

The synthesis of novel heterocyclic systems based on 3-pyrazolidinones

Abstract

In dissertation The synthesis of novel heterocyclic systems based on 3-pyrazolidinones, we investigated possibility of synthesis of the new heterocyclic systems from the 3-pyrazolidinone derivatives, and researched the potential of optimizing reaction conditions to expand chemical libraries of already known compounds.

In the first part we focused on optimizing synthesis conditions and the preparation of saturated tetrahydropyrazolo[1,5-*c*]pyrimidin-2,7-(1*H*,3*H*)-diones of which, prior to our work, only a few representatives were known and prepared by our reaserch group. We were able to reduce the synthetic steps from twelve to five.

We also optimized the synthesis conditions of bicyclic products such as pyrazolo[1,2-*a*]pyrazolones, resulting in a reaction between azomethine imines and dipolarophiles. Optimized conditions allow the reaction of azomethine imines with terminal acetylenes as dipolarphiles, being carried out at room temperature with the addition of CuI and a base, or simply with the addition of elemental copper. To expand the library of bicyclic products, we also searched for conditions which enabled the introduction of aliphatic groups at position 3 of the bicyclic products. So far, synthesis of such derivatives was underexplored.

The second part of our research was about preparation of some unknown heterocyclic frameworks. Initially we focused on the preparation of 7-methyl and 7-phenyl-2-oxo-2,3,3*a*,4,5,6-hexahydropyrazolo[1,5-*a*]pyridine azomethine imine as the key-intermediate in the preparation of two new heterocyclic frameworks: saturated pyrazolo[1,5-*a*]pyridinones and tricyclic systems, diazacyclopenta[*cd*]indene-2-ones.

Later on, we continued with the preparation of an unknown bridged system, triazabicyclo[3.2.1]octanone. Furthermore, we focused on the N–N bond cleavage in pyrazolo[1,2-*a*]pyrazolones, that would lead to formation of a less known 8-membered heterocyclic framework, 1,5-diazocan-2-ones.

Keywords: 3-pyrazolidinone, 1,2-dipolar cycloaddition, saturated pyrazolo[1,5-*c*]pyrimidines, saturated pyrazolo[1,5-*a*]pyridines, tricyclic systems, pyrazolo[1,2-*a*]pyrazolones, triazabicyclo[3.2.1]oktanone.