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Assessing a double silicon decorated fullerene for the delivery of interacting flurbiprofen and salicylic acid drugs: A DFT approach

Çatal, Esin^a; Bağlayan, Özge^a; Körögölü, Ahmet^b;Parlak, Cemal^c; Alver, Özgür^a

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SciVal Topics

Chemicals and CAS Registry Numbers

Abstract

Since the number of drugs increases constantly, drug interactions appear as a critical issue to handle. The effective use of multiple drugs appears as another important subject to discuss and the use of targeted and selective delivery of drugs is becoming more important. Impurity doped C₆₀ fullerenes with various dopant atoms such as silicon or boron appear as promising drug delivery vehicles. Therefore, in the framework of this study, we investigated the interaction between salicylic acid and flurbiprofen and their controlled delivery by using double silicon decorated C₆₀ fullerene using density functional theory. Stability and reactivity considerations were also examined by investigating some important structural parameters, interaction energies and frontier molecular orbitals. The interactions were also monitored by examining important diagnostic vibrational bands. The strength of the interactions between atoms at the interaction sites was also identified by using the quantum theory of atoms in molecules. © 2023 Indian Chemical Society

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DFT; Flurbiprofen; Fullerene; QTAIM; Salicylic acid

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