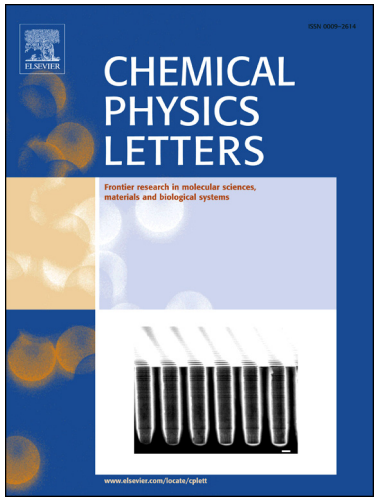

Research paper

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Molecular Inclusion Process of Urease Inhibitors into Cyclodextrins: A Theoretical Study

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ABSTRACT

This paper reports a theoretical investigation on formation of *host/guest* inclusion complexes of two urease inhibitors into cyclodextrins. The main goals were to modeling and propose new supramolecular delivery systems of urease inhibitors. Structures and stabilization energies were calculated, in 1:1 and 2:1 molar ratios, by DFT calculations. It was found that the hydrogen bonds formed between two CDs molecules play an important role in the complexes stabilization. With this work we are able to propose by a molecular modeling study new *host/guest* inclusion compound, being the BGA-1 and the *β*-CD the most suitable *guest* and *host*, respectively.

INTRODUCTION