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

Sayron Reis,^a Ângelo de Fátima,^b Luciana Guimarães,^a Clebio S. Nascimento Jr.^{a*}

^a Laboratório de Química Teórica e Computacional (LQTC), Departamento de Ciências Naturais (DCNAT), Universidade Federal de São João Del-Rei (UFSJ), Campus Dom Bosco, São João Del Rei, 36301-160, MG, Brazil.

^b Grupo de Estudos em Química Orgânica e Biológica (GEQOB), Departamento de Química (DQ), Instituto de Ciências Exatas (ICEEx), Universidade Federal de Minas Gerais (UFMG), Av. Pres. Antônio Carlos, 6627, Pampulha, Belo Horizonte, 31270-901, MG, Brazil.

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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

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