

## عنوان مقاله:

ONIOM studies of interaction between single-walled carbon nanotube and gallates derivatives as anticancer agents

## محل انتشار:

مجله علوم نانو، دوره 4، شماره 1 (سال: 1396)

تعداد صفحات اصل مقاله: 6

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## خلاصه مقاله:

**Objective(s):** The novel 7-hydroxycoumarinyl gallates derivatives are detected in many pharmaceutical compounds like anticancer and antimicrobial agents. Whereas carbon nanotubes (CNTs) have been discussed for nanomedicine applications and in particular as drug delivery systems. The capability of armchair (5, 5) SWCNT -based drug delivery system in the therapy of anticancer has been investigated by quantum mechanics/molecular mechanics method. **Materials and Methods:** Theoretical investigation of the interaction between armchair (5, 5) SWCNT with gallates derivatives has been fulfilled by quantum mechanics/molecular mechanics (QM/MM) method by ONIOM2 (DFT: UFF) using the program of GAUSSIAN 03 suite. **Results:** The results derived from this study, demonstrate that armchair (5, 5) SWCNT has weak interaction that these interactions contain Vander Waals interactions and indicated clearly that these systems have relatively low durability and so armchair (5, 5) SWCNT is appropriate drug delivery that have been investigated for anti-cancer drug. **Conclusion:** Analysis of ONIOM2 calculations and the interaction energies of the armchair (5, 5) SWCNT and gallates derivatives represented that this carrier can be utilized to improve the biological and anti-cancer activity of gallates derivatives.

## کلمات کلیدی:

Anticancer, Armchair (5, 5) SWCNT, Drug Delivery, Gallates derivatives, ONIOM2, Quantum Mechanics/Molecular Mechanics

## لینک ثابت مقاله در پایگاه سیویلیکا:

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