عنوان مقاله:

Interaction of Graphene with Amoxicillin Antibiotic by in Silico Study

محل انتشار:

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تعداد صفحات اصل مقاله: 11

نویسندگان:

Somayeh Pour Karim - *Department of Chemistry, College of Basic Sciences, Yadegar-e-Imam Khomeini (RAH) Shahre Rey Branch, Islamic Azad University, Tehran, Iran*

Roya Ahmadi - *Department of Chemistry, College of Basic Sciences, Yadegar-e-Imam Khomeini (RAH) Shahre Rey Branch, Islamic Azad University, Tehran, Iran*

Mohammad Yousefi - *Department of Chemistry, Faculty of Pharmaceutical Chemistry, Tehran Medical Sciences, Islamic Azad University, Tehran, Iran*

Khadijeh Kalateh - *Department of Chemistry, College of Basic Sciences, Yadegar-e-Imam Khomeini (RAH) Shahre Rey Branch, Islamic Azad University, Tehran, Iran*

Goldasteh Zarei - *Department of Chemistry, College of Basic Sciences, Yadegar-e-Imam Khomeini (RAH) Shahre Rey Branch, Islamic Azad University, Tehran, Iran*

خلاصه مقاله:

This paper examined interaction of Graphene with Amoxicillin antibiotic through density functional theory (DFT) and by using molecular docking method. For this, the structures of Amoxicillin and, Graphene were initially optimized with Gaussian program. Then, by using the molecular docking strategy and its grading system, we computed the arrangement of ۱۰ structures with additional negative binding energy and a fixed state compared with other samples. Finally, for the most fixed arrangement with Graphene, molecular orbitals evaluations were conducted, and binding energy along with thermodynamic evaluated, the results indicated that the adsorption of Amoxicillin antibiotic on Graphene was an exothermic. Finally, the QTAIM calculations were performed to evaluate the type of interaction and .bonds created between amoxicillin and graphene

کلمات کلیدی:

In Silico, Molecular docking, graphene, Amoxicillin, QTAIM