

Assessment of the Biological Effects of Nanomaterials Symposium

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Interaction of fullerene with model membranes: Computer simulation studies

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Carbon nanoparticles are biologically active and can enter easily different kinds of cells. It is not clear how these materials enter cell membranes and what are the mechanisms of cell damage. Recently it has been found that natural organic matter (NOM) interacts strongly with fullerene and carbon nanotubes, altering their interaction with cells. Gallic acid is one of the main components of NOM. The mixture of fullerene and gallic acid can cause cell membrane damage and cell death by unknown mechanisms [1]. Our goal is to investigate the molecular interactions between fullerene and model membranes, in the absence and in the presence of NOM, and to explore different possible mechanisms of cell damage, using computer simulations.

We have developed a coarse-grained (CG) model for simple carbon nanoparticles (fullerenes and nanotubes) compatible with the MARTINI CG force field for lipids and proteins [2-4]. Our CG model reproduces reasonably well partitioning of fullerene between different organic solvents. We use both unbiased and non-equilibrium MD techniques to characterize the thermodynamics and the mechanism of permeation of fullerene clusters through DOPC lipid bilayers. We show that high fullerene concentrations induce changes in the structural and elastic properties of the lipid bilayer, but these are not large enough to cause a direct mechanical damage to the membrane [5]. In order to study the combined effect of fullerene and gallic acid on membranes properties, we use molecular dynamics simulations with an atomistic representation. Our results suggest that gallic acid significantly changes the distribution of fullerene and its interaction with cell membranes. We hypothesize that changes in the membrane elastic properties could alter membrane

protein functioning and therefore cause cell damage.

[1] E Salonen et al., *Small*, 4 (2008) 1986.

[2] SJ Marrink et al., *J Phys Chem B*, 108 (2004) 750.

[3] SJ Marrink et al., *J Phys Chem B*, 111 (2007) 7812.

[4] L Monticelli et al., *J Chem Theory Comput*, 4 (2008) 819.

[5] J Wong-ekkabut et al., *Nature Nanotech*, 3 (2008), 363.

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