Academy of Sciences of the Republic of Uzbekistan

S.Yu. Yunusov Institute of the Chemistry of Plant Substances AS RUz

INTERNATIONAL SCIENTIFIC AND TECHNICAL CONFERENCE

Actual Problems of the Chemistry of Natural Compounds

ABSTRACTS

September 19–20, 2024
Tashkent

CONFERENCE TOPICS

1. Chemistry, biology, pharmacology, and technology of natural compounds and their derivatives.
2. Successes and problems of creation of new drugs.

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X-RAY ANALYSIS AND MOLECULAR DOCKING OF THE ETHYL 2-(4-(DIMETHYLAMINO)BENZOYL)-3-HYDROXY-5-METHYLPYRAZOLIDINE-3-CARBOXYLATE

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The interest in the fine structure of acylhydrazones is primarily due to the fact that they are capable of being in various tautomeric forms. Depending on the structural features of the dicarbonyl component in the series of acylhydrazones of 1,3-diketones, a triple ring chain equilibrium can be expected between linear (hydrazone, enhydrazine) and cyclic 5-hydroxy-2-hydroxypyrazoline tautomeric forms. It should be noted at once that paired prototropic equilibrium was observed for acylhydrazones of both 1,3-ketoesters and 1,3-ketoaldehyde derivatives. We have studied the structure of condensation products of 2,4-dioxopentanoic acid (I) ethyl ether with hydrazides of para-substituted aromatic acids. We report herein the synthesis, crystal structure, DFT calculation and Molecular docking analysis for a new ethyl ester of 2,4-dioxopentanoic acid derivative, 4-dimethylaminobenzoylhydrazone ethyl ester of 2,4-dioxopentanoic acid (H_2L).

The molecular structure of the title compound is illustrated in Fig. 1. Five membered heterocyclic pyrazoline rings, consisting of atoms C(1)C(2)C(3)N(2)N(1) flat. The maximum deviation of atoms from the plane of heterocycles is 0.0036–0.0067 Å (H_2L), respectively, and for phenyl rings these deviations are 0.0067 Å. The phenyl ring of the benzoylhydrazide residue in the molecule (H_2L) is rotated relative to the pyrazoline ring in space by 45.66°. The angle between the ester group of the β-diketone part of the molecule and the hydroxypyrazoline ring is 136.42° and they lie outside the same plane, although the ester group itself is sufficiently coplanar, as indicated by the value of the dihedral angle O(1)C(4)O(2)C (5) - 4.38°. An analysis of the bond lengths of the molecule shows that this molecule has double bonds N(2)=C(3) 1.27 Å, O(1)=C(4) 1.20 Å and O(4)=C(8) 1.23 Å. The slight difference between the double bonds O(1)=C(4) and O(4)=C(8) is explained, as was determined above, by the inclusion of the oxygen atom O(4) in the p-π-conjugation by the free pair of the p-electron with the π-orbital of the aromatic nucleus.

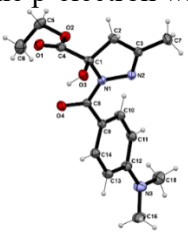

Fig. 1. Crystal structure of the H_2L

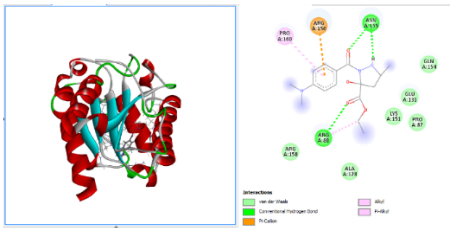

Fig. 2. Molecular docking results of the H_2L

In the case of the molecular docking analysis of H_2L -3QPC, the position with the highest binding affinity, determined by various interactions at the binding site, has a binding energy of -6.97462 kcal/mol.