عنوان مقاله:

An Iron-enhanced nanocone assisted drug delivery of Aspirin : DFT assessments

محل انتشار:

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خلاصه مقاله:

By the importance of customizing appropriate carriers for the specific drugs to approach a successful drug delivery process, the drug delivery of aspirin (ASP) was assessed by the assistance of an iron-enhanced nanocone (FCONE), using density functional theory (DFT) calculations. ASP, CONE, and FCONE models were optimized to be prepared for involving in bimolecular interactions to form ASP@CONE and ASP@FCONE complexes along with re-optimization calculations and vibrational frequency confirmations. Benefits of the enhanced FCONE model were seen for better interacting with the ASP counterpart comparing with the CONE and ASP interactions within the evaluated values of -۲۶.۳۵ and -۱۰.۰۷ kcal/mol for the corrected binding energies to yield a meaningful "recovery time" term. Additionally, the electronic molecular orbital features showed a priority for a better detection of ASP counterpart by the FCONE, in which the variations of energy gap values yielded a meaningful "conductance rate" especially for the ASP@FCONE complex. As a consequence, the recognized models of ASP@CONE and ASP@FCONE complexes were learned by a better advantage of enhanced FCONE model to be worked a s better proposed carrier for the ASP drug delivery process.

کلمات کلیدی:

Adsorption, DFT, Drug delivery, Molecular Interaction, Nanocone