

The hydrophobic solvation of halogenated compounds. Thermodynamic study on contribution of halogen bonding in intermolecular complexes.

An increasing number of halogenated compounds become potential drugs or drug candidates. Also, a still increasing amount of the already approved drugs contains at least a single halogen atom (i.e. Fluorine, Chlorine, Bromine or Iodine). Such compounds are usually highly hydrophobic, which means that their solubility in aqueous solvents is very limited. Bearing in mind that a vast majority of drugs is administered in an aqueous suspension, the methods enabling accurate description of the interactions of such hydrophobic substances with aqueous solvent are sought.

The initial steps of searching for new drug usually takes place virtually, using powerful computers. Such a procedure is much simpler, and furthermore cheaper, than blindly testing hundreds of thousands of available chemicals. However, for this purpose an accurate model that describe in a quantitative manner not only interactions with a target biomolecule, but also interactions of free solute with a solvent, before it can be caught by its partners.

And this is the main issue of the presented project, whose the most important feature is the combination of precise methods used in pure science to objects belonging to the world of Life Science. We are going to define how individual compounds affects the surrounding solvent molecules, and also to define the effect of addition of cyclodextrin molecules, various derivatives of which are becoming widely used as carriers for already available drugs.

The obtained results will also be analyzed in the structural context, and therefore we intend to study the intermolecular interactions at atomic level. In particular, we are ready to measure, and then describe, how strong the halogen atom interacts with its surroundings.

We hope that the results obtained will help in a deeper understanding how potential drug interact with their partners, and thus also how improve computer-aided drug design procedures.