Molecular simulation of Dendritic Core-Multi-Shell (CMS) Nano transporter

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Our research focused on molecular simulation of Core Multi-Shell (CMS) Nano transporter. CMS is a novel nano transporter with lots of compatibilities that makes this nano carrier distinct from the others.

Limited matrix compatibility is one of the basic problems of such a carrier systems. They can either transport non-polar molecules into an aqueous environment or, if the system relies on inverted micellar architecture, transfer polar molecules into a hydrophobic environment such as an organic medium. Therefore, the generation of nano compartments that are compatible with various environments such CMS should solve many solubility and stability problems of active agents.

New multi shell design and properties are based on a hyperbranched polymeric core surrounded by double layered shells. This type of system can encapsulate and transport a wide variety of compounds ranging from non-polar to ionic molecules in a broad matrix spectrum including non-polar and polar organic as well as aqueous environments. This CMS consist of three different part, Poly Glycerol (PG) Core which is hydrophilic, surrounded by hydrophobic parts of alkyl chain and monomethyl poly ethylene glycol (mPEG). Single size of this structure is about 8-10 nm and when it gets aggregated as a carrier in a different size between 20-50 nm.

To simulation of this novel nano carrier, Molecular Dynamic in Gromacs and methods of Conformational dynamic has been used. All the simulations are in (NVT) ensemble. Single parts of the structures and Surface simulated with the solvent (water) and intended drug(Morphine) is also located into the simulations. For the preliminary results and progressing the coarse-grained model, the morphine location on the CMS Nano carrier has been detected by calculating Free energies and entropies of morphine in different places of the structure.

References:

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Figures:

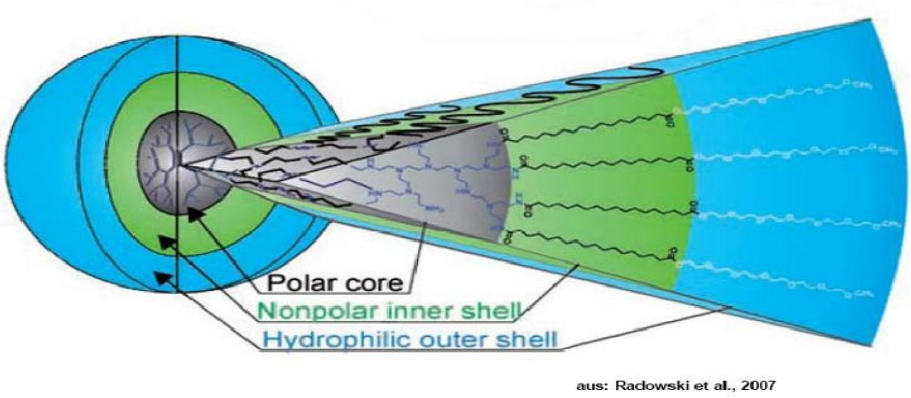

Figure-1: Single structure of CMS which content of three different parts; Two Polar and a Non polar in the middle of the structure.

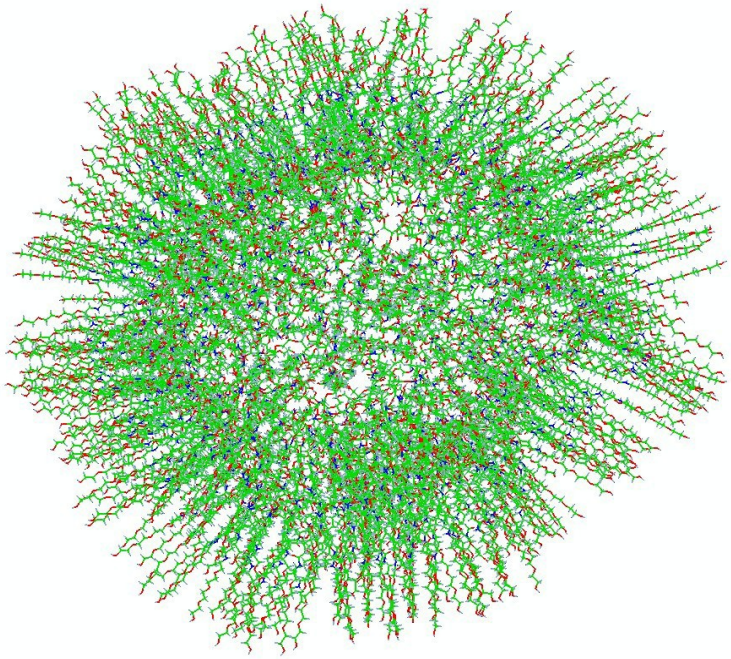

Figure-2: CMS coarse-grained model

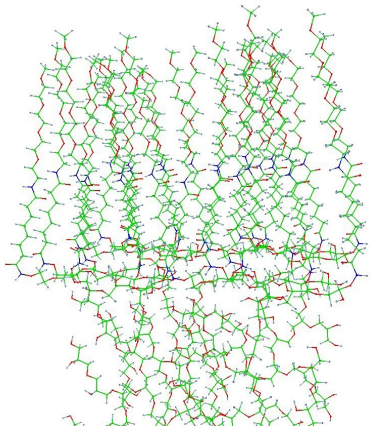

Figure-3: Surface model of CMS