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Computer Simulations of Protein Interactions with Lipid Domains RONALD DAVENPORT-DENDY, KWAN CHENG, Trinity University — Protein interactions with multi-component lipid bilayers are major molecular events in cell membranes. Using coarse-grained (CG) molecular dynamics simulations, we have studied the binding behavior and membrane disruption mechanics of a protein dimer on phase separated lipid rafts consisting of cholesterol, saturated and unsaturated lipids. Large size (50,000 CG-atoms) and long (3000 ns) simulations have been performed. We observed that the protein prefers to bind at the interface of liquid-ordered (Lo) and liquid-disordered (Ld) coexisting phases. When the polarity of cholesterol is increased, this interface becomes more distinct, and binding occurs sooner than normal; conversely, reducing the polarity of the cholesterol within the lipid raft leads to an unorganized Lo/Ld interface, and no binding occurs. We quantified our data by analyzing: 1) the extent to which dimer-lipid interaction affects the domains' sizes, 2) the minimum distance between the protein and various lipids during the binding event, and 3) the average transverse density profile of the dimer-lipid system.

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