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**Molecular Insights into Phospholipid – NSAID Interactions** MOHAN BABU BOGGARA, RAMANAN KRISHNAMOORTI, Dept of Chemical and Biomolecular Engg., Univ 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. Using all atomistic simulations and two different methodologies, we studied the partitioning behavior of two model NSAIDs (Aspirin and Ibuprofen) as a function of pH and drug loading. The results from two methodologies are consistent in describing the equilibrium drug distribution in the bilayers. Additionally, the heterogeneity in density and polarity of the bilayer in the normal direction along with the fact that NSAIDs are amphiphilic (all of them have a carboxylic acid group and a non-polar part consisting of aromatic moieties), indicate that the diffusion mechanism in the bilayer is far different compared to the same in a bulk medium. This study summarizes the various effects of NSAIDs and their behavior inside the lipid bilayer both as a function of pH and drug concentration.

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