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Coarse Graining to Investigate Membrane Induced Peptide Folding of Anticancer Peptides SAI GANESAN, HONGCHENG XU, SILVINA MATYSIAK, Univ of Maryland-College Park — Information about membrane induced peptide folding mechanisms using all-atom molecular dynamics simulations is a challenge due to time and length scale issues.We recently developed a low resolution Water Explicit Polarizable PROtein coarse-grained Model by adding oppositely charged dummy particles inside protein backbone beads.These two dummy particles represent a fluctuating dipole,thus introducing structural polarization into the coarse-grained model.With this model,we were able to achieve significant α-β secondary structure content de novo,without any added bias.We extended the model to zwitterionic and anionic lipids,by adding oppositely charged dummy particles inside polar beads, to capture the ability of the head group region to form hydrogen bonds.We use zwitterionic POPC and anionic POPS as our model lipids, and a cationic anticancer peptide,SVS1,as our model peptide.We have characterized the driving forces for SVS1 folding on lipid bilayers with varying anionic and zwitterionic lipid compositions.Based on our results, dipolar interactions between peptide backbone and lipid head groups contribute to stabilize folded conformations.Cooperativity in folding is induced by both intra peptide and membrane-peptide interaction.

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