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SYNTHESIS OF A NEW HETEROCYCLIC SYSTEM, 5H-BENZ[4,5]IMIDAZO[1,2-*c*]-PYRAZINO[2',3':4,5]PYRROLO[3,2-*e*]PYRIMIDINE

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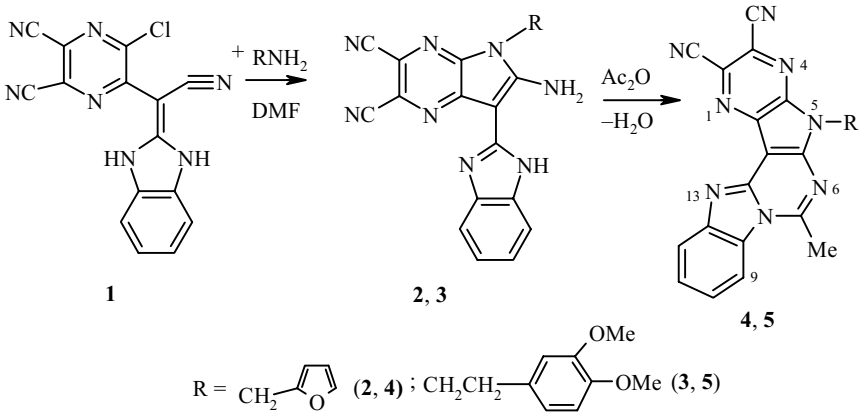
Keywords: 1H-benz[4,5]imidazo[1,2-*c*]pyrazino[2',3':4,5]pyrrolo[3,2-*e*]pyrimidine, synthesis and acylation of 6-amino-7-(1H-benz[*d*]imidazol-2-yl)-5-R-5H-pyrrolo[2,3-*b*]pyrazin-2,3-dicarbonitriles.

The interaction of 2,3-dichloro-5,6-dicyanopyrazines with α-azahetarylacetonitriles led to products of substitution of one of the chlorine atoms **1** [1].



When 5 mmol of compound **1** in 8 ml of DMF reacted with 10 mmol of a primary amine at 50-60°C for 5 h replacement of the chlorine atom by an amine group occurred with subsequent addition of the secondary amine formed to a nitrile group to give compounds **2** and **3**. When 5 mmol of compounds **2** and **3** were heated in 30 ml of acetic anhydride for 8 h acylation occurred at the amino group with subsequent cyclization to give 5-substituted 5H-benz[4,5]imidazo[1,2-*c*]pyrazino[2',3':4,5]pyrrolo[3,2-*e*]pyrimidines **4** and **5**.

6-Amino-7-(1H-benz[*d*]imidazol-2-yl)-5-(2-furylmethyl)-5H-pyrrolo[2,3-*b*]pyrazin-2,3-dicarbonitrile (2). Yield 86%; mp > 300°C (DMF). ^{1}H NMR spectrum (DMSO-d_6, 100 MHz), δ, ppm: 5.54 (2H, s, CH_2); 6.5 (2H, m, 3',4'-H_{fur}); 7.2 (2H, m, H_{arom}); 7.62 (3H, m, 5'-H_{fur} + H_{arom}); 9.3 (2H, s, NH_2); 11.92 (1H, br. s, N–H). IR spectrum (KBr), ν, cm^{-1}: 3520, 3340 (NH_2), 2220 (av.) (CN), 1625 (C=N), 1600 (δ NH_2). Found, %: N 29.02. $C_{20}H_{12}N_8O$. Calculated, %: N 29.46.

6-Amino-7-(1H-benz[*d*]imidazol-2-yl)-5-(3,4-dimethoxyphenethyl)-5H-pyrrolo[2,3-*b*]pyrazin-2,3-dicarbonitrile (3). Yield 81%; mp > 300°C (DMF). ^{1}H NMR spectrum (DMSO-d_6, 100 MHz), δ, ppm.: 3.0 (2H, t, CH_2); 3.66 (6H, s, CH_3); 4.50 (2H, t, CH_2); 6.6-6.8 (3H, m, H_{arom}); 7.15-7.25 (2H, m, H_{arom}); 7.6-7.62 (2H, m, H_{arom}); 9.17 (2H, s, NH_2); 11.86 (1H, br. s, N–H). IR spectrum (KBr), ν, cm^{-1}: 3300-3450 (NH_2), 2220 (av.) (CN), 1625 (C=N), 1600 (δ NH_2). Found, %: N 23.88. $C_{25}H_{20}N_8O_2$. Calculated, %: N 24.12.

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5-(2-Furylmethyl)-7-methyl-5H-benz[4,5]imidazo[1,2-*c*]pyrazino[2',3':4,5]pyrrolo[3,2-*e*]pyrimidin-2,3-dicarbonitrile (4). Yield 87%; mp > 300°C (DMF). ^{1}H NMR spectrum (DMSO-d_6, 100 MHz), δ, ppm: 3.37 (3H, s, CH_3); 5.81 (2H, s, CH_2); 6.42 (1H, dd, 4'-H_{fur}); 6.55 (1H, d, J = 3.5, 3'-H_{fur}); 7.47-7.56 (3H, m, 10-, 11-H + 5'-H_{fur}); 7.88 (1H, d, J = 7.5, 9- or 11-H); 8.25 (1H, d, J = 8, 9- or 11-H). IR spectrum (KBr), ν, cm^{-1}: 2220 (w) (CN), 1650 (C=N). Found, %: N 27.39. $C_{22}H_{12}N_8O$. Calculated, %: N 27.71.

5-(3,4-Dimethoxyphenethyl)-7-methyl-5H-benz[4,5]imidazo[1,2-*c*]pyrazino[2',3':4,5]pyrrolo[3,2-*e*]-pyrimidin-2,3-dicarbonitrile (5). Yield 88%; mp > 300°C (DMF). ^{1}H NMR spectrum (DMSO-d_6, 100 MHz), δ, ppm: 3.08 (2H, t, CH_2); 3.32 (3H, s, CH_3); 3.64 (6H, s, O–CH_3); 4.83 (2H, t, N–CH_2); 6.5-6.7 (3H, m, H_{arom}); 7.63 (2H, m, 10-, 11-H); 7.95 (1H, d, J = 8 Hz, 9- or 11-H); 8.29 (1H, d, J = 8 Hz, 9- or 11-H). IR spectrum, ν, cm^{-1}: 2220 (w) (CN), 1640 (C=N). Found, %: N 23.20. $C_{27}H_{20}N_8O_2$. Calculated, %: N 22.94.

REFERENCES

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