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

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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