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Toward a Discrete Molecular Dynamics Coarse-Grained Lipid Bilayer Model for Studies of amyloid beta -Membrane Interactions BLAKE ANTOS, Drexel University, DR. BRIGITA URBANC, Drexel Universty — Despite being the focus of intense study, the exact mechanism underlying Alzheimers disease is not well understood. Soluble, low molecular weight assemblies formed by amyloid beta-protein (Abeta), called oligomers, are hypothesized to trigger the Alzheimers disease pathology by causing synaptic failure that involves interactions between Abeta and the membrane. Several studies using a computational method called discrete molecular dynamics (DMD) combined with a coarse-grained protein model have demonstrated that many aspects of Abeta oligomer formation and structure can be captured and predicted by this efficient approach. Here, we aim to expand this DMD approach to include a model of a lipid bilayer to be combined with the protein model in an effort to examine Abeta -membrane interactions. We have developed a course-grained lipid model which can self-assemble into a membrane-like structure. Next, this lipid bilayer model will be characterized and the parameters of the model adjusted to achieve the correct cross-layer density and diffusion constant, and to capture multiple phases transitions observed in real membranes. Finally, we will investigate interactions of a lipid bilayer with Abeta oligomers which are expected to disrupt the lipid bilayer. This research will provide insights into the possible mechanisms underlying Abeta oligomer-mediated cytotoxicity.

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