Molecular dynamics and density functional theory studies of conformational stability of bilirubin and biliverdin

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Rok wydania

2023

Czasopismo

Journal of Molecular Liquids

Numer woluminu

391

Strony

123287/1-123287/7

DOI

10.1016/j.molliq.2023.123287

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Molecular Dynamics (MD) and Density Functional Theory (DFT) simulations have been employed for the research of the influence of the intramolecular and intermolecular hydrogen bonds on the conformational stability of bilirubin and biliverdin (bilins). On the grounds of the MD and DFT calculated results, the crucial difference in the motives responsible for the conformational stability of biliverdin and bilirubin has been shown. The presented studies have revealed that the intramolecular hydrogen bonds and π-electronic conjugation are in charge of the conformational stability of bilins, whereas the intermolecular hydrogen bond leads to their conformational instability (significant dynamics). The biliverdin and bilirubin conformational stability originates in π-electronic conjugation between dipyrromethene moieties and intramolecular hydrogen bonding, respectively.

Słowa kluczowe

Bilirubin, Biliverdin, Hydrogen bond, MD, DFT

Adres publiczny

http://dx.doi.org/10.1016/j.molliq.2023.123287

Strona internetowa wydawcy

http://www.elsevier.com