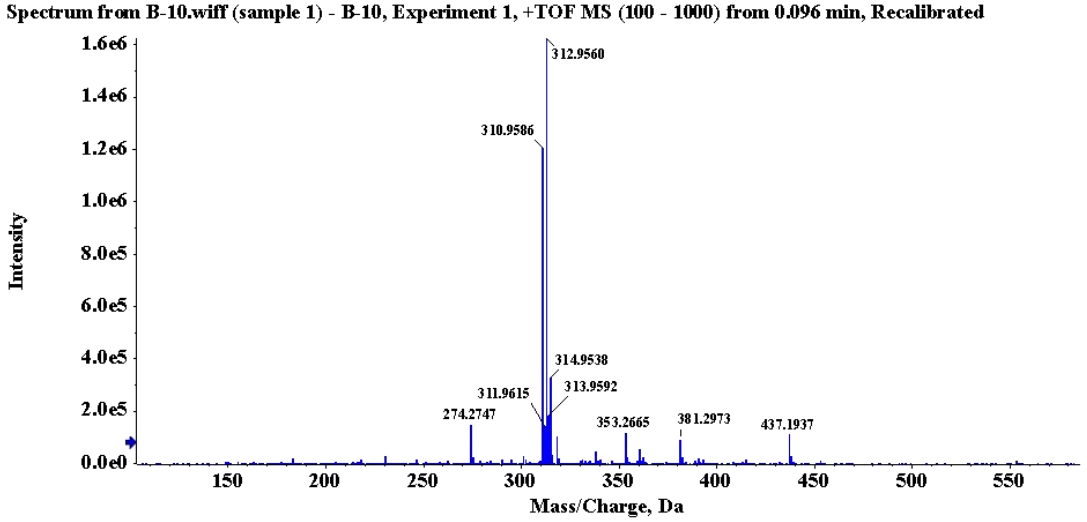
Compound 9i



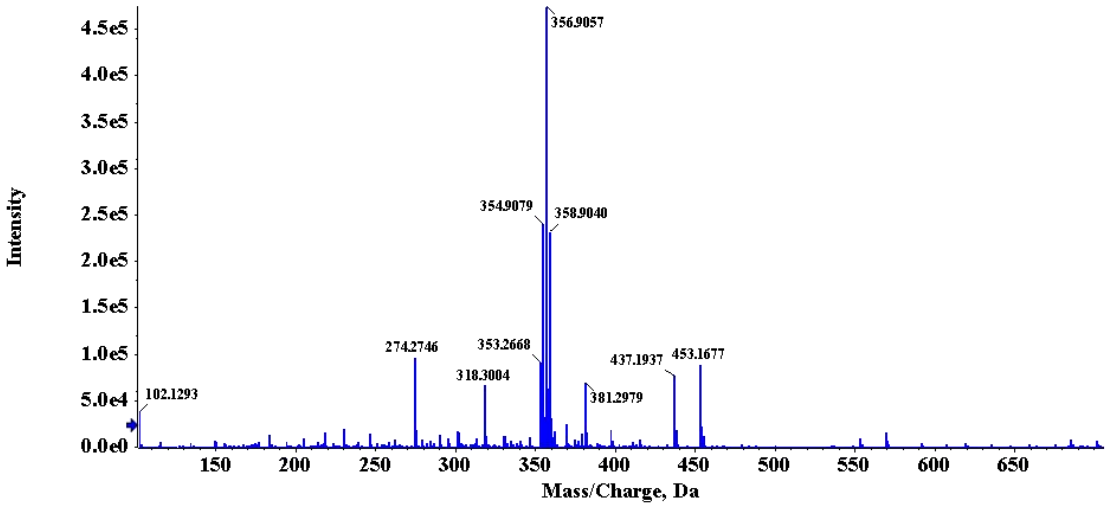
Compound 10a



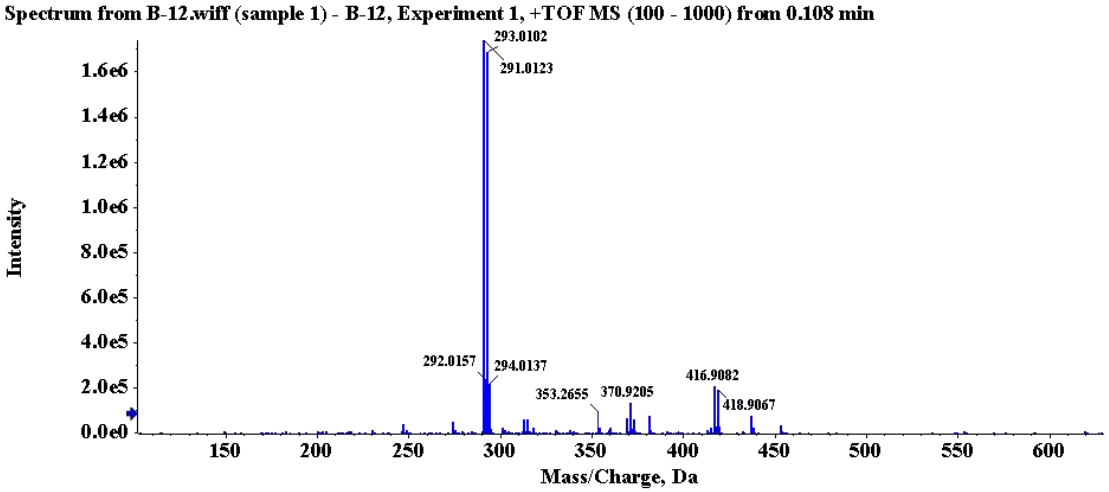
Compound 10b



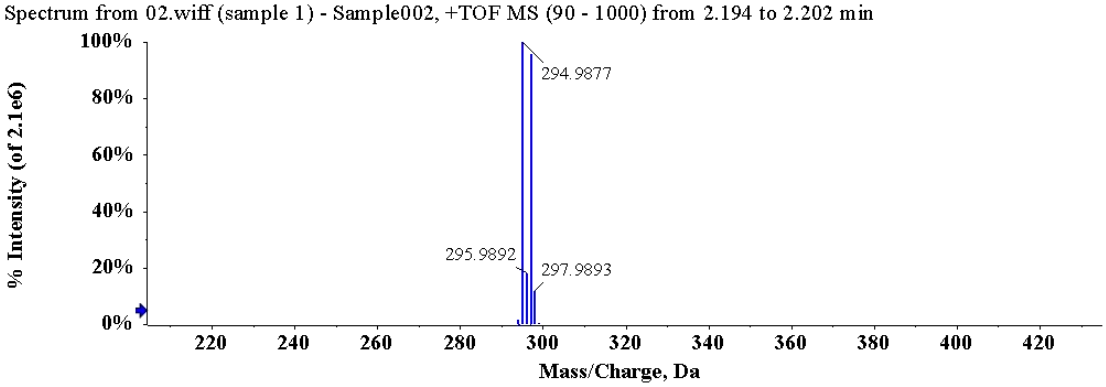
Compound 10c



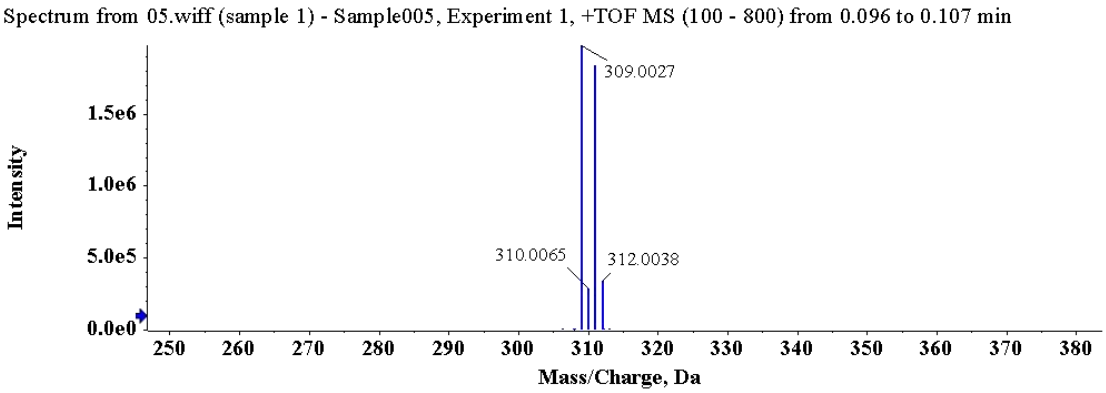
Compound 10d



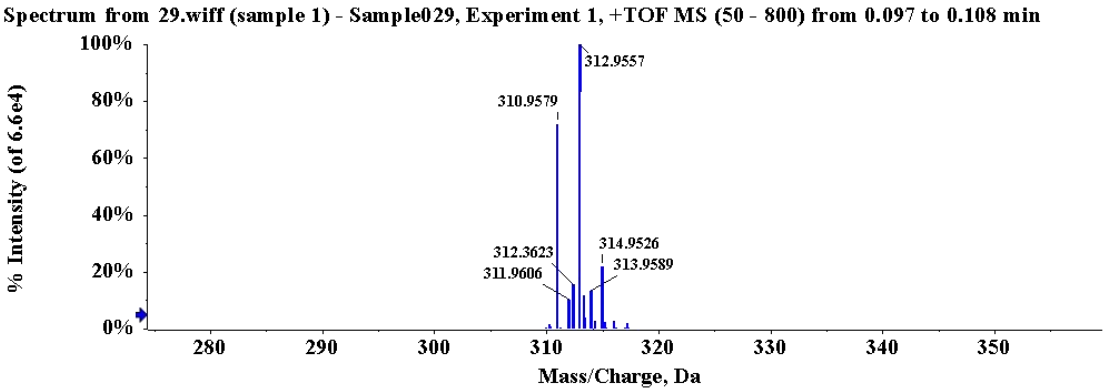
Compound 10e



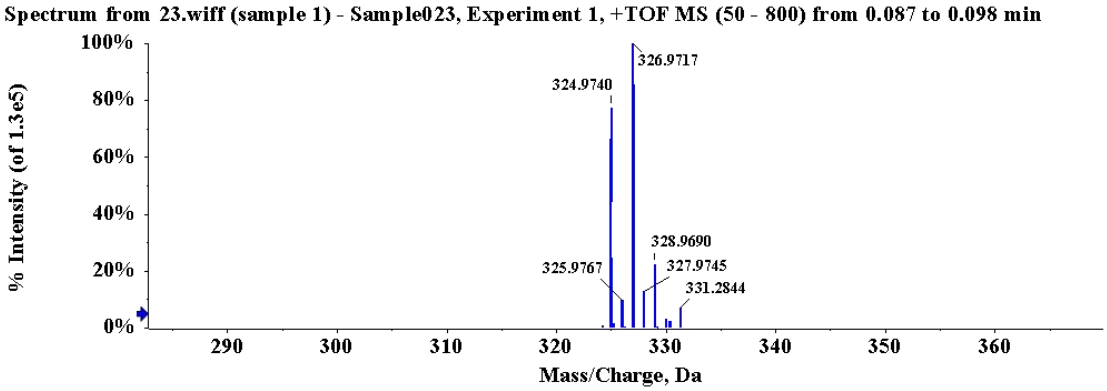
Compound 10f



Compound 10g



Compound 10h



Compound 10i