Supporting Information

Facile Synthesis of *N*-Dialkylaminomethyl-substituted Heterocycles

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Characterization Data for Compounds **4**, **6** & **7**

NMR spectra obtained in CDCl₃ at either 300 or 500 MHz (¹H) and either 75 or 125 MHz (¹³C)

1-[(Dimethylamino)methyl]imidazole 4a¹ ¹H NMR: δ 7.50 (s, 1H), 7.07 (s, 1H), 6.96 (s, 1H), 4.67 (s, 2H), 2.29 (s, 6H); ¹³C NMR: δ 137.1, 128.4, 119.4, 68.7, 41.4; LRMS(EI) *m/z* (rel intensity) 125 ([M]⁺ 2%), 68 (65%), 58 (100%).

1-(1-Pyrrolidinomethyl)imidazole 4b² ¹H NMR: δ 7.50 (s, 1H), 7.01 (s, 1H), 6.96 (s, 1H), 4.79 (s, 2H), 2.6-2.5 (m, 4H), 1.8-1.7 (m, 4H); ¹³C NMR: δ 137.0, 128.4, 119.2, 64.1, 49.6, 23.0; LRMS(EI) *m/z* (rel intensity) 84 ([M-Im]⁺ 87%), 68 (100%).

1-(1H-Imidazol-1-ylmethyl)piperidine 4c³ ¹H NMR: δ 7.47 (s, 1H), 7.03 (s, 1H), 6.93 (s, 1H), 4.68 (s, 2H), 2.5-2.4 (m, 4H), 1.6-1.5 (m, 4H), 1.4-1.3 (m, 2H); ¹³C NMR: δ 137.1, 128.3, 119.4, 68.8, 50.5, 25.2, 23.2; LRMS(EI) *m/z* (rel intensity) 98 ([M-Im]⁺ 88%), 68 (100%).

4-(1H-Imidazol-1-ylmethyl)morpholine 4d³ ¹H NMR: δ 7.51 (s, 1H), 7.07 (s, 1H), 6.97 (s, 1H), 4.67 (s, 2H), 3.7-3.6 (m, 4H), 2.5-2.4 (m, 4H); ¹³C NMR: δ 137.2, 128.9, 119.3, 68.3, 66.2, 49.8; mp 68-71 °C (lit³ 69-71).

1-(1H-Imidazol-1-ylmethyl)-4-methylpiperazine 4e² ¹H NMR: δ 7.48 (s, 1H), 7.02 (s, 1H), 6.94 (s, 1H), 4.67 (s, 2H), 2.6-2.4 (m, 8H), 2.25 (s, 3H); ¹³C NMR: δ 137.1, 128.7, 119.2, 67.9, 54.2, 49.3, 45.5; LRMS(EI) *m/z* (rel intensity) 113 ([M-Im]⁺ 100%), 68 (85%); mp 70-77°C.

1-(Dimethylamino)methyl-2-methylimidazole 6a⁴ ¹H NMR: δ 6.89 (s, 1H), 6.88 (s, 1H), 4.46 (s, 2H), 2.40 (s, 3H), 2.28 (s, 6H); ¹³C NMR: δ 144.6, 126.0, 119.6, 67.8, 41.7, 12.6; LRMS(EI) *m/z* (rel intensity) 139 ([M]⁺ 5%), 82 (92%), 58 (100%).

3,5-Dimethyl-1-[(dimethylamino)methyl]pyrazole 6b⁵ ¹H NMR: δ 5.81 (s, 1H), 4.58 (s, 2H), 2.30 (s, 6H), 2.27 (s, 3H), 2.22 (s, 3H); ¹³C NMR: δ 147.1, 139.5, 105.2, 70.1, 42.3, 13.3, 10.9; LRMS(EI) *m/z* (rel intensity) 153 ([M]⁺ 2%), 96 (11%), 58 (100%).

1-[(Dimethylamino)methyl]benzimidazole 6d⁶ ¹H NMR: δ 7.91 (s, 1H), 7.85-7.75 (m, 1H), 7.5-7.4 (m, 1H), 7.3-7.2 (m, 2H) 4.81 (s, 2H), 2.31 (s, 6H); ¹³C NMR: δ 143.5, 143.4, 134.3, 123.0, 122.0, 120.0, 110.2, 67.2, 42.3; LRMS(EI) *m/z* (rel intensity) 118 ([M-Me₂NCH]⁺ 7%), 58 (100%); mp 38-49 °C.

1-(Dimethylamino)methyl-2-methylbenzimidazole 6e⁷ ¹H NMR: δ 7.7-7.6 (m, 1H), 7.4-7.3 (m, 1H), 7.2-7.1 (m, 2H) 4.44 (s, 2H), 2.54 (s, 3H), 2.21 (s, 6H); ¹³C NMR: δ 151.9, 141.9, 135.3, 121.7, 121.4, 118.3, 109.4, 65.7, 42.2, 13.6; LRMS(EI) *m/z* (rel intensity) 132 ([M-Me₂NCH]⁺ 100%).

1-[(Dimethylamino)methyl]-1H-indole-3-carboxaldehyde 6f⁸ ¹H NMR: δ 10.02 (s, 1H), 8.4-8.3 (m, 1H), 7.76 (s, 1H), 7.5-7.4 (m, 1H), 7.4-7.3 (m, 2H), 4.80 (s, 2H), 2.34 (s, 6H); ¹³C NMR: δ 184.7, 138.8, 137.8, 125.1, 124.0, 122.8, 121.8, 118.1, 110.7, 69.4, 42.5; mp 58-59 °C (lit⁸ 60-60.5).

1-[1-(Dimethylamino)methyl]-(1H-indol-3-yl)ethanone 6g⁸ ¹H NMR: δ 8.4-8.3 (m, 1H), 7.78 (s, 1H), 7.5-7.4 (m, 1H), 7.3-7.2 (m, 2H), 4.76 (s, 2H), 2.52 (s, 3H), 2.33 (s, 6H); ¹³C NMR: δ 193.0, 137.3, 135.1, 126.0, 123.1, 122.3, 122.1, 116.9, 110.3, 69.1, 42.4, 27.3; LRMS(EI) *m/z* (rel intensity) 216 ([M]⁺ 4%), 159 (36%), 144 (72%), 58 (100%); mp 72-79 °C.

1-(Dimethylamino)methyl-3-(2-phenylethenyl)-1H-indole 6h⁸ ¹H NMR: δ 7.97 (d, *J* = 8.1 Hz, 1H), 7.6-7.1 (m, 11H), 4.72 (s, 2H), 2.31 (s, 6H); ¹³C NMR: δ 138.5, 137.9, 128.6, 128.0, 126.5, 126.3, 125.7, 125.3, 122.4, 121.4, 120.3, 120.1, 114.4, 110.3, 68.8, 42.7; LRMS(EI) *m/z* (rel intensity) 276 ([M]⁺ 58%), 217 (20%), 58 (100%); mp 81-84 °C.

3-(Dimethylamino)methyl-2(3H)-benzothiazolethione 6j⁹ ¹H NMR: δ 7.5-7.2 (m, 4H), 5.05 (s, 2H), 2.44 (s, 6H); ¹³C NMR: δ 190.6, 141.9, 126.9, 126.6, 124.6, 120.7, 113.6, 67.4, 43.0; mp 74-77 °C (lit⁹ 79-80).

9-(Dimethylamino)methyl-9H-carbazole 6k¹⁰ ¹H NMR: δ 8.05 (d, J = 7.8 Hz, 2H), 7.5-7.4 (m, 4H), 7.3-7.2 (m, 2H), 4.77 (s, 2H), 2.31 (s, 6H); ¹³C NMR: δ 141.0, 125.7, 123.0, 120.1, 119.3, 109.4, 66.0, 43.0; LRMS(EI) m/z (rel intensity) 224 ($[M]^+$ 5%), 167 (49%), 58 (100%); mp 68-70 °C (lit¹⁰ 68-70).

1,3-Bis[(dimethylamino)methyl]indole 7a¹¹ ¹H NMR: δ 7.66 (d, J = 7.5 Hz, 1H), 7.39 (d, J = 7.5 Hz, 1H), 7.19 (dd, J = 7.5 Hz, 1H), 7.10 (dd, J = 7.5 Hz, 1H), 7.08 (s, 1H), 4.68 (s, 2H), 3.62 (s, 2H), 2.27 (s, 6H), 2.26 (s, 6H); ¹³C NMR: δ 137.1, 128.3, 128.0, 121.6, 119.3, 119.1, 111.7, 109.8, 68.5, 54.2, 45.1, 42.6; LRMS(EI) m/z (rel intensity) 231 ($[M]^+$ 7%), 129 (100%), 102 (70%), 58 (83%).

1,3-Bis[(dimethylamino)methyl]-1,3-dihydro-2H-benzimidazole-2-thione 7c¹² ¹H NMR: δ 7.4-7.3 (m, 2H), 7.3-7.2 (m, 2H), 5.03 (s, 4H), 2.43 (s, 12H); ¹³C NMR: δ 171.6, 132.5, 123.0, 110.2, 67.1, 43.3; mp 78-80 °C (lit¹² 80-81).

1,3-Bis[(dimethylamino)methyl]-2-benzimidazolinone 7d¹³ ¹H NMR: δ 7.05-6.95 (m, 4H), 4.48 (s, 4H), 2.28 (s, 12H); ¹³C NMR: δ 155.1, 129.8, 121.2, 108.4, 63.6, 42.6; LRMS(EI) m/z (rel intensity) 248 ($[M]^+$ 9%), 58 (100%).

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