

## New Type of T-Reactions in the Synthesis of Zwitterionic Heterocycles

V.G.Kartsev<sup>1</sup>, K.A.Krasnov<sup>2</sup>

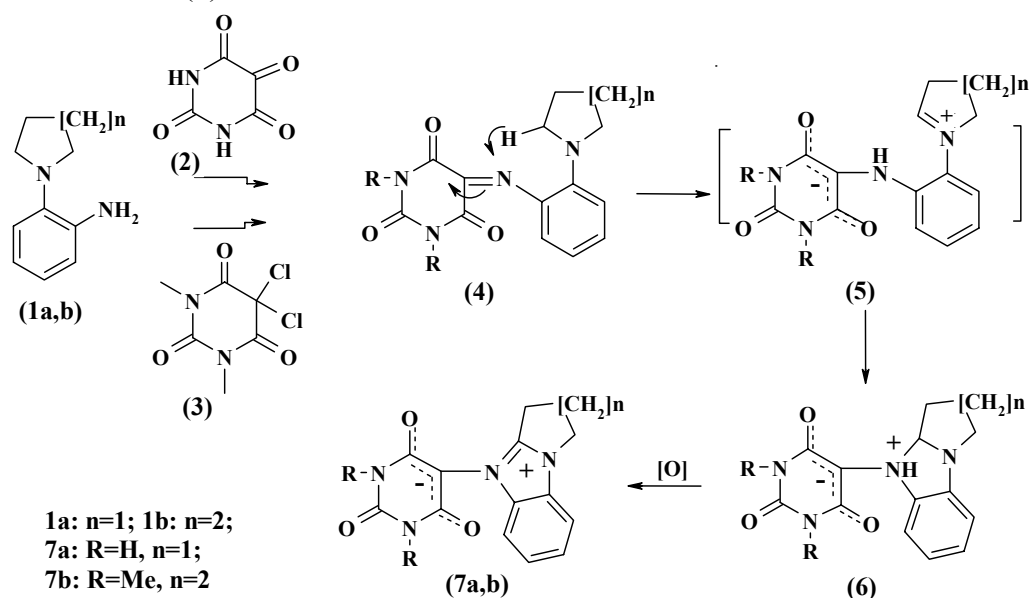
<sup>1</sup>InterBioScreen Ltd., Institutskii pr. 7a, Chernogolovka, Moscow, 143432 Russia

Fax: (095) 7880651,

[screen@ibscreen.chg.ru](mailto:screen@ibscreen.chg.ru)

<sup>2</sup>Mechnikov State Medical Academy, Piskarevskii pr. 47, St. Petersburg, 195067 Russia

Condensation of substituted *o*-phenylenediamines (**1a,b**) with alloxan (**2**) as well as with 5,5-dichloro-1,3-dimethylbarbituric acid (**3**) could be expected to yield respective 5-imino derivatives (**4**).



We have found that the above reactions yield benzimidazole derivatives (**7a,b**) via unstable intermediates **4** which could not be isolated. The rearrangement of intermediates **4** can be regarded as a new example of the so-called T-reaction. Tentatively, this rearrangement involves also the stage of 1,5-hydride shift (by analogy with [1]) followed by cyclization of derivatives **5** into compounds **6**. The latter ones could be readily oxidized with starting substrates (**2** or **3**) into respective zwitterionic benzimidazoles **7**.

The structure of synthesized compounds was confirmed by <sup>1</sup>H NMR, <sup>13</sup>C NMR, and mass spectra. Compounds **7a,b** are mesomeric betaines with a positive charge distributed over the N–C–N triad in the benzimidazole moiety and a negative charge, over the β-dicarbonyl system in the pyrimidine cycle.