Micelle/water partition coefficients prediction in aqueous solutions – a proper drug delivery platform based on Molecular dynamics simulations

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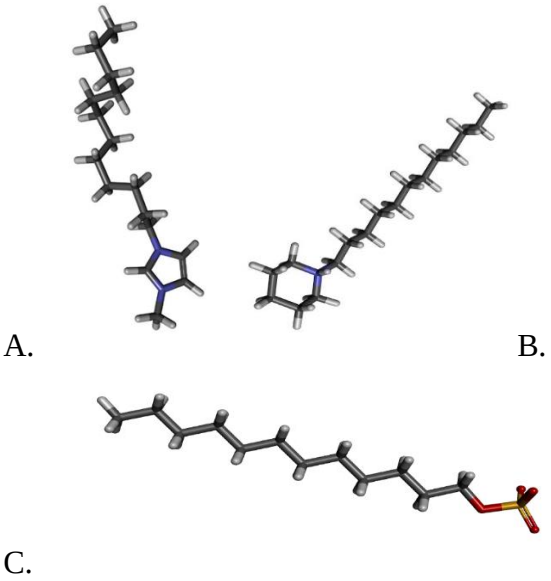

Figure 1: Atomistic representation of A - 1-Decyl-3-methylimidazolium cation, B - 1-Dodecylpyridinium cation, C – sodium dodecyle sulfate (SDS)

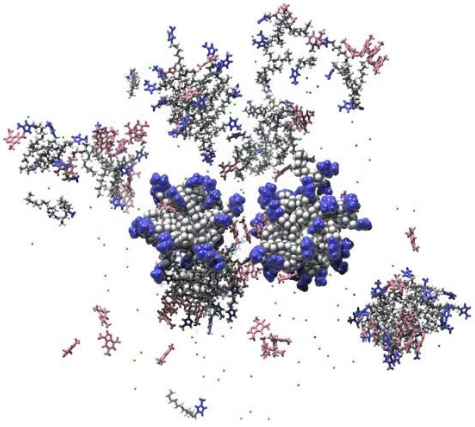

Figure 2: Snapshot from MD simulation of $[C_{12}MIM]^+$ and Cl^- and caffeine in presence of water molecules.

Description of the problem

In silico logP models (partition coefficients models) based solely on chemical structures have become an essential part of modern drug discovery. Moderate and low water solubility is a feature for more than 40% of the new chemicals developed from the current drug discovery programs. The restricted dissolution of the drugs in the gastrointestinal fluids is crucial in drug development for bioavailability issues and enhancement of bioavailability. The classical method for increasing the solubility and permeability in drug discovery of hydrophobic drugs is by solubilization in surfactant micelles. Predicting log P between the micelle/water in the frame of MD simulation is the main focus of the proposed study. A team from Sofia University Faculty of Chemistry and Pharmacy works mainly on this task in cooperation with a team from the University of Maryland, Baltimore, which is part of Computer-aided drug design, University of Maryland.

❖ Use of HPC Infrastructure

The Physon was used to obtain the presented exhausted and long simulation results. PHYSON is a compact 216 core high performance linux cluster, dedicated to support scientific research and education. The machine was built as part of Modeling and analysis of complex systems grant financed by National Scientific Research Fund

Results and Future Work

The results obtained can be summarized as follows:

- A simulation of the encapsulation of five drugs within three micelles with different structures (two ionic liquids and SDS);
- The 2D density map approach was developed for better insight into the structural and transport properties of explored systems.

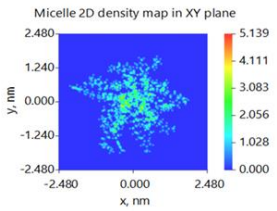

Figure 3: 2D density map for the micelles