Supporting information

A General and Efficient Five-Step One-Pot Procedure Leading to Nitrogen-bridgehead Heterocycles Containing an Imidazole Ring

Alexis Parenty, Yu-Fei Song, Craig Richmond and Leroy Cronin*

*WestCHEM, University of Glasgow, Chemistry Department, Glasgow, G12 8QQ, UK
L.Cronin@chem.gla.ac.uk*

Table of contents

Instruments and Materials.....	S2
Methodology.....	S3
Synthetic procedures and analytical data.....	S3
General procedure for the synthesis of 2-bromoethyl-pyridinium derivatives (Activation step of Method 1).....	S3
General procedure for the synthesis of acetyl-pyridinium derivatives (Activation step of Method 2).....	S7
General procedure for the synthesis of Imidazo[1,2-a]pyridine derivatives (Ips) with unsubstituted imidazole moiety (Method 1).....	S10
General procedure for the synthesis of Imidazo[1,2-a]pyridine derivatives (Ips) with substituted imidazole moiety (Method 2).....	S14
Copies of NMR spectra.....	S17

1. Instruments and Materials

All reactions were carried out using oven-dried glassware. All starting materials and solvents were commercially available (reagent grade) and used as supplied, from Aldrich Chemical Co., without further purification.

^1H NMR and ^{13}C NMR were recorded using a Bruker DPX 400 spectrometer operating at 400 and 100 MHz, respectively. Chemical shifts (δ) are given in ppm relative to residual solvent peak. Coupling constants (J) are given in Hz. The multiplicities are expressed as follows: s = singlet, d = doublet, t = triplet, q = quartet. Infra-red spectral analyses were performed on a JASCO 410 spectrophotometer, using a KBr disc; peaks are quoted in wavenumbers (cm^{-1}) and their relative intensity are reported as follows: s = strong, m = medium, w = weak. UV-Vis spectroscopy was performed on Shimadzu UV-310PC UV-VIS-NIR scanning spectrophotometer. Mass spectra were obtained using a JEOL JMS 700 spectrometer operating, in FAB, EI or CI mode. Microanalyses were performed on a CE-440 elemental analyzer. Melting points were determined on a digital IA9000 series melting point apparatus, using capillary tubes.

2. Methodology

a. Synthetic procedures and analytical data

i. General procedure for the synthesis of 2-bromoethyl-pyridinium derivatives (Activation step of Method 1), **1a-f**

Pyridine derivative (30 mmol) was dissolved in 1,2-dibromoethane (114.2 g; 50 mL; 608 mmol) and stirred at 90 °C for five days. Any precipitate formed during the reaction was recovered by filtration daily. After each filtration, the precipitate was rinsed with an additional 5 mL of 1,2-dibromoethane and the mother liquor stirred at 90 °C until the next filtration. The reaction was complete when no more precipitate formed. The precipitates were combined and washed with acetone to give, after drying, the corresponding 2-bromoethyl-pyridinium derivative **1a-f**, as a beige powder.

1. 2-bromo-ethyl-phenanthridinium bromide, **1a**

2-bromo-ethyl-phenanthridinium **1a** (10.45 g; 28.5 mmol), was isolated as a beige powder in a 95% yield; **mp**: 234-235 °C (dec.); ¹H NMR (D₂O, 400 MHz): δ 9.81 (s, 1H), 8.72 (d, 1H, *J*=7.2 Hz), 8.63 (d, 1H, *J*=7.2 Hz), 8.37 (d, 1H, *J*=7.2 Hz), 8.26 (d, 1H, *J*=7.2 Hz), 8.18 (t, 1H, *J*=7.2 Hz), 7.98 (t, 1H, *J*=7.2 Hz), 7.90 (m, 2H), 5.37 (t, 2H, *J*=5.8 Hz), 4.05 (t, 2H, *J*=5.8 Hz); ¹³C NMR (D₂O, 100 MHz): δ 155.27 (CH), 139.03 (CH),

135.59 (C), 133.18 (CH), 132.78 (C), 132.58 (CH), 130.85 (CH), 130.72 (CH), 126.57 (C), 125.13 (CH), 123.32 (C), 123.00 (CH), 118.91 (CH), 58.87 (CH₂), 29.41 (CH₂); **IR** (KBr, cm⁻¹): 2947(w), 1620(m), 763(s), 717(m); **MS** (EI): 288.1 (M-Br) (100), 206.2 (8); **Anal. Calcd** for C₁₅H₁₃NBr₂: C, 49.32; H, 3.59; N, 3.84. Found: C, 49.15; H, 3.48; N, 3.76.

2. 2-bromo-ethyl-quinolinium bromide, 1b

2-bromo-ethyl-quinolinium bromide **1b** (9.05 g; 28.6 mmol), was isolated as a beige powder, in a 95 % yield; **mp**: 289-290 °C (dec.); **¹H NMR** (D₂O, 400 MHz): δ 9.24 (d, 1H, *J*=8.4 Hz), 9.12 (d, 1H, *J*=8.4 Hz), 8.87 (d, 1H, *J*=8.4 Hz), 8.33 (d, 1H, *J*=8.4 Hz), 8.20 (t, 1H, *J*=8.4 Hz), 7.98 (m, 2H), 5.41 (t, 2H, *J*=5.8 Hz), 4.05 (t, 2H, *J*=5.8 Hz); **¹³C NMR** (D₂O, 100 MHz): δ 149.80 (C), 149.20 (CH), 138.08 (C), 136.66 (CH), 131.43 (CH), 130.68 (CH), 130.55 (CH), 121.59 (CH), 118.08 (CH), 58.59 (CH₂), 29.28 (CH₂); **IR** (KBr, cm⁻¹): 3437 (s), 3045 (w), 2981 (m), 2947 (m), 1624 (s), 1599 (m), 1585 (m), 1525 (s), 1489 (w), 1450 (m), 1400 (m), 1363 (s), 1242 (s), 1126 (m), 1161 (m), 1144 (m), 1049 (w), 874 (w), 816 (m), 800 (m), 775 (s); **MS** (FAB): 237 (M-Br) (98), 236 (100), 209.9 (2), 172 (2), 156 (12), 129.1 (6), 107.2 (2), 89.5 (2), 72.7 (1), 59.9 (1); **Anal. Calcd** for C₁₁H₁₁NBr₂: C, 41.67; H, 3.49; N, 4.42. Found: C, 41.75; H, 3.50; N, 4.51.

3. 2-bromo-ethyl-isoquinolinium bromide, 1c

2-bromo-ethyl-isoquinolinium bromide **1c** (8.56 g; 27 mmol), was isolated as a beige powder, in a 90 % yield; **mp**: 280-281 °C (dec.); **¹H NMR** (D₂O, 400 MHz): δ 9.65 (s, 1H), 8.47 (d, 1H, *J*=6.4 Hz), 8.35 (d, 2H, *J*=7.6 Hz), 8.15 (m, 2H), 7.95 (t, 1H, *J*=6.4 Hz), 5.09 (t, 2H, *J*=5.6 Hz), 4.01 (t, 2H, *J*=5.6 Hz); **¹³C NMR** (D₂O, 100 MHz): δ 150.15 (CH), 138.21 (C), 137.94 (CH), 134.21 (CH), 131.90 (CH), 130.75 (CH), 127.74 (C), 127.62 (CH), 126.93 (CH), 62.15 (CH₂), 30.86 (CH₂); **IR** (KBr, cm⁻¹): 3373 (s), 2985 (s), 2904 (s), 2152 (m), 2105 (s), 2083 (m), 1635 (s), 1602 (s), 1560 (m), 1509 (m), 1427 (m),

1272 (s), 1107 (s), 875 (s), 833 (s). **MS** (FAB): 237 (M-Br) (98), 236 (100), 209.9 (2), 172 (2), 156 (12), 129.1 (6), 107.2 (2), 89.5 (2), 72.7 (1), 59.9 (1).

4. 2-bromo-ethyl-4-methyl-quinolinium bromide, **1d**

2-bromo-ethyl-4-methyl-quinolinium bromide **1d** (8.75 g; 26.4 mmol), was isolated as a beige powder, in a 88 % yield. **mp**: 271-272 °C; **¹H NMR** (D₂O, 400 MHz): δ 8.97 (d, 1H, *J*=6.0 Hz), δ 8.37 (d, 1H, *J*=8.0 Hz), δ 8.25 (d, 1H, *J*=8.0 Hz), δ 8.08 (t, 1H, *J*=8.0 Hz), δ 7.87 (t, 1H, *J*=8.0 Hz), δ 7.79 (d, 1H, *J*=6.0 Hz), δ 5.27 (t, 2H, *J*=5.5 Hz), δ 3.94 (t, 2H, *J*=5.5 Hz), δ 2.89 (s, 3H); **¹³C NMR** (D₂O, 100MHz): δ 149.80 (C), 149.20 (CH), 138.08 (C), 136.66 (CH), 131.43 (CH), 130.68 (CH), 130.55 (CH), 121.59 (CH), 118.08 (CH), 58.59 (CH₂), 29.28 (CH₂); **IR** (KBr, cm⁻¹): 3437 (s), 3045 (w), 2981 (m), 2947 (m), 1624 (s), 1599 (m), 1585 (m), 1525 (s), 1489 (w), 1450 (m), 1400 (m), 1363 (s), 1242 (s), 1126 (m), 1161 (m), 1144 (m), 1049 (w), 874 (w), 816 (m), 800 (m), 775 (s); **MS** (FAB): 237 (M-Br) (98), 236 (100), 209.9 (2), 172 (2), 156 (12), 129.1 (6), 107.2 (2), 89.5 (2), 72.7 (1), 59.9 (1).

5. 2-bromo-ethyl-phthalazinium bromide, **1e**

2-bromo-ethyl-phthalazinium bromide **1e** (8.96 g; 28.2 mmol), was isolated as a beige powder in a 94 % yield. **mp**: 170-171 °C (dec.); **¹H NMR** (D₂O, 400 MHz): δ 10.25 (s, 1H), δ 9.74 (s, 1H), δ 8.47 (d, 1H, *J*=8.0 Hz), δ 8.39 (m, 2H), δ 8.26 (t, 1H, *J*=8.0 Hz), δ 5.14 (t, 2H, *J*=5.6 Hz), δ 4.01 (t, 2H, *J*=5.6 Hz); **¹³C NMR** (D₂O, 100 MHz): δ 155.54 (CH), δ 151.84 (CH), δ 140.11 (CH), δ 136.76 (CH), δ 130.66 (CH), δ 128.44 (CH), δ 128.18 (C), δ 127.55 (C), δ 64.63 (CH₂), δ 29.42 (CH₂); **IR** (KBr, cm⁻¹): 3240 (w), 3069 (w), 3025 (w), 2968 (s), 1619 (m), 1593 (s), 1578 (m), 1485 (s), 1440 (s), 1400 (s), 1367 (s), 1329 (s), 1279 (s), 1229 (s), 1229 (s), 1178 (s), 1144 (w), 1097 (w), 943 (s); **MS** (CI): 239 (M-Cl) (20), 201.2 (2), 169.1 (5), 159.1 (10), 131.1 (100), 85.1 (10), 69.1 (10).

6. 3-acetylamino-1-(2-bromo-ethyl)-quinolinium bromide, **1f**

3-acetylamino-1-(2-bromo-ethyl)-quinolinium bromide **1f** (9.98 g; 26.7 mmol), was isolated as a beige powder, in a 89 % yield. **mp**: 201-201 °C (dec.); **¹H NMR** (D₂O, 400 MHz): δ 9.55 (s, 1H), δ 8.95 (s, 1H), δ 8.25 (d, 1H, *J*=8.4 Hz), δ 8.17 (d, 1H, *J*=8.4 Hz), δ 8.03 (t, 1H, *J*=8.4 Hz), δ 7.84 (t, 1H, *J*=8.4 Hz), δ 5.36 (t, 2H, *J*=5.8 Hz), δ 3.98 (t, 2H, *J*=5.8 Hz), δ 2.17 (s, 3H); **¹³C NMR** (D₂O, 100 MHz): δ 173.36 (C), δ 143.64 (CH), δ 136.61 (CH), δ 135.04 (C), δ 134.96 (CH), δ 131.92 (C), δ 130.44 (CH), δ 130.40 (CH), δ 130.18 (C), δ 117.55 (CH), δ 58.61 (CH₂), δ 28.85 (CH₂), δ 22.88 (CH₃); **IR (KBr, cm⁻¹)**: 3475 (s), 3129 (m), 2955 (s), 1697 (s), 1514 (s), 1464 (m), 1376 (s), 1263 (s), 1152 (m), 1052 (m), 1017 (m), 908 (m), 893 (m); **MS** (FAB): 295 (M-Br) (5), 293 (5), 277.2 (5), 221.3 (2), 207.4 (3), 185.7 (35), 94.8 (100), 77.1 (32).

ii. General procedure for the synthesis of acetylpyridinium derivatives (Activation step of Method 2), **1g-i**

Pyridine derivative (30 mmol) was dissolved in acetonitrile (40 mL) and the 2-halogenoacetyl derivative (33 mmol) was added to the stirred solution. The reaction mixture was refluxed overnight and left to cool down to room temperature before adding diethyl ether (20 mL). The resulting precipitate was recovered by filtration, washed with acetone and dried under vacuum to give the corresponding acetylpyridinium derivatives as a beige powder.

1. 5-(2-oxo-propyl)-phenanthridinium chloride, **1g**

5-(2-oxo-propyl)-phenanthridinium chloride **1g** (7.17 g; 26.4 mmol), was isolated as a brown powder, in a 88 % yield. **mp**: 139-141 °C (dec.); **¹H NMR** (D₂O, 400 MHz): δ 9.50 (s, 1H), δ 8.50 (d, 1H, *J*=8.0 Hz), δ 8.45 (d, 1H, *J*=8.0 Hz), δ 8.17 (d, 1H, *J*=8.0 Hz), δ 8.03 (t, 1H, *J*=8.0 Hz), δ 7.85 (t, 1H, *J*=9.0 Hz), δ 7.80 (d, 1H, *J*=9.0 Hz), δ 7.74 (m, 2H), δ 6.05 (s, 2H), δ 2.47 (s, 3H); **¹³C NMR** (D₂O, 100 MHz): δ 202.36 (C), δ 155.52 (CH), δ 138.76 (CH), δ 135.03 (C), δ 133.20 (C), δ 132.68 (CH), δ 132.15 (CH), δ 130.39 (CH), δ 130.33 (CH), δ 125.56 (C), δ 124.40 (CH), δ 123.03 (C), δ 122.56 (CH), δ 118.67 (CH), δ 68.00 (CH₂), δ 26.99 (CH₃); **IR (KBr, cm⁻¹)**: 3465 (s), 3415 (s), 3238 (w), 3066 (m), 3019 (m), 2963 (m), 2672 (w), 1851 (w), 1735 (s), 1625 (s), 1578 (m), 1533 (m), 1447 (s), 1347 (s), 1264 (m), 1170 (s), 1039 (w); **MS** (CI): 236.13 (M-Cl) (20), 180.12 (40), 139.14 (5), 127.15 (10), 113.17 (15), 85.14 (70), 69.08 (100).

2. 5-[2-(4-methoxy-phenyl)-2-oxo-ethyl]-phenanthridinium bromide, **1h**

5-[2-(4-methoxy-phenyl)-2-oxo-ethyl]-phenanthridinium bromide **1h** (12.24 g; 30 mmol), was isolated as a white powder, in a quantitative yield. **mp**: 235-236 °C (dec.); **¹H NMR** (DMSO-*d*₆, 400 MHz): δ 10.40 (s, 1H), δ 9.26 (t, 2H, *J*=8.2 Hz), δ 8.62 (d, 1H, *J*=8.2 Hz), δ 8.50 (t, 1H, *J*=8.2 Hz), δ 8.44 (d, 1H, *J*=8.2 Hz), δ 8.18 (d, 2H, *J*=9.2 Hz), δ 8.11 (m, 3H), δ 7.25 (d, 2H, *J*=9.2 Hz), δ 7.05 (s, 2H), δ 3.94 (s, 3H); **¹³C NMR** (DMSO-*d*₆, 100 MHz): δ 188.99 (C), δ 164.50 (C), δ 157.10 (CH), δ 138.74 (CH), δ 134.72 (C), δ 134.03 (C), δ 133.08 (CH), δ 132.17 (C), δ 131.15 (CH), δ 130.64 (CH), δ 130.39 (C), δ 126.38 (C), δ 125.44 (C), δ 124.94 (CH), δ 123.43 (CH), δ 123.26 (C), δ 120.02 (CH), δ 114.42 (CH), δ 63.02 (CH₂), δ 55.88 (CH₃); **IR (KBr, cm⁻¹)**: 3555 (s), 3393 (s), 3239 (m), 2959 (s), 2584 (w), 2472 (w), 2039 (w), 1900 (w), 1856 (w), 1687 (s), 1598 (s), 1507 (s), 1450 (s), 1422 (s), 1355 (s), 1240 (s), 1183 (s), 1021 (s), 966 (s), 837 (s); **MS (FAB)**: 328.1 (M-Br) (100), 298.1 (2), 254.1 (2), 193.6 (10), 154.9 (20), 137.2 (20), 122.4 (10), 79.0 (10).

3. 5-(1-methyl-2-oxo-propyl)-phenanthridinium bromide, **1i**

5-(1-methyl-2-oxo-propyl)-phenanthridinium bromide **1i** (8.91 g; 27 mmol), was isolated as a beige powder, in a 90 % yield. **mp**: 209-211 °C (dec.); **¹H NMR** (DMSO, 400 MHz): δ 10.25 (s, 1H), δ 9.26-9.24 (m, 1H), δ 9.20 (d, 1H, *J*=7.8 Hz), δ 8.76 (d, 1H, *J*=7.8 Hz), δ 8.56 (brd, 1H), δ 8.48 (t, 1H, *J*=7.8 Hz), δ 8.17 (t, 1H, *J*=7.8 Hz), δ 8.16-8.11 (m, 2H), δ 6.92 (brd, 1H), δ 2.57 (s, 3H), δ 2.22 (d, 3H, *J*=7.2 Hz); **¹³C NMR** (DMSO, 100 MHz): δ 202.31 (C), δ 154.61 (CH), δ 138.67 (CH), δ 134.39 (C), δ 133.82 (C), δ 133.41 (CH), δ 132.15 (CH), δ 130.43 (CH), δ 130.26 (CH), δ 125.61 (CH), δ 125.17 (CH), δ 123.45 (C), δ 123.20 (CH), δ 27.09 (CH₃), δ 16.43 (CH₃); **IR (KBr, cm⁻¹)**: 3423 (m), 3021 (w), 2936

(w), 1719 (s), 1625 (s), 1534 (m), 1503 (m), 1456 (m), 1425 (m), 1357 (m), 1288 (w), 1263 (m), 1169 (m), 1150 (m), 1092 (m), 967 (m), 926, 877 (w) (m); **MS** (CI): 252.2 (100) (M+1), 180.1 (78), 151 (10), 123.1 (8), 69.1 (40).

iii. General procedure for the synthesis of Imidazo[1,2-a]pyridine derivatives (Ips) with unsubstituted imidazole moiety (Method 1), 6a-f

Under stirring, liquid ammonia (40 ml) was added to an opened round bottom flask containing 40 ml of toluene. To the resulting cool biphasic solution, was added under stirring the 2-bromo-ethyl-pyridinium bromide derivative **1a-f** (4 mmol), followed by addition of 10 equivalents of MnO₂ (3.5 g; 40 mmol) and 5 equivalents of Na₂CO₃ (2.12g; 20 mmol). The reaction mixture was left stirring until complete evaporation of the ammonia phase (i.e. 1 to 2 hours, until the reaction mixture reaches room temperature) and the toluene was brought to reflux for 4 hours. The reaction mixture was then filtered on glass frit n° 4 and the residue was rinsed extensively with acetone. Finally, the mother liquor was concentrated to dryness to afford analytically pure **Ips 6a-f**, without further purification.

1. Imidazo[1,2-f]phenanthridine, 6a

Imidazo[1,2-f]phenanthridine **6a**, (870 mg; 4 mmol), was isolated as a yellow powder, in a quantitative yield. **mp**: 77-78 °C; **R_f** = 0.3 in ethyl acetate; **¹H NMR** (CDCl₃, 400 MHz): δ 8.79 (m, 1H), δ 8.51 (dd, 1H, *J*=8.0 and 1.0 Hz), δ 8.42 (m, 1H), δ 8.05 (d, 1H, *J*=1.2 Hz), δ 7.93 (dd, 1H, *J*=8.0 and 1.0 Hz), δ 7.7 (m, 3H), δ 7.68 (d, 1H, *J*=1.2 Hz), δ 7.58 (td, 1H, *J*=8.0 and 1.0 Hz); **¹³C NMR** (CDCl₃, 100 MHz): δ 142.08 (C), δ 131.49 (C), δ 130.45 (C), δ 129.19 (CH), δ 129.06 (CH), δ 128.86 (CH), δ 127.68 (C), δ 125.53 (CH), δ 124.59 (CH), δ 124.29 (CH), δ 122.42 (CH), δ 121.91 (C), δ 115.94 (CH), δ 112.15 (CH); **IR** (KBr, cm⁻¹): 3432 (s), 1629 (m), 1532 (m), 1495 (w), 1463 (m), 1439 (m), 1316 (m), 1262 (s), 1104 (s), 803 (m), 719 (s); **MS** (FAB): 219.4 (M+1) (100), 178.7 (3), 164.9 (2), 98.8 (5), 71.2 (7), 57.4 (10); Anal. Calcd for C₁₅H₁₀N₂: C, 82.55; H, 4.62; N, 12.84; Found: C, 82.40; H, 4.65; N, 12.90.

2. Imidazo[1,2-a]quinoline, 6b

Imidazo[1,2-a]quinoline **6b** (440 mg; 2.6 mmol), was isolated as a brown oil, in a 65 % yield; **Rf** = 0.2 in ethyl acetate; **¹H NMR** (CDCl₃, 400 MHz): δ 7.98 (d, 1H, *J*=1.6 Hz), δ 7.84 (d, 1H, *J*=8.0 Hz), δ 7.74 (d, 1H, *J*=8.0 Hz), δ 7.58 (d, 1H, *J*=1.6 Hz), δ 7.57 (t, 1H, *J*=8.0 Hz), δ 7.50 (d, 1H, *J*=9.6 Hz), δ 7.43 (d, 1H, *J*=9.6 Hz), δ 7.39 (t, 1H, *J*=8.0 Hz); **¹³C NMR** (CDCl₃, 100 MHz): δ 143.98 (C), δ 132.73 (C), δ 132.52 (CH), δ 129.15 (CH), δ 128.78 (CH), δ 126.06 (CH), δ 124.76 (CH), δ 123.43 (C), δ 117.33 (CH), δ 115.16 (CH), δ 111.05 (CH); **IR** (KBr, cm⁻¹): 3367 (s), 1613 (s), 1557 (s), 1536 (s), 1487 (m), 1446 (s), 1419 (s), 1317 (s), 1279 (m), 1217 (s), 1088 (s), 870 (m); **MS** (EI): 168.1 (M⁺) (100), 140 (12), 128 (28), 114 (20), 84 (11), 63 (8), 51 (5); **HRMS** (EI) for C₁₁H₈N₂ calcd 168.0687 (M⁺), obsd 168.0689.

3. Imidazo[2,1-a]isoquinoline, 6c

Imidazo[2,1-a]isoquinoline **6c** (670 mg; 4 mmol), was isolated as a brown powder, in a quantitative yield. **mp**: 69-70 °C; **Rf** = 0.25 in ethyl acetate; **¹H NMR** (CDCl₃, 400 MHz): δ 8.63 (d, 1H, *J*=8.0 Hz), δ 7.86 (d, 1H, *J*=7.2 Hz), δ 7.65 (d, 1H, *J*=8.0 Hz), δ 7.59 (t, 1H, *J*=8.0 Hz), δ 7.55 (d, 1H, *J*=1.2 Hz), δ 7.54 (t, 1H, *J*=8.0 Hz), δ 7.51 (d, 1H, *J*=1.2 Hz), δ 7.02 (d, 1H, *J*=7.2 Hz); **¹³C NMR** (CDCl₃, 100 MHz): δ 143.05 (C), δ 131.22 (CH), δ 129.46 (C), δ 128.30 (CH), δ 128.25 (CH), δ 126.94 (CH), δ 123.85 (C), δ 123.29 (CH), δ 123.09 (CH), δ 114.28 (CH), δ 113.27 (CH); **IR** (KBr, cm⁻¹): 3444 (s), 3069 (s), 2743 (s), 2451 (w), 1960 (m), 1934 (m), 1725 (m), 1638 (s), 1607 (s), 1518 (s), 1449 (s), 1385 (s), 1317 (s), 1224 (s), 1141 (s), 1095 (s), 953 (s), 910 (s), 882 (s); **MS** (EI): 168.1 (M⁺) (100), 141 (12), 114 (30), 113 (5), 70.5 (10), 63 (5), 49 (3); **HRMS** for C₁₁H₈N₂ calcd 168.0687 (M⁺), obsd 168.0689.

4. 5-Methyl-imidazo[1,2-a]quinoline, **6d**

5-Methyl-imidazo[1,2-a]quinoline **6d** (730 mg; 4 mmol), was isolated as a brown oil, in a quantitative yield; **Rf** = 0.2 in ethyl acetate; $^1\text{H NMR}$ (CDCl_3 , 400 MHz): δ 7.90 (s, 1H), δ 7.83 (d, 1H, $J=7.8$ Hz), δ 7.81 (d, 1H, $J=7.8$ Hz), δ 7.55 (t, 1H, $J=7.8$ Hz), δ 7.50 (d, 1H, $J=1.2$ Hz), δ 7.41 (t, 1H, $J=7.8$ Hz), δ 7.32 (d, 1H, $J=1.2$ Hz), δ 2.53 (s, 3H); $^{13}\text{C NMR}$ (CDCl_3 , 100 MHz): δ 133.04 (C), δ 128.62 (CH), δ 128.28 (C), δ 125.81 (CH), δ 124.59 (CH), δ 123.88 (C), δ 121.87 (CH), δ 116.51 (CH), δ 115.36 (CH), δ 110.58 (CH), δ 19.29 (CH_3); **IR** (KBr, cm^{-1}): 3407 (s), 2912 (w), 1621 (s), 1455 (s), 1420 (s), 1325 (s), 1198 (s), 1148 (m), 865 (m); **MS** (EI): 182.1 (M^+) (100), 181.1 (98), 154.1 (20), 127 (29), 91 (19), 77 (12), 63 (11), 51 (10); **HRMS** (EI) for $\text{C}_{12}\text{H}_{10}\text{N}_2$ calcd 182.0844 (M^+), obsd 182.0840.

5. Imidazo[2,1-a]phthalazine, **6e**

Imidazo[2,1-a]phthalazine **6e** (620 mg; 3.68 mmol), was isolated as a yellow powder, in a 92 % yield. **mp**: 74-75 °C; **Rf** = 0.3 in ethyl acetate; $^1\text{H NMR}$ (CDCl_3 , 400 MHz): δ 8.59 (s, 1H), δ 8.56 (d, 1H, $J=8.0$ Hz), δ 7.85 (d, 2H, $J=1.6$ Hz), δ 7.83 (m, 2H), δ 7.65 (t, 1H, $J=8.0$ Hz), δ 7.58 (d, 1H, $J=1.6$ Hz); $^{13}\text{C NMR}$ (CDCl_3 , 100 MHz): δ 145.78 (CH), δ 133.31 (CH), δ 131.88 (C), δ 129.73 (CH), δ 129.11 (CH), δ 127.65 (CH), δ 125.45 (C), δ 122.86 (C), δ 122.49 (CH), δ 117.54 (CH); **IR** (KBr, cm^{-1}): 3110 (s), 2382 (m), 1984 (m), 1964 (m), 1855 (m), 1721 (m), 1656 (s), 1557 (s), 1523 (s), 1449 (s), 1337 (s), 1240 (s), 1141 (s), 1068 (s), 904 (s), 862 (s); **MS** (CI $^+$): 170.12 ($\text{M}+\text{H}$) (100), 169.12 (25), 147.11 (20), 131.12 (12), 115.10 (3); **HRMS** (EI) for $\text{C}_{10}\text{H}_7\text{N}_3$ calcd 169.0640 (M^+), obsd 169.0637.

N-Imidazo[1,2-a]quinolin-4-yl-acetamide, 6f

N-Imidazo[1,2-a]quinolin-4-yl-acetamide **6f** (880 mg; 3.92 mmol), was isolated as a pale yellow powder, in a 98 % yield. **mp**: 153-154 °C; **R_f** = 0.2 in ethyl acetate; **¹H NMR** (CDCl₃, 400 MHz): δ 9.2 (s, 1H), δ 8.61 (s, 1H), δ 8.04 (d, 1H, *J*=1.6 Hz), δ 7.81 (t, 2H, *J*=7.8 Hz), δ 7.58 (d, 1H, *J*=1.6 Hz), δ 7.54 (t, 1H, *J*=7.8 Hz), δ 7.45 (t, 1H, *J*=7.8 Hz), δ 2.31 (s, 3H); **¹³C NMR** (CDCl₃, 100 MHz): δ 130.13 (CH), δ 129.79 (CH), δ 128.42 (CH), δ 121.50 (CH), δ 119.56 (CH), δ 114.68 (CH), δ 75 (CH₃); **IR** (KBr, cm⁻¹): 3446 (w), 3147 (m), 2924 (m), 2770 (w), 1681 (s), 1557 (s), 1520 (s), 1458 (m), 1421 (s), 1369 (m), 1331 (s), 1310 (m), 1260 (s), 1142 (m), 1003 (w) 872 (m), 846 (m); **MS** (EI): 225.1 (M⁺) (35), 183.1 (100), 155.1 (20), 128 (5), 101 (5), 82.9 (5), 49 (3); **Anal. Calcd** for **C₁₃H₁₁N₃O**: C, 69.32; H, 4.92; N, 18.66; Found: C, 69.12; H, 4.83; N, 18.45.

iv. General procedure for the synthesis of Imidazo[1,2-a]pyridine derivatives (**Ips**) with substituted imidazole moiety (Method 2), **6g-i**

To a stirred suspension of acetyl-pyridinium **1g-i** (4 mmol) in 1,4-dioxane (40 ml) at room temperature, were added 4 equivalents of ammonium acetate (1.23 g; 16 mmol), followed by 10 equivalents of MnO₂ (3.5 g; 40 mmol). The reaction mixture was refluxed for 4 hours before adding 10 equivalents of Na₂CO₃ (4.24 g; 40 mmol). The suspension was then cooled down to room temperature and diethyl ether (10 ml) added to precipitate any inorganic side products. The reaction mixture was filtered on glass frit n° 4 and the residue was rinsed extensively with acetone. Finally, the mother liquor was concentrated to dryness to afford analytically pure **Ips 6g-i**, without further purification.

1. 2-Methyl-imidazo[1,2-f]phenanthridine, **6g**

2-Methyl-imidazo[1,2-f]phenanthridine **6g** (790 mg; 3.4 mmol), was isolated as a brown powder, in a 85 % yield. **mp**: 130-131 °C; **R_f** = 0.4 in ethyl acetate; **¹H NMR** (CDCl₃, 400 MHz): δ 8.46 (d, 1H, *J*=8.0 Hz), δ 8.14 (d, 1H, *J*=8.0 Hz), δ 8.10 (d, 1H, *J*=8.0 Hz), δ 7.48 (t, 1H, *J*=8.0 Hz), δ 7.44 (m, 3H), δ 7.34 (t, 1H, *J*=8.0 Hz), δ 7.22 (t, 1H, *J*=8.0 Hz), δ 2.38 (s, 3H); **¹³C NMR** CDCl₃, 100 MHz): δ 141.73 (C), δ 140.86 (C), δ 131.39 (C), δ 128.55 (CH), δ 128.23 (CH), δ 127.21 (C), δ 124.51 (CH), δ 123.89 (CH), δ 123.86 (CH), δ 123.22 (C), δ 122.44 (CH), δ 122.20 (CH), δ 121.26 (CH), δ 115.49 (CH), δ 108.86 (CH), δ 14.31 (CH₃); **IR** (KBr, cm⁻¹): 3372 (w), 3146 (m), 3067 (w), 2915 (m), 1607 (m), 1591 (s), 1550 (s), 1591 (s), 1550 (s), 1530 (s), 1460 (s), 1433 (s), 1392 (s), 1349 (m), 1313 (s) 1233 (w), 1109 (m), 1036 (w); **MS** (EI): 232.1 (M⁺) (100), 204.1 (10), 178.1

(11), 177.1 (10), 116 (15), 82.9 (12), 76 (5), 49 (5); **HRMS** (EI) for C₁₆H₁₂N₂ calcd 232.1000 (M⁺), obsd 232.0998.

2. 2-(4-Methoxy-phenyl)-imidazo[1,2-f]phenanthridine, **6h**

2-(4-Methoxy-phenyl)-imidazo[1,2-f]phenanthridine **6h** (1.14 g; 3.52 mmol), was isolated as a beige powder, in a 88 % yield. **mp**: 160-161 °C; **R_f** = 0.7 in ethyl acetate; **¹H NMR** (CDCl₃, 400 MHz): δ 8.69 (d, 1H, *J*=7.2 Hz), δ 8.40 (d, 1H, *J*=8.0 Hz), δ 8.32 (d, 1H, *J*=7.2 Hz), δ 8.09 (s, 1H), δ 7.91 (d, 2H, *J*=8.8 Hz), δ 7.83 (d, 1H, *J*=8.0 Hz), δ 7.57 (m, 3H), δ 7.44 (t, 1H, *J*=7.2 Hz), δ 6.94 (d, 2H, *J*=8.8 Hz), δ 3.80 (s, 3H); **¹³C NMR** (CDCl₃, 100 MHz): δ 159.35 (C), δ 144.03 (C), δ 142.61 (C), δ 131.70 (C), δ 128.84 (CH), δ 128.58 (CH), δ 128.51 (CH), δ 127.52 (C), δ 127.05 (CH), δ 126.75 (C), δ 124.94 (CH), δ 124.45 (CH), δ 124.21 (C), δ 123.59 (C), δ 123.59 (C), δ 122.35 (CH), δ 121.76 (C), δ 115.80 (CH), δ 114.18 (CH), δ 106.69 (CH), δ 55.36 (CH₃); **IR** (KBr, cm⁻¹): 3442 (s), 3143 (w), 2939 (w), 2837 (w), 2898 (m), 1561 (m), 1462 (s), 1436 (s), 1399 (m), 1295 (w), 1245 (s), 1033 (s), 943 (w), 828 (s); **MS** (EI): 324.1 (M⁺) (100), 309.1 (22), 281.1 (20), 246.1 (25), 245.1 (18), 179.1 (20), 178.1 (15), 162.1 (11), 140.1 (10), 69 (10), 44 (50); **HRMS** (EI) for C₂₂H₁₆ON₂ calcd 324.1263 (M⁺), obsd 324.1264.

3. 2,3-Dimethyl-imidazo[1,2-f]phenanthridine, **6i**

2,3-Dimethyl-imidazo[1,2-f]phenanthridine **6i** (985 mg; 4 mmol), was isolated as a beige powder, in a 100 % yield. **mp**: 135-136 °C; **R_f** = 0.4 in ethyl acetate; **¹H NMR** (CDCl₃, 400 MHz): δ 8.61 (d, 1H, *J*=8.0 Hz), δ 8.37 (d, 1H, *J*=8.0 Hz), δ 7.47 (t, 1H, *J*=8.0 Hz), δ 7.39 (t, 1H, *J*=8.0 Hz), δ 2.75 (s, 3H), δ 2.39 (s, 3H); **¹³C NMR** (CDCl₃, 100 MHz): δ 140.90 (C), δ 136.97 (C), δ 133.80 (C), δ 128.58 (CH), δ 128.44 (CH), δ 128.22 (CH), δ

127.13 (C), δ 124.56 (CH), δ 124.18 (CH), δ 124.13 (CH), δ 122.49 (C), δ 122.05 (C), δ 120.88 (C), δ 116.29 (CH), δ 14.30 (CH₃), δ 12.92 (CH₃); **IR** (KBr, cm⁻¹): 3383 (m), 3054 (m), 2975 (m), 2919 (m), 2858 (m), 1945 (m), 1664 (m), 1595 (s), 1573 (s), 1531 (s), 1542 (s), 1398 (s), 1372 (s), 1040 (m), 945 (m), 817 (m); **MS** (EI): 246.1 (M⁺) (100), 245.1 (50), 231.1 (10), 204.1 (10), 178.1 (10), 177.1 (10), 123.1 (9), 122.1 (3), 84 (4), 82.9 (4), 49 (4); HRMS (EI) for C₁₇H₁₄N₂ calcd 246.1157 (M⁺), obsd 246.1158.

3. Copies of NMR Spectra (^1H NMR and ^{13}C NMR DEPT 135)
a. 2-Bromoethyl pyridinium derivatives (1a-f)

Alexis Puriony
D9
E135 A3.gla D2O u alexisp 1

b. Acetyl-pyridinium derivatives (1g-i)

User - Craig Richmond
Dimethyl Phen bromide
C13DE135_A3.gfa DMSO-d₆ u cratic 4

c. Imidazo[1,2-a]pyridine derivatives (Ips) with unsubstituted imidazole moiety (6a-f)

User: Alexis Paverly
 AP19-65
 CHSE135_A3 gla COC3 u serisp 4

12.00
 11.99
 11.98
 11.97
 11.96
 11.95
 11.94
 11.93
 11.92
 11.91
 11.90
 11.89
 11.88
 11.87
 11.86
 11.85
 11.84
 11.83
 11.82
 11.81
 11.80
 11.79
 11.78
 11.77
 11.76
 11.75
 11.74
 11.73
 11.72
 11.71
 11.70
 11.69
 11.68
 11.67
 11.66
 11.65
 11.64
 11.63
 11.62
 11.61
 11.60
 11.59
 11.58
 11.57
 11.56
 11.55
 11.54
 11.53
 11.52
 11.51
 11.50
 11.49
 11.48
 11.47
 11.46
 11.45
 11.44
 11.43
 11.42
 11.41
 11.40
 11.39
 11.38
 11.37
 11.36
 11.35
 11.34
 11.33
 11.32
 11.31
 11.30
 11.29
 11.28
 11.27
 11.26
 11.25
 11.24
 11.23
 11.22
 11.21
 11.20
 11.19
 11.18
 11.17
 11.16
 11.15
 11.14
 11.13
 11.12
 11.11
 11.10
 11.09
 11.08
 11.07
 11.06
 11.05
 11.04
 11.03
 11.02
 11.01
 11.00
 10.99
 10.98
 10.97
 10.96
 10.95
 10.94
 10.93
 10.92
 10.91
 10.90
 10.89
 10.88
 10.87
 10.86
 10.85
 10.84
 10.83
 10.82
 10.81
 10.80
 10.79
 10.78
 10.77
 10.76
 10.75
 10.74
 10.73
 10.72
 10.71
 10.70
 10.69
 10.68
 10.67
 10.66
 10.65
 10.64
 10.63
 10.62
 10.61
 10.60
 10.59
 10.58
 10.57
 10.56
 10.55
 10.54
 10.53
 10.52
 10.51
 10.50
 10.49
 10.48
 10.47
 10.46
 10.45
 10.44
 10.43
 10.42
 10.41
 10.40
 10.39
 10.38
 10.37
 10.36
 10.35
 10.34
 10.33
 10.32
 10.31
 10.30
 10.29
 10.28
 10.27
 10.26
 10.25
 10.24
 10.23
 10.22
 10.21
 10.20
 10.19
 10.18
 10.17
 10.16
 10.15
 10.14
 10.13
 10.12
 10.11
 10.10
 10.09
 10.08
 10.07
 10.06
 10.05
 10.04
 10.03
 10.02
 10.01
 10.00
 9.99
 9.98
 9.97
 9.96
 9.95
 9.94
 9.93
 9.92
 9.91
 9.90
 9.89
 9.88
 9.87
 9.86
 9.85
 9.84
 9.83
 9.82
 9.81
 9.80
 9.79
 9.78
 9.77
 9.76
 9.75
 9.74
 9.73
 9.72
 9.71
 9.70
 9.69
 9.68
 9.67
 9.66
 9.65
 9.64
 9.63
 9.62
 9.61
 9.60
 9.59
 9.58
 9.57
 9.56
 9.55
 9.54
 9.53
 9.52
 9.51
 9.50
 9.49
 9.48
 9.47
 9.46
 9.45
 9.44
 9.43
 9.42
 9.41
 9.40
 9.39
 9.38
 9.37
 9.36
 9.35
 9.34
 9.33
 9.32
 9.31
 9.30
 9.29
 9.28
 9.27
 9.26
 9.25
 9.24
 9.23
 9.22
 9.21
 9.20
 9.19
 9.18
 9.17
 9.16
 9.15
 9.14
 9.13
 9.12
 9.11
 9.10
 9.09
 9.08
 9.07
 9.06
 9.05
 9.04
 9.03
 9.02
 9.01
 9.00
 8.99
 8.98
 8.97
 8.96
 8.95
 8.94
 8.93
 8.92
 8.91
 8.90
 8.89
 8.88
 8.87
 8.86
 8.85
 8.84
 8.83
 8.82
 8.81
 8.80
 8.79
 8.78
 8.77
 8.76
 8.75
 8.74
 8.73
 8.72
 8.71
 8.70
 8.69
 8.68
 8.67
 8.66
 8.65
 8.64
 8.63
 8.62
 8.61
 8.60
 8.59
 8.58
 8.57
 8.56
 8.55
 8.54
 8.53
 8.52
 8.51
 8.50
 8.49
 8.48
 8.47
 8.46
 8.45
 8.44
 8.43
 8.42
 8.41
 8.40
 8.39
 8.38
 8.37
 8.36
 8.35
 8.34
 8.33
 8.32
 8.31
 8.30
 8.29
 8.28
 8.27
 8.26
 8.25
 8.24
 8.23
 8.22
 8.21
 8.20
 8.19
 8.18
 8.17
 8.16
 8.15
 8.14
 8.13
 8.12
 8.11
 8.10
 8.09
 8.08
 8.07
 8.06
 8.05
 8.04
 8.03
 8.02
 8.01
 8.00
 7.99
 7.98
 7.97
 7.96
 7.95
 7.94
 7.93
 7.92
 7.91
 7.90
 7.89
 7.88
 7.87
 7.86
 7.85
 7.84
 7.83
 7.82
 7.81
 7.80
 7.79
 7.78
 7.77
 7.76
 7.75
 7.74
 7.73
 7.72
 7.71
 7.70
 7.69
 7.68
 7.67
 7.66
 7.65
 7.64
 7.63
 7.62
 7.61
 7.60
 7.59
 7.58
 7.57
 7.56
 7.55
 7.54
 7.53
 7.52
 7.51
 7.50
 7.49
 7.48
 7.47
 7.46
 7.45
 7.44
 7.43
 7.42
 7.41
 7.40
 7.39
 7.38
 7.37
 7.36
 7.35
 7.34
 7.33
 7.32
 7.31
 7.30
 7.29
 7.28
 7.27
 7.26
 7.25
 7.24
 7.23
 7.22
 7.21
 7.20
 7.19
 7.18
 7.17
 7.16
 7.15
 7.14
 7.13
 7.12
 7.11
 7.10
 7.09
 7.08
 7.07
 7.06
 7.05
 7.04
 7.03
 7.02
 7.01
 7.00
 6.99
 6.98
 6.97
 6.96
 6.95
 6.94
 6.93
 6.92
 6.91
 6.90
 6.89
 6.88
 6.87
 6.86
 6.85
 6.84
 6.83
 6.82
 6.81
 6.80
 6.79
 6.78
 6.77
 6.76
 6.75
 6.74
 6.73
 6.72
 6.71
 6.70
 6.69
 6.68
 6.67
 6.66
 6.65
 6.64
 6.63
 6.62
 6.61
 6.60
 6.59
 6.58
 6.57
 6.56
 6.55
 6.54
 6.53
 6.52
 6.51
 6.50
 6.49
 6.48
 6.47
 6.46
 6.45
 6.44
 6.43
 6.42
 6.41
 6.40
 6.39
 6.38
 6.37
 6.36
 6.35
 6.34
 6.33
 6.32
 6.31
 6.30
 6.29
 6.28
 6.27
 6.26
 6.25
 6.24
 6.23
 6.22
 6.21
 6.20
 6.19
 6.18
 6.17
 6.16
 6.15
 6.14
 6.13
 6.12
 6.11
 6.10
 6.09
 6.08
 6.07
 6.06
 6.05
 6.04
 6.03
 6.02
 6.01
 6.00
 5.99
 5.98
 5.97
 5.96
 5.95
 5.94
 5.93
 5.92
 5.91
 5.90
 5.89
 5.88
 5.87
 5.86
 5.85
 5.84
 5.83
 5.82
 5.81
 5.80
 5.79
 5.78
 5.77
 5.76
 5.75
 5.74
 5.73
 5.72
 5.71
 5.70
 5.69
 5.68
 5.67
 5.66
 5.65
 5.64
 5.63
 5.62
 5.61
 5.60
 5.59
 5.58
 5.57
 5.56
 5.55
 5.54
 5.53
 5.52
 5.51
 5.50
 5.49
 5.48
 5.47
 5.46
 5.45
 5.44
 5.43
 5.42
 5.41
 5.40
 5.39
 5.38
 5.37
 5.36
 5.35
 5.34
 5.33
 5.32
 5.31
 5.30
 5.29
 5.28
 5.27
 5.26
 5.25
 5.24
 5.23
 5.22
 5.21
 5.20
 5.19
 5.18
 5.17
 5.16
 5.15
 5.14
 5.13
 5.12
 5.11
 5.10
 5.09
 5.08
 5.07
 5.06
 5.05
 5.04
 5.03
 5.02
 5.01
 5.00
 4.99
 4.98
 4.97
 4.96
 4.95
 4.94
 4.93
 4.92
 4.91
 4.90
 4.89
 4.88
 4.87
 4.86
 4.85
 4.84
 4.83
 4.82
 4.81
 4.80
 4.79
 4.78
 4.77
 4.76
 4.75
 4.74
 4.73
 4.72
 4.71
 4.70
 4.69
 4.68
 4.67
 4.66
 4.65
 4.64
 4.63
 4.62
 4.61
 4.60
 4.59
 4.58
 4.57
 4.56
 4.55
 4.54
 4.53
 4.52
 4.51
 4.50
 4.49
 4.48
 4.47
 4.46
 4.45
 4.44
 4.43
 4.42
 4.41
 4.40
 4.39
 4.38
 4.37
 4.36
 4.35
 4.34
 4.33
 4.32
 4.31
 4.30
 4.29
 4.28
 4.27
 4.26
 4.25
 4.24
 4.23
 4.22
 4.21
 4.20
 4.19
 4.18
 4.17
 4.16
 4.15
 4.14
 4.13
 4.12
 4.11
 4.10
 4.09
 4.08
 4.07
 4.06
 4.05
 4.04
 4.03
 4.02
 4.01
 4.00
 3.99
 3.98
 3.97
 3.96
 3.95
 3.94
 3.93
 3.92
 3.91
 3.90
 3.89
 3.88
 3.87
 3.86
 3.85
 3.84
 3.83
 3.82
 3.81
 3.80
 3.79
 3.78
 3.77
 3.76
 3.75
 3.74
 3.73
 3.72
 3.71
 3.70
 3.69
 3.68
 3.67
 3.66
 3.65
 3.64
 3.63
 3.62
 3.61
 3.60
 3.59
 3.58
 3.57
 3.56
 3.55
 3.54
 3.53
 3.52
 3.51
 3.50
 3.49
 3.48
 3.47
 3.46
 3.45
 3.44
 3.43
 3.42
 3.41
 3.40
 3.39
 3.38
 3.37
 3.36
 3.35
 3.34
 3.33
 3.32
 3.31
 3.30
 3.29
 3.28
 3.27
 3.26
 3.25
 3.24
 3.23
 3.22
 3.21
 3.20
 3.19
 3.18
 3.17
 3.16
 3.15
 3.14
 3.13
 3.12
 3.11
 3.10
 3.09
 3.08
 3.07
 3.06
 3.05
 3.04
 3.03
 3.02
 3.01
 3.00
 2.99
 2.98
 2.97
 2.96
 2.95
 2.94
 2.93
 2.92
 2.91
 2.90
 2.89
 2.88
 2.87
 2.86
 2.85
 2.84
 2.83
 2.82
 2.81
 2.80
 2.79
 2.78
 2.77
 2.76
 2.75
 2.74
 2.73
 2.72
 2.71
 2.70
 2.69
 2.68
 2.67
 2.66
 2.65
 2.64
 2.63
 2.62
 2.61
 2.60
 2.59
 2.58
 2.57
 2.56
 2.55
 2.54
 2.53
 2.52
 2.51
 2.50
 2.49
 2.48
 2.47
 2.46
 2.45
 2.44
 2.43
 2.42
 2.41
 2.40
 2.39
 2.38
 2.37
 2.36
 2.35
 2.34
 2.33
 2.32
 2.31
 2.30
 2.29
 2.28
 2.27
 2.26
 2.25
 2.24
 2.23
 2.22
 2.21
 2.20
 2.19
 2.18
 2.17
 2.16
 2.15
 2.14
 2.13
 2.12
 2.11
 2.10
 2.09
 2.08
 2.07
 2.06
 2.05
 2.04
 2.03
 2.02
 2.01
 2.00
 1.99
 1.98
 1.97
 1.96
 1.95
 1.94
 1.93
 1.92
 1.91
 1.90
 1.89
 1.88
 1.87
 1.86
 1.85
 1.84
 1.83
 1.82
 1.81
 1.80
 1.79
 1.78
 1.77
 1.76
 1.75
 1.74
 1.73
 1.72
 1.71
 1.70
 1.69
 1.68
 1.67
 1.66
 1.65
 1.64
 1.63
 1.62
 1.61
 1.60
 1.59
 1.58
 1.57
 1.56
 1.55
 1.54
 1.53
 1.52
 1.51
 1.50
 1.49
 1.48
 1.47
 1.46
 1.45
 1.44
 1.43
 1.42
 1.41
 1.40
 1.39
 1.38
 1.37
 1.36
 1.35
 1.34
 1.33
 1.32
 1.31
 1.30
 1.29
 1.28
 1.27
 1.26
 1.25
 1.24
 1.23
 1.22
 1.21
 1.20
 1.19
 1.18
 1.17
 1.16
 1.15
 1.14
 1.13
 1.12
 1.11
 1.10
 1.09
 1.08
 1.07
 1.06
 1.05
 1.04
 1.03
 1.02
 1.01
 1.00
 0.99
 0.98
 0.97
 0.96
 0.95
 0.94
 0.93
 0.92
 0.91
 0.90
 0.89
 0.88
 0.87
 0.86
 0.85
 0.84
 0.83
 0.82
 0.81
 0.80
 0.79
 0.78
 0.77
 0.76
 0.75
 0.74
 0.73
 0.72
 0.71
 0.70
 0.69
 0.68
 0.67
 0.66
 0.65
 0.64
 0.63
 0.62
 0.61
 0.60
 0.59
 0.58
 0.57
 0.56
 0.55
 0.54
 0.53
 0.52
 0.51
 0.50
 0.49
 0.48
 0.47
 0.46
 0.45
 0.44
 0.43
 0.42
 0.41
 0.40
 0.39
 0.38
 0.37
 0.36
 0.35
 0.34
 0.33
 0.32
 0.31
 0.30
 0.29
 0.28
 0.27
 0.26
 0.25
 0.24
 0.23
 0.22
 0.21
 0.20
 0.19
 0.18
 0.17
 0.16
 0.15
 0.14
 0.13
 0.12
 0.11
 0.10
 0.09
 0.08
 0.07
 0.06
 0.05
 0.04
 0.03
 0.02
 0.01
 0.00
 -0.01
 -0.02
 -0.03
 -0.04
 -0.05
 -0.06
 -0.07
 -0.08
 -0.09
 -0.10
 -0.11
 -0.12
 -0.13
 -0.14
 -0.15
 -0.16
 -0.17
 -0.18
 -0.19
 -0.20
 -0.21
 -0.22
 -0.23
 -0.24
 -0.25
 -0.26
 -0.27
 -0.28
 -0.29
 -0.30
 -0.31
 -0.32
 -0.33
 -0.34
 -0.35
 -0.36
 -0.37
 -0.38
 -0.39
 -0.40
 -0.41
 -0.42
 -0.43
 -0.44
 -0.45
 -0.46
 -0.47
 -0.48
 -0.49
 -0.50
 -0.51
 -0.52
 -0.53
 -0.54
 -0.55
 -0.56
 -0.57
 -0.58
 -0.59
 -0.60
 -0.61
 -0.62
 -0.63
 -0.64
 -0.65
 -0.66
 -0.67
 -0.68
 -0.69
 -0.70
 -0.71
 -0.72
 -0.73
 -0.74
 -0.75
 -0.76
 -0.77
 -0.78
 -0.79
 -0.80
 -0.81
 -0.82
 -0.83
 -0.84
 -0.85
 -0.86
 -0.87
 -0.88
 -0.89
 -0.90
 -0.91
 -0.92
 -0.93
 -0.94
 -0.95
 -0.96
 -0.97
 -0.98
 -0.99
 -1.00
 -1.01
 -1.02
 -1.03
 -1.04
 -1.05
 -1.06
 -1.07
 -1.08
 -1.09
 -1.10
 -1.11
 -1.12
 -1.13
 -1.14
 -1.15
 -1.16
 -1.17
 -1.18
 -1.19
 -1.20
 -1.21
 -1.22
 -1.23
 -1.24
 -1.25
 -1.26
 -1.27
 -1.28
 -1.29
 -1.30
 -1.31
 -1.32
 -1.33
 -1.34
 -1.35
 -1.3

d. Imidazo[1,2-a]pyridine derivatives (Ips) with substituted imidazole moiety (6g-i)

User: Alexis Pareny
 AP24-15
 C:\30E135_A3.gia CDC13 u alexisp 5

129.84 C
 128.58 C
 127.04 C
 124.44 C
 122.35 C
 115.80 C
 114.18 F
 106.69 C

Current Data Parameters
 NAME: A006075AP23-15
 EXPNO: 1
 PROCNO: 1
 P2 - Acquisition Parameters
 INSTRUM: spect
 F2 - 13C
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 4
 DS: 4
 SWH: 31871.13 Hz
 AQ: 0.000000 sec
 RG: 16384
 INJ: 15.00 usec
 TE: 298.4 K
 P1: 14.00 usec
 PC: 14.00 usec
 PD: 0.000000 sec
 PR: 0.000000 sec
 DE: 0.000000 sec
 DELT: 0.000000 sec
 ACQ: 0.000000 sec
 NUC1: 13C
 NUC2: 13C
 P1: 14.00 usec
 P2: 14.00 usec
 P3: 14.00 usec
 P4: 0.00 dB
 SF: 100.6254642 MHz
 ===== CHANNEL f2 =====
 CPDPRG2: waltz16
 NU2: 13C
 P1: 14.00 usec
 P2: 14.00 usec
 P3: 14.00 usec
 P4: 25.20 usec
 PCPD2: 94.00 usec
 P1: 14.00 dB
 P2: 14.00 dB
 P3: 14.00 dB
 P4: 18.00 dB
 SF2: 400.1116005 MHz
 P2 - Processing parameters
 SI: 32768
 SF: 100.6127400 MHz
 AS: 0
 SD: 0
 LB: 1.00 Hz
 GB: 0
 PC: 2.00
 PR: 30
 ISM: 153K