

X-Ray mapping in heterocyclic design. X-Ray diffraction study of the derivatives 5-amide-4,6-dimethylpyridone-2

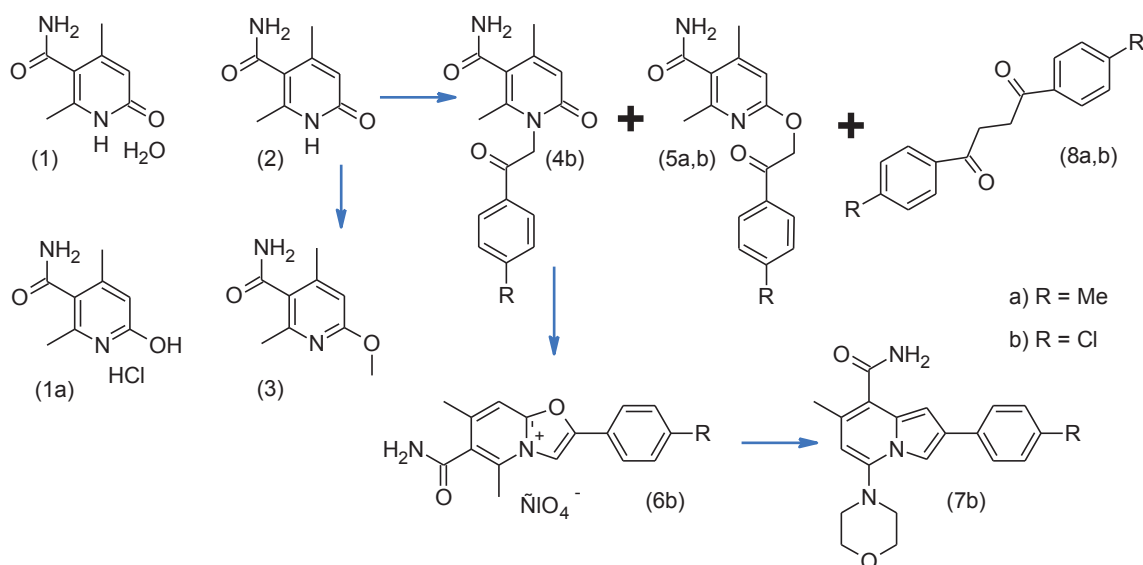
E.M. Feklicheva (Okul)¹, A.A. Kononenko², E.V. Babaev¹, V.B. Rybakov¹

¹ M.V. Lomonosov Moscow State University, Chemistry Department, Vorob'evy Gory, 1-3, 119991, Moscow, Russia.

² Gubkin Russian State University of Oil and Gas (National Research University), Leninsky Prospect, 65-1, 119991, Moscow, Russia.

E-mail: anjakononenko1994@gmail.com

Crystal and molecular structures of 9 target (**1-7**) and 2 incidental (**8a**, **8b**) compounds were studied by single crystal X-Ray analysis. All samples were characterized by ¹H NMR spectra. A comparative analysis is performed for bond lengths, bond and torsion angles with similar fragments of the parent molecules. In many structures the H-bonds were localized that influence the strength of molecular packing in crystals. Different rotation angles of amide group from the pyridine heterocycle were registered in the polymorph crystals of compounds **1** and **2**. Chemical problems of preparation and full description of studied molecular and crystal structures will be discussed.



Keywords: molecular structure, heterocycles, pyridone-2, indolizine