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, 117.21, 118.20, 120.19, 120.34, 125.79, 133.31 IR (KBr) ν max/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 (s,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 (s,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) ν max/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) ν max/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).

2-[hydroxyl(2-pyridinyl)methyl] acrylate (6). ¹H NMR (200 MHz, CDCl₃) δ 3.71 (s, 3H); 5.61 (s, 1H); 5.31 (s, 1H); 6.06 (s,1H,OH), 8.27 (d, 1H J 6, Hz), 8.05 (s, 1H), 7.19 (ddd, 1H, J 7.8/5.6 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 (s, 1H); 5.31 (s, 1H); 5.06 (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 74.36, 117.88, 119.53, 126.80, 133.42; IR (KBr) ν max/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).
Figure S1. $^1$H NMR spectrum of compound 6.

Figure S2. $^{13}$C NMR spectrum of compound 6.
2-[Hydroxy(pyridin-2-yl)methyl] acrylonitrile (7)

Figure S3. FTIR spectrum of compound 7.

Figure S4. $^1$H NMR spectrum of compound 7.
Figure S5. $^{13}$C NMR spectrum of compound 7.

Indolizine-2-carbonitrile (1)

Figure S6. FTIR spectrum of compound 1.
Figure S7. $^1$H NMR spectrum of compound 1.

Figure S8. $^{13}$C NMR spectrum of compound 1.

Figure S9. HRGC Chromatogram of compound 1.
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Figure S10. EI-MS spectra of compound 1.

Methyl indolizine-2-carboxylate (2)

Figure S11. FTIR spectrum of compound 2.

Figure S12. $^1$H NMR spectrum of compound 2.
Figure S13. $^{13}$C NMR spectrum of compound 2.

Figure S14. HRGC Chromatogram of compound 2.

Figure S15. El-MS spectra of compound 2.
Indolizine-2-carboxylic acid (3)

Figure S16. FTIR spectrum of compound 3.

Figure S17. $^1$H NMR spectrum of compound 3.
Figure S18. $^{13}$C NMR spectrum of compound 3.

Indolizin-2-ylmethanamine (4)

Figure S19. FTIR spectrum of compound 4.
Figure S20. $^1$H NMR spectrum of compound 4.

Figure S21. $^{13}$C NMR spectrum of compound 4.

Figure S22. HRGC Chromatogram of compound 4.
Figure S23. EI-MS spectra of compound 4.

Indolizin-2-ylmethanol (5)

Figure S24. FTIR spectrum of compound 5.
Figure S25. $^{13}$C NMR spectrum of compound 5.

Figure S26. HRGC Chromatogram of compound 5.
Figure S27. EI-MS spectra of compound 5.