

A complex study of 5-amino-3-methyl-4-[2-(5-amino-1,3,4-oxadiazolo)]-isoxazole monohydrate: A new low-molecular-weight immune response modifier.

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A new potential lead structure with immunological activity, 5-amino-3-methyl-4-[2-(5-amino-1,3,4-oxadiazolo)]-isoxazole monohydrate, was synthesized. A detailed description of synthesis is presented together with X-ray structural analysis. *In vitro* assays showed that the compound had a potent immunosuppressive activity. Next, Density Functional Theory (DFT) was employed to shed a light on molecular properties of the investigated isoxazole derivative. The molecular modeling part included geometric as well as electronic structure descriptions: (i) the conformational analysis was performed to localize the most appropriate conformation; (ii) the coordination energy and Basis Set Superposition Error (BSSE) were estimated for the complex of the isoxazole derivative interacting with water molecule; (iii) the potential energy distribution was used to assign molecular vibrations, and NBO population analysis served to describe the electronic structure; (iv) the electrostatic potential map was generated to provide the graphical presentation of regions exposed for intermolecular interactions. The contacts between the water molecule and the nitrogen atom of the isoxazole ring edge were present in the solid phase. On the other hand, the theoretical DFT prediction was that the oxygen atom of the edge should form a more stable complex with the water molecule.

Słowa kluczowe

Isoxazole derivatives, X-ray structure analysis, Immunological activity, DFT, BSSE, Natural bond orbitals

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