Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Information

Visible-Light-Induced Intermolecular [3+2] Alkenylation–Cyclization Strategy: Metal-Free Construction of Pyrrolo[2,1,5-*cd*]indolizine Rings

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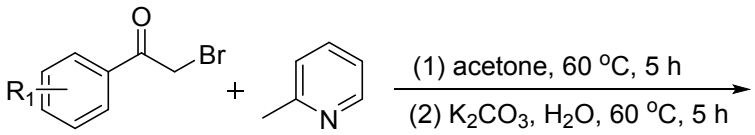
List of Contents

A. General consideration

Analytical thin layer chromatography was carried out using silica gel GF254, visualized under UV light (at 254 nm). Proton NMR (^{1}H) were recorded at 400 MHz, and Carbon NMR (^{13}C) at 100 MHz NMR spectrometer. Multiplicities are abbreviated as: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet. The data of HRMS was carried out on a high-resolution mass spectrometer (LCMS-IT-TOF). IR spectra were obtained either as potassium bromide pellets or as liquid films between two potassium bromide pellets with a Bruker TENSOR 27 spectrometer.

B. General procedure

Synthesis of 1a according to the following procedure:



A solution of 2-picoline (0.93 g, 10 mmol, 1.0 equiv.) and 2 bromoacetophenone (1.99 g, 10 mmol, 1.0 equiv) in acetone (50 mL) were added to a 100 mL round bottom flask and heated at 60 °C for 5 hours. The precipitate obtained by filtration separation was redissolved in 20 mL of hot water (60 °C). Then, K_2CO_3 (1.38 g, 10 mmol, 1.0 equiv) was added and heated at 60 °C for 5 hours. After filtration and drying in vacuo, a white solid compound 1a was obtained in 50% overall yield (965 mg, 5 mmol) without further purification.

Synthesis of 3a according to the following procedure:

A 25 mL sealed tube was charged with a stirring bar, and added 2-phenylindolizine 1a (0.039g, 1.0 equiv), methyl acrylate 2a (0.026g, 1.5 equiv), TFA (0.023g, 1 equiv), rose bengal (0.006g, 0.03 equiv), CH_2Cl_2 (2 mL). The reaction was irradiated with a 20W blue LED at room temperature stirring for 10 h and monitored by TLC. The reaction mixture was then diluted with EtOAc and water, extracted with EtOAc. The organic layers were washed with brine and dried over $MgSO_4$, evaporated under reduced pressure. The crude mixture was purified by Thin layer chromatography silica gel plate (eluted with petroleum ether : ethyl acetate = 15 : 1) to give 3a in 80% yield (44.0 mg).

C. X-ray Structure and Data of 3g

Single-crystal X-ray diffraction data for **3g** were collected at low temperature (100.00 K) with graphite-monochromatized MoKα radiation (λ= 0.71073 Å). absorption corrections were performed using SADABS. A suitable crystal was selected and the cell parameters were obtained from the least squares refinement of the spots using the SMART program. The structure was solved by a direct method and followed by several cycles of full-matrix least-squares refinement using SHELXS-97 program package. In the final refinement, all non-hydrogen atoms were refined with anisotropic thermal coefficients. Crystallographic data for compound **3g** is given in Table S1.

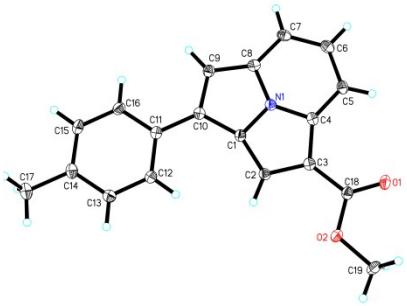


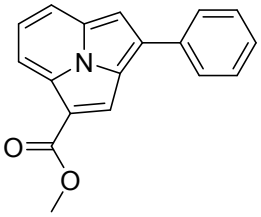
Figure S1. X-Ray crystal structure of **3g**

Table S1. Crystal data and structure refinement for **3g**

Identification code	1
Empirical formula	$C_{19}H_{15}NO_2$
Formula weight	289.32
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	3.9198(2)
b/Å	25.3323(11)
c/Å	7.1542(3)
α/°	90
β/°	97.305(5)
γ/°	90
Volume/Å^3	704.62(6)
Z	2
ρ_{calc}g/cm^3	1.364
μ/mm^{-1}	0.709
F(000)	304.0
Crystal size/mm^3	0.13 × 0.12 × 0.11
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	12.474 to 146.678
Index ranges	-4 ≤ h ≤ 4, -31 ≤ k ≤ 30, -6 ≤ l ≤ 8
Reflections collected	3274
Independent reflections	2230 [R_{int} = 0.0177, R_{sigma} = 0.0212]
Data/restraints/parameters	2230/1/201
Goodness-of-fit on F^2	1.067
Final R indexes [I>=2σ (I)]	R_1 = 0.0367, wR_2 = 0.0949
Final R indexes [all data]	R_1 = 0.0385, wR_2 = 0.0966
Largest diff. peak/hole / e Å^{-3}	0.20/-0.29
Flack/Hooft parameter	-0.08(15)/-0.10(9)

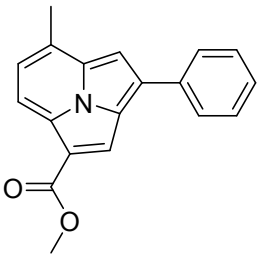
D. Analytical data for 3a-3P, 4a-4f, 5a-5d

Methyl 3-phenylpyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3a)



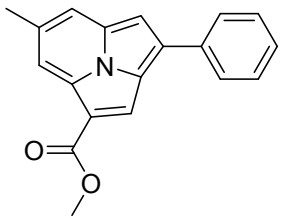
Yellow solid (44.0 mg, 80%); m.p. 100-101 °C. IR (KBr): 3054, 2969, 1554, 1462, 1221, 1132, 782 cm^{-1}.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, J = 8.0 Hz, 1H), 8.29 (s, 1H), 8.01 (d, J = 7.2 Hz, 2H), 7.84 (dt, J = 15.2, 7.6 Hz, 2H), 7.55-7.49 (m, 3H), 7.41 (t, J = 7.4 Hz, 1H), 4.03 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 135.6, 134.0, 131.9, 129.8, 129.1, 128.5, 127.6, 124.4, 124.4, 119.6, 114.7, 113.9, 113.0, 109.1, 51.4. HRMS ESI (m/z): calcd for $C_{18}H_{13}NO_2$ $[M + H]^+$: 276.1019, found: 276.1017.

Methyl 5-methyl-3-phenylpyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3b)



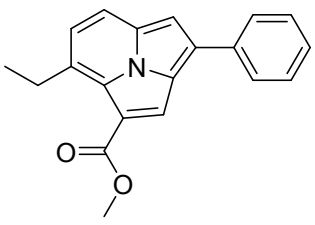
Yellow solid (45.1 mg, 78%); m.p. 114-116 °C. IR (KBr): 3034, 2973, 1507, 1456, 1221, 1147, 779 cm^{-1}.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (dd, J = 5.0, 2.6 Hz, 2H), 8.00 (d, J = 7.8 Hz, 2H), 7.59 (d, J = 8.0 Hz, 1H), 7.52 (s, 1H), 7.50 (d, J = 7.8 Hz, 2H), 7.39 (t, J = 7.4 Hz, 1H), 4.01 (s, 3H), 2.83 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 134.3, 131.3, 129.1, 128.2, 127.5, 126.2, 124.5, 124.2, 118.9, 114.7, 113.9, 107.7, 51.4, 17.2. IR (KBr): 3054, 2969, 1554, 1462, 1221, 1132, 782 cm^{-1} . HRMS ESI (m/z): calcd for $C_{19}H_{16}NO_2$ $[M + H]^+$: 290.1176, found: 276.1180.

Methyl 6-methyl-3-phenylpyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3c)



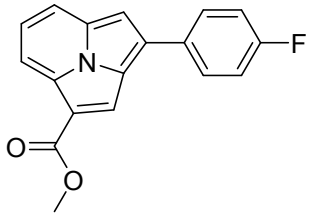
Yellow solid (44.5 mg, 77%); m.p. 93-95 °C. IR (KBr): 3034, 2929, 1553, 1460, 1236 1127, 765 cm^{-1}.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (s, 1H), 8.14 (s, 1H), 7.99 (d, J = 7.2 Hz, 2H), 7.65 (s, 1H), 7.51 (t, J = 7.6 Hz, 2H), 7.39 (d, J = 11.8 Hz, 2H), 4.02 (s, 3H), 2.77 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 135.8, 135.7, 134.1, 131.7, 129.8, 129.0, 128.3, 127.4, 123.9, 119.4, 115.4, 114.1, 112.8, 108.38, 51.3, 22.6. HRMS ESI (m/z): calcd for $C_{19}H_{15}NaNO_2$ $[M + Na]^+$: 312.0995, found: 312.0991.

Methyl 7-ethyl-3-phenylpyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3d)



Yellow solid (42.4 mg, 70%); m.p. 94-96 °C. IR (KBr): 3057, 2930, 1550, 1460, 1392 1117, 794 cm^{-1}.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.99 (d, J = 7.4 Hz, 2H), 7.76 (d, J = 7.8 Hz, 1H), 7.62 (d, J = 7.8 Hz, 1H), 7.51 (t, J = 7.8 Hz, 2H), 7.47 (s, 1H), 7.39 (t, J = 7.4 Hz, 1H), 4.00 (s, 3H), 3.61 (q, J = 7.4 Hz, 2H), 1.44 (t, J = 7.6 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 165.0, 134.2, 133.8, 133.8, 130.6, 129.0, 128.2, 128.0, 127.3, 125.9, 124.2, 120.0, 114.4, 113.3, 108.8, 51.3, 26.8, 17.2. HRMS ESI (m/z): calcd for $C_{20}H_{17}NaNO_2$ $[M + Na]^+$: 326.1151, found: 326.1148.

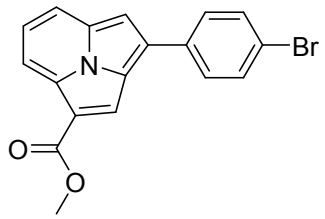
Methyl 3-(4-fluorophenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3e)



Yellow solid (44.0 mg, 75%); m.p. 94-96 °C. IR (KBr): 3063, 2932, 1537, 1341 1201,1064, 776 cm^{-1}.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, J = 7.6 Hz, 1H), 8.26 (s, 1H), 7.97 (d, J = 8.8 Hz, 2H), 7.88-7.83 (m,

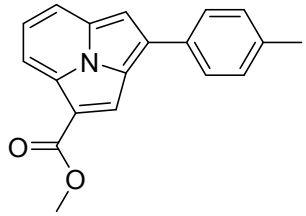
2H), 7.48 (s, 1H), 7.22 (d, *J* = 8.8 Hz, 2H), 4.03 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 164.2 (*J* = 247.2 Hz), 134.6, 131.9, 130.3, 130.3, 129.9, 129.3, 129.2, 124.6, 124.2, 119.4, 116.3, 116.1, 114.8, 114.18, 113.1, 108.9, 51.46. HRMS ESI (m/z): calcd for $C_{18}H_{13}FNO_2$ $[M + H]^+$: 294.0925, found: 294.0922.

Methyl 3-(4-bromophenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3f)



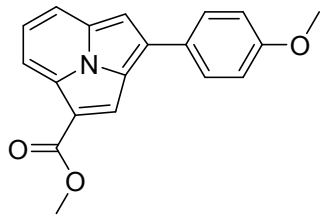
Yellow solid (55.1 mg, 78%); m.p. 165-167 °C. IR (KBr): 3061, 2926, 1688, 1554, 1263, 695 cm^{-1}.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 7.6 Hz, 1H), 8.26 (s, 1H), 7.88 (dd, *J* = 15.8, 7.8 Hz, 4H), 7.63 (d, *J* = 8.6 Hz, 2H), 7.52 (s, 1H), 4.03 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4, 134.3, 133.0, 132.3, 131.8, 129.9, 128.9, 124.6, 124.1, 122.5, 119.4, 115.1, 114.3, 113.4, 109.2, 51.5. HRMS ESI (m/z): calcd for $C_{18}H_{13}BrNO_2$ $[M + H]^+$: 354.0124, found: 354.0118.

Methyl 3-(*p*-tolyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3g)



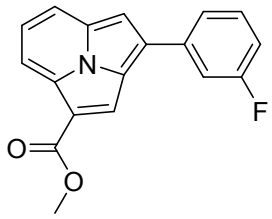
Yellow solid (42.8 mg, 74%); m.p. 107-108 °C. IR (KBr): 3049, 2970, 1532, 1383 1024, 887 cm^{-1}.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (dd, *J* = 7.0, 1.6 Hz, 1H), 8.29 (s, 1H), 7.91 (d, *J* = 8.2 Hz, 2H), 7.85-7.80 (m, 2H), 7.50 (s, 1H), 7.32 (d, *J* = 7.8 Hz, 2H), 4.03 (s, 3H), 2.44 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 138.5, 135.8, 132.1, 131.2, 129.8, 127.4, 124.4, 119.5, 114.5, 113.8, 112.8, 108.6, 51.4, 21.3. HRMS ESI (m/z): calcd for $C_{19}H_{15}NaNO_2$ $[M + Na]^+$: 312.0995, found: 312.0993.

Methyl 3-(4-methoxyphenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3h)



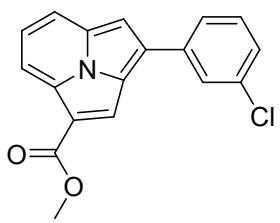
Yellow solid (43.3 mg, 71%); m.p. 103-104 °C. IR (KBr): 3046, 2963, 1699, 1583, 1224, 780 cm^{-1}.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (dd, *J* = 5.6, 3.0 Hz, 1H), 8.26 (s, 1H), 7.95 (d, *J* = 8.8 Hz, 2H), 7.84-7.79 (m, 2H), 7.44 (s, 1H), 7.06-7.02 (m, 2H), 4.03 (s, 3H), 3.89 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 159.9, 135.6, 132.2, 129.9, 128.8, 126.7, 124.4, 124.3, 119.3, 114.6, 114.3, 113.7, 112.5, 108.0, 55.3, 51.4. HRMS ESI (m/z): calcd for $C_{19}H_{15}NO_3$ $[M + H]^+$: 305.1042, found: 305.10464.

Methyl 3-(3-fluorophenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3i)



Yellow solid (44.0 mg, 75%); m.p. 125-126 °C. IR (KBr): 3043, 2894, 1521, 1365, 1179, 764 cm^{-1}.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 7.8 Hz, 1H), 8.25 (s, 1H), 7.88 (d, *J* = 7.6 Hz, 1H), 7.83 (t, *J* = 7.8 Hz, 1H), 7.77 (d, *J* = 7.6 Hz, 1H), 7.66 (d, *J* = 9.8 Hz, 1H), 7.51 (s, 1H), 7.49-7.44 (m, 1H), 7.10 (t, *J* = 8.4 Hz, 1H), 4.03 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.3, 164.5 (*J* = 245.0 Hz), 136.2 (*J* = 8.0 Hz), 134.1, 131.7, 130.7, 130.5, 129.8, 124.5, 124.1, 123.2, 119.50, 115.3 (*J* = 13.0 Hz), 114.3, 114.1, 113.5, 109.5, 51.4. HRMS ESI (m/z): calcd for $C_{18}H_{12}FNO_2$ $[M + H]^+$: 293.0847, found: 293.08411.

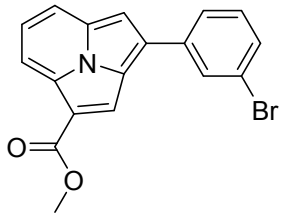
Methyl 3-(3-chlorophenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3j)



Yellow solid (40.8 mg, 66%); m.p. 126-128 °C. IR (KBr): 3057, 2899,

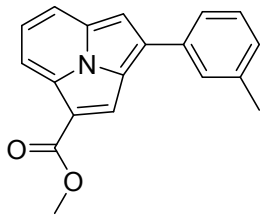
1554, 1440, 1201, 1122, 810 cm $^{-1}$. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, J = 7.8 Hz, 1H), 8.30 (s, 1H), 7.99-7.85 (m, 4H), 7.56 (s, 1H), 7.41 (dd, J = 26.9, 8.2 Hz, 2H), 4.04 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4, 135.9, 135.1, 134.0, 131.7, 130.3, 129.9, 128.3, 127.5, 125.6, 124.6, 124.1, 119.5, 115.2, 114.5, 113.5, 109.5, 51.5. HRMS ESI (m/z): calcd for $C_{18}H_{13}ClNO_2$ $[M + H]^+$: 310.0629, found: 310.0620.

Methyl 3-(3-bromophenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3k)



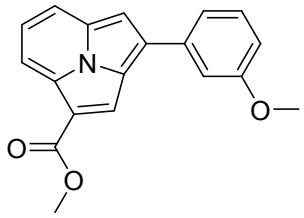
Yellow solid (49.4 mg, 70%); m.p. 95-97 °C. IR (KBr): 3034, 2912, 1552, 1375, 1221, 1130, 715 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, J = 7.4 Hz, 1H), 8.29 (s, 1H), 8.13 (t, J = 1.7 Hz, 1H), 7.94-7.86 (m, 3H), 7.53 (d, J = 9.4 Hz, 2H), 7.38 (t, J = 7.8 Hz, 1H), 4.04 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4, 136.2, 133.8, 131.3, 130.6, 130.4, 129.9, 126.1, 124.6, 123.2, 119.5, 115.3, 114.5, 113.6, 109.6, 51.5. HRMS ESI (m/z): calcd for $C_{18}H_{13}BrNO_2$ $[M + H]^+$: 354.0124, found: 310.0118.

Methyl 3-(*m*-tolyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3l)



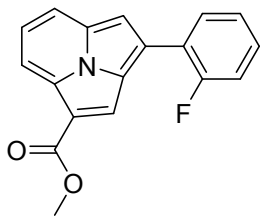
Yellow oil (41.1 mg, 71%); IR (KBr): 3054, 2924, 1543, 1324, 1183, 765 cm $^{-1}$. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, J = 7.6 Hz, 1H), 8.31 (s, 1H), 7.84 (dd, J = 13.6, 6.4 Hz, 4H), 7.54 (s, 1H), 7.41 (t, J = 7.6 Hz, 1H), 7.23 (d, J = 7.6 Hz, 1H), 4.04 (s, 3H), 2.49 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 138.7, 135.8, 133.9, 132.0, 129.8, 129.3, 129.0, 128.2, 124.7, 124.5, 124.4, 119.6, 114.7, 113.9, 112.9, 109.1, 51.4, 21.6. HRMS ESI (m/z): calcd for $C_{19}H_{15}NNaO_2$ $[M + Na]^+$: 312.0995, found: 312.0991.

Methyl 3-(3-methoxyphenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3m)



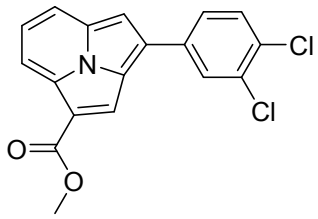
Yellow solid (41.5 mg, 68%); m.p. 90-92 °C. IR (KBr): 3042, 2964, 1692, 1521, 1365, 1179, 790 cm^{-1}.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, J = 7.6 Hz, 1H), 8.29 (s, 1H), 7.88 (d, J = 7.6 Hz, 1H), 7.84 (d, J = 7.8 Hz, 1H), 7.61 (d, J = 7.8 Hz, 1H), 7.54 (s, 2H), 7.43 (t, J = 7.8 Hz, 1H), 6.96 (d, J = 8.2 Hz, 1H), 4.03 (s, 3H), 3.93 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 160.1, 135.5, 135.3, 131.9, 130.1, 129.8, 124.4, 120.1, 119.5, 114.8, 114.0, 113.8, 113.2, 113.1, 109.3, 55.3, 51.4. HRMS ESI (m/z): calcd for $C_{19}H_{15}NNaO_3$ $[M + Na]^+$: 328.0944, found: 328.0945.

Methyl 3-(2-fluorophenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3n)



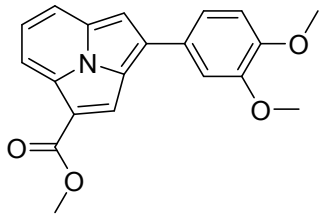
Yellow solid (38.1 mg, 65%); m.p. 122-123 °C. IR (KBr): 3068, 2958, 1621, 1322, 1221, 1107, 780 cm^{-1}.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, J = 7.8 Hz, 1H), 8.31 (d, J = 2.2 Hz, 1H), 8.05 (td, J = 7.8, 1.8 Hz, 1H), 7.93 (d, J = 7.8 Hz, 1H), 7.86 (t, J = 7.8 Hz, 1H), 7.72 (d, J = 1.8 Hz, 1H), 7.41-7.36 (m, 1H), 7.33-7.29 (m, 1H), 4.03 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4, 164.5(J = 245.0 Hz), 137.3, 134.2, 131.7, 130.6(J = 9.0 Hz), 129.85, 124.55, 123.26, 119.50, 115.33(J = 22.0 Hz), 115.20, 114.13(J = 22.0 Hz), 113.51, 109.54, 51.48. HRMS ESI (m/z): calcd for $C_{18}H_{13}FNO_2$ $[M + Na]^+$: 294.0925, found: 294.0919.

Methyl 3-(3,4-dichlorophenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3o)



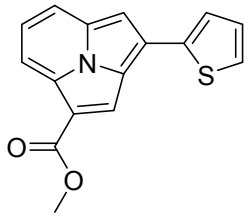
Yellow solid (48.0 mg, 70%); m.p. 113-115 °C. IR (KBr): 3075, 2899, 1576, 1407, 1311, 885 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 7.8 Hz, 1H), 8.23 (s, 1H), 8.03 (d, *J* = 2.2 Hz, 1H), 7.88 (dt, *J* = 15.6, 7.8 Hz, 2H), 7.78 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.54 (d, *J* = 8.2 Hz, 1H), 7.49 (s, 1H), 4.03 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) *δ* 165.3, 134.1, 133.2, 132.8, 132.3, 131.6, 131.0, 129.9, 129.0, 126.5, 124.7, 123.8, 119.3, 115.4, 114.6, 113.7, 109.5, 51.5. HRMS ESI (m/z): calcd for $C_{18}H_{12}Cl_2NO_2$ $[M + H]^+$: 344.0240, found: 344.0238.

Methyl 3-(3,4-dimethoxyphenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3p)



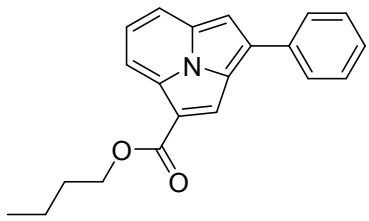
Yellow solid (44.2 mg, 66%); m.p. 153-154 °C. IR (KBr): 3072, 2982, 1565, 1477, 1328, 770 cm^{-1}.^1H NMR (400 MHz, $CDCl_3$) *δ* 8.33-8.30 (m, 1H), 8.24 (s, 1H), 7.84-7.81 (m, 2H), 7.60 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.49 (d, *J* = 2.0 Hz, 1H), 7.45 (s, 1H), 7.00 (d, *J* = 8.4 Hz, 1H), 4.03 (d, *J* = 3.8 Hz, 6H), 3.97 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) *δ* ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 165.6, 149.6, 149.4, 135.8, 132.1, 129.8, 127.0, 124.5, 124.3, 120.5, 119.2, 114.5, 113.7, 112.5, 111.6, 110.5, 108.2, 56.0, 55.9, 51.4. HRMS ESI (m/z): calcd for $C_{20}H_{18}NO_4$ $[M + H]^+$: 336.1230, found: 336.1223.

Methyl 3-(thiophen-2-yl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3q)



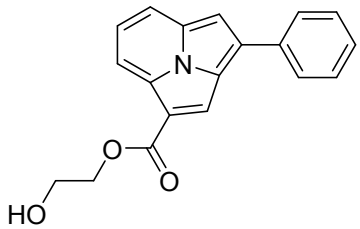
Yellow solid (38.8 mg, 69%); m.p. 75-77 °C. IR (KBr): 3067, 2964, 1521, 1481, 1221, 776 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$) *δ* 8.35 (dd, *J* = 22.4, 6.8 Hz, 2H), 8.24 (s, 1H), 7.81 (d, *J* = 5.8 Hz, 2H), 7.64 (d, *J* = 3.2 Hz, 1H), 7.41 (s, 1H), 7.18 (d, *J* = 3.6 Hz, 1H), 4.02 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) *δ* 165.4, 137.2, 131.9, 131.0, 129.2, 129.1, 128.3, 126.4, 126.0, 124.6, 118.8, 114.9, 112.9, 109.5, 108.4, 51.4. HRMS ESI (m/z): calcd for $C_{16}H_{11}NNaO_2S$ $[M + H]^+$: 304.0403, found: 304.0404.

Butyl 3-phenylpyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (4a)



Yellow solid (43.8 mg, 69%); m.p. 62-64 °C. IR (KBr): 3043, 2965, 1565, 1464, 1221, 770 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$) *δ* 8.33 (d, *J* = 7.4 Hz, 1H), 8.30 (s, 1H), 8.02 (d, *J* = 7.4 Hz, 2H), 7.84 (dd, *J* = 11.0, 7.4 Hz, 2H), 7.54 -7.50 (m, 3H), 7.41 (t, *J* = 7.2 Hz, 1H), 4.46 (t, *J* = 6.6 Hz, 2H), 1.90-1.85 (m, 2H), 1.59 (dd, *J* = 15.0, 7.6 Hz, 2H), 1.05 (t, *J* = 7.4 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$) *δ* 165.2, 135.6, 134.0, 131.9, 129.8, 129.0, 128.4, 127.6, 124.3, 119.5, 114.7, 114.4, 112.9, 108.9, 64.0, 31.0, 19.4, 13.8. HRMS ESI (m/z): calcd for $C_{21}H_{20}NO_2$ $[M + H]^+$: 318.1489, found: 318.1484.

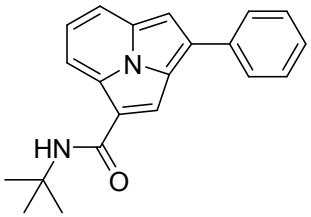
2-Hydroxyethyl 3-phenylpyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (4b)



Yellow solid (41.5 mg, 68%); m.p. 128-129 °C. IR (KBr): 3640, 1677, 1376, 1250, 1123, 1052, 786 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$) *δ* 8.29 (d, *J* = 7.4 Hz, 1H), 8.24 (s, 1H), 8.00-7.96 (m, 2H),

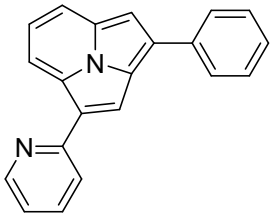
7.81 (dd, *J* = 9.8, 7.2 Hz, 2H), 7.53-7.48 (m, 3H), 7.40 (t, *J* = 7.4 Hz, 1H), 4.61-4.57 (m, 2H), 4.09-4.04 (m, 2H).^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4, 135.7, 133.9, 132.0, 129.8, 129.1, 128.5, 127.5, 124.6, 124.4, 119.6, 114.7, 113.5, 113.0, 109.2, 66.0, 61.8. HRMS ESI (m/z): calcd for $C_{19}H_{15}NNaO_3$ [M + H]$^+$: 328.0944, found: 328.0941.

_N_-(_tert_-butyl)-3-phenylpyrrolo[2,1,5-_cd_]indolizine-1-carboxamide (4c)



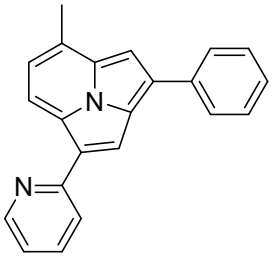
Yellow solid. (42.4 mg, 67%); m.p. 158-160 °C. IR (KBr): 3523, 3035, 2806, 1640, 1345, 790 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.42 (d, *J* = 7.8 Hz, 1H), 8.03 (d, *J* = 7.0 Hz, 2H), 7.97 (s, 1H), 7.91 (d, *J* = 7.6 Hz, 1H), 7.82 (t, *J* = 7.8 Hz, 1H), 7.55 -7.51 (m, 3H), 7.41 (t, *J* = 7.4 Hz, 1H), 1.59 (s, 9H).^{13}C NMR (100 MHz, $CDCl_3$) *δ* 164.59, 135.0, 134.4, 131.6, 129.3, 129.1, 128.3, 127.6, 123.5, 121.9, 115.3, 114.9, 113.2, 108.3, 51.6, 29.3. HRMS ESI (m/z): calcd for $C_{21}H_{21}NO_2$ [M + H]$^+$: 317.1648, found: 317.1643.

3-Phenyl-1-(pyridin-2-yl)pyrrolo[2,1,5-_cd_]indolizine (4d)



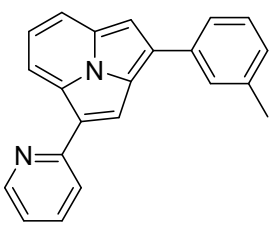
Yellow solid (38.2 mg, 65%); m.p. 124-126 °C. IR (KBr): 3048, 2965, 1571, 1482, 1175, 901 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, *J* = 4.8 Hz, 1H), 8.61 (d, *J* = 7.8 Hz, 1H), 8.33 (s, 1H), 8.10 (d, *J* = 7.6 Hz, 2H), 7.93 (t, *J* = 8.2 Hz, 2H), 7.81 (d, *J* = 7.8 Hz, 1H), 7.78-7.74 (m, 1H), 7.55 (d, *J* = 7.6 Hz, 2H), 7.52 (d, *J* = 2.8 Hz, 1H), 7.40 (t, *J* = 7.4 Hz, 1H), 7.16 (dd, *J* = 7.2, 5.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.7, 149.0, 137.1, 134.7, 134.1, 131.5, 129.0, 128.6, 128.0, 127.6, 124.9, 122.9, 120.6, 120.5, 115.2, 115.1, 113.2, 107.1. HRMS ESI (m/z): calcd for $C_{21}H_{15}N_2$ [M + H]$^+$: 295.1230, found: 295.1225.

5-Methyl-3-phenyl-1-(pyridin-2-yl)pyrrolo[2,1,5-_cd_]indolizine (4e)



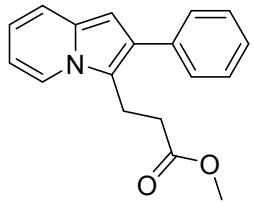
Yellow solid (42.5 mg, 69%); m.p. 126-128 °C. IR (KBr): 3055, 2972, 1551, 1392, 1165, 877 cm^{-1}.^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.72 (d, *J* = 4.8 Hz, 1H), 8.46 (d, *J* = 8.0 Hz, 1H), 8.23 (s, 1H), 8.09 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.74 (td, *J* = 7.8, 1.8 Hz, 1H), 7.57-7.50 (m, 4H), 7.38 (t, *J* = 7.4 Hz, 1H), 7.15-7.12 (m, 1H), 2.88 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.2, 149.6, 136.5, 135.1, 132.5, 130.9, 129.0, 127.7, 127.5, 127.3, 124.9, 124.8, 124.3, 124.1, 120.4, 120.3, 115.2, 114.2, 105.4, 17.3. HRMS ESI (m/z): calcd for $C_{22}H_{16}N_2$ [M + H]$^+$: 309.1386, found: 309.1391.

1-(Pyridin-2-yl)-3-(*m*-tolyl)pyrrolo[2,1,5-_cd_]indolizine (4f)



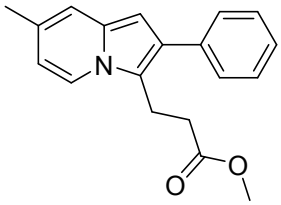
Yellow solid (40.7 mg, 66%); m.p. 126-128 °C. IR (KBr): 3054, 2922, 1541, 1332, 1185, 779 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.74 (d, *J* = 4.8 Hz, 1H), 8.58 (d, *J* = 7.8 Hz, 1H), 8.36 (s, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.91 (d, *J* = 7.4 Hz, 3H), 7.81-7.75 (m, 2H), 7.51 (s, 1H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.22 (d, *J* = 7.6 Hz, 1H), 7.18-7.14 (m, 1H), 2.51 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.0, 149.4, 138.7, 136.8, 134.7, 134.2, 131.5, 129.0, 128.9, 128.6, 128.3, 124.8, 122.7, 120.5, 120.5, 115.1, 115.1, 113.1, 107.0, 21.61. HRMS ESI (m/z): calcd for $C_{22}H_{16}N_2$ [M + H]$^+$: 309.1386, found: 309.1391.

Methyl 3-(2-Phenylindolizin-3-yl)propanoate (5a)



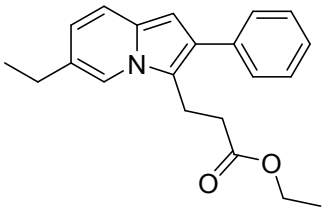
Yellow oil. (42.4 mg, 76%); IR (KBr): 3050, 1678, 1507, 1450, 1332, 759 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 4.6 Hz, 1H), 7.65 (t, *J* = 7.6 Hz, 1H), 7.51 (d, *J* = 6.8 Hz, 2H), 7.41-7.34 (m, 3H), 7.28 (d, *J* = 7.8 Hz, 1H), 7.13-7.08 (m, 1H), 6.81 (s, 1H), 3.67 (s, 3H), 3.03 (t, *J* = 7.2 Hz, 2H), 2.82 (t, *J* = 7.0 Hz, 2H).^{13}C NMR (100 MHz, $CDCl_3$) δ 173.5, 153.2, 148.7, 136.8, 135.1, 129.3, 128.8, 126.3, 125.1, 124.0, 122.0, 51.6, 38.2, 28.2. HRMS ESI (m/z): calcd for $C_{18}H_{17}NO_2$ $[M + H]^+$: 279.1254, found: 279.1254.

Methyl 3-(7-Methyl-2-phenylindolizin-3-yl)propanoate (5b)



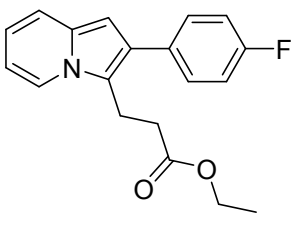
Yellow oil (45.7 mg, 78%); IR (KBr): 3047, 1699, 1550, 1402, 1327, 780 cm^{-1}.^1H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 4.8 Hz, 1H), 7.51 (d, *J* = 7.4 Hz, 2H), 7.38 (s, 1H), 7.37-7.32 (m, 2H), 7.11 (s, 1H), 6.94 (d, *J* = 4.8 Hz, 1H), 6.78 (s, 1H), 3.67 (s, 3H), 3.00 (d, *J* = 7.0 Hz, 2H), 2.80 (t, *J* = 7.2 Hz, 2H), 2.33 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 173.5, 153.1, 148.6, 147.8, 146.0, 135.4, 128.8, 128.7, 126.3, 125.4, 124.9, 122.9, 51.6, 38.4, 28.3, 20.9. HRMS ESI (m/z): calcd for $C_{19}H_{19}NO_2$ $[M + H]^+$:293.1413, found: 293.1413.

Ethyl 3-(6-Ethyl-2-phenylindolizin-3-yl)propanoate (5c)



Yellow oil (44.3 mg, 69%); IR (KBr): 3055, 1683, 1563, 1455, 1347, 792 cm^{-1}.^1H NMR (400 MHz, $CDCl_3$) δ 8.39 (s, 1H), 7.51 (dd, *J* = 6.8, 1.5 Hz, 2H), 7.47 (d, *J* = 5.8 Hz, 1H), 7.38 (s, 1H), 7.37-.32 (m, 2H), 7.20 (d, *J* = 7.8 Hz, 1H), 6.80 (d, *J* = 2.8 Hz, 1H), 4.13 (q, *J* = 7.2 Hz, 2H), 3.03 (t, *J* = 7.2 Hz, 2H), 2.80 (t, *J* = 7.0 Hz, 2H), 2.62 (d, *J* = 7.6 Hz, 2H), 1.24 (dd, *J* = 7.2, 3.0 Hz, 6H).^{13}C NMR (100 MHz, $CDCl_3$) δ 173.2, 151.0, 148.8, 145.3, 137.9, 136.0, 135.5, 128.8, 128.7, 126.3, 125.23, 123.8, 60.5, 38.5, 28.7, 25.9, 15.2, 14.2. HRMS ESI (m/z): calcd for $C_{21}H_{23}NO_2$ $[M + H]^+$:321.1723, found: 321.1723.

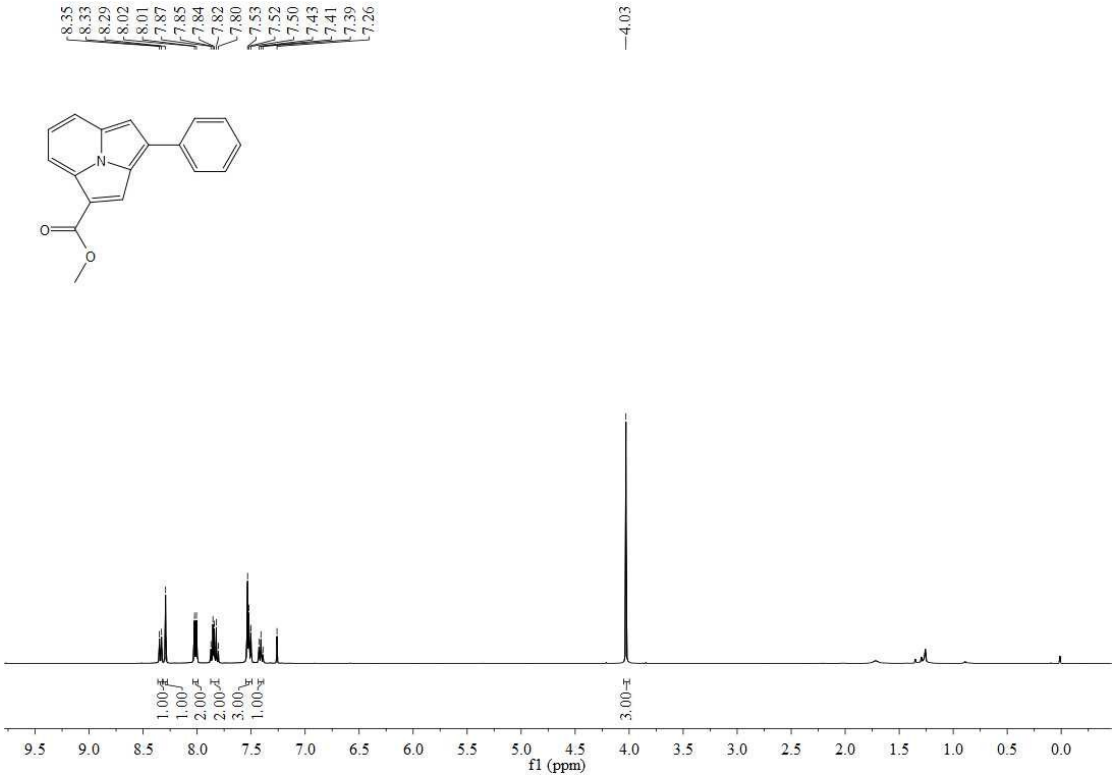
Ethyl 3-(2-(4-Fluorophenyl)indolizin-3-yl)propanoate (5d)

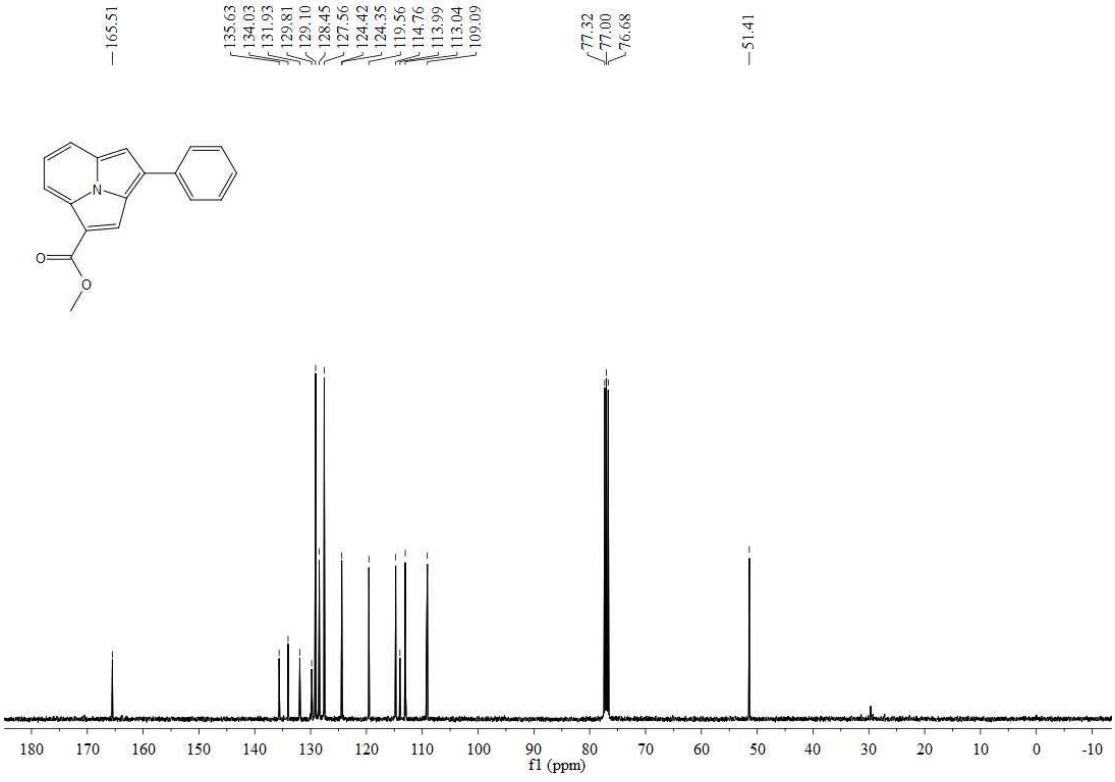


Yellow oil (44.8 mg, 72%); IR (KBr): 3077, 1674, 1532, 1449, 1322, 756 cm^{-1}.^1H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, *J* = 3.6 Hz, 1H), 7.67 (t, *J* = 7.8 Hz, 1H), 7.56 - 7.47 (m, 2H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.14 (dd, *J* = 7.0, 5.2 Hz, 1H), 7.08 (t, *J* = 8.8 Hz, 2H), 6.76 (s, 1H), 4.13 (q, *J* = 7.2 Hz, 2H), 3.00 (t, *J* = 7.0 Hz, 2H), 2.76 (t, *J* = 6.8 Hz, 2H), 1.26 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.0, 164.4 (*J* = 248.0 Hz,), 153.2, 148.70, 137.0, 131.3, 128.3 (*J* = 9.0 Hz,), 124.9, 123.9, 122.1, 115.9(*J* = 22.0 Hz,), 60.52, 38.19, 28.47, 14.16. HRMS ESI (m/z): calcd for $C_{19}H_{18}FNO_2$ $[M + H]^+$:311.1316, found: 311.1316.

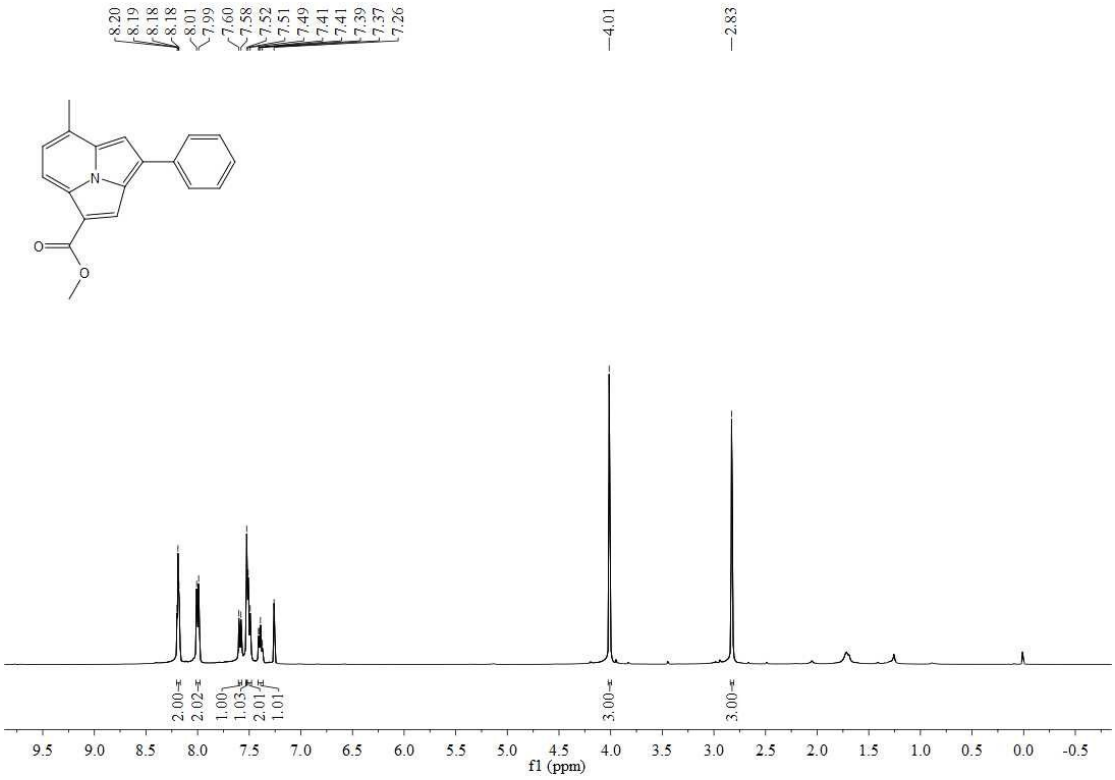
E. NMR Spectra

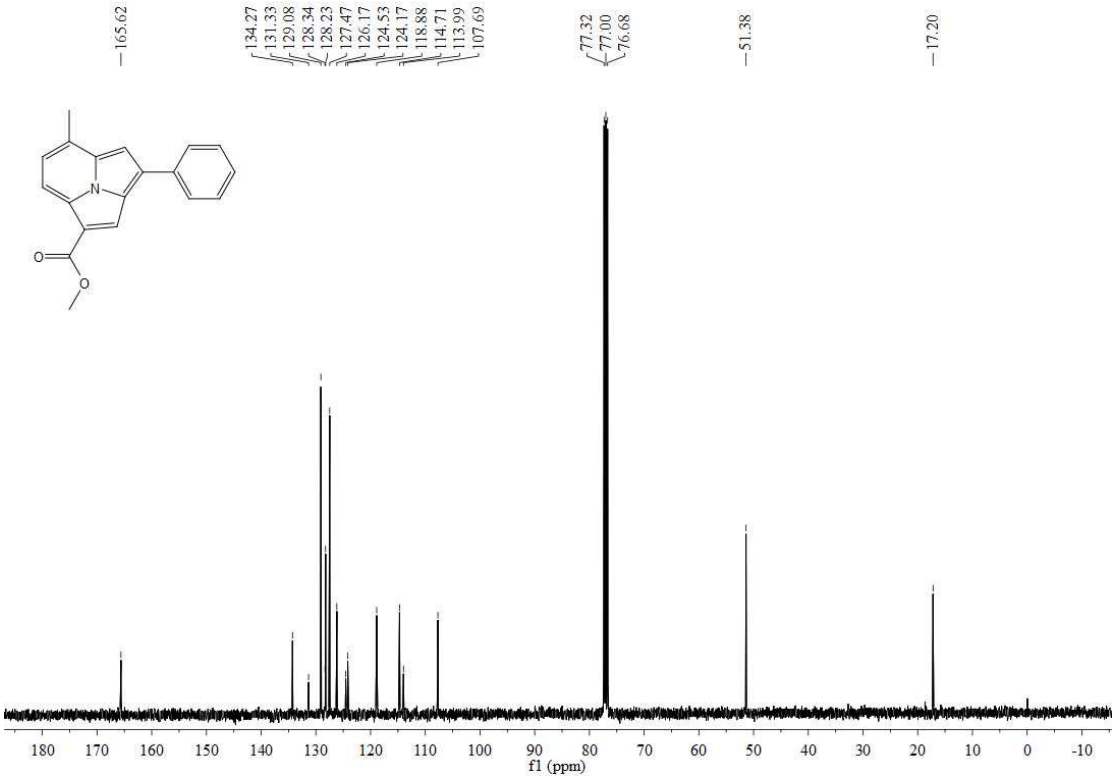
Methyl 3-phenylpyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3a)



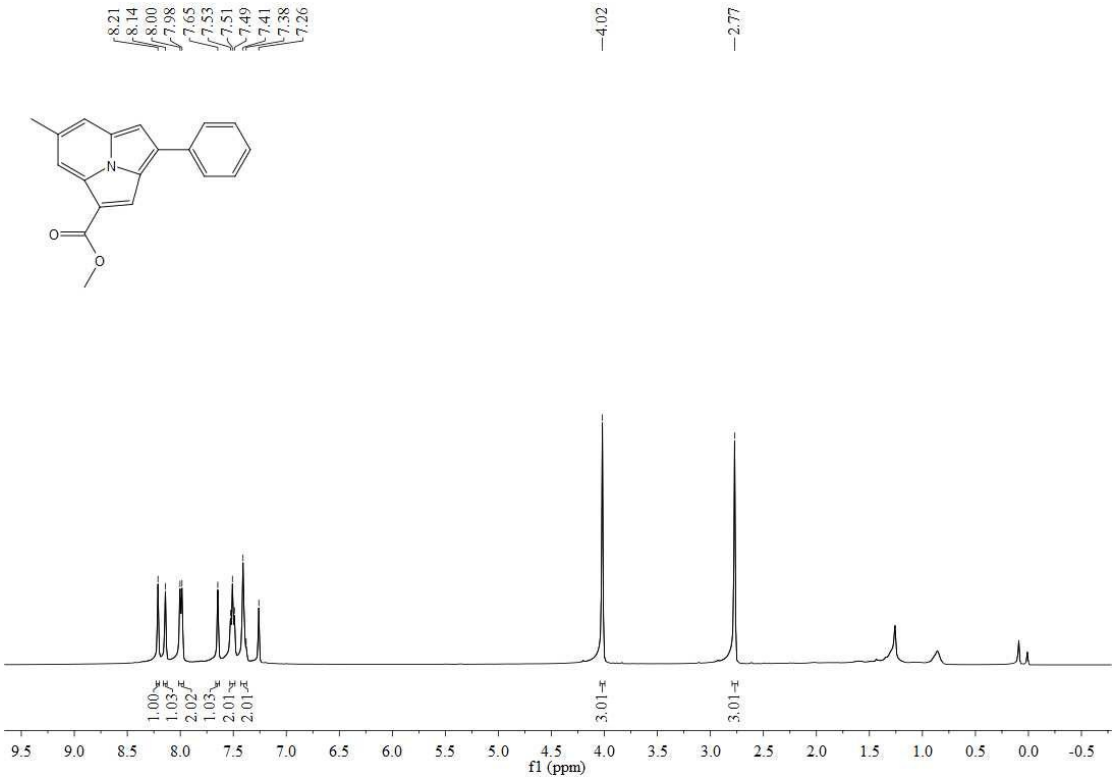


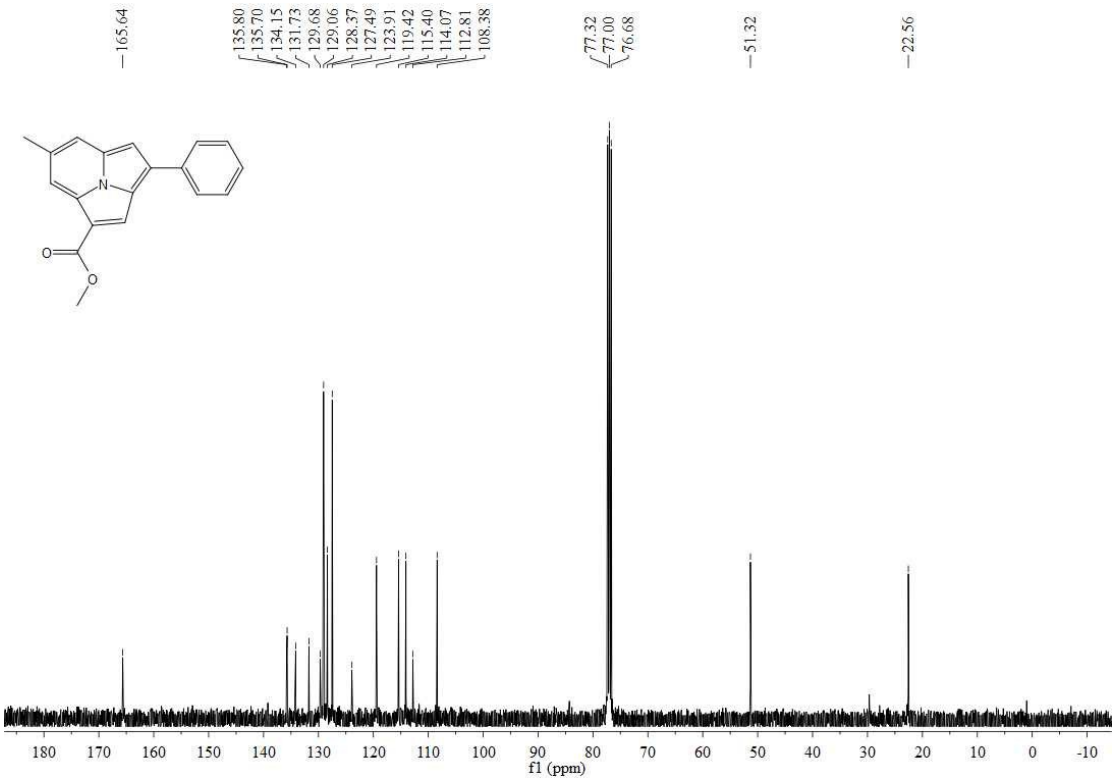
Methyl 5-methyl-3-phenylpyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3b)



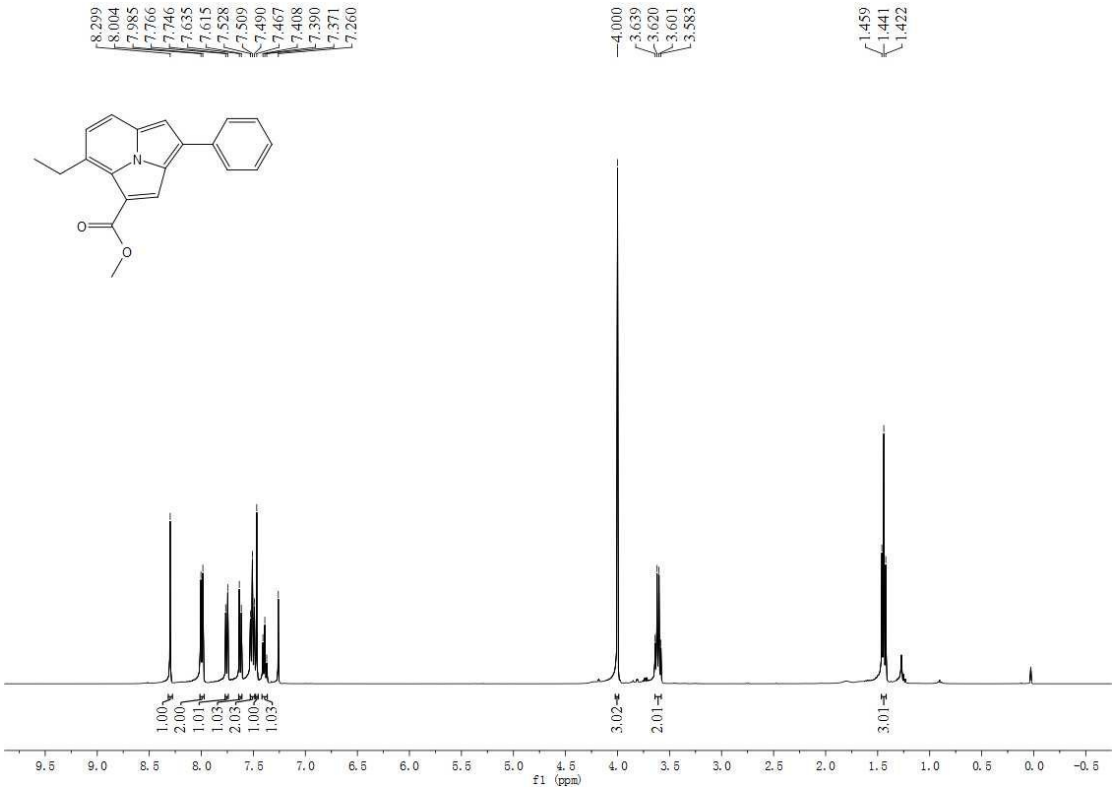


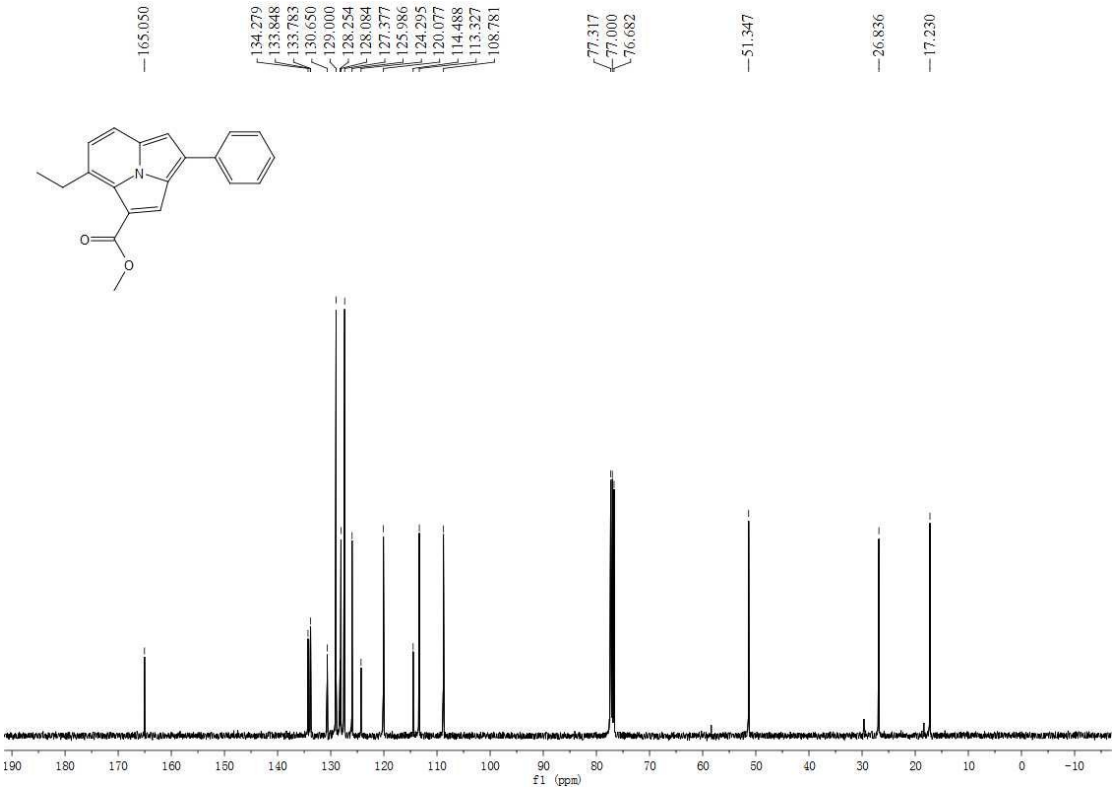
Methyl 6-methyl-3-phenylpyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3c)



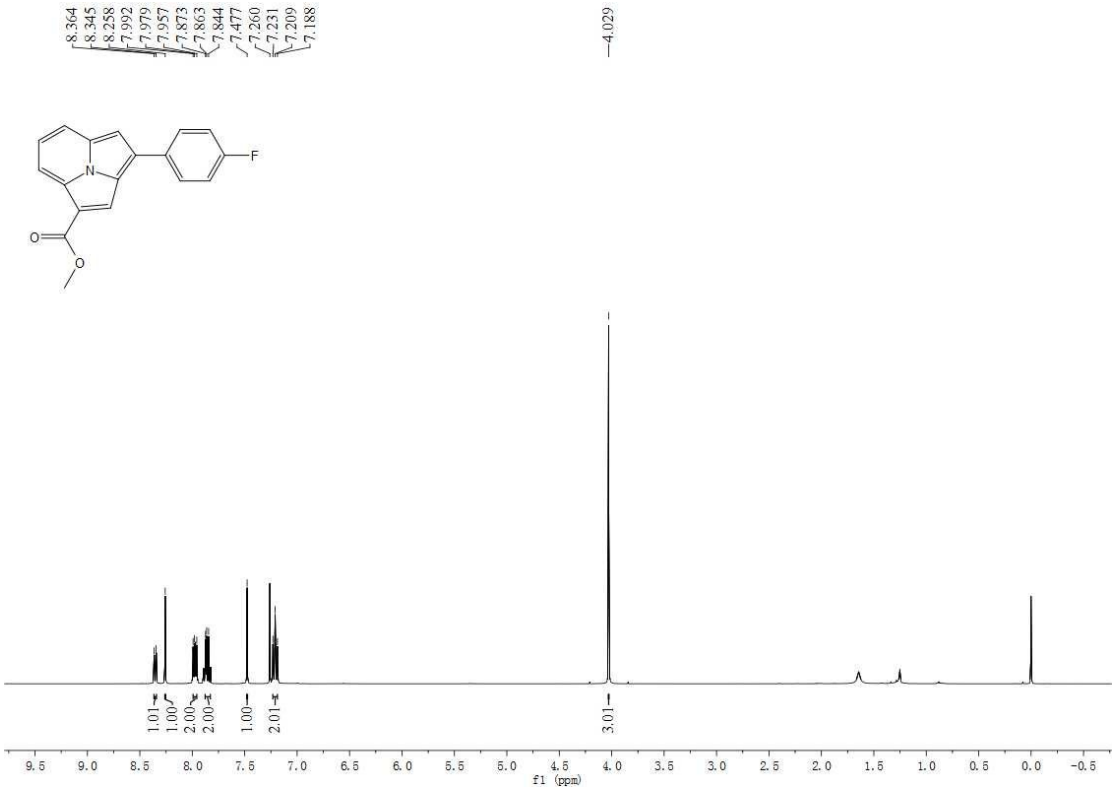


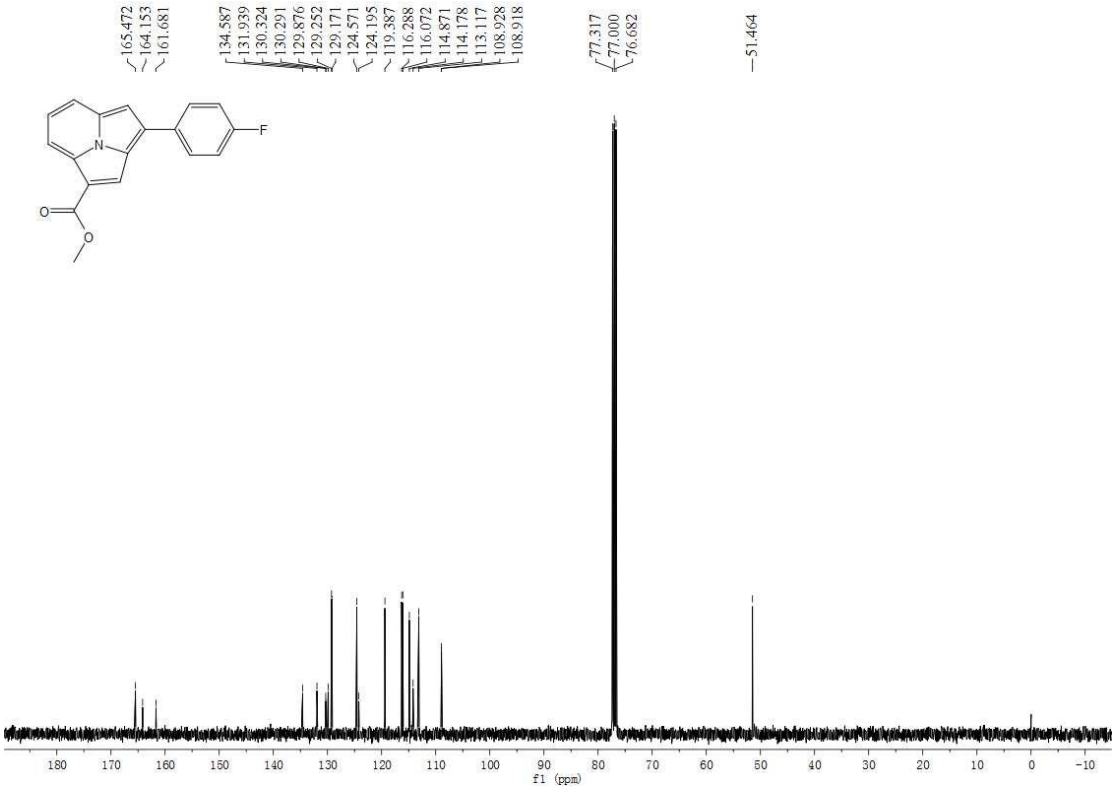
Methyl 7-ethyl-3-phenylpyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3d)



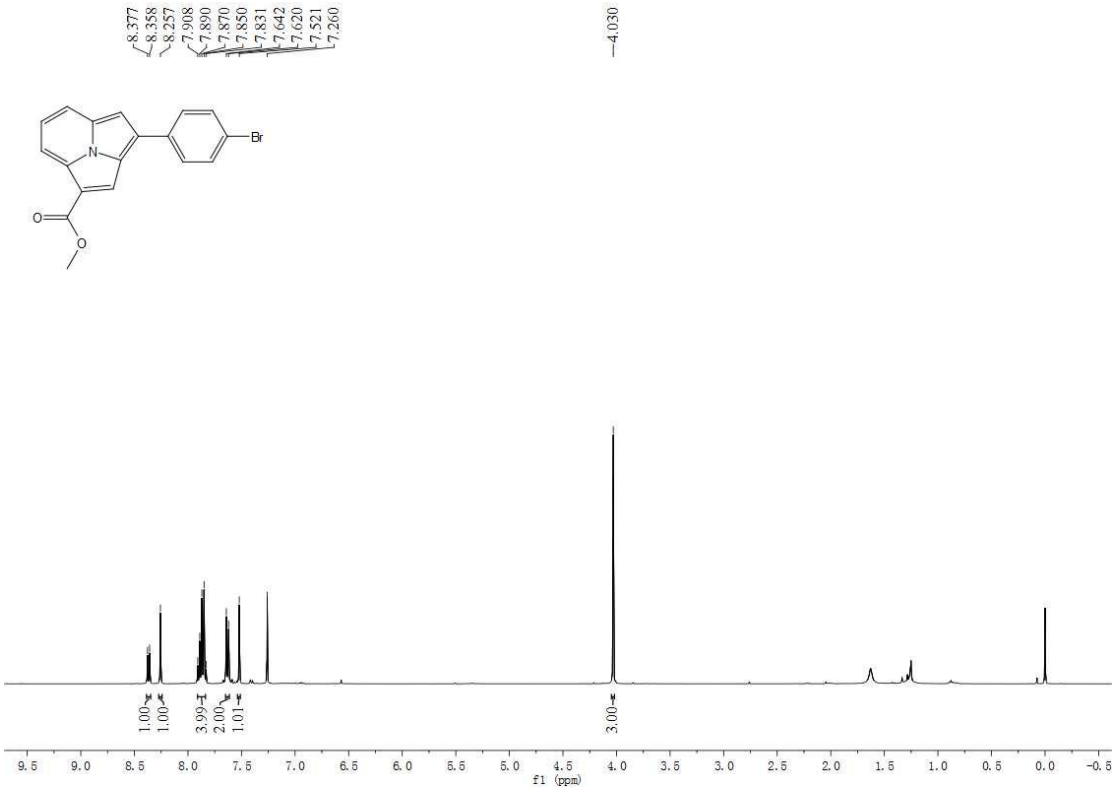


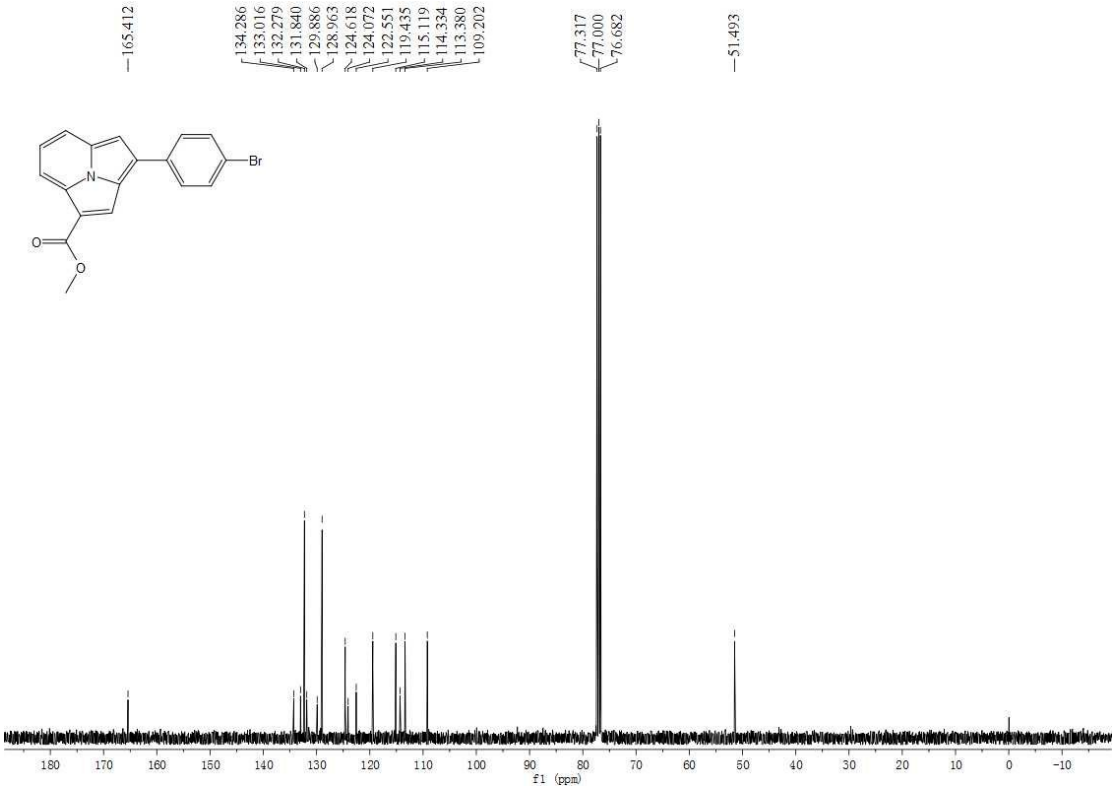
Methyl 3-(4-fluorophenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3e)



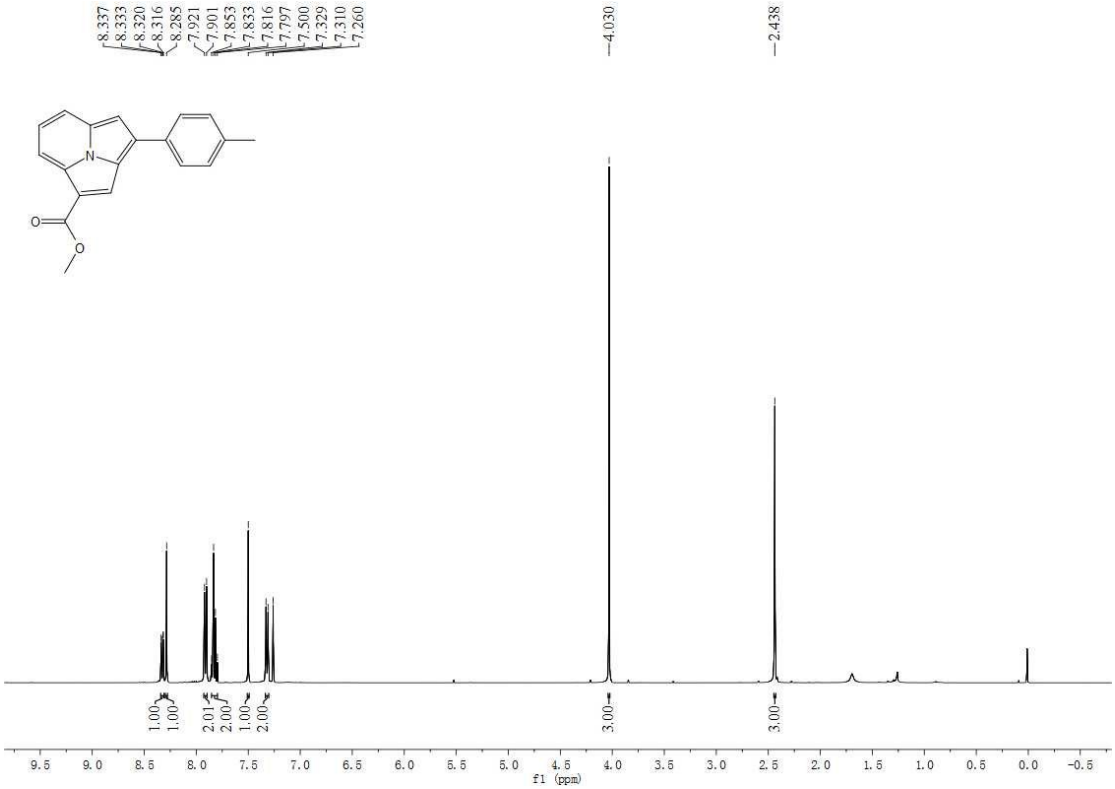


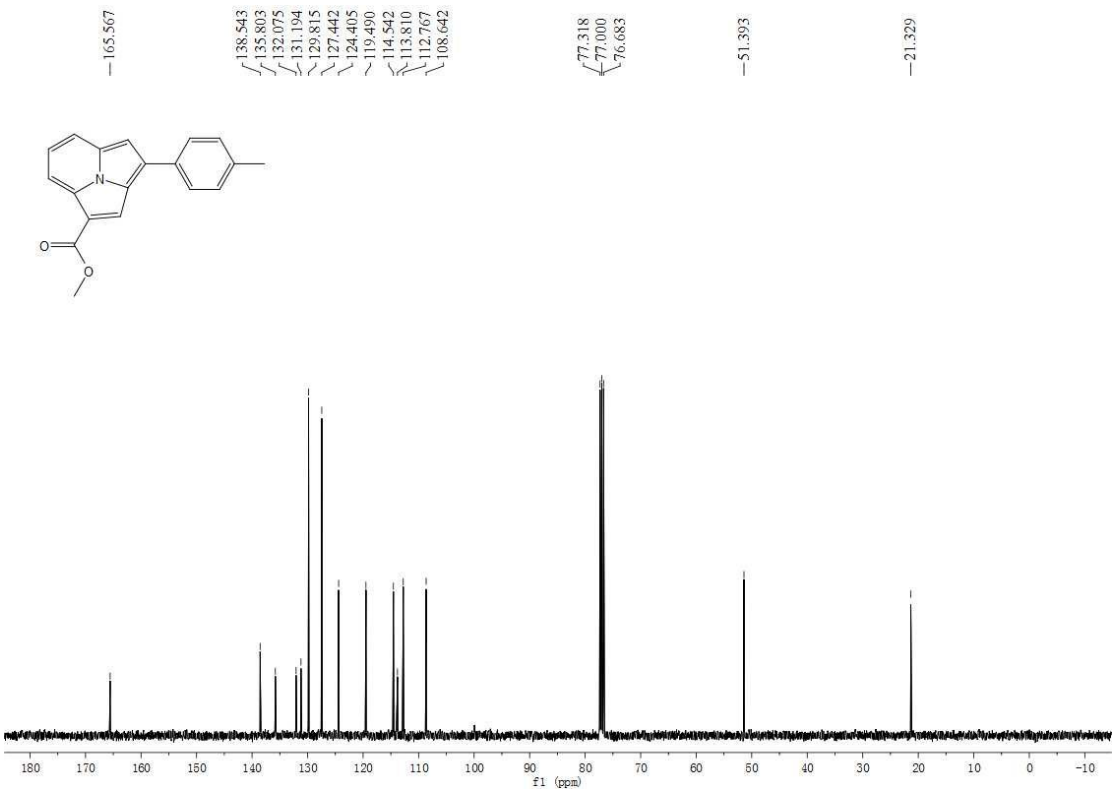
Methyl 3-(4-bromophenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3f)



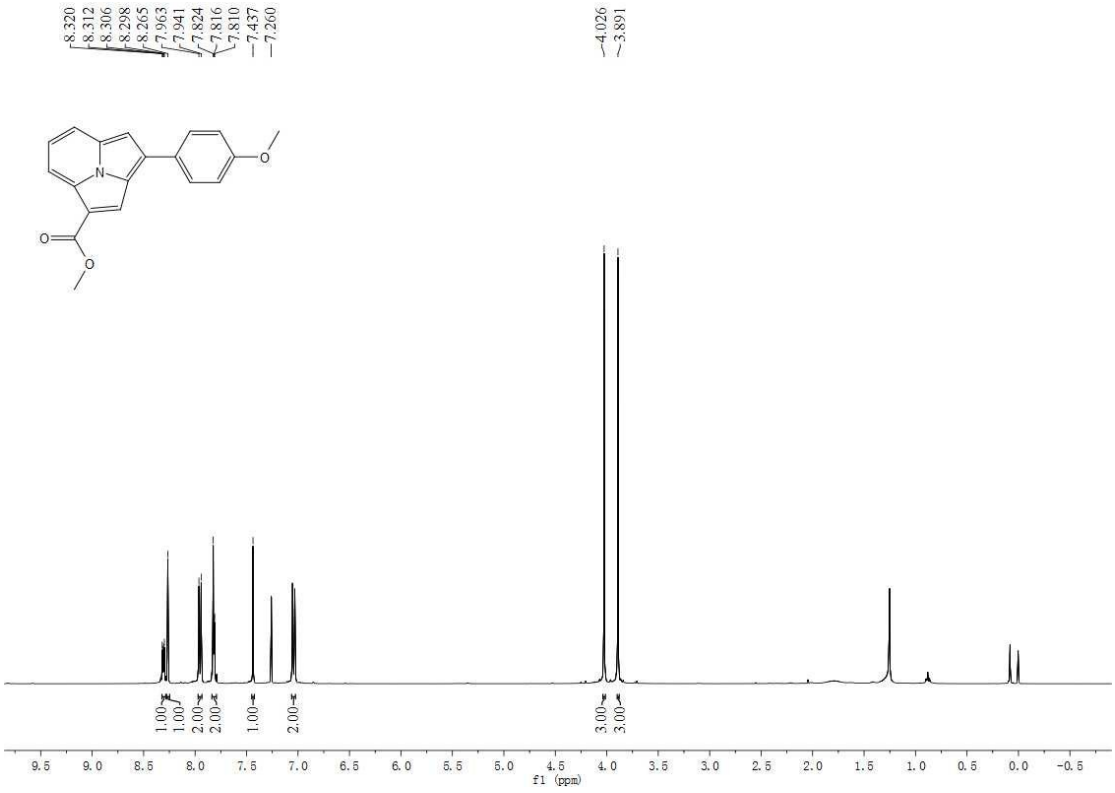


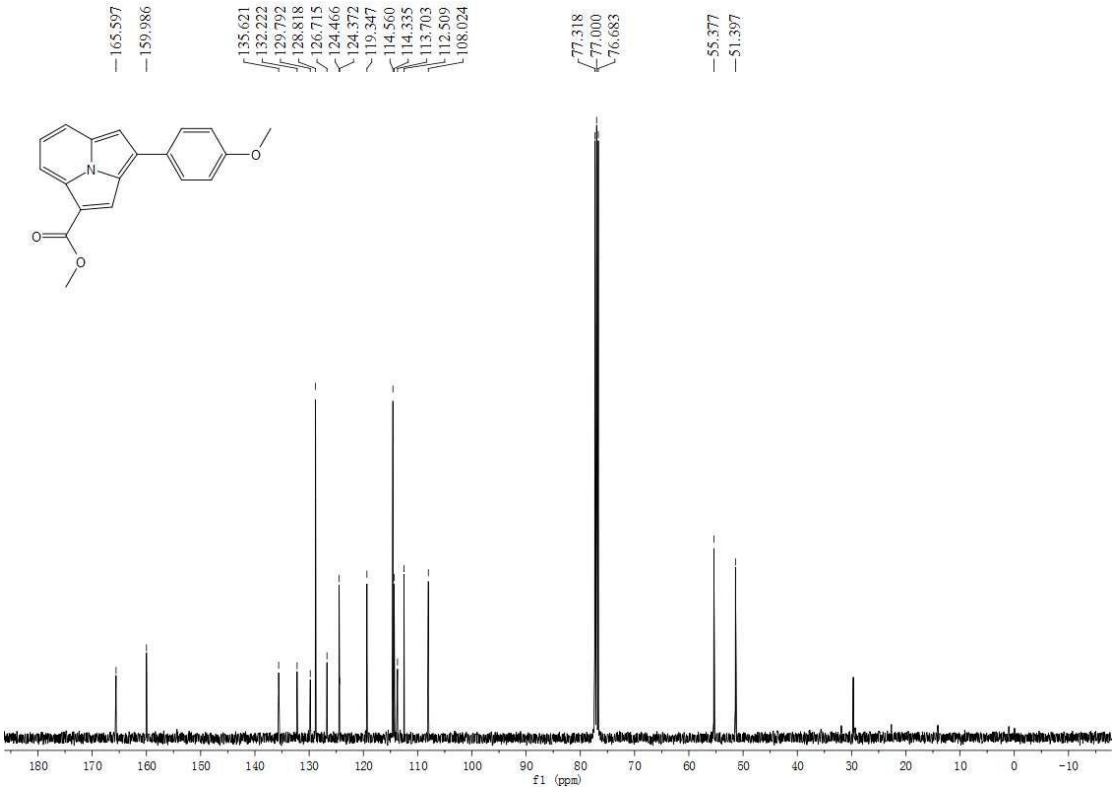
Methyl 3-(*p*-tolyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3g)



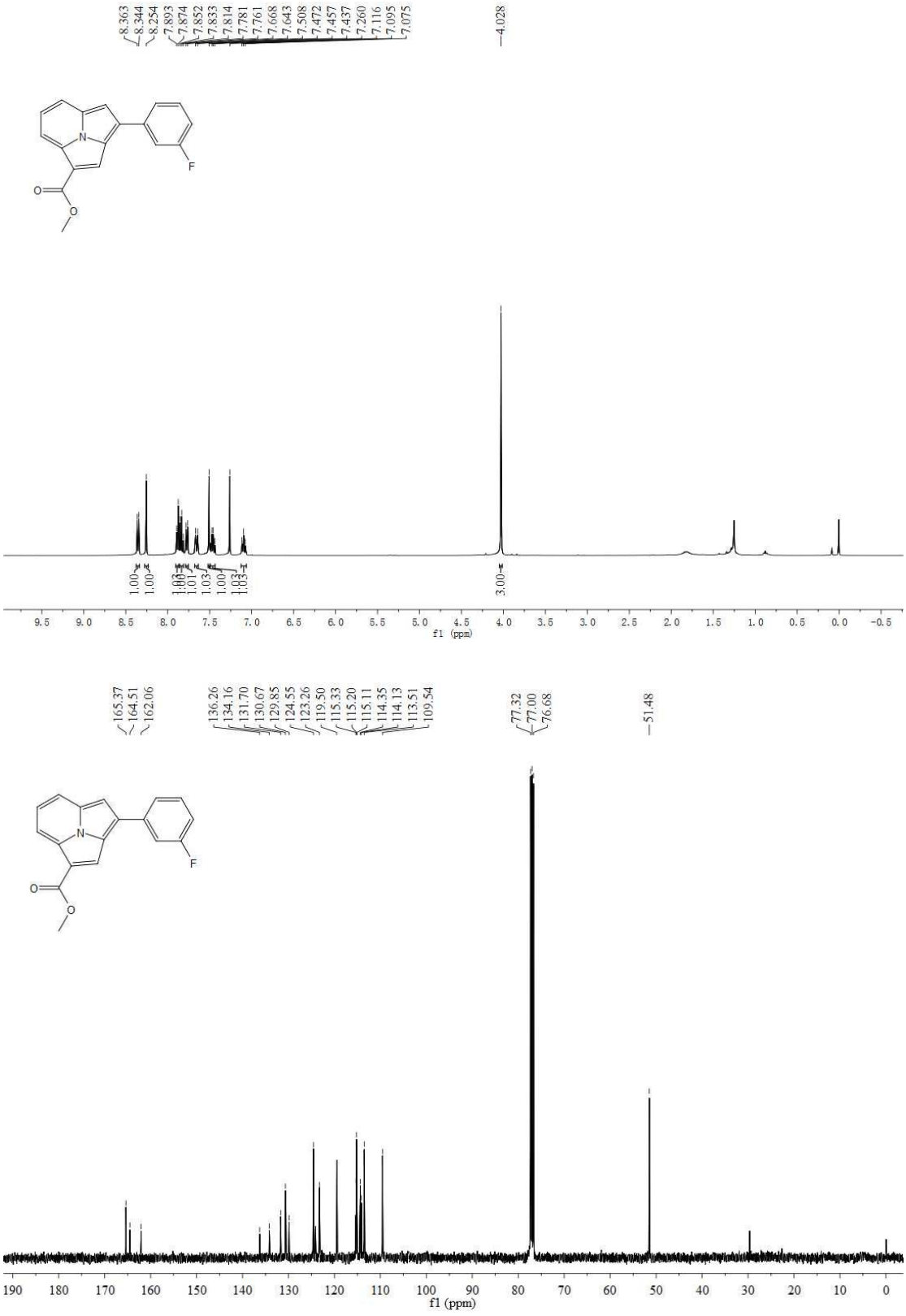


Methyl 3-(4-methoxyphenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3h)

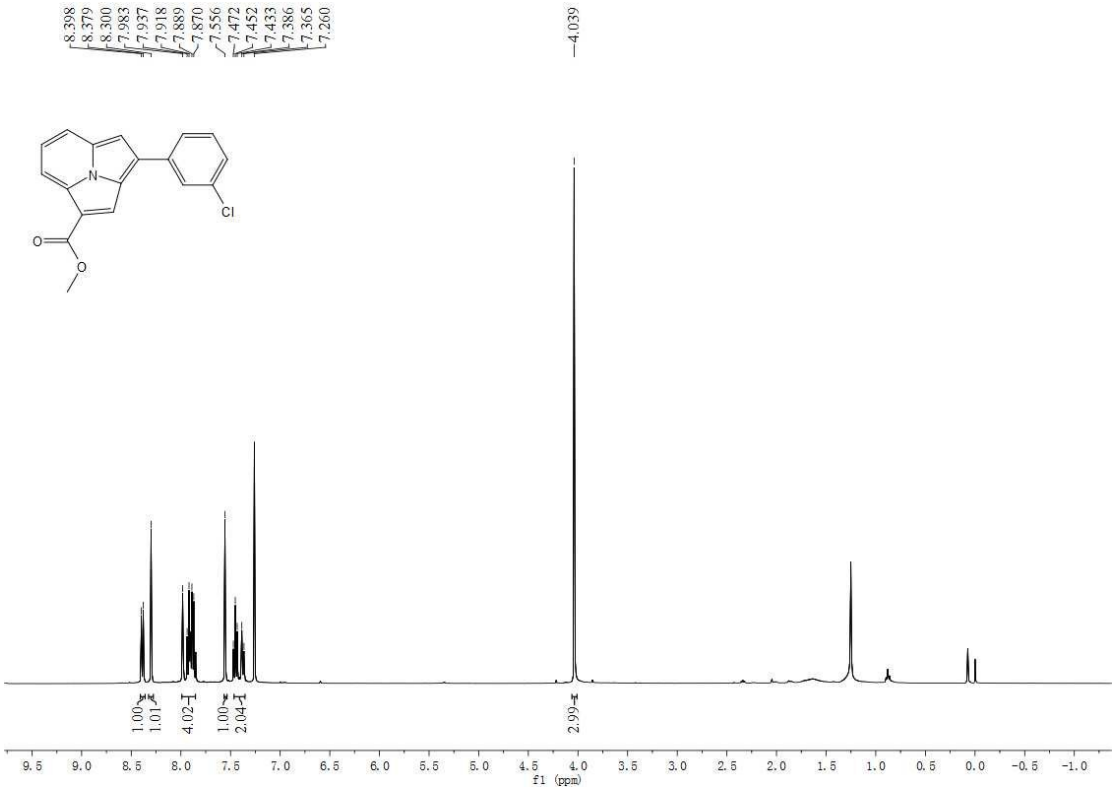


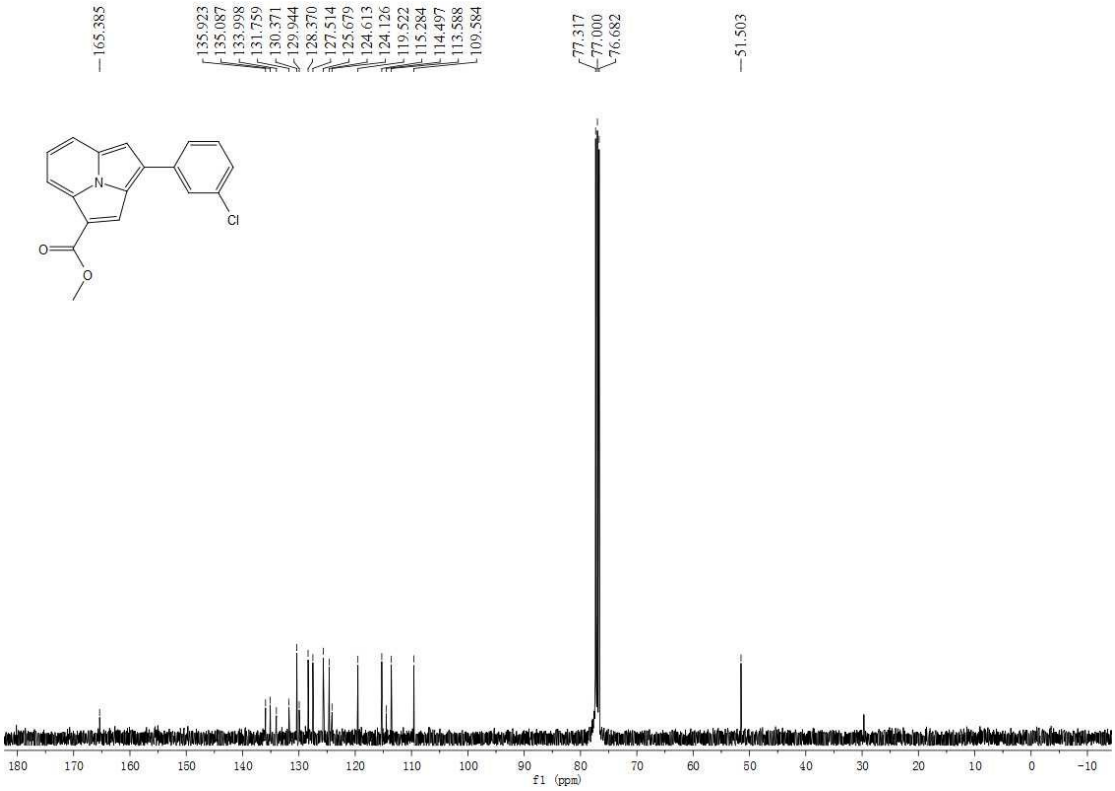


Methyl 3-(3-fluorophenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3i)

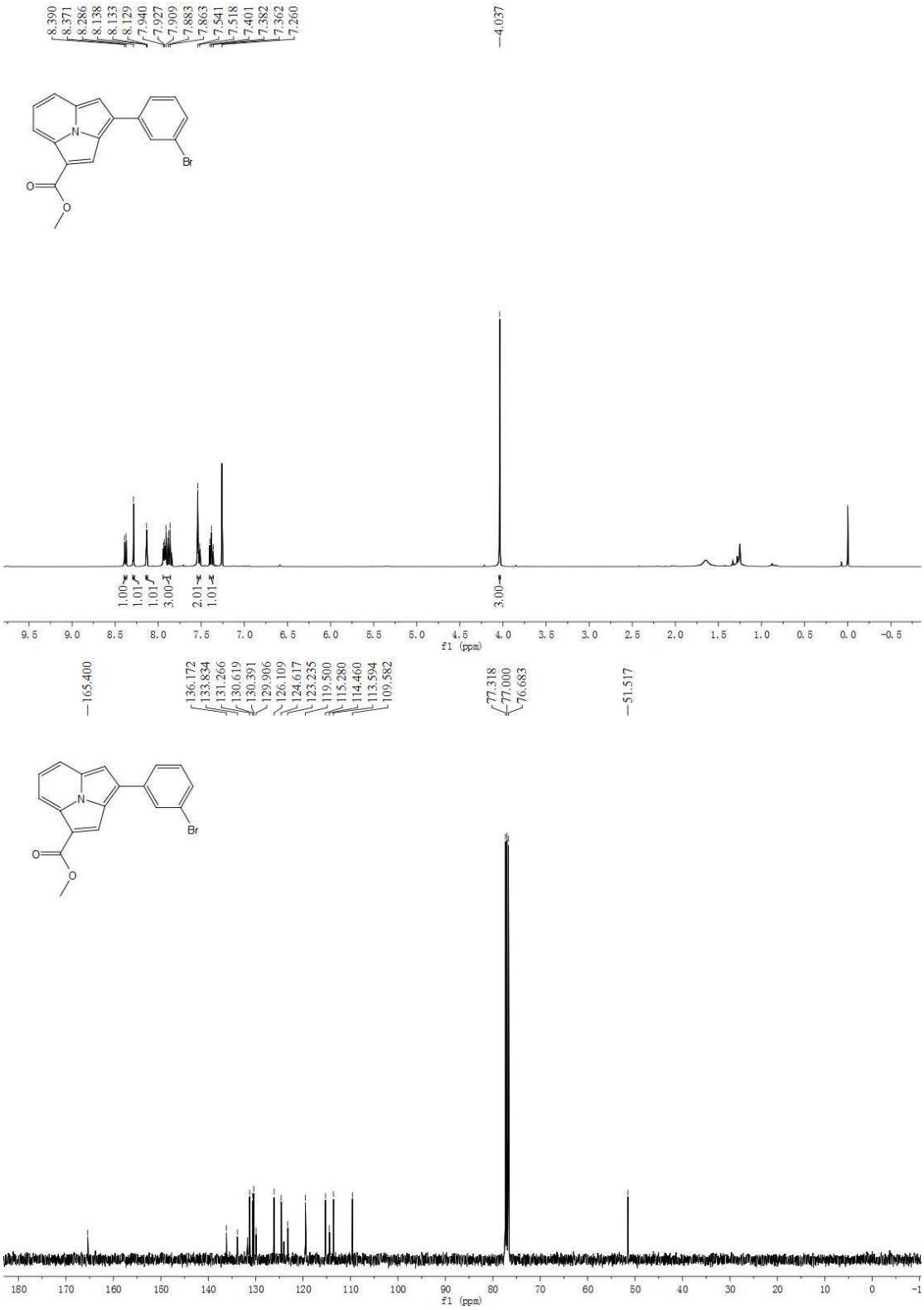


Methyl 3-(3-chlorophenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3j)

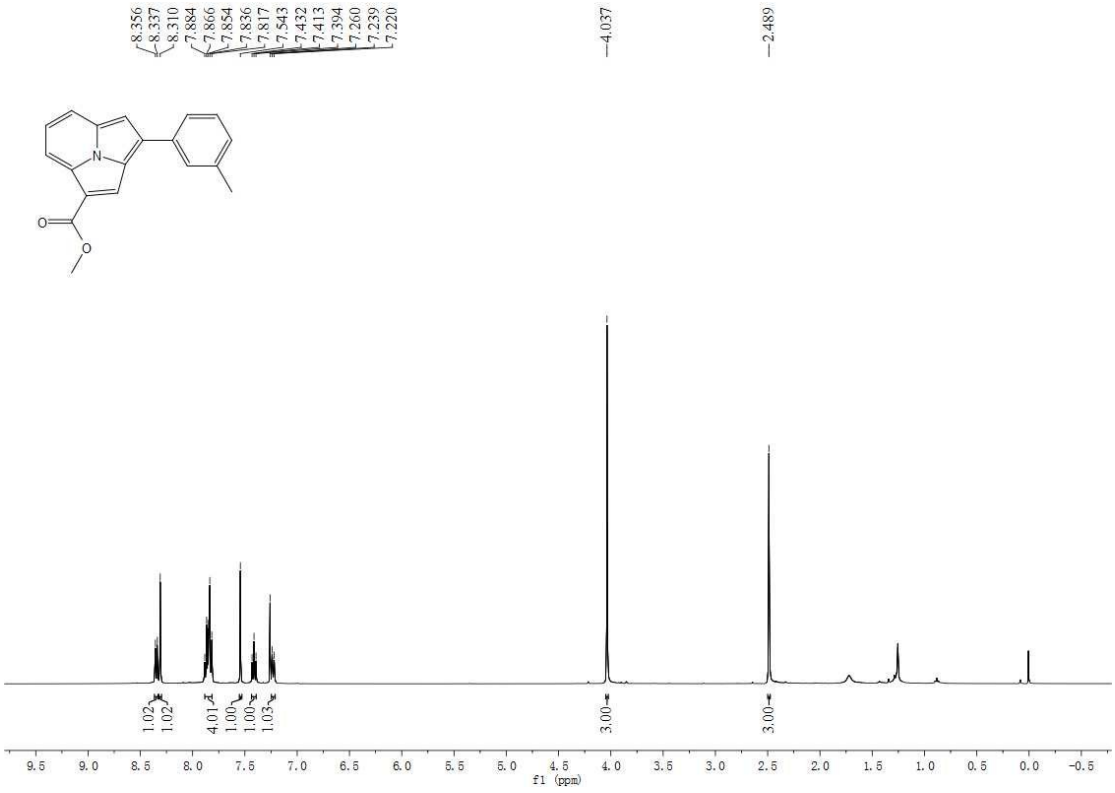


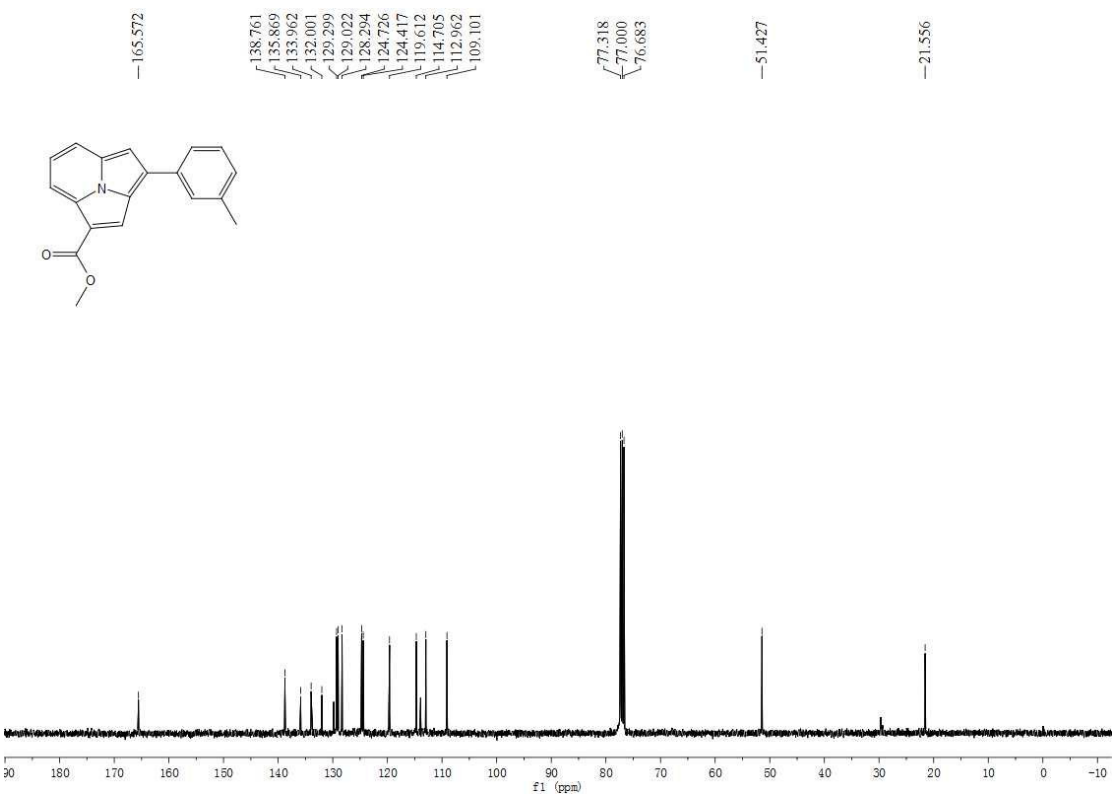


Methyl 3-(3-bromophenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3k)

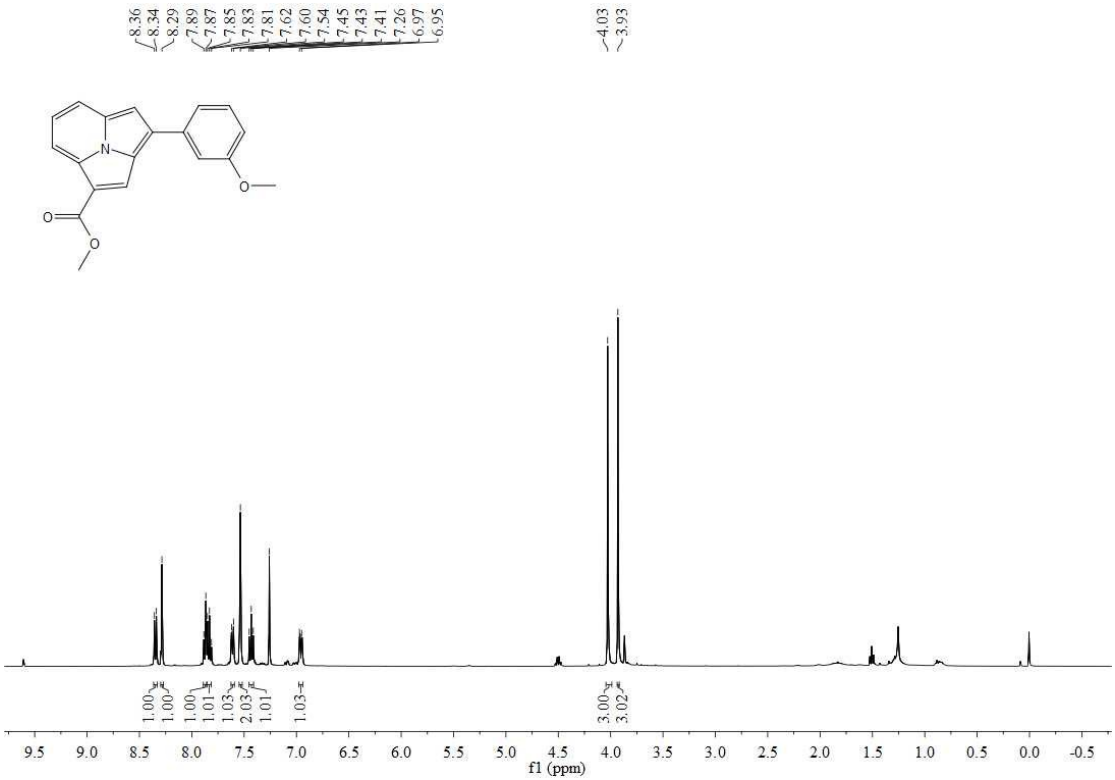


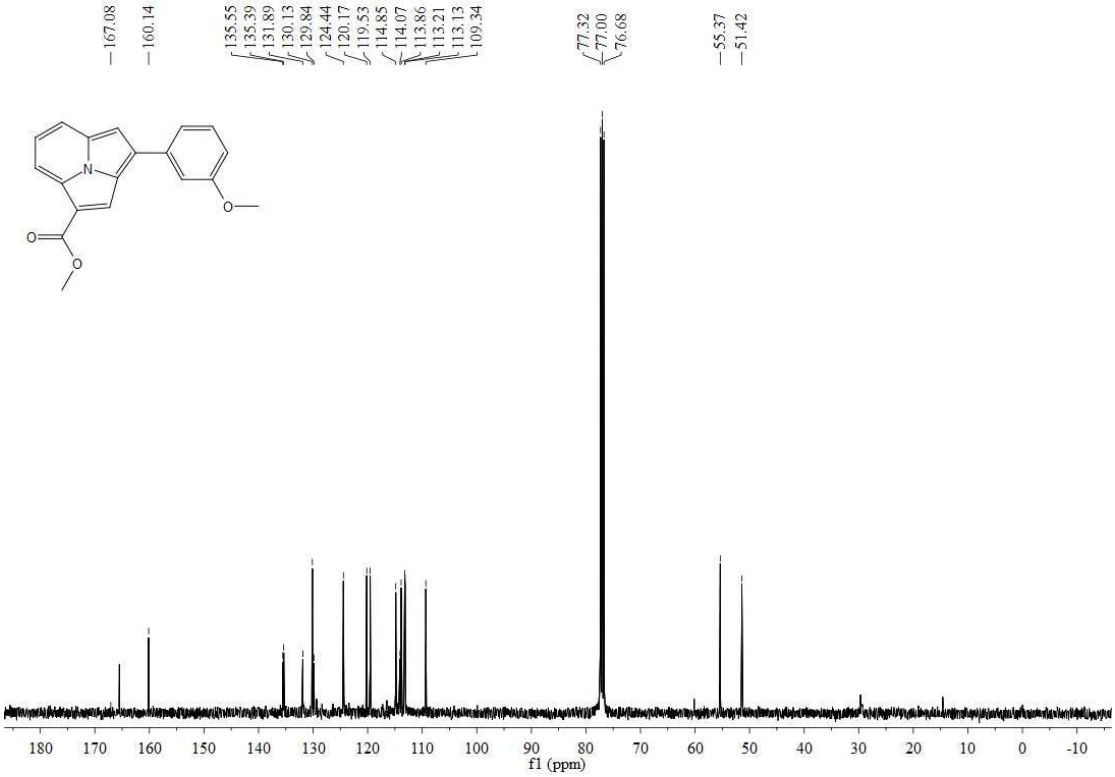
Methyl 3-(*m*-tolyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3l)



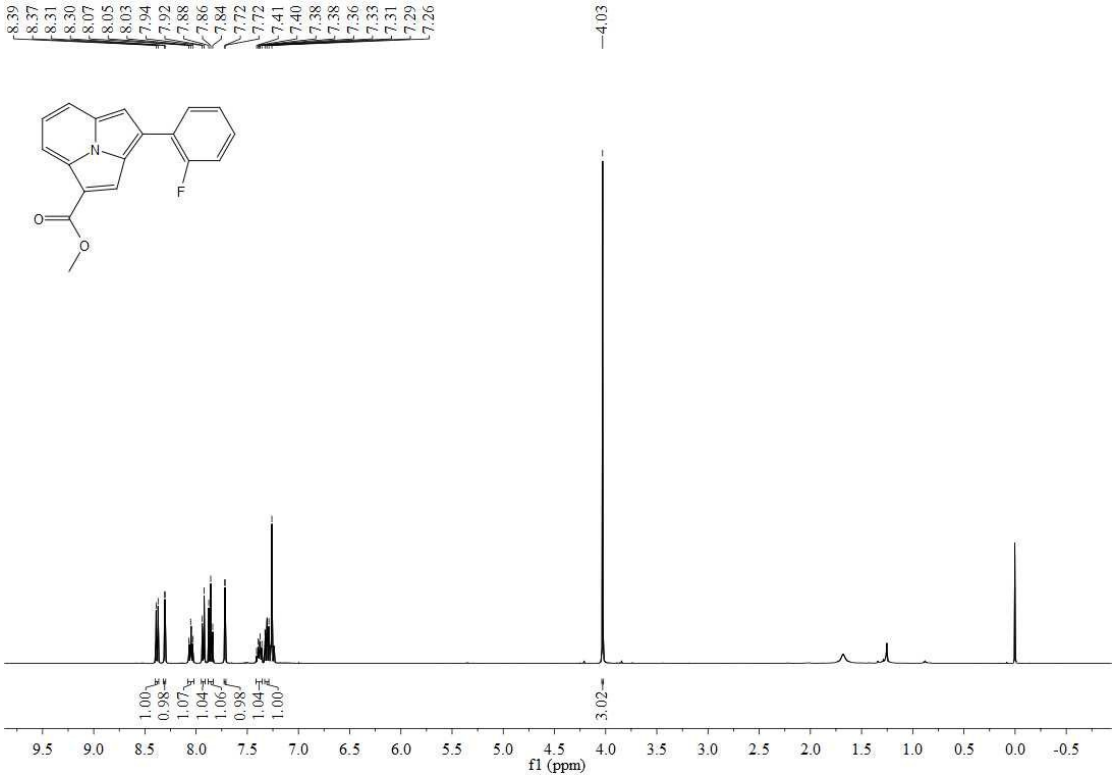


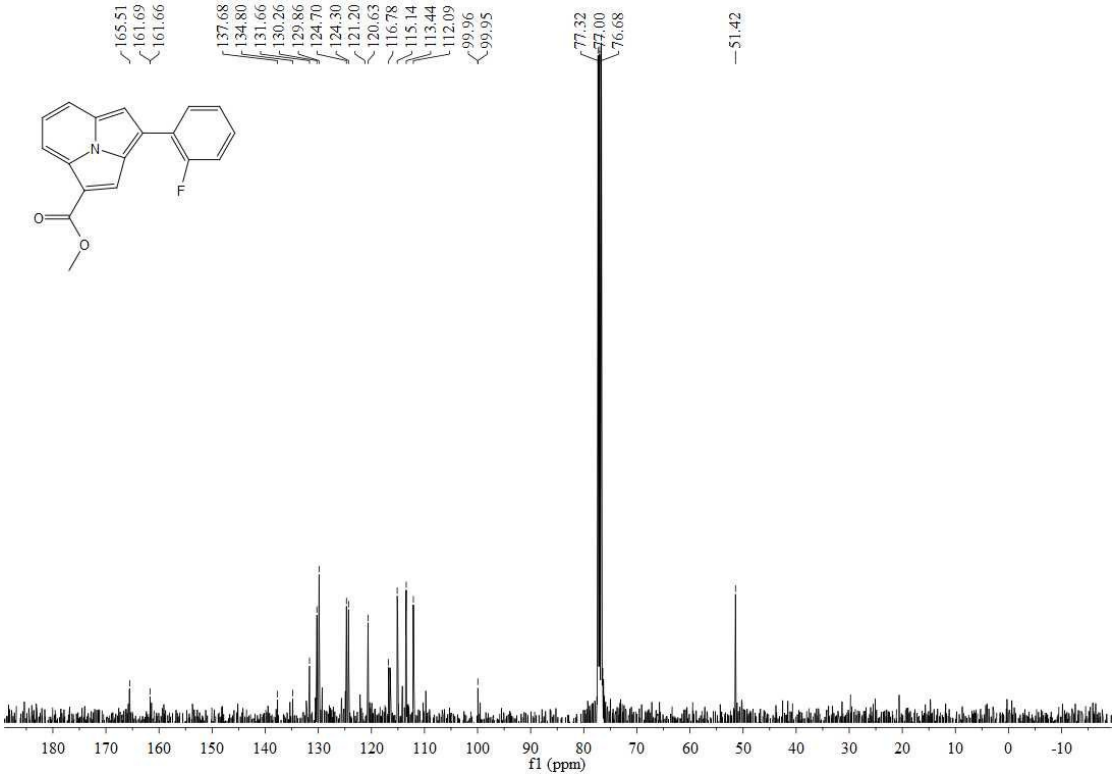
Methyl 3-(3-methoxyphenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3m)



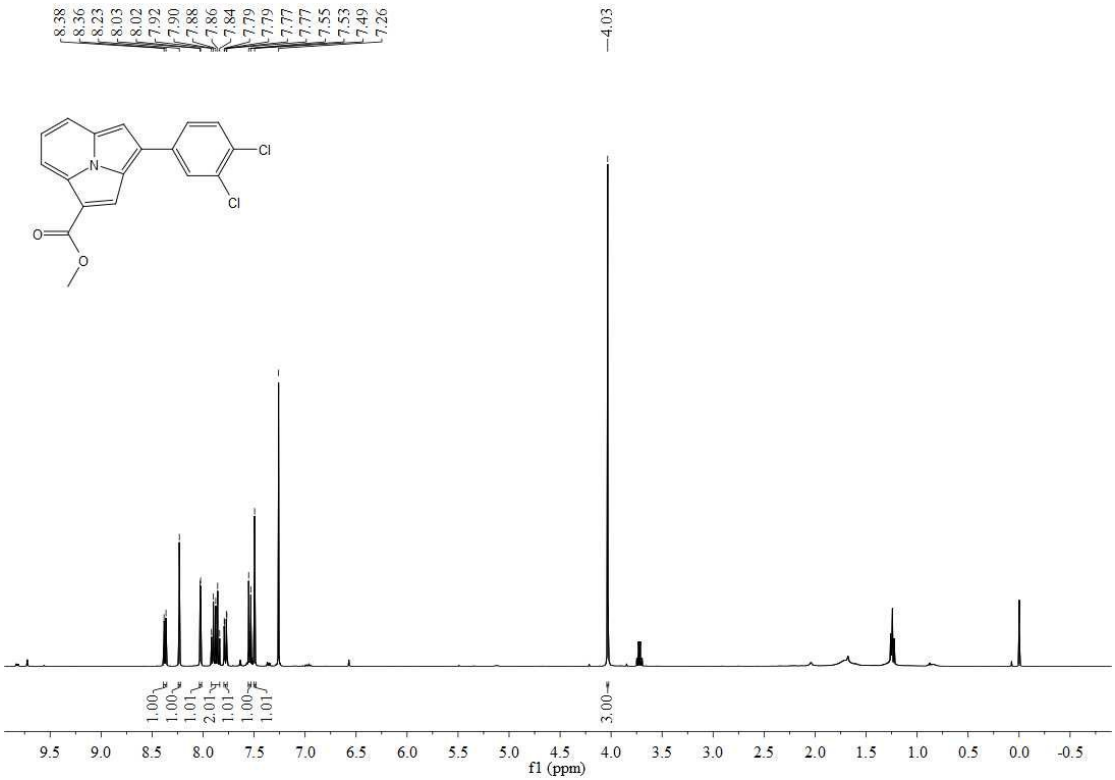


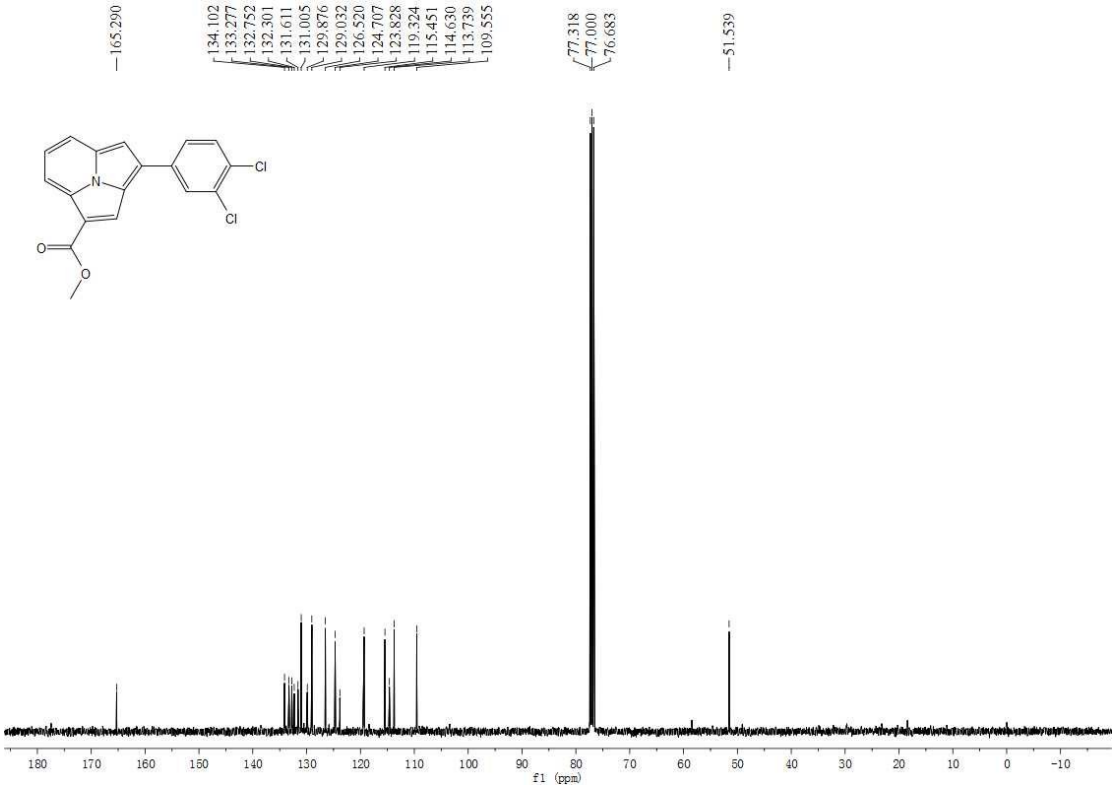
Methyl 3-(2-fluorophenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3n)



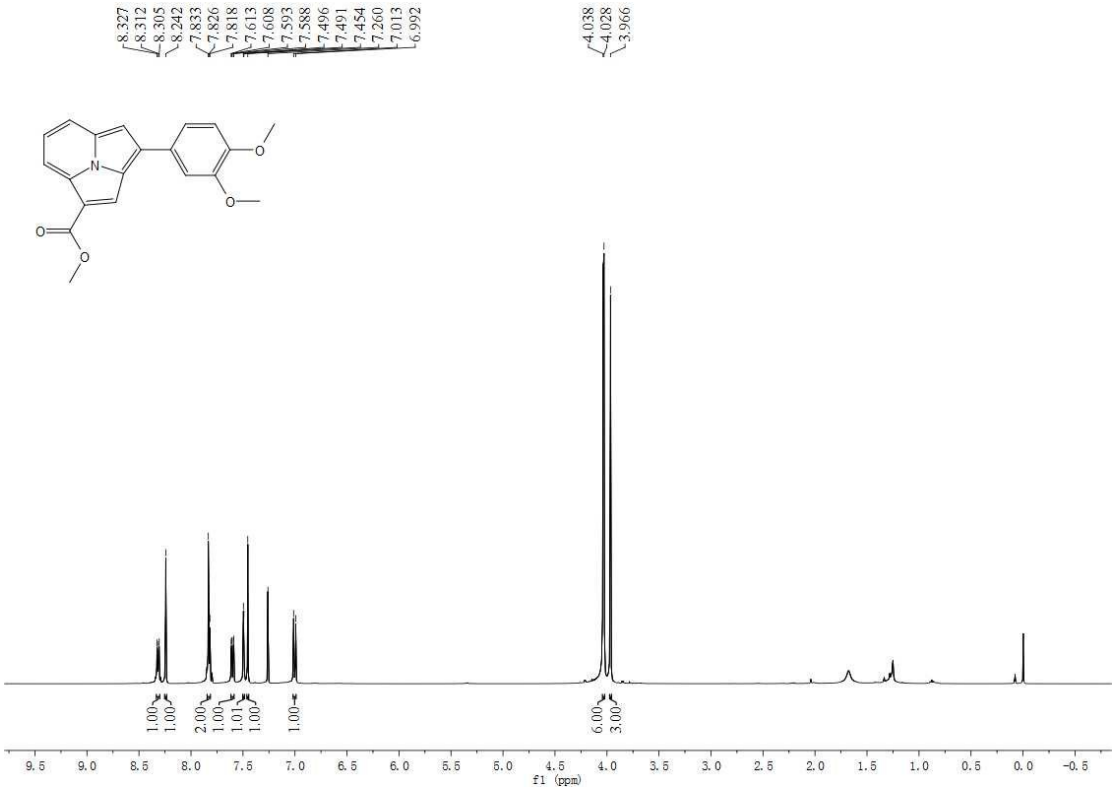


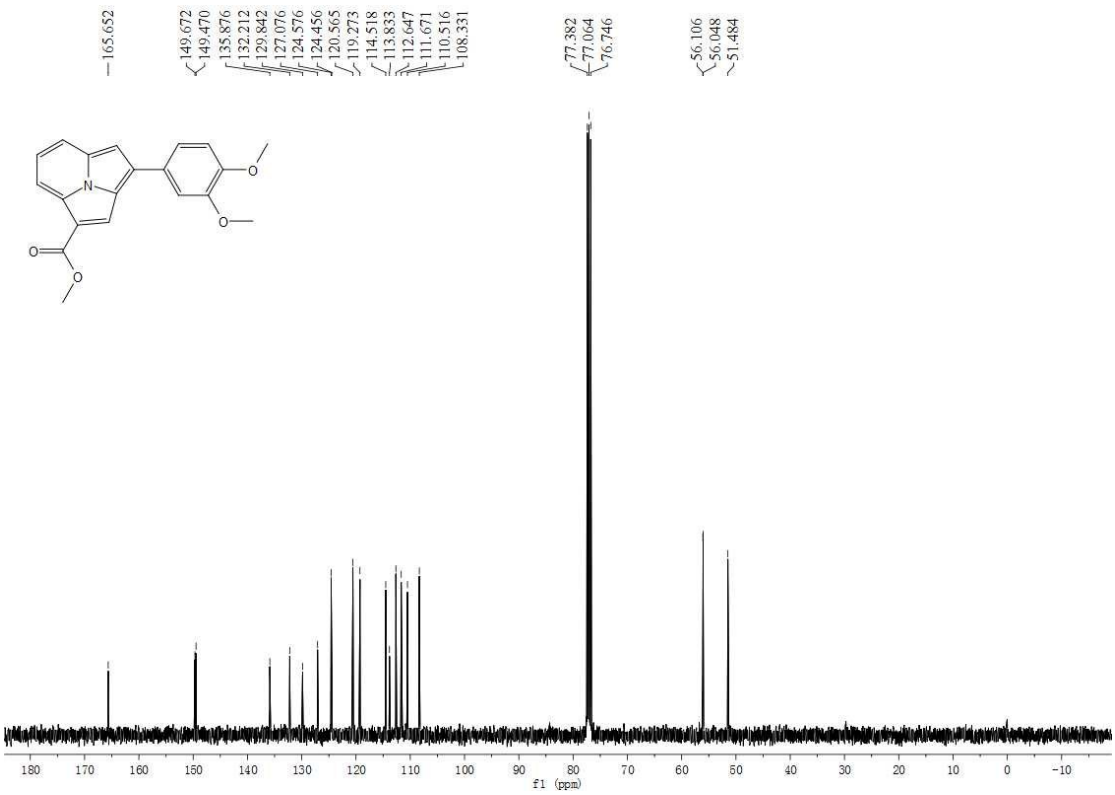
Methyl 3-(3,4-dichlorophenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3o)



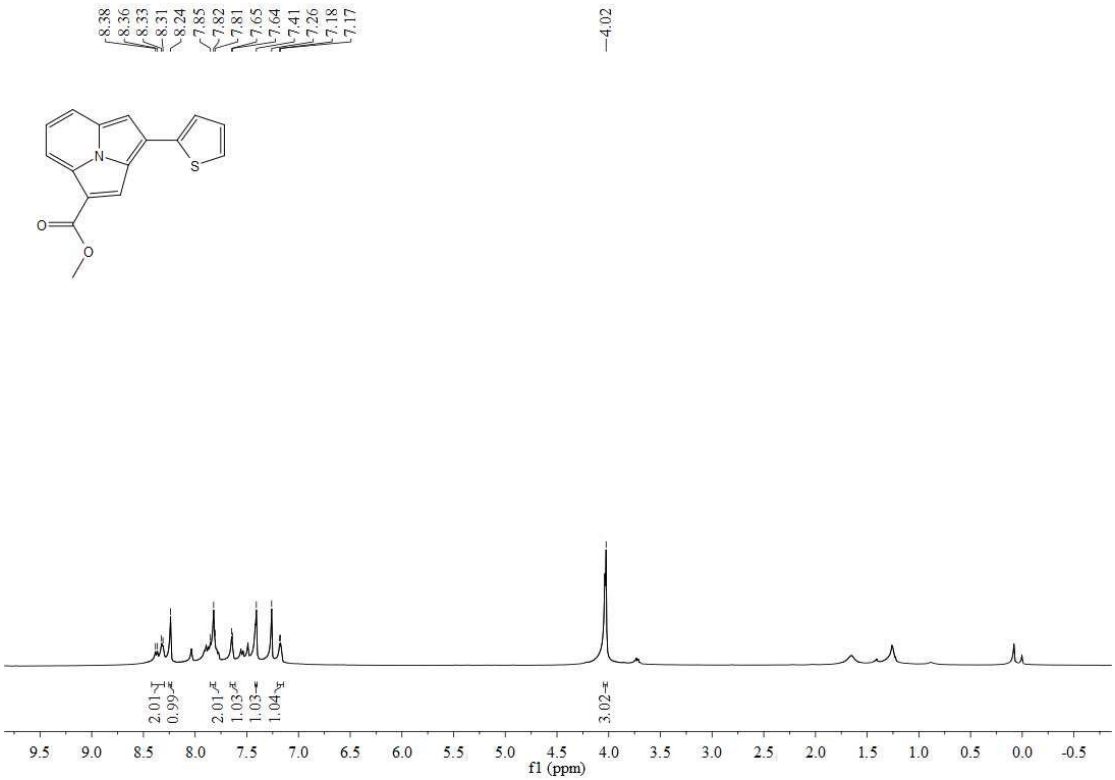


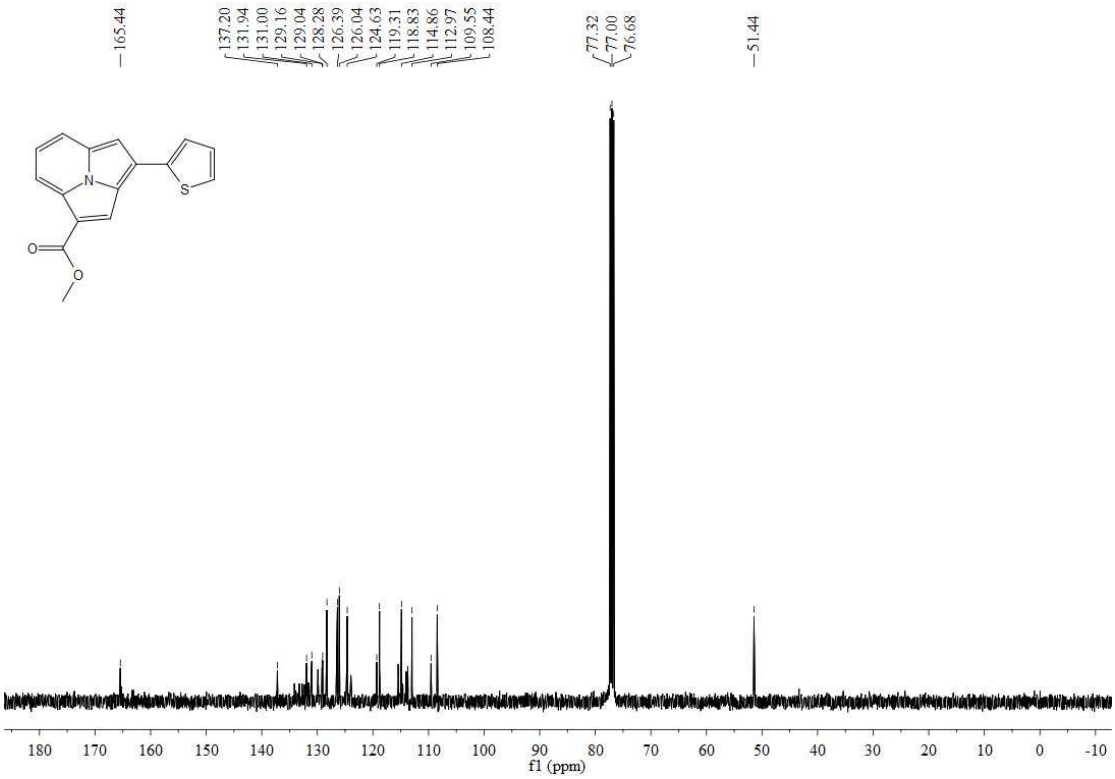
Methyl 3-(3,4-dimethoxyphenyl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3p)



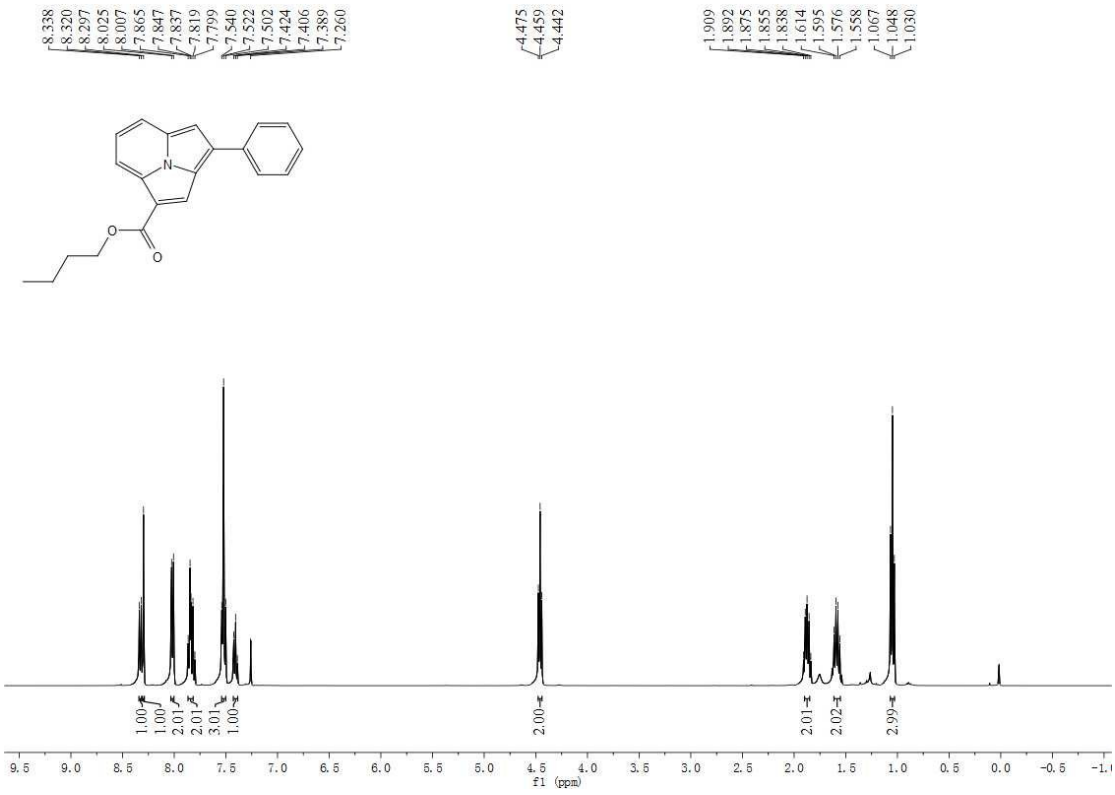


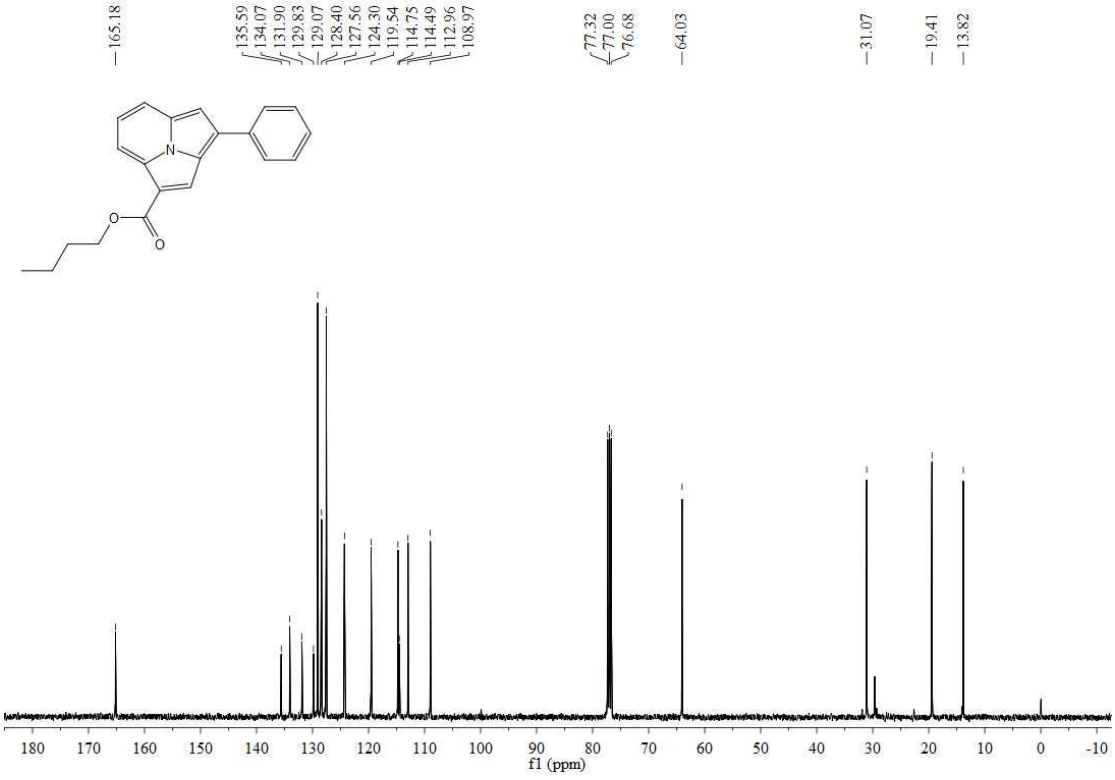
Methyl 3-(thiophen-2-yl)pyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (3q)



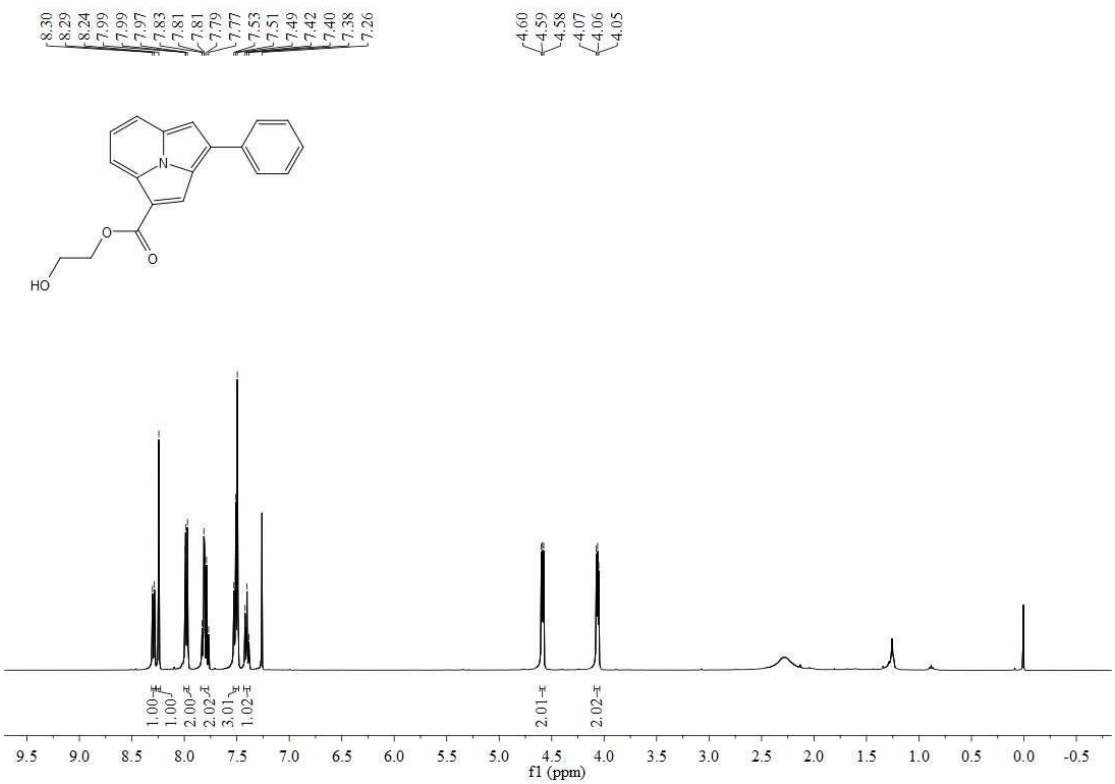


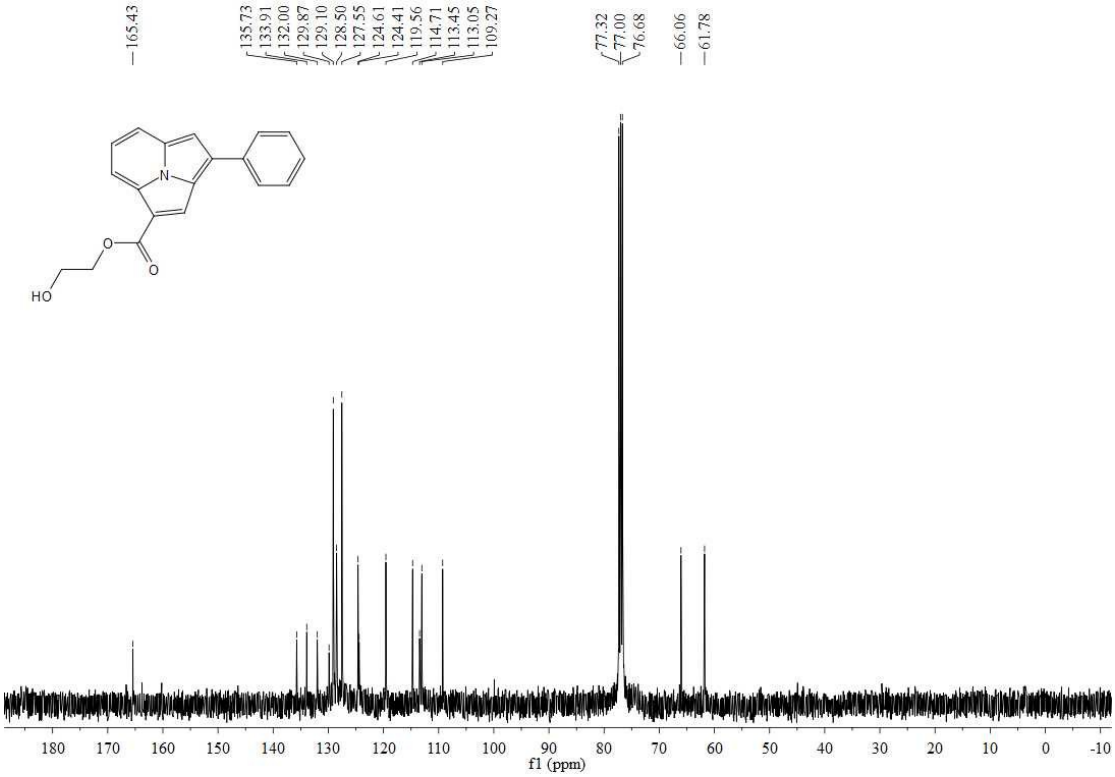
Butyl 3-phenylpyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (4a)



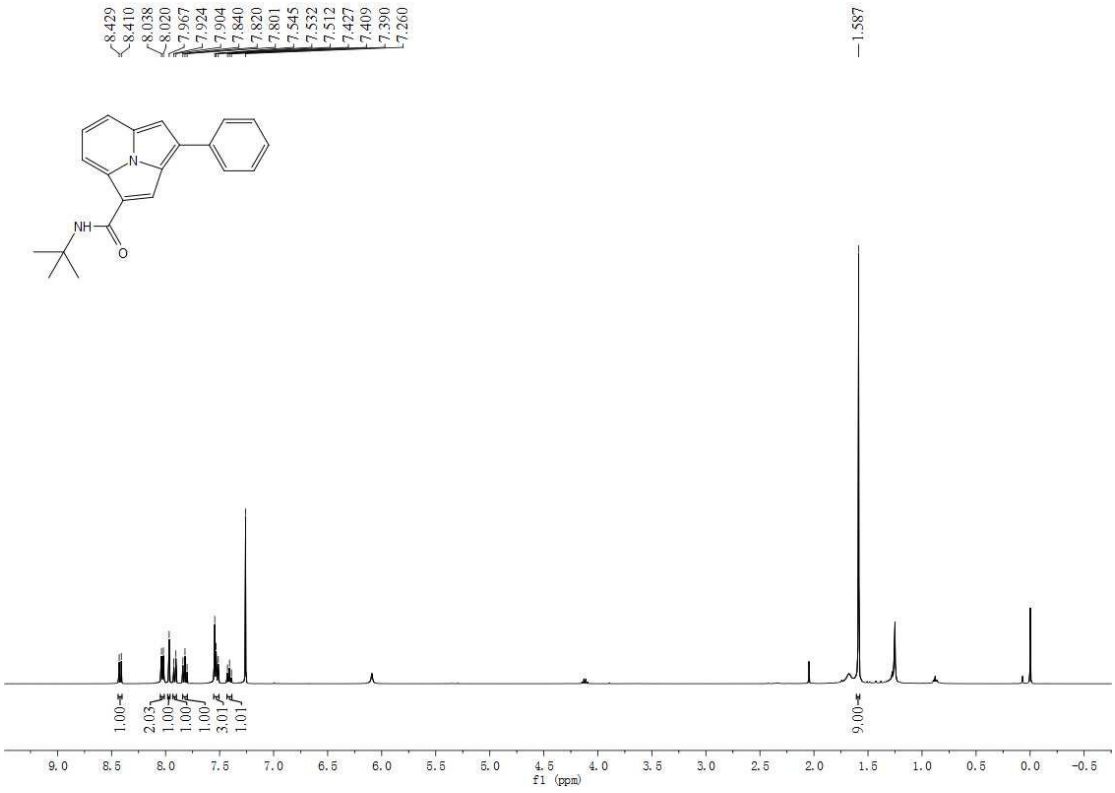


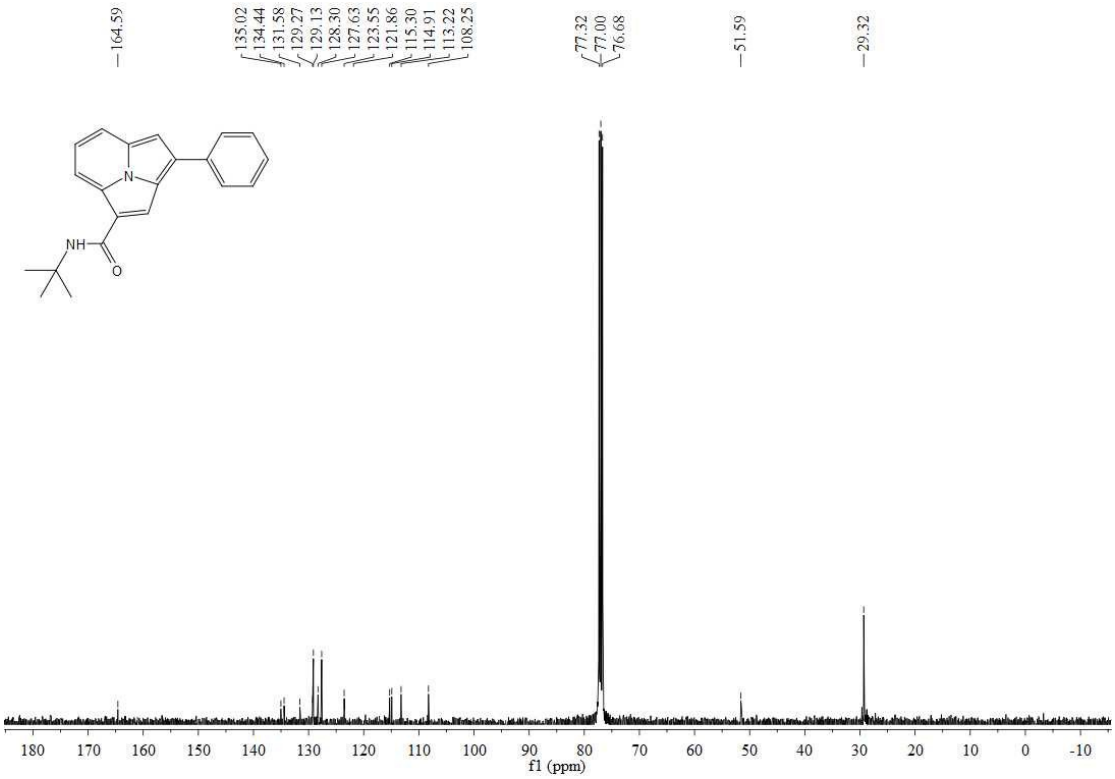
2-Hydroxyethyl 3-phenylpyrrolo[2,1,5-*cd*]indolizine-1-carboxylate (4b)



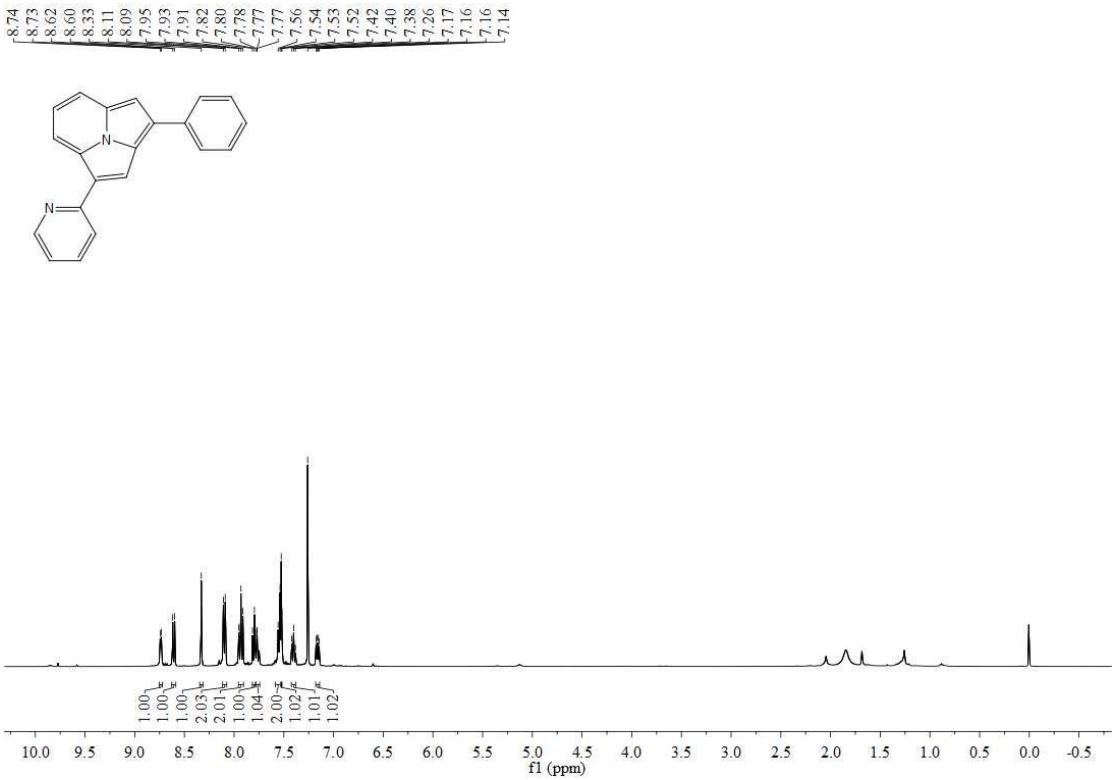


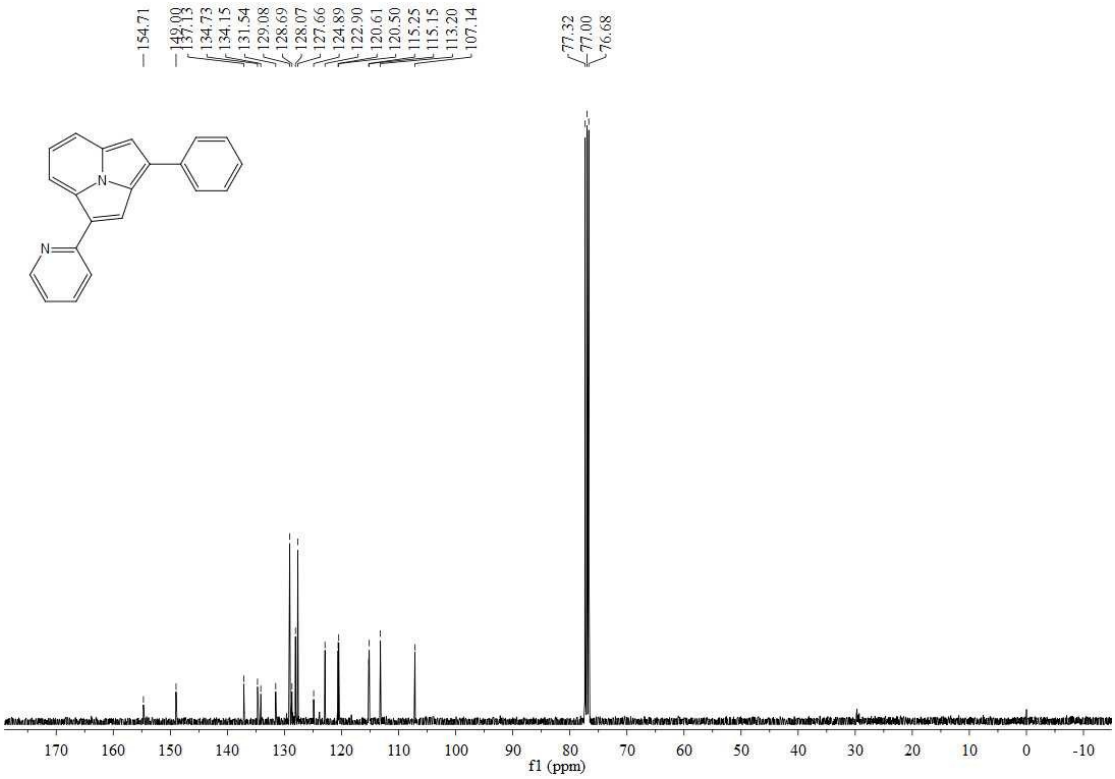
***N*-(*tert*-butyl)-3-phenylpyrrolo[2,1,5-*cd*]indolizine-1-carboxamide (4c)**



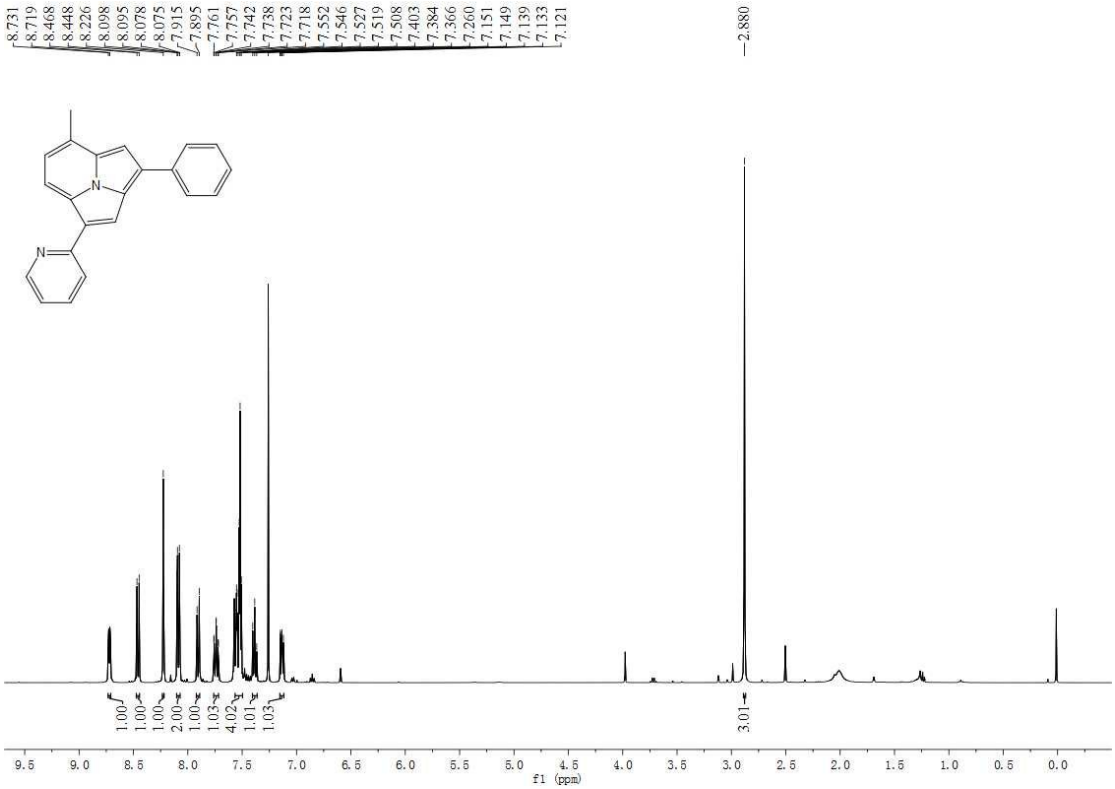


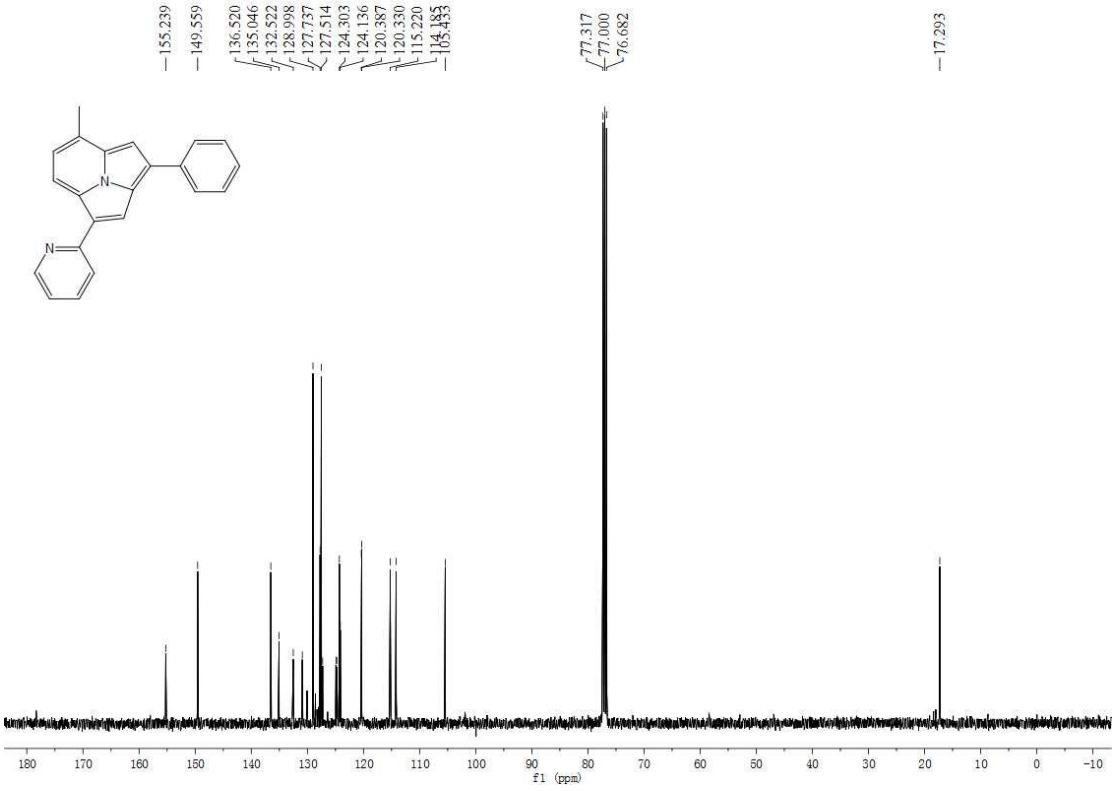
3-Phenyl-1-(pyridin-2-yl)pyrrolo[2,1,5-*cd*]indolizine (4d)



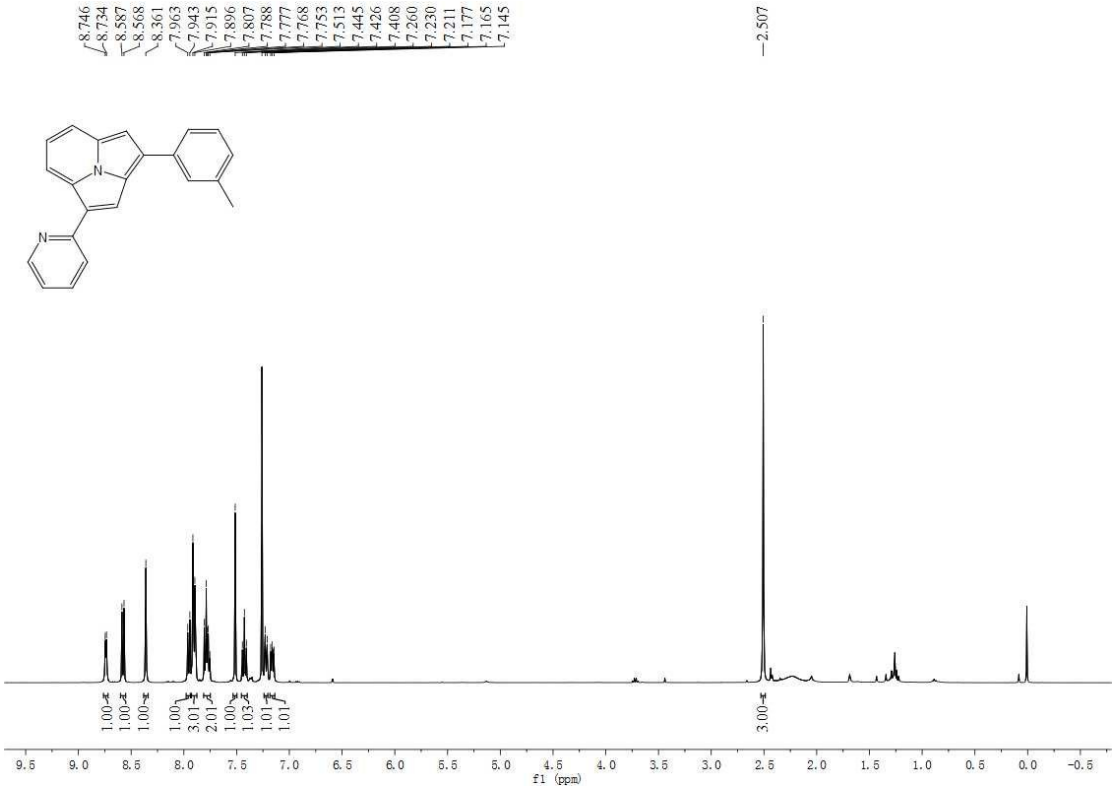


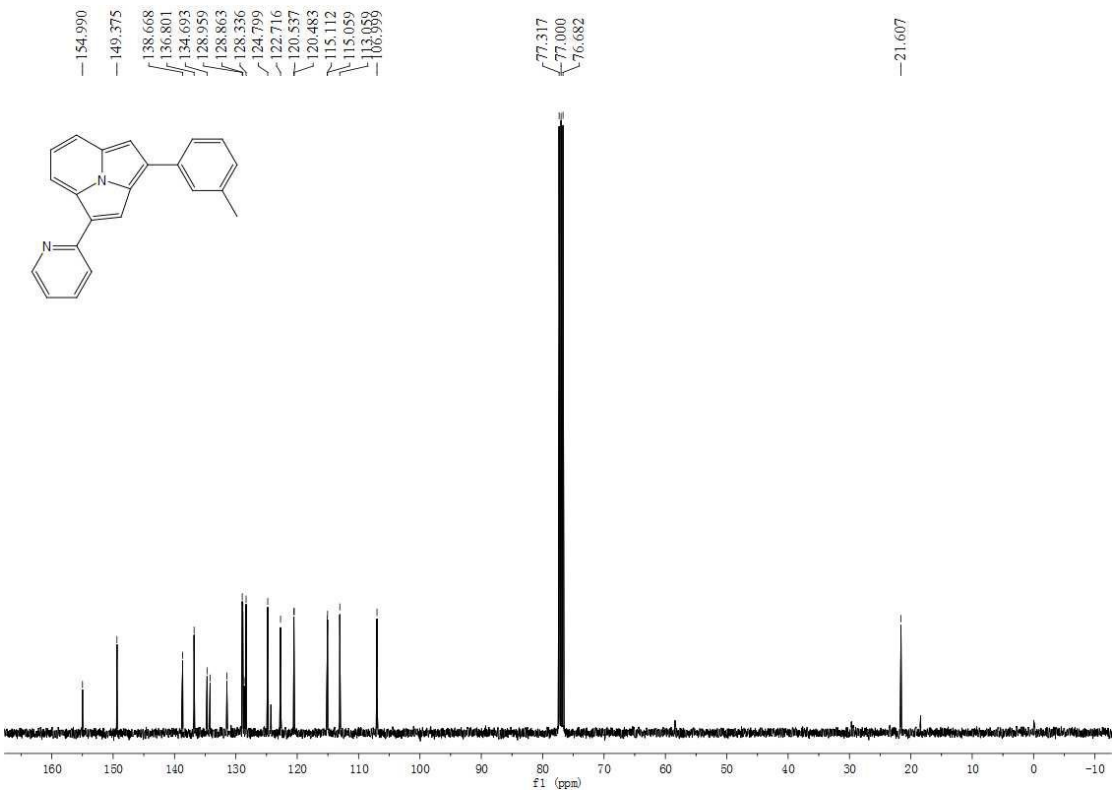
5-Methyl-3-phenyl-1-(pyridin-2-yl)pyrrolo[2,1,5-*cd*]indolizine (4e)



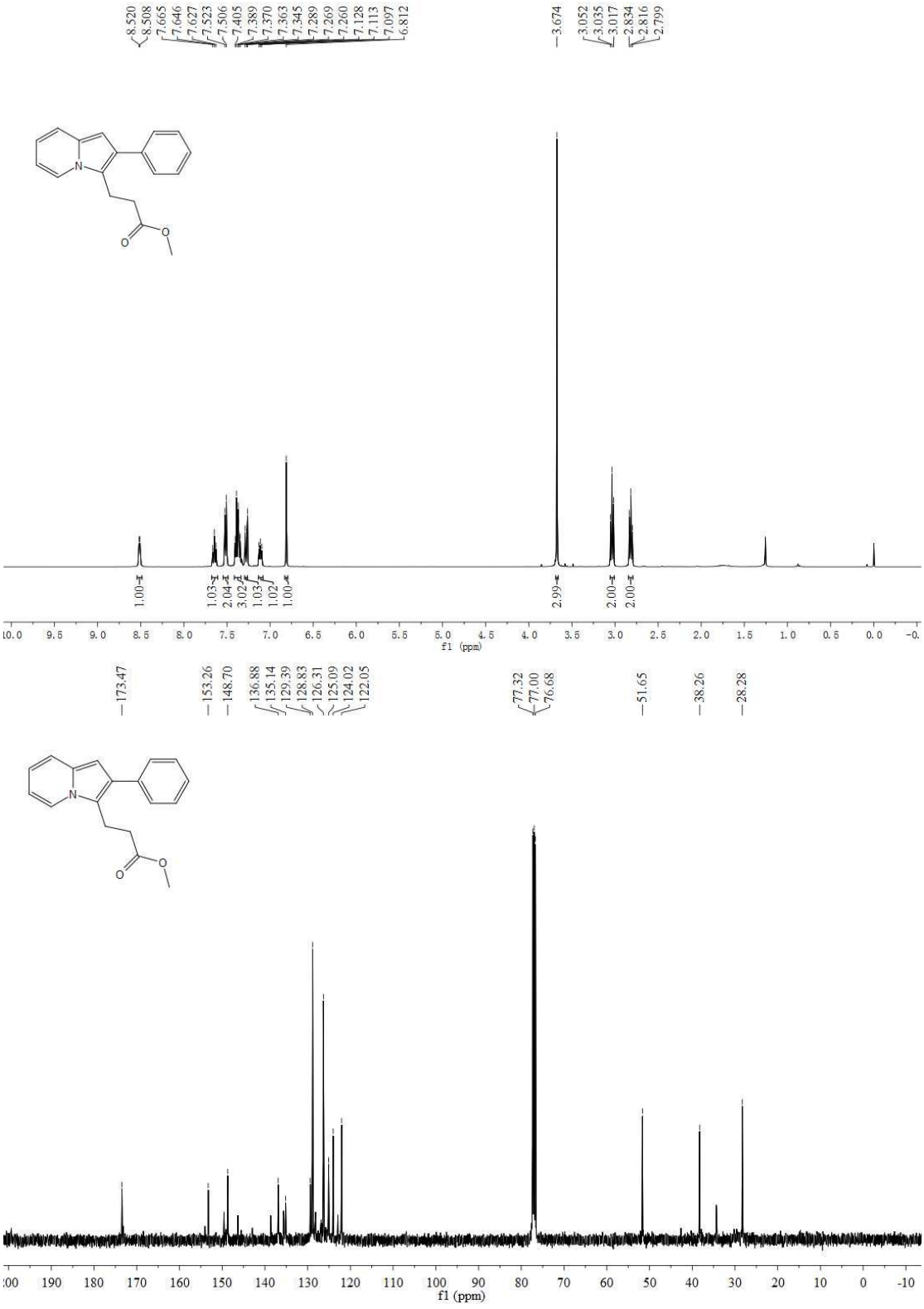


1-(Pyridin-2-yl)-3-(*m*-tolyl)pyrrolo[2,1,5-*cd*]indolizine (4f)

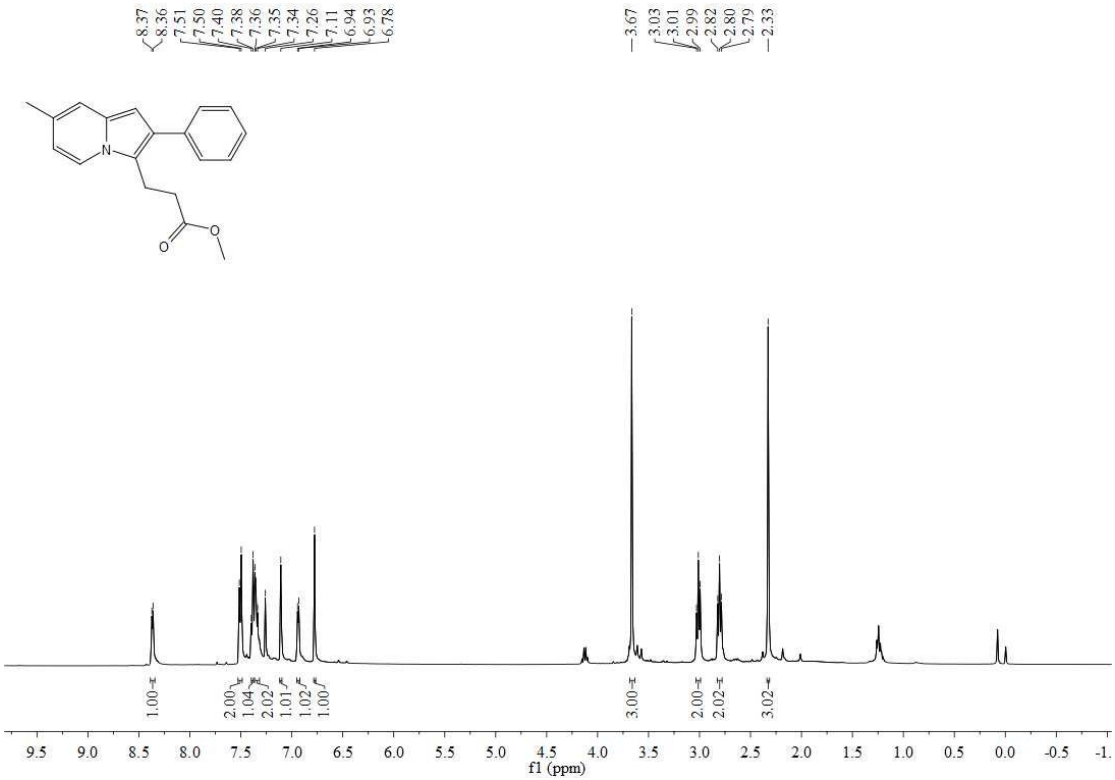


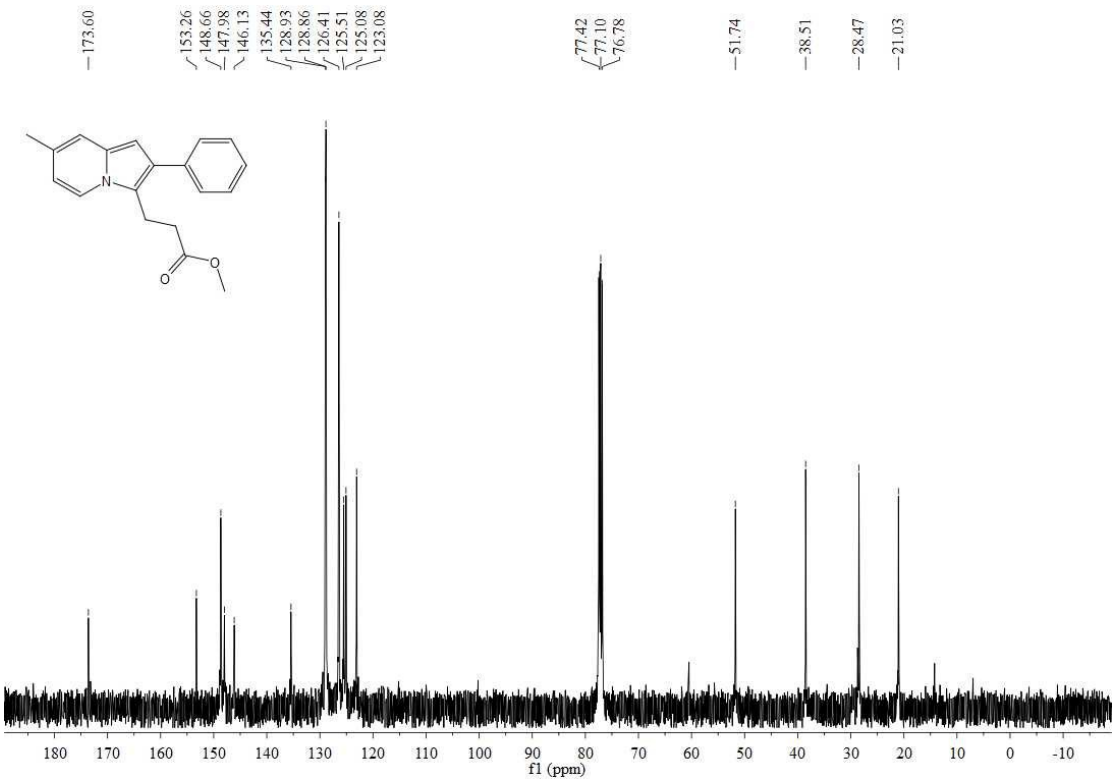


Methyl 3-(2-Phenylindolizin-3-yl)propanoate (5a)

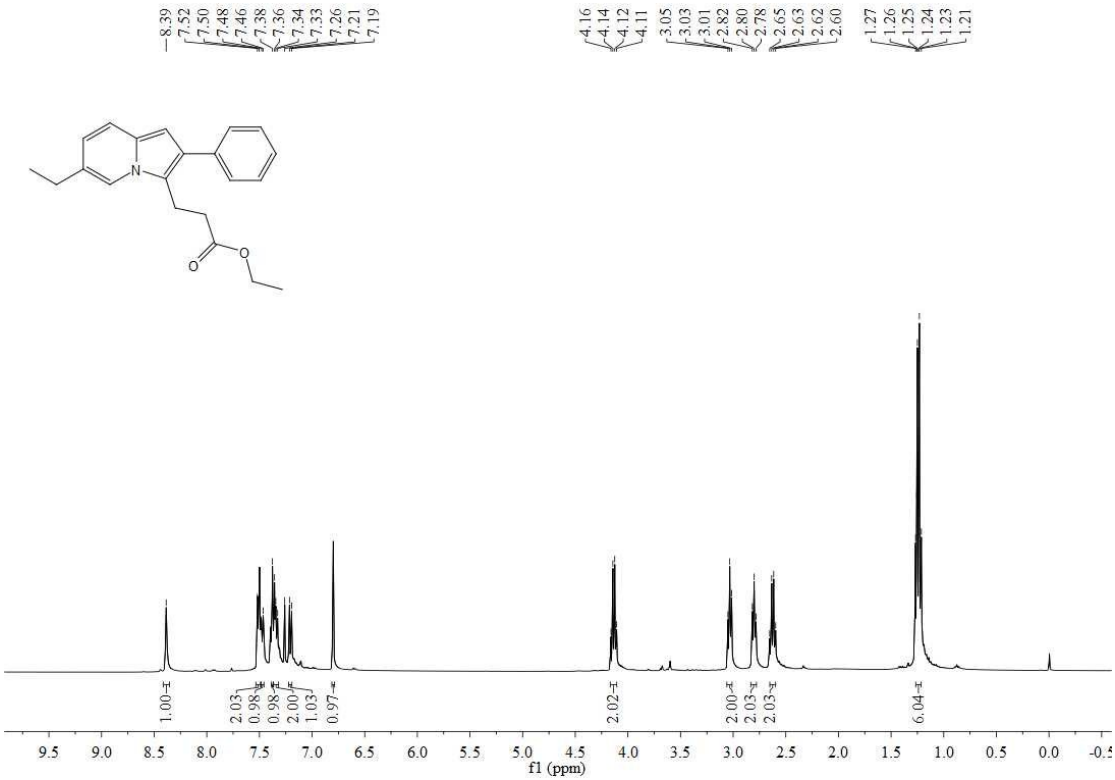


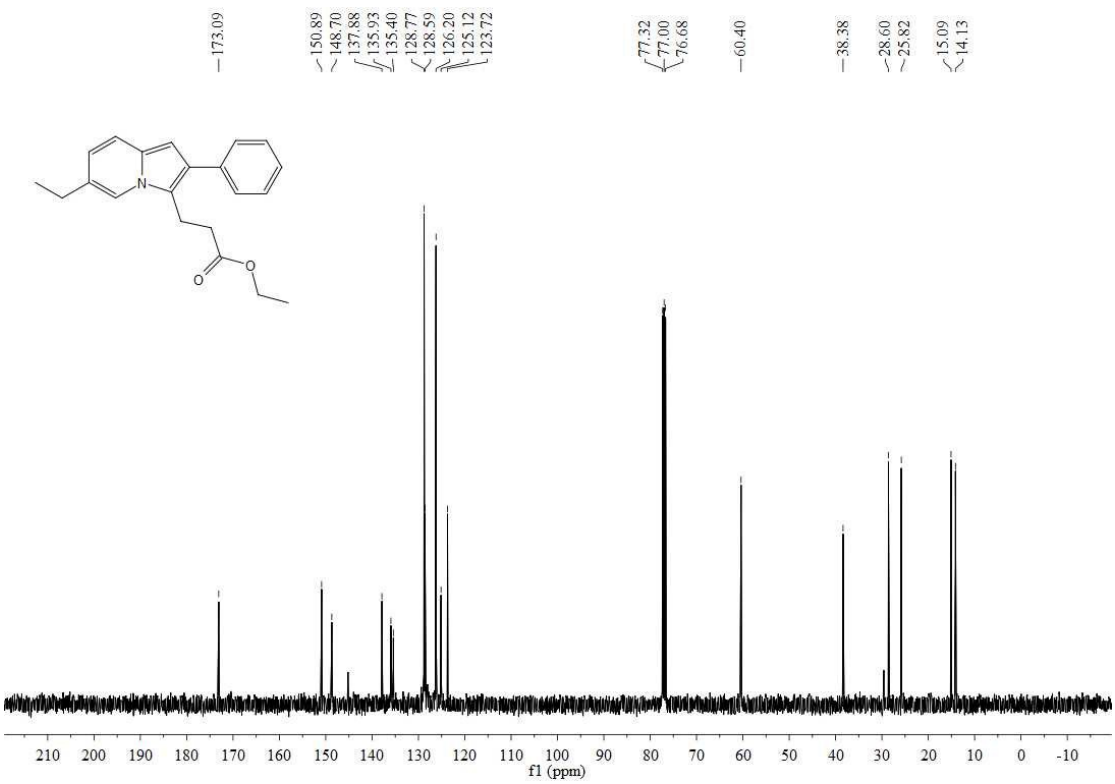
Methyl 3-(7-Methyl-2-phenylindolizin-3-yl)propanoate (5b)



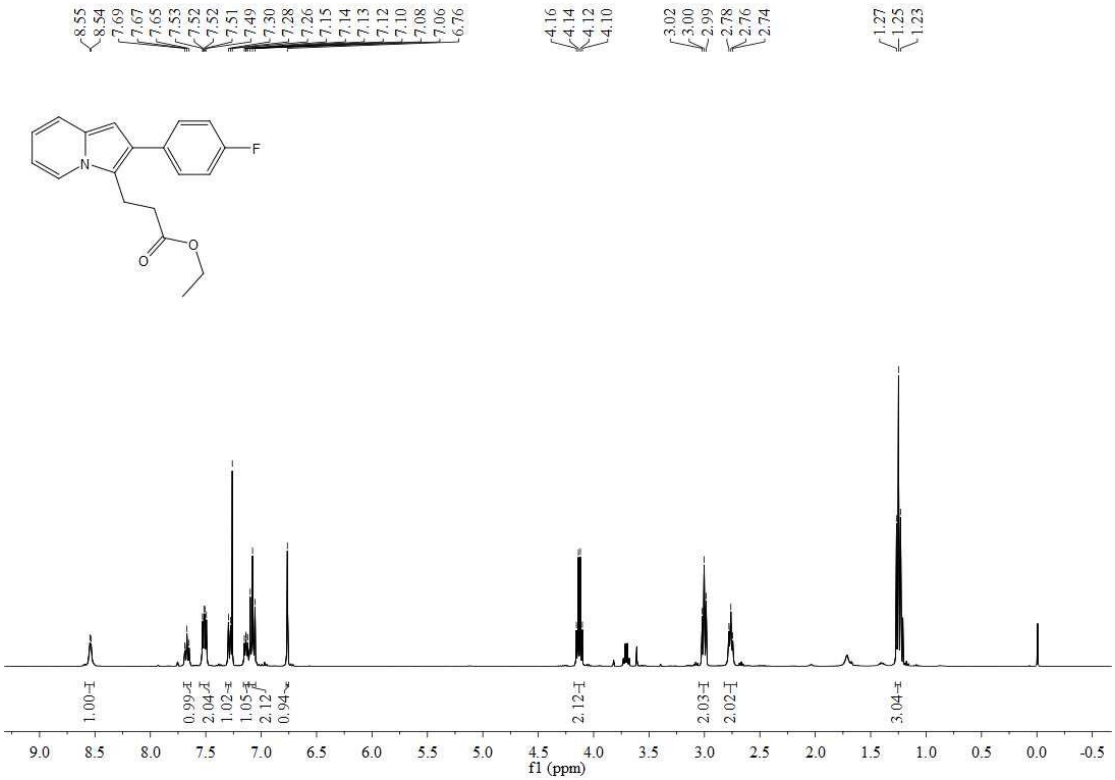


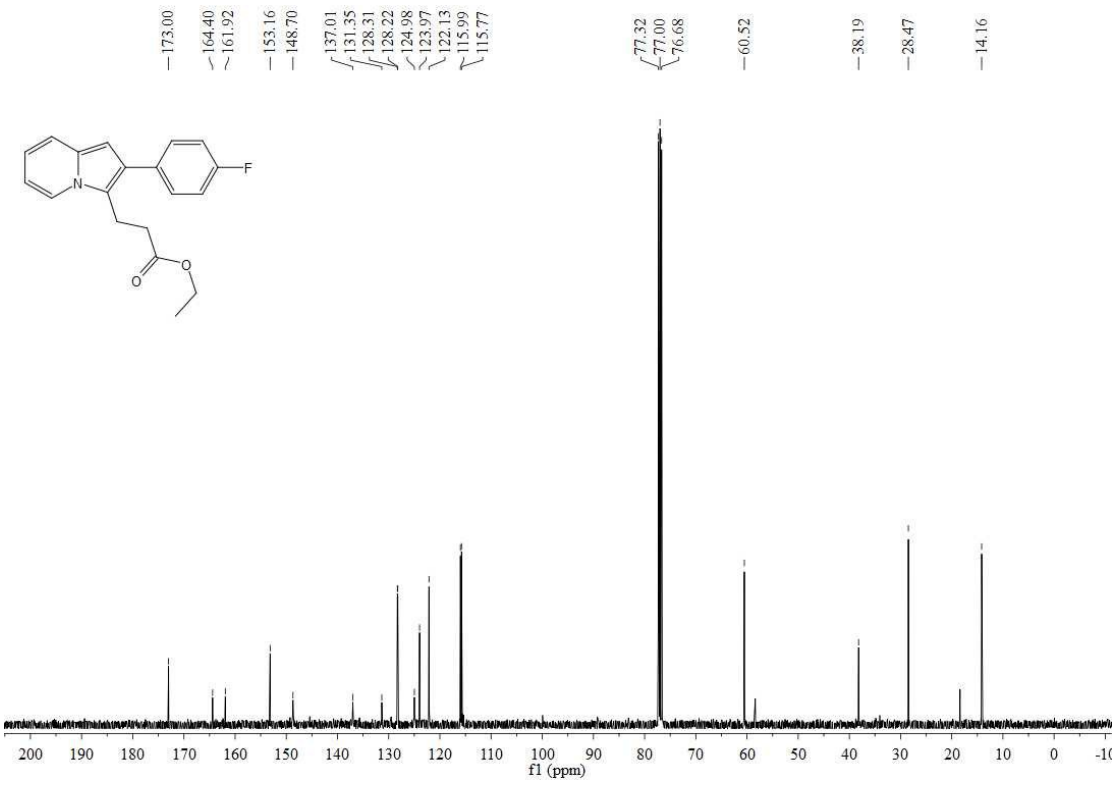
Ethyl 3-(6-Ethyl-2-phenylindolizin-3-yl)propanoate (5c)





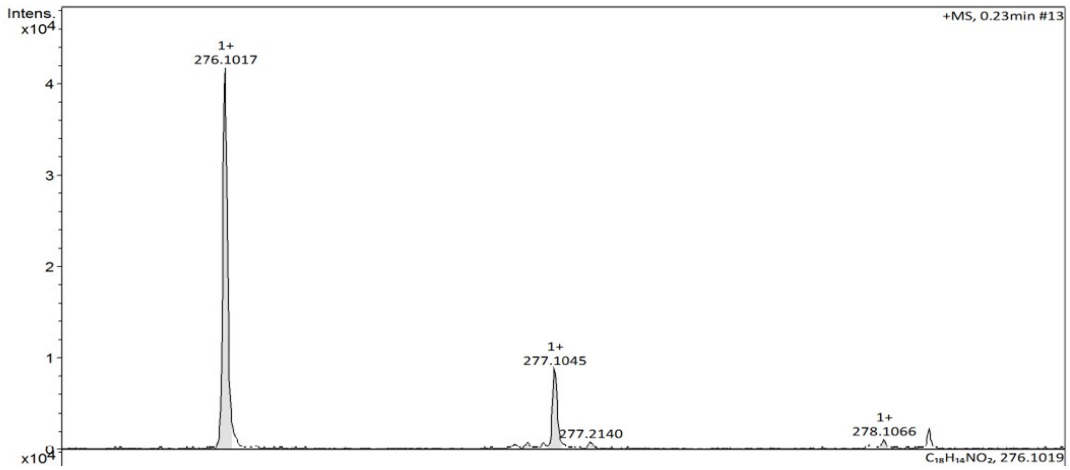
Ethyl 3-(2-(4-Fluorophenyl)indolizin-3-yl)propanoate (5d)



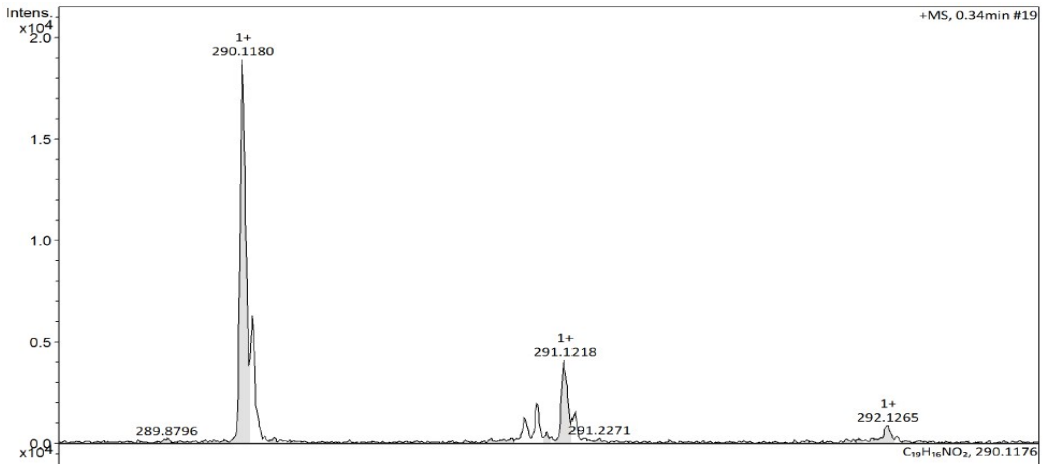


F. HRMS Spectra

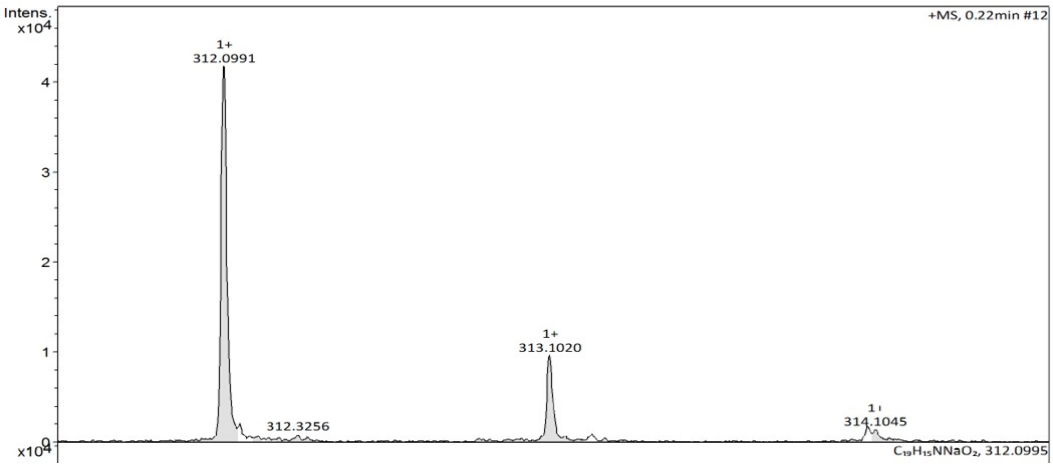
3a



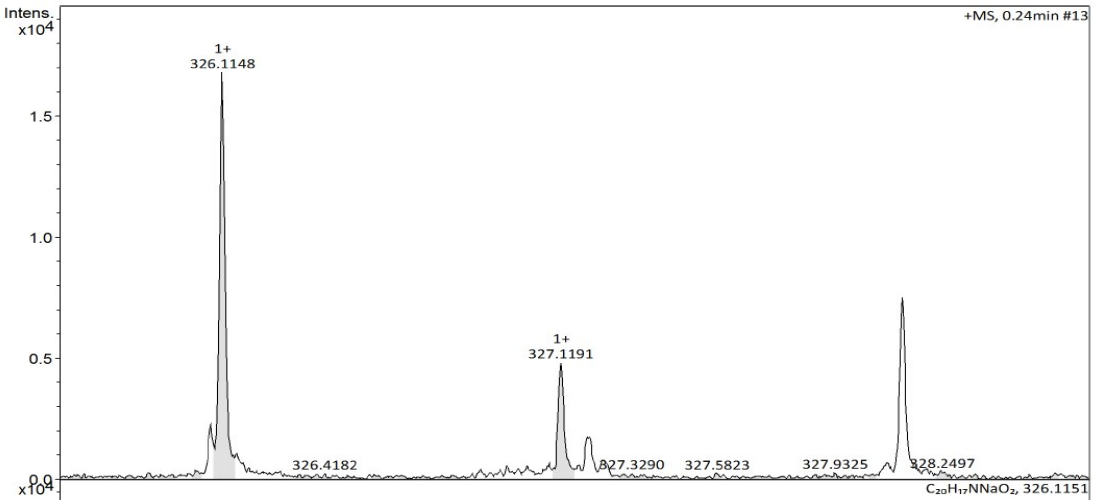
3b



3c



3d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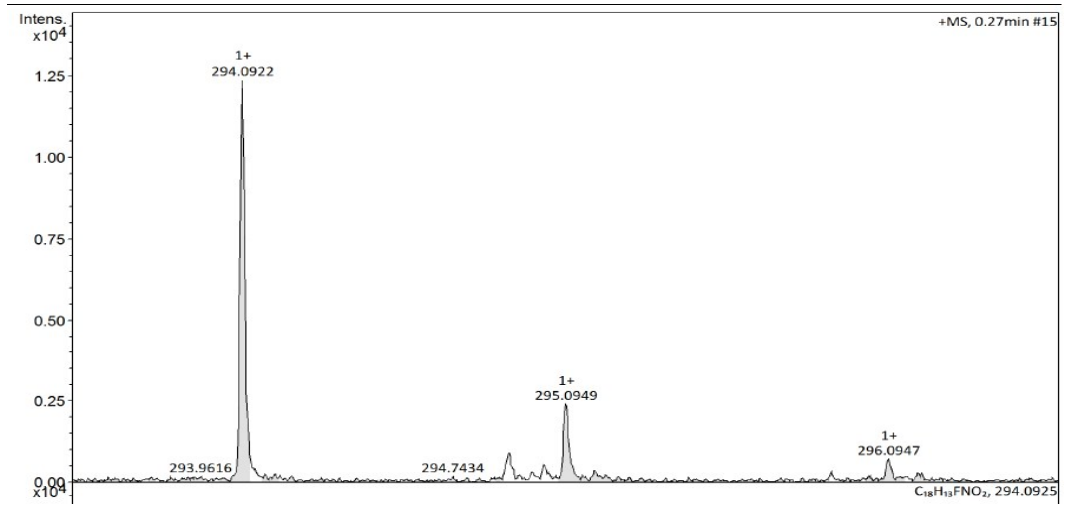
x10^4
+MS, 0.24min #13
1+
326.1148
1+
327.1191
326.4182
327.3290
327.5823
327.9325
328.2497
C20H17NNaO2, 326.1151

3e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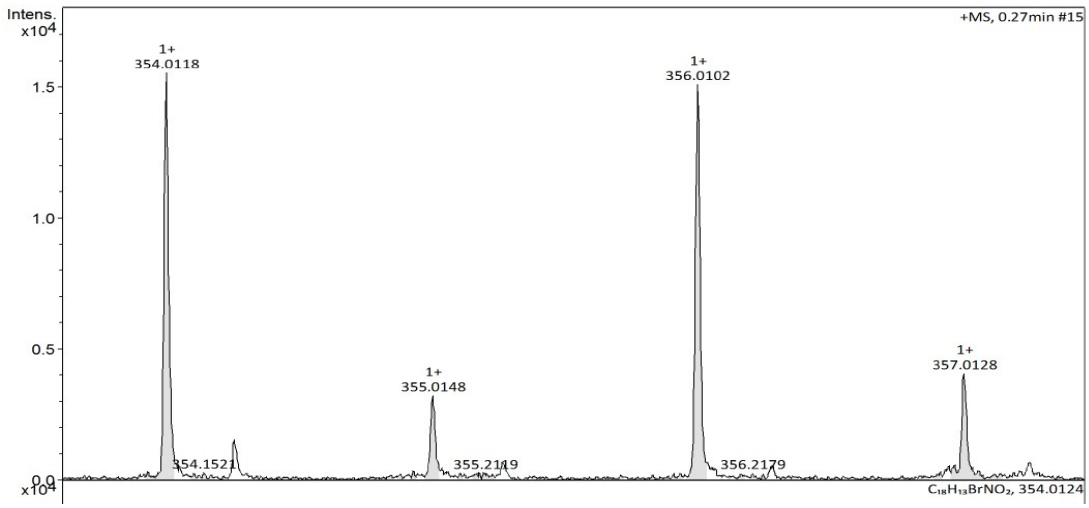
C18H13FNO2, 294.0925

3f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x10^4
+MS, 0.27min #15
1+
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1+
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356.2179
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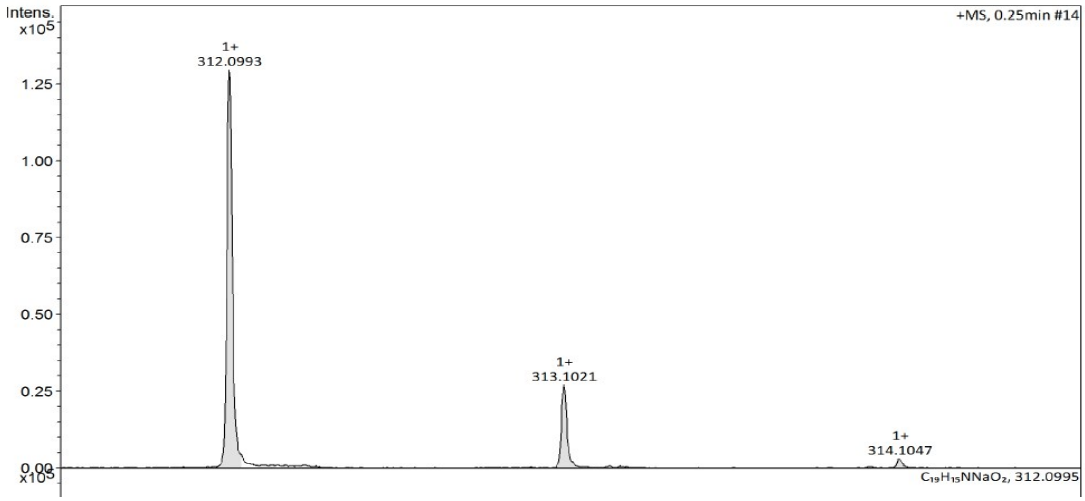
3g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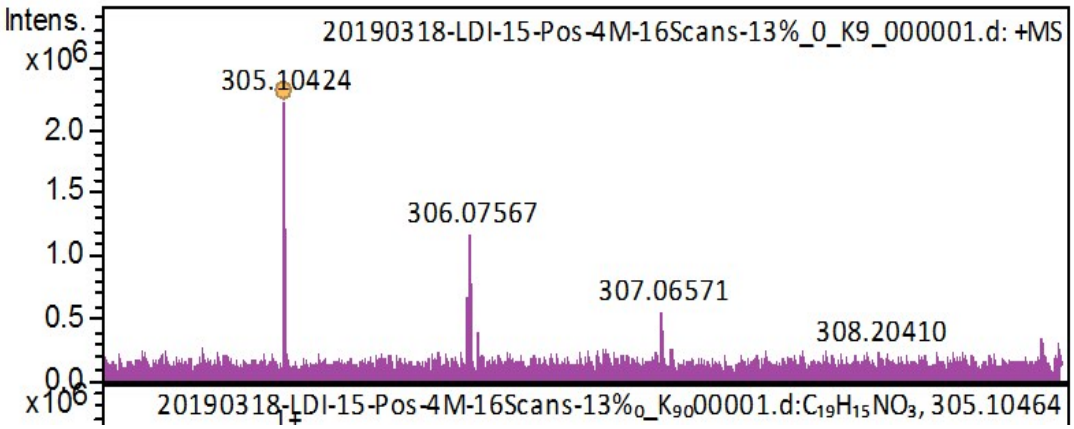
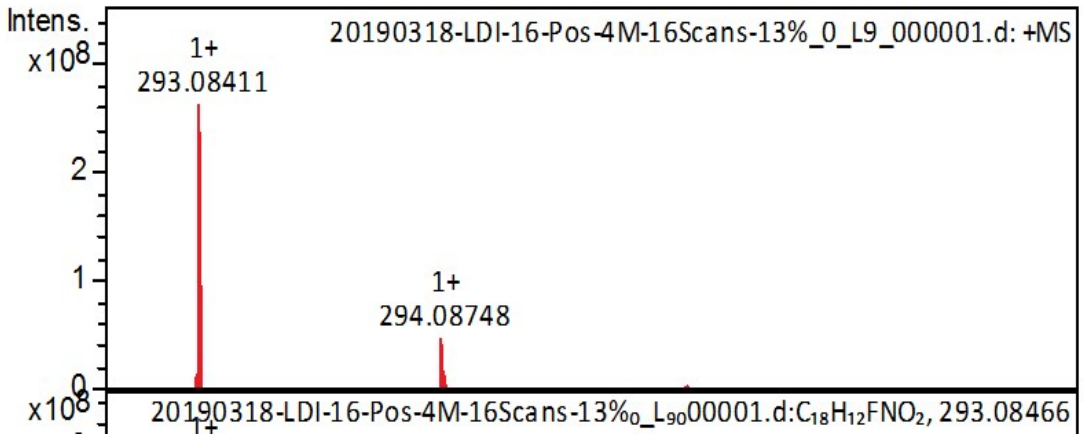
+MS, 0.25min #14
1+
312.0993
1.25
1.00
0.75
0.50
1+
313.1021
0.25
1+
314.1047
0.00
x10^5
C19H15NNaO2, 312.0995

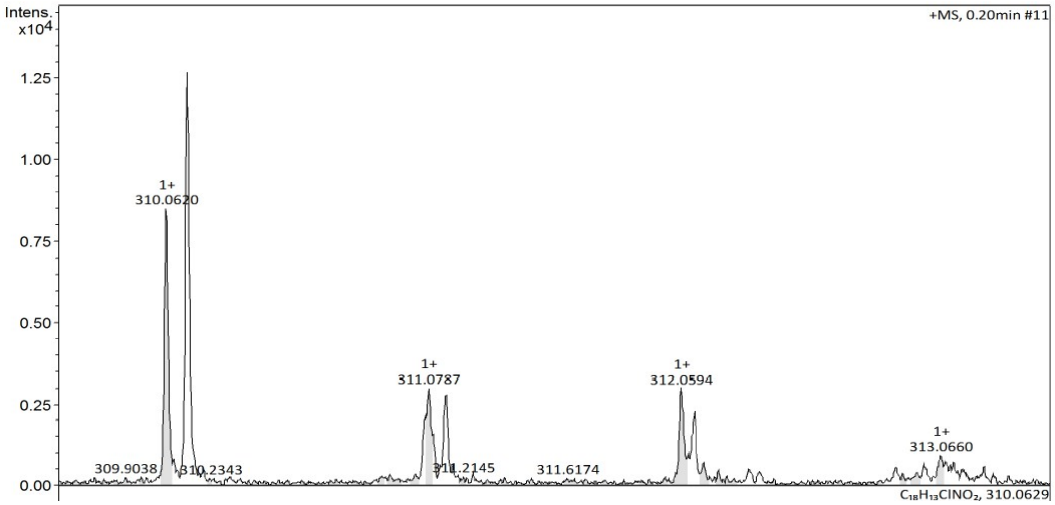
3h


Intens.
x10^6
20190318-LDI-15-Pos-4M-16Scans-13%_0_K9_000001.d: +MS
305.10424
2.0
1.5
306.07567
1.0
307.06571
0.5
308.20410
0.0
x10^6
1+
20190318-LDI-15-Pos-4M-16Scans-13%_0_K900001.d:C19H15NO3, 305.10464

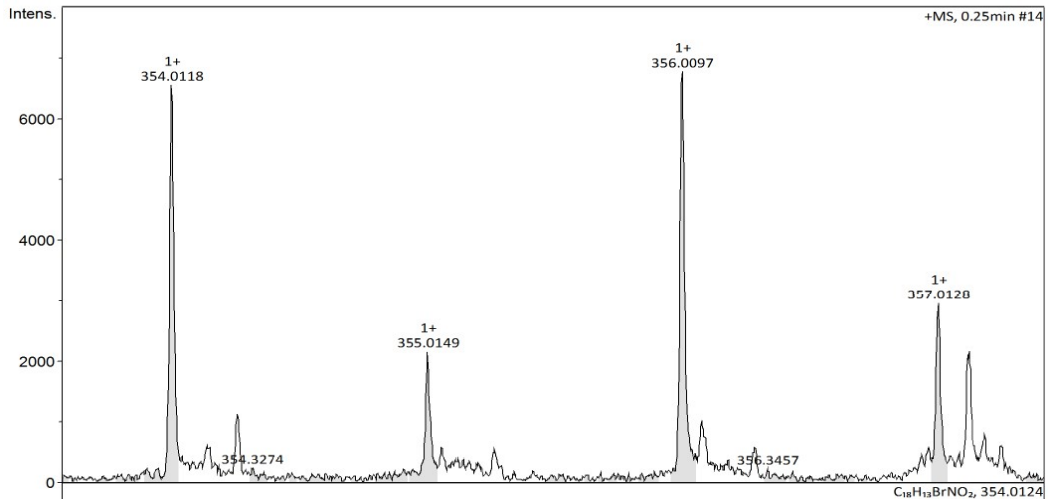
3i


Intens.
x10^8
20190318-LDI-16-Pos-4M-16Scans-13%_0_L9_000001.d: +MS
1+
293.08411
2
1
1+
294.08748
0
x10^8
1+
20190318-LDI-16-Pos-4M-16Scans-13%_0_L900001.d:C18H12FNO2, 293.08466

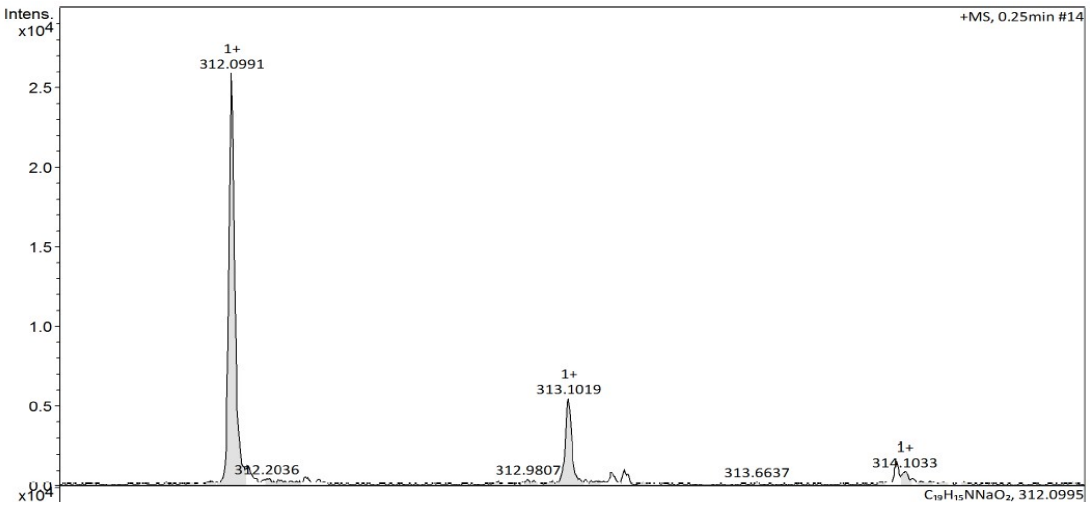
3j


Intens.
x10^4
+MS, 0.20min #11
1.25
1.00
0.75
0.50
0.25
0.00
1+
310.0620
1+
311.0787
1+
312.0594
1+
313.0660
309.9038
310.2343
311.2145
311.6174
C18H13ClNO2, 310.0629

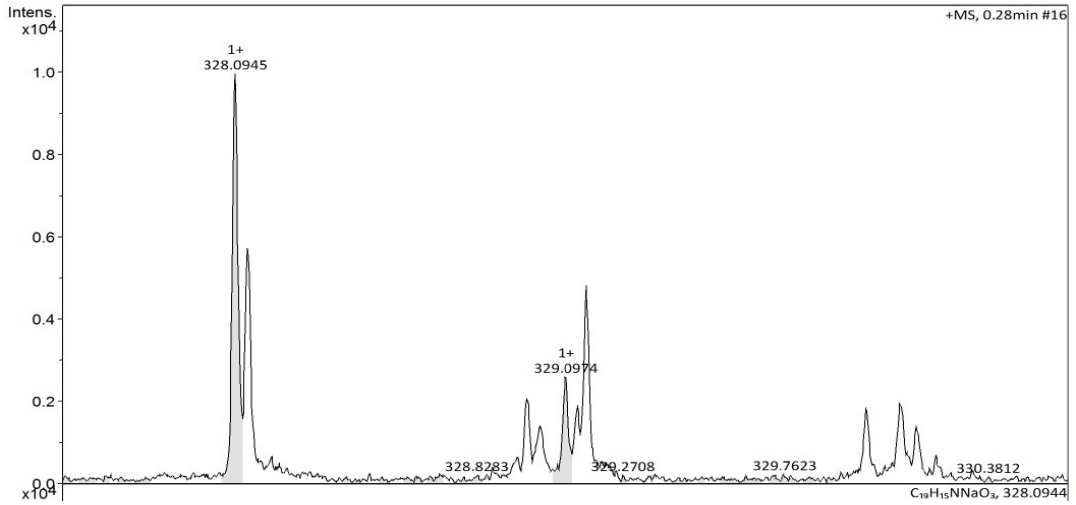
3k


Intens.
+MS, 0.25min #14
6000
4000
2000
0
1+
354.0118
1+
355.0149
1+
356.0097
1+
357.0128
354.3274
356.3457
C18H13BrNO2, 354.0124

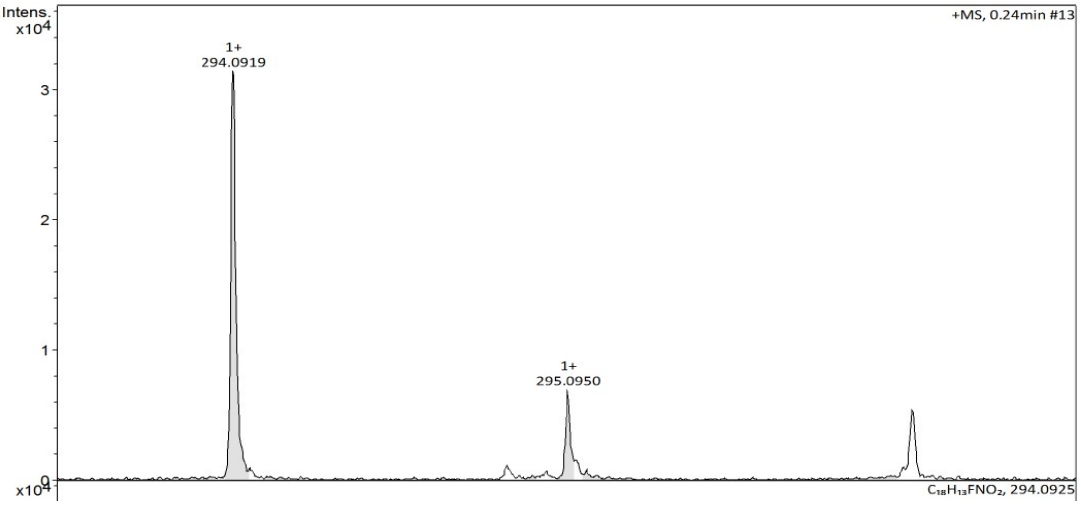
3l


Intens.
x10^4
+MS, 0.25min #14
2.5
2.0
1.5
1.0
0.5
0.0
1+
312.0991
1+
313.1019
1+
314.1033
312.2036
312.9807
313.6637
C19H15NNaO2, 312.0995

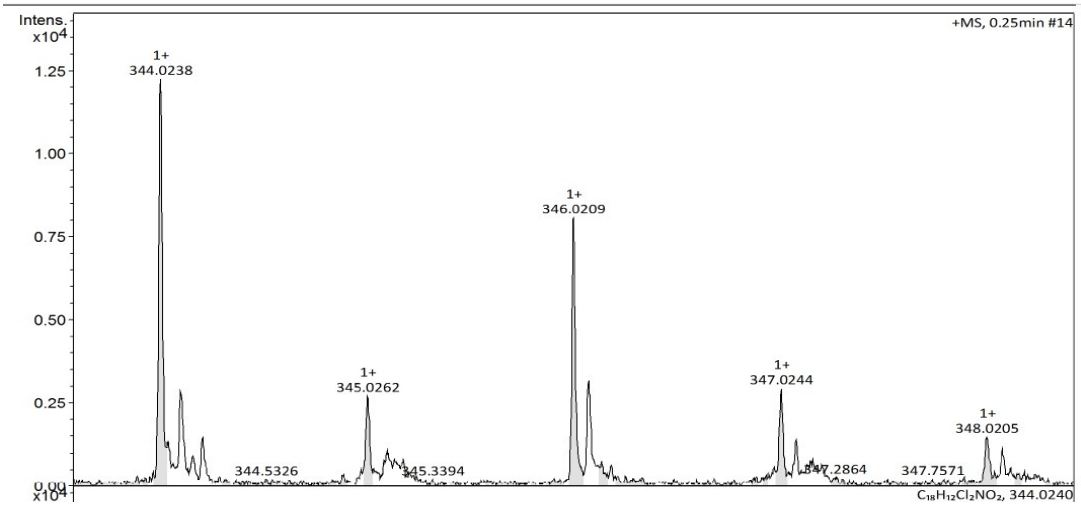
3m


Intens.
x10^4
+MS, 0.28min #16
1+
328.0945
1+
329.0974
328.8283
329.2708
329.7623
330.3812
C19H15NNaO3, 328.0944

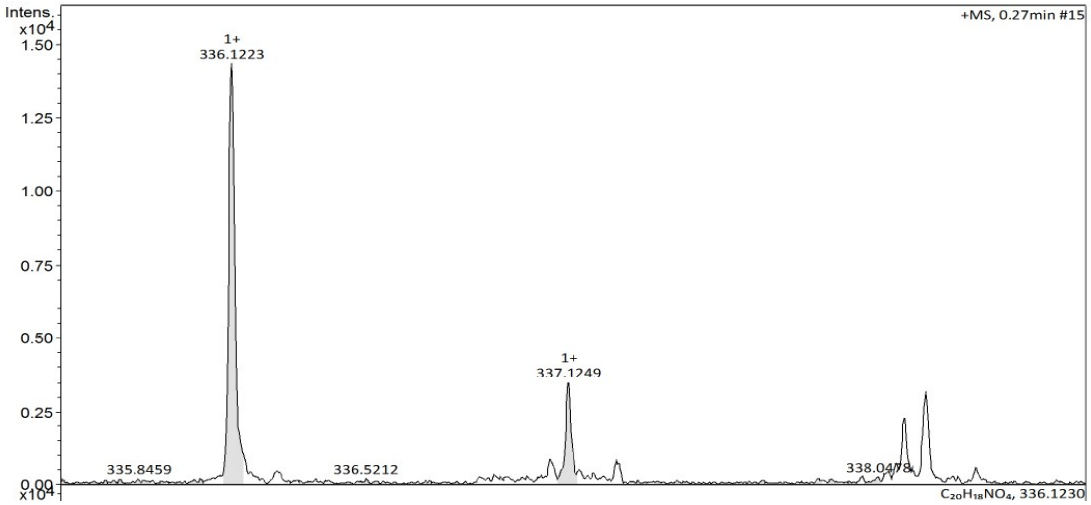
3n


Intens.
x10^4
+MS, 0.24min #13
1+
294.0919
1+
295.0950
C18H13FNO2, 294.0925

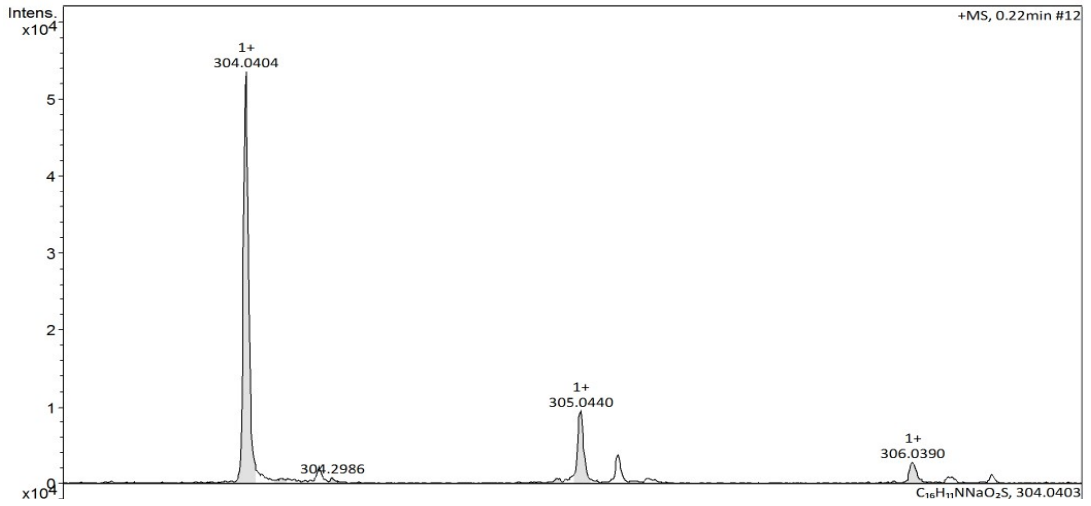
3o


Intens.
x10^4
+MS, 0.25min #14
1+
344.0238
1+
345.0262
1+
346.0209
1+
347.0244
1+
348.0205
344.5326
345.3394
347.2864
347.7571
C18H12Cl2NO2, 344.0240

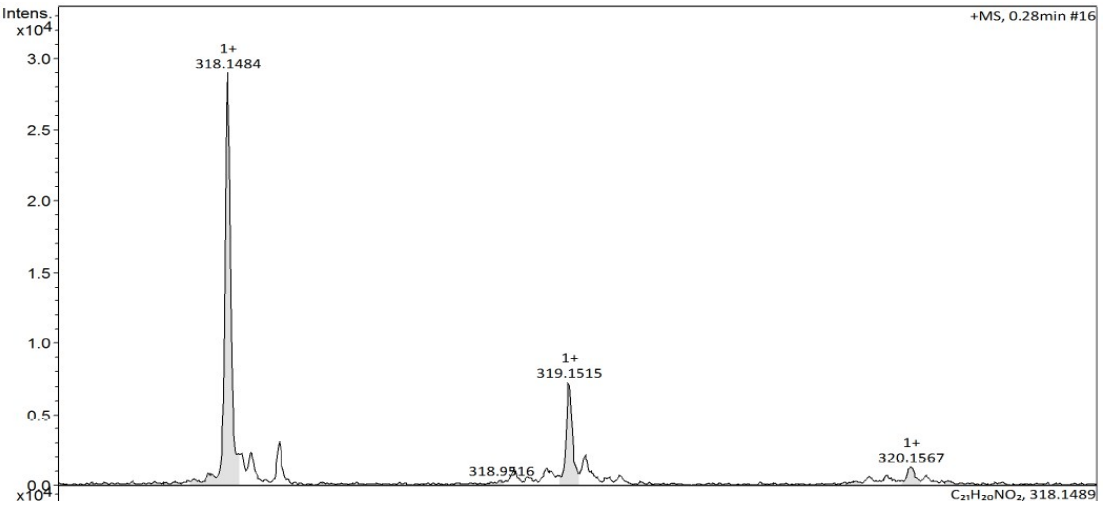
3p


Intens.
x10^4
1.50
1.25
1.00
0.75
0.50
0.25
0.00
x10^4
+MS, 0.27min #15
1+
336.1223
1+
337.1249
335.8459
336.5212
338.0478
C20H18NO4, 336.1230

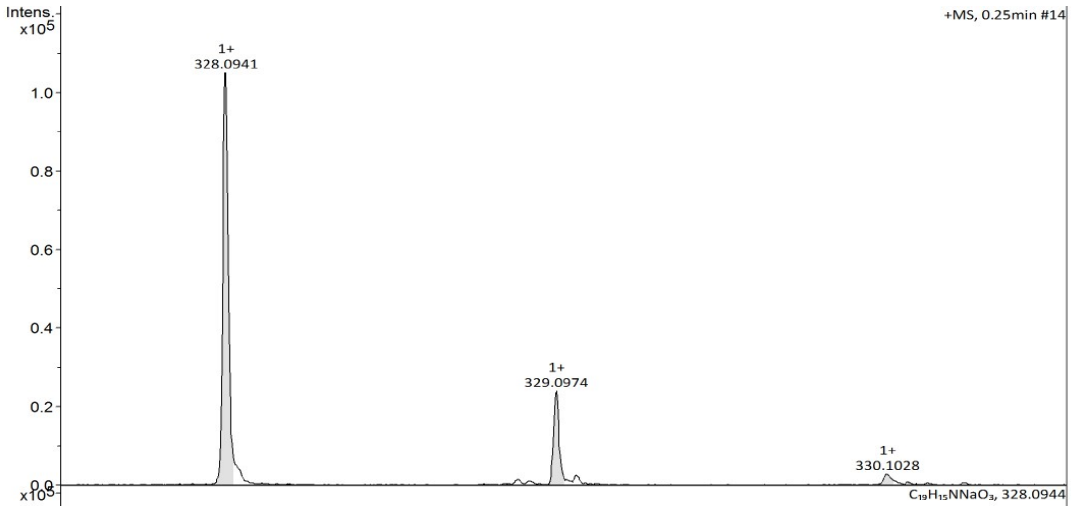
3q


Intens.
x10^4
5
4
3
2
1
0
x10^4
+MS, 0.22min #12
1+
304.0404
1+
305.0440
1+
306.0390
304.2986
C16H11NNaO2S, 304.0403

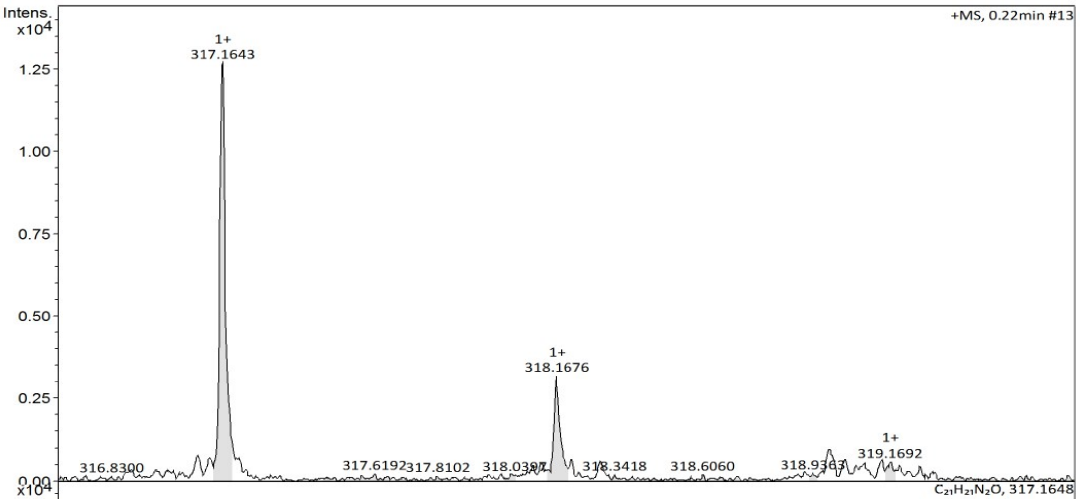
4a


Intens.
x10^4
3.0
2.5
2.0
1.5
1.0
0.5
0.0
x10^4
+MS, 0.28min #16
1+
318.1484
1+
319.1515
1+
320.1567
318.9516
C21H20NO2, 318.1489

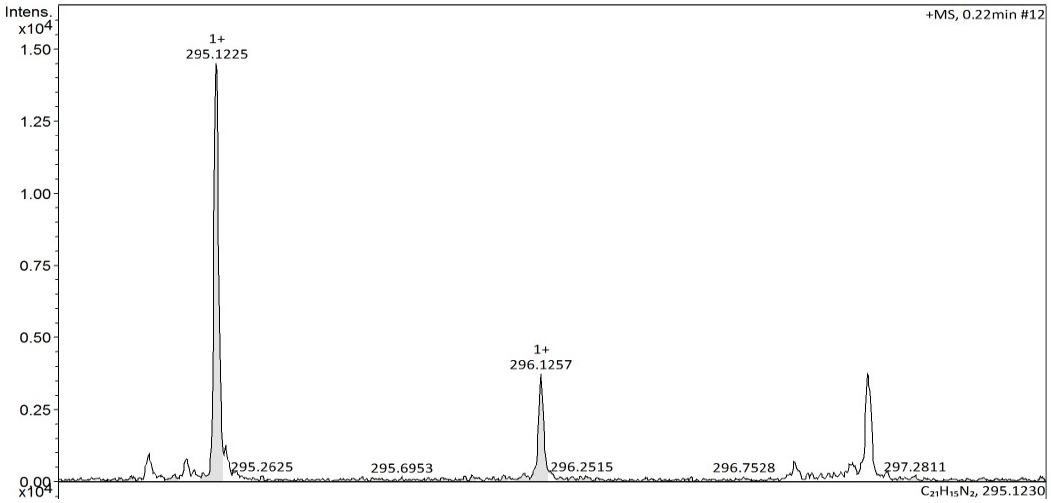
4b


Intens.
x10^5
+MS, 0.25min #14
1+
328.0941
1+
329.0974
1+
330.1028
C19H15NNaO3, 328.0944

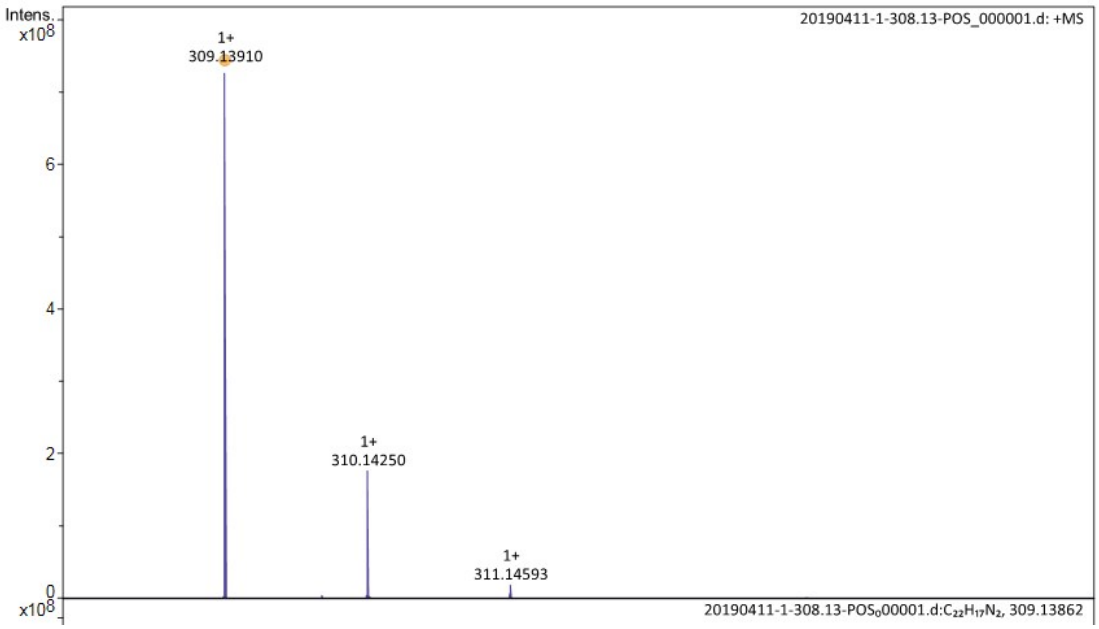
4c


Intens.
x10^4
+MS, 0.22min #13
1+
317.1643
1+
318.1676
1+
319.1692
316.8300
317.6192
317.8102
318.3418
318.6060
C21H21N2O, 317.1648

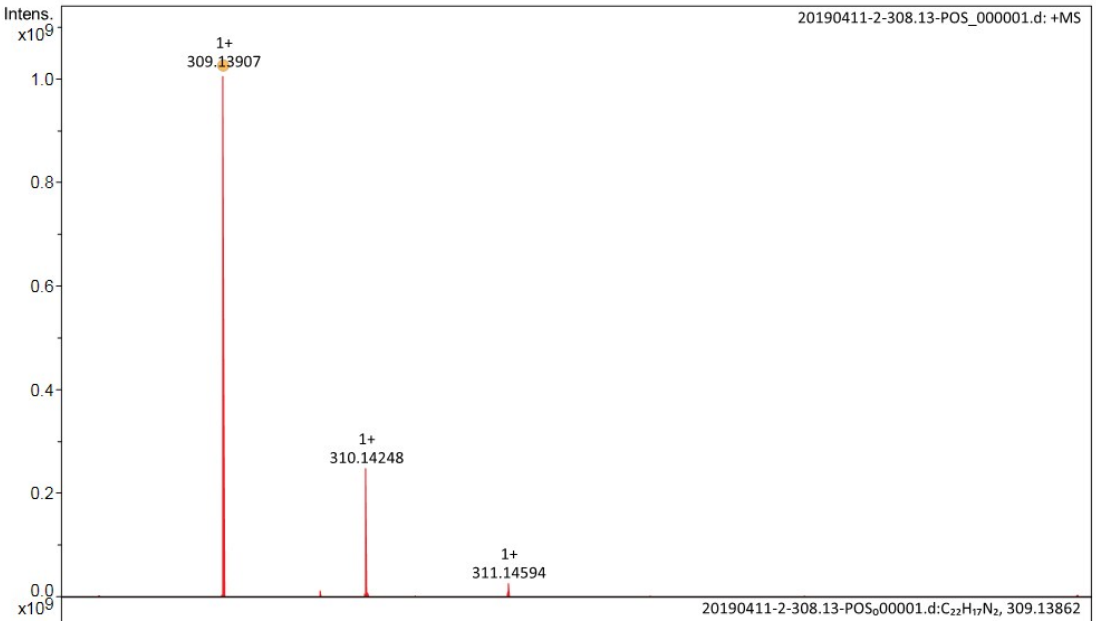
4d


Intens.
x10^4
+MS, 0.22min #12
1+
295.1225
1+
296.1257
295.2625
295.6953
296.2515
296.7528
297.2811
C21H15N2, 295.1230

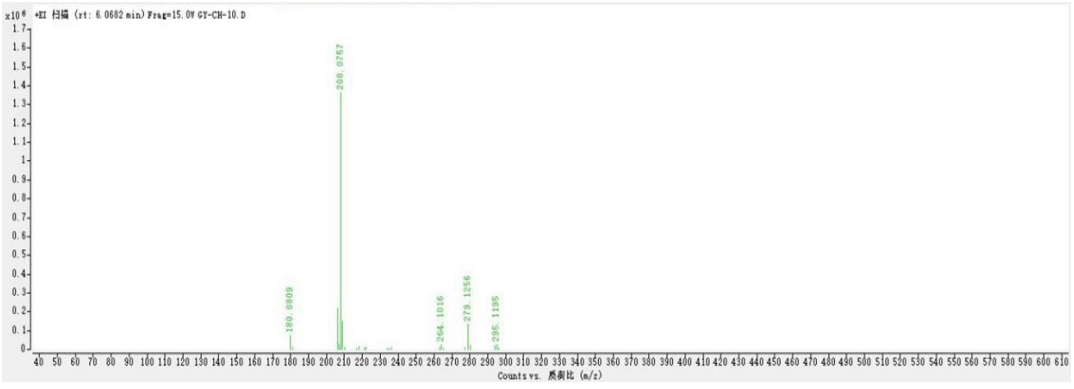
4e


Intens.
x10^8
20190411-1-308.13-POS_000001.d: +MS
1+
309.13910
1+
310.14250
1+
311.14593
20190411-1-308.13-POS_00001.d:C22H17N2, 309.13862

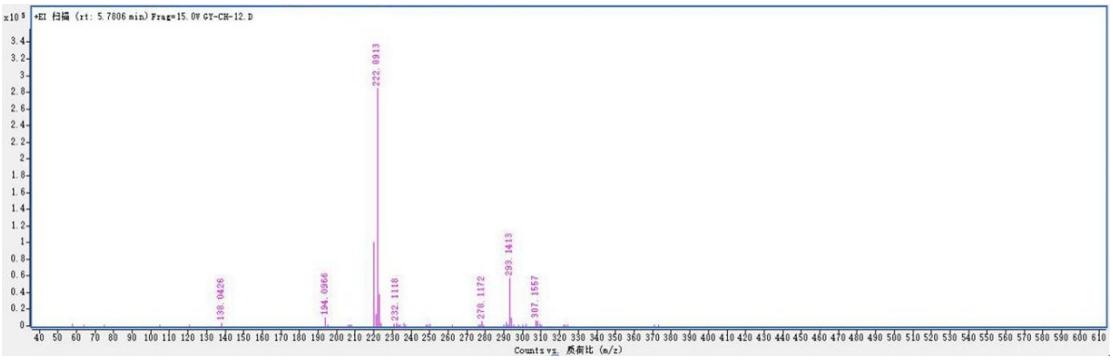
4f


Intens.
x10^9
20190411-2-308.13-POS_000001.d: +MS
1+
309.13907
1+
310.14248
1+
311.14594
20190411-2-308.13-POS_00001.d:C22H17N2, 309.13862

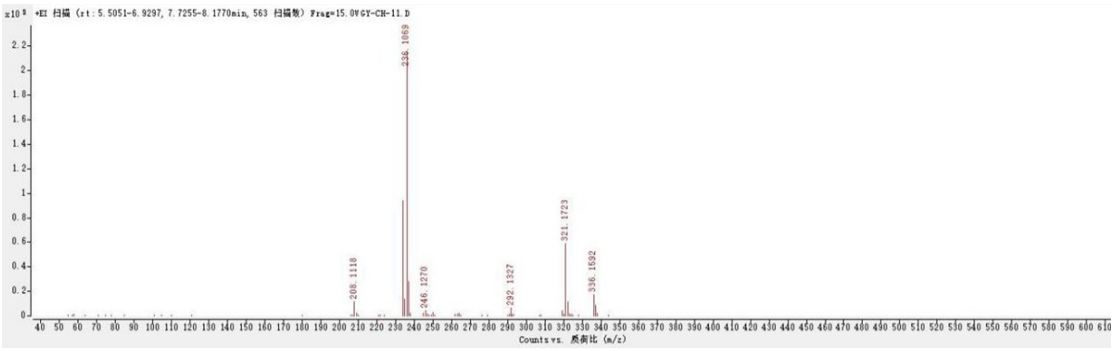
5a


208.0757
180.0808
264.1016
279.1256
295.1195
Counts vs. 质荷比 (m/z)

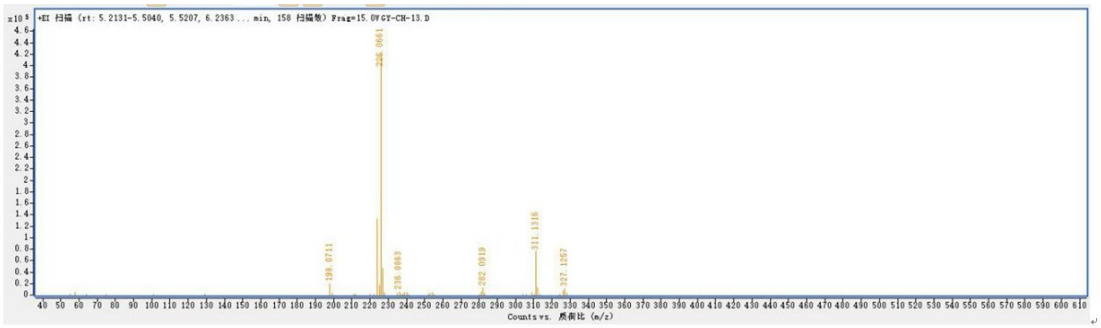
5b


x10 5
+EI 扫描 (rt: 5.7806 min) Frag=15.0V GY-CH-12.D
222.0913
299.1413
138.0426
194.0966
232.1118
270.1172
307.1557
Counts vs. 质荷比 (m/z)

5c


x10 5
+EI 扫描 (rt: 5.5051-6.9297, 7.7255-8.1770min, 563 扫描数) Frag=15.0VGY-CH-11.D
236.1069
321.1723
208.1118
246.1270
292.1527
336.1932
Counts vs. 质荷比 (m/z)

5d


x10 5
+EI 扫描 (rt: 5.2131-5.5040, 5.5207, 6.2363 ... min, 158 扫描数) Frag=15.0VGY-CH-13.D
226.0661
311.1316
198.0711
236.0883
282.0919
327.1257
Counts vs. 质荷比 (m/z)