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THEORETICAL INVESTIGATION ON B-CYCLODEXTRIN INCLUSION COMPOUNDS WITH PROTONATED SULCONAZOLE BY SEMI-EMPIRICAL AM1 AND PM3 CALCULATIONS

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Dedicated to Professor Alexandru T. Balaban on the occasion of the 50*th anniversary of his election to the Romanian Academy*

Abstract

PM3 and AM1 semi-empirical quantum mechanical calculations methods were applied to investigate the inclusion complexation of β-cyclodextrin with protonated sulconazole. The affinity of the different parts of protonated sulconazole and cyclodextrin cavity was studied to determine the inclusion pathways of the guest. The results revealed that the most stable inclusion compound was formed when the protonated imidazole ring of the sulconazole enters into cyclodextrin cavity through the narrow hydroxyls rim, which confirms our previous experimental data.

Introduction

A significant number of scientific papers and excellent reviews describe the host-guest interaction between cyclodextrins (CDs) and their derivatives, as hosts, and poorly water-soluble molecules, as guests. Such inclusion complexes are intended to enhance the solubility and dissolution rate, as well as the light and heat stability of the guest molecules [1,2]. That is why a large variety of drugs encapsulated through noncovalent interactions into higher

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