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Theoretical study on β-cyclodextrin inclusion complexes with propiconazole and protonated propiconazole

Adrian Fifere[1], Narcisa Marangoci[1], Stelian Maier[2], Adina Coroaba[1], Dan Maftei[3] and Mariana Pinteala[*1]

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Address:
[1]Centre of Advance Research in Bionanoconjugates and Biopolymers, "Petru Poni" Institute of Macromolecular Chemistry, 700487 Iasi, Romania, [2]Faculty of Textiles & Leather Engineering and Industrial Management, "Gheorghe Asachi" Technical University of Iasi, 700050 Iasi, Romania and [3]Faculty of Chemistry, "Al. I. Cuza" University Iasi, Iasi 700506, Romania

Email:
Mariana Pinteala* - pinteala@icmpp.ro

* Corresponding author

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Abstract

The synthesis of the β-cyclodextrin/propiconazole nitrate inclusion complex and the advantages of the encapsulation of this drug were recently reported, but the experimental data only partially revealed the structure of the supramolecular complex due to the limitations in understanding the intermolecular association mechanism. The present work describes the equilibrium molecular geometries of β-cyclodextrin/propiconazole and β-cyclodextrin/protonated propiconazole, established by the AM1 and PM3 semi-empirical methods. The affinity between different parts of the guest molecule and the cyclodextrin cavity was studied considering that propiconazole possesses three residues able to be included into the host cavity through primary or secondary hydroxyl rims. The results have revealed that the most stable complex is formed when the azole residue of the propiconazole enters the cavity of the cyclodextrin through the narrow hydroxyl's rim.

Introduction

The occurrence of fungal diseases has dramatically increased during the past 20 years. Extremely rare ten years ago, nowadays, antifungal drug resistance has become an important problem in treatment of fungal diseases for various categories of patients, especially those infected with HIV. Excessive and prolonged treatment with azole-containing medicines has led to fungal resistance to this class of compounds, especially in the case of HIV patients with repeated recurrent episodes [1,2]. Today, the number of reported cases of clinic resistance to antifungal drugs is growing and mycologists have warned about an