Molecular prediction of water transfer in water-octanol interfaces for liquid-liquid extraction

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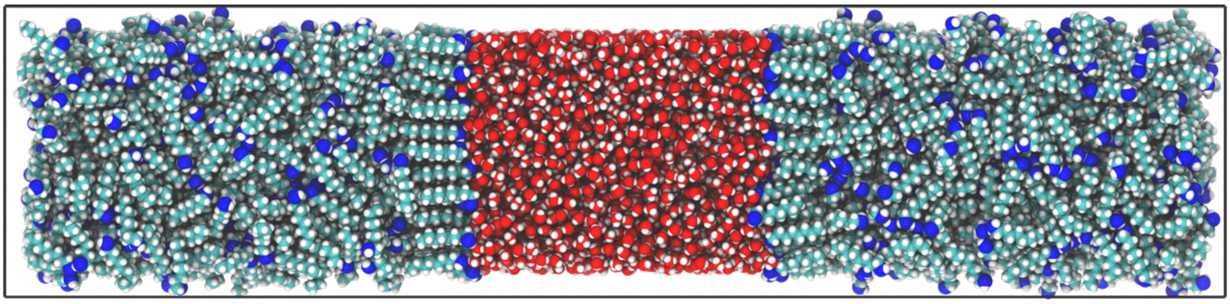
Liquid-liquid extraction is a key extraction process used to selectively separate different solutes. One of the most important extraction systems is the water-octanol interface used in the industry to classify solutes based on their hydrophilicity [1]. The hydrophilicity of a solute, measured experimentally by its partition coefficient log(P), is linked to the Gibbs energy of transfer, which governs the solute transfer between the aqueous and the organic octanol phases [2].

This work deals with the prediction of the Gibbs energy of transfer of water molecules in water-octanol interfaces using Steered Molecular Dynamics (SMD), an out-of-equilibrium simulation technique for Molecular Dynamics. The SMD methodology uses a moving biasing harmonic potential to steer the water molecules from the aqueous phase to the organic phase, allowing for accurate sampling of the free energy landscape of the interface [3,4].

Calculating the molecular orientation revealed that the octanol molecules at the interface organize themselves in a rigid bilayer structure, as previously observed [5] (Fig. 1), preventing the water transfer toward octanol. SMD simulations were carried out to determine the Gibbs energy barrier of this interface, allowing a preliminary calculation of the water solubility in octanol.



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