

POSTER PRESENTATIONS

SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF UNSYMMETRICAL ARYL-HETERYL UREA HYBRIDS

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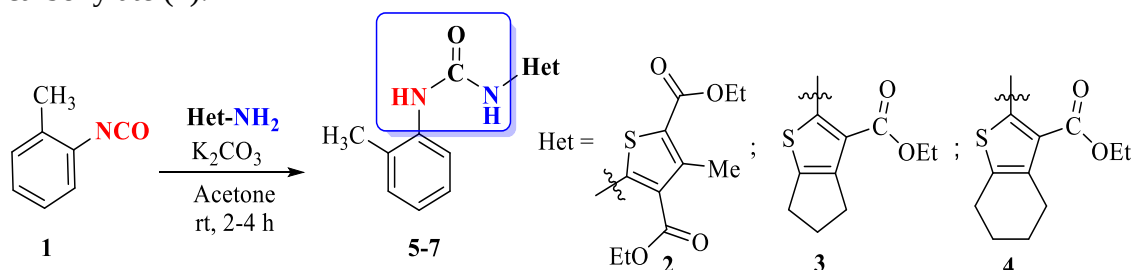
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Urea derivatives constitute an important class of pharmacophoric motifs in organic and pharmaceutical chemistry. Their —NH—C(=O)—NH— group can simultaneously function as both a hydrogen-bond donor and acceptor. This feature enhances the selective interaction of urea-containing molecules with the active sites of enzymes, receptors and other biomacromolecules [1,2]. The urea scaffold is also found in several clinically used antitumor, antidiabetic, and central nervous system-active drugs [1,3].

The urea fragment promotes a relatively planar molecular conformation and provides the ability to form hydrogen bonds through two N–H groups. These characteristics make the aryl urea scaffold a valuable molecular-recognition element in protein–ligand complexes. Urea-based drug candidates have been extensively investigated, particularly in the field of kinase inhibitors, where this structural motif is considered an important pharmacophore for the development of antitumor agents [1,3,4].

In the present study, o-tolylisocyanate was reacted with 2-amino-4-methyl-3,5-diethoxycarbonylthiophene (2), ethyl 2-amino-5,6-dihydro-4H-cyclopenta[b]thiophene-3-carboxylate (3), and ethyl 2-amino-4,5,6,7-tetrahydrobenzo[b]thiophene-3-carboxylate (4):



As a result of these reactions aryl-heteryl urea hybrids (5-7) were isolated in 60-68% yields. The structures of the synthesized compounds were confirmed by IR, ¹H NMR spectroscopy and mass spectrometry.

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