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A General Method for the Preparation of 4- and 6-Azaindoles

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Supporting Materials

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Page S7-S17 ¹H and ¹³C of Azaindoles

HRMS Results

Compound Number	Formula [M+H]	Theoretic m/z.	Observed m/z	Deviation in ppm
4a	C ₈ H ₉ N ₂ O	149.0715	149.0720	3.4
4b	C ₁₃ H ₁₀ FN ₂ O	229.0777	229.0787	4.3
4c	C ₇ H ₆ ClN ₂	153.0220	153.0225	3.6
4f	C ₈ H ₉ N ₂	133.0766	133.0767	1.0
4h	C ₁₄ H ₁₃ N ₂ O	225.1028	225.1029	0.5
4i	C ₈ H ₉ N ₂ O	149.0715	149.0721	-3.9
4j	C ₇ H ₆ ClN ₂	153.0220	153.0216	-2.3
5	C ₇ H ₇ N ₂	119.0609	119.0612	-2.1
Compound Number	Formula [M-H]	Theoretic m/z.	Observed m/z	Deviation in ppm
4d	C ₈ H ₆ BrN ₂ O	224.9664	224.9666	-1.1
4e	C ₇ H ₃ BrClN ₂	228.9168	228.9173	-1.9
4g	C ₈ H ₆ ClN ₂	165.0220	165.0221	-1.1

Supporting Material: Spectra

7-Methoxy-6-azaindole 4a. ^1H NMR (500 MHz, CD_3OD) δ 7.81 (d, 1H, $J = 2.85$ Hz), 7.63 (d, 1H, $J = 6.55$ Hz), 7.55 (d, 1H, $J = 6.65$ Hz), 6.77 (d, 1H, $J = 2.90$ Hz), 4.39 (s, 3H); ^{13}C NMR (125 MHz, CD_3OD) δ 151.5, 139.0, 135.2, 127.0, 121.1, 112.6, 105.2, 58.3; HRMS m/z : ($\text{M}+\text{H}$) $^+$ calcd for $\text{C}_8\text{H}_9\text{N}_2\text{O}$ 149.0715, found 149.0720.

7-(2-Fluoro-phenyloxy)-6-azaindole 4b. ^1H NMR (500 MHz, CD_3OD) δ 7.61 (d, 1H, $J = 2.95$ Hz), 7.54 (d, 1H, $J = 5.85$ Hz), 7.41 (d, 1H, $J = 5.90$ Hz), 7.29 (m, 4H), 6.66 (d, 1H, $J = 2.90$ Hz); ^{13}C NMR (125 MHz, CD_3OD) δ 156.9, 154.9, 150.0, 138.8, 132.6, 132.4, 128.2, 126.4, 124.7, 122.0, 118.2, 113.6, 103.9; HRMS m/z : ($\text{M}+\text{H}$) $^+$ calcd for $\text{C}_{13}\text{H}_{10}\text{FN}_2\text{O}$ 229.0777, found 229.0787.

7-Chloro-6-azaindole 4c. ^1H NMR (500 MHz, CD_3OD) δ 7.84 (d, 1H, $J = 7.95$ Hz), 7.76 (m, 2H), 6.61 (d, 1H, $J = 5.45$ Hz); ^{13}C NMR (125 MHz, CD_3OD) δ 137.6, 136.7, 135.3, 131.6, 131.3, 116.3, 103.6; HRMS m/z : ($\text{M}+\text{H}$) $^+$ calcd for $\text{C}_7\text{H}_6\text{ClN}_2$ 153.0220, found 153.0225.

4-Bromo-7-methoxy-6-azaindole 4d. ^1H NMR (500 MHz, CDCl_3) δ 8.85 (b, 1H), 7.84 (s, 1H), 7.31 (d, 1H, $J = 5.5$ Hz), 6.57 (d, 1H, $J = 5.15$ Hz), 4.08 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 158.5, 135.7, 134.3, 126.4, 120.9, 105.5, 103.3, 53.4; HRMS m/z : ($\text{M}-\text{H}$) calcd for $\text{C}_8\text{H}_6\text{BrN}_2\text{O}$ 224.9664, found 224.9666.

4-Bromo-7-chloro-6-azaindole 4e. ^1H NMR (500 MHz, DMSO- d_6) δ 8.05 (s, 1H), 7.79 (d, 1H, J = 3.00 Hz), 6.58 (d, 1H, J = 3.00 Hz), 3.40 (b, 1H); ^{13}C NMR (125 MHz, DMSO- d_6) δ 137.2, 134.3, 132.9, 131.6, 129.3, 110.9, 102.2; HRMS m/z : (M-H) $^-$ calcd for $\text{C}_7\text{H}_3\text{BrClN}_2$ 228.9168, found 228.9173.

7-Methyl-4-azaindole 4f. ^1H NMR (500 MHz, CD_3OD) δ 8.41 (d, 1H, J = 6.00 Hz), 8.07 (d, 1H, J = 3.25 Hz), 7.49 (d, 1H, J = 6.05 Hz), 6.84 (d, 1H, J = 3.2 Hz), 2.84 (s, 3H); ^{13}C NMR (125 MHz, CD_3OD) δ 143.2, 137.2, 136.8, 135.0, 133.6, 119.0, 97.9, 17.6; HRMS m/z : (M+H) $^+$ calcd for $\text{C}_8\text{H}_9\text{N}_2$ 133.0766 found 133.0767.

5-Chloro-7-methyl-4-azaindole 4g. ^1H NMR (500 MHz, DMSO- d_6) δ 7.67 (d, 1H, J = 5.95 Hz), 6.97 (s, 1H), 6.50 (d, 1H, J = 4.85 Hz), 2.50 (s, 3H); ^{13}C NMR (125 MHz, DMSO- d_6) δ 144.8, 142.5, 133.0, 129.6, 127.4, 116.1, 101.4, 16.0; HRMS m/z : (M-H) $^-$ calcd for $\text{C}_8\text{H}_6\text{ClN}_2$ 165.0220, found 165.0221.

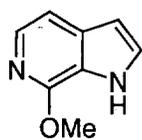
7-Benzyloxy-4-azaindole 4h. ^1H NMR (500 MHz, CDCl_3) δ 8.64 (b, 1H), 8.34 (d, 1H, J = 5.35 Hz), 7.40 (m, 6H), 6.72 (d, 1H, J = 3.25 Hz), 6.67 (d, 1H, J = 5.45 Hz), 5.35 (s, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 151.1, 147.9, 145.2, 135.8, 128.8, 128.6, 127.9, 126.3, 119.6, 103.9, 99.6, 70.2.; HRMS m/z : (M+H) $^+$ calcd for $\text{C}_{14}\text{H}_{13}\text{N}_2\text{O}$ 225.1028, found 225.1029.

7-Methoxy-4-azaindole 4i. ^1H NMR (500 MHz, CD_3OD) δ 8.16 (d, 1H, $J = 5.55$ Hz), 7.41 (d, 1H, $J = 3.20$ Hz), 6.74 (d, 1H, $J = 5.55$ Hz), 6.52 (d, 1H, $J = 3.15$ Hz), 4.04 (s, 3H); ^{13}C NMR (125 MHz, CD_3OD) δ 154.5, 148.3, 145.0, 128.6, 102.4, 99.5, 56.2; HRMS m/z : $(\text{M}+\text{H})^+$ calcd for $\text{C}_8\text{H}_9\text{N}_2\text{O}$ 149.0715, found 149.0721.

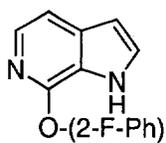
7-Chloro-4-azaindole 4j. ^1H NMR (500 MHz, CD_3OD) δ 8.50 (d, 1H, $J = 6.20$ Hz), 8.10 (d, 1H, $J = 3.20$ Hz), 7.71 (d, 1H, $J = 6.30$ Hz), 6.91 (d, 1H, $J = 3.25$ Hz); ^{13}C NMR (125 MHz, CD_3OD) δ 148.5, 143.6, 131.5, 128.5, 128.1, 117.5, 103.4; HRMS m/z : $(\text{M}+\text{H})^+$ calcd for $\text{C}_7\text{H}_6\text{ClN}_2$ 153.0220, found 153.0216.

6-Azaindole 5. ^1H NMR (500 MHz, CD_3OD) δ 8.67 (s, 1H), 8.03 (d, 1H, $J = 5.55$ Hz), 7.58 (d, 1H, $J = 5.55$ Hz), 7.53 (d, 1H, $J = 3.05$ Hz), 6.54 (d, 1H, $J = 3.00$ Hz); ^{13}C NMR (125 MHz, CD_3OD) δ 137.9, 134.9, 134.8, 134.6, 131.0, 116.5, 102.1; HRMS m/z : $(\text{M}+\text{H})^+$ calcd for $\text{C}_7\text{H}_7\text{N}_2$ 119.0609, found 119.0612.

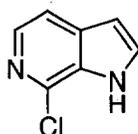
Figures



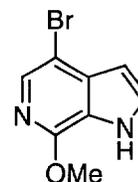
4a



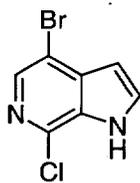
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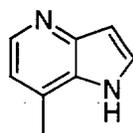
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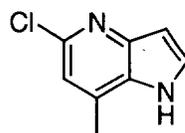
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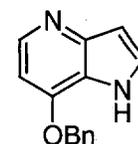
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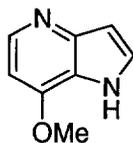
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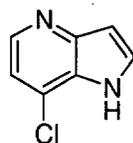
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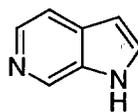
4h



4i



4j



5

