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Inclusion complexes of propiconazole nitrate with substituted β -cyclodextrins: Synthesis, characterization and in silico assessment

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Propiconazole is a triazole developed and marketed by Janssen Pharmaceuticals (Belgium) as an antifungal pesticide. Protonated propiconazole nitrate (PCZH NO₃), a derivative of propiconazole, was proved to have a better antifungal activity and lower acute toxicity, comparable to those of commercial azole drugs, which makes it a good candidate for clinical use. As most clinical azoles, PCZH NO₃ has the major inconvenient of being hydrophobic, which severely reduces its bioavailability. To address this issue, the formation of a host guest inclusion complex with β Cyclodextrin (β CD) as a host carrier molecule was investigated, with good results. The main purpose of this study is to report the synthesis and characterization of the inclusion complexes formed by PCZH-NO₃ with three substituted cyclodextrin (CD) derivatives, namely namely sulfobutylether β CD (SBE7 β CD), sulfated β CD (β CD SNa) and monochlorotriazinyl β CD (MCT β CD) and to investigate them as new antifungal systems. The inclusion complexes were prepared using the freeze-drying method. The structures were confirmed by Nuclear Magnetic Resonance spectroscopy (NMR), Differential Scanning Calorimetry (DSC) and in silico docking and molecular dynamics simulations. This study demonstrates the coexistence of two types of PCZH-NO₃ inclusion into the CD cavity. The complexes with SBE7 β CD had the lowest dissociation constant values. Inclusion efficiency was close to 100%. Comparative in silico docking and molecular dynamics simulations were performed. The antifungal activity was assessed on *Candida* spp. and the cytotoxicity was assessed on Normal Human Dermal Fibroblasts (NHDF).

Biography

Narcisa Laura Marangoci has completed her PhD in Chemistry at the Romanian Academy, and, since 2005, has been a Scientific Researcher at Centre of Advanced Research in Bionanoconjugates and Biopolymers at Petru Poni Institute of Macromolecular Chemistry from Iasi. Her professional experience includes synthesis, characterization and applications of functional polymers, supramolecular compounds, "host-guest" inclusion complexes (25 ISI scientific papers) and also design and implementation of national and international projects.

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