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Simulations of Oppositely Charged Peptides

Polyelectrolyte complexes (PECS) are nano-sized aggregates of oppositely charged polymers forming from the electrostatic attraction between the charged groups. Variations of these complexes have been studied extensively and have found a wide range of uses in pharmaceuticals, cosmetics and biomedicine. Given the applicability of peptide-based PECs towards biomedicine, it would be advantageous to understand the sequence-dependent phase behavior of oppositely charged peptides. Using model polypeptide sequences, characterized by collaborators [1], we are studying the effect of hydrophobicity on complex phase behavior by performing microsecond simulation studies of oppositely charged peptide pairs, each varying in hydrophobicity. From these simulations, we were able to observe sensible trends between the peptide size, conformation and degree of hydrogen bonding. These results align with experimental observations of secondary structure.

1.Tabandeh, S., & Leon, L. (2019). Engineering peptide-based polyelectrolyte complexes with increased hydrophobicity. Molecules, 24(5), 868 .https://doi.org/10.3390/molecules24050868