PP5. SYNTHIS OF NEW DERIVATE OF MERCAPTO-3-PHENYL-1,3,4-THIADIAZOL-2-THIONE AND ESTIMATION OF ITS BIOLOGICAL ACTIVITY ON PASS.

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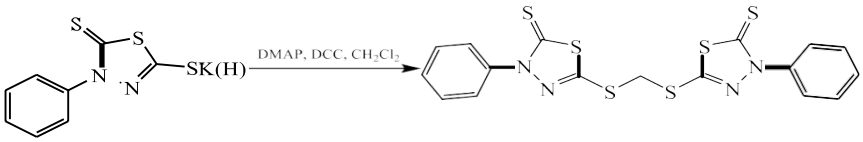
Heterocyclic compounds of 1,3,4-thiadiazole are the important class of substances with a wide spectrum of biological activity. The sulfur atom of thiadiazole givesthese compounds lipophilic properties, which allow to better penetrating through biological membranes. Thiadiazole fragments have potential activity with G- receptors, through enzyme binding, at the active final cysteine (for example, bacterialenzymes are part of non- steroidal anti-inflammatory drugs. For the synthesis of new heterocyclic derivatives with a wide spectrum of biological activity, we study the formation of various derivatives based on 5-mercapto-3-phenyl-1,3,4-thiadiazol-2-thione. The experiment was carried out in the presence of a mixture of DMAP and DCC catalysts according to the general procedure [1].



Scheme 1. Reaction

We report here the synthesis of 5-mercapto-3-phenyl-1,3,4-thiadiazol-2-thione, in the presence of a mixture of DMAP and DCC catalysts. The presence of a mixture of catalysts promotes the formation of a methylene bridge in the structure of the resulting compound - 5,5'-(methylenebis(sulfanediyl))bis(3-phenyl-1,3,4-thiadiazole- 2(3H)-thione). The crystal structure has been determined by X-ray diffraction and intermolecular interactions have been analyzed by HS. We studied the "biological activity spectrum" of 5,5'- (methylenebis(sulfanediyl))bis(3-phenyl-1,3,4-thiadiazole-2(3H)-thione) by PASS on line software, and described biological activity properties in a depending of its structure [2].

In the future, PASS on screening should help to test biological activity of 5,5'-(methylenebis(sulfanediyl))bis(3-phenyl-1,3,4-thiadiazole-2(3H)-thione) on amyloid beta precursor protein antagonist, 5-O-(4-coumaroyl)-D-quinate 3'-monooxygenase inhibitor or Glycosylphosphatidylinositol phospholipase D inhibitor, according their most significant values Pa.

REFERENCES

[1] Md. Ch. Sheikh, Sh.Takagi, T.Yoshimura, H.Morita Mechanistic studies of DCC/HOBt-mediated reaction of 3-phenylpropionic acid with benzyl alcohol and studies on the reactivities of 'active ester' and the related derivatives with nucleophiles. Tetrahedron. 2010;66:7272–7278. https://doi.org/10.1016/j.tet.2010.07.011.

[2] K.J.Tidke, P.R.Solanki Microwave assisted synthesis of (substitutedbenzilidene)-4-amino dihydrothiophen-3(2H)-one (IA-IH) and their biological activities on PASS/JETIR. 2020; 7:(3), 1-12.