Bridging Theory and Practice
Enhancing Drug Design Through Molecular Simulations and Solvent Stability Analysis

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This project aims to advance molecular modeling through computational chemistry by predicting octanol: water partition coefficients that are crucial for the design of new medications.

The octanol:water partition coefficients are vital as drug-like molecules need a balanced distribution between oil and water to dissolve in blood and permeate oily cell membranes of the target efficiently. By using computational design of new medicines and employing predictive computational screening methods we assess the oil: water partitioning of candidate molecules, and so we avoid unfavorable candidates before investing in lab synthesis.

Collaborating with Prof. Simanek's group, this study focuses on synthesizing potential "smart drugs," these are large and flexible cyclic molecules with diverse properties in different environments. The current computational pre-screening methods struggle to accurately predict the octanol: water partitioning of these complex molecules. As so, we are testing a more sophisticated computational screening method that combines conformational screening using DFT structure refinement. The goal of this is to determine whether these innovative methods outperform industry-standard approaches for these novel molecules, and so providing insights into their behavior at the hydrophobic-hydrophilic interactions and enhancing drug design precision.

References:

Adaptation of Empirical Methods to Predict the LogD of Triazine Macrocycles
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