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UNVEILING THE UREASE INHIBITORY MECHANISM OF FLAVONOIDS THROUGH GFN2-xTB AND aISS DOCKING STUDIES

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ABSTRACT

UNVEILING THE UREASE INHIBITORY MECHANISM OF FLAVONOIDS THROUGH GFN2-xTB AND aISS DOCKING STUDIES

The current study aims to address environmental and health issues arising from urease overactivity, which leads to nitrogen loss, soil erosion, and health ailments. The overall goal is to delve, at the molecular level, into the urease-flavonoids active site interactions for four specific urease inhibitors which are catechin, quercetin, apigenin, and mangiferin. Adopting advanced computational chemistry methodologies, automatic Interaction Site Screening (aISS) docking simulations and GFN2-xTB semi-empirical quantum mechanics calculations, the study assesses the complexity, binding energies, and electron density allocations of the urease-flavonoid complexes for the four specific urease inhibitor-flavonoids studied. Through geometry optimization and topological evaluation, it becomes evident that quercetin at position 2 of nickel 116, is the nearest inhibitor at the nickel centers in urease, exhibitings the strongest binding capacity, reflected by drastically negative interaction energies. Hence revealing its highest inhibitory potential in comparison to the other flavonoids studied. The finding highlights the vital role structural features, such as hydroxyl group placement, planarity, and glycosylation, play in the inhibitory mechanism. Lastly, the study presents the complete molecular insight into the flavonoids as a natural urease inhibitor propelling the eco-friendly alternative compared to commercial urease inhibitors. The finding bears important information for future applications in sustainable agriculture, environmental conservation, and medical therapies for urease-related ailments, hence facilitating the achievement of global sustainability goals by advocating for natural compounds to reduce the ecological footprint and maximize nitrogen use efficiency.

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