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Title	Prediction of Enantioseparation of Econazole on the Cyclodextrin Derivatives as Chiral Selectors by Molecular Docking Approach
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Title and Abstract

Title	Prediction of Enantioseparation of Econazole on the Cyclodextrin Derivatives as Chiral Selectors by Molecular Docking Approach
Abstract	Molecular docking approach has been successfully developed for prediction of enantioseparation of econazole on the cyclodextrin derivatives namely sulfated-β-cyclodextrin (S-β-CD) and hydroxypropyl-γ-cyclodextrin (HP-γ-CD) as chiral selectors. Molecular docking was performed using AutoDock Vina software and the root mean square deviation (RMSD) was calculated using PyMol software. Molecular docking shows that R-Econazole forms more stable interaction with all cyclodextrin derivatives than S-Econazole forms, suggesting that S-econazole will be eluted earlier than R-econazole. In addition, the stability level of cyclodextrin derivatives as chiral selectors was S-β-CD > HP-γ-CD.

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Prediction of Enantioseparation of Econazole on the Cyclodextrin Derivatives as Chiral Selectors by Molecular Docking Approach

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Keywords

Cyclodextrin; Enantioseparation; Econazole; Molecular docking

Abstract

Molecular docking approach has been successfully developed for predic of enantioseparation of econazole on the cyclodextrin derivatives namely sulfated-β-cyclodextrin (S-β-CD) and hydroxypropyl-γ-cyclodextrin (HP-γ-CD) as chiral selectors. Molecular docking was performed using AutoDock Vina software and the root mean square deviation (RMSD) was calculated using PyMol software. Molecular docking shows that R-Econazole forms more stable interaction with all cyclodextrin derivatives than S-Econazole forms, suggesting that S-econazole will be eluted earlier than R-econazole. In addition, the stability level of cyclodextrin derivatives as chiral selectors was S-β-CD > HP-γ-CD.

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