

Supporting Information

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Two new pyrrolo[2,3-*d*]pyrimidines (7-deazapurines): Ultrasonic-assisted synthesis, experimental and theoretical characterizations as well as antibacterial evaluation

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Contents

S2–S3: Short explanation for the spectra of compounds **3** and **4**

S4: FT-IR spectrum of compound **3**

S5: ¹H NMR spectrum of compound **3**

S6: ¹³C NMR spectrum of compound **3**

S7–S9: 2D-NOESY spectrum of compound **3**

S10: FT-IR spectrum of compound **4**

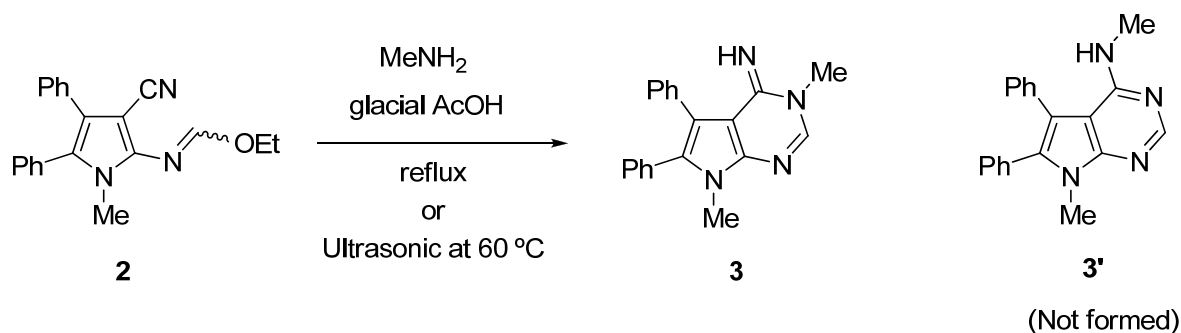
S11–S12: ¹H NMR spectrum of compound **4**

S13: ¹³C NMR spectrum of compound **4**

S14–S16: 2D-NOESY spectrum of compound **4**

Short explanation for the spectra of compounds 3 and 4

The reaction of compound **2** with methyl amine gave a product identified as structure **3**. As shown in the 2D-NOESY spectrum in S7–S9, the interaction between pyrimidine CH at $\delta = 7.70$ with the Me group at $\delta = 3.52$ ppm indicates that these groups are close together and therefore the correct structure is **3**.

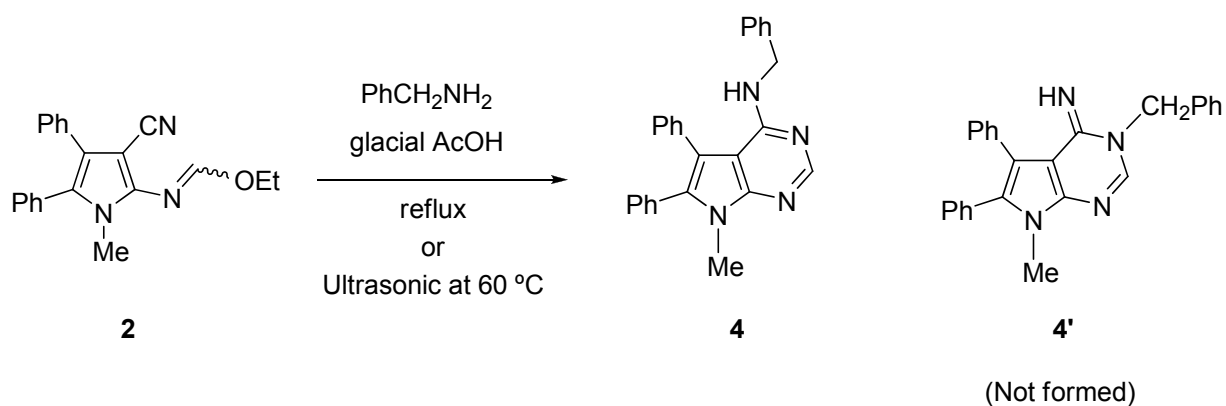


3,7-Dimethyl-5,6-diphenyl-3H-pyrrolo[2,3-d]pyrimidin-4(7H)-imine (**3**)

The colors are in accord with the spectra (S5–S9).

IR (KBr disk): $\nu = 3318, 3026, 2949, 1632, 1565, 1502, 1325, 1181, 1077, 791, 758, 703\text{ cm}^{-1}$. – ^1H NMR (300 MHz, CDCl_3 , 25°C , TMS): $\delta = 3.52$ (s, 3H, CH_3), 3.64 (s, 3H, CH_3), $7.18\text{--}7.31$ (m, 11H, arom-H and NH), 7.70 (s, 1H, pyrimidine CH). – ^{13}C NMR (75 MHz, CDCl_3 , 25°C , TMS): $\delta = 29.92, 35.56, 103.19, 117.43, 126.85, 127.86, 128.30, 128.34, 130.52, 130.66, 130.84, 132.79, 134.06, 143.22, 145.59, 156.25$. – Anal. Calcd for $\text{C}_{20}\text{H}_{18}\text{N}_4$: C, 76.41; H, 5.77; N, 17.82. Found: C, 76.12; H, 5.69; N, 17.91.

The reaction of compound **2** with benzyl amine gave a product identified as structure **4**. As shown in the 2D-NOESY spectrum in S14–S16, there is no interaction between pyrimidine CH at $\delta = 8.54$ ppm with the methylene group at $\delta = 4.70$ ppm, which indicates these groups are not close together and confirms the structure **4**.



4-Benzylamino-7-methyl-5,6-diphenyl-7H-pyrrolo[2,3-d]pyrimidine (**4**)

The colors are in accord with the spectra (S11–S16).

IR (KBr disk): $\nu = 3429, 3025, 2910, 1660, 1584, 1454, 1412, 1334, 1265, 1180, 1134, 1071, 825, 795, 766\text{ cm}^{-1}$. – ^1H NMR (300 MHz, CDCl_3 , 25 $^{\circ}\text{C}$, TMS): $\delta = 3.37$ (s, 3H, CH_3), 4.70 (d, 2H, $J = 5.7\text{ Hz}$, CH_2), 5.38 (br, 1H, NH), 7.17–7.42 (m, 15H, arom-H), 8.54 (d, 1H, $J = 3.6\text{ Hz}$, pyrimidine CH). – ^{13}C NMR (75 MHz, CDCl_3 , 25 $^{\circ}\text{C}$, TMS): $\delta = 29.88, 44.61, 101.80, 113.30, 127.03, 127.15, 127.17, 128.14, 128.37, 128.53, 128.58, 130.57, 130.87, 134.47, 134.61, 138.82, 150.15, 151.97, 156.27$. – Anal. Calcd for $\text{C}_{26}\text{H}_{22}\text{N}_4$: C, 79.97; H, 5.68; N, 14.35. Found: C, 80.27; H, 5.57; N, 14.21.

