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<th>ID: 6635</th>
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<td><strong>Congress:</strong> 1st Tabriz International Life Science Conference and 12th Iran Biophysical Chemistry Conference</td>
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<td><strong>Title:</strong> A Computational Study on Anticancer Drug Camptothecin Interaction with Single Walled Carbon Nanotube</td>
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<td><strong>Authors:</strong> Maryam Malekzadeh1, Aida Amidi2</td>
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<td><strong>Abstract:</strong> Camptothecin demonstrated strong anticancer activity in preliminary clinical trials but also low solubility and adverse drug reaction. CPT is believed to be a potent topoisomerase inhibitor that interferes with the essential function of topoisomerase in DNA replication. Since carbon nanotubes discovery in 1991 by Ijima, it have been considered as the ideal material for a variety of applications. Carbon nanotubes own unique sets of properties such as biocompatibility in pharmaceutical drug delivery systems, they also play an excellent role as drug carries with a highly site-selective delivery and sensitivity for particular diseases like cancer. This work reports an investigation of the combination of CPT and SWCNTs with DFTB method. We calculated stabilization energies and physiochemical properties. The results show the interaction of CPT and SWCNTs has stabilization energies and structural stability in solvent. What we think is that our results are helpful for drug design and drug delivery.</td>
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<td><strong>Camptothecin, SWCNTs, DFTB, AntiCancer drug</strong></td>
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<td><strong>Presentation:</strong> Poster</td>
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