Abstract Submitted
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**Distribution of Drug Molecules in Lipid Membranes: Neutron Diffraction and MD Simulations.**[1] MOHAN BOGGARA, University of Houston, ELLA MIHAILESCU, University of California, Irvine, RAMANAN KRISHNAMOORTI, University of Houston — Non-steroidal anti-inflammatory drugs (NSAIDs) e.g. Aspirin and Ibuprofen, with chronic usage cause gastro intestinal (GI) toxicity. It has been shown experimentally that NSAIDs pre-associated with phospholipids reduce the GI toxicity and also increase the therapeutic activity of these drugs compared to the unmodified ones. In this study, using neutron diffraction, the DOPC lipid bilayer structure (with and without drug) as well as the distribution of a model NSAID (Ibuprofen) as a function of its position along the membrane normal was obtained at sub-nanometer resolution. It was found that the bilayer thickness reduces as the drug is added. Further, the results are successfully compared with atomistic Molecular Dynamics simulations. Based on this successful comparison and motivated by atomic details from MD, quasi-molecular modeling of the lipid membrane is being carried out and will be presented. The above study is expected to provide an effective methodology to design drug delivery nanoparticles based on a variety of soft condensed matter such as lipids or polymers.

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