

Computational Exploration of Reactivity of 6-Methyluracil/Imidazole-2-Carbaldehyde Oxime Conjugate

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Abstract

© 2016, Springer Science+Business Media New York. Molecular docking and ab initio quantum mechanical calculations were used to assess the nucleophilic reactivity of conjugates of 6-methyluracil and imidazole-2-carbaldehyde oxime. Minimum energy profiles for oxime group rotation and proton transfer were calculated for isolated conjugate. Results indicated that proton transfer and activation are possible. Results suggests that the compound can be active itself, reacting with esters in a way, similar to enzymatic histidine-containing catalytic triad. Thus, this compound is of potential interest for direct scavenging organophosphorus inhibitors of cholinesterases and/or as co-reagent in cholinesterase-based pseudocatalytic bioscavengers.

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Keywords

Acetylcholinesterase, Oxime, Quantum chemistry, Reactivation

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