عنوان مقاله:

Theoretical Design of Aptasensor Based on the Gold nanoparticles

محل انتشار:

اولین کنفرانس ملی شیمی کاربردی و نانوشیمی (سال: 1397)

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خلاصه مقاله:

In this article, immobilized RNA aptamer on the gold nano particle surface was theoretically designed for selective detection of the neomycin B, neomycin C and paromomycin. Several molecular dynamic (MD) simulations on the pure aptamer, aptamer with –S(CH2)6- linker and immobilized aptamer on the gold nanoparticles surface were performed in the presence Neomycin B (NB). The obtained results indicate that the linker does not perturb the structure of the RNA aptamer. Also, full atomistic MD simulations on the immobilized RNA aptamer, as a biosensor, reveals a good sensing ability to ward neomycin B. On the basis of the DFT-D3 calculations, neomycin B forms a most stable complex with the aptamer binding site, due to the strong hydrogen bond formation. Moreover, the obtained results .indicate that electrostatic interactions are the driving forces of complex formation

کلمات کلیدی:

Neomycin B, Aptamer, Sensor, MD simulation, Electrostatic interaction