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Supplementary Materials

Design, Synthesis and Antifungal/Nematicidal Activity of Novel 1,2,4-Oxadiazole Derivatives Containing Amide Fragments

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1. The characterization data of the not known intermediated

The characterization data of the not known intermediated including ^{1}H NMR and ^{13}C NMR were shown as below.

Data for 3-Chloro-*N*-hydroxy-5-(trifluoromethyl)picolinimidamide (**a6**), m.p. 120–121 ℃, yield 86.7%, ^{1}H NMR (400 MHz, DMSO-*d6*) δ 10.05 (s, 1H), 8.98 (d, J = 1.2 Hz, 1H), 8.53 (d, J = 1.2 Hz, 1H), 5.97 (s, 2H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 153.08, 149.43, 144.16 (d, J = 4.0 Hz), 136.51 (d, J = 3.5 Hz), 130.53, 126.27 (d, J = 33.1 Hz), 123.13 (d, J = 271.4 Hz).

Data for Ethyl 3-(3-chloro-5-(trifluoromethyl)pyridin-2-yl)-1,2,4-oxadiazole-5-carboxylate (**b6**), white solid, m.p. 43–44 ℃, yield 75.8%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.97 (d, J = 1.2 Hz, 1H), 8.19 (d, J = 1.6 Hz, 1H), 4.59 (q, J = 7.2 Hz, 2H), 1.50 (t, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.99, 166.90, 153.65, 146.37, 144.71 (d, J = 4.0 Hz), 136.21 (d, J = 3.5 Hz), 132.64, 129.66–128.46 (m), 122.10 (q, J = 274.8 Hz), 64.21, 13.99.

Data for 3-(4-Thlorophenyl)-1,2,4-oxadiazole-5-carboxylic acid (**c3**), white solid, m.p. 85–86 ℃, yield 56.7%, ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.77 (s, 1H), 8.06 (d, J = 8.4 Hz, 2H), 7.67 (d, J = 8.4 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 168.16, 166.50, 136.87, 134.61, 129.97, 129.97, 129.40, 129.40, 125.22.

Data for 3-(Thiophen-2-yl)-1,2,4-oxadiazole-5-carboxylic acid (**c4**), m.p. 76–77 ℃, yield 60.3%, ^{1}H NMR (400 MHz, DMSO-*d6*) δ 11.17 (s, 1H), 8.09 (d, J = 6.2 Hz, 1H), 7.99 (d, J = 3.8 Hz, 1H), 7.30 (dd, J = 5.0, 3.8 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 150.43, 139.43, 135.49, 128.81, 124.67, 114.99, 108.73.

Data for 3-(6-Bromopyridin-3-yl)-1,2,4-oxadiazole-5-carboxylic acid (**c5**) m.p. 111–112 ℃, yield 57.8%, ^{1}H NMR (400 MHz, DMSO-*d6*) δ 11.16 (s, 1H), 8.92–8.87 (m, 1H), 8.27 (dd, J = 8.3, 2.4 Hz, 1H), 7.98–7.90 (m, 1H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 153.94, 150.45, 146.29, 142.99, 129.19, 124.67, 116.78, 109.30.

Data for 3-(3-Chloro-5-(trifluoromethyl)pyridin-2-yl)-1,2,4-oxadiazole-5-carboxylic acid (**c6**) m.p. 60–61 ℃, yield 50.9%, ^{1}H NMR (400 MHz, DMSO-*d6*) δ 10.57 (s, 1H), 9.16 (d, J = 0.8 Hz, 1H), 8.90 (d, J = 0.8 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 150.42, 146.42 (d, J = 4.0 Hz), 136.74 (d, J = 3.7 Hz), 136.09, 129.45 (d, J = 19.8 Hz), 124.67, 123.88, 121.15, 114.95.

2. The characterization data of the target compound

The characterization data of the target compound including ^{1}H NMR, ^{13}C NMR and HRMS were shown as below.

Data for 3-Phenyl-*N*-(2-(pyridin-2-yl)ethyl)-1,2,4-oxadiazole-5-carboxamide (**F1**), white solid, m.p. 110–112 ℃, yield 67.3%, purity 96.1%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (s, 2H), 8.28 (s, 1H), 8.08 (d, J = 6.0 Hz, 2H), 7.78 (d, J = 36.0 Hz, 2H), 7.49 (d, J = 6.8 Hz, 3H), 4.10 (s, 2H), 3.67 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.88, 168.73, 157.49, 153.41, 146.56, 140.00, 131.84, 129.08, 129.08, 127.68, 127.68, 125.87, 125.14, 123.10, 39.08, 34.95. HRMS (ESI): calcd for $C_{16}H_{15}N_4O_2$ ([M+H]$^+$), 295.11895; found, 295.11966.

Data for *N*-(2-(3-chloro-5-(trifluoromethyl)pyridin-2-yl)ethyl)-3-phenyl-1,2,4-oxadiazole-5-carboxamide (**F2**), white solid, m.p. 81–82 ℃, yield 52.6%, purity 99.0%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, *J* = 0.8 Hz, 1H), 8.09 (dd, *J* = 7.6, 1.2 Hz, 3H), 7.94 (d, *J* = 1.2 Hz, 1H), 7.56–7.47 (m, 3H), 4.07 (dd, *J* = 12.0, 6.0 Hz, 2H), 3.35 (t, *J* = 5.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.76, 168.66, 160.20,

153.05, 143.78 (d, *J* = 4.1 Hz), 134.01 (d, *J* = 3.5 Hz), 131.95, 131.81, 129.01, 129.01, 127.55, 127.55, 126.73, 125.74, 123.85 (dd, *J* = 239.37, 33.84 Hz), 36.78, 33.93. HRMS (ESI): calcd for $C_{17}H_{13}ClF_3N_4O_2$ ([M+H]$^+$), 396.06736; found, 396.06738.

Data for *N*-(2,4-difluorobenzyl)-3-phenyl-1,2,4-oxadiazole-5-carboxamide (**F3**), white solid, m.p. 92–93 ℃, yield 52.9%, purity 98.7%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 6.8 Hz, 2H), 7.60 (s, 1H), 7.53–7.42 (m, 4H), 6.87 (dd, *J* = 18.0, 8.8 Hz, 2H), 4.69 (d, *J* = 6.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.77, 168.38, 163.26 (dd, *J* = 174.9, 12.1 Hz), 160.78 (dd, *J* = 174.5, 12.1 Hz), 153.07, 131.87, 131.62 (dd, *J* = 9.9, 5.7 Hz), 129.03, 129.03, 127.55, 127.55, 125.65, 119.65 (dd, *J* = 15.2, 3.8 Hz), 111.73 (dd, *J* = 21.3, 3.8 Hz), 104.20, 37.50. HRMS (ESI): calcd for $C_{16}H_{13}F_2N_3O_2$ ([M+H]$^+$), 316.08921; found, 316.08899.

Data for *N*-(2,4-dichlorophenyl)-3-phenyl-1,2,4-oxadiazole-5-carboxamide (**F4**), white solid, m.p. 163–164 ℃, yield 50.0%, purity 98.4%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.45 (s, 1H), 8.48 (d, *J* = 8.8 Hz, 1H), 8.14 (d, *J* = 6.8 Hz, 2H), 7.60–7.50 (m, 3H), 7.48 (d, *J* = 2.0 Hz, 1H), 7.35 (dd, *J* = 8.8, 2.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.88, 168.27, 150.43, 132.06, 131.88, 131.03, 129.21, 129.11, 129.11, 128.32, 127.65, 127.65, 125.44, 124.10, 122.25. HRMS (ESI): calcd for $C_{15}H_9Cl_2N_3O_2Na$ ([M+Na]$^+$), 355.99640; found, 355.99606.

Data for *N*-(2-(pyridin-2-yl)ethyl)-3-(p-tolyl)-1,2,4-oxadiazole-5-carboxamide (**F5**), yellow solid, m.p. 126–128 ℃, yield 43.3%, purity 97.3%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (d, *J* = 4.4 Hz, 1H), 8.56 (s, 1H), 7.99 (d, *J* = 8.0 Hz, 2H), 7.65 (td, *J* = 7.6, 1.6 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.21 (dd, *J* = 7.6, 0.8 Hz, 2H), 3.94 (dd, *J* = 12.4, 6.0 Hz, 2H), 3.14 (t, *J* = 6.0 Hz, 2H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.40, 157.57, 151.69, 147.89, 140.76, 135.49, 128.29, 128.29, 126.12, 126.12, 122.13, 122.13, 121.72, 120.52, 37.51, 34.59, 20.23. HRMS (ESI): calcd for $C_{17}H_{17}N_4O_2$ ([M+H]$^+$), 309.13460; found, 309.13394.

Data for *N*-(2-(3-chloro-5-(trifluoromethyl)pyridin-2-yl)ethyl)-3-(p-tolyl)-1,2,4-oxadiazole-5-carboxamide (**F6**), white solid, m.p. 96–98 ℃, yield 58.1%, purity 98.9%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (s, 1H), 8.05 (s, 1H), 7.97 (d, *J* = 8.2 Hz, 2H), 7.93 (t, *J* = 5.6 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 2H), 4.06 (dd, *J* = 12.1, 6.1 Hz, 2H), 3.35 (t, *J* = 5.9 Hz, 2H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.78, 168.53, 160.22, 153.13, 143.79 (d, J = 4.1 Hz), 142.27, 134.01 (d, J = 3.5 Hz), 131.95, 129.71, 127.49, 126.42, 126.08, 124.04, 122.96, 121.32, 36.80, 33.96, 21.62. HRMS (ESI): calcd for $C_{18}H_{15}ClF_3N_4O_2$ ([M+H]$^+$), 411.08301; found, 411.08237.

Data for *N*-(2,4-difluorobenzyl)-3-(p-tolyl)-1,2,4-oxadiazole-5-carboxamide (**F7**), white solid, m.p. 119–120 ℃, yield 45.9%, purity 99.2%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.4 Hz, 2H), 7.55 (s, 1H), 7.48–7.40 (m, 1H), 7.29 (d, *J* = 8.0 Hz, 2H), 6.93–6.83 (m, 2H), 4.69 (d, *J* = 6.2 Hz, 2H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.78, 168.20, 164.17, 162.39 (d, *J* = 12.2 Hz), 161.69, 159.91 (d, *J* = 12.1 Hz), 153.13, 142.39, 131.64 (dd, *J* = 9.7, 5.5 Hz), 129.75, 127.49, 122.80, 119.66 (d, *J* = 19.0 Hz), 111.74 (dd, *J* = 21.6, 3.8 Hz), 104.21, 37.44, 21.65. HRMS (ESI): calcd for $C_{17}H_{14}F_2N_3O_2$ ([M+H]$^+$), 330.10486; found, 330.10410.

Data for *N*-(2,4-dichlorophenyl)-3-(p-tolyl)-1,2,4-oxadiazole-5-carboxamide (**F8**), white solid, m.p. 163–165 ℃, yield 62.8%, purity 99.1%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.43 (s, 1H), 8.48 (d, *J* = 8.8 Hz, 1H), 8.02 (d, *J* = 8.4 Hz, 2H), 7.48 (d, *J* = 2.4 Hz, 1H), 7.34 (dd, *J* = 10.0, 2.4 Hz, 3H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.89, 168.11, 150.50, 142.59, 131.91, 130.98, 129.80, 129.80, 129.20, 128.30, 127.58, 127.58, 124.09, 122.60, 122.25, 21.67. HRMS (ESI): calcd for $C_{16}H_{11}Cl_2N_3O_2Na$ ([M+Na]$^+$), 370.01205; found, 370.01202.

Data for 3-(4-chlorophenyl)-*N*-(2-(pyridin-2-yl)ethyl)-1,2,4-oxadiazole-5-carboxamide (**F9**), white solid, m.p. 129–131 ℃, yield 55.5%, purity 98.4%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (s, 1H, Py-H), 8.63–8.58 (m, 1H), 8.10–8.01 (m, 2H), 7.67 (td, *J* = 7.7, 1.8 Hz, 1H), 7.52–7.44 (m, 2H), 7.22 (dd, *J* = 7.6, 4.4 Hz, 2H), 3.99–3.89 (m, 2H), 3.19–3.11 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.06, 167.97, 158.92, 152.79, 149.18, 137.93, 136.96, 129.33, 129.33, 128.86, 128.86, 124.36, 123.55, 121.96, 38.88, 35.78. HRMS (ESI): calcd for $C_{16}H_{14}ClN_4O_2$ ([M+H]$^+$), 329.07998; found, 329.07922.

Data for *N*-(2-(3-chloro-5-(trifluoromethyl)pyridin-2-yl)ethyl)-3-(4-chlorophenyl)-1,2,4-oxadiazole-5-carboxamide (**F10**), white solid, m.p. 109–110 ℃, yield 43.7%, purity 99.5%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.77 (s, 1H), 8.07 (s, 1H), 8.00 (d, *J* = 8.6 Hz, 2H), 7.92 (d, *J* = 1.8 Hz, 1H), 7.48–7.43 (m, 2H), 4.04 (dd, *J* = 9.6 Hz, *J* = 8.8 Hz, 2H), 3.33 (t, *J* = 4.8 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.88, 168.06, 160.26, 152.95, 143.84 (d, *J* = 3.0 Hz), 138.13, 134.11 (d, *J* = 2.1 Hz), 132.04, 129.46, 129.46, 128.93, 128.93, 126.33 (q, *J* = 54.3 Hz), 124.29, 122.73 (d, *J* = 272.9 Hz), 36.88, 33.98. HR MS (ESI): calcd for $C_{17}H_{12}Cl_2F_3N_4O_2$ ([M+H]$^+$), 431.02839; found, 431.02731.

Data for 3-(4-chlorophenyl)-*N*-(2,4-difluorobenzyl)-1,2,4-oxadiazole-5-carboxamide (**F11**), white solid, m.p. 97–98 ℃, yield 54.2%, purity 98.5%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.4 Hz, 2H), 7.55 (s, 1H), 7.47 (d, *J* = 8.4 Hz, 2H), 7.43 (dd, *J* = 8.8, 6.4 Hz, 1H), 6.92–6.83 (m, 2H), 4.69 (d, *J* = 6.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.51, 167.99, 163.22 (d, *J* = 176.2 Hz), 160.80 (d, *J* = 185.5 Hz), 152.89, 138.16, 131.65 (dd, *J* = 9.1, 5.2 Hz), 129.41, 129.41, 128.86, 128.86, 124.12, 119.59 (d, *J* = 15.2 Hz), 111.75 (dd, *J* = 21.4, 3.7 Hz), 104.23, 37.56. HRMS (ESI): calcd for $C_{16}H_{10}ClF_2N_3O_2Na$ ([M+Na]$^+$), 372.03218; found, 372.03220.

Data for 3-(4-chlorophenyl)-N-(2,4-dichlorophenyl)-1,2,4-oxadiazole-5-carboxamide (**F12**), white solid, m.p. 169–171 ℃, yield 57.3%, purity 98.5%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.41 (s, 1H), 8.48 (d, *J* = 9.2 Hz, 1H), 8.09 (d, *J* = 8.4 Hz, 2H), 7.51 (d, *J* = 8.8 Hz, 2H), 7.49 (d, *J* = 2.4 Hz, 1H), 7.35 (dd, *J* = 8.8, 2.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.43, 168.12, 150.26, 138.38, 131.79, 131.14, 131.14, 129.50, 129.50, 129.23, 128.96, 128.96, 128.35, 124.00, 122.28. HRMS (ESI): calcd for $C_{15}H_7Cl_3N_3O_2$ ([M-H]$^-$), 365.96984; found, 365.96996.

Data for *N*-(2-(pyridin-2-yl)ethyl)-3-(thiophen-2-yl)-1,2,4-oxadiazole-5-carboxamide (**F13**), yellow solid, m.p. 133–135 ℃, yield 57.2%, purity 98.7%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.62 (s, 1H), 8.58 (d, *J* = 4.5 Hz, 1H), 7.82 (d, *J* = 4.5 Hz, 1H), 7.64 (t, *J* = 17.5 Hz, 1H), 7.53 (d, *J* = 6.0 Hz, 1H), 7.19 (t, *J* = 2.5 Hz, 2H), 7.15 (dd, *J* = 5.0, 4.0 Hz, 1H), 3.91 (dd, *J* = 12.5, 11.0Hz, 2H), 3.14–3.09 (m, 2H). ^{13}C NMR (126

MHz, $CDCl_3$) δ 168.82, 164.91, 158.99, 152.82, 149.32, 137.01, 130.48, 130.16, 128.22, 127.33, 123.62, 122.03, 38.99, 35.90. HRMS (ESI): calcd for $C_{14}H_{13}N_4O_2S$ ([M+H]$^+$), 310.07537; found, 310.07428.

Data for *N*-(2-(3-chloro-5-(trifluoromethyl)pyridin-2-yl)ethyl)-3-(thiophen-2-yl)-1,2,4-oxadiazole-5-carboxamide (**F14**), yellow solid, m.p. 94–96 ℃, yield 56.0%, purity 99.4%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.76 (s, 1H), 8.07 (s, 1H), 7.92 (s, 1H), 7.80 (d, *J* = 3.5 Hz, 1H), 7.53 (d, *J* = 6.0 Hz, 1H), 7.15 (dd, *J* = 5.0, 3.8 Hz, 1H), 4.03 (dd, *J* = 12.0, 6.2 Hz, 2H), 3.32 (t, *J* = 5.9 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.55, 164.88, 160.24, 152.89, 143.84 (d, *J* = 3.9 Hz), 134.09 (d, *J* = 3.3 Hz), 132.01, 130.52, 130.26, 128.26, 127.14, 126.30 (d, *J* = 33.9 Hz), 122.74 (d, *J* = 272.9 Hz), 36.91, 33.96. HRMS (ESI): calcd for $C_{15}H_{11}ClF_3N_4O_2S$ ([M+H]$^+$), 403.02379; found, 403.02222.

Data for *N*-(2,4-difluorobenzyl)-3-(thiophen-2-yl)-1,2,4-oxadiazole-5-carboxamide (**F15**), yellow solid, m.p. 102–103 ℃, yield 63.7%, purity 98.8%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 3.6, 0.8 Hz, 1H), 7.55 (dd, *J* = 4.8, 1.2 Hz, 2H), 7.47–7.39 (m, 1H), 7.17 (dd, *J* = 4.8, 3.6 Hz, 1H), 6.92–6.82 (m, 2H), 4.68 (d, *J* = 6.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.17, 164.79, 163.26 (d, *J* = 164.9 Hz), 160.72 (d, *J* = 176.4 Hz), 152.83, 131.64 (dd, *J* = 9.8, 5.6 Hz), 130.46, 130.26, 128.22, 126.96, 119.56 (d, J = 15.2 Hz), 111.74 (d, J = 25.3 Hz), 104.22, 37.48. HRMS (ESI): calcd for $C_{14}H_{10}F_2N_3O_2S$ ([M+H]$^+$), 322.04563; found, 322.04425.

Data for *N*-(2,4-dichlorophenyl)-3-(thiophen-2-yl)-1,2,4-oxadiazole-5-carboxamide (**F16**), white solid, m.p. 147–148 ℃, yield 53.7%, purity 99.3%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.38 (s, 1H), 8.46 (d, *J* = 9.2 Hz, 1H), 7.90 (dd, *J* = 4.0, 1.2 Hz, 1H), 7.59 (dd, *J* = 5.2, 1.2 Hz, 1H), 7.49 (d, *J* = 2.4 Hz, 1H), 7.35 (dd, *J* = 8.8, 2.4Hz, 1H), 7.20 (dd, *J* = 4.8, 3.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.06, 164.97, 150.23, 131.80, 131.12, 130.85, 130.53, 129.23, 128.31, 128.24, 126.70, 124.19, 122.35. HRMS (ESI): calcd for $C_{13}H_7Cl_2N_3O_2SNa$ ([M+Na]$^+$), 361;95282; found, 361;95276.

Data for 3-(6-bromopyridin-3-yl)-*N*-(2-(pyridin-2-yl)ethyl)-1,2,4-oxadiazole-5-carboxamide (**F17**), white solid, m.p. 135–137 ℃, yield 53.0%, purity 93.8%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.15–9.12 (m, 1H), 8.80 (s, 1H), 8.60 (d, *J* = 4.4 Hz, 1H), 8.36 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.67 (td, *J* = 7.6, 1.6 Hz, 1H), 7.50 (dd, *J* = 8.4, 0.4 Hz, 1H), 7.25–7.19 (m, 2H), 3.99–3.91 (m, 2H), 3.19–3.11 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.56, 166.09, 158.97, 154.58, 152.46, 149.20, 148.79, 137.29, 137.00, 124.75, 123.57, 122.01, 121.26, 38.94, 35.68. HRMS (ESI): calcd for $C_{15}H_{12}BrN_5O_2$ ([M-H]$^-$), 407.98574; found, 407.98596.

Data for 3-(6-bromopyridin-3-yl)-*N*-(2-(3-chloro-5-(trifluoromethyl)pyridin-2-yl)ethyl)-1,2,4-oxadiazole-5-carboxamide (**F18**), white solid, m.p. 118–120 ℃, yield 43.8%, purity 99.6%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.10 (d, *J* = 2.4 Hz, 1H), 8.78 (s, 1H), 8.34 (dd, *J* = 8.2, 2.4 Hz, 1H), 8.13 (s, 1H), 7.95 (d, *J* = 1.6 Hz, 1H), 7.50 (d, *J* = 8.2 Hz, 1H), 4.07 (dd, *J* = 12.0, 6.0 Hz, 2H), 3.36 (t, *J* = 6.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.25, 166.11, 160.14, 154.69, 152.54, 148.75, 143.76 (d, *J* = 3.9 Hz), 137.27, 134.05, 131.97, 126.51, 126.18, 124.78, 121.11, 36.92, 33.84. HRMS (ESI): calcd for $C_{16}H_{10}BrClF_3N_5O_2$ ([M-H]$^-$), 509.93415; found, 509.93390.

Data for 3-(6-bromopyridin-3-yl)-*N*-(2,4-difluorobenzyl)-1,2,4-oxadiazole-5-carboxamide (**F19**), white solid, m.p. 128–129 ℃, yield 53.1%, purity 98.5%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.08 (d, *J* = 2.0 Hz, 1H), 8.34 (dd, *J* = 8.2, 2.4 Hz, 1H), 7.60 (s, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.48–7.40 (m, 1H), 7.01–6.78 (m, 2H), 4.71 (d, *J* = 6.0 Hz, 2H). ^{113}C NMR (101 MHz, $CDCl_3$) δ 168.94, 166.11, 163.30 (dd, *J* = 178.1, 11.9 Hz), 160.81 (dd, *J* = 177.8, 12.2 Hz), 154.76, 152.59, 148.71, 137.28, 131.68 (dd, *J* = 9.8, 6.4 Hz), 124.82, 121.01, 119.47 (dd, *J* = 14.9, 3.7 Hz), 111.77 (dd, *J* = 21.5, 3.9 Hz), 104.26, 37.62. HRMS (ESI): calcd for $C_{15}H_9BrF_2N_4O_2$ ([M-H]$^-$), 428.95600; found, 428.95587.

Data for 3-(6-bromopyridin-3-yl)-*N*-(2,4-dichlorophenyl)-1,2,4-oxadiazole-5-carboxamide (**F20**), white solid, m.p. 201–202 ℃, yield 53.8%, purity 99.0%; ^{1}H NMR (400 MHz, DMSO-*d6*) δ 11.18 (s, 1H), 9.10 (d, *J* = 2.2 Hz, 1H), 8.50 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.82 (d, *J* = 6.1 Hz, 1H), 7.81 (s, 1H), 7.70 (d, *J* = 8.6 Hz, 1H), 7.55 (dd, *J* = 8.6, 2.4 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 169.65, 166.28, 153.88, 152.01, 148.84, 138.74, 132.73, 132.53, 130.78, 129.86, 129.51, 128.52, 125.80, 121.82. HRMS (ESI): calcd for $C_{14}H_6BrCl_2N_4O_2$ ([M-H]$^-$), 410.90457; found, 410.90454

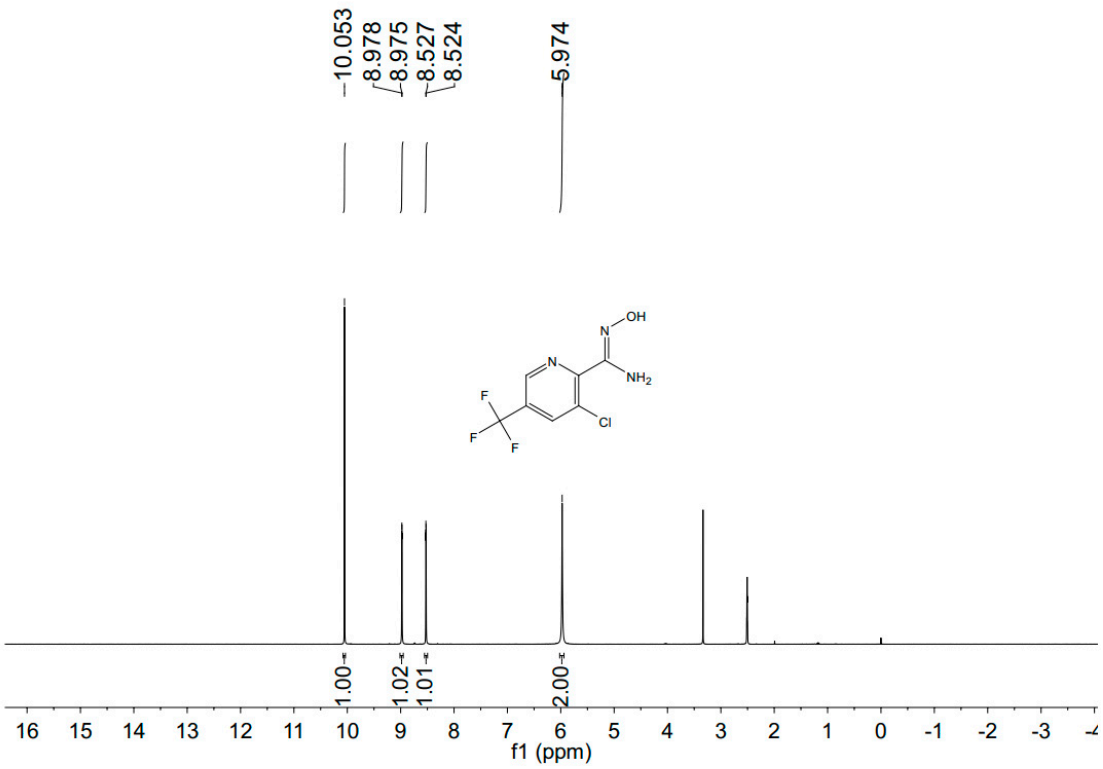
Data for 3-(3-chloro-5-(trifluoromethyl)pyridin-2-yl)-*N*-(2-(pyridin-2-yl)ethyl)-1,2,4-oxadiazole-5-carboxamide (**F21**), yellow solid, m.p. 140–141 ℃, yield 56.5%, purity 92.4%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.96 (d, *J* = 1.22 Hz, 1H), 8.56 (dd, *J* = 4.8, 0.8 Hz, 1H), 8.87 (s, 1H), 8.18 (d, *J* = 2.4 Hz, 1H), 7.46 (td, *J* = 8.0, 2.0 Hz, 1H), 7.21–7.17 (m, 1H), 3.96 (dd, *J* = 12.4, 7.0 Hz, 2H), 3.14 (t, *J* = 6.4 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.37, 166.17, 158.73, 152.42, 149.33, 146.60, 144.64 (d, *J* = 3.8 Hz), 136.81, 136.32 (d, *J* = 3.5 Hz), 132.70, 129.01 (d, *J* = 34.2 Hz), 123.47, 121.88, 120.75, 39.00, 35.99. HRMS (ESI): calcd for $C_{16}H_{12}ClF_3N_5O_2$ ([M+H]$^+$), 398.06261; found, 398.06070.

Data for 3-(3-chloro-5-(trifluoromethyl)pyridin-2-yl)-*N*-(2-(3-chloro-5-(trifluoromethyl)pyridin-2-yl)ethyl)-1,2,4-oxadiazole-5-carboxamide (**F22**), white solid, m.p. 158–159 ℃, yield 49.9%, purity 99.4%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.96 (d, *J* = 0.8 Hz, 1H), 8.74 (s, 1H), 8.19 (d, *J* = 1.2 Hz, 1H), 8.08 (s, 1H), 7.93 (d, *J* = 1.6 Hz, 1H), 4.07 (m, 2H), 3.35 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.13, 166.09, 159.98, 152.48, 146.44, 144.66 (d, *J* = 3.8 Hz), 143.82 (d, *J* = 4.0 Hz), 136.39 (d, *J* = 3.5 Hz), 133.97 (d, *J* = 3.6 Hz), 132.75, 131.91, 129.09 (d, *J* = 34.3 Hz), 126.23 (d, *J* = 33.7 Hz), 123.72 (d, *J* = 57.3 Hz), 121.00 (d, *J* = 57.8 Hz), 36.90, 33.89. HRMS (ESI): calcd for $C_{17}H_{10}Cl_2F_6N_5O_2$ ([M+H]$^+$), 500.01103; found, 500.00858.

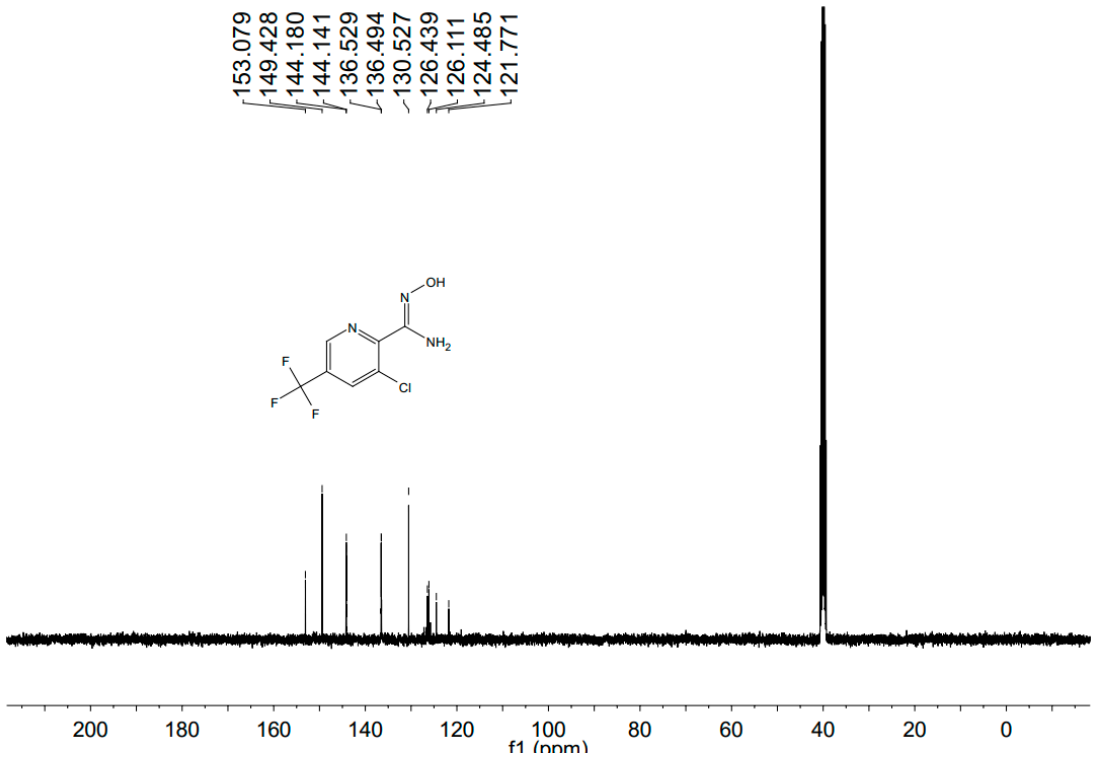
Data for 3-(3-chloro-5-(trifluoromethyl)pyridin-2-yl)-*N*-(2,4-difluorobenzyl)-1,2,4-oxadiazole-5-carboxamide (**F23**), white solid, m.p. 112–114 ℃, yield 47.7%, purity 98.6%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (s, 1H), 8.19 (s, 1H), 7.64 (s, 1H), 7.46–7.37 (m, 1H), 6.92–6.81 (m, 2H), 4.68 (d, *J* = 6.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.82, 166.08, 164.13, 161.64, 152.41,

146.19, 144.67 (d, *J* = 3.8 Hz), 136.53 (d, *J* = 3.6 Hz), 132.82, 131.79 (dd, *J* = 9.9, 5.5 Hz), 129.12 (d, *J* = 34.3 Hz), 122.04 (d, *J* = 274.6 Hz), 119.27, 111.73 (dd, *J* = 21.4, 3.6 Hz), 104.22, 37.57. HRMS (ESI): calcd for $C_{16}H_9ClF_5N_4O_2$ ([M+H]$^+$), 419.03287; found, 419.03104.

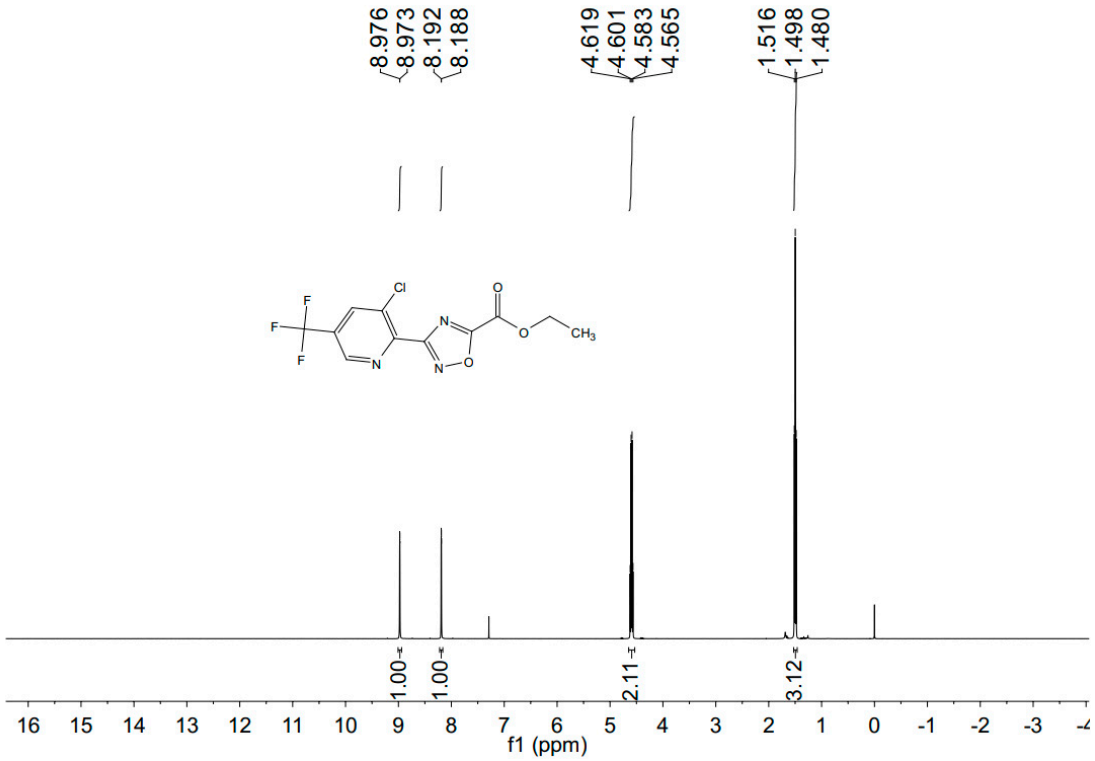
Data for 3-(3-chloro-5-(trifluoromethyl)pyridin-2-yl)-*N*-(2,4-dichlorophenyl)-1,2,4-oxadiazole-5-carboxamide (**F24**), white solid, m.p. 137–138 ℃, yield 55.0%, purity 92.3%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.41 (s, 1H), 8.99 (d, *J* = 0.8 Hz, 1H), 8.44 (d, *J* = 8.8 Hz, 1H), 8.21 (d, *J* = 1.2 Hz, 1H), 7.49 (d, *J* = 2.0 Hz, 1H), 7.37 (dd, *J* = 8.8, 2.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.72, 166.30, 149.94, 146.29, 144.76 (d, *J* = 3.7 Hz), 136.32 (d, *J* = 3.5 Hz), 132.84, 131.59, 131.41, 129.31, 128.31, 124.47, 123.45, 122.62, 120.73. HRMS (ESI): calcd for $C_{15}H_6Cl_3F_3N_4O_2Na$ ([M+Na]$^+$), 458.94006; found, 458.93991.



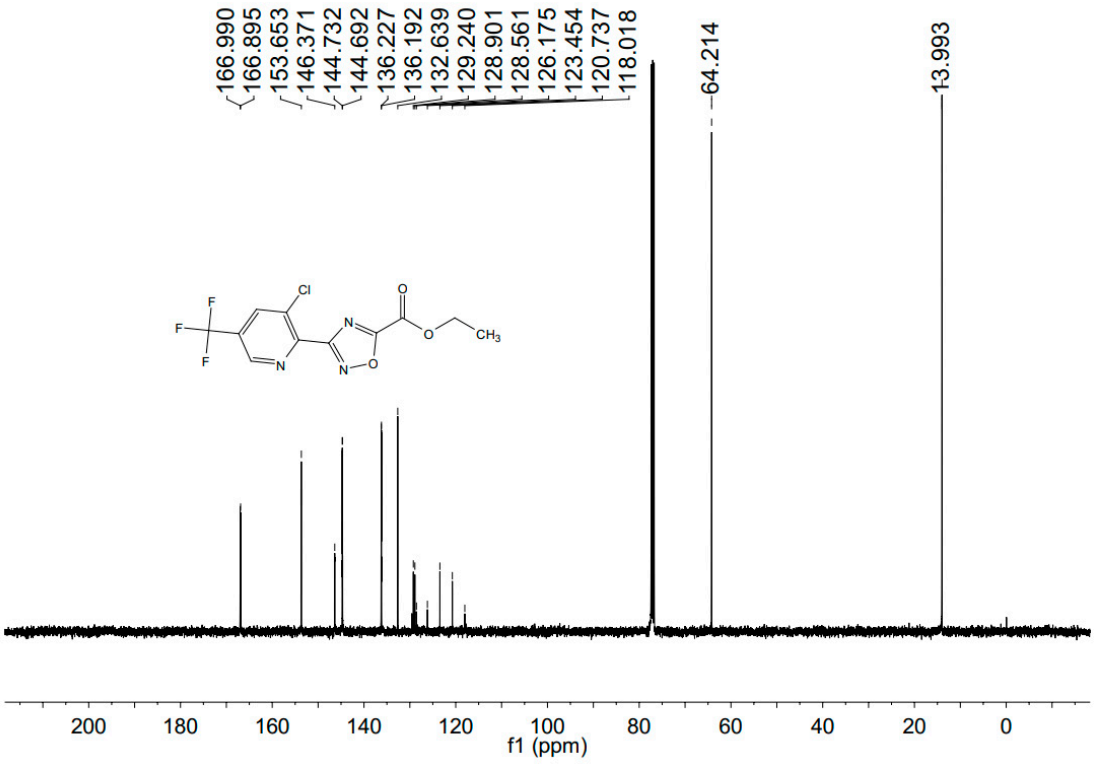
^{1}H NMR of intermediate **a6**



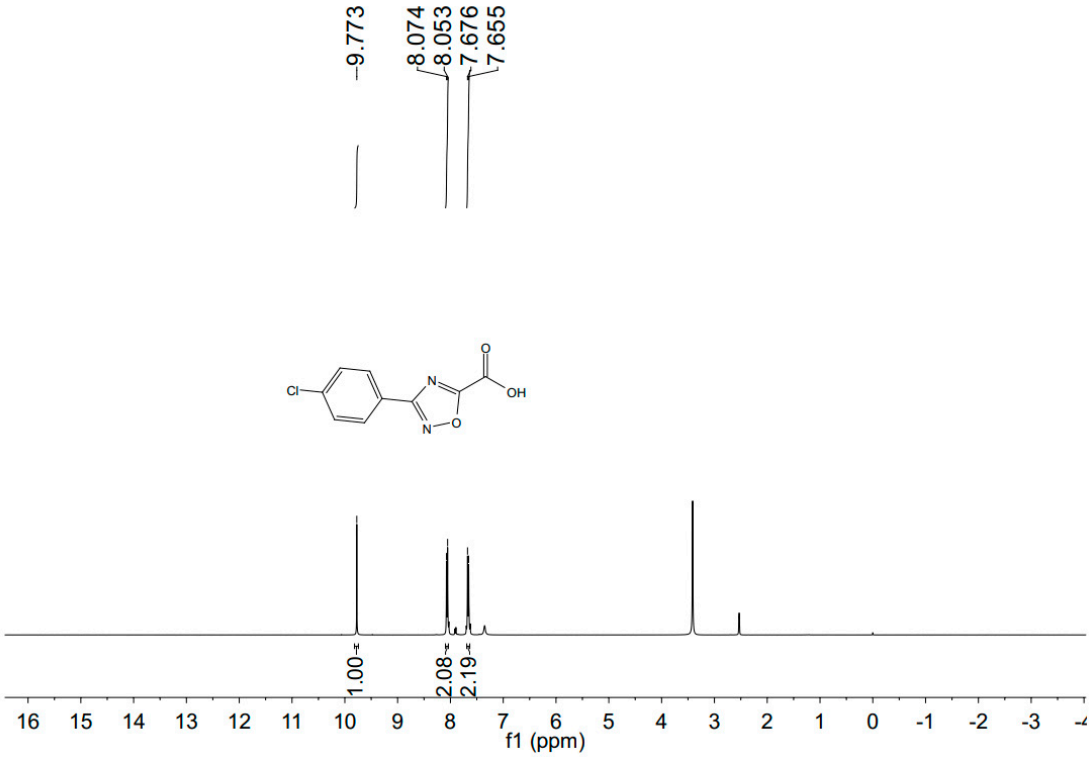
^{13}C NMR of intermediate **a6**



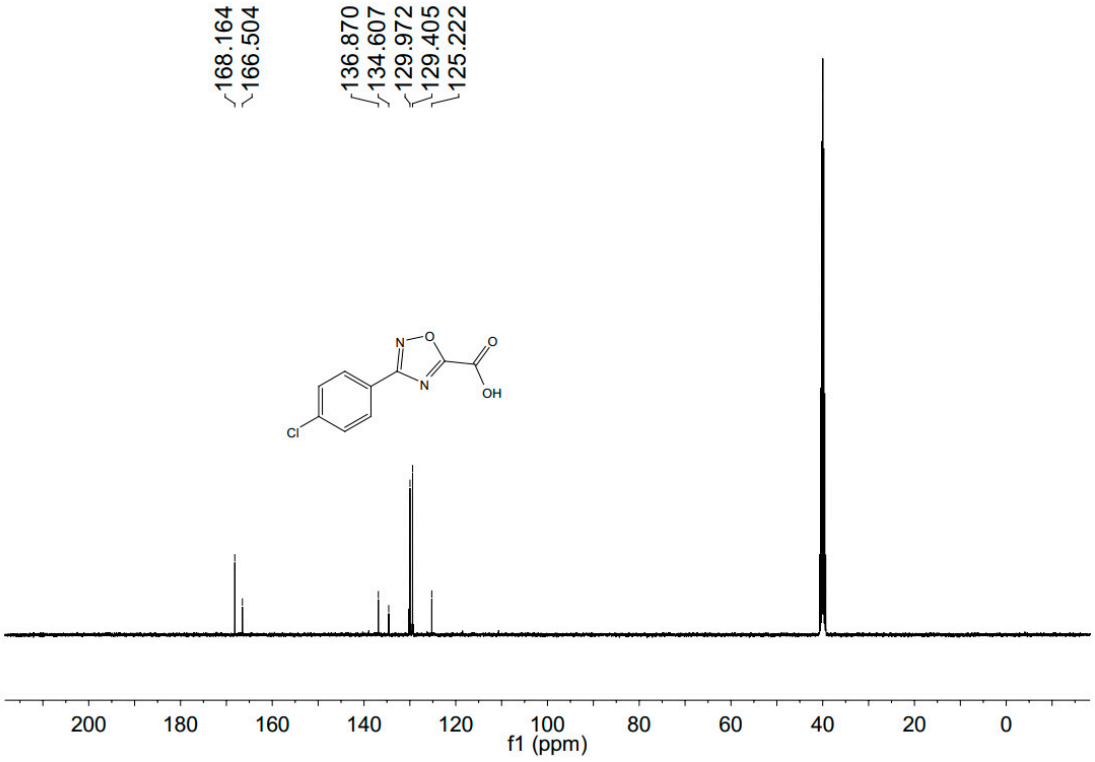
^{1}H NMR of intermediate **b6**



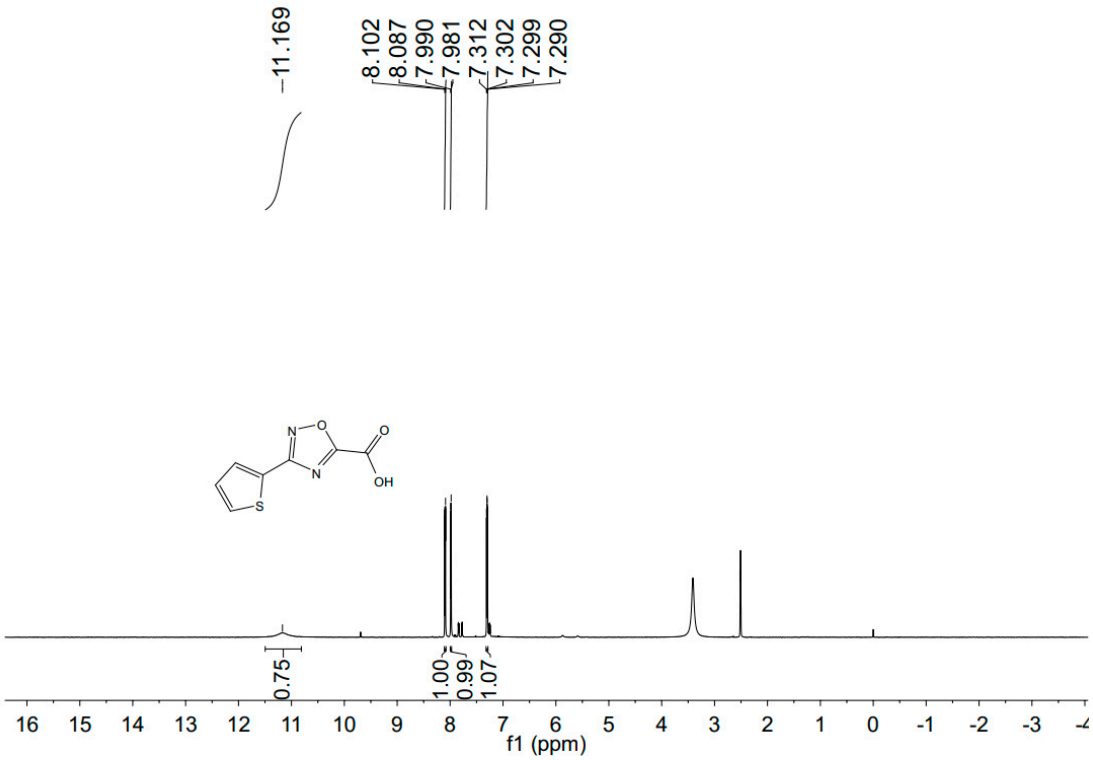
^{13}C NMR of intermediate **b6**



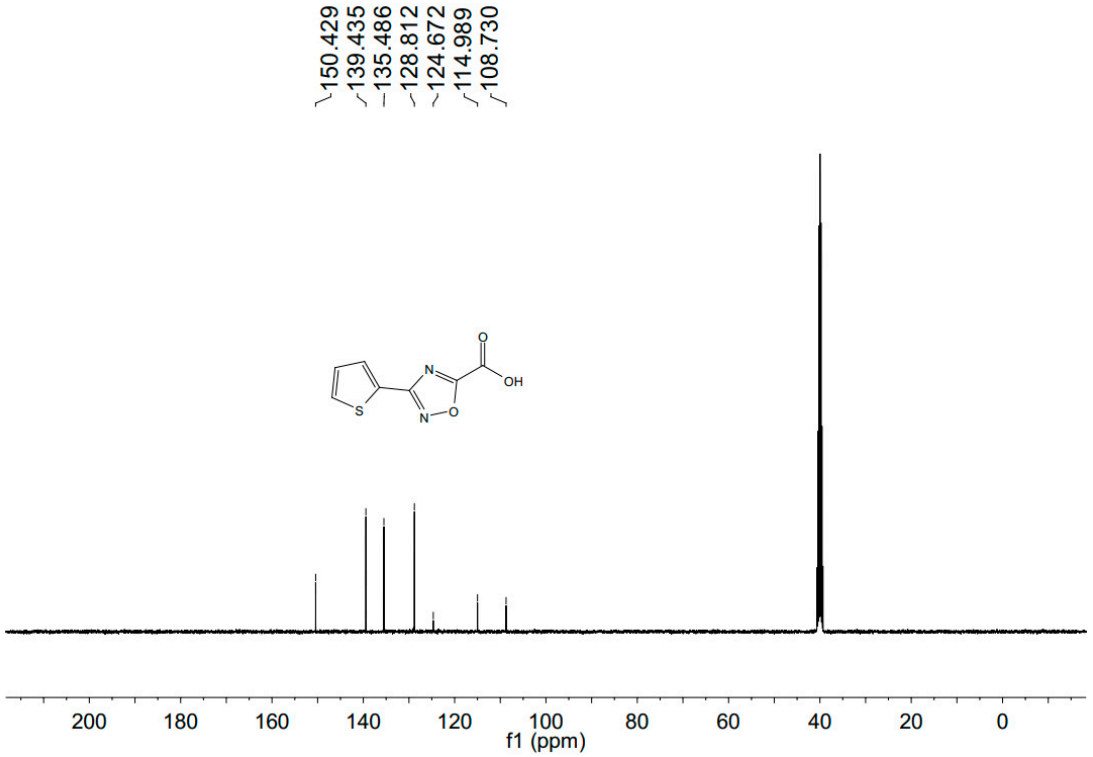
^{1}H NMR of intermediate **c3**



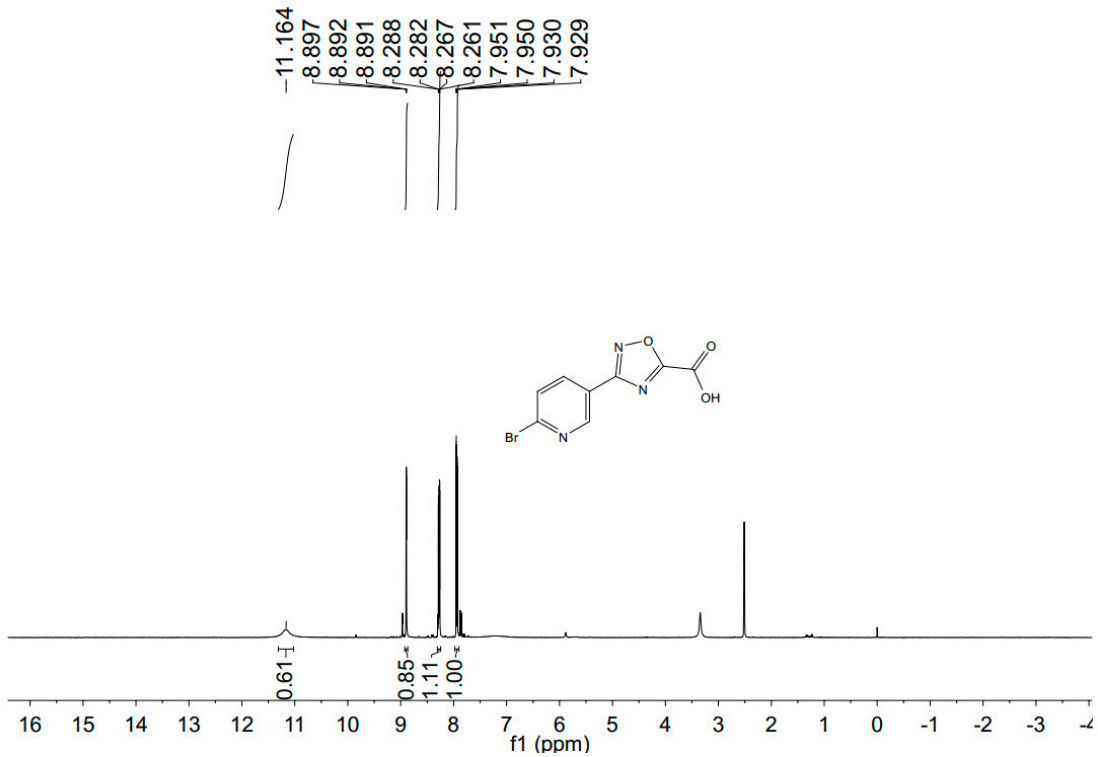
^{13}C NMR of intermediate **c3**



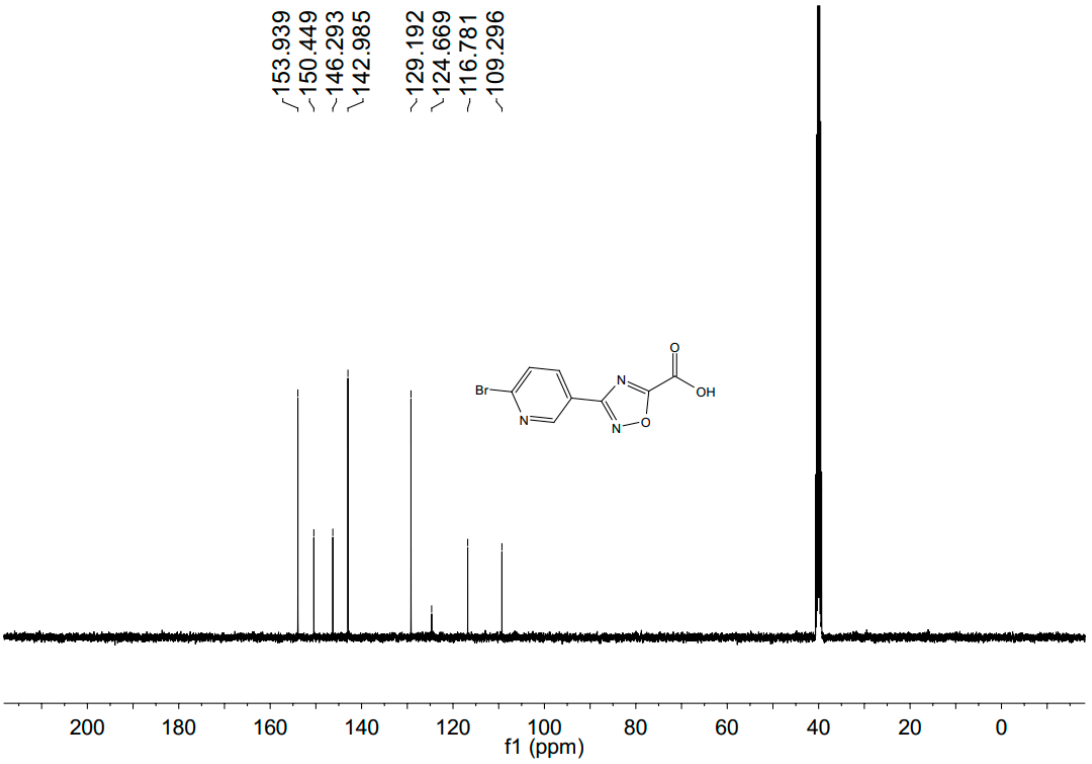
^{1}H NMR of intermediate **c4**



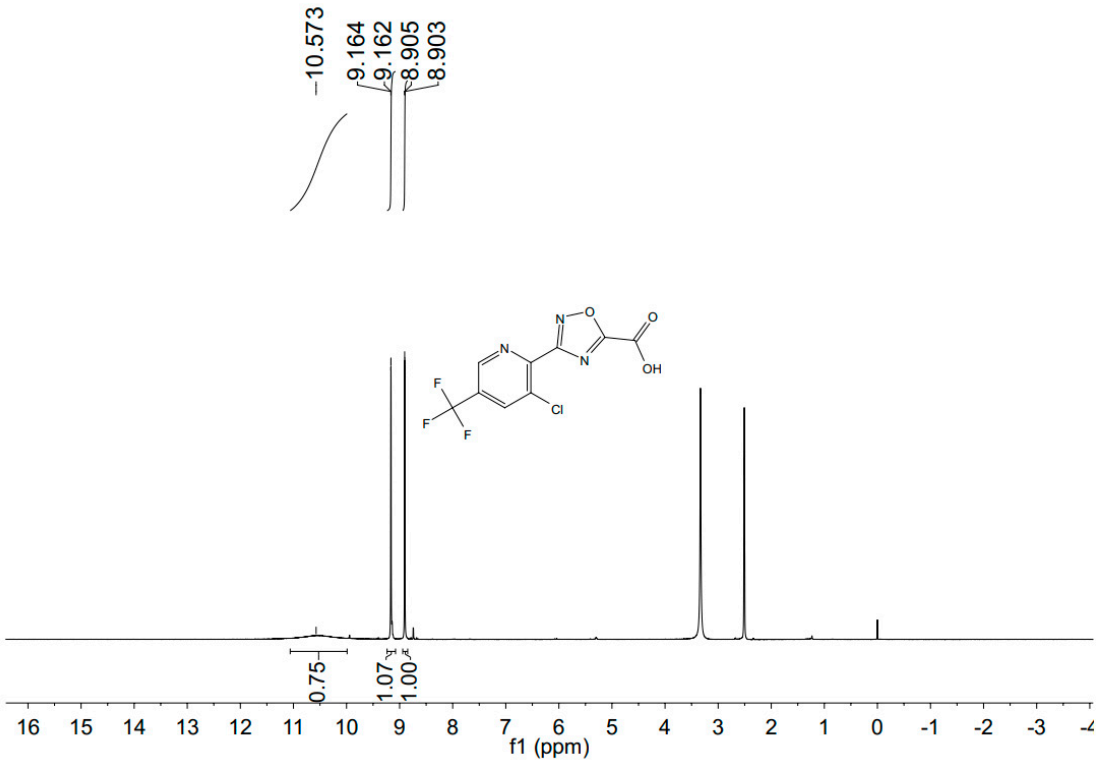
^{13}C NMR of intermediate **c4**



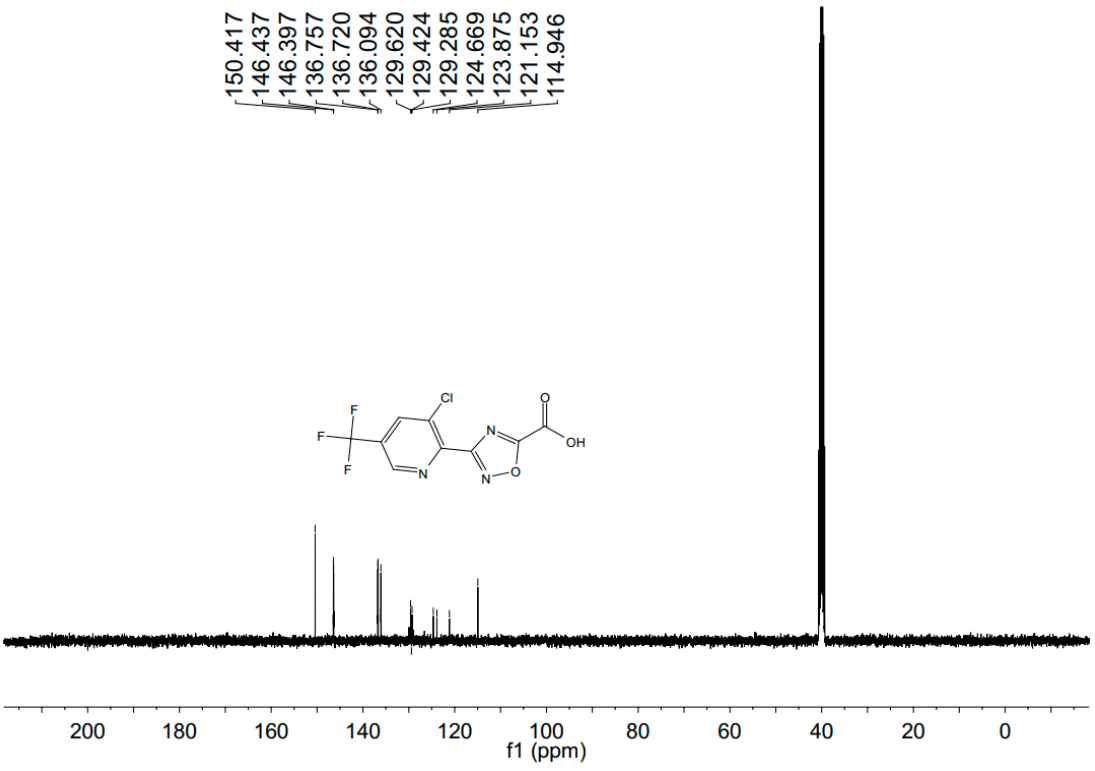
^{1}H NMR of intermediate **c5**



^{13}C NMR of intermediate **c5**



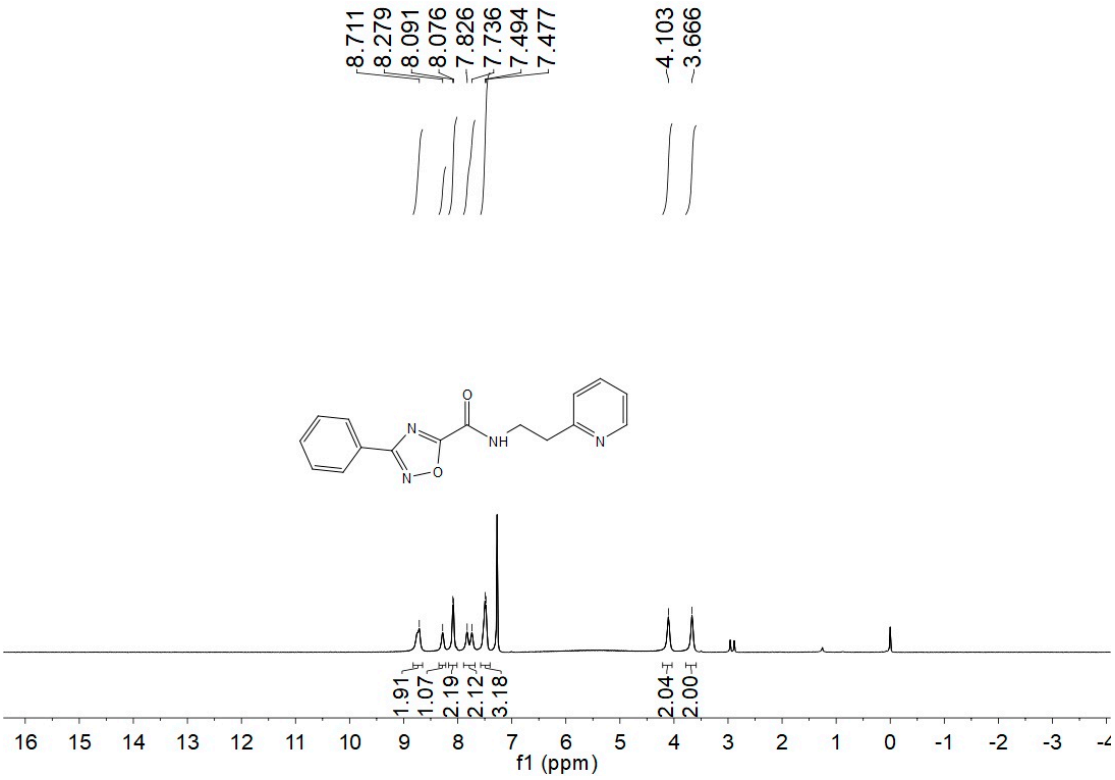
^{1}H NMR of intermediate **c6**



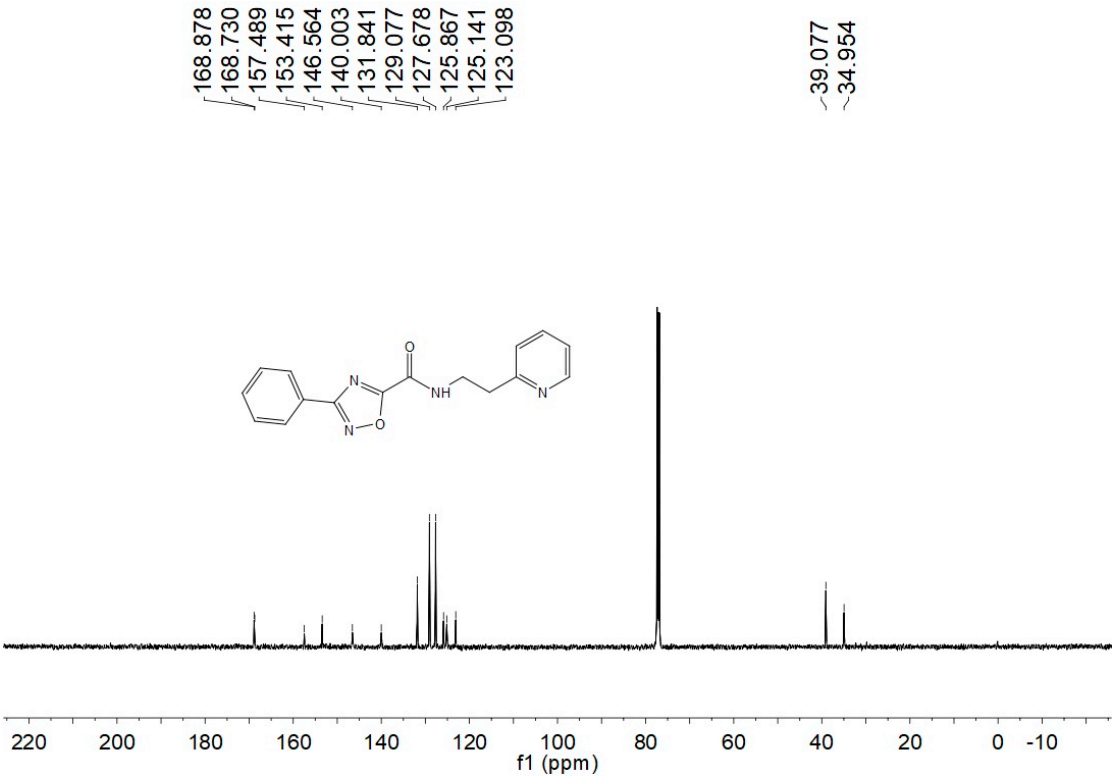
^{13}C NMR of intermediate **c6**

峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
1	3.063	164380	10086		0.331				0.331
2	3.709	307338	34093	V	0.620				0.620
3	5.308	1271064	121568		2.563				2.563
4	9.385	198761	13408		0.401				0.401
5	13.209	47654171	1658626	M	96.085				96.085
总计		49595713	1837781		100.000				100.000

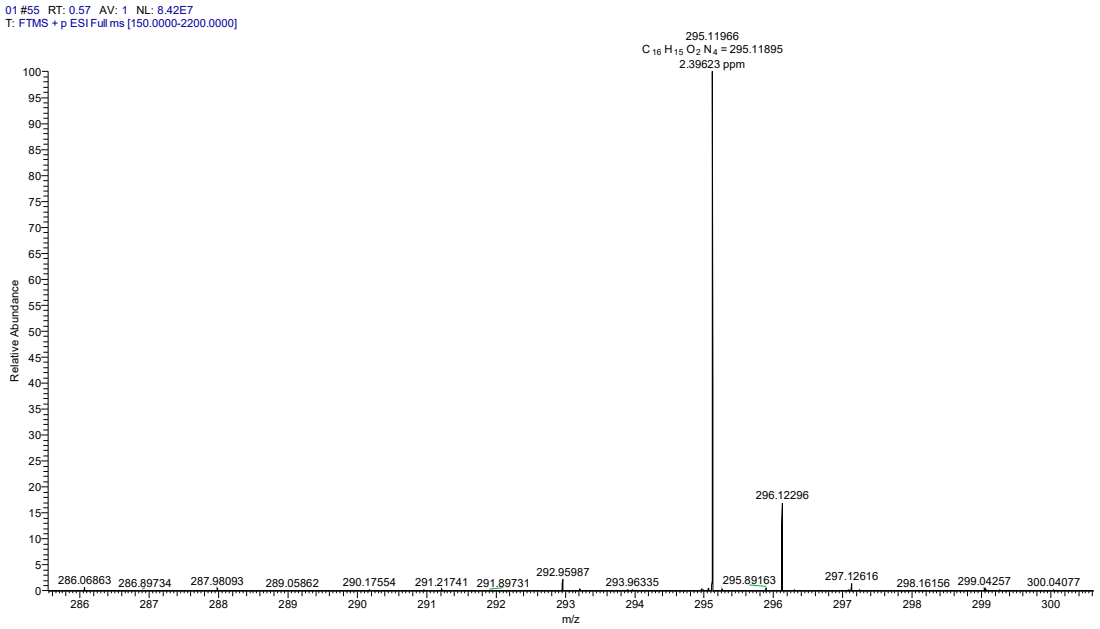
HPLC of compound **F1**



^{1}H NMR of compound **F1**



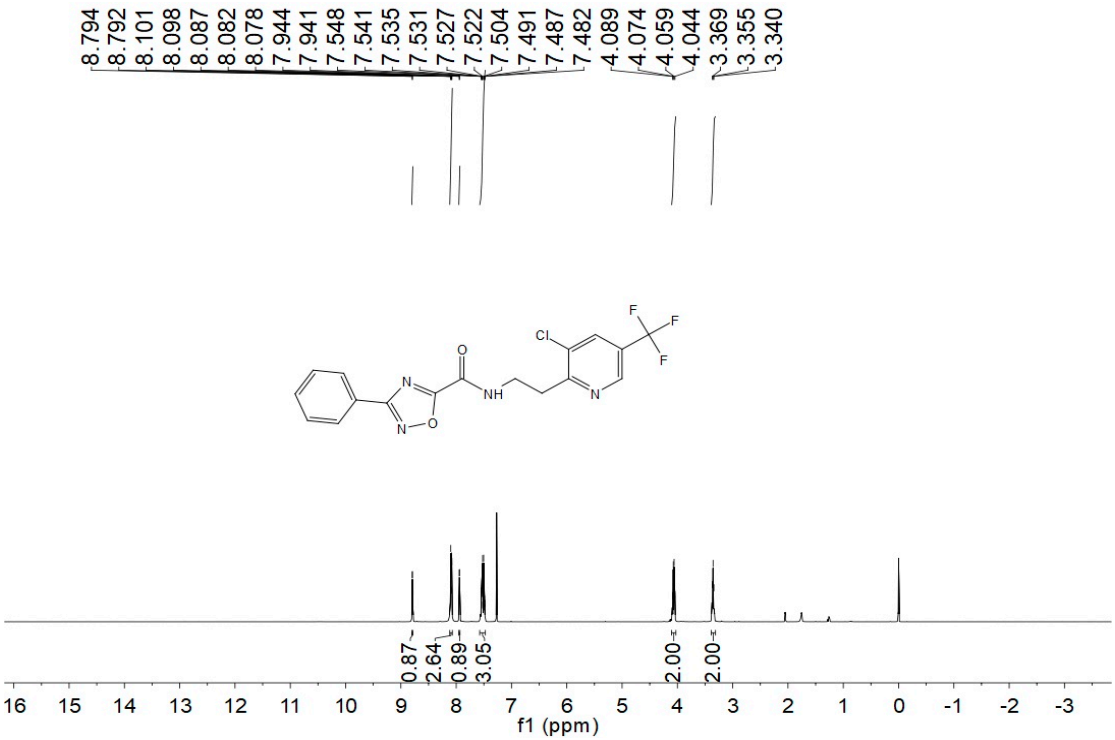
^{13}C NMR of compound **F1**



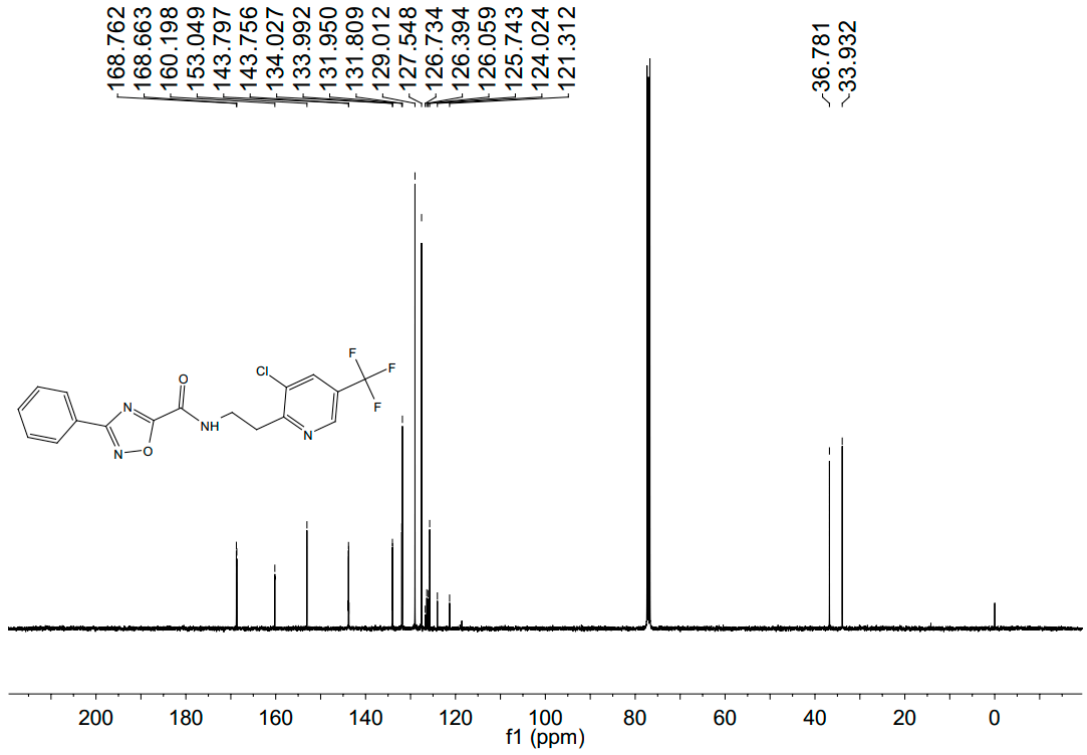
HRMS of compound **F1**

峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
5	5.238	39691	4984	V	0.166				0.166
6	6.367	10281	641		0.043				0.043
7	6.692	1322	125	V	0.006				0.006
8	7.066	46219	3182	V	0.193				0.193
9	7.706	3163	237		0.013				0.013
10	9.481	23693183	1539843		98.989				98.989
总计		23936176	1560214		100.000				100.000

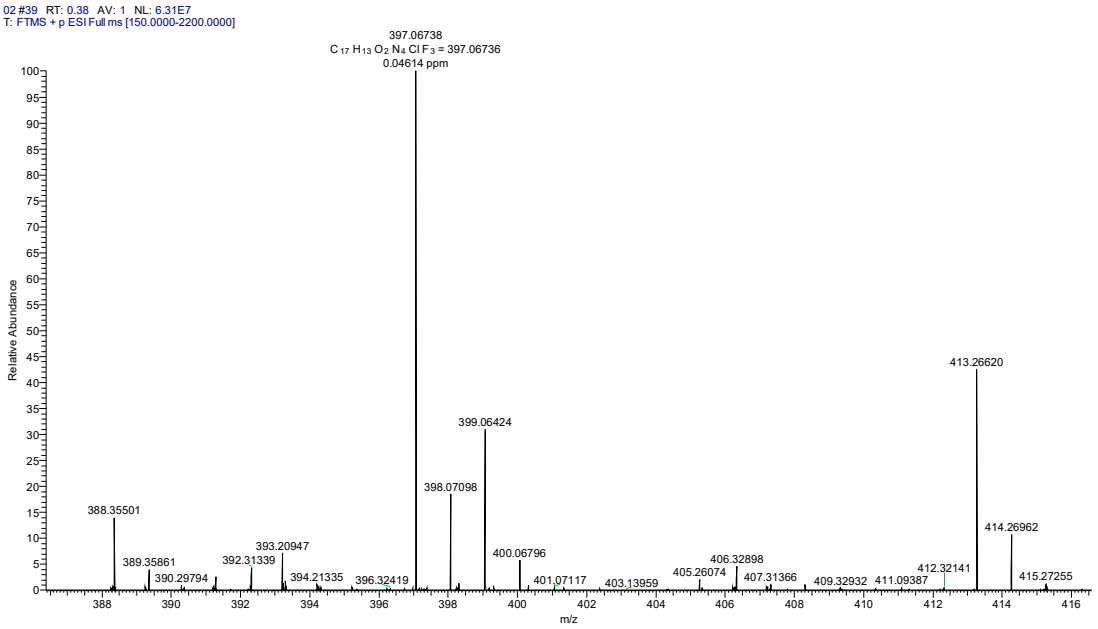
HPLC of compound **F2**



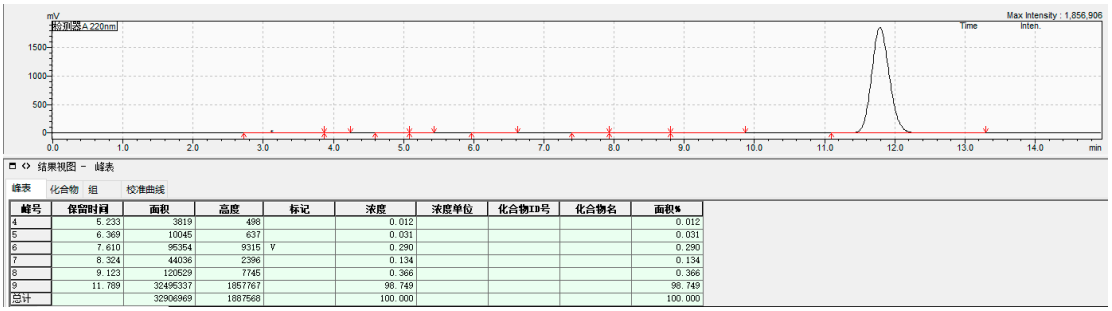
^{1}H NMR of compound **F2**



^{13}C NMR of compound **F2**

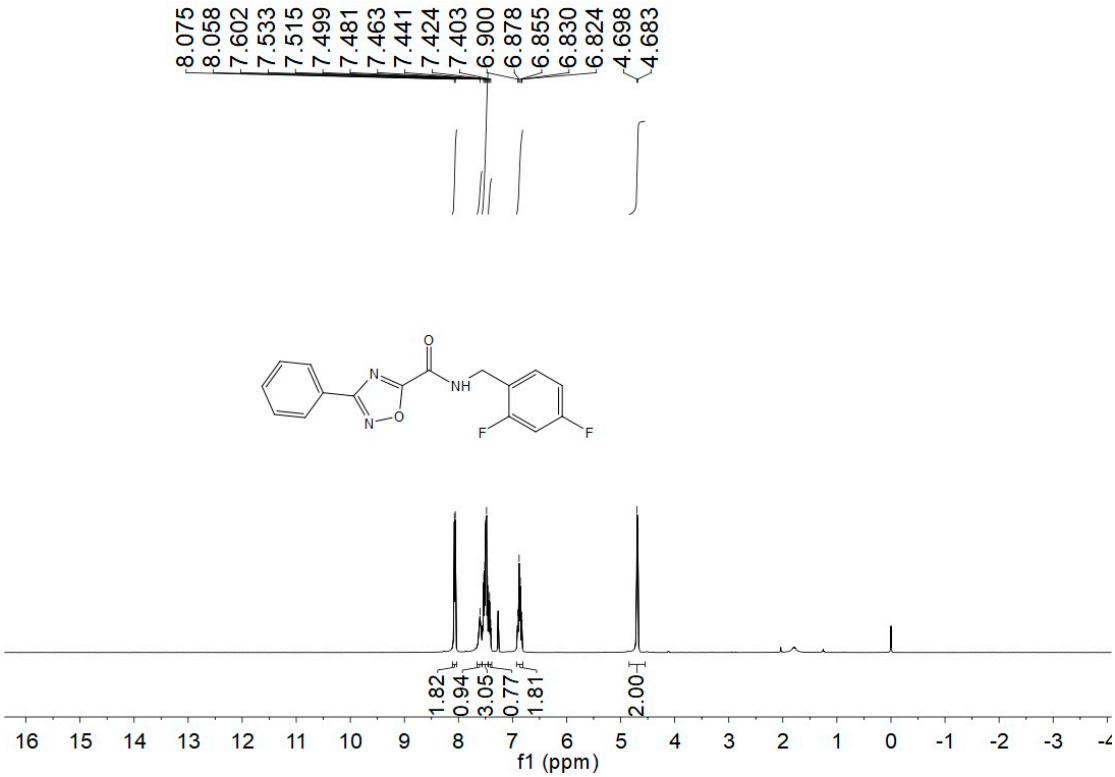


HRMS of compound **F2**

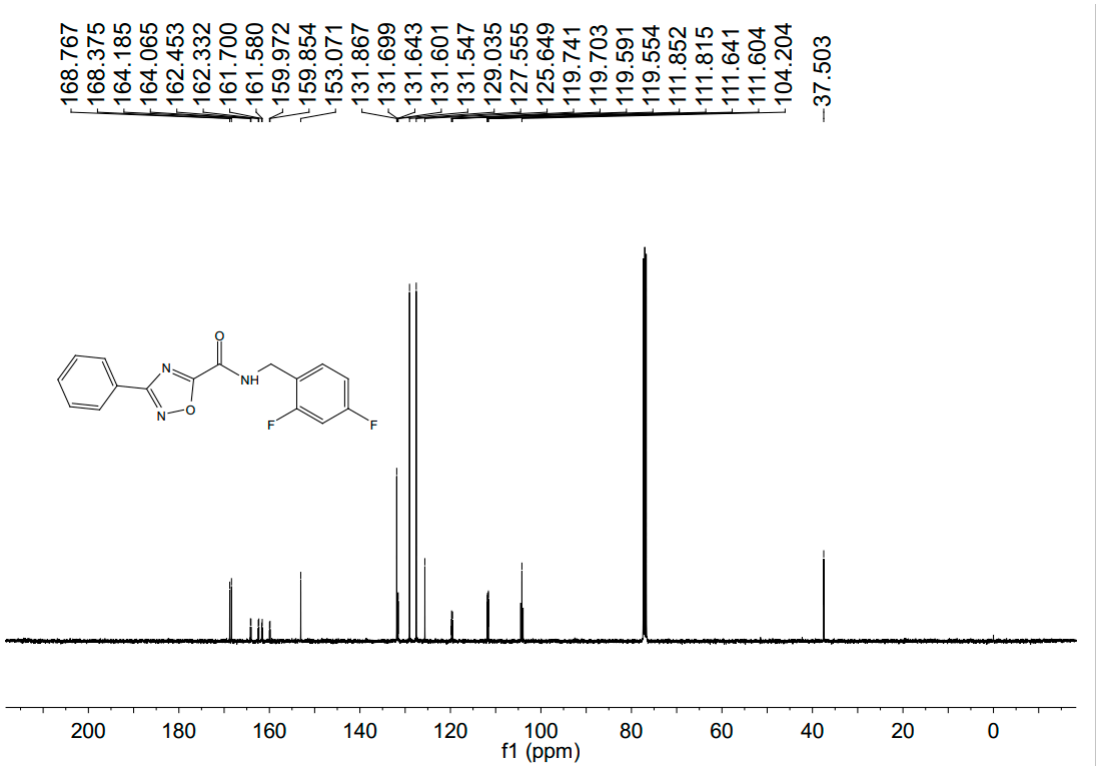


峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
4	5.233	3819	498		0.012				0.012
5	6.369	10045	637		0.031				0.031
6	7.610	96354	9315	V	0.290				0.290
7	8.324	44036	2396		0.134				0.134
8	9.123	120529	7745		0.366				0.366
9	11.789	32495337	1857767		98.749				98.749
总计		32906969	1887568		100.000				100.000

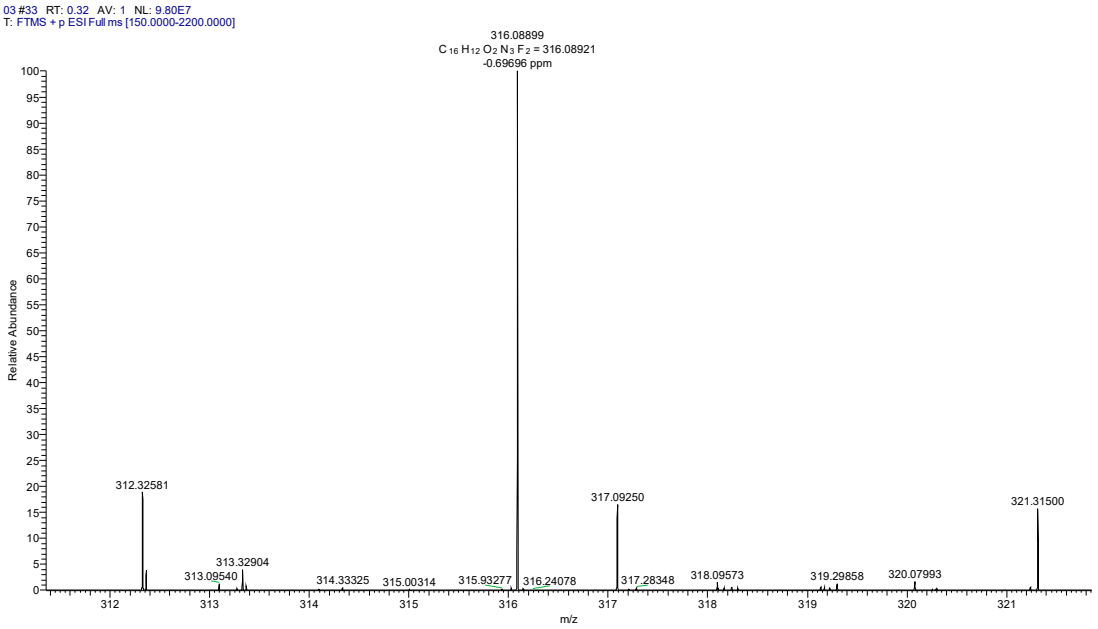
HPLC of compound **F3**



^{1}H NMR of compound **F3**



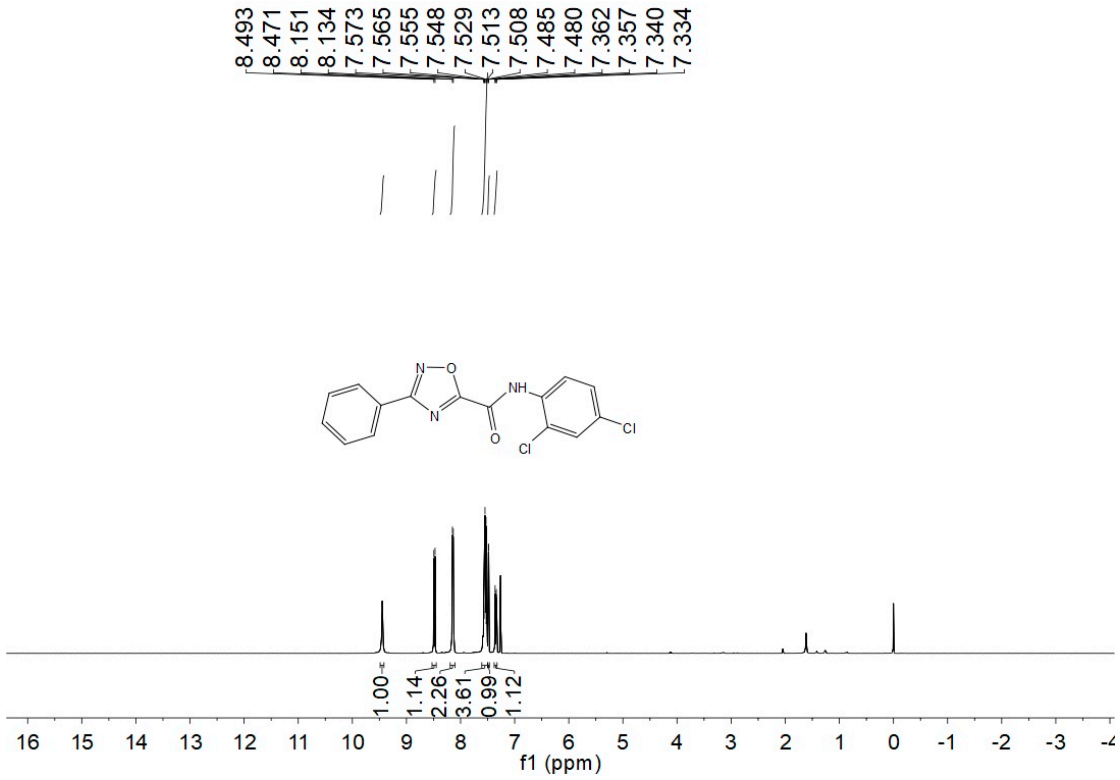
^{13}C NMR of compound **F3**



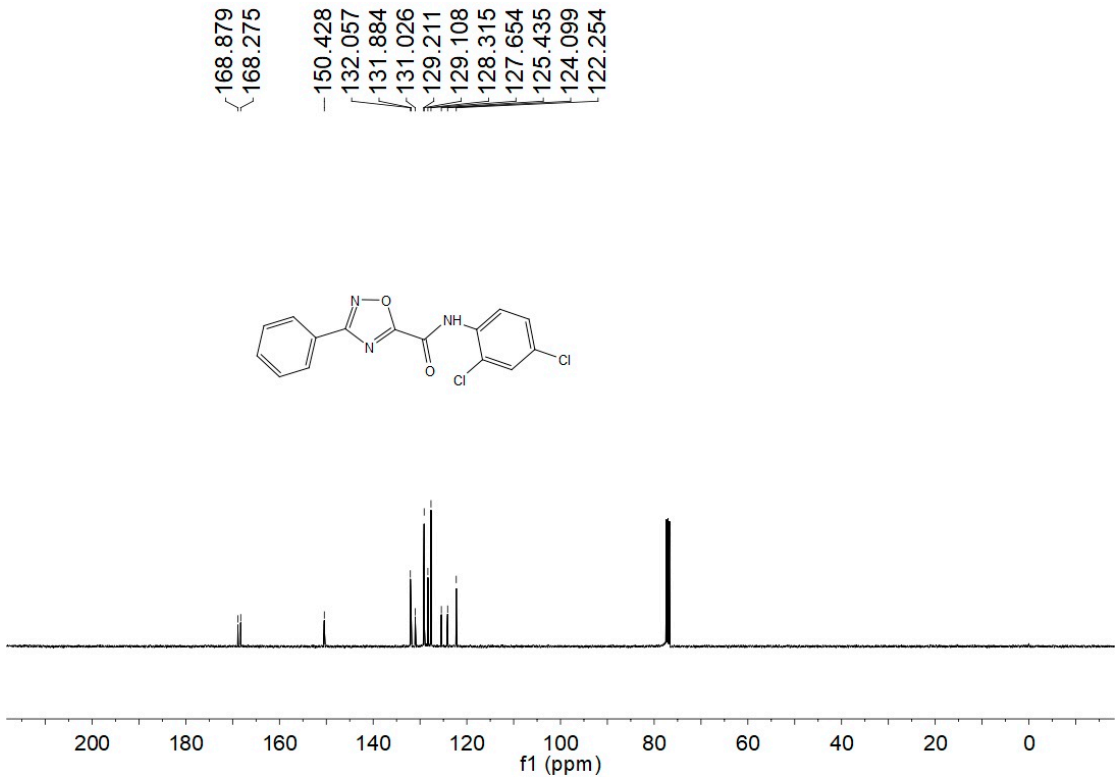
HRMS of compound **F3**

峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
1	3.068	82863	5776		1.559				1.559
2	4.785	1265	191		0.024				0.024
3	7.147	2529	116		0.048				0.048
4	7.827	5230096	498066	M	98.370				98.370
总计		5316753	504148		100.000				100.000

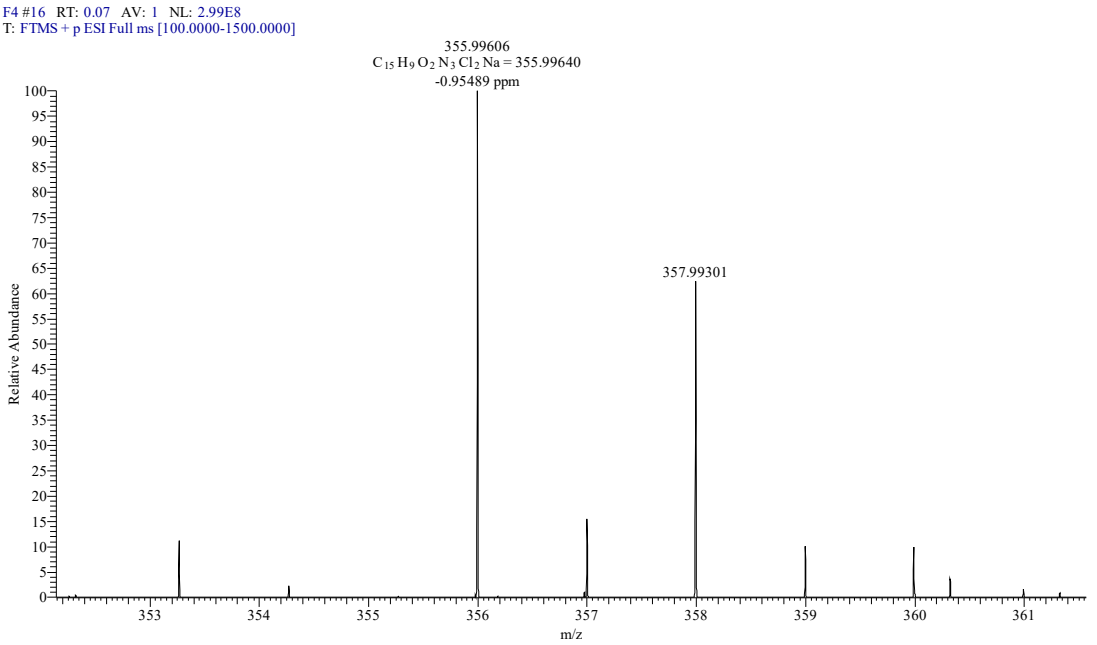
HPLC of compound **F4**



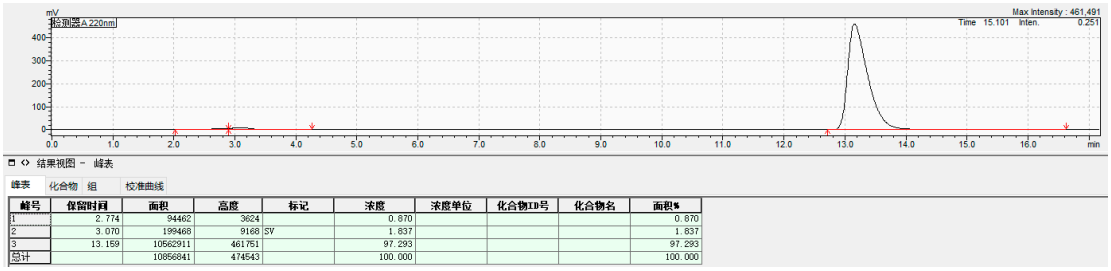
^{1}H NMR of compound **F4**



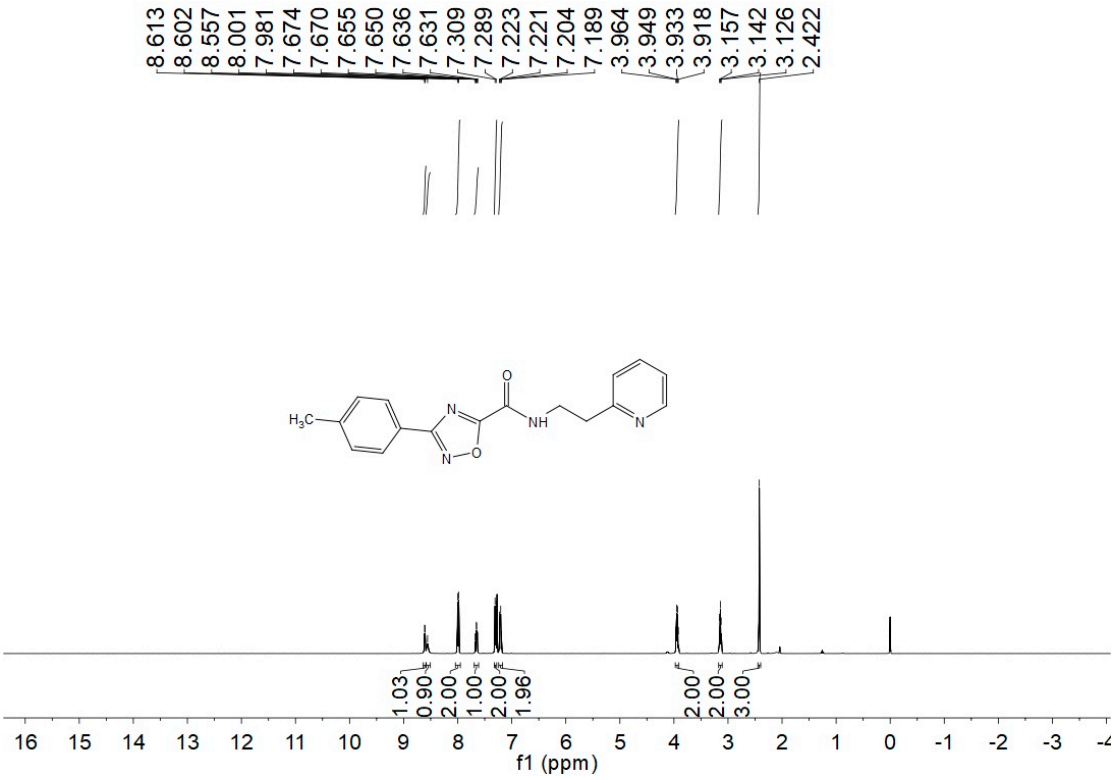
^{13}C NMR of compound **F4**



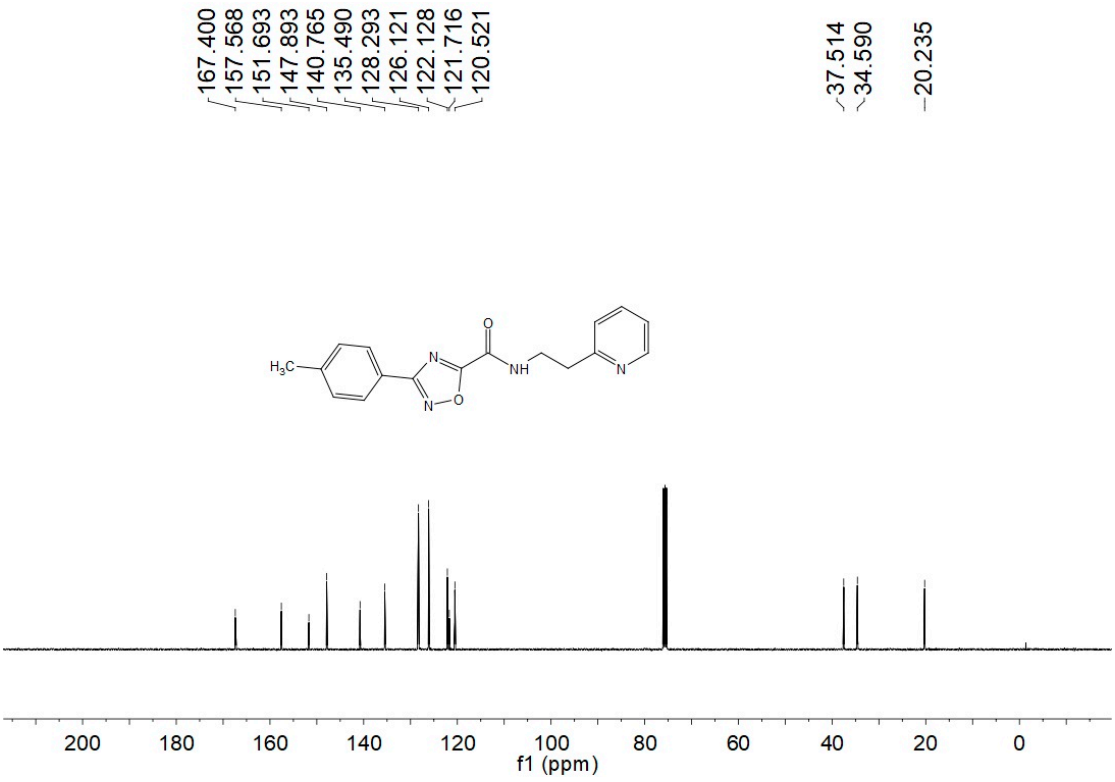
HRMS of compound **F4**



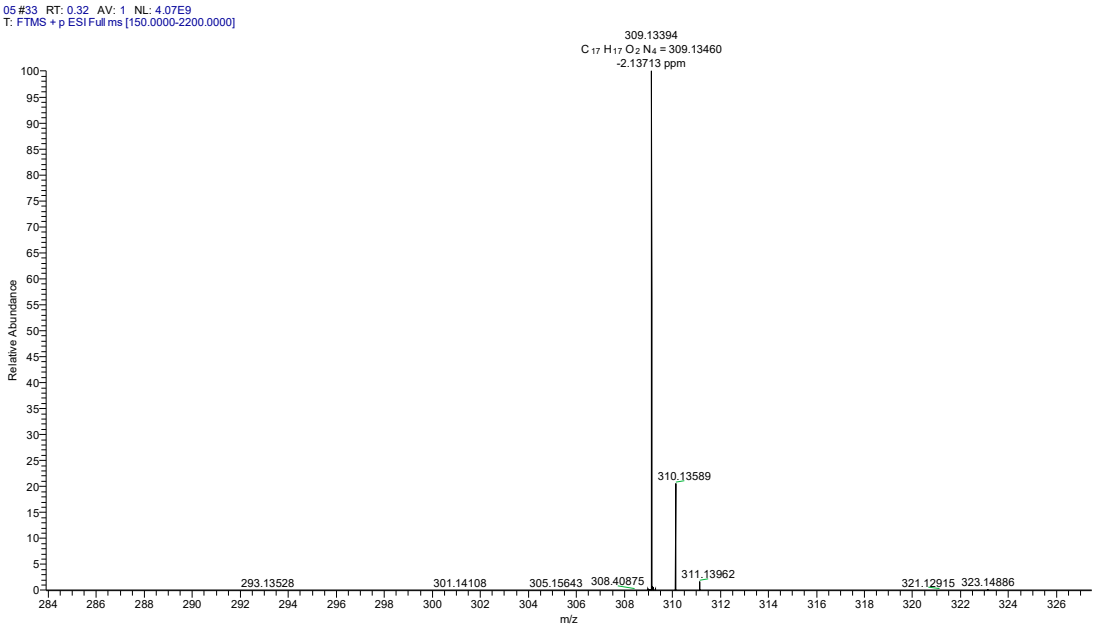
HPLC of compound **F5**



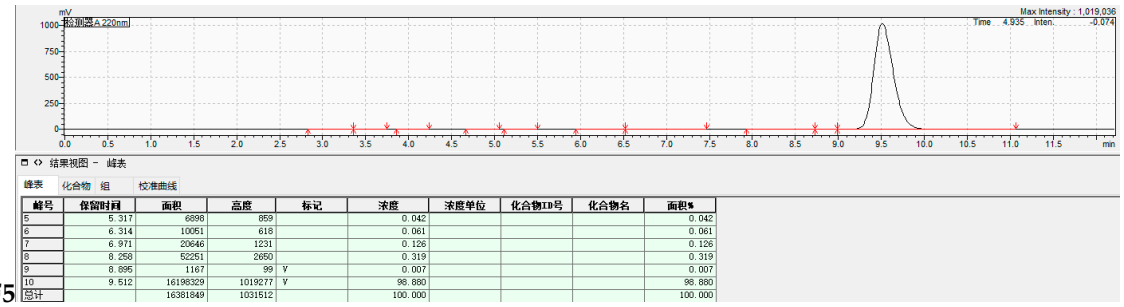
^{1}H NMR of compound **F5**



^{13}C NMR of compound **F5**

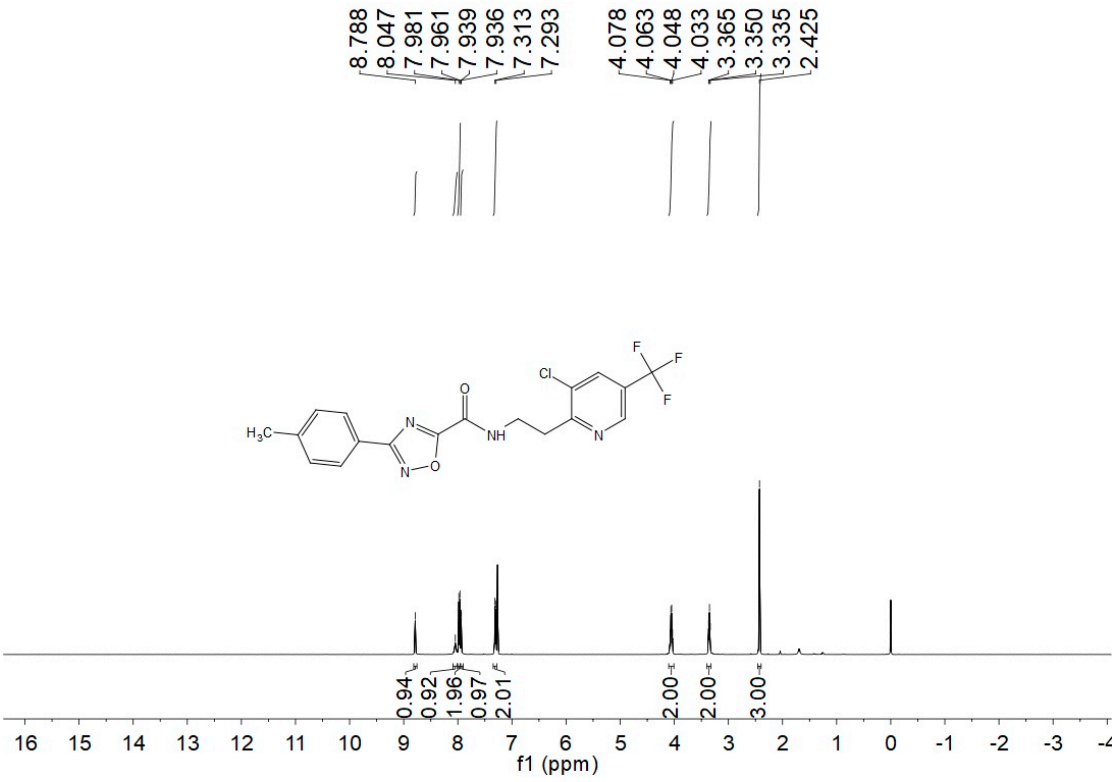


HRMS of compound **F5**

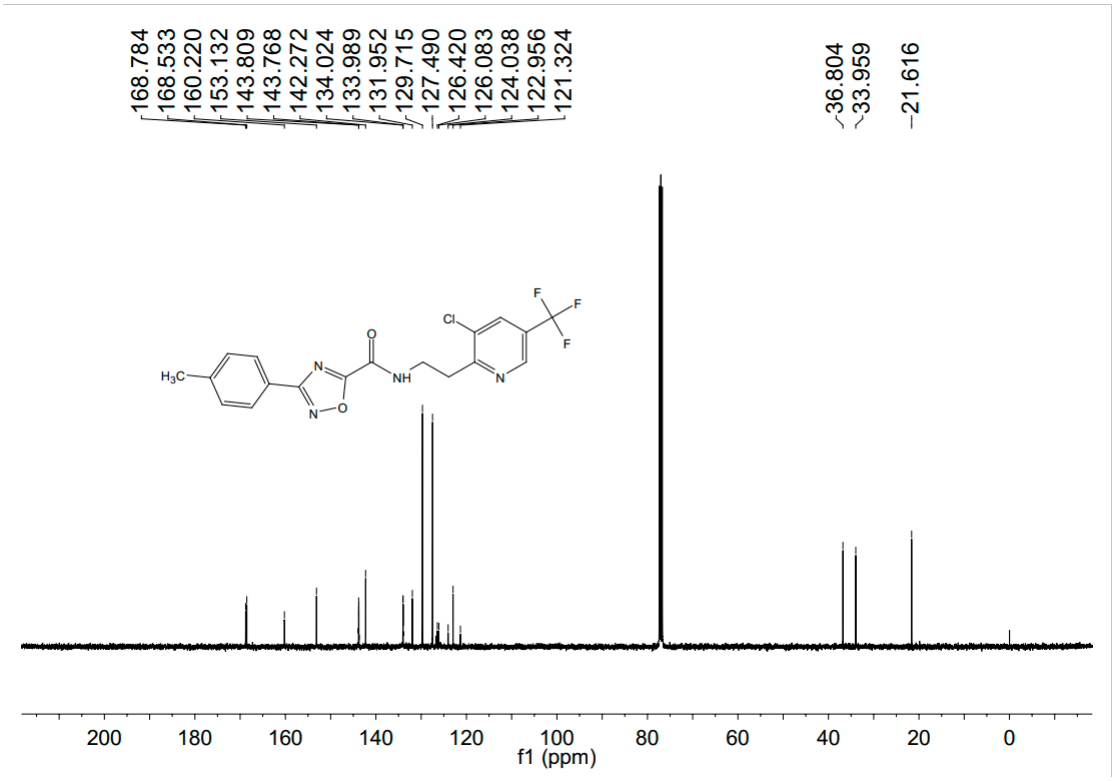


峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
5	5.317	6898	859		0.042				0.042
6	6.314	10051	618		0.061				0.061
7	6.971	20646	1231		0.126				0.126
8	8.268	52251	2650		0.319				0.319
9	8.895	1167	99	V	0.007				0.007
10	9.512	16198329	1019277	V	98.880				98.880
总计		16381849	1031512		100.000				100.000

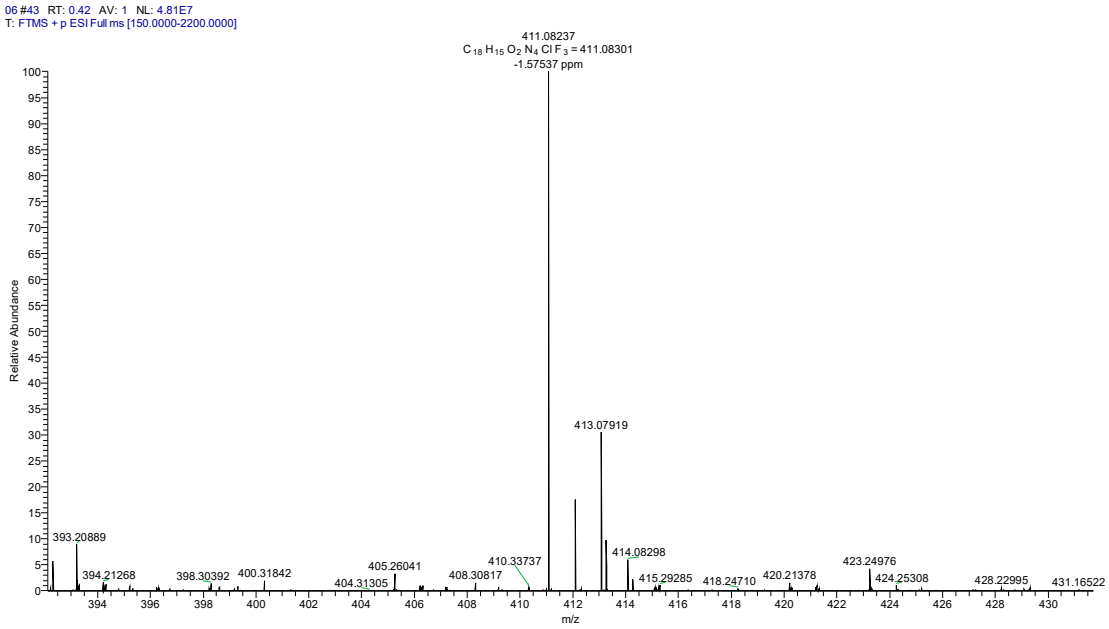
HPLC of compound **F6**

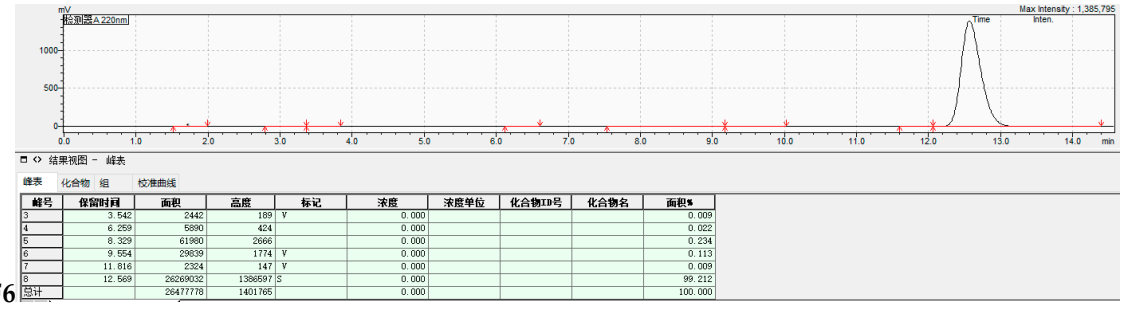


^{1}H NMR of compound **F6**



^{13}C NMR of compound **F6**

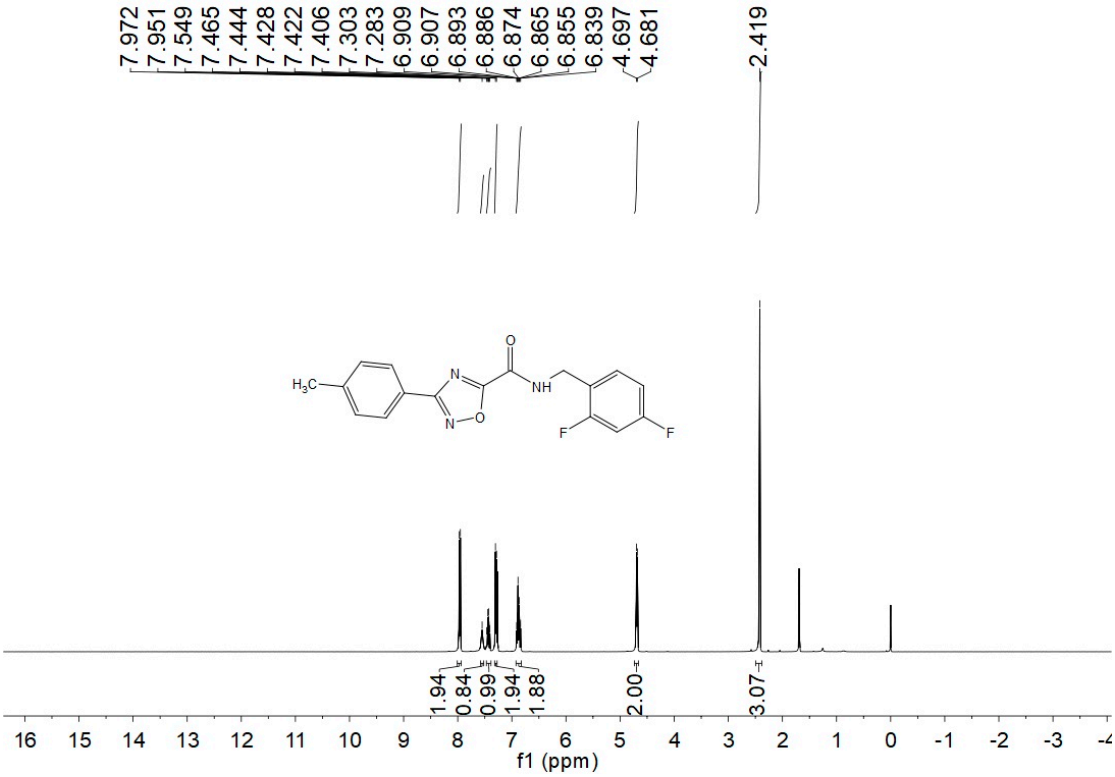




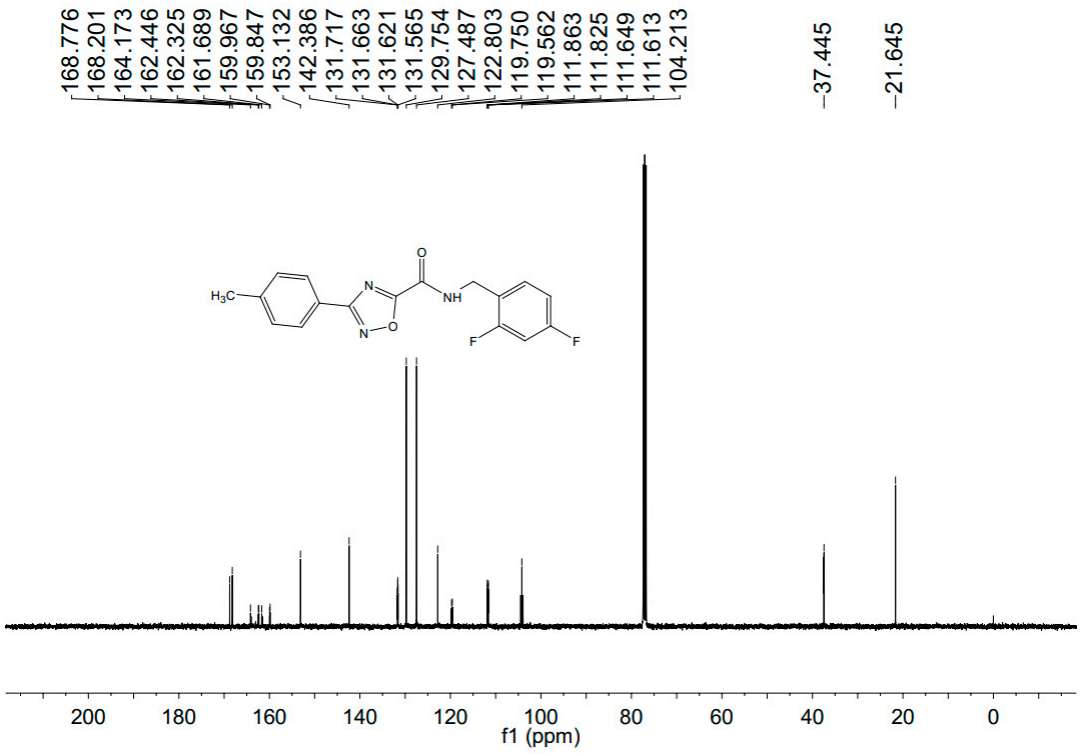
峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
3	3.542	2442	189	V	0.000				0.009
4	6.259	5890	424		0.000				0.022
5	8.329	61980	2666		0.000				0.234
6	9.554	29839	1774	V	0.000				0.113
7	11.816	2324	147	V	0.000				0.009
8	12.569	26269032	1386597	S	0.000				99.212
总计		26477778	1401765		0.000				100.000

HRMS of compound **F6**

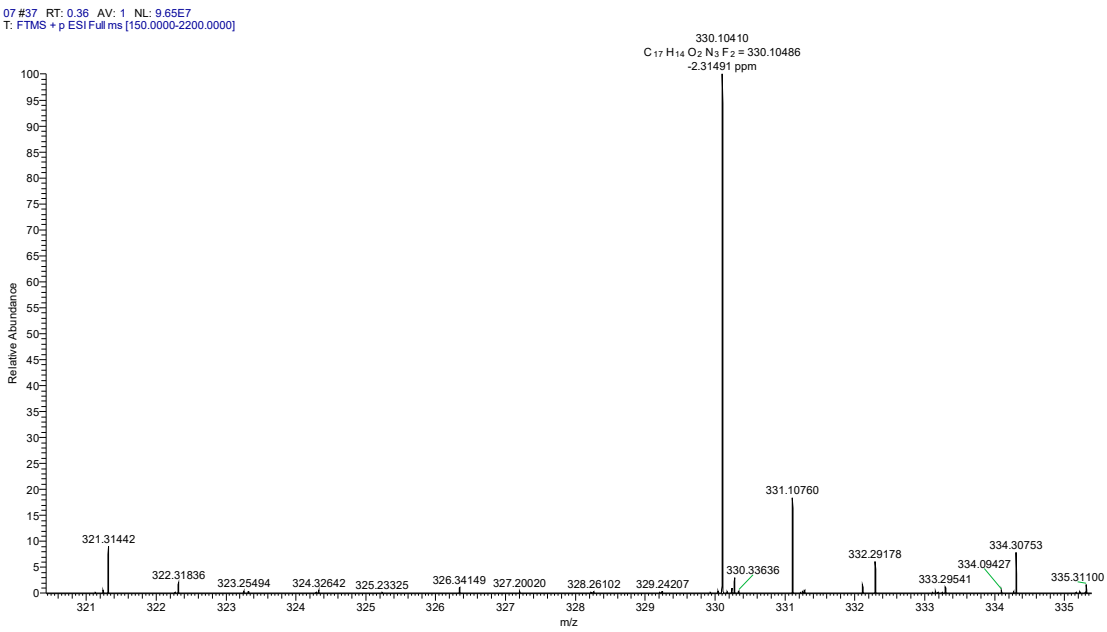
HPLC of compound **F7**



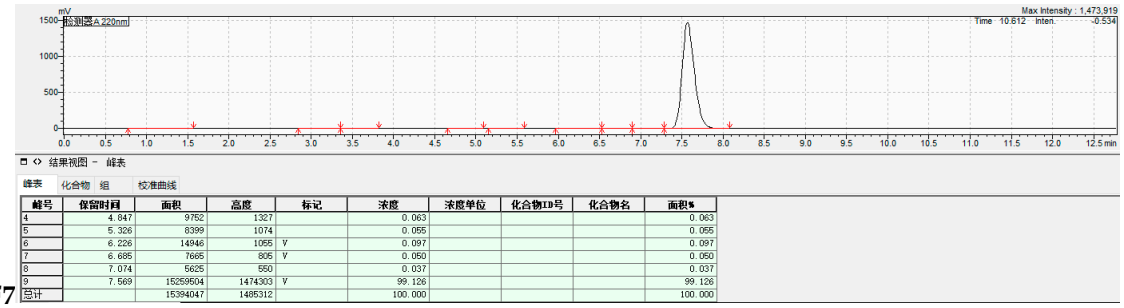
^{1}H NMR of compound **F7**



^{13}C NMR of compound **F7**

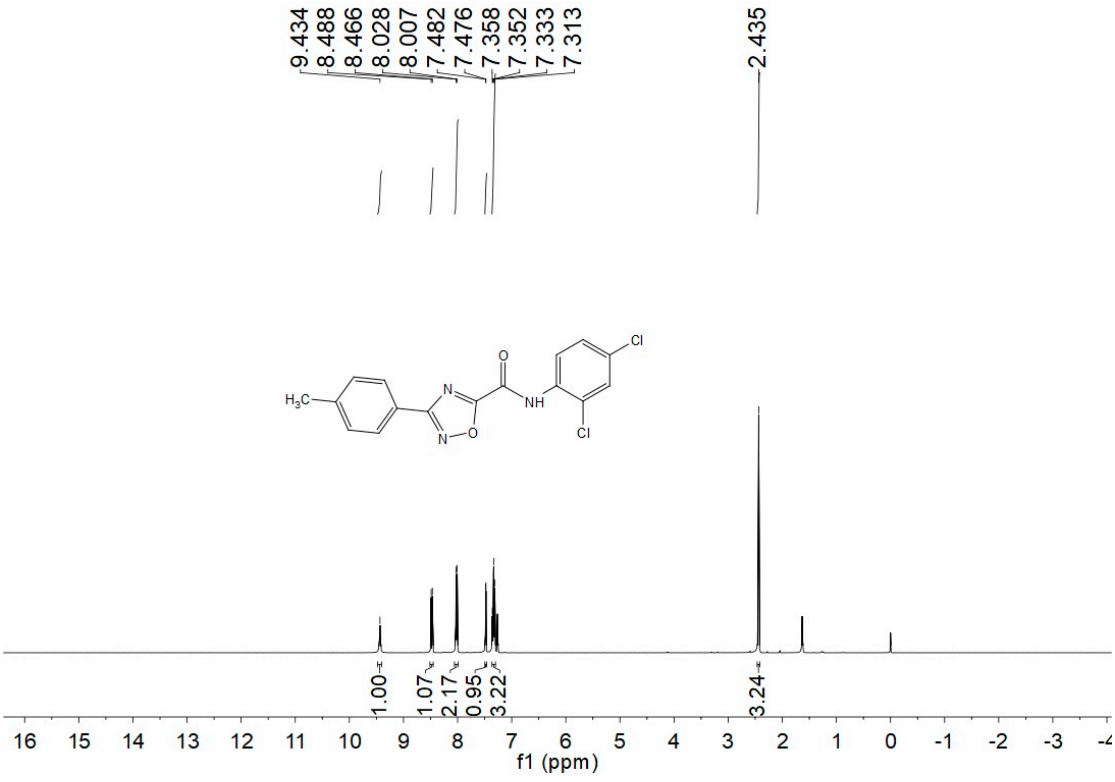


HRMS of compound **F7**

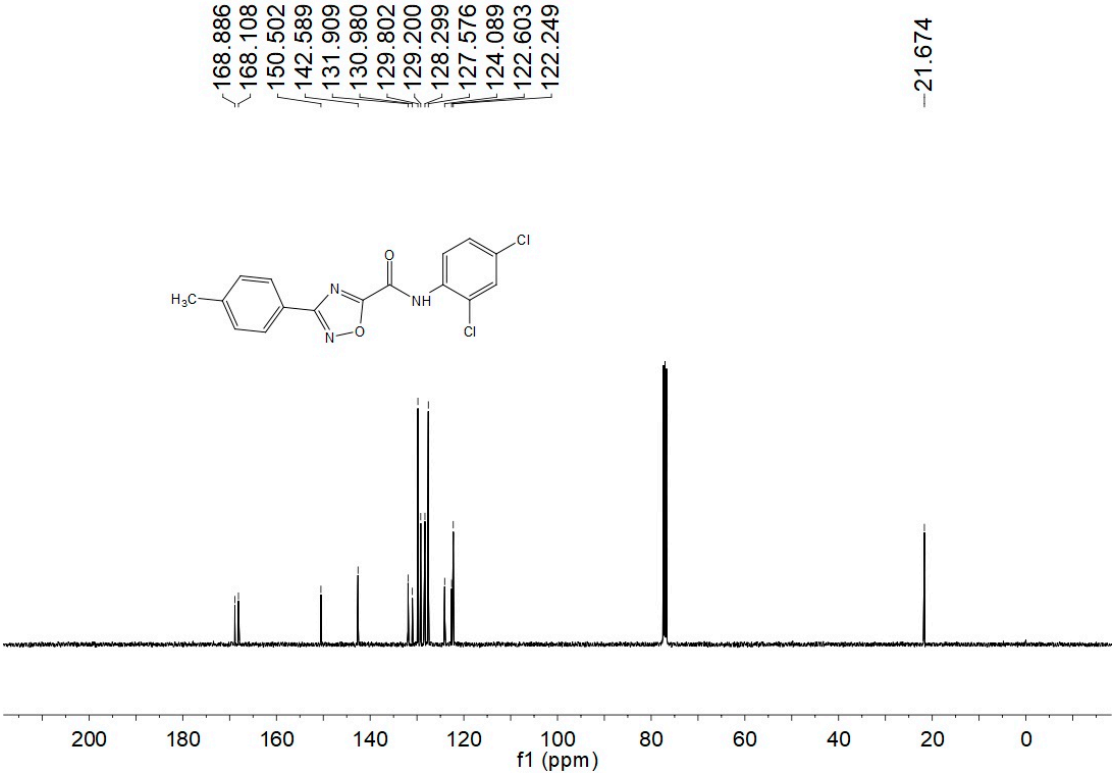


峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
4	4.847	9752	1327		0.063				0.063
5	5.326	8399	1074		0.055				0.055
6	6.226	14946	1055	V	0.097				0.097
7	6.685	7665	805	V	0.050				0.050
8	7.074	5625	550		0.037				0.037
9	7.569	15259504	1474303	V	99.126				99.126
总计		15394047	1486312		100.000				100.000

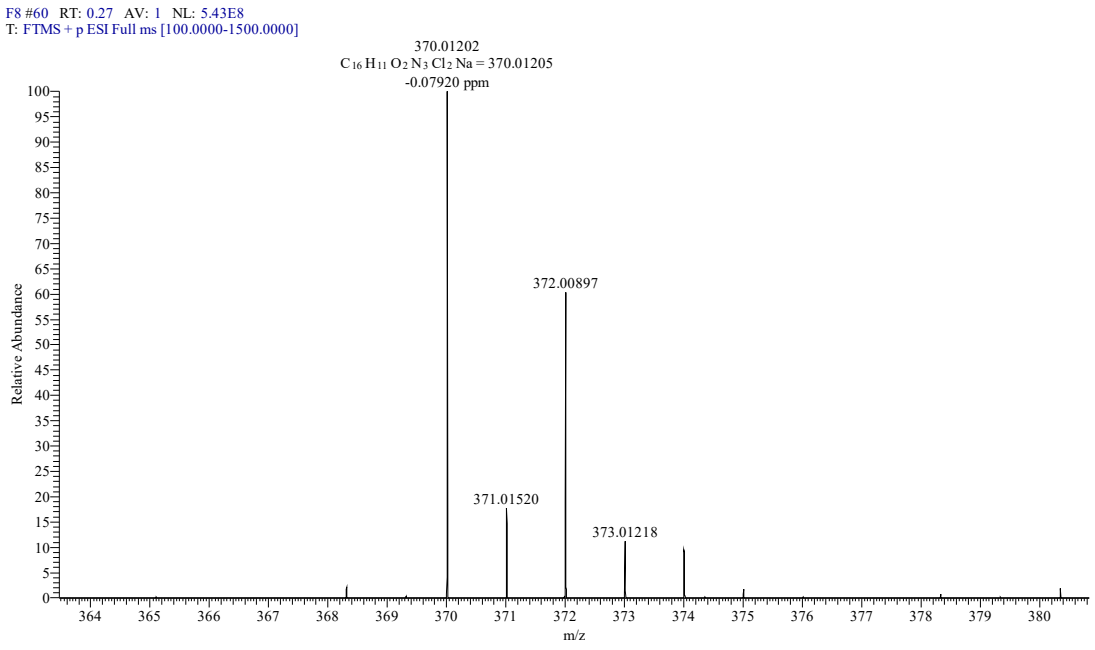
HPLC of compound **F8**



^{1}H NMR of compound **F8**



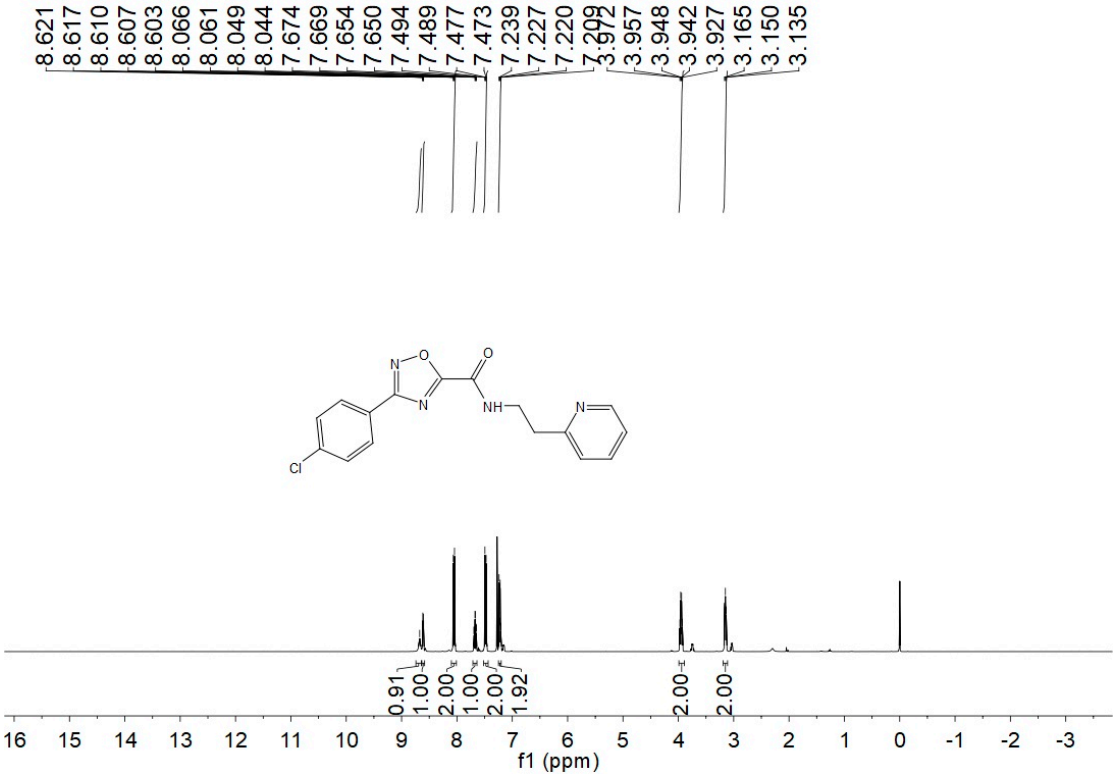
^{13}C NMR of compound **F8**



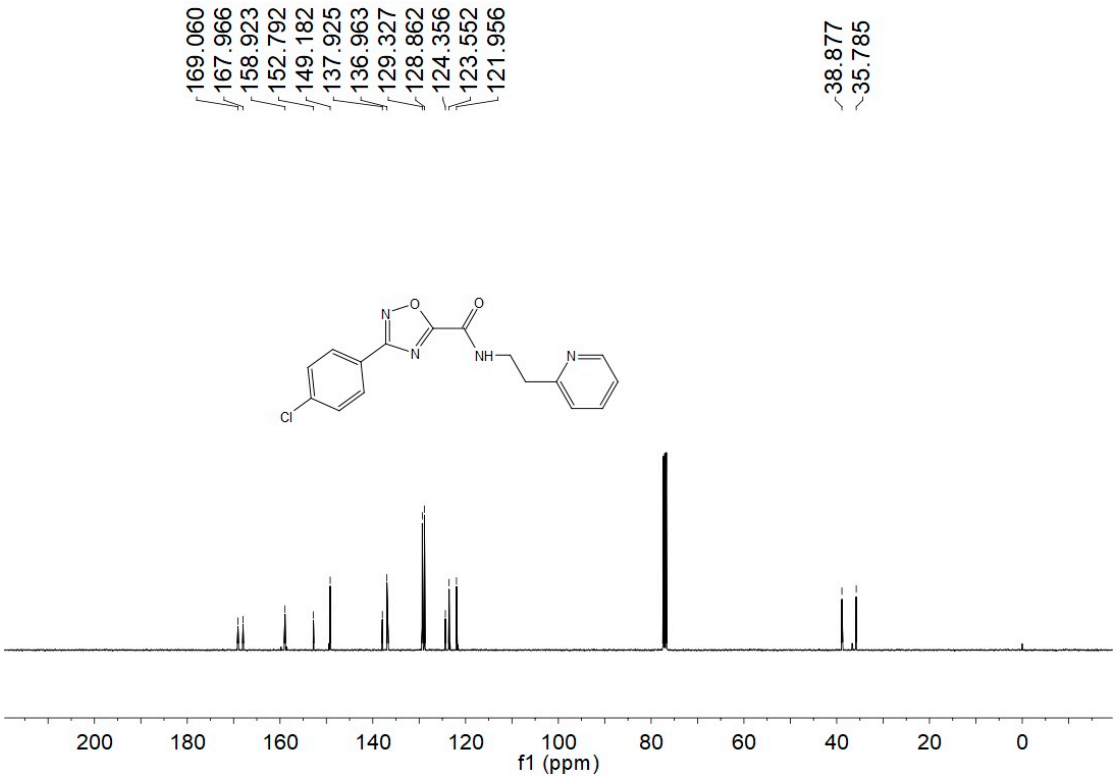
峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
1	3.049	91415	6692		0.627				0.627
2	4.456	39424	3272		0.270				0.270
3	6.233	56772	5731		0.389				0.389
4	8.246	50672	2696		0.348				0.348
5	16.913	14338524	410651		98.365				98.365
总计		14576808	429042		100.000				100.000

HRMS of compound **F8**

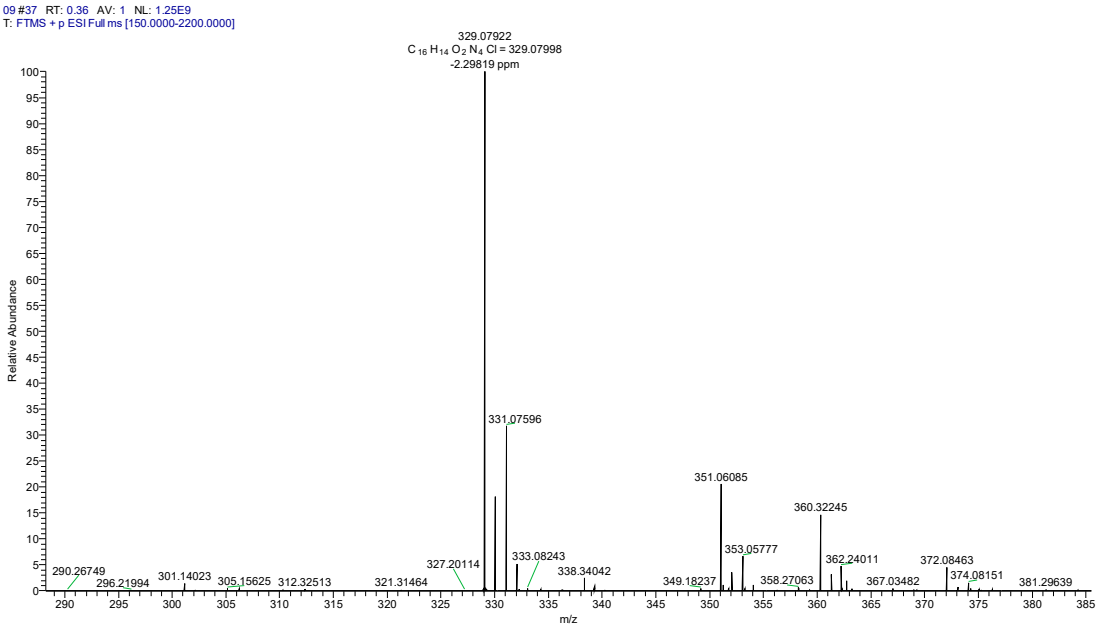
HPLC of compound **F9**



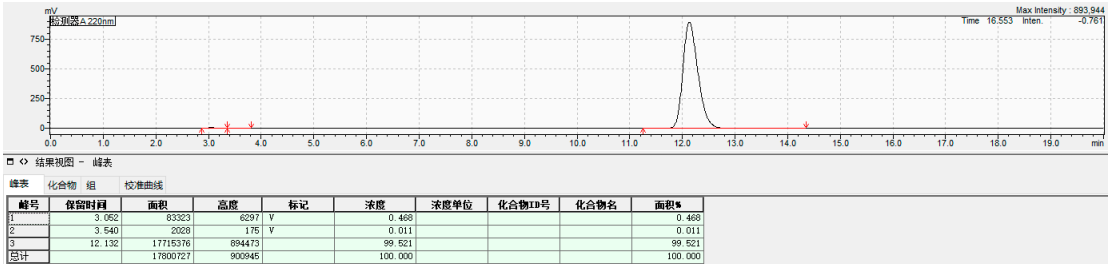
^{1}H NMR of compound **F9**



^{13}C NMR of compound **F9**

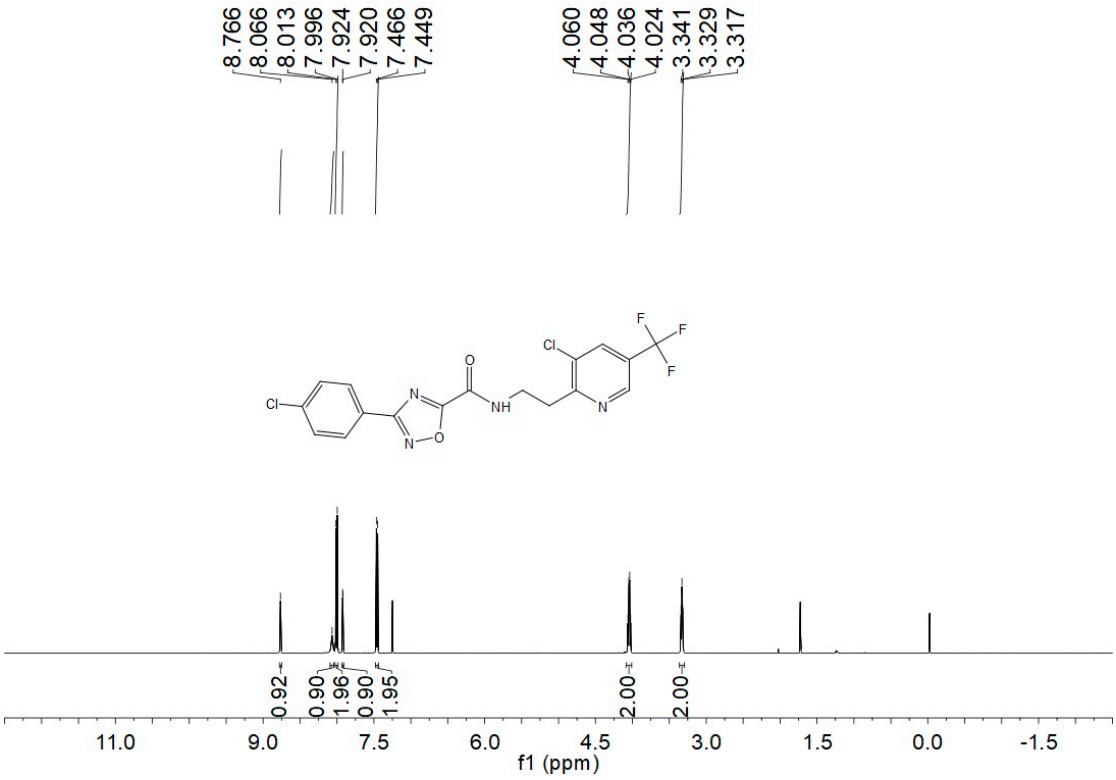


HRMS of compound **F9**

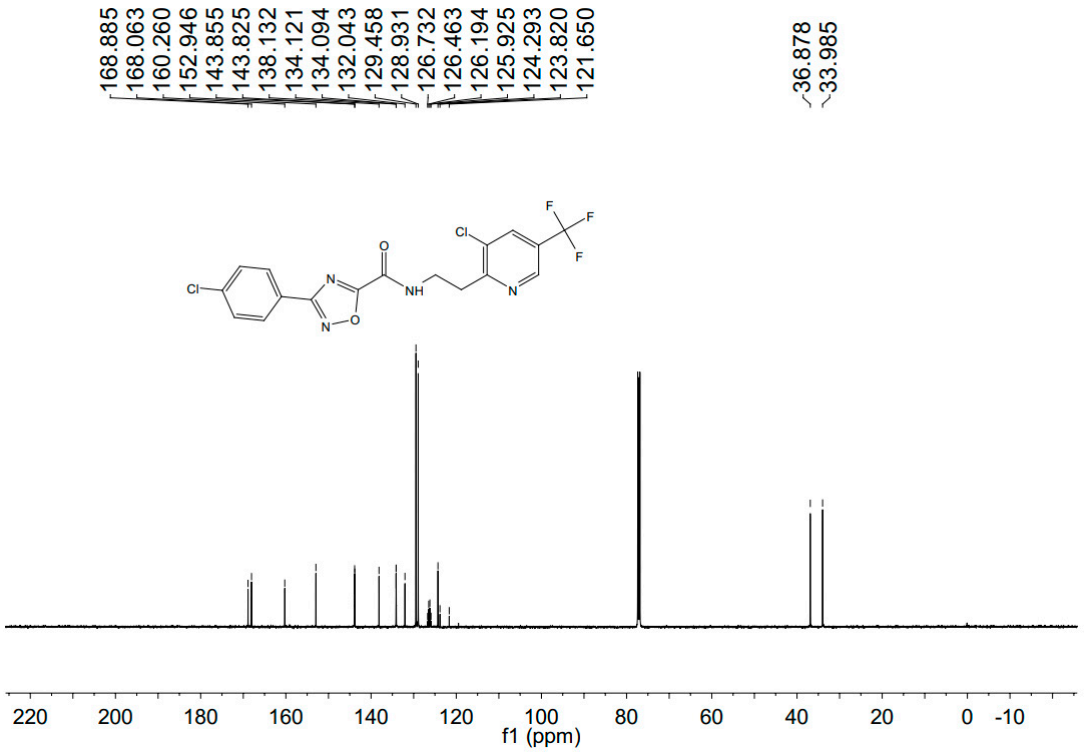


峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
1	3.062	83323	6297	V	0.468				0.468
2	3.540	2028	175	V	0.011				0.011
3	12.132	17715376	894473		99.521				99.521
总计		17800727	900945		100.000				100.000

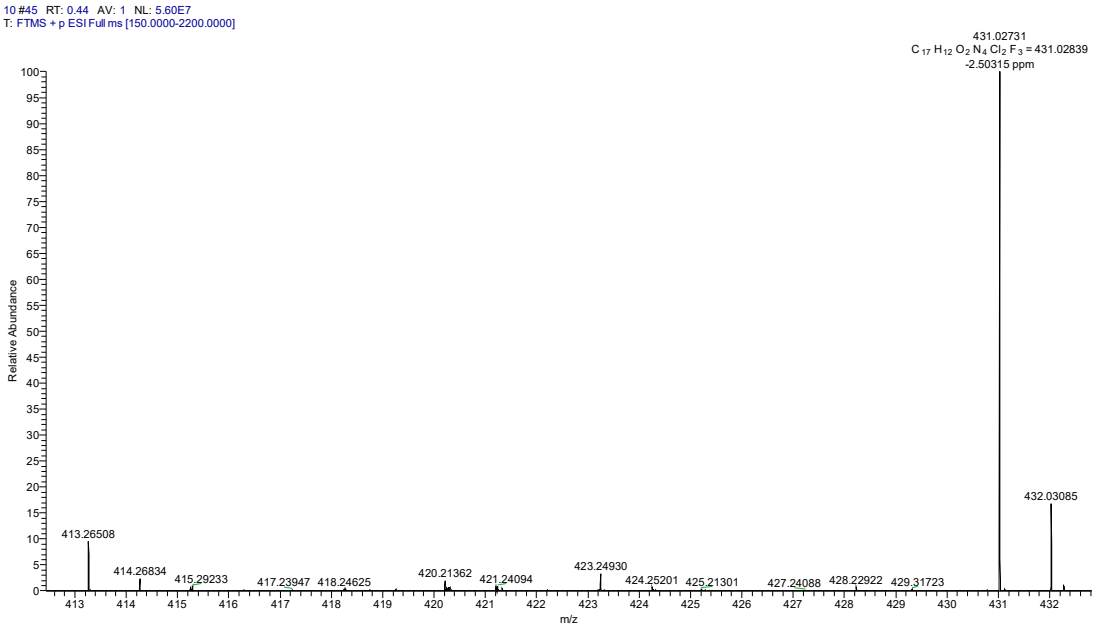
HPLC of compound **F10**



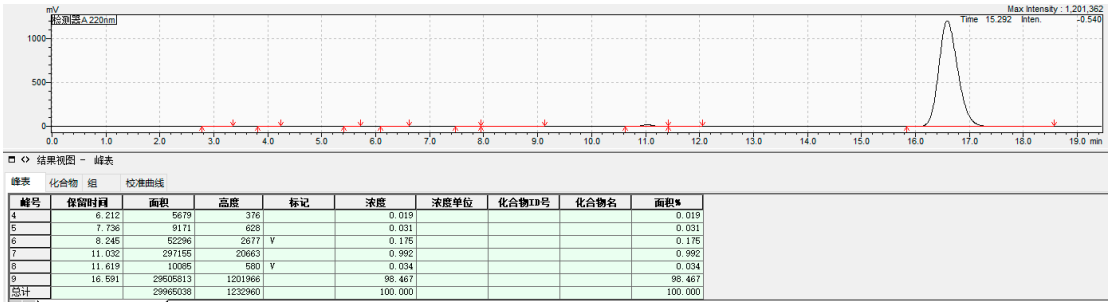
^{1}H NMR of compound **F10**



^{13}C NMR of compound **F10**

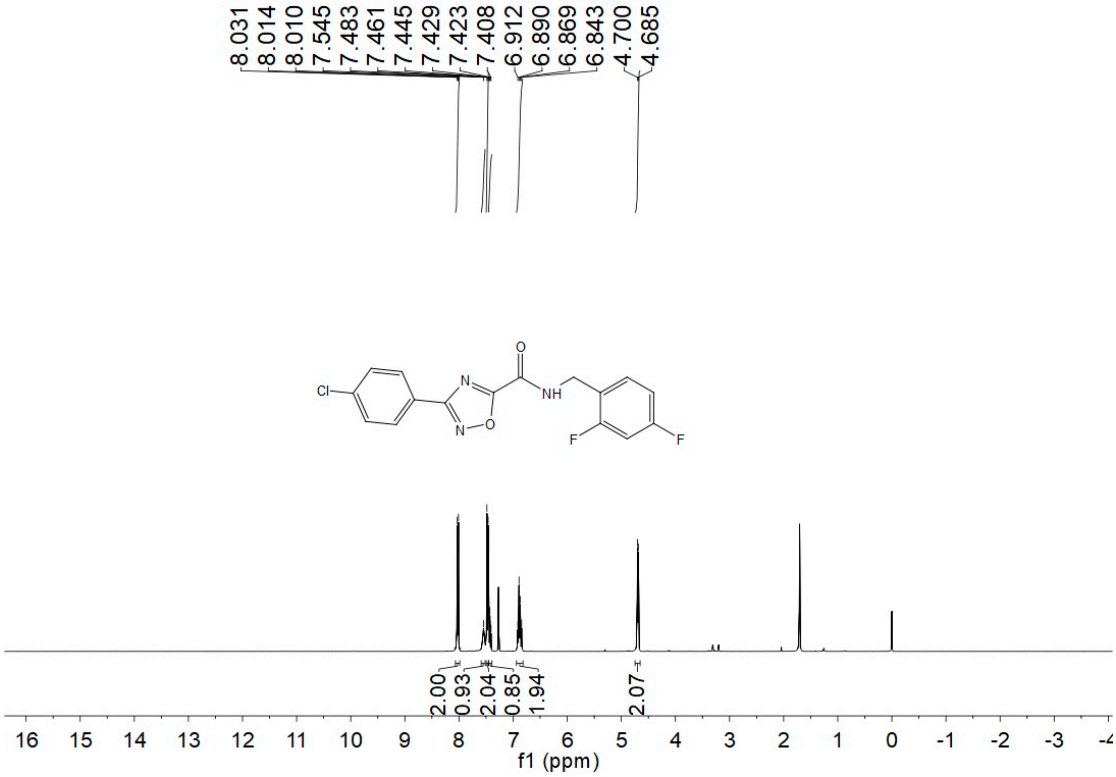


HRMS of compound **F10**

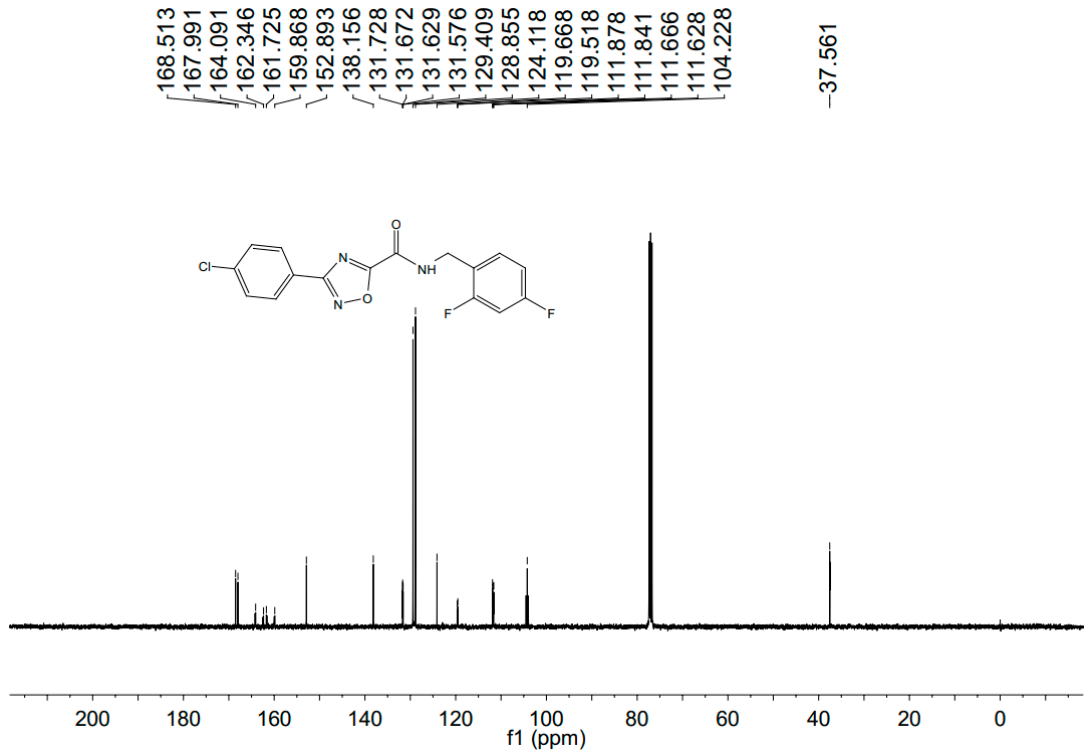


峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
4	6.212	5679	376		0.019				0.019
5	7.736	9171	628		0.031				0.031
6	8.245	52296	2677	V	0.175				0.175
7	11.032	297155	20663		0.992				0.992
8	11.619	10085	580	V	0.034				0.034
9	16.591	29505813	1201966		98.467				98.467
总计		29965038	1232960		100.000				100.000

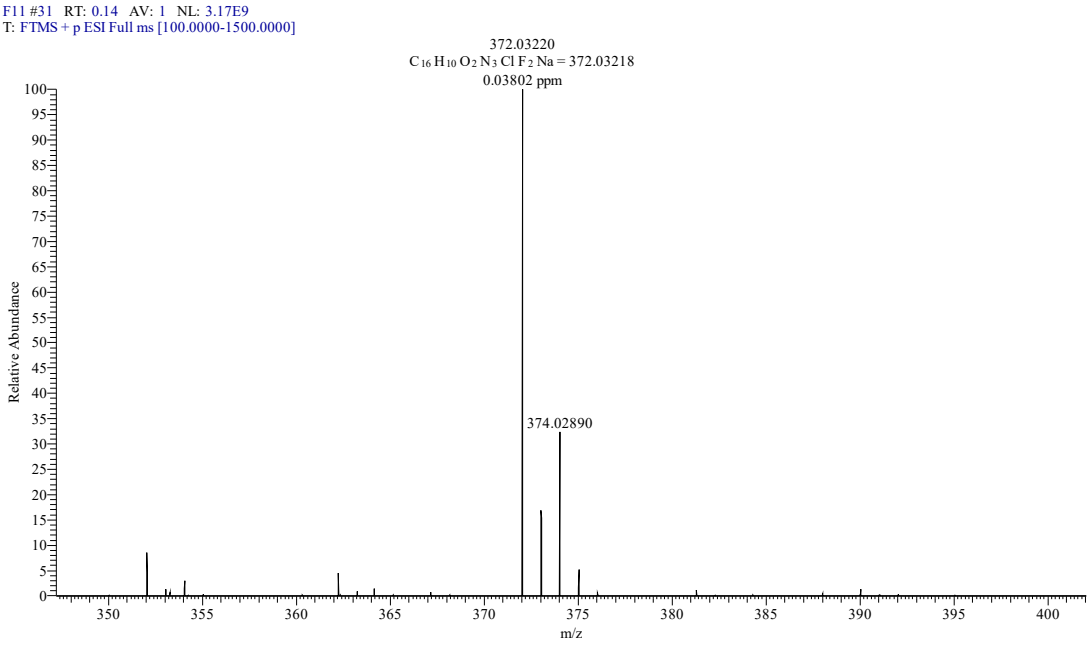
HPLC of compound **F11**



^{1}H NMR of compound **F11**



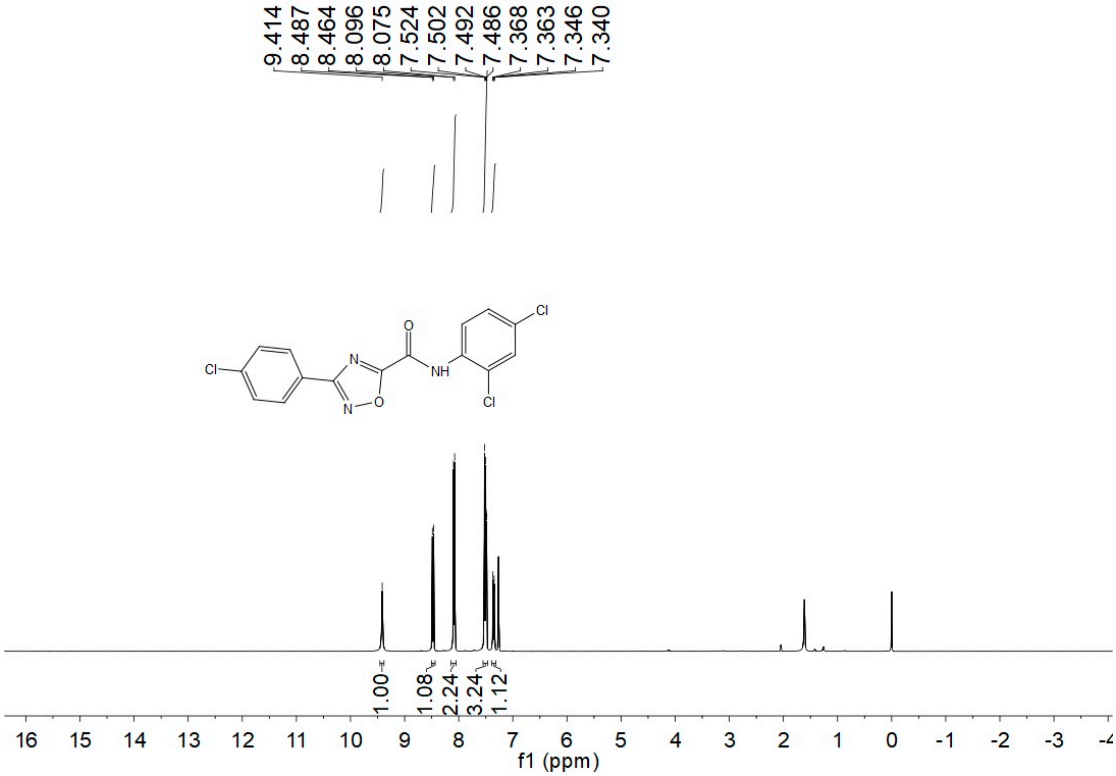
^{13}C NMR of compound **F11**



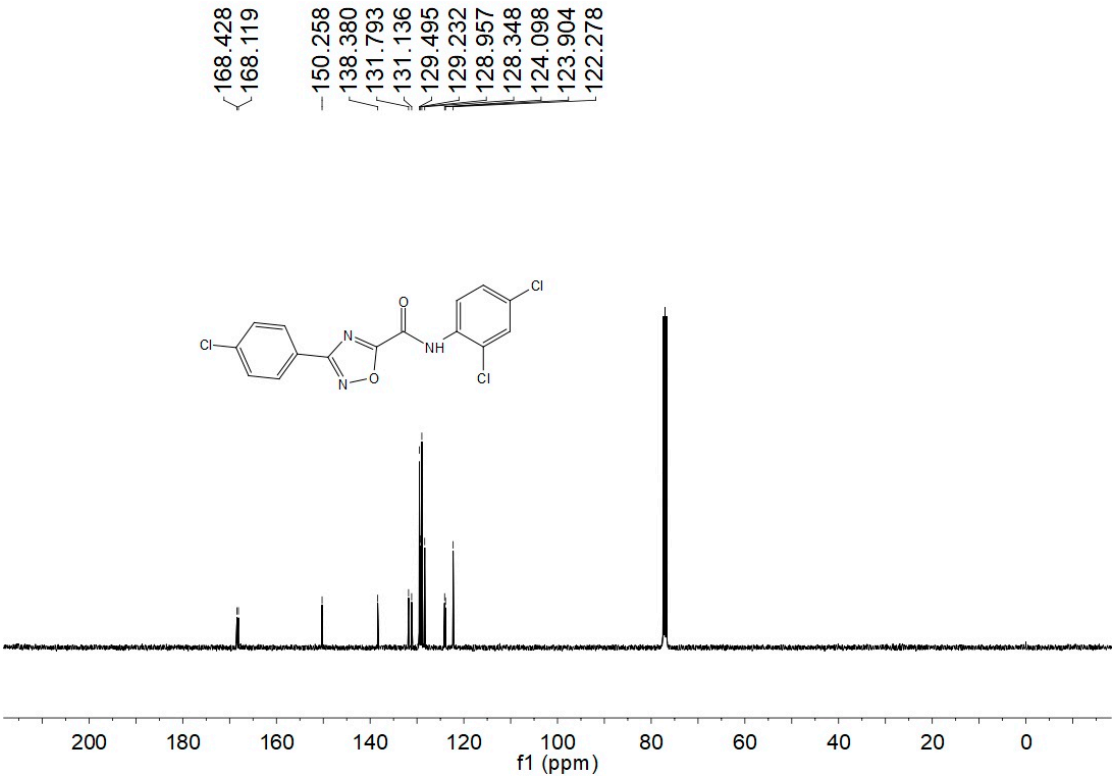
HRMS of compound **F11**

峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
2	5.594	1921	258		0.016				0.016
3	5.794	4398	547	V	0.036				0.036
4	6.040	63228	8004	V	0.517				0.517
5	6.303	38811	3403	V	0.317				0.317
6	9.177	1696	170	V	0.014				0.014
7	9.700	12051844	923246		98.460				98.460
总计		12240386	941152		100.000				100.000

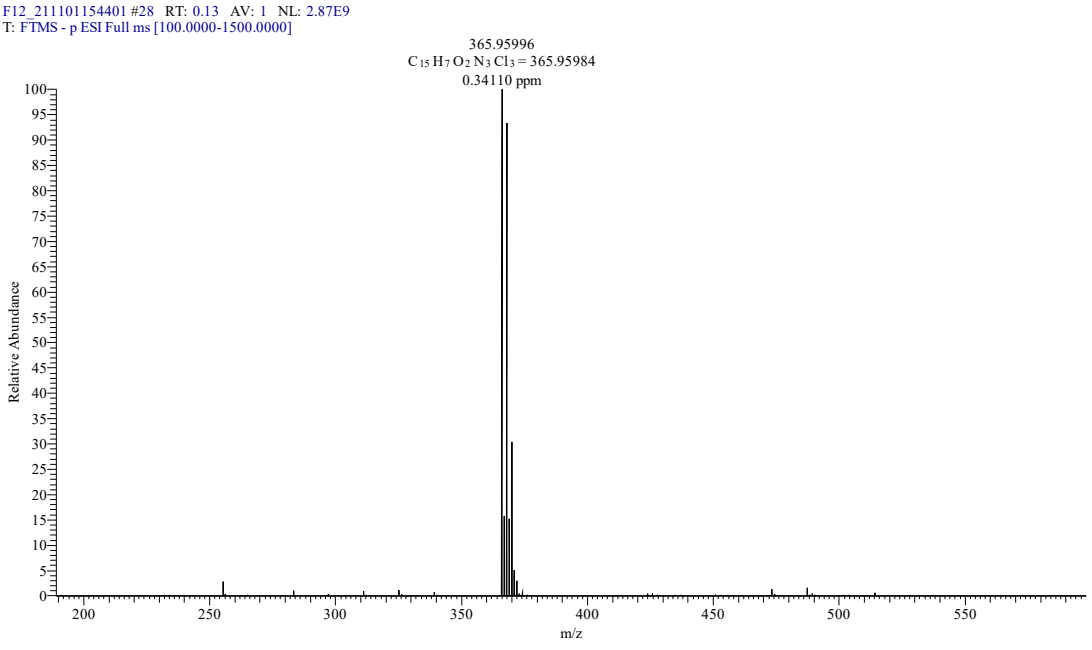
HPLC of compound **F12**



^{1}H NMR of compound **F12**



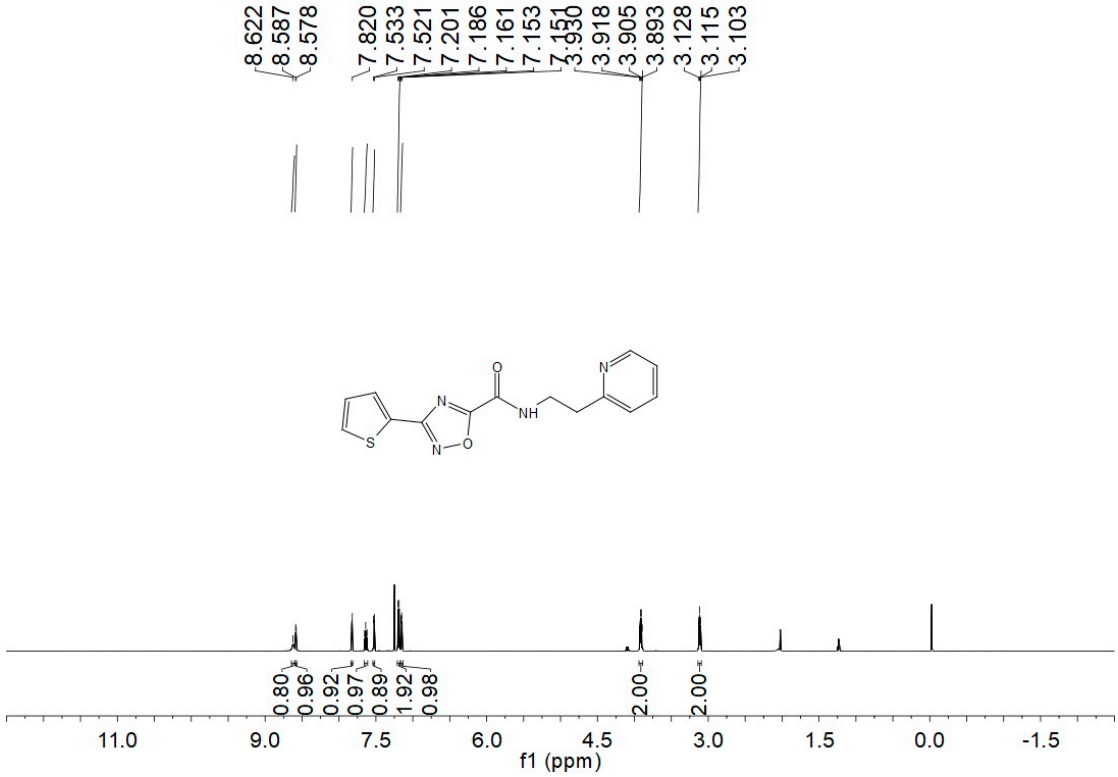
^{13}C NMR of compound **F12**



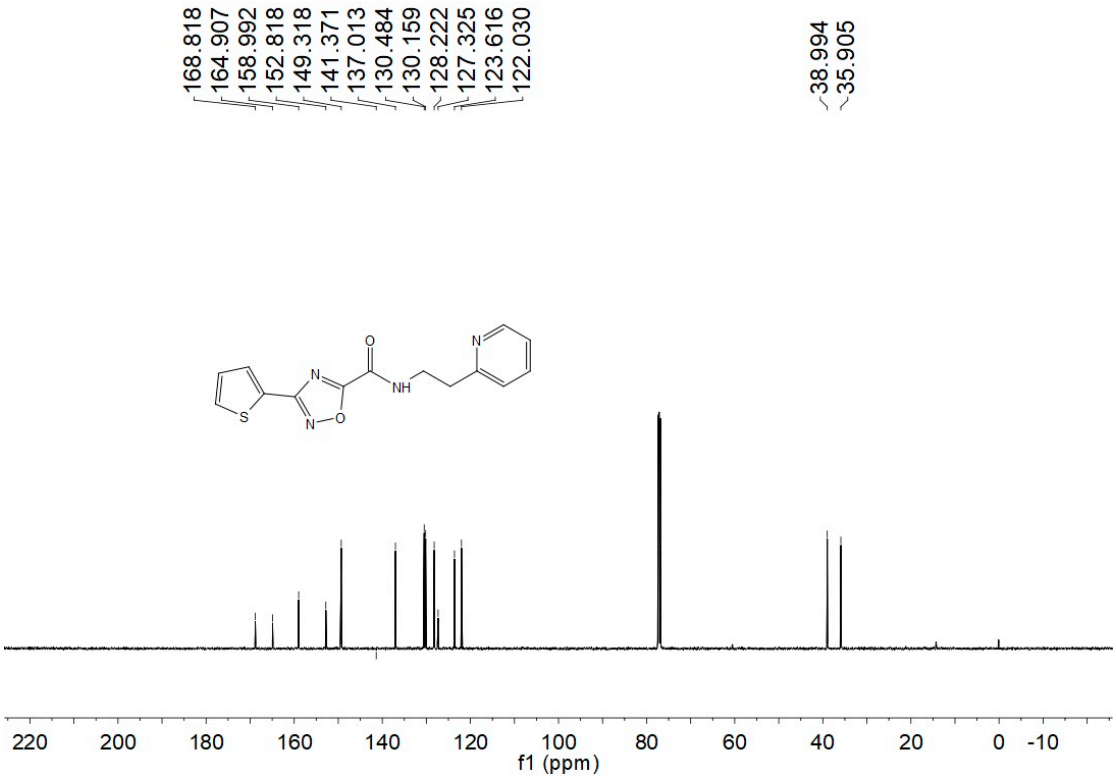
HRMS of compound **F12**

峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
5	8.259	67028	2714		0.287				0.287
6	9.261	5487	306	V	0.024				0.024
7	10.440	84672	5148		0.363				0.363
8	13.182	14790	769		0.063				0.063
9	13.594	17515	798	V	0.075				0.075
10	14.790	23036245	756552		98.748				98.748
总计		23328412	773986		100.000				100.000

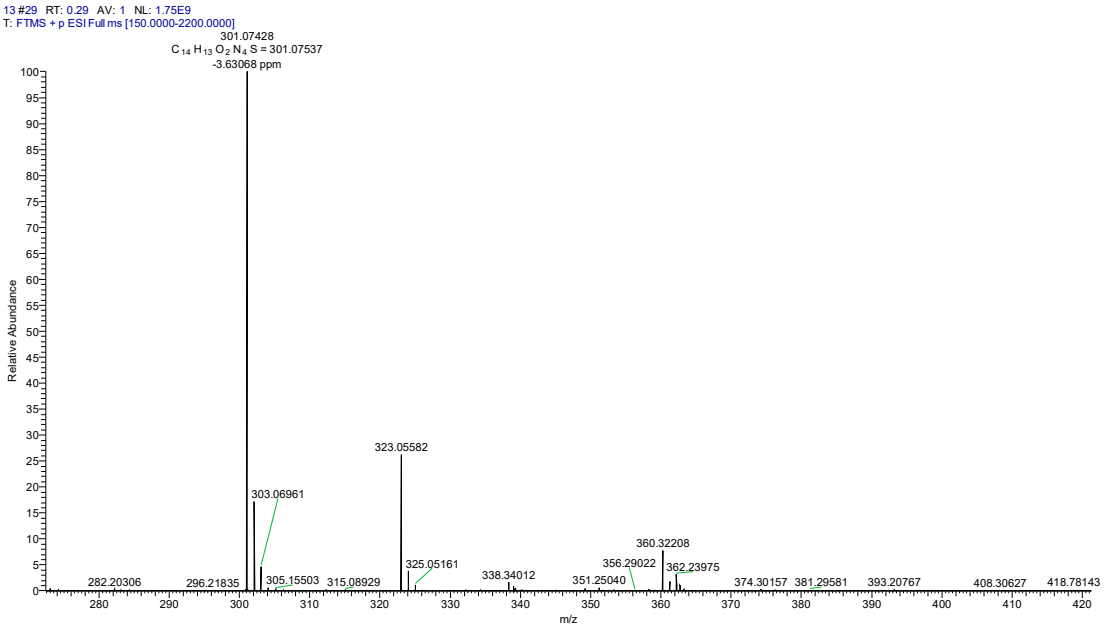
HPLC of compound **F13**



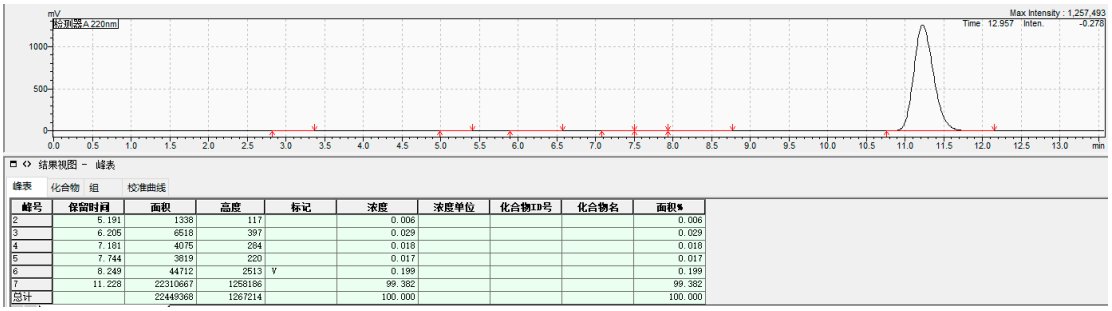
^{1}H NMR of compound **F13**



^{13}C NMR of compound **F13**

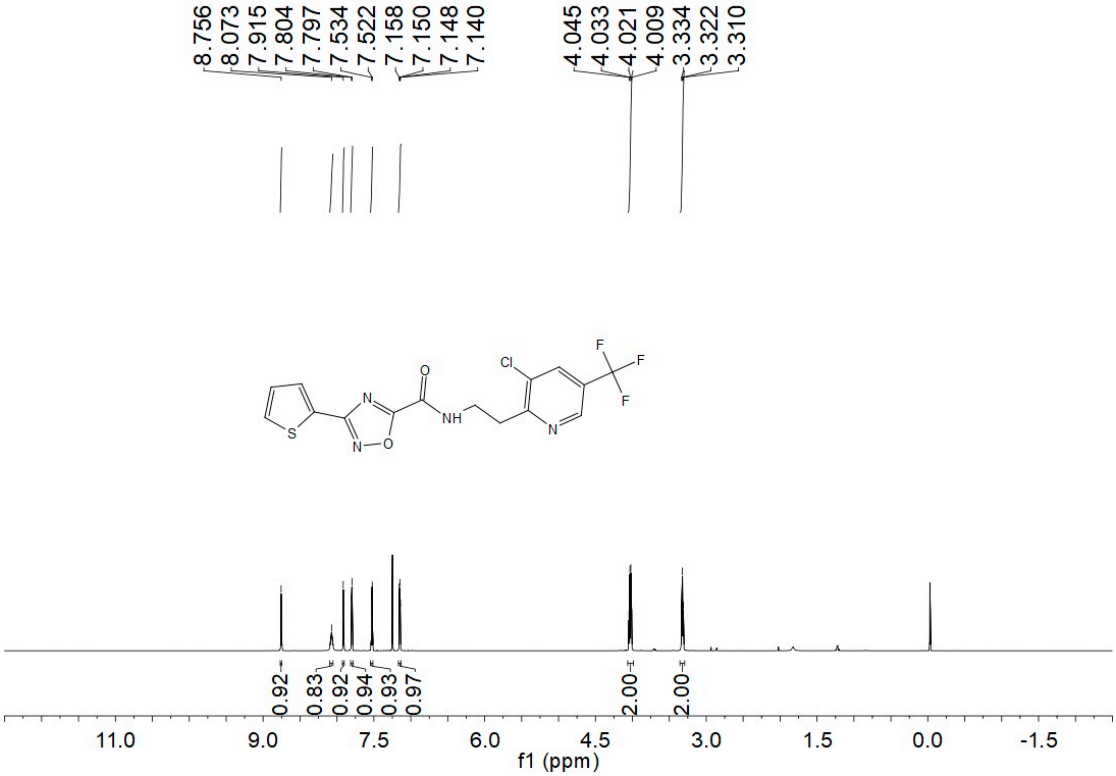


HRMS of compound **F13**

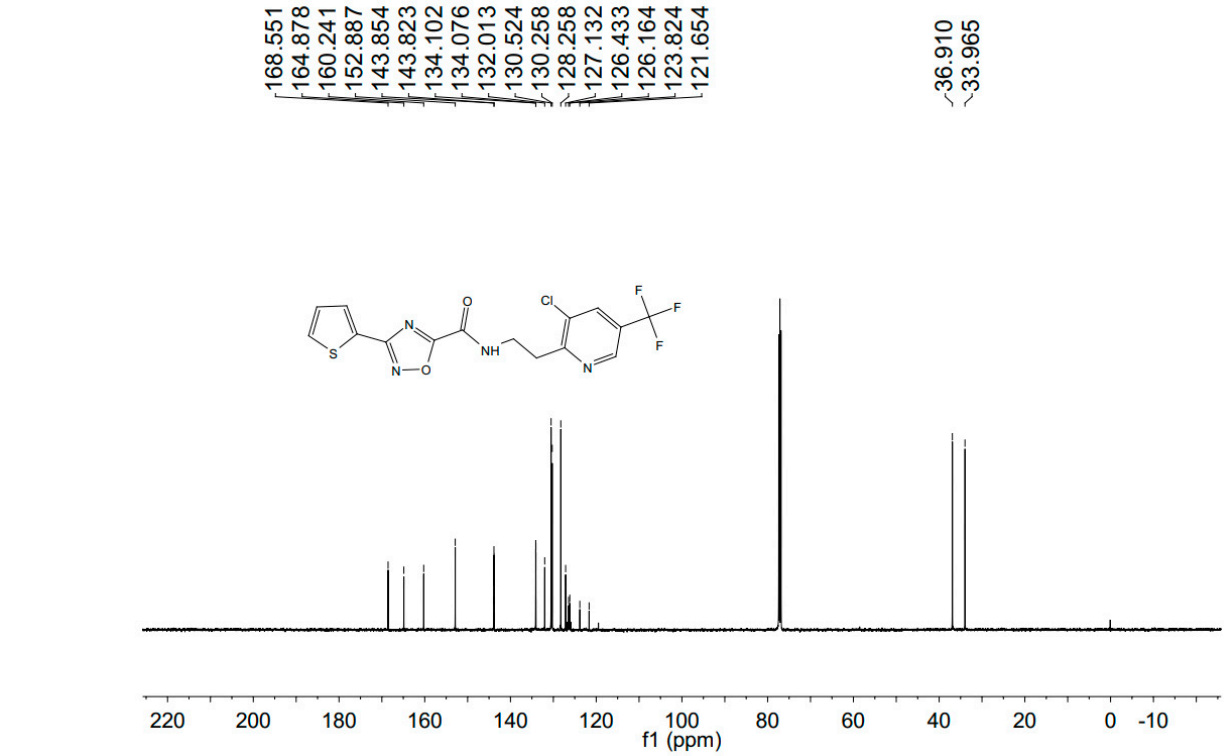


峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
2	5.191	1338	117		0.006				0.006
3	6.206	6518	397		0.029				0.029
4	7.181	4075	284		0.018				0.018
5	7.744	3819	220		0.017				0.017
6	8.249	44712	2513	V	0.199				0.199
7	11.228	22310667	1258186		99.382				99.382
总计		22449368	1267214		100.000				100.000

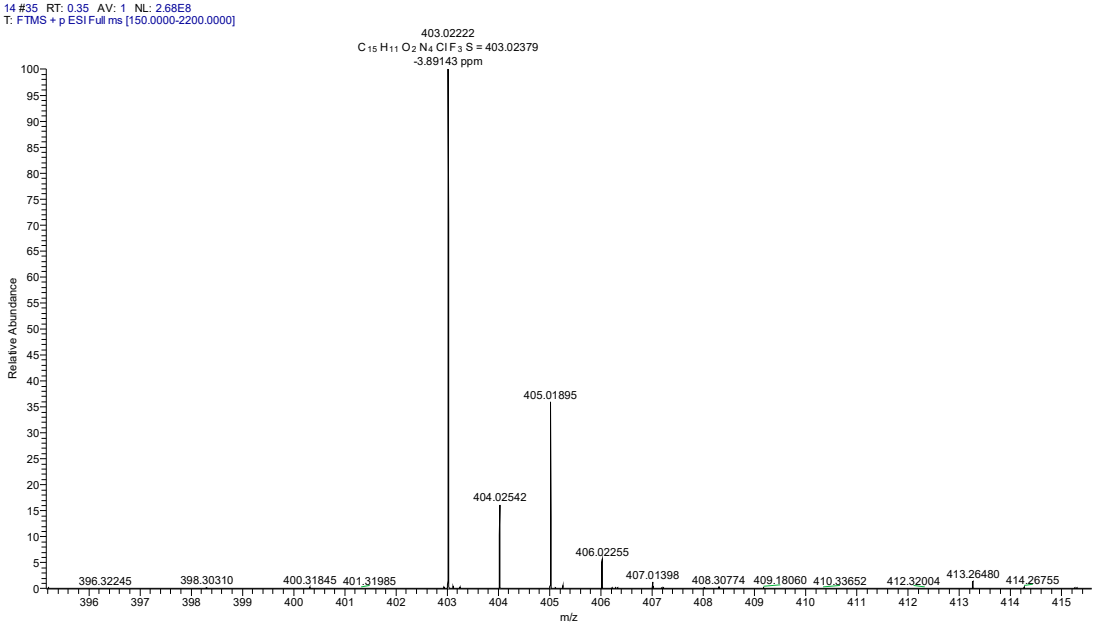
HPLC of compound **F14**



^{1}H NMR of compound **F14**



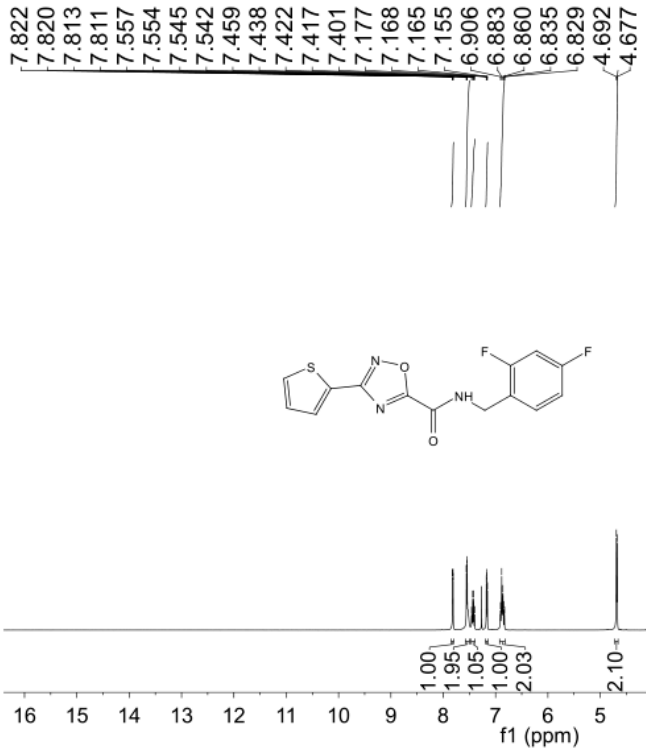
^{13}C NMR of compound **F14**



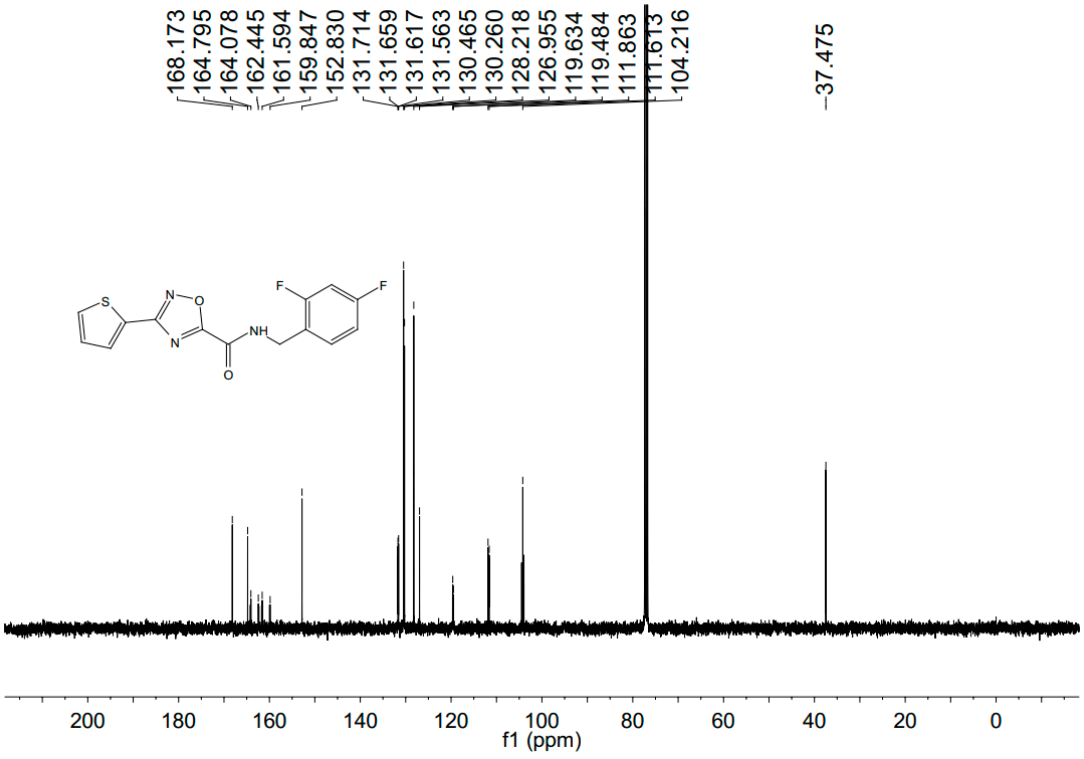
HRMS of compound **F14**

峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
2	3.754	4689	580		0.029				0.029
3	5.514	14651	1646		0.091				0.091
4	9.189	2580	180		0.016				0.016
5	9.685	43406	2074	V	0.270				0.270
6	11.828	13313	626		0.083				0.083
7	15.199	15915322	722723		98.832				98.832
总计		16103409	736366		100.000				100.000

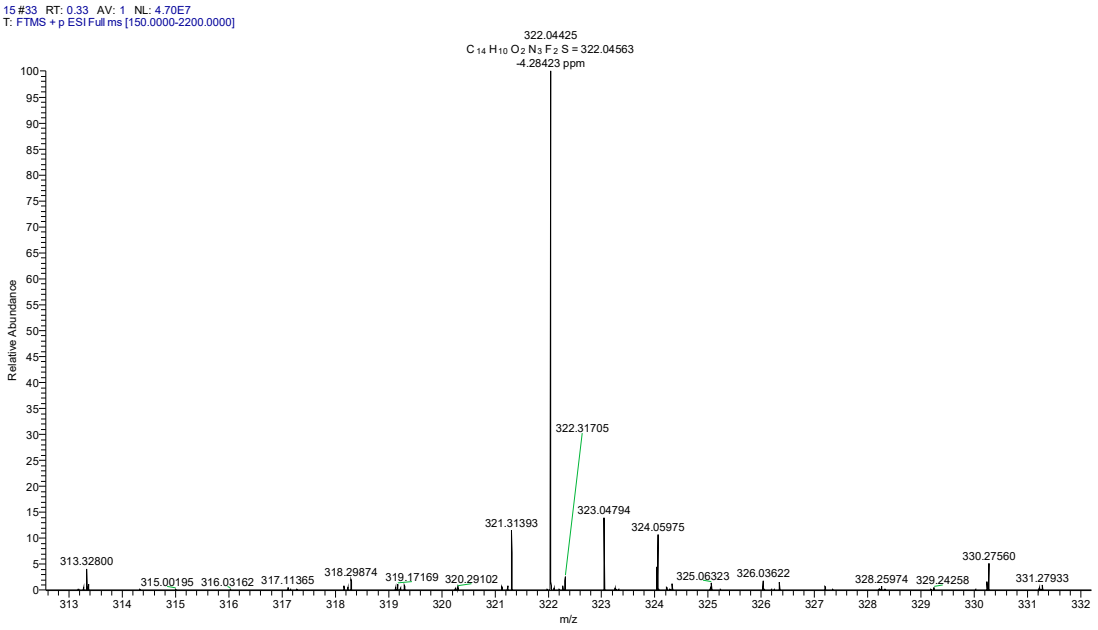
HPLC of compound **F15**



^{1}H NMR of compound **F15**



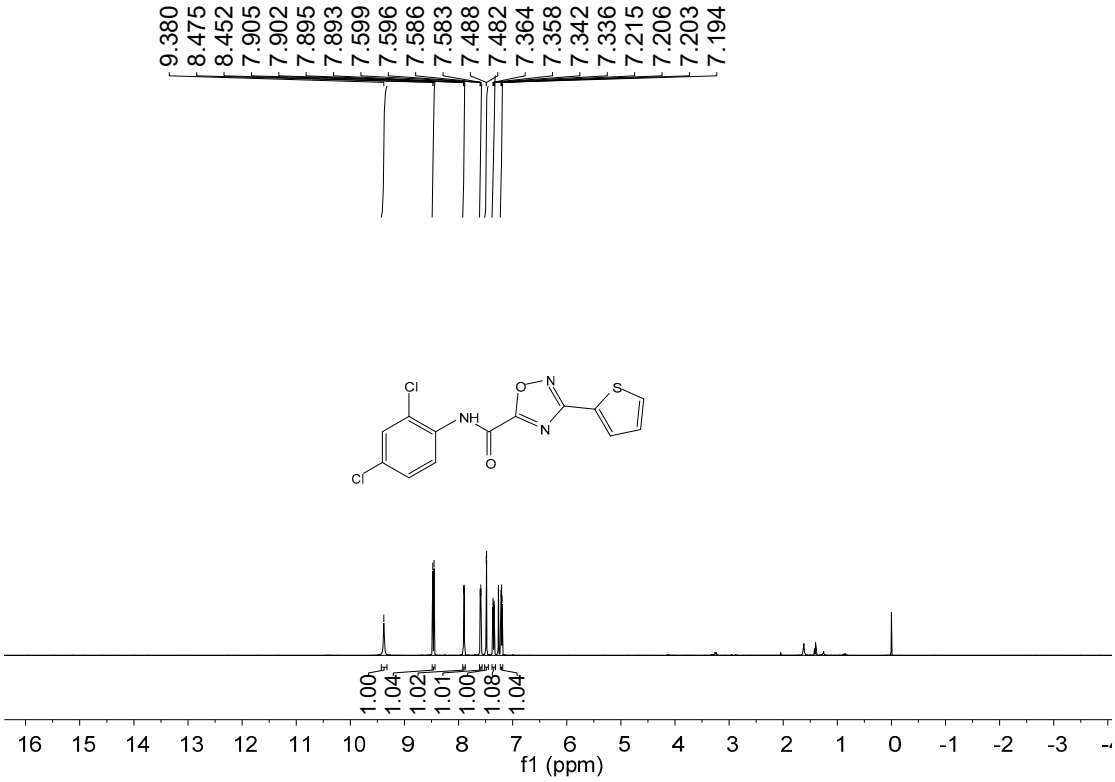
^{13}C NMR of compound **F15**



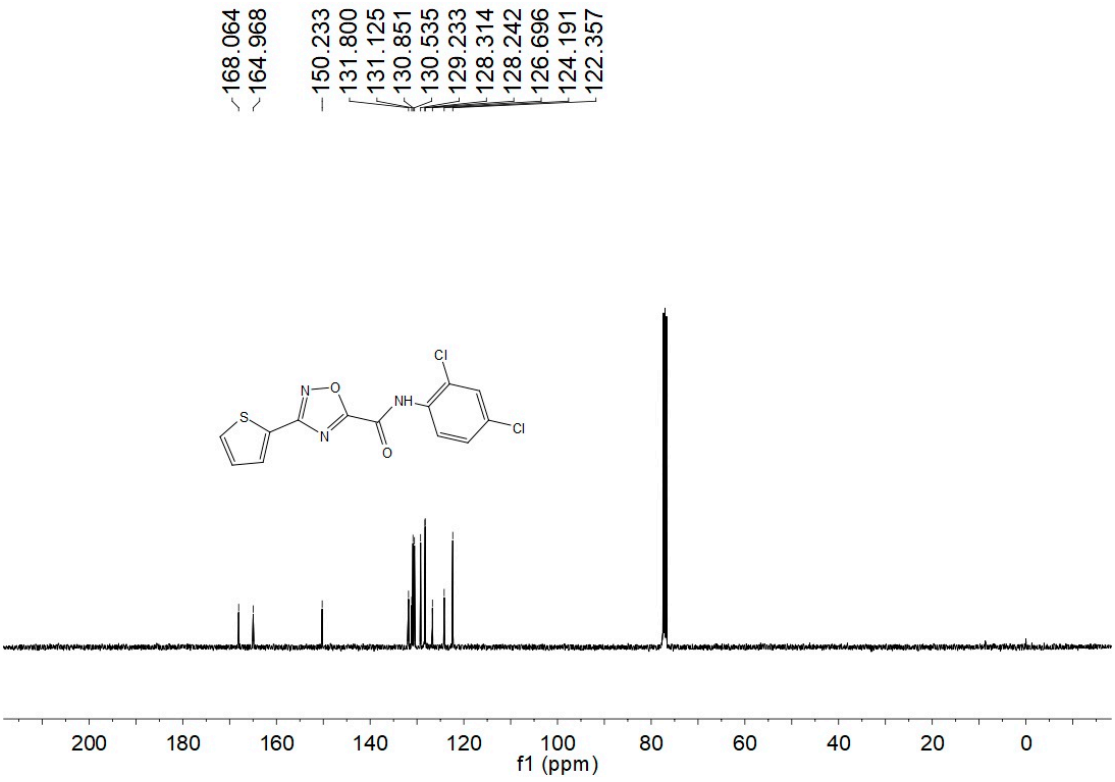
HRMS of compound **F15**

峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
1	2.485	2416	100		0.010				0.010
2	3.055	84899	5944	S	0.350				0.350
3	6.722	13524	840		0.056				0.056
4	9.222	72732	2506		0.300				0.300
5	10.369	24063001	1765350	V	99.284				99.284
总计		24256572	1774739		100.000				100.000

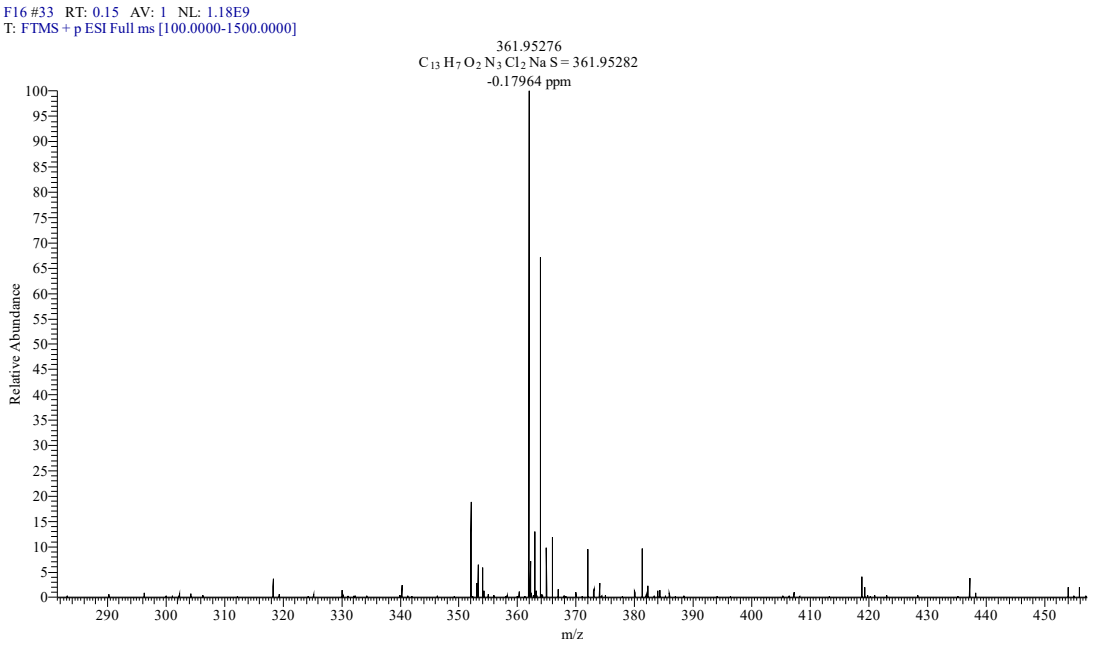
HPLC of compound **F16**



^{1}H NMR of compound **F16**



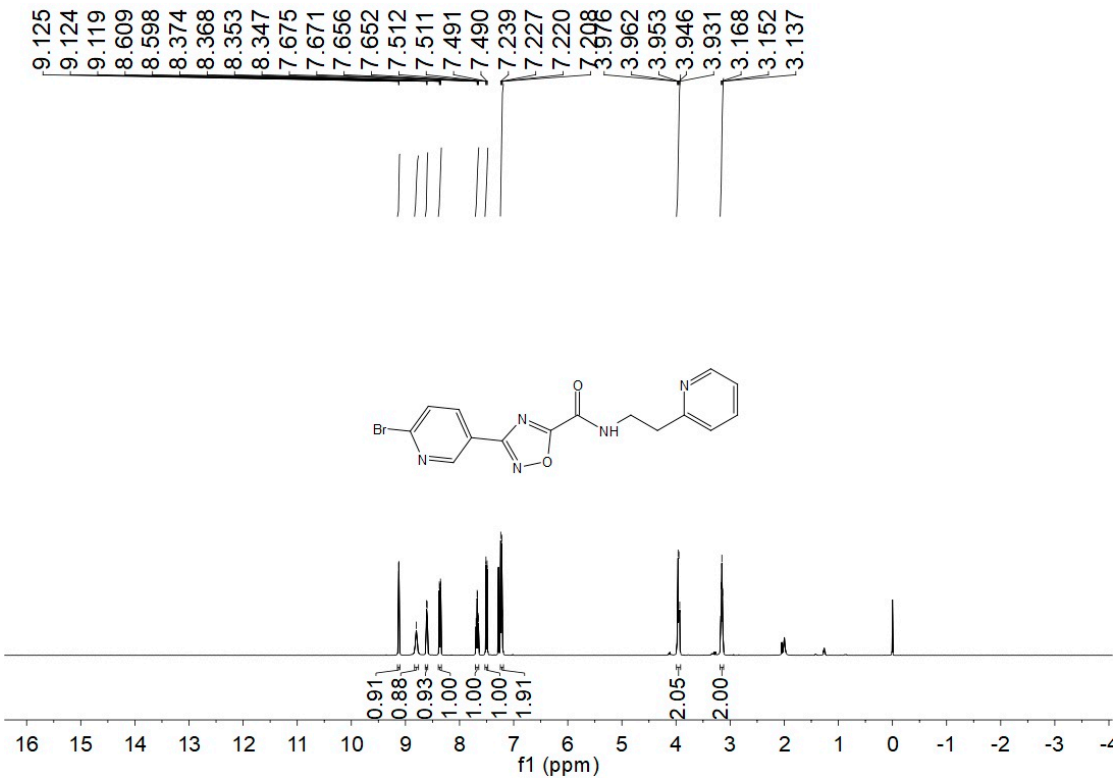
^{13}C NMR of compound **F16**



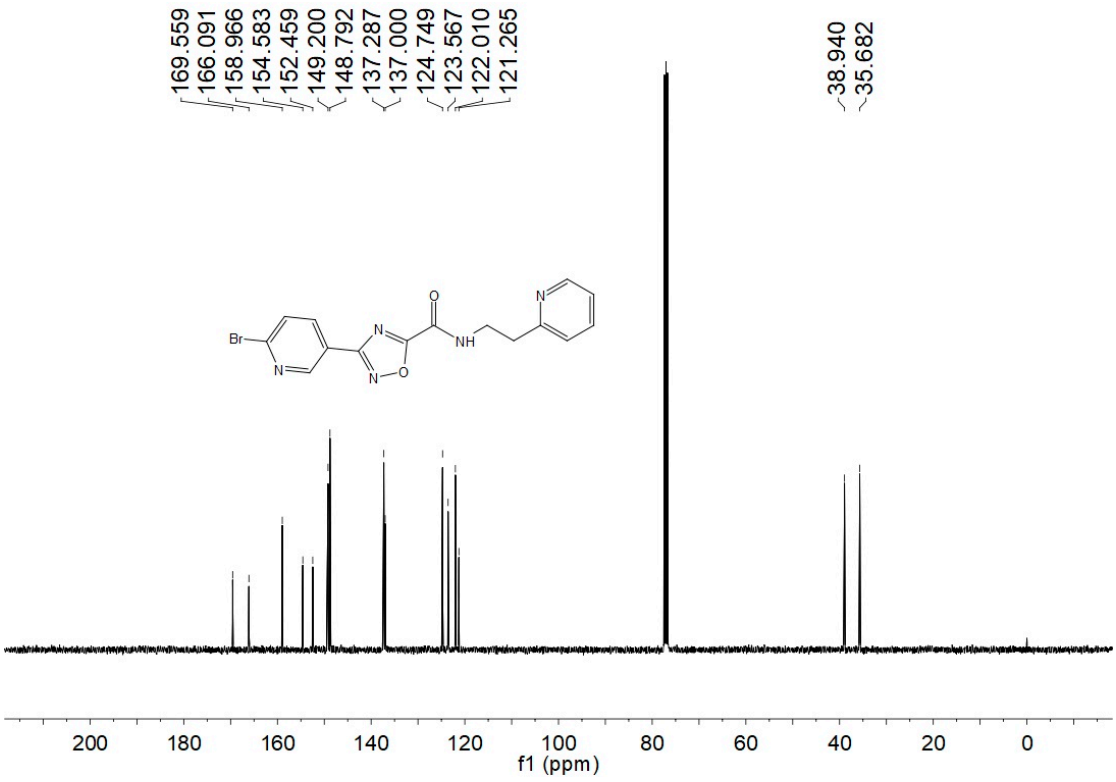
HRMS of compound **F16**

峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
1	1.458	12346	682		0.476				0.476
2	3.052	90749	6370		3.498				3.498
3	7.767	3232	194		0.125				0.125
4	8.251	53659	2709	V	2.065				2.065
5	21.059	2434144	48080		93.836				93.836
总计		2594031	58035		100.000				100.000

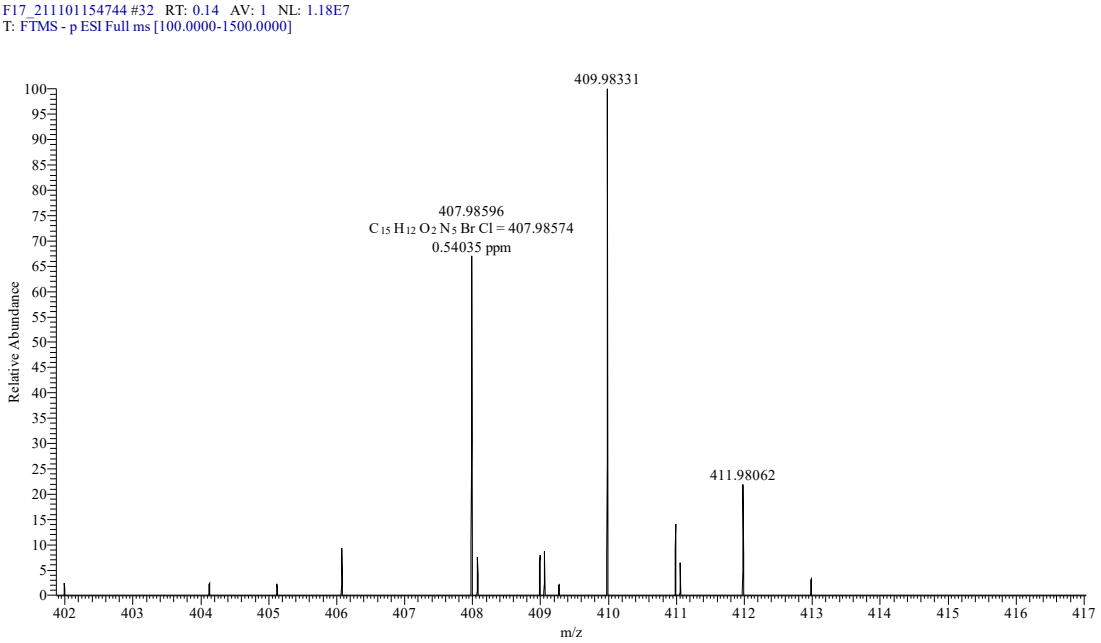
HPLC of compound **F17**



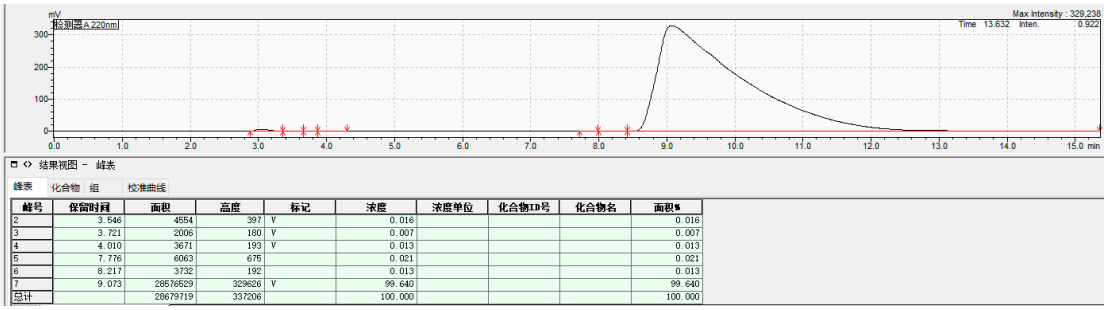
^{1}H NMR of compound **F17**



^{13}C NMR of compound **F17**

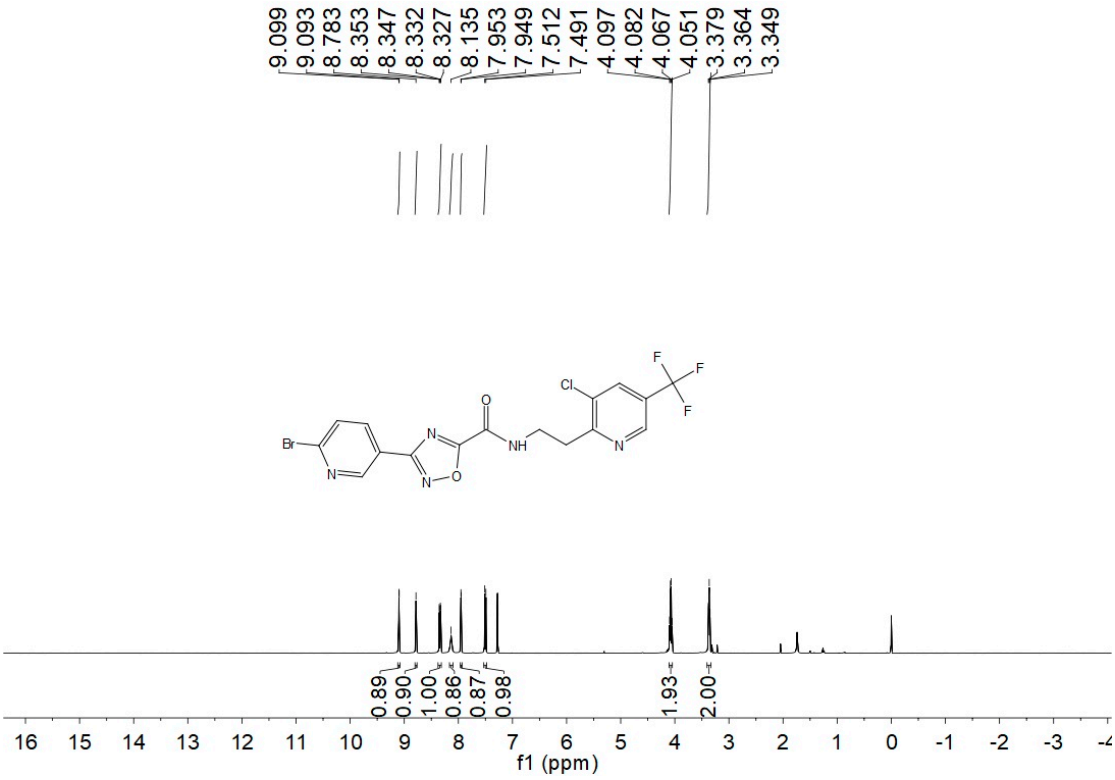


HRMS of compound **F17**

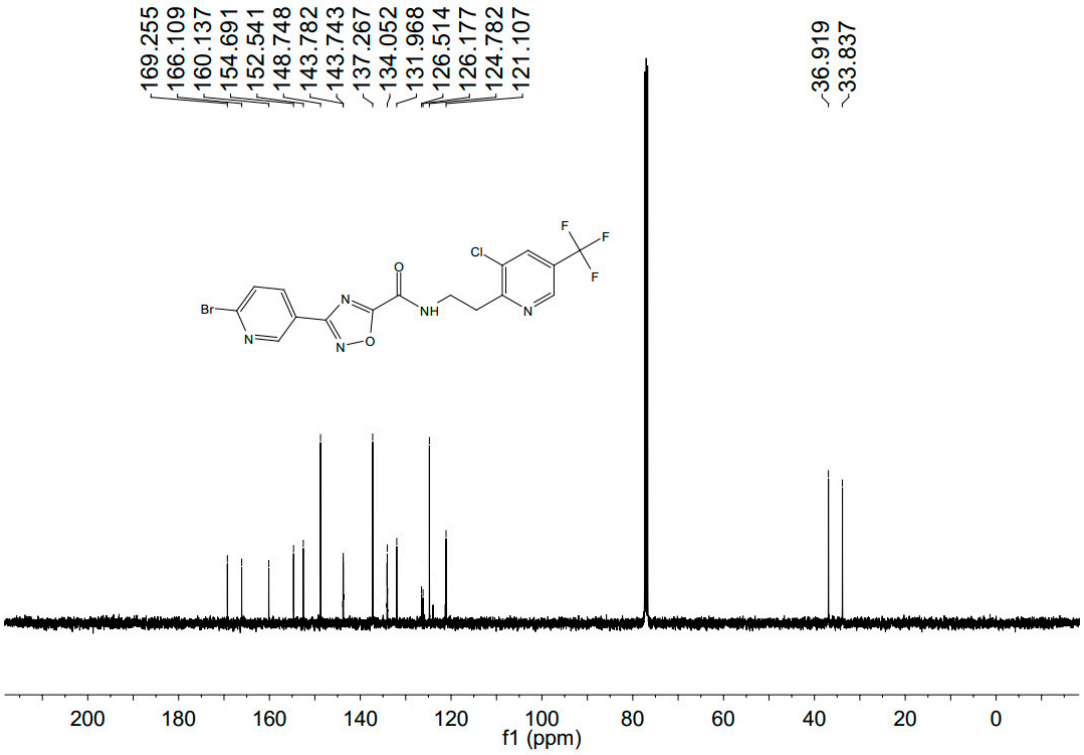


峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
2	3.546	4554	397	V	0.016				0.016
3	3.721	2006	180	V	0.007				0.007
4	4.010	3671	193	V	0.013				0.013
5	7.776	6063	675		0.021				0.021
6	8.217	3732	192		0.013				0.013
7	9.073	28576529	329626	V	99.640				99.640
总计		28679719	337206		100.000				100.000

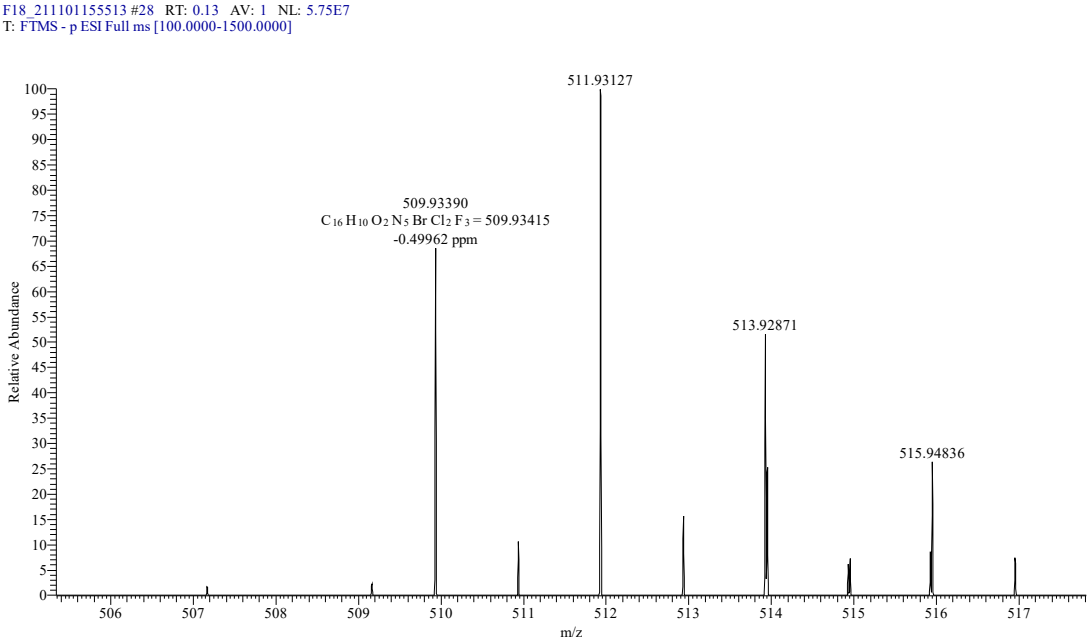
HPLC of compound **F18**



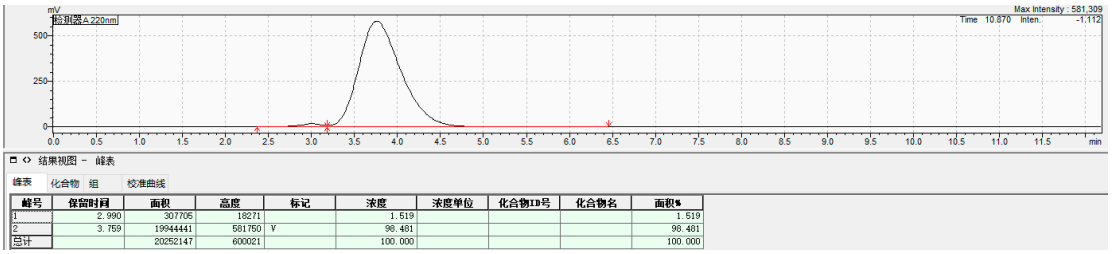
^{1}H NMR of compound **F18**



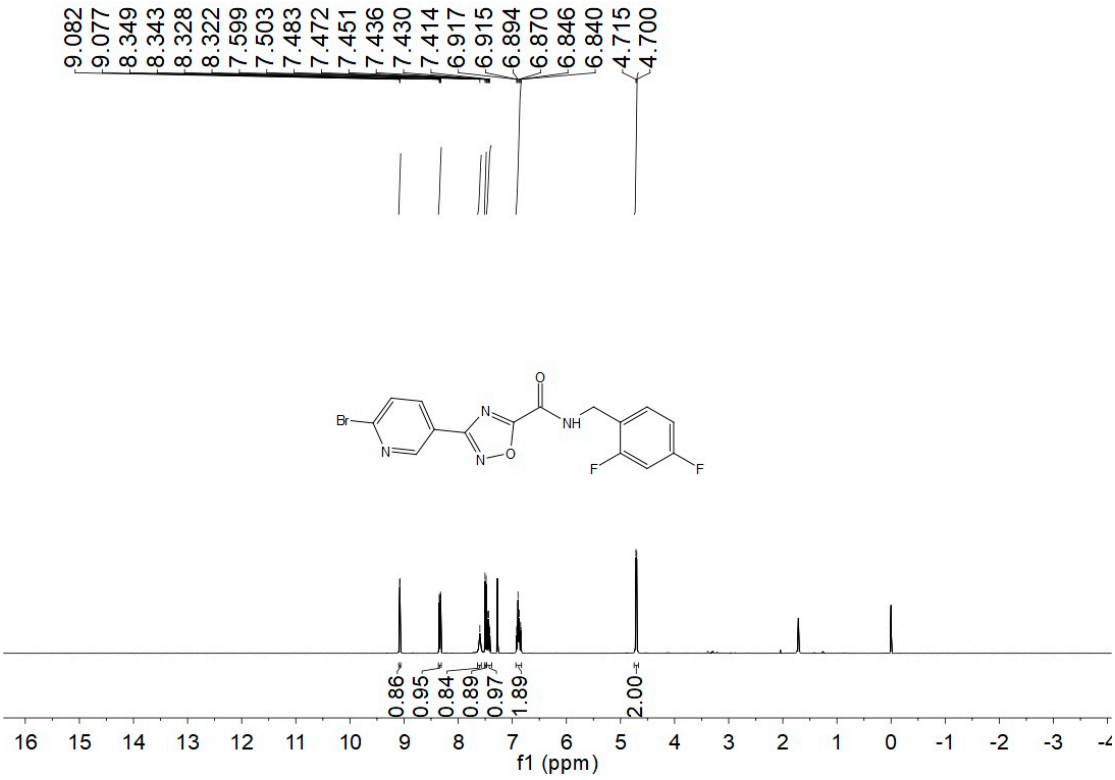
^{13}C NMR of compound **F18**



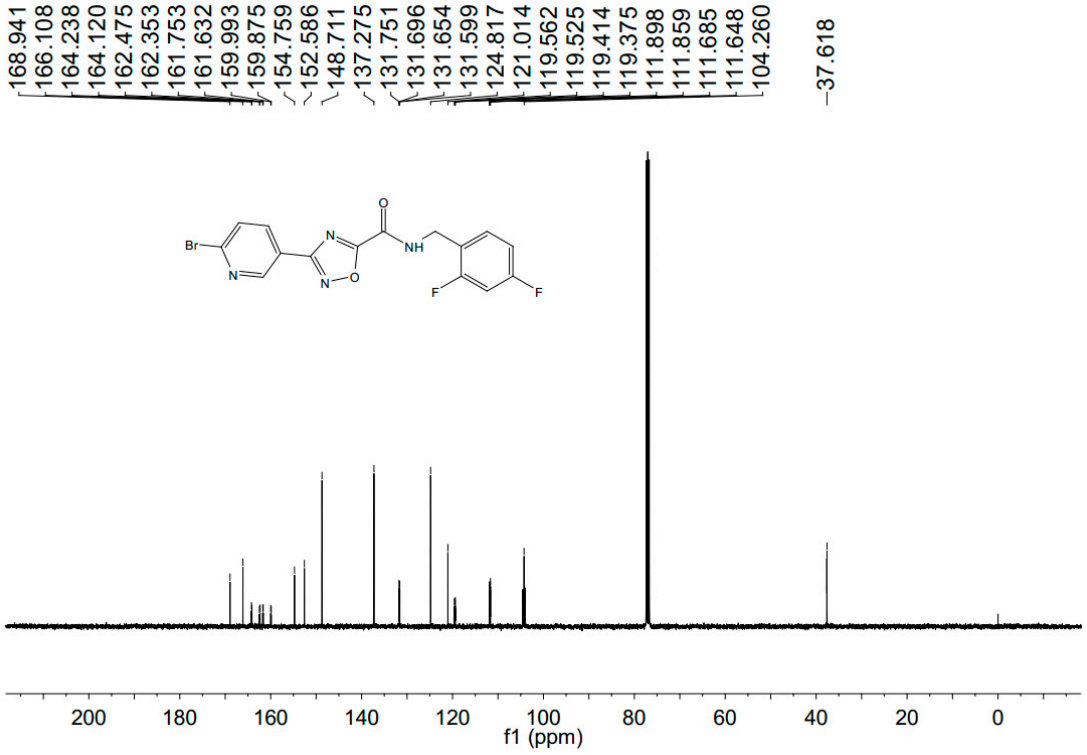
HRMS of compound **F18**



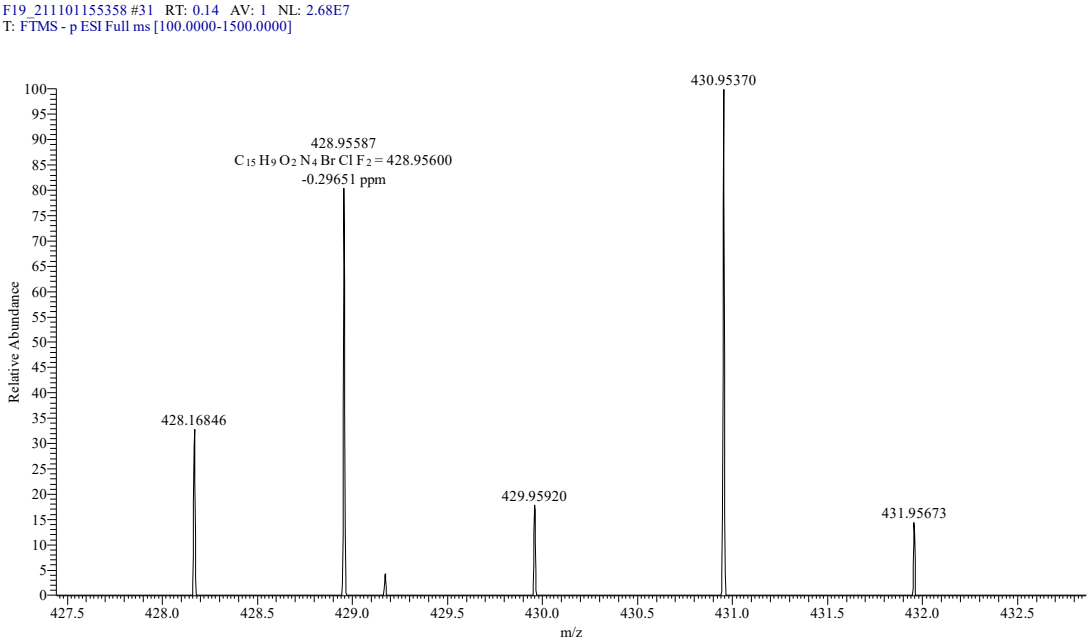
HPLC of compound **F19**



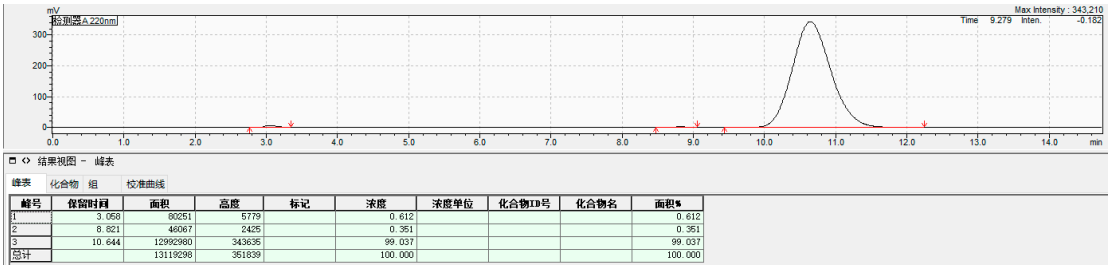
^{1}H NMR of compound **F19**



^{13}C NMR of compound **F19**

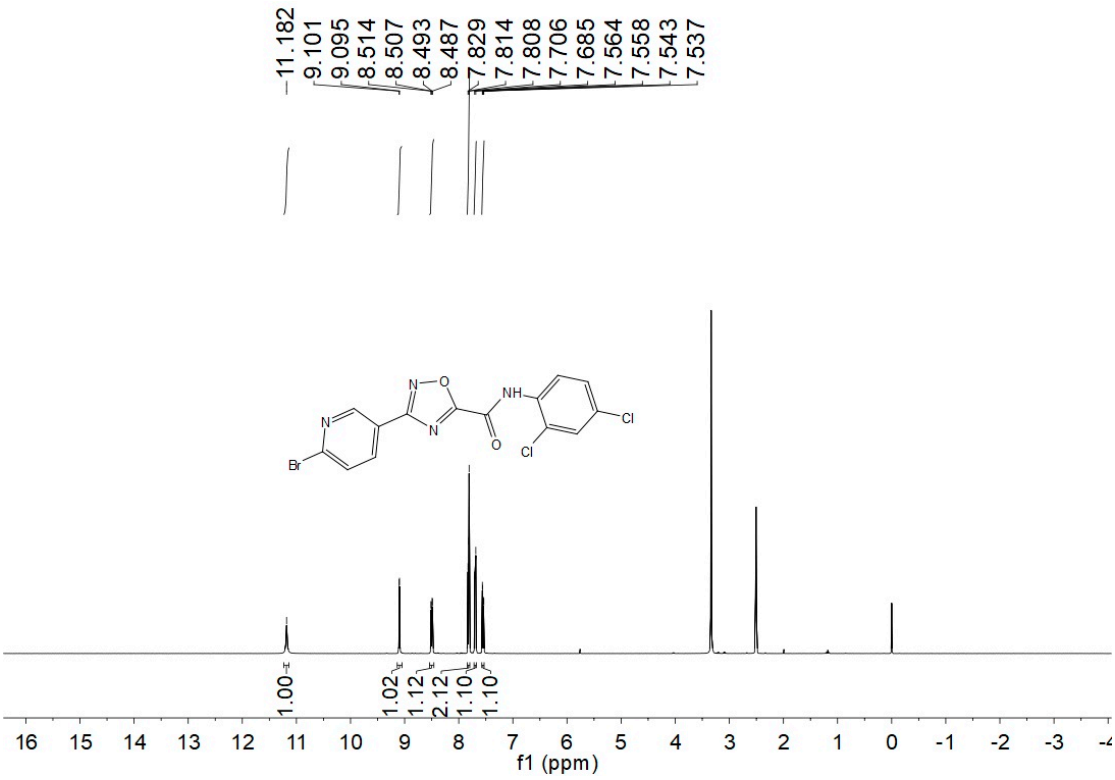


HRMS of compound **F19**

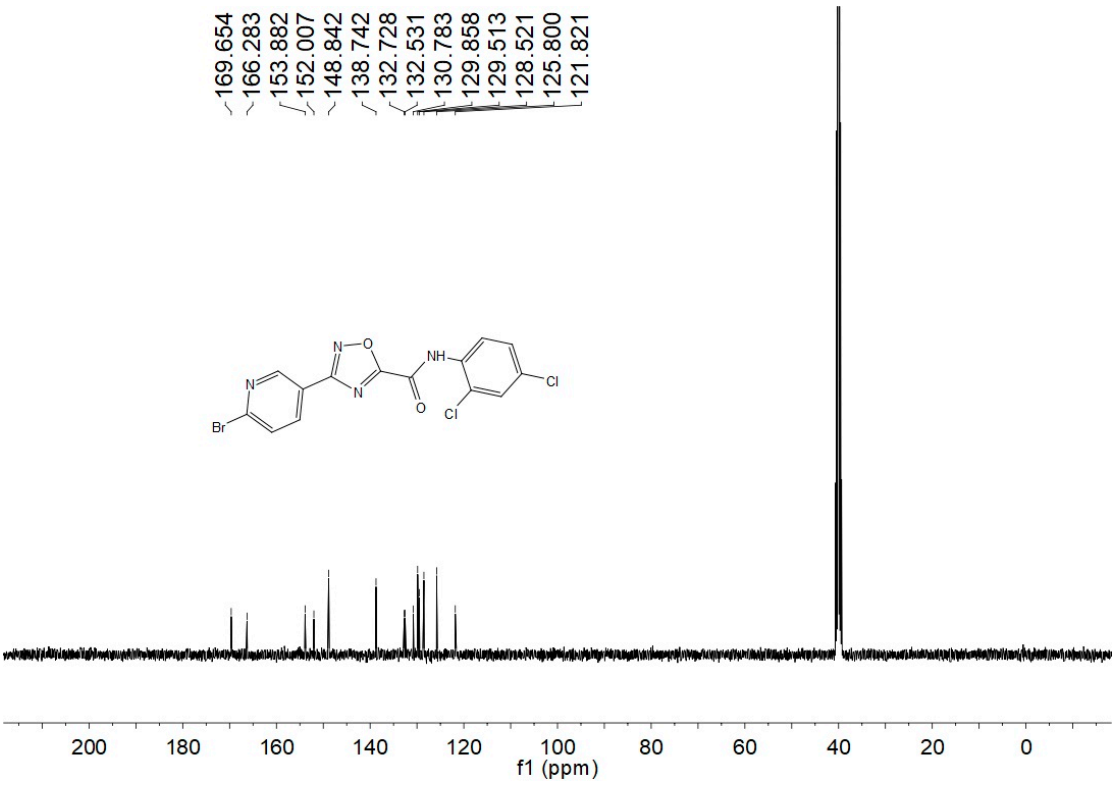


峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
1	3.058	80251	5779		0.612				0.612
2	8.821	46067	2425		0.351				0.351
3	10.644	12992980	343635		99.037				99.037
总计		13119298	351839		100.000				100.000

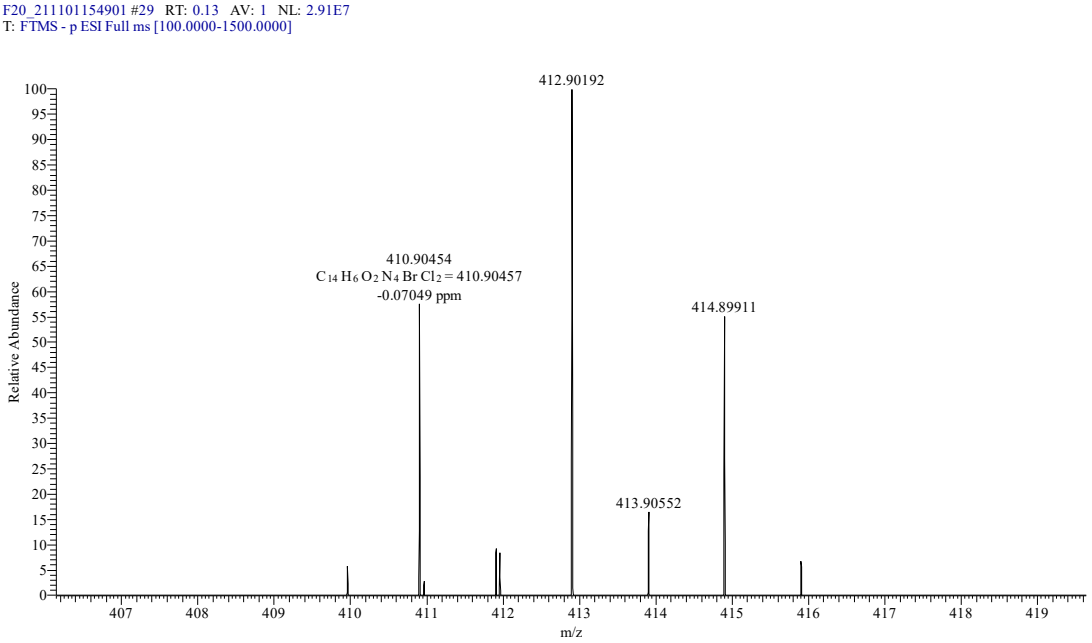
HPLC of compound **F20**



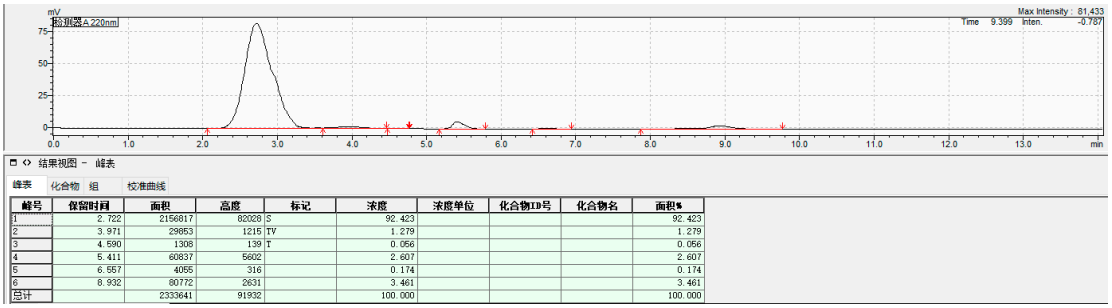
^{1}H NMR of compound **F20**



^{13}C NMR of compound **F20**



HRMS of compound **F20**

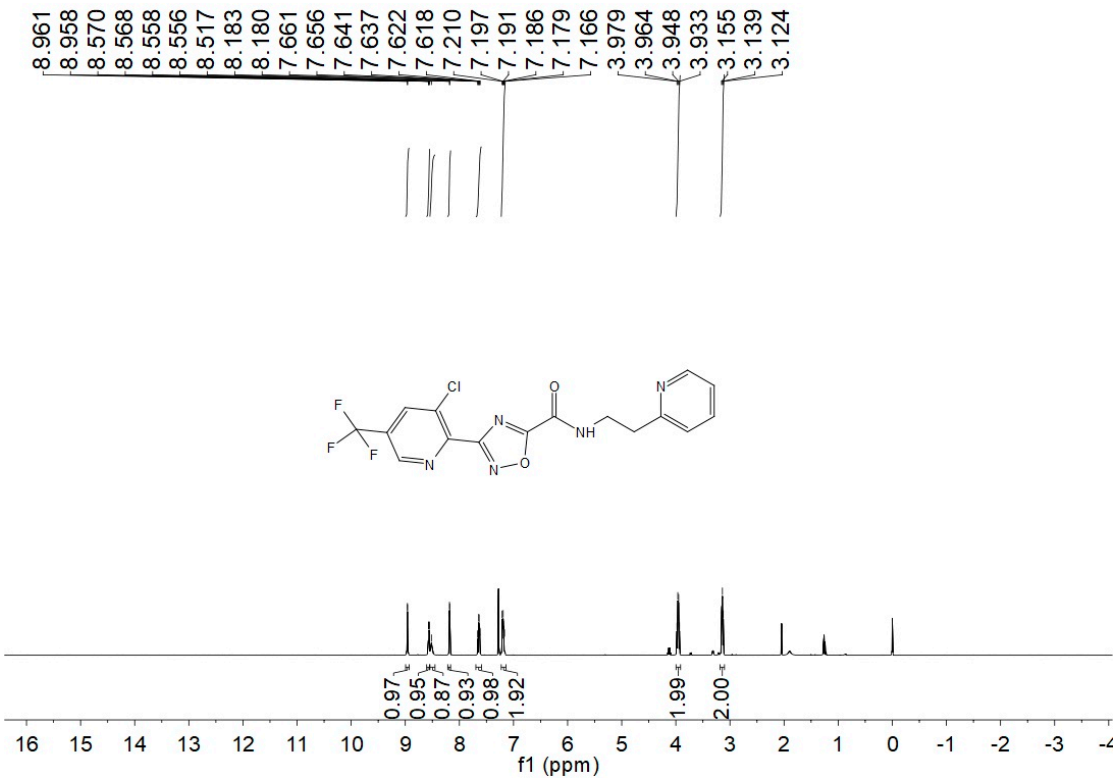


结果视图 - 峰表

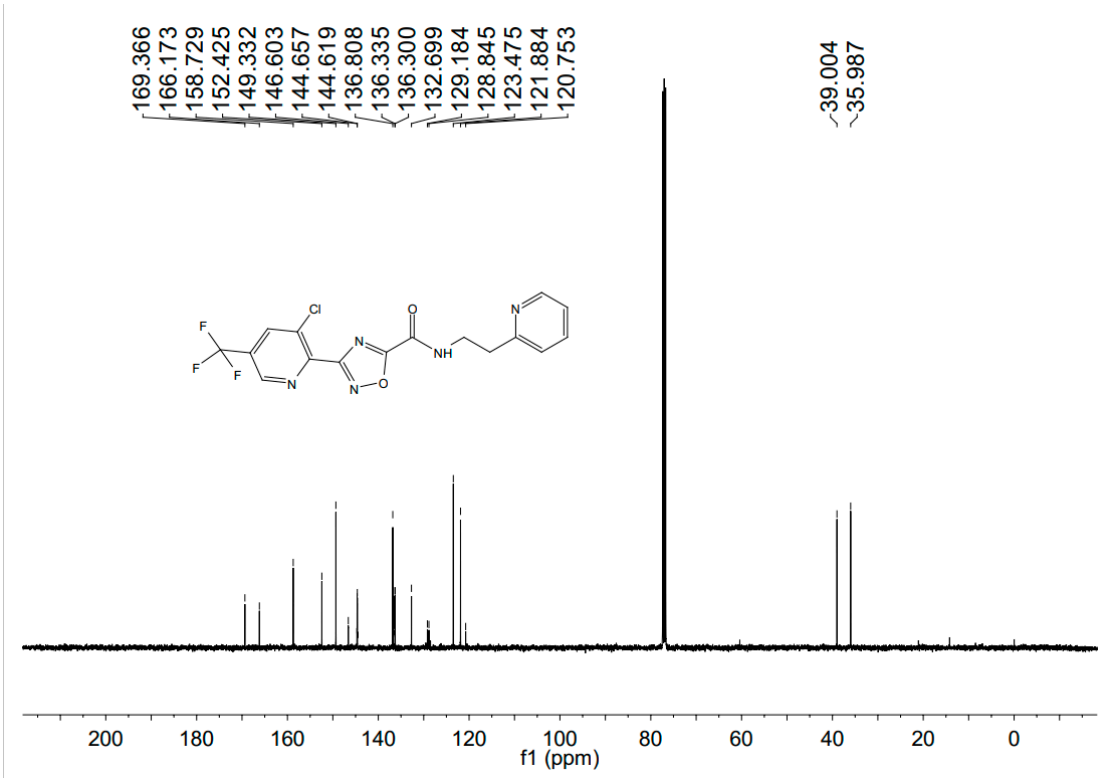
峰表 化合物 组 校准曲线

峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
1	2.722	2156817	82028	S	92.423				92.423
2	3.971	29853	1215	TV	1.279				1.279
3	4.590	1308	139	T	0.056				0.056
4	5.411	60837	5602		2.607				2.607
5	6.557	4055	316		0.174				0.174
6	8.932	80772	2631		3.461				3.461
总计		2333641	91932		100.000				100.000

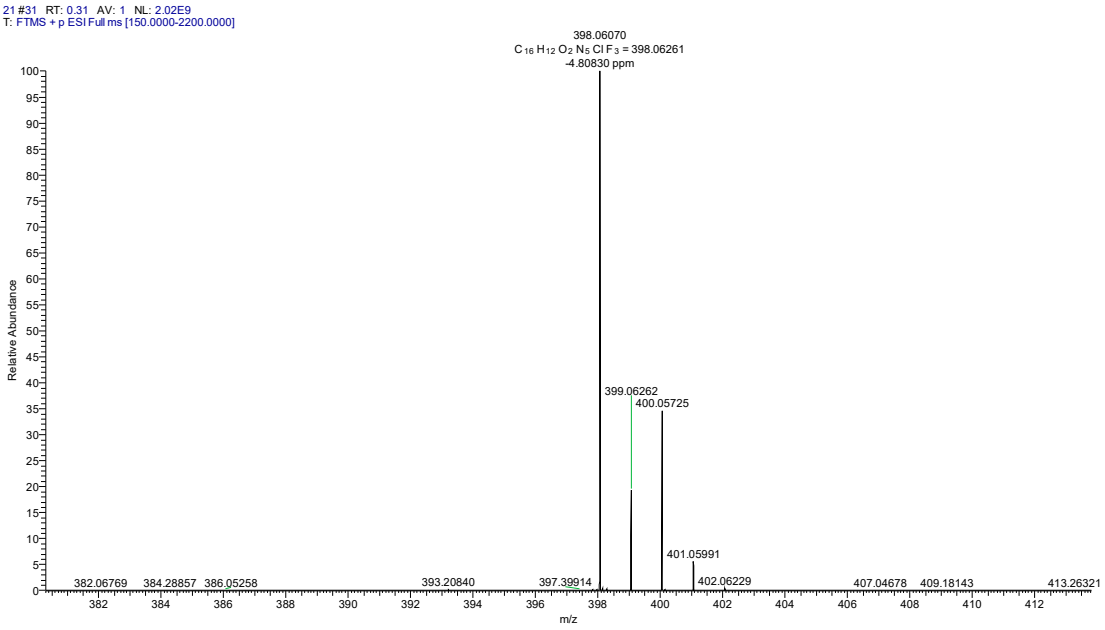
HPLC of compound **F21**



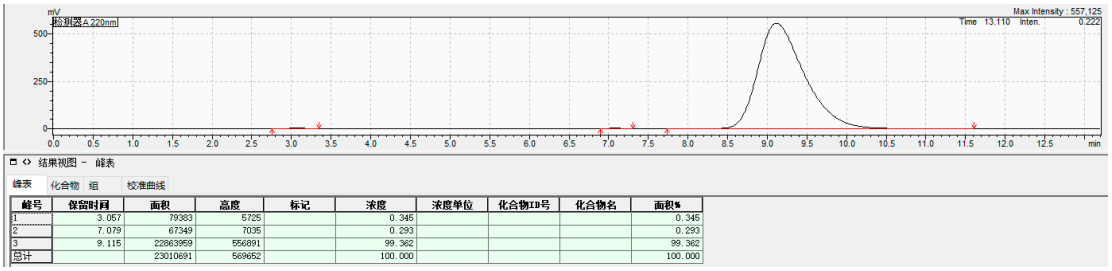
^{1}H NMR of compound **F21**



^{13}C NMR of compound **F21**

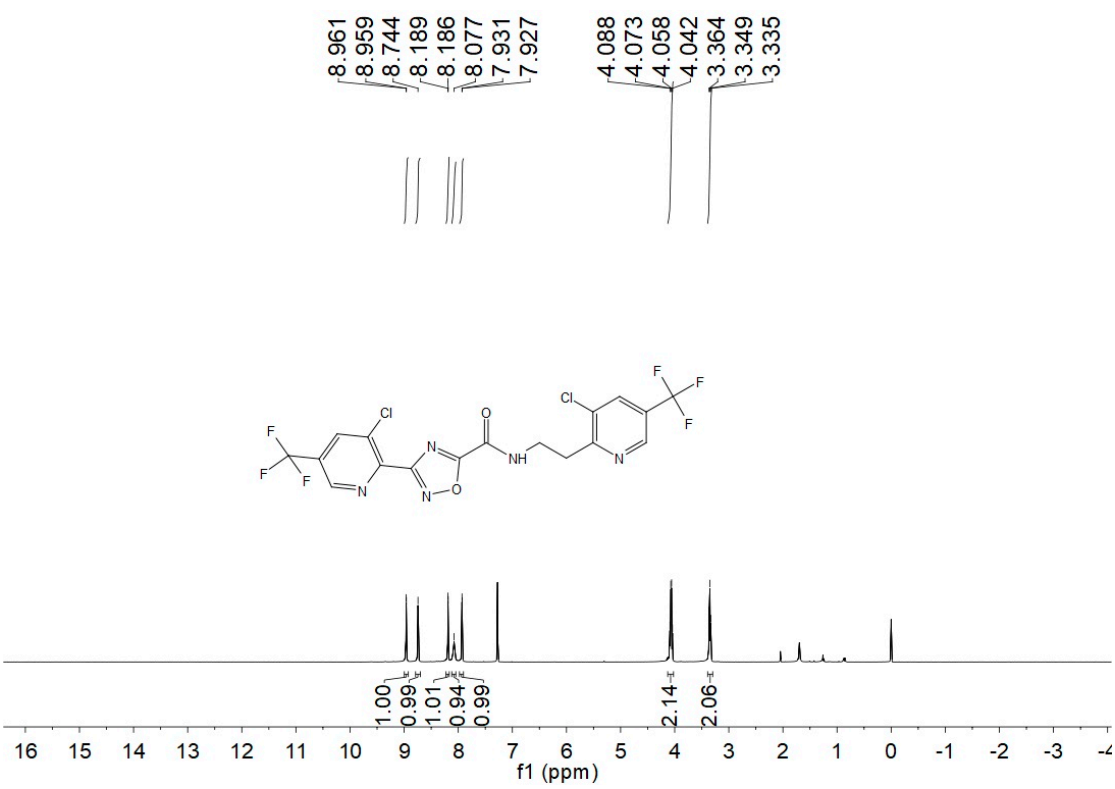


HRMS of compound **F21**

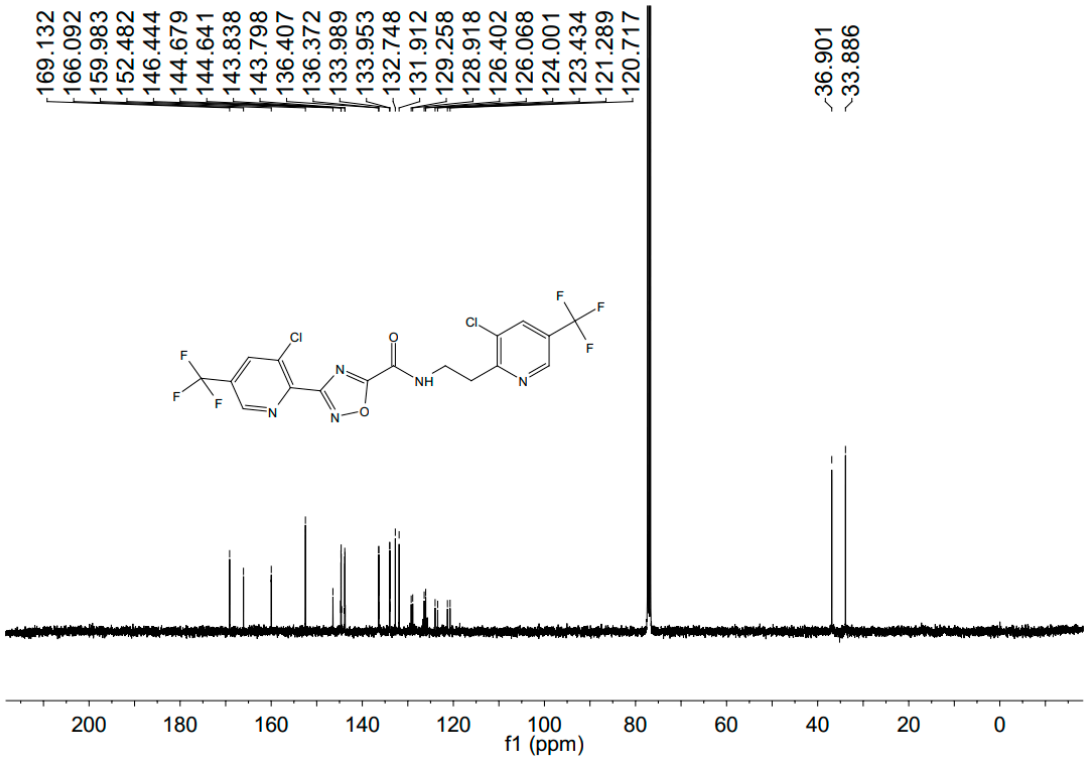


峰号	保留时间	面积	高度	标记	浓度	浓度单位	化合物ID号	化合物名	面积%
1	3.057	79383	5725		0.345				0.345
2	7.079	67349	7035		0.293				0.293
3	9.115	22863959	556891		99.362				99.362
总计		23010691	569652		100.000				100.000

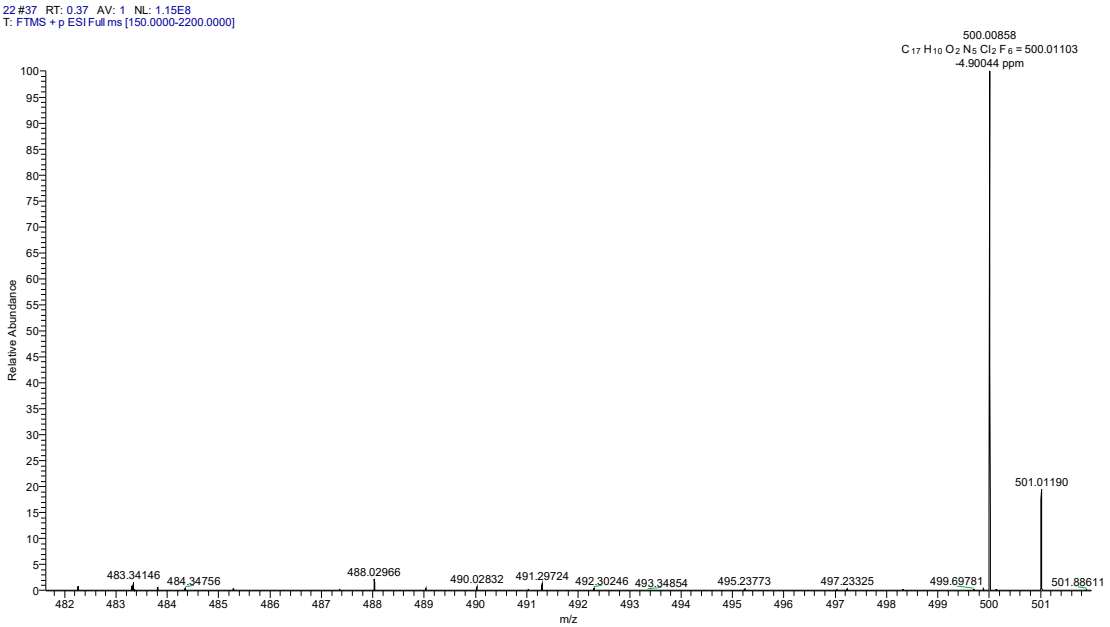
HPLC of compound **F22**



^{1}H NMR of compound **F22**

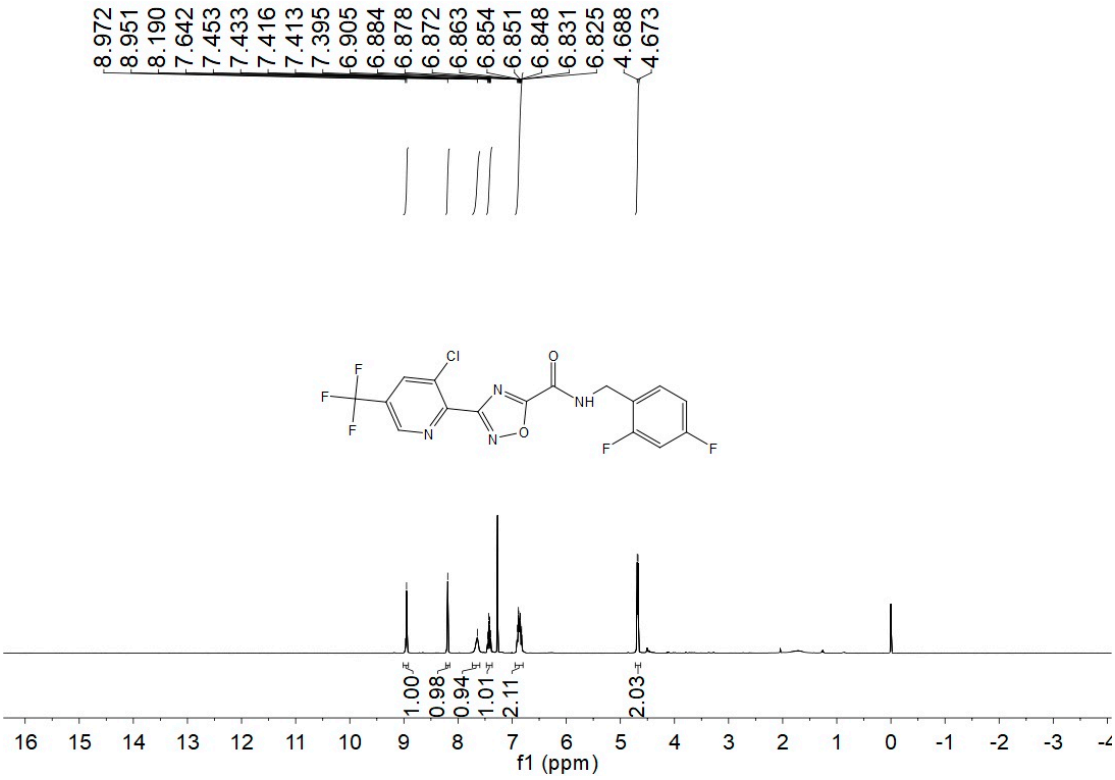


^{13}C NMR of compound **F22**

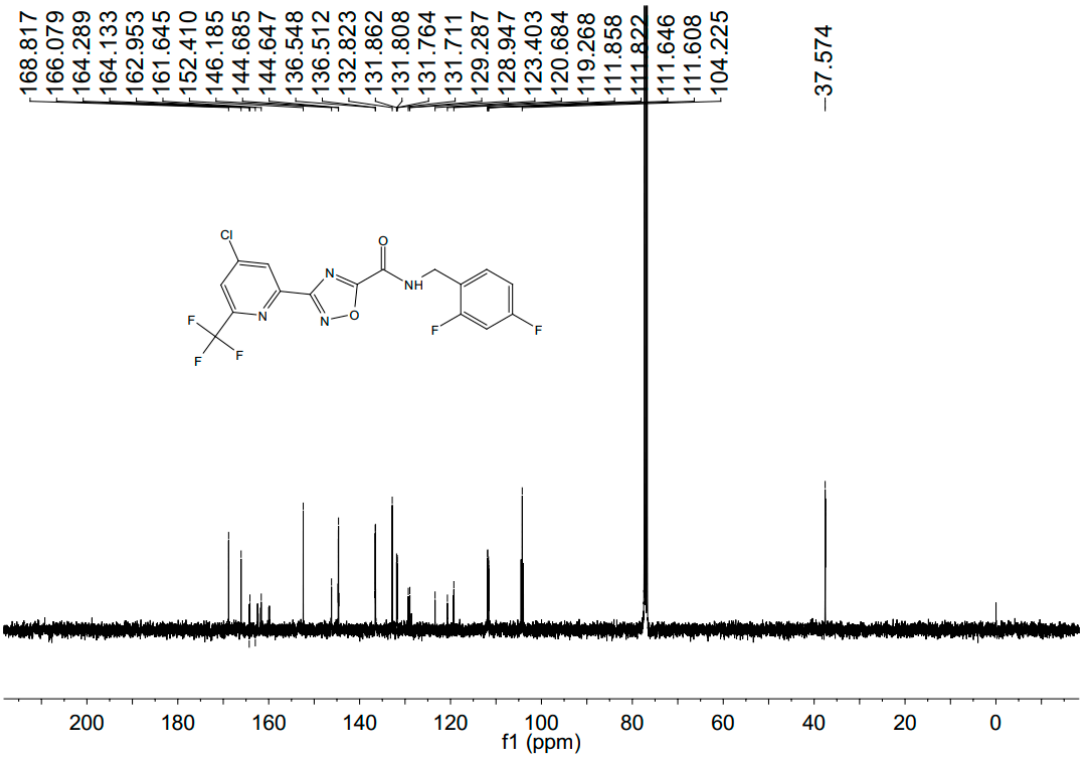


HRMS of compound **F22**

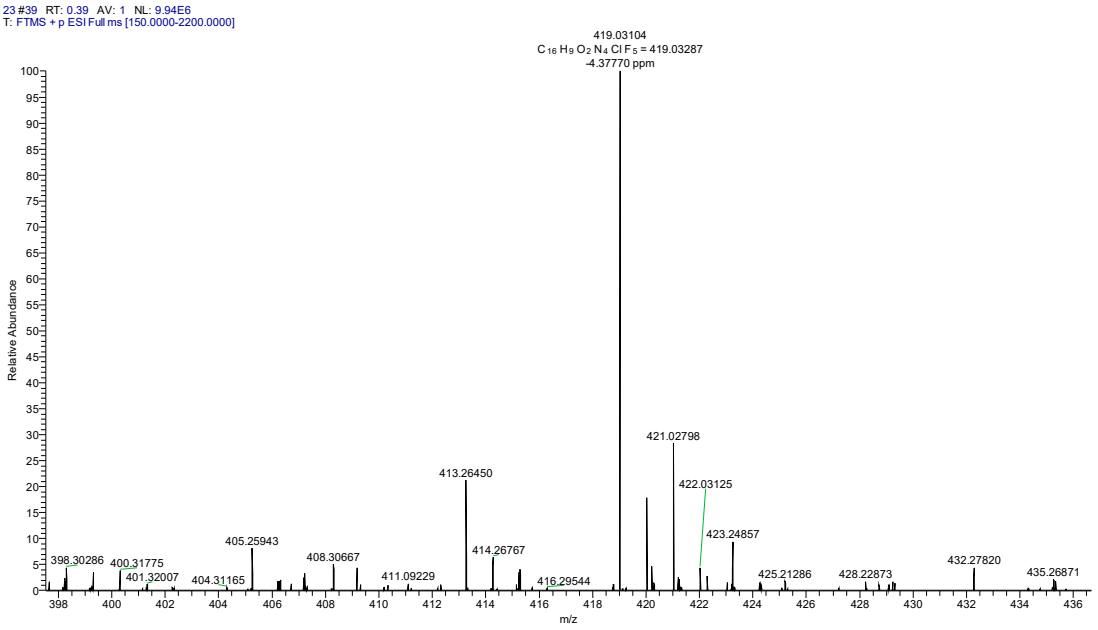
HPLC of compound **F23**



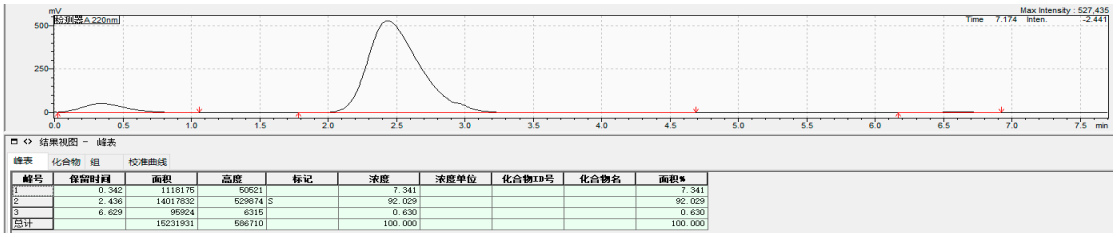
^{1}H NMR of compound **F23**



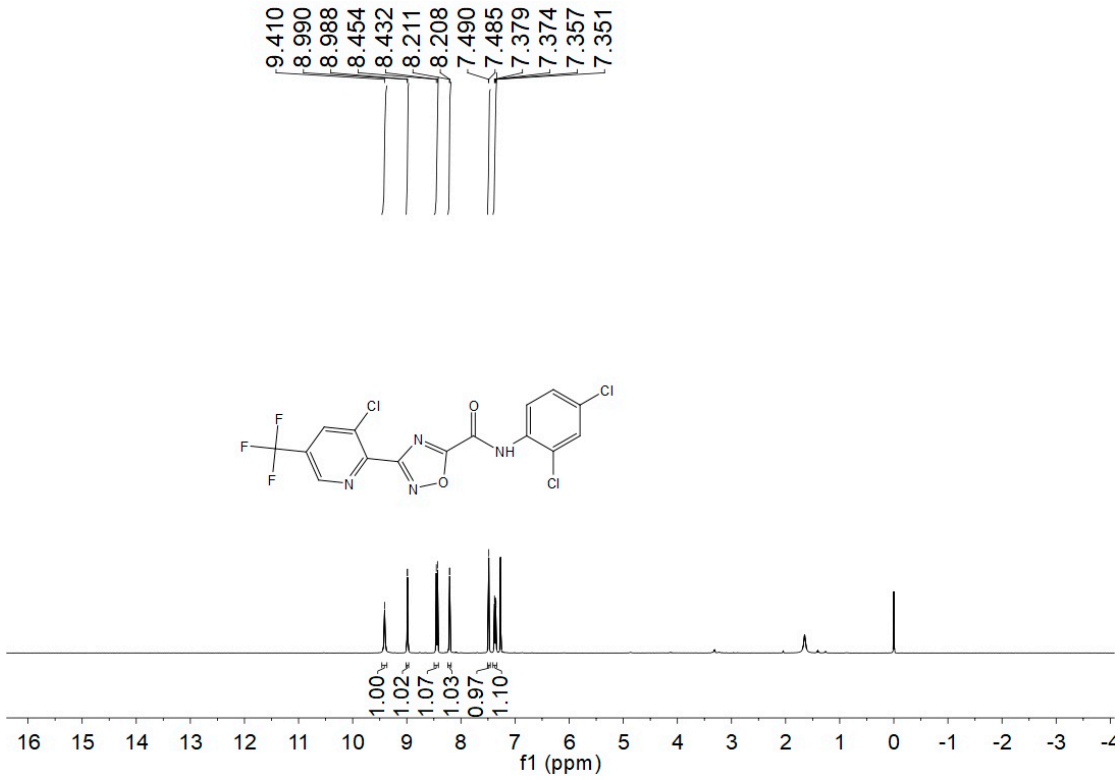
^{13}C NMR of compound **F23**



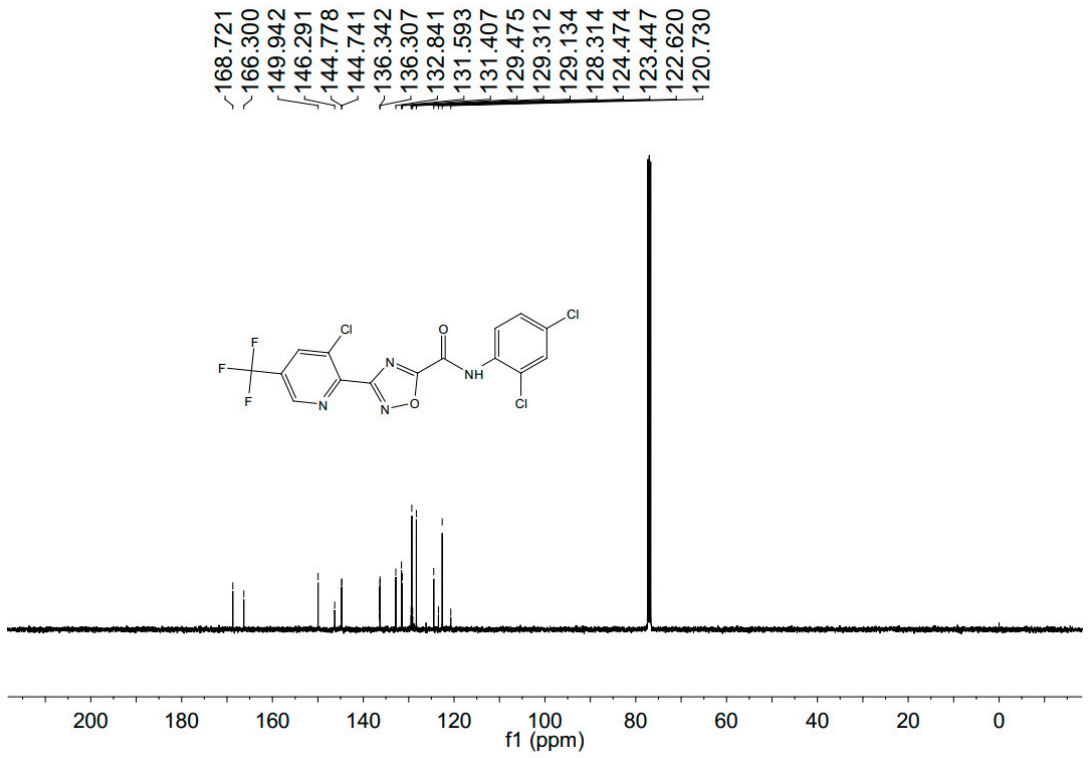
HRMS of compound **F23**



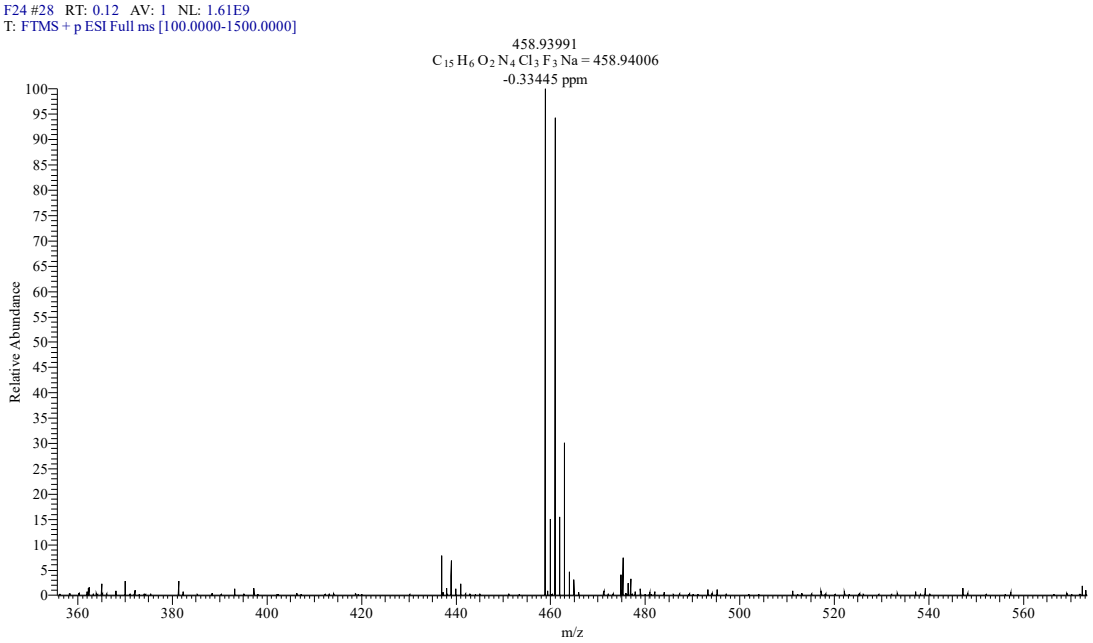
HPLC of compound **F24**



^{1}H NMR of compound **F24**



^{13}C NMR of compound F24



HRMS of compound **F24**