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Nanostudy and simulation of carbon nanotube binding to amino acids using by molecular mechanics method

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Background and Aims: Carbon nanotubes due to many advantages such as small size, ability to target, enhance treatment effects and reduced toxicity as of drug delivery systems have been investigated. Mitochondrial transfer RNAs genes are essential components of protein biosynthesis that hotspot for mutations so the mutation is associated with a wide range of human diseases. These tRNAs mutations can alter their steady state level and affect the structure of tRNAs and result in protein synthesis defects. So to resolve this problem we propose substitution of tRNA with carbon nanotubes .
Methods: In this work, we have investigated temperature effect on the potential energy complex of amino acids- nanotube carbon 6/0/3 and 7/0/3, and studied the structural properties of water surrounding single-walled carbon nanotube (SWCNT) and mixtures of them as well using Molecular mechanics simulation.
Results: The results of these calculations showed that the performance of carbon nanotubes 7/0/3 is better than 6/0/3 nanotube as a carrier for transport of amino acids; because the average range at different temperatures were lower and showed more stability. Also, according to the change the stability of carbon nanotube-amino acids complex at different temperatures may be necessary to break this complex of changes in temperature.
Conclusions: These findings confirm that 7/0/3 carbon nanotube-amino acids complex at different temperatures is better than 6/0/3 nanotube as a carrier for transport of amino acids.

Keywords: Amino acids; Single-walled carbon nanotubes; Molecular mechanic; tRNA; Temperature