

## Calculation of hydration networks mediating target-ligand interactions

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Precise determination of interaction networks of target-ligand interfaces is a pre-requisite of structure-based drug design. Crystallography and other methods produce high quality target-ligand structures at an increasing rate. However, development of calculation techniques for the interface structure is necessary for drug design projects with thousands of candidate ligands. In many cases, interactions between the target and ligand molecules are mediated by numerous water molecules filling the space and bridging between the two partners. Determination of the position of such mediating water molecules in the target-ligand interface is very challenging due to their mobility and promiscuous interaction profile. To overcome the limitations of rational design related to such structural uncertainty of hydration, we develop a new technique for the determination of the position of essential water molecules in the binding interface. The technique will be useful for precise calculation of hydration networks of molecular interfaces helping further calculations of binding thermodynamics of target-ligand complexes. It will be also useful for experimentalists helping the assignation of positions of water molecules in problematic situations.

### Biography

Csaba Hetényi is Research Associate Professor at the Molecular Biophysics Research Group of the Hungarian Academy of Sciences. He is a qualified chemist and a Ph.D. in Pharmacy. He has co-authored research articles in prestigious journals such as *J Am Chem Soc*, *EMBO Reports*, *FASEB J*, etc. and has already received more than one thousand citations for his research results. His works were favorably evaluated by several review articles. He is also co-inventor in three US patents. In 2011, he received the prestigious Talentum Academy Award of the Central-European Talent Search Foundation. His primary research interests focus on chemical biophysics, computational and medicinal chemistry, structural bioinformatics, molecular pathomechanisms of diseases, and he has also published works in the fields of chromatography and capillary electrophoresis.

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