

عنوان مقاله:

Adsorption of Flavonoid Molecules on Carbon Nanotubes by Molecular Dynamics Simulation

محل انتشار:

هجدهمین همایش شیمی فیزیک ایران (سال: 1394)

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خلاصه مقاله:

Carbon nanotubes (CNTs) have shown great promise in biomedical, environmental applications and as nanoscaled vehicles for targeted drug delivery. One of the main advantages of the CNT is its ability to deliver drugs directly to cancer cells [1]. Flavonoids are polyphenolic compounds comprising fifteen carbons, with two aromatic rings connected by a three-carbon bridge [2]. Natural polyphenols, the most abundant antioxidants in human diet, have many potential benefits in human health [3]. The main subclasses of flavonoids are the flavones, flavonols, flavan-3-ols, isoflavones, flavanones and anthocyanidins [2]. We have investigated the adsorption of these six compounds on carbon nanotube (6,6).

کلمات کلیدی:

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