



SUPPLEMENTARY MATERIAL TO  
**Microwave-assisted synthesis of azepines via  
nucleophilic aromatic substitution**

NINA BOŽINOVIĆ, BOGDAN A. ŠOLAJA\* and IGOR M. OPSENICA\*\*

*Faculty of Chemistry, University of Belgrade, Studentski trg 16, P. O. Box 51,  
11158 Belgrade, Serbia*

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CHARACTERIZATION DATA FOR COMPOUNDS 5–8

*N,N*-dimethyl-5H-dipyrido[4,3-b:3',4'-f]azepine-5-propanamine (**5**).<sup>1</sup> Yield: 61 %; yellow oil; <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>, δ / ppm): 8.39 (2H, *d*, *J* = 5.5 Hz), 8.18 (2H, *s*), 6.78 (2H, *d*, *J* = 6.0 Hz), 6.66 (2H, *s*), 3.82–3.75 (2H, *m*), 2.46–2.39 (2H, *m*), 2.22 (6H, *s*), 1.84–1.76 (2H, *m*); (+)ESI-HRMS *m/z*: calcd. for [M+H<sup>+</sup>]: 281.17607. Found: 281.17612.

5-[3-(Morpholin-4-yl)propyl]-5H-dipyrido[4,3-b:3',4'-f]azepine (**6**).<sup>1</sup> Yield: 62 %; yellow oil; <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>, δ / ppm): 8.39 (2H, *d*, *J* = 5.5 Hz), 8.16 (2H, *s*), 6.76 (2H, *d*, *J* = 6.0 Hz), 6.64 (2H, *s*), 3.81–3.76 (2H, *m*), 3.67–3.61 (4H, *m*), 2.47–2.41 (2H, *m*), 2.39–2.34 (4H, *m*), 1.82–1.78 (2H, *m*); (+)ESI-HRMS *m/z*: Calcd. for [M+H<sup>+</sup>]: 323.18664. Found: 323.18700.

*N,N*-dimethyl-5H-dipyrido[4,3-b:3',4'-f]azepine-5-ethanamine (**7**). Yield: 56 %; yellow oil; IR (ATR, cm<sup>-1</sup>): 3393, 2946, 2867, 2827, 2780, 1674, 1579, 1480, 1399, 1172, 1053, 928, 840; <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>, δ / ppm): 8.41 (2H, *d*, *J* = 5.5 Hz), 8.18 (2H, *s*), 6.79 (2H, *d*, *J* = 5.5 Hz), 6.65 (2H, *s*), 3.90–3.83 (2H, *m*), 2.60–2.52 (2H, *m*), 2.28 (6H, *s*); <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>, δ / ppm): 156.94, 150.90, 150.81, 131.23, 128.64, 115.19, 56.41, 48.54, 45.79; (+)ESI-HRMS *m/z*: Calcd. for [M+H<sup>+</sup>]: 267.16042. Found: 267.16018.

5H-Dipyrido[4,3-b:3',4'-f]azepine-5-propanol (**8**). Yield: 45 %; yellow oil; IR (ATR, cm<sup>-1</sup>): 3172, 2920, 2867, 2480, 1660, 1569, 1477, 1399, 1323, 1249, 1168, 1071, 908, 844, 789, 755, 729; <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>, δ / ppm): 8.39 (2H, *d*, *J* = 5.5 Hz), 8.17 (2H, *s*), 6.79 (2H, *d*, *J* = 5.5 Hz), 6.66 (2H, *s*), 3.94–3.86 (2H, *m*), 3.82–3.74 (2H, *m*), 1.93–1.84 (2H, *m*); <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>, δ / ppm): 156.92, 150.74, 150.68, 131.23, 128.68, 115.38, 60.02, 46.59, 29.50; (+)ESI-HRMS *m/z*: calcd. for [M+H<sup>+</sup>]: 254.12879. Found: 254.12827.

\* Corresponding authors. E-mail: (\*)bsolaja@chem.bg.ac.rs; (\*\*)igorop@chem.bg.ac.rs

REFERENCE

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