

Supplementary Information

Microwave-Assisted Convenient Syntheses of 2-Indolizine Derivatives from Morita-Baylis-Hillman Adducts: New *in silico* Potential Ion Channel Modulators

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Spectroscopy data

2-[hydroxy(pyridine-2-yl)methyl] acrylonitrile (1). ¹H NMR (200 MHz, CDCl₃) δ 7.84(d, 1H, *J* 8 Hz), 7.65 (s, 1H), 7.32(d, 1H, *J* 8 Hz), 6.78 (m, 1H), 6.61(m, 2H). ¹³C NMR (50 MHz, CDCl₃) δ 97.90, 103.14, 113.75, 117.21, 118.20, 120.19, 120.34, 125.79, 133.31 IR (KBr) $\nu_{\max}/\text{cm}^{-1}$ 3128.54(C-H sp²), 2229.71(CN), 1635.64 and 1404.18(C=C).

Methyl indolizine-2-carboxylate (2) ¹H NMR (200 MHz, CDCl₃) δ 7.80 (m, 2H), 7.31(d, 1H *J* 8 Hz), 6.81 (sl, 1H), 6.66 (m, 1H), 6.50 (m, 1H), 3.87 (s, 1H). ¹³C NMR (50 MHz, CDCl₃) δ 52.13, 101.08, 112.95, 116.60, 118.85, 120.29, 120.96, 126.06, 133.46, 166.29.

Indolizine-2-carboxylic acid (3) ¹H NMR (200 MHz, CDCl₃) δ 12.36 (sl, 1H, OH), 8.27 (d, 1H *J* 6, Hz), 8.05 (s, 1H), 7.44 (d, 1H, *J* 8 Hz), 6.74 (m, 3H). ¹³C NMR (50 MHz, CDCl₃) δ 101.25, 113.22, 117.73, 119.68, 121.03, 121.29, 127.46, 133.43, 167.10 IR (KBr) $\nu_{\max}/\text{cm}^{-1}$ 2920.23(O-H), 1670.35(C=O).

Indolizin-2-ylmethanamine (4) ¹H NMR (200 MHz, CDCl₃) δ 7.86 (m, 1H), 7.14 (s, 1H), 7.05 (d, 1H, *J* 8), 6.37 (m, 1H), 6.20 (m, 1H), 6.03 (s, 1H), 3.51 (s, 2H).

¹³C NMR (50 MHz, CDCl₃) δ 98.98, 105.86, 110.64, 111.61, 117.88, 119.53, 126.80, 133.42; IR (KBr) $\nu_{\max}/\text{cm}^{-1}$ 3275.13(NH), 3109.25, 2920.23(C-H sp²), 2850.79(C-H sp³), 1589.34(N-H), 1300.02(C-N).

Indolizin-2-ylmethanol (5) ¹H NMR (200 MHz, CDCl₃) δ 7.86 (m, 1H), 7.14 (s, 1H), 7.05 (d, 1H, *J* 8), 6.37 (m, 1H), 6.20 (m, 1H), 6.03 (s, 1H), 3.51(s, 2H). ¹³C NMR (50 MHz, CDCl₃) δ 142.73, 141.19, 136.29, 129.39, 127.53, 121.61, 119.94, 108.47, 68.01; IR (KBr) $\nu_{\max}/\text{cm}^{-1}$ 3290.56(O-H), 2916.37(C-H sp³), 2866.22(C-H sp³), 1458.18(-CH₂-), 1138.00(C-O).

2-[hydroxyl(2-pyridinyl)methyl] acrylate (6) ¹H NMR (200 MHz, CDCl₃) δ 3.71 (s, 3H); 5.61 (s, 1H); 5.96 (s, 1H); 6.34 (s, 1H); 7.19 (ddd, 1H, *J* 7.6/5/0.6 Hz); 7.40 (d, 1H, *J* 8 Hz); 7.66 (ddd, 1H, *J* 7.8/7.6/1.6 Hz); 8.51 (m, 1H). ¹³C NMR (50 MHz, CDCl₃) δ 51.82; 72.01; 121.22; 122.61; 126.83; 136.82; 141.56; 148.16; 159.40; 166.47.

2-[Hydroxy(pyridin-2-yl)methyl] acrylonitrile (7) ¹H NMR (200 MHz, CDCl₃) δ 5.00 (sl, 1H); 5.31 (sl, 1H); 6.06 (s, 1H); 6.23 (s, 1H); 7.31 (m, 1H); 7.41 (d, 1H, *J* 7.8 Hz); 7.77 (ddd, 1H, *J* 7.8/7.6/1.6 Hz); 8.57 (m, 1H). ¹³C NMR (50 MHz, CDCl₃) δ 74.31; 118.15; 122.69; 125.16; 127.07; 132.54; 139.01; 149.80; 157.48.

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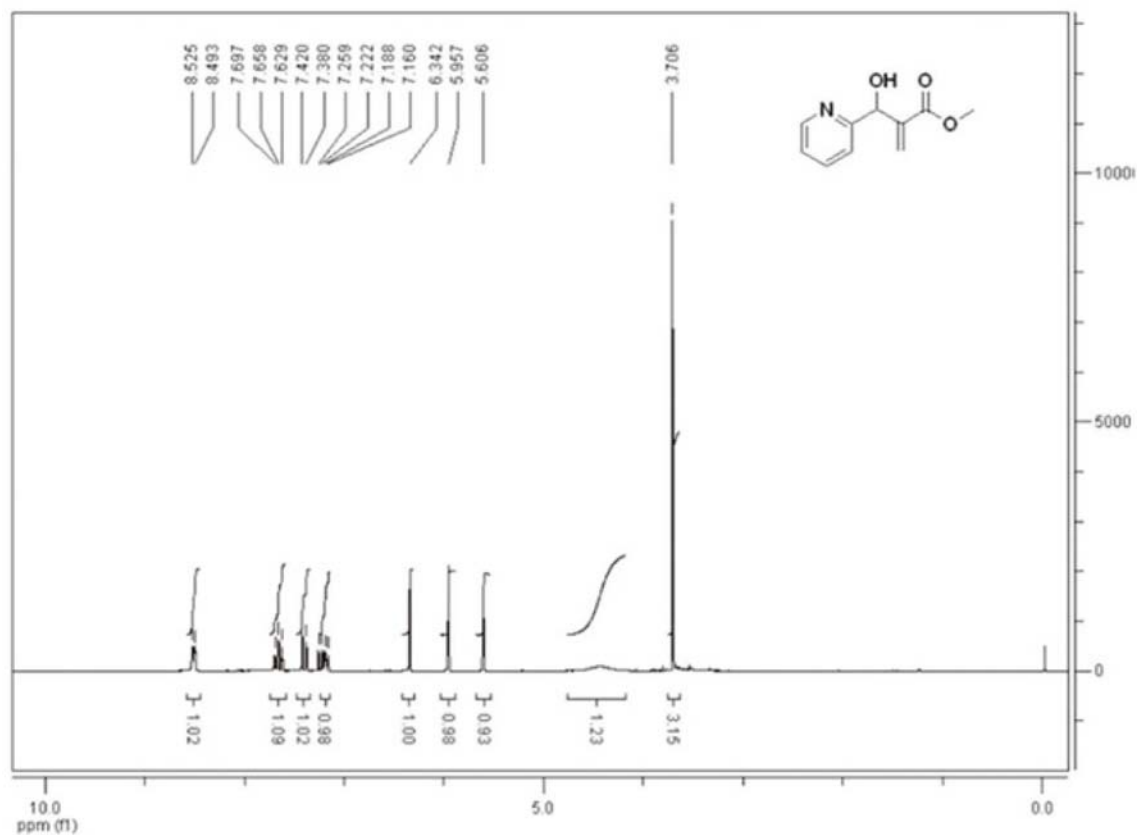


Figure S1. ¹H NMR spectrum of compound 6.

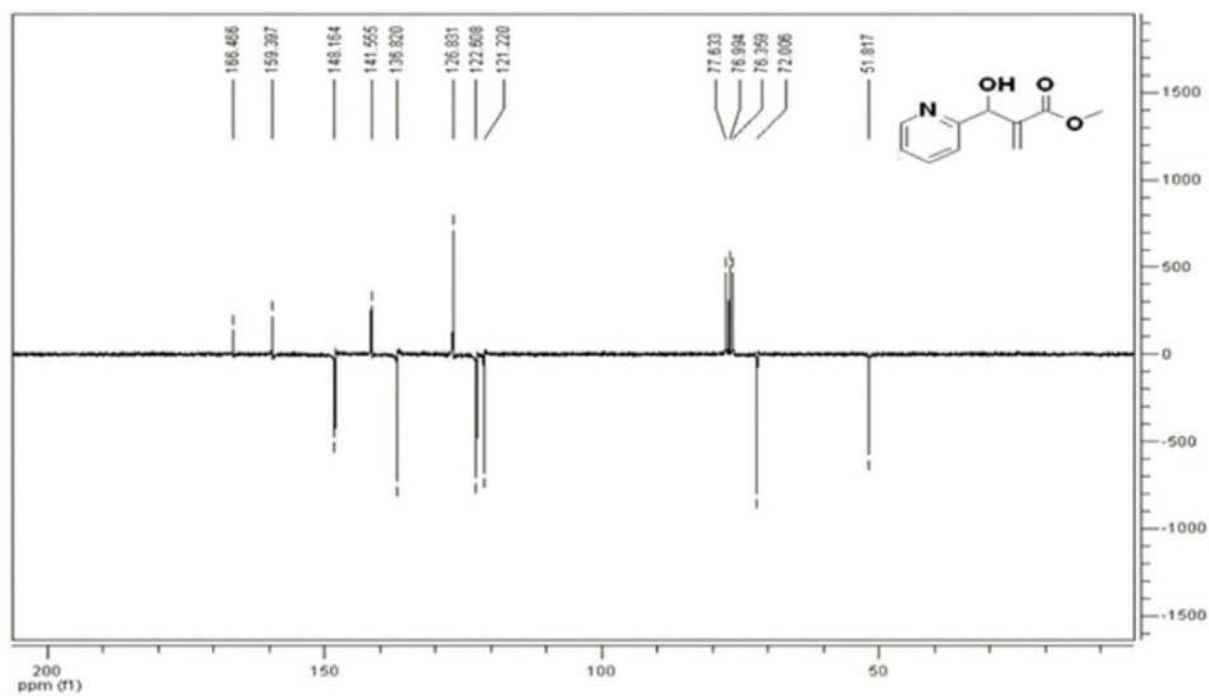


Figure S2. ¹³C NMR spectrum of compound 6.

2-[Hydroxy(pyridin-2-yl)methyl] acrylonitrile (7)

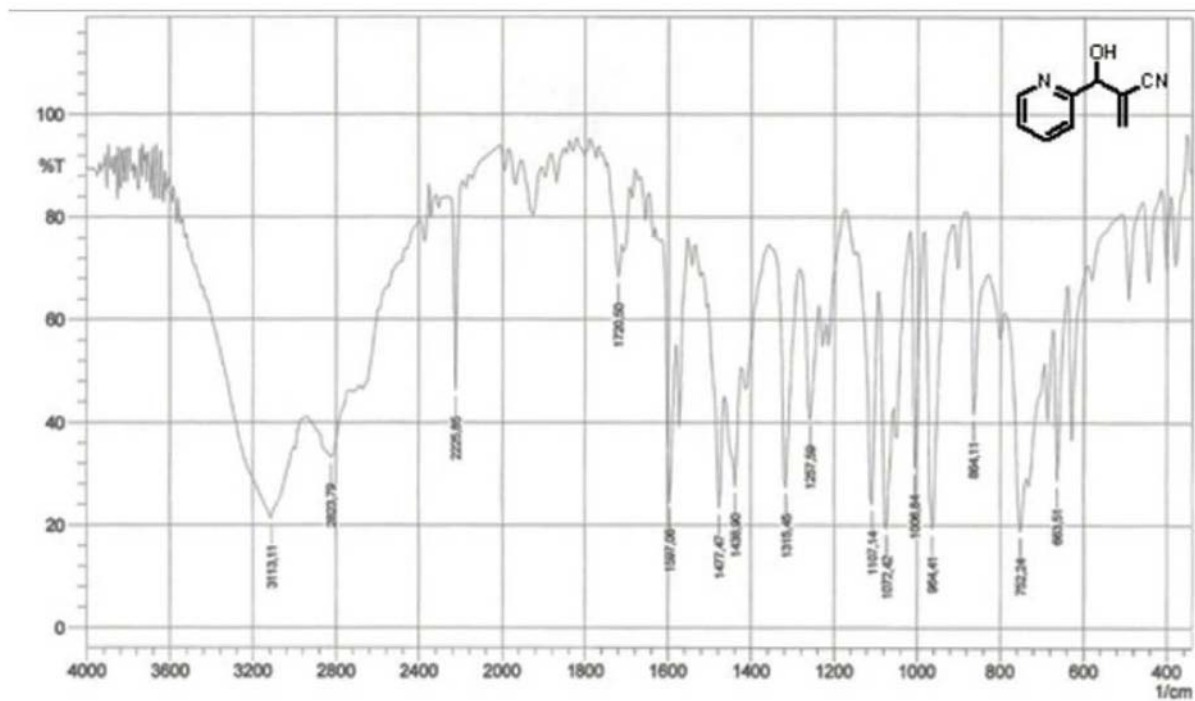
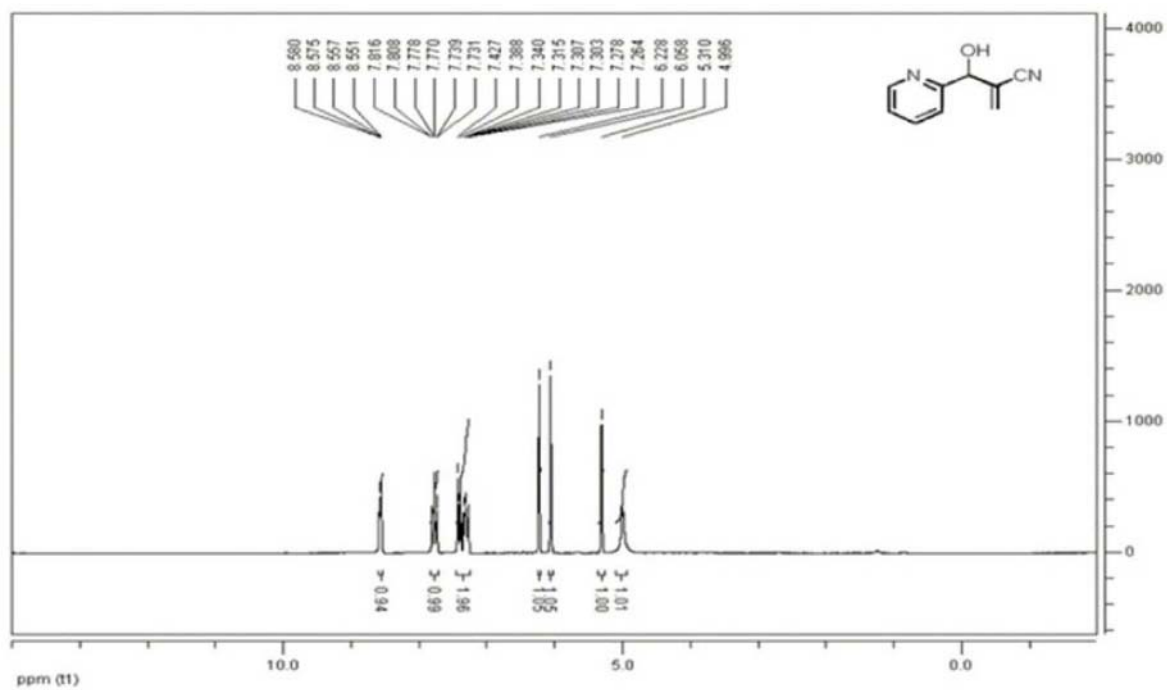


Figure S3. FTIR spectrum of compound 7.

Figure S4. ¹H NMR spectrum of compound 7.

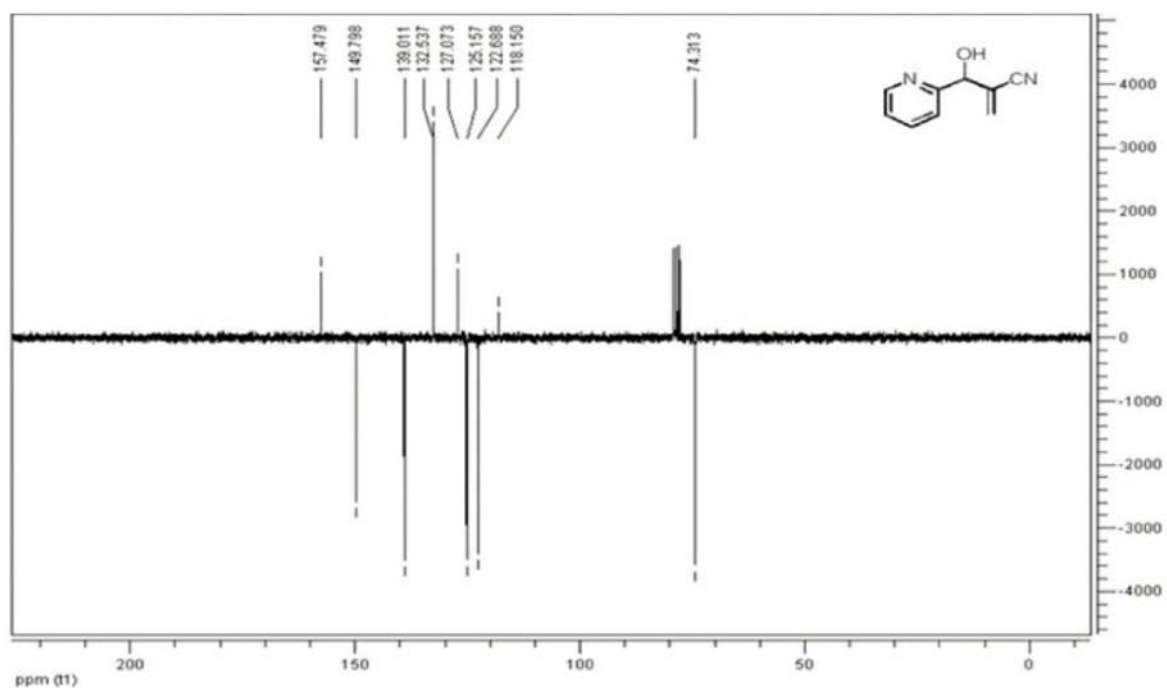


Figure S5. ¹³C NMR spectrum of compound 7.

Indolizine-2-carbonitrile (1)

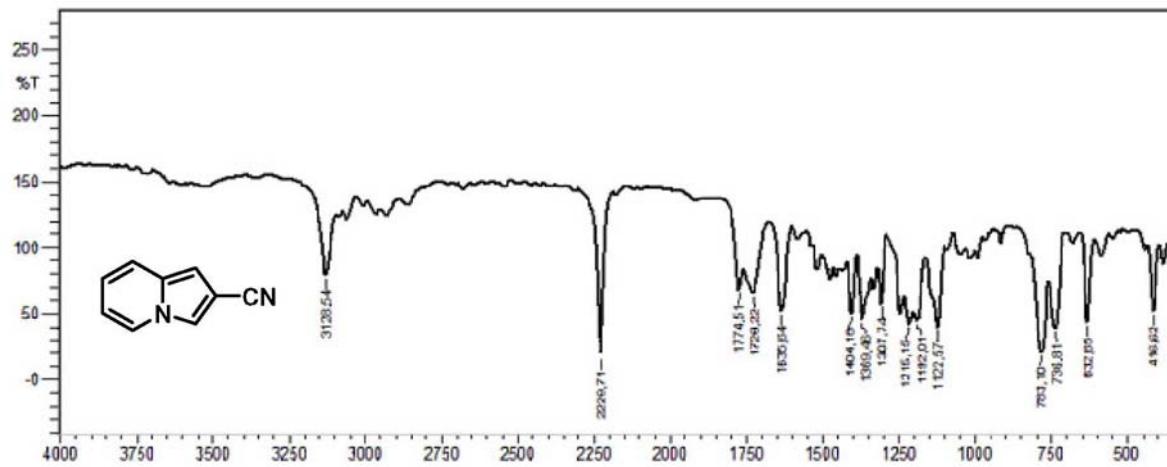


Figure S6. FTIR spectrum of compound 1.

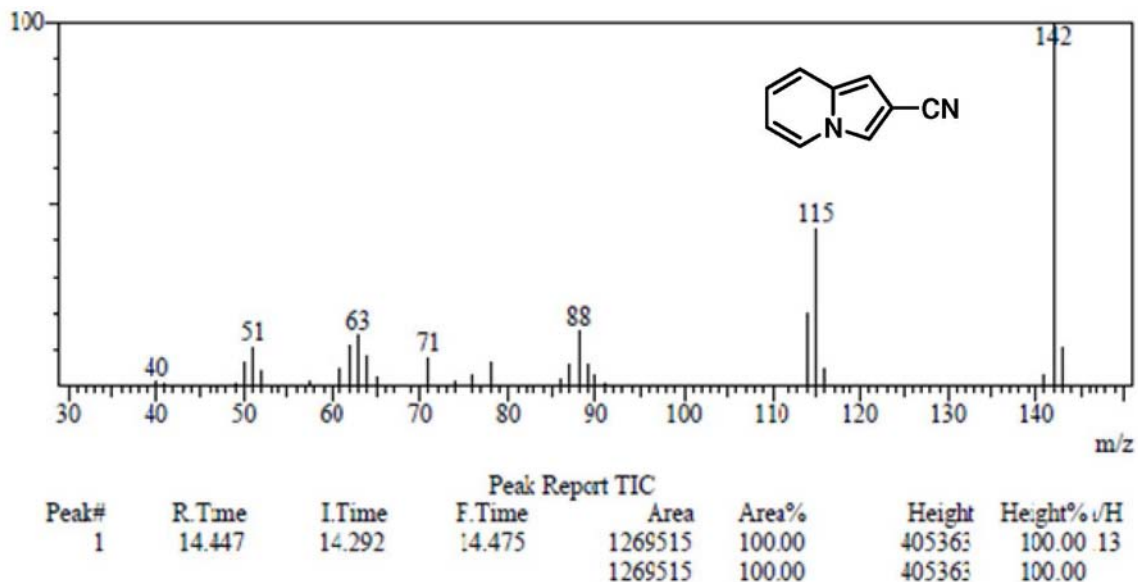


Figure S10. EI-MS spectra of compound 1.

Methyl indolizine-2-carboxylate (2)

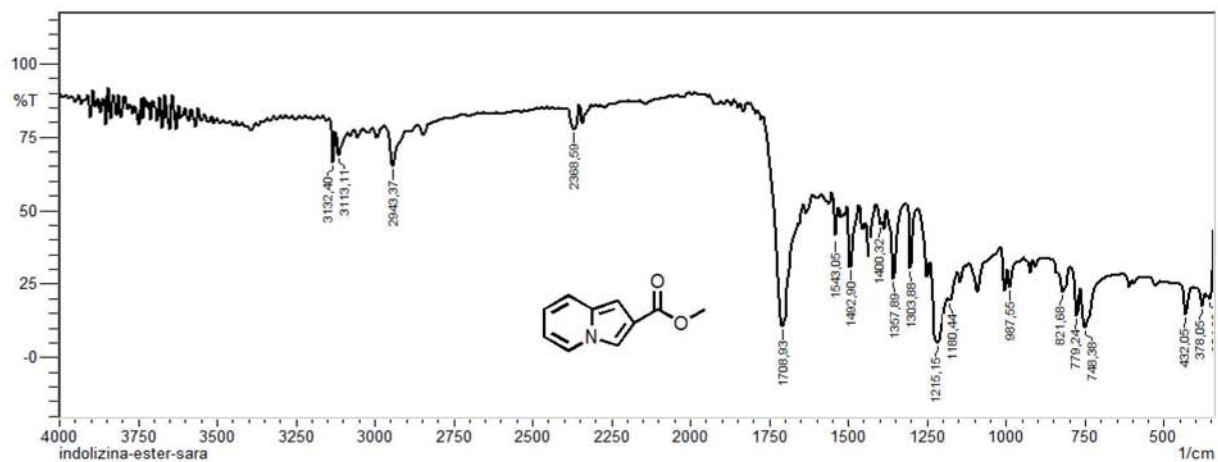
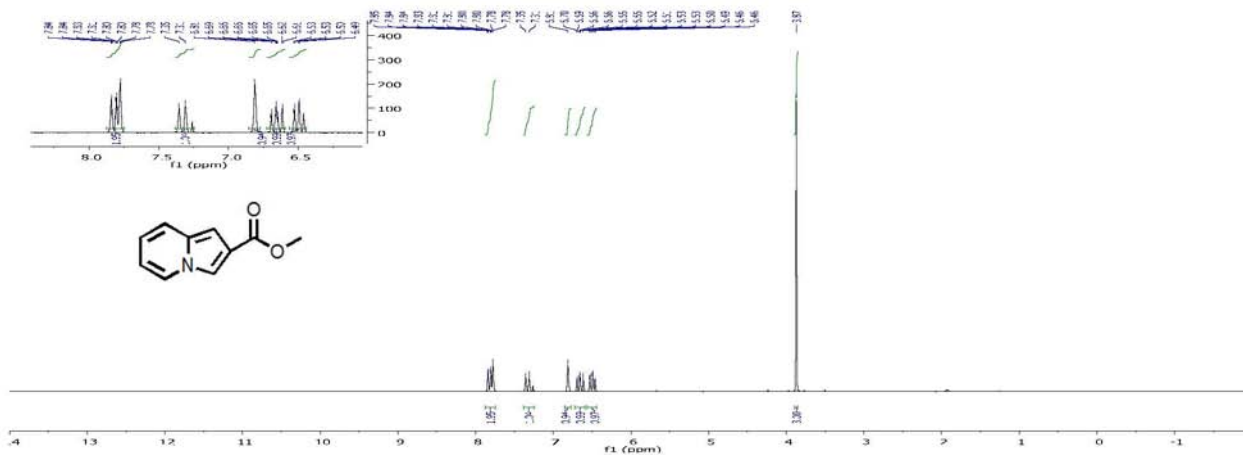


Figure S11. FTIR spectrum of compound 2.

Figure S12. ¹H NMR spectrum of compound 2.

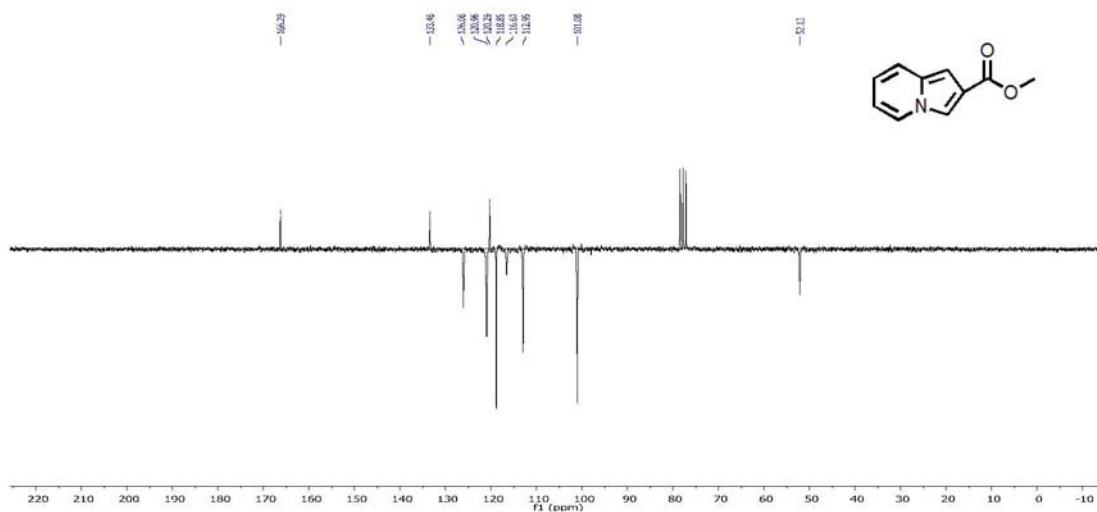
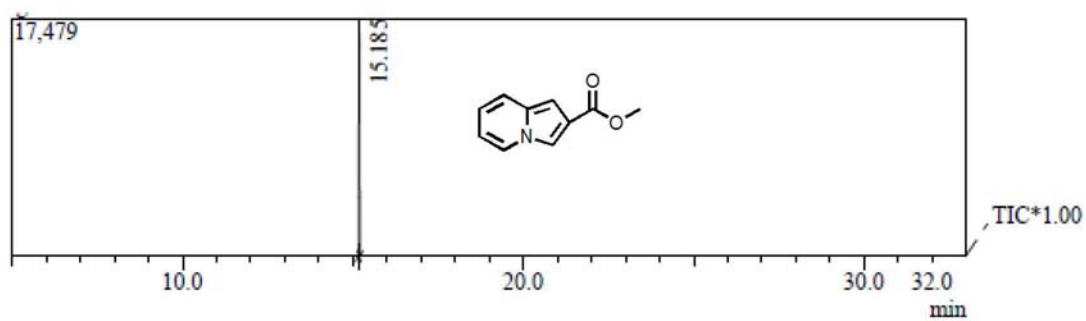
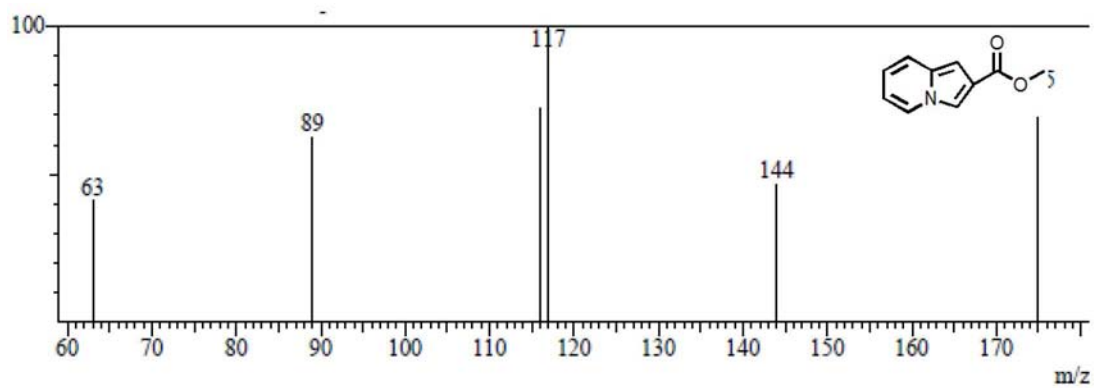
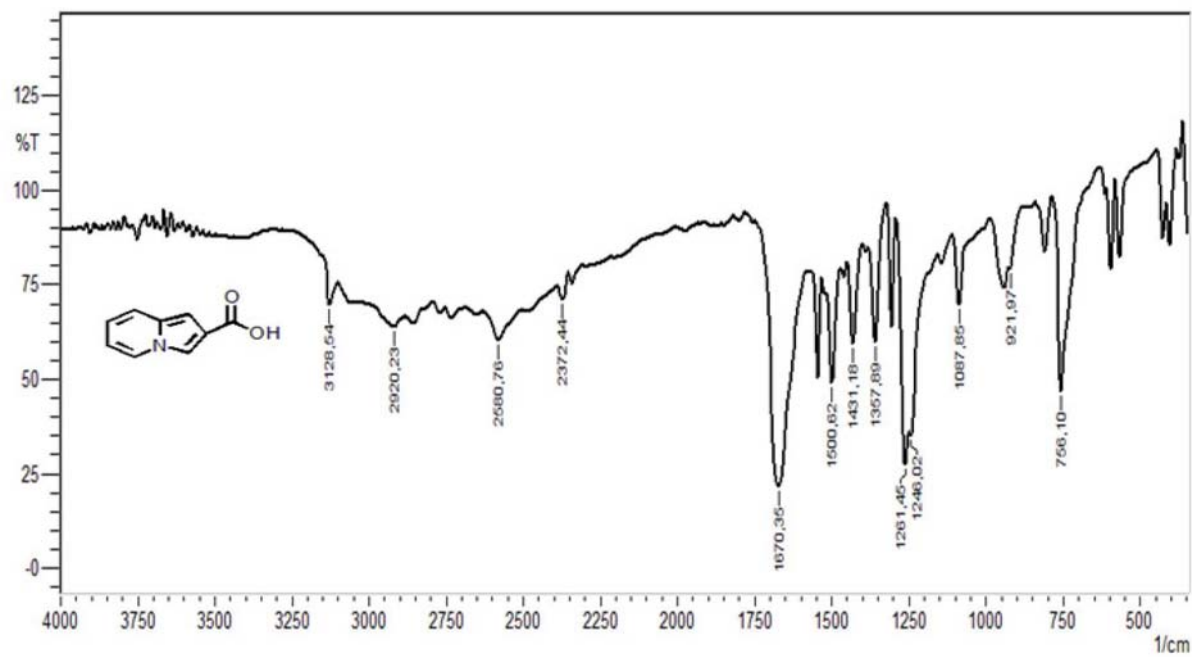
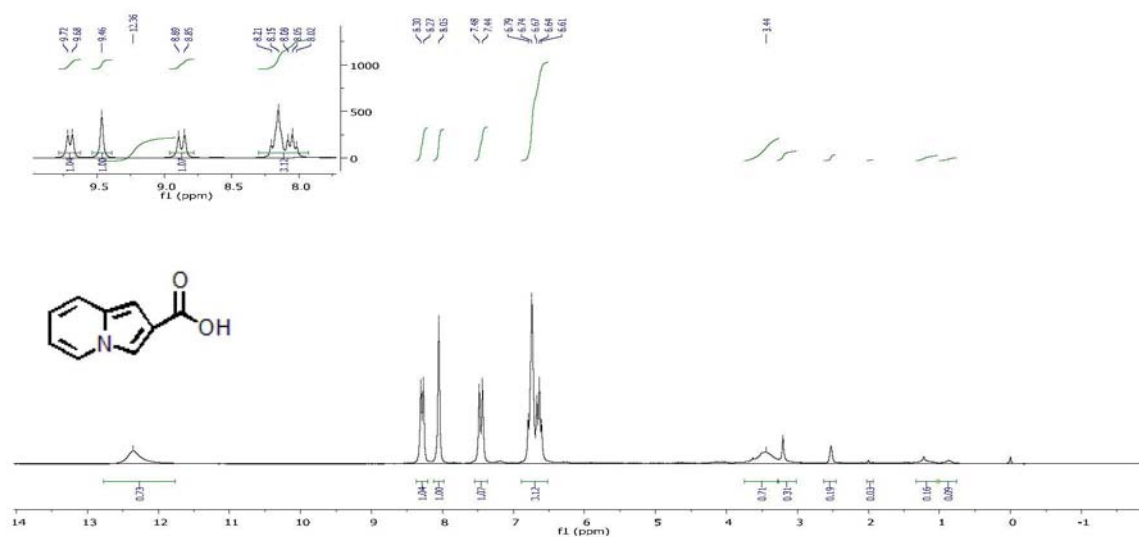
Figure S13. ^{13}C NMR spectrum of compound 2.

Figure S14. HRGC Chromatogram of compound 2.



Peak Report TIC							
Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height% A/H
1	15.185	15.158	15.200	24623	100.00	17479	100.00 1.41
				24623	100.00	17479	100.00

Figure S15. EI-MS spectra of compound 2.

Indolizine-2-carboxylic acid (**3**)Figure S16. FTIR spectrum of compound **3**.Figure S17. ^1H NMR spectrum of compound **3**.

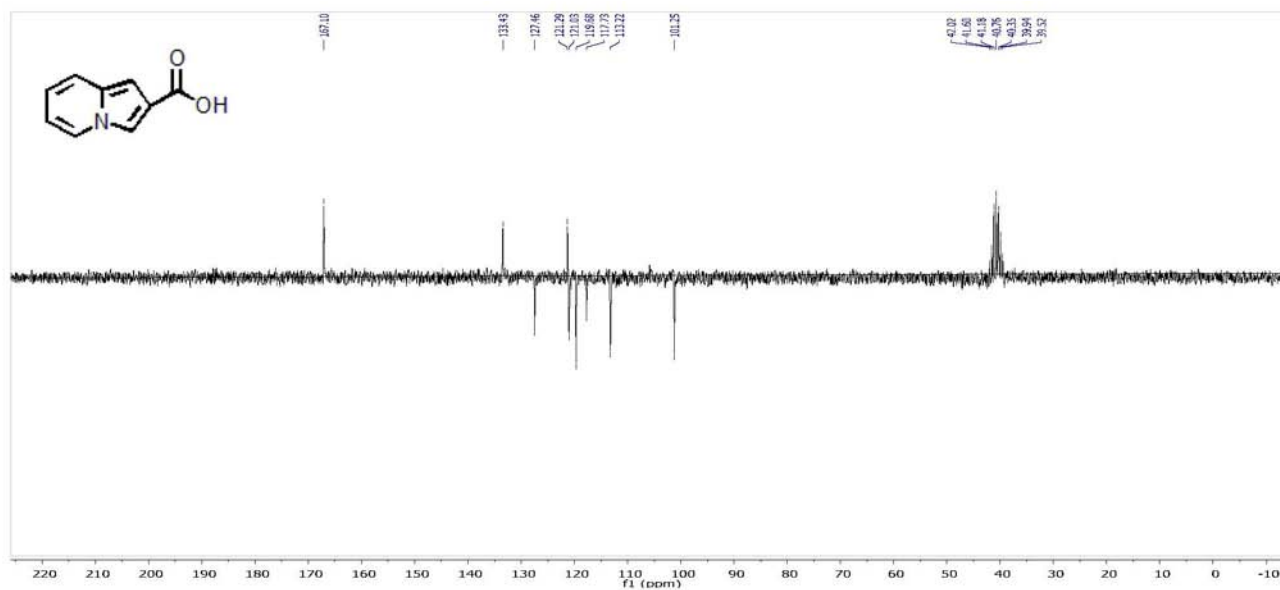


Figure S18. ¹³C NMR spectrum of compound 3.

Indolizin-2-ylmethanamine (4)

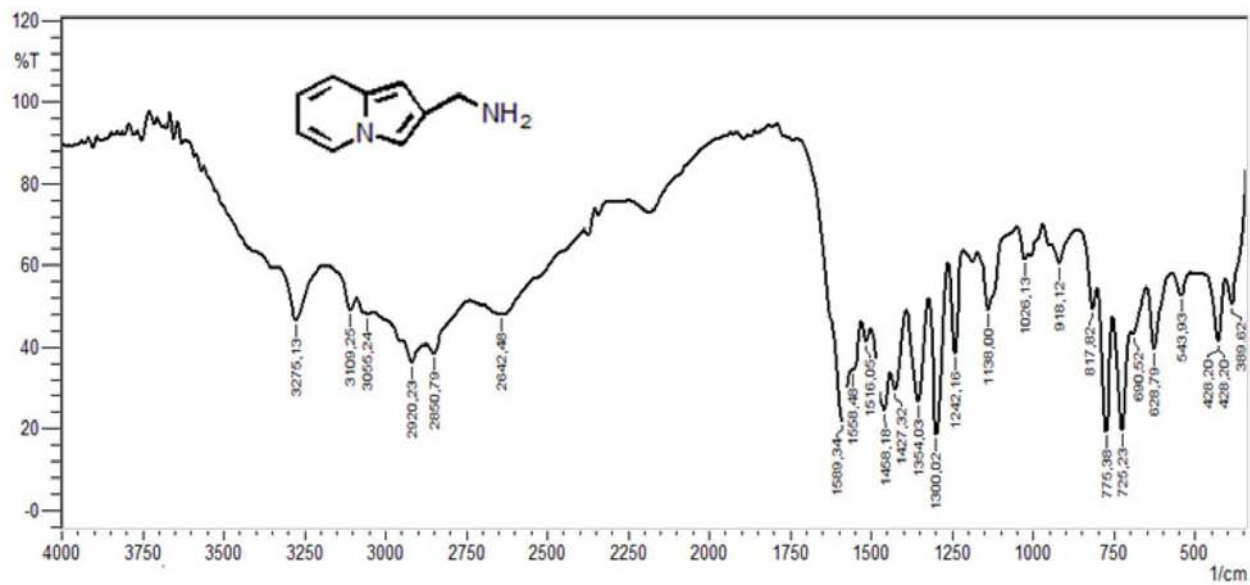


Figure S19. FTIR spectrum of compound 4.

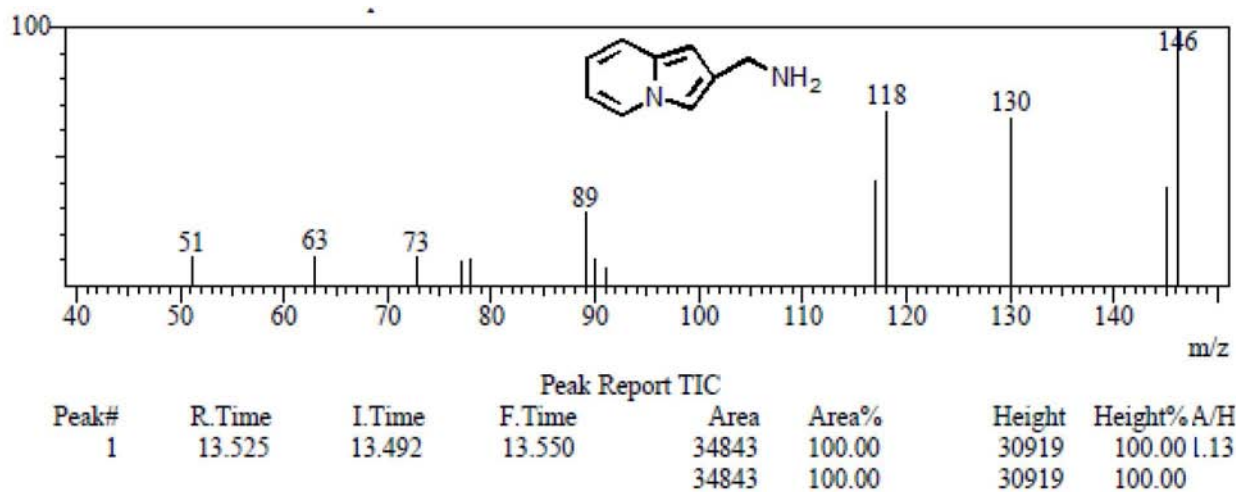


Figure S23. EI-MS spectra of compound 4.

Indolizin-2-ylmethanol (5)

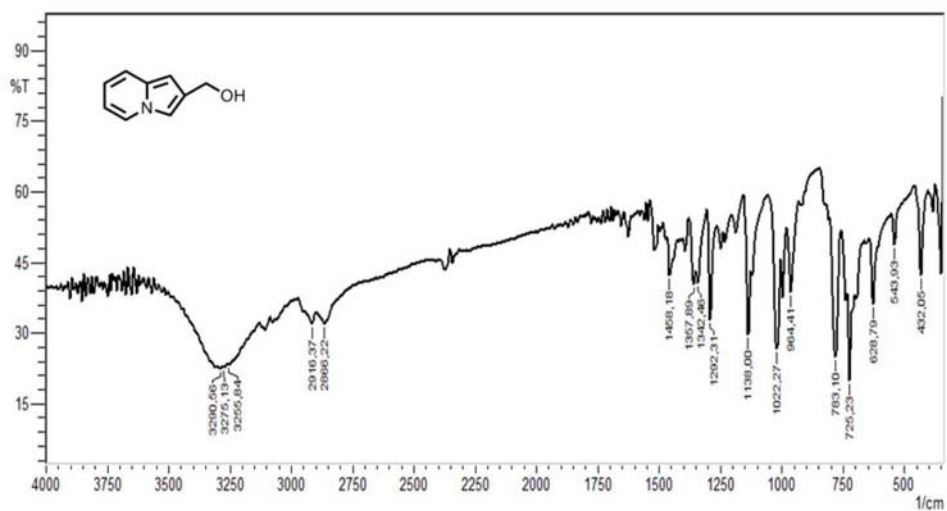


Figure S24. FTIR spectrum of compound 5.

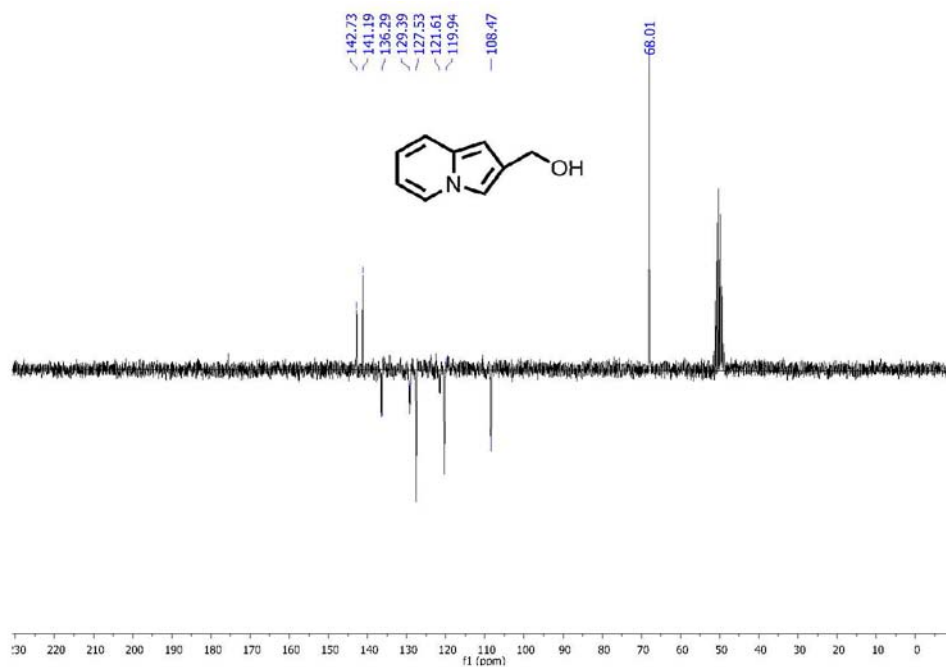


Figure S25. ¹³C NMR spectrum of compound 5.

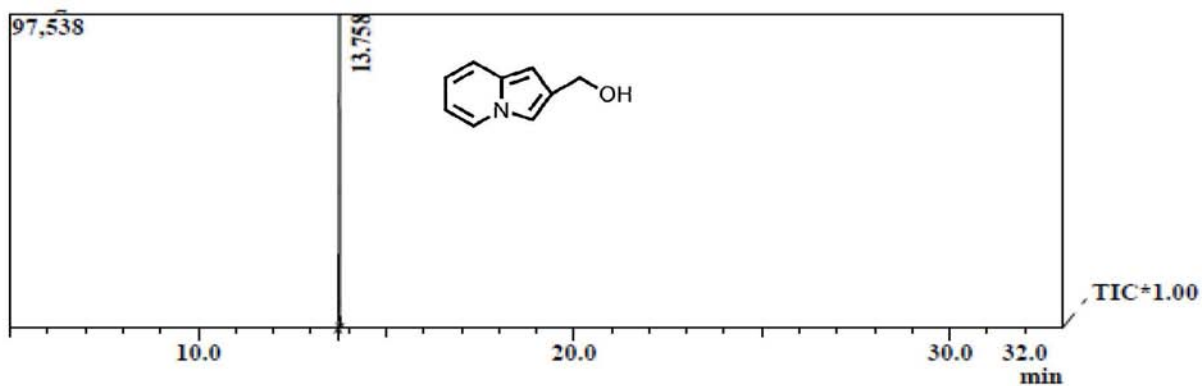


Figure S26. HRGC Chromatogram of compound 5.

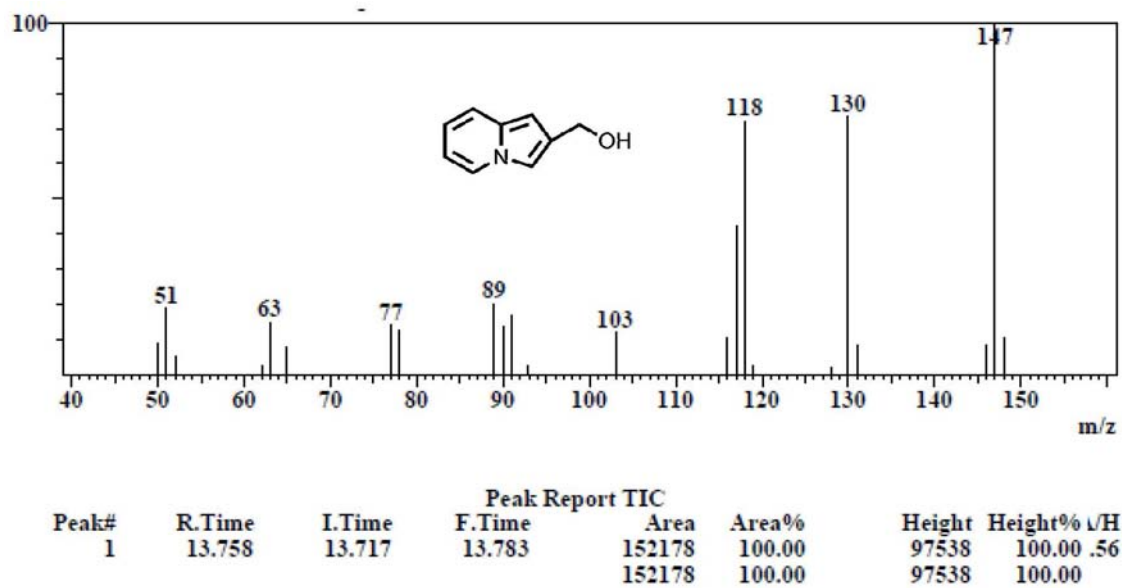


Figure S27. EI-MS spectra of compound 5.