Interactions between pollutants and biomolecules – 30 hp

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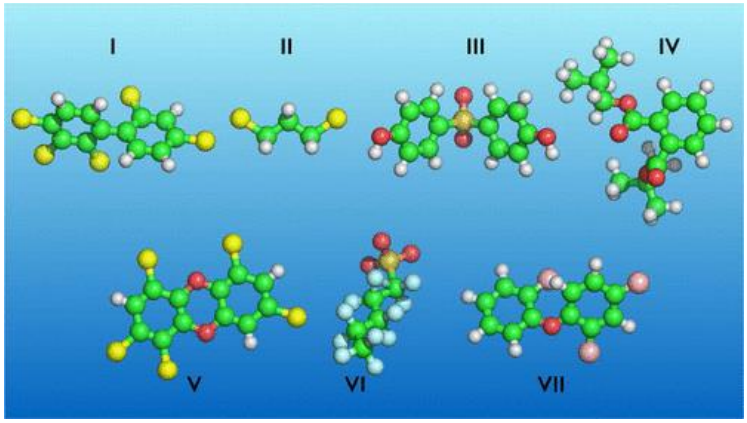
For the development of computational methods for simulation of biosystems, adequate reference benchmark data is necessary [1]. The persistent organic pollutants is a broad class of molecules potentially harmful to humans and environment alike to various degrees [2]. Being able to reliably predict the interactions of these molecules with biomolecules would be very advantageous in studying their hazard risk. Part of such predictions could be the propensity to cross biological membranes [3].

The objective of this computational project is to construct a benchmark dataset – a library of pollutant structures (or of their complexes with biomolecule representatives) and their corresponding properties, such as interaction energies. Firstly, the appropriate representative structures will be chosen and their structure optimized (relaxed) by a density functional theory (DFT) method. DFT and higher level quantum mechanical calculations will be then used to obtain the benchmark properties. The performance of different force fields or DFT methods will then be tested against the dataset. The outcomes of this work will be published in a peer-reviewed scientific journal.

Skills required: knowledge of biochemistry or organic chemistry.

Good to have: familiarity with Linux and/or Python programming.



References

1. Kristian Kříž et al. In: J. Chem. Inf. Model. Submitted, Nov. 2022 https://doi.org/10.26434/chemrxiv-2022-ggzd3
2. Sergio Manzetti et al. In: Chem. Res. Toxicol. 27 (2014), pp. 713–737, https://doi.org/10.1021/tx500014w
3. David van der Spoel et al. ACS Omega 4 (2019) pp 13772-13781 https://doi.org/10.1021/acsomega.9b01277