**Protein kinases in 4D**

Our co-operation is based on the three-dimensional, atomic resolution structure of protein kinases determined by X-ray crystallography in the research group of Attila Reményi. The measured proteins and their ligand-binding is further investigated by structural bioinformatics methods such as docking and molecular dynamics. Molecular dynamics investigations allow exploration of time-dependence of the meachanism of protein kinases. In this way, the three dimensions of experimental structural determination can be completed with a fourth (time) dimension via application of theoretical methods of molecular modeling. The latter investigations are based on the experience of the work group of Csaba Hetényi, which extensively applies and develops methods for the research of structure and energetics of proteins and their complexes. Such approaches uncovering the dynamic nature of protein kinases are essential for full understanding of their function, and also for planning biochemical measurements to be accomplished by the research group of Attila Reményi. Our common publications can lead to original discoveries in various aspects of the regulation of activity of protein kinases, and the specificity of their interactions, as well. In summary, our project aims at a complete, 4D investigation of protein kinases using a winning synergy of experimental and theoretical approaches.

