**Protein kinases in 4D**

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In the first part of our common project we planned a detailed analysis of the molecular motions of protein-protein complexes involving signaling relevant protein kinases. We used molecular dynamic simulations where the starting structural models were the ERK2-RSK1 and Cbk1-Mob2 crystallographic complexes, which were formally determined by the Reményi Group. We were able to reveal the structural determinants which drive the assembly of a cellular growth promoting molecular switch, and showed how the catalytically competent ERK2-RSK1 heterodimeric complex forms. We also demonstrated how co-activator protein (Mob2) binds to an NDR/LATS kinase (Cbk1) exerts allosteric control on the the activity of a unique group of protein kinases, which had not been structurally characterized earlier [2]. We found that exploration of the role of structural water molecules located on protein surfaces and in the interface regions would be essential. Thus, in the next half year period we plan to extend our investigations to the field of hydration structure too.

1. Anita Alexa, Gergő Gógl, Gábor Glatz, Ágnes Garai, András Zeke, János Varga, Erika Dudás, Norbert Jeszenői, Andrea Bodor, **Csaba Hetényi and Attila Reményi**.

Structural assembly of the signaling competent ERK2–RSK1 heterodimeric protein kinase complex. *PNAS 112:2711-6, 2015*

2. Gergő Gógl, Kyle D. Schneider, Brian J. Yeh, Nashida Alam, Alex N. Nguyen Ba, Alan M. Moses, **Csaba Hetényi, Attila Reményi\*** and Eric L. Weiss.\* *(*\*Shared senior authors)

The structure of an NDR/LATS kinase – Mob complex reveals a novel kinase-coactivator system and substrate docking mechanism.

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