Abstract Submitted
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**An Experiment-Driven Molecular Dynamics Study of GAG in Water/Ethanol Mixtures**[1] SHUTING ZHANG[2], BRIAN ANDREWS, REINHARD SCHWEITZER-STENNER, BRIGITA URBANC, Drexel Univ — Cationic glycylalanylglycine (GAG) is reported to form a hydrogel in binary mixtures of water and ethanol in vitro. Alanine residue in GAG adopts high polyproline II (pPII) content in water. Spectroscopic data, including three J coupling constants and amide I' profiles, indicate that if the ethanol fraction in the aqueous solution exceeds 42%, the pPII content of alanine residue in GAG is significantly reduced. Here, the experiment-based Gaussian model of Ramachandran distributions and three molecular dynamics (MD) force fields (Amber ff14SB, OPLS-AA/M, and CHARMM36m), are evaluated according to their ability to capture the ethanol-induced conformational changes observed in the experiments. MD simulations on monomeric GAG in eight water/ethanol mixtures reveal that only Amber ff14SB partially reproduces the conformational change in experiments due to ethanol. Further simulations of 200 mM GAG in the aqueous solution with 42% ethanol and pure water reveal the capacity of CHARMM36m to capture the ethanol-induced pPII content change of alanine in GAG. These findings provide a possible explanation of the failure of MD force fields in simulations of monomeric GAG and suggest that the above ethanol-induced conformational changes emerge from GAG self-assembly induced by ethanol.

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