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A METHOD FOR CONSTRUCTION OF NEW CONDENSED SYSTEM – QUINOXALINO[1,2-*a*]PYRROLO-[2,3-*b*][1,5]PYRIDODIAZEPIN

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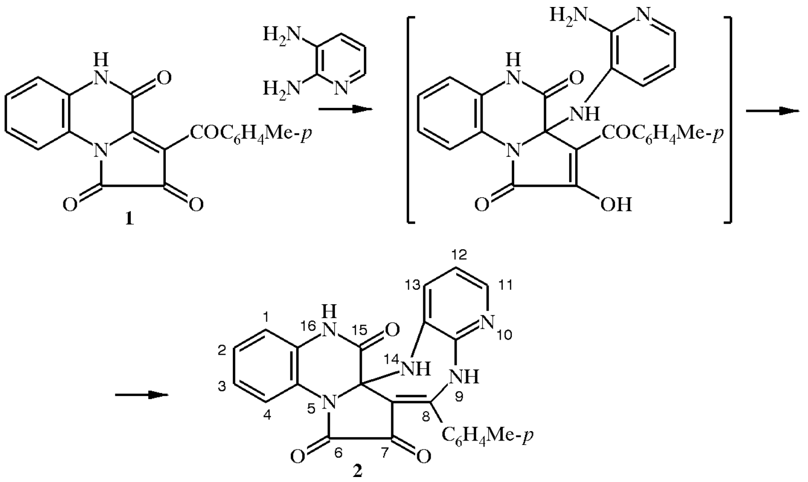
We are the first to report the reaction of 3-*p*-toluyl-1,2,3,4-tetrahydropyrrolo[1,2-*a*]quinoxaline-1,2,4-trione (**1**) [1] with 2,3-diaminopyridine, leading to the formation of 8-*p*-tolyl-6,7,9,14,15,16-hexahydroquinoxalino[1,2-*a*]pyrrolo[2,3-*b*][1,5]pyridodiazepin-6,7,15-trione (**2**).



This reaction proceeds similarly to the reaction of 3-aroyl-1,2,3,4-tetrahydropyrrolo[1,2-*a*]quinoxaline-1,2,4-triones with *o*-phenylenediamine [2] with successive nucleophilic attack of $C_{(5)}$ and the carbonyl group of the aroyl fragment at position 4 of the pyrroledione ring by the amino groups of 2,3-diaminopyridine.

Quantum chemical calculations of the 2,3-diaminopyridine molecule by semi-empirical and nonempirical methods do not provide the correct explanation of the observed direction of the reaction of this compound with pyrroloquinoxalinetrione **1**. Furthermore, the significant downfield shift for $N_{(9)}H$ in the ^1H NMR spectrum of **2** relative to the spectral data for model compound 8-*p*-tolyl-6,7,9,14,15,16-hexahydroquinoxalino[1,2-*a*]pyrrolo-[2,3-*b*][1,5]benzdiazepin-6,7,15-trione (from 12.58 [2] to 13.70 ppm) along with the lack of shift for $N_{(14)}H$ (6.87 ppm for **2** and 6.90 ppm for the model compound) suggests specific initial nucleophilic attack by $N_{(3)}$ in 2,3-diaminopyridine and supports the structure proposed for **2**.

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This reaction is a method for constructing quinoxalino[1,2-*a*]pyrrolo[2,3-*b*][1,5]pyridodiazepin, which had previously been an unavailable functionalized condensed heterocyclic system.

8-*p*-Tolyl-6,7,9,14,15,16-hexahydroquinoxalino[1,2-*a*]pyrrolo[2,3-*b*][1,5]pyridodiazepin-6,7,15-trione (2). A solution of 2,3-diaminopyridine (1.09 g, 10 mmol) in absolute dioxane (20 ml) was added to a solution of **1** (3.3 g, 10 mmol) in absolute dioxane (50 ml). The mixture was heated at reflux for 5 min and cooled. The precipitate formed was filtered off to give 3.81 g (90%) of compound **2**; mp 275-276°C (dioxane–acetonitrile, 1:1). IR spectrum, cm^{-1}: 3220 ($N_{(5)}HCO$), 3160 br (NH), 1700 ($C_{(6)}=O$), 1680 ($C_{(7)}=O$, $C_{(15)}=O$). ^1H NMR spectrum (DMSO-d_6), δ, ppm: 2.39 (3H, s, CH_3); 6.87 (1H, s, $N_{(14)}H$); 7.05-8.15 (11H, m, $2C_6H_4 + C_6H_3$); 11.85 (1H, s, $N_{(16)}H$); 13.70 (1H, s, $N_{(9)}H$). Found, %: C 68.15; H 4.17; N 16.38. $C_{24}H_{17}N_5O_3$. Calculated, %: C 68.08; H 4.05; N 16.54.

REFERENCES

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