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SYNTHESIS OF A NOVEL HETEROCYCLIC SYSTEM 6H-PYRROLO[2',3',4':4,5]NAPHTHO[1,8-*de*][1,2,3]TRIAZINES

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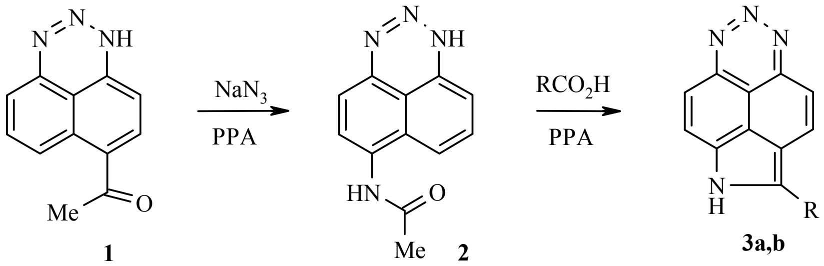
Keywords: 6H-pyrrolo[2',3',4':4,5]naphtho[1,8-*de*][1,2,3]triazines, PPA, sodium azide, 1H-1,5,6,7-tetraazacyclopenta[*c*,*d*]phenalenes, *peri* annelation, Schmidt reaction.

We have previously developed a series of methods of *peri* annelation of six-membered rings to a 1H-naptho[1,8-*de*][1,2,3]triazine [1, 2]. With the high biological activity of a significant number of indole derivatives we have now developed a method for the *peri* annelation of a pyrrole ring to this compound. It was found that the reaction of 1 mmole of ketone **1** and NaN_3 (0.07 g, 1.08 mmol) in PPA* (2-3 g; the PPA used had an 86% P_2O_5 content and was prepared by method [3]) at 60-70ºC for 1 h followed by addition of acetic or benzoic acid (2 mmol) with heating at 100-110ºC for 4 h (monitoring by TLC) gave the previously unknown 1H-1,5,6,7-tetraazacyclopenta[*c,d*]phenalenes **3a,b** in 41 and 34% yield respectively



3 **a** R = Me, **b** R = Ph

The reaction included an intermediate formation of the amide **2** which could be separated.

^1H NMR spectra were recorded on a Bruker WP-200 (200 MHz) instrument using DMSO-d_6 with TMS as internal standard. Monitoring of the reaction course and the purity of the synthesized compounds was carried out on Silufol UV-254 plates with ethyl acetate as solvent. The reaction mixture was treated with water (50 ml) and basified with ammonia solution to pH 8-9. The precipitate formed was filtered off. The mother liquor was extracted with hot benzene (3×50 ml). The solvent was evaporated and the residue was combined with the precipitate. The compounds obtained were purified by recrystallization.

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N-(1H-Naphtho[1,8-*de*][1,2,3]triazin-6(7)-yl)acetamide (2). Yield 0.147 g (65%); mp 225-226ºC (decomp., ethyl acetate). ^{1}H NMR spectrum, δ, ppm (*J*, Hz): 2.13 (3H, s, $COCH_3$); 6.93 (1H, d, *J* = 7.7, H-9(4)); 7.31 (1H, dd, *J* = 8.4 and *J* = 7.7, H-8(5)); 7.38 (1H, d, *J* = 8.1, H-4(9)); 7.46 (1H, d, *J* = 8.4, H-7(6)); 8.31 (1H, d, *J* = 8.1, H-5(8)); 9.60 (1H, br. s, NHCO); 11.0 (1H, br. s, NH). Found, %: C 63.87; H 4.42; N 24.68. $C_{12}H_{10}N_4O$. Calculated, %: C 63.71; H 4.46; N 24.76.

7-Methyl-6H-pyrrolo[2',3',4':4,5]naphtho[1,8-*de*][1,2,3]triazine (3a). Yield 0.085 g (41%); mp 271-273ºC (decomp., benzene). ^{1}H NMR spectrum, δ, ppm (*J*, Hz): 2.96 (3H, s, CH_3); 7.63 (1H, d, *J* = 9.0, H-9); 7.82 (1H, d, *J* = 9.0, H-3); 8.34 (1H, d, *J* = 9.0, H-4); 8.54 (1H, d, *J* = 9.0, H-8); 13.1 (1H, br. s, NH). Found, %: C 69.38; H 3.79; N 26.83. $C_{12}H_8N_4$. Calculated, %: C 69.22; H 3.87; N 26.91.

7-Phenyl-6H-pyrrolo[2',3',4':4,5]naphtho[1,8-*de*][1,2,3]triazine (3b). Yield 0.092 g (34%); mp 284-286ºC (decomp., benzene). ^{1}H NMR spectrum, δ, ppm (*J*, Hz): 7.55 (3H, m, H-3,4,5 Ph); 7.69 (1H, d, *J* = 9.0, H-3); 7.82 (1H, d, *J* = 8.8, H-9); 8.21 (2H, d, *J* = 7.7, H-2,6 Ph); 8.38 (1H, d, *J* = 8.8, H-8); 8.74 (1H, d, *J* = 9.0, H-4); 12.8 (1H, br. s, NH). Found, %: C 75.71; H 3.65; N 20.64. $C_{17}H_{10}N_4$. Calculated, %: C 75.54; H 3.73; N 20.73.

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