Abstract Submitted
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Self-Assemblies of novel molecules, VECAR[1] BIJAY SHRESTHA, HYE-YOUNG KIM, Department of Chemistry and Physics, Southeastern Louisiana University, SOOJIN LEE, Mechanical Engineering, Georgia Institute of Technology, BRIAN NOVAK, DOREL MOLDOVAN, Department of Mechanical & Industrial Engineering, Louisiana State University — VECAR is a newly synthesized molecule [1], which is an amphiphilic antioxidant molecule that consists of two molecular groups, vitamin-E and Carnosine, linked by a hydrocarbon chain. The hydrocarbon chain is hydrophobic and both vitamin-E and Carnosine ends are hydrophilic. In the synthesis process, the length of the hydrophobic chain of VECAR molecules can vary from the shortest (n=0) to the longest (n=18), where n indicates the number of carbon atoms in the chain. We conducted MD simulation studies of self-assembly of VECAR molecules in water using GROMACS on LONI HPC resources. Our study shows that there is a strong correlation between the shape and atomistic structure of the self-assembled nano-structures (SANs) and the chain-length (n) of VECAR molecules. We will report the results of data analyses including the atomistic structure of each SANs and the dynamic and energetic mechanisms of their formation as function of time. In summary, both VECAR molecules of chain-length n=18 and 9 form worm-like micelles, which may be used as a drug delivery system.

[1] C. E. Astete, D. S. Meador, D. Spivak, C. Sabliov, Synthetic Commun. 43, 1299 (2013).

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