

DFT study of a novel lead structure in the isoxazole heterocyclic system.

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Streszczenie

5- β -Hydroxyethylaminomethinimino-3-methyl-4-isoxazolecarboxylic acid 4'-chlorophenylamide was used previously as a lead structure in the synthesis of a new series of compounds with similar properties. The compound exhibits strong immunosuppressive activity, investigated experimentally in in vivo and in vitro assays. Various theoretical techniques were used in order to find the structure-activity relationship between immunological activity and molecular properties. Topological analysis and electrostatic properties showed the most reactive places in the molecule, which are crucial in drug-receptor interactions. The quantum-chemical (gas-phase and solid-state) calculations are in good agreement with the available X-ray diffraction data. Car-Parrinello molecular dynamics was used for the solid-state case in order to investigate the dynamic behaviour of the compound. Additionally, the Polarizable Continuum (SCRF/PCM) solvent model served as a tool to reproduce environmental influence on the properties of the molecule.

Adres publiczny

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