



SUPPLEMENTARY MATERIAL TO  
**Electrocatalytic multicomponent assembling of aminouracils,  
aldehydes and malonitrile: An efficient approach to  
7-aminopyrido[2,3-*d*]pyrimidine-6-carbonitrile derivatives**

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PHYSICAL AND SPECTRAL DATA FOR COMPOUNDS **4a–j**

*7-Amino-5-(4-chlorophenyl)-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-*d*]pyrimidine-6-carbonitrile (4a)*. Yield: 80 %; m.p.: >300 °C dec. (Lit.: >300 °C<sup>1</sup>); IR (KBr, cm<sup>-1</sup>): 3395, 3336 (–NH stretching of primary amine), 3200 (–NH stretching of secondary amide), 2200 (C–N stretch), 1705, 1645 (–C=O stretching of amide group); <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 7.30 (2H, *d*, *J* = 8.4 Hz, Ar-H), 7.48 (2H, *d*, *J* = 8.4 Hz, Ar-H), 7.69–7.71 (2H, *brs*, NH<sub>2</sub>), 10.97 (1H, *s*, NH), 11.51 (1H, *s*, NH); <sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 80.3 (CN), 114.0, 114.9, 116.5, 122.8, 130.0, 133.5, 135.8, 154.8, 156.9 (Ar-C), 161.1 (C=N), 161.8 (C=N), 163.7(C=O), 165.0 (C=O).

*7-Amino-5-(4-methoxyphenyl)-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-*d*]pyrimidine-6-carbonitrile (4b)*. Yield: 78 %; m.p.: >300 °C dec. (Lit.: >300 °C dec.<sup>2</sup>); IR (KBr, cm<sup>-1</sup>): 3400, 3385 (–NH stretching of primary amine), 3190 (–NH stretching of secondary amide), 2205 (C–N stretch), 1700, 1645 (–C=O stretching of amide group). <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 3.84 (3H, *s*, CH<sub>3</sub>), 6.80 (2H, *d*, *J* = 8.7 Hz, Ar-H), 7.43 (2H, *d*, *J* = 8.7 Hz, Ar-H), 7.68 (2H, *s*, NH<sub>2</sub>), 10.95 (1H, *s*, NH), 11.50 (1H, *s*, NH); <sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 54.6 (OCH<sub>3</sub>), 115.4 (CN), 115.8, 116.4, 124.2, 132.4, 133.6, 134.5, 134.4, 149.1, 153.6 (Ar-C), 159.1 (C=N), 160.5 (C=N), 164.4 (C=O), 164.9 (C=O).

*7-Amino-5-(3-nitrophenyl)-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-*d*]pyrimidine-6-carbonitrile (4c)*. Yield: 85 %; m.p.: > 300 °C dec. (Lit.: >300 °C dec.<sup>2</sup>); IR (KBr, cm<sup>-1</sup>): 3400, 3333 (–NH stretching of primary amine), 3186 (–NH stretching of secondary amide), 2223 (C–N stretch), 1705, 1647 (–C=O stretching of amide group); <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 7.74–7.81 (4H,

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*m*, Ar-H & NH<sub>2</sub>), 8.21–8.22 (1H, *m*, Ar-H), 8.30–8.32 (1H, *m*, Ar-H), 11.02 (1H, *s*, NH), 11.56 (1H, *s*, NH); <sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 87.9 (CN), 99.3, 116.1, 122.6, 123.3, 129.2, 135.0, 138.3, 147.2, 149.9 (Ar-C), 155.6 (C=N), 156.3 (C=N), 160.0 (C=O), 160.8 (C=O).

*7-Amino-5-(4-nitrophenyl)-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile (4d)*. Yield: 84 %; m.p.: >300 °C (Lit.: >300 °C dec.<sup>2</sup>); IR (KBr, cm<sup>-1</sup>): 3410, 3300 (–NH stretching of primary amine), 3197 (–NH stretching of secondary amide), 2205 (C–N stretch), 1704, 1645 (–C=O stretching of amide group); <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 7.74 (2H, *s*, NH<sub>2</sub>), 7.78 (2H, *d*, *J* = 6.8 Hz, Ar-H), 8.27 (2H, *d*, *J* = 6.8 Hz, Ar-H), 11.02 (1H, *s*, NH), 11.57 (1H, *s*, NH); <sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 88.0 (CN), 98.7, 115.4, 122.8, 129.2, 144.2, 146.9, 150.1, 155.7 (Ar-C), 156.6 (C=N), 160.3 (C=N), 160.8 (C=O), 166.5 (C=O).

*7-Amino-5-(4-chlorophenyl)-4-oxo-2-thioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile (4e)*. Yield: 82 %; m.p.: >300 °C (Lit.: >300 °C dec.<sup>1</sup>); IR (KBr, cm<sup>-1</sup>): 3415, 3305 (–NH stretching of primary amine), 3202 (–NH stretching of secondary amide), 2210 (C–N stretch), 1695, 1650 (–C=O stretching of amide group); <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 6.45 (2H, *s*, NH<sub>2</sub>), 7.73 (2H, *d*, *J* = 8.4 Hz, Ar-H), 8.10 (2H, *d*, *J* = 8.4 Hz, Ar-H), 11.45 (1H, *s*, NH), 11.52 (1H, *s*, NH); <sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 89.8 (CN), 114.1, 115.3, 116.9, 123.3, 129.5, 134.0, 143.9, 152.4, 154.9 (Ar-C), 160.9 (C=N), 162.0 (C=N), 164.2 (C=O), 174.5 (C=S).

*7-Amino-5-(4-nitrophenyl)-4-oxo-2-thioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile (4f)*. Yield: 86 %; m.p.: > 300 °C dec. (Lit.: >300 °C dec.<sup>1</sup>); IR (KBr, cm<sup>-1</sup>): 3410, 3305 (–NH stretching of primary amine), 3215 (–NH stretching of secondary amide), 2210 (C–N stretch), 1687, 1640 (–C=O stretching of amide group); <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 6.36 (2H, *s*, NH<sub>2</sub>), 8.14 (2H, *d*, *J* = 8.8 Hz, Ar-H), 8.30 (2H, *d*, *J* = 8.8 Hz, Ar-H), 12.49 (1H, *s*, NH), 13.10 (1H, *s*, NH); <sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 89.9 (CN), 108.1, 114.2, 115.3, 116.7, 123.0, 129.3, 132.9, 152.1, 154.2 (Ar-C), 160.6 (C=N), 161.7 (C=N), 163.9 (C=O), 174.7 (C=S).

*7-Amino-5-(4-chlorophenyl)-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile (4g)*. Yield: 71 %; m.p.: 282–283 °C (Lit.:<sup>3</sup> 280–281 °C); IR (KBr, cm<sup>-1</sup>): 3415, 3315 (–NH stretching of primary amine), 2215 (C–N stretch), 1715, 1665 (–C=O stretching of amide group); <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 3.09 (3H, *s*, CH<sub>3</sub>), 3.51 (3H, *s*, CH<sub>3</sub>), 7.28 (2H, *d*, *J* = 8.4 Hz, Ar-H), 7.51 (2H, *d*, *J* = 8.4 Hz, Ar-H), 7.90–7.94 (2H, *brs*, NH<sub>2</sub>).

*7-Amino-5-(3-bromophenyl)-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile (4h)*. Yield: 70 %; m.p.: 297–299 °C (Lit.:<sup>4</sup> >300 °C); IR (KBr, cm<sup>-1</sup>): 3314, 3219 (–NH stretching of primary amine), 2214 (C–N stretch), 1716, 1662 (–C=O stretching of amide group); <sup>1</sup>H-NMR (400

MHz, DMSO-*d*<sub>6</sub>,  $\delta$  / ppm): 3.32 (3H, *s*, CH<sub>3</sub>), 3.67 (3H, *s*, CH<sub>3</sub>), 5.74 (2H, *s*, NH<sub>2</sub>), 7.20–7.23 (1H, *m*, Ar-H), 7.40 (1H, *t*, *J* = 8.0 Hz, Ar-H), 7.41 (1H, *s*, Ar-H), 7.63–7.65 (1H, *m*, Ar-H); <sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>,  $\delta$  / ppm): 28.4 (CH<sub>3</sub>), 30.2 (CH<sub>3</sub>), 90.0 (CN), 114.8, 122.4, 124.6, 129.9, 132.2, 134.9, 138.1, 148.1, 151.1 (Ar-C), 154.0 (C=N), 158.3 (C=N), 158.9 (C=O), 159.8 (C=O).

*7-Amino-1,3-dimethyl-5-(3-nitrophenyl)-2,4-dioxo-1,2,3,4-tetrahydropyrido-[2,3-d]pyrimidine-6-carbonitrile (4i)*. Yield 76%; m.p.: 312–314 °C (Lit.:<sup>3</sup> 298–299 °C); IR (KBr, cm<sup>-1</sup>): 3388, 3336 (–NH stretching of primary amine), 2224 (C–N stretch), 1709, 1668 (–C=O stretching of amide group); <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>,  $\delta$  / ppm): 3.30 (3H, *s*, CH<sub>3</sub>), 3.68 (3H, *s*, CH<sub>3</sub>), 5.82 (2H, *s*, NH<sub>2</sub>), 7.61–7.64 (1H, *m*, Ar-H), 7.71 (1H, *t*, *J* = 7.6 Hz, Ar-H), 8.17 (1H, *t*, *J* = 2.0 Hz, Ar-H), 8.37–8.40 (1H, *m*, Ar-H); <sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>,  $\delta$  / ppm): 28.4 (CH<sub>3</sub>), 30.3 (CH<sub>3</sub>), 89.7 (CN), 100.2, 114.6, 122.7, 124.0, 129.5, 133.2, 137.7, 148.0, 151.0 (Ar-C), 154.1 (C=N), 157.2 (C=N), 159.0 (C=O), 159.9 (C=O).

*7-Amino-1,3-dimethyl-5-(4-nitrophenyl)-2,4-dioxo-1,2,3,4-tetrahydropyrido-[2,3-d]pyrimidine-6-carbonitrile (4j)*. Yield 72 %; m.p.: >300 °C (Lit.:<sup>3</sup> >300 °C); IR (KBr, cm<sup>-1</sup>): 3445, 3313 (–NH stretching of primary amine), 2218 (C–N stretch), 1711, 1637 (–C=O stretching of amide group). <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>,  $\delta$  / ppm): 3.08 (3H, *s*, CH<sub>3</sub>), 3.51 (3H, *s*, CH<sub>3</sub>), 7.57 (2H, *d*, *J* = 8.8 Hz, Ar-H), 8.01–8.04 (2H, *brs*, NH<sub>2</sub>), 8.32 (2H, *d*, *J* = 8.8 Hz, Ar-H); <sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>,  $\delta$  / ppm): 27.7 (CH<sub>3</sub>), 29.6 (CH<sub>3</sub>), 87.8 (CN), 98.3, 115.0, 123.0, 128.9, 144.4, 147.3, 150.8 (Ar-C), 153.5 (C=N), 157.0 (C=N), 158.6 (C=O), 160.2 (C=O).

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