

عنوان مقاله:

In silico Analysis of Molecular Interactions of Vitamin D₃ with Cellulose Nanofiber Assemblies

محل انتشار:

اولین همایش ملی داده کاوی در علوم مهندسی و زیستی (سال: 1402)

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خلاصه مقاله:

Cellulose nanofibers (CNFs) have various applications in varieties of fields including pharmaceutical and aerospace industries due to their lightness and temperature resistance. CNFs are biocompatible and biodegradable, and have extremely low immunogenicity. Healthy diet with suitable amounts of fat-soluble vitamin D lowers the onset and progression of many diseases. Here, molecular interactions of CNFs with vitamin D investigated computationally to envisage CNFs as a supplementary drug delivery system. Cylindrical and plane arrangements of CNFs were put into scrutiny to decipher the types of interactions. The results showed that the plane structure with higher binding affinity score to vitamin D was a better candidate

کلمات کلیدی:

drug delivery, molecular modeling, molecular docking, supplementary drug

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