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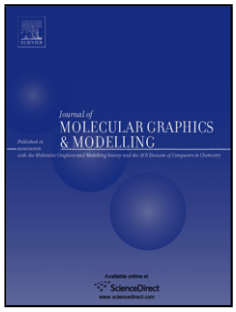


Title: Designing New Surfactant Peptides for Binding to Carbon Nanotubes via Computational Approaches

Authors: Alireza Mansouri, Karim Mahnam

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**Highlights**

The most important finding in this study is that among aromatic residues, the peptides containing Trp residues have higher binding affinity to nanotube compared to the peptides with Phe or Tyr residue. Steric hindrance between bulky aromatic residues in peptide sequence has a negative influence in the binding peptide to nanotube and in designing a surfactant peptide, the number and distance of aromatic residue and polarity of them should be taken into account. Our results also show that in docking peptides to the nanotube, full-flexible docking leads to incorrect results.

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