Computational Study of the Self-Assembly of Surfactants

Camera Whicker[1], Dhruva K, Chakravorty[2]
University of New Orleans, Department of Chemistry

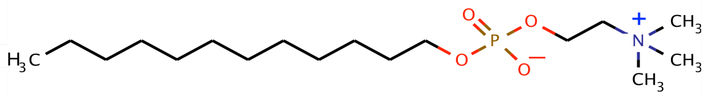
LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

Abstract

Understanding the nature of interactions between surfactant molecules will provide molecular insight into the structure-property relationships that are responsible for surfactant action. In this study, we present an analysis of the conformational dynamics study of surfactant molecules in different solvent models and salinity conditions using molecular dynamics (MD) simulations. Towards this, we performed MD simulations on the well-characterized dodecyldiphosphocholine (DPC) surfactant. Our simulations provide atomistic insights into the conformational ensembles sampled by the surfactant molecules in the commonly used SPC/E, TIP3P, TIP4P and TIP5P water models. We further study the influence of Na^+Cl^- and K^+Cl^- ions on the conformational dynamics of surfactants molecules. We are currently expanding our studies to investigate the self-assembly of 54 randomly dispersed monomers in similar conditions. Determining the self-assembly pathways will help us understand inter-monomer interactions and provide a means to develop a theoretical surfactant model for prediction of solubility of large molecules.

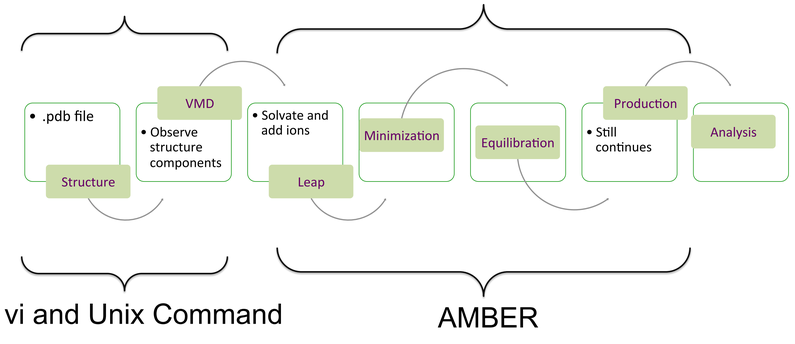
Dodecylphosphocholine

- DPC is a polar surfactant used for membrane protein solubilization and purification
- It is a structural analog of lauroyl lysophosphatidylcholine that is more stable to hydrolytic degradation.
- DPC is an extensively studied system with available kinetics and thermodynamic data that may be used to validate our simulations.



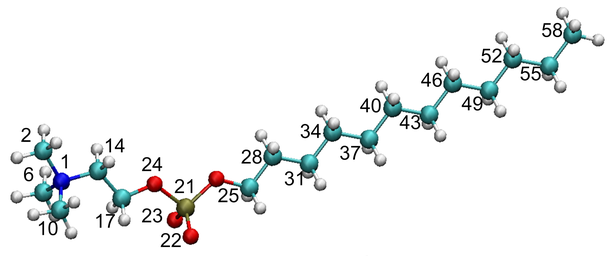
Methods

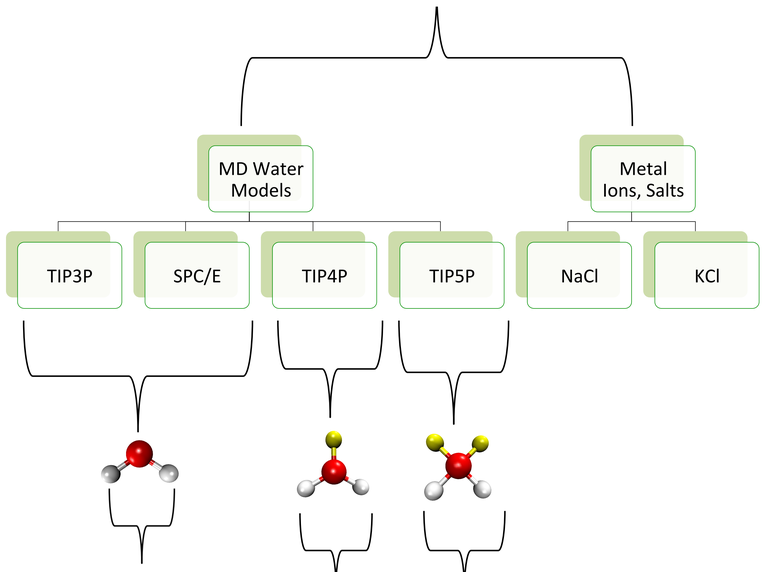
LONI- Super Computing



References

1. *AMBER Tools Manual, 2014.*
2. S100: *Thorsten Ostendorp, et al. EMBO J., 2007, 3868.*
3. *Deborah A. Kallick, et al. J. Magn. Res., 1995, 60.*
4. *Stephane Abel, et al. JCTC, 2012, 4610.*

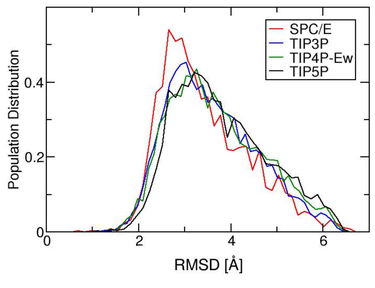


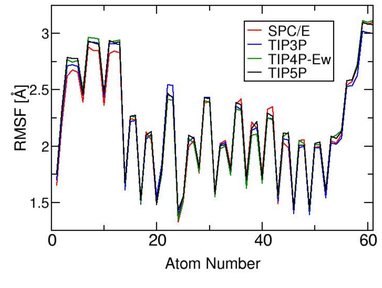


- Simple Point Charge
- 4-site
- 5-site

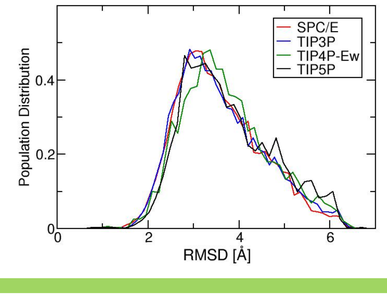
Results

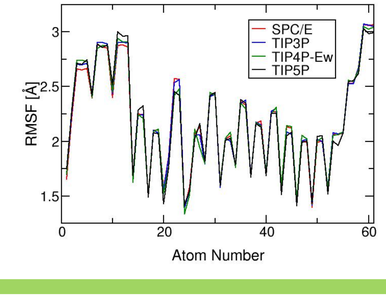
Water



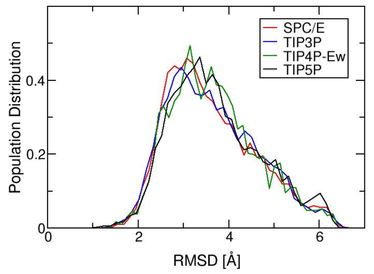


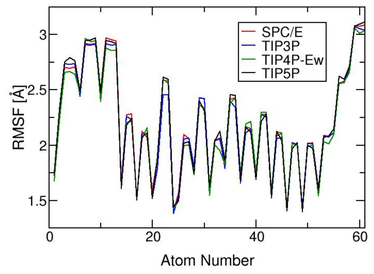
0.4 M NaCl





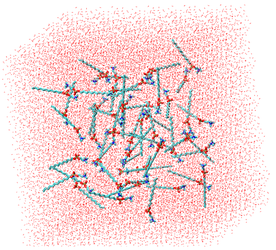
0.4 M KCl



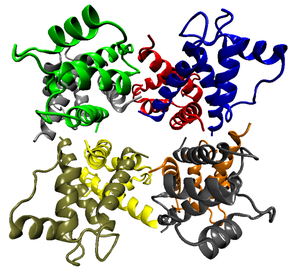


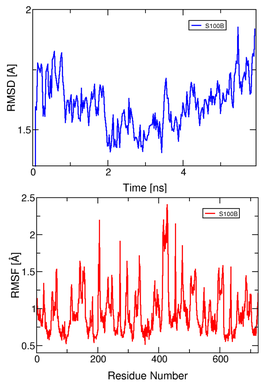
Conclusions

- Different water models and presence of salts appear to have a minimal influence on conformational sampling of the DPC surfactant by itself.
- *Future work involves simulating the self-assembly of multiple DPC molecules in solution.*



S100b Protein





- S100B is a member of the S100 protein family.
- RAGE activation by S100B represents the major pro-inflammatory pathway in acute and chronic inflammatory diseases. including diabetes, Alzheimer disease, and inflammations.

Acknowledgements

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