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

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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**).¹ Yield: 61 %; yellow oil; ¹H-NMR (500 MHz, CDCl₃, 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⁺]: 281.17607. Found: 281.17612.

5-[3-(Morpholin-4-yl)propyl]-5H-dipyrido[4,3-b:3',4'-f]azepine (**6**).¹ Yield: 62 %; yellow oil; ¹H-NMR (500 MHz, CDCl₃, 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⁺]: 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⁻¹): 3393, 2946, 2867, 2827, 2780, 1674, 1579, 1480, 1399, 1172, 1053, 928, 840; ¹H-NMR (500 MHz, CDCl₃, 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*); ¹³C-NMR (125 MHz, CDCl₃, 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⁺]: 267.16042. Found: 267.16018.

5H-Dipyrido[4,3-b:3',4'-f]azepine-5-propanol (**8**). Yield: 45 %; yellow oil; IR (ATR, cm⁻¹): 3172, 2920, 2867, 2480, 1660, 1569, 1477, 1399, 1323, 1249, 1168, 1071, 908, 844, 789, 755, 729; ¹H-NMR (500 MHz, CDCl₃, 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*); ¹³C-NMR (125 MHz, CDCl₃, 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⁺]: 254.12879. Found: 254.12827.

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REFERENCE

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