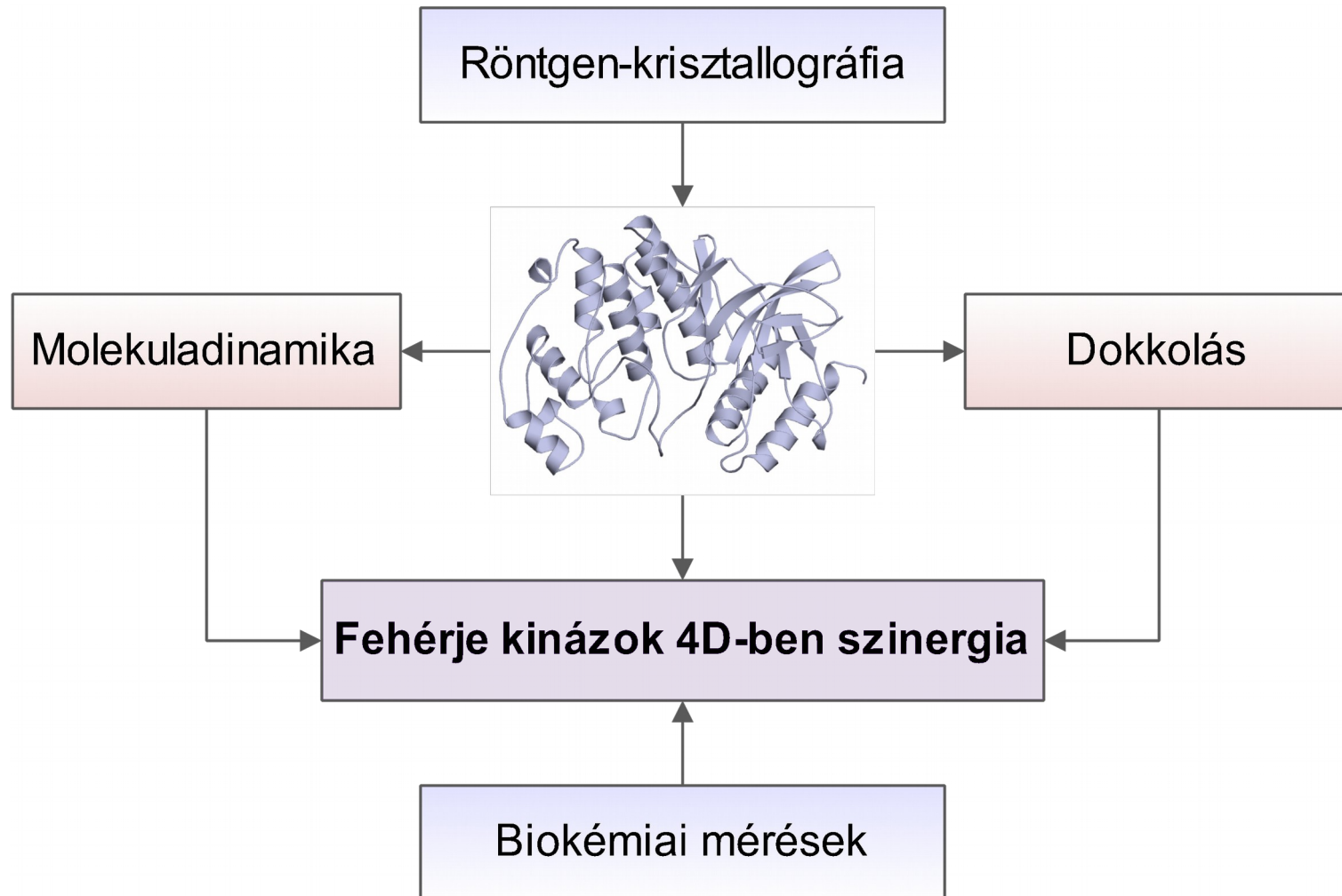


Fehérje Kinázok 4D-ben

Hetényi Csaba, ELTE Biokémiai Tanszék
Reményi Attila, MTA TTK, Enzimológiai Intézet

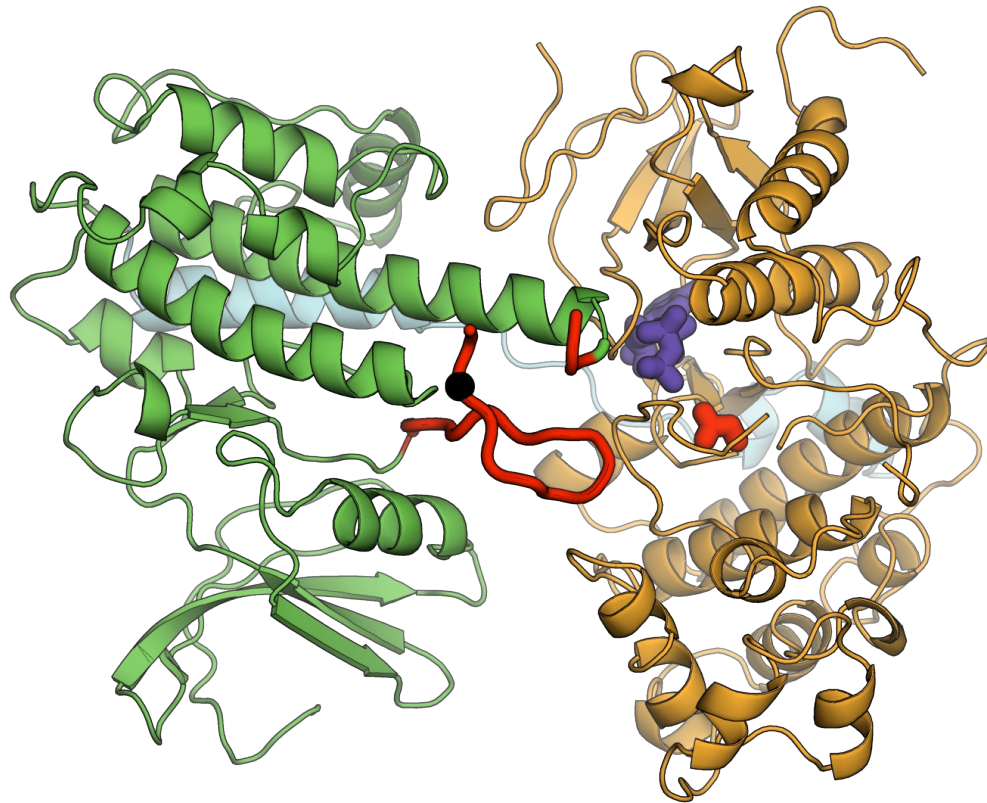
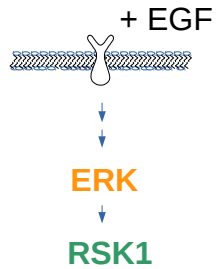
A szinergia lényege



Kérdések

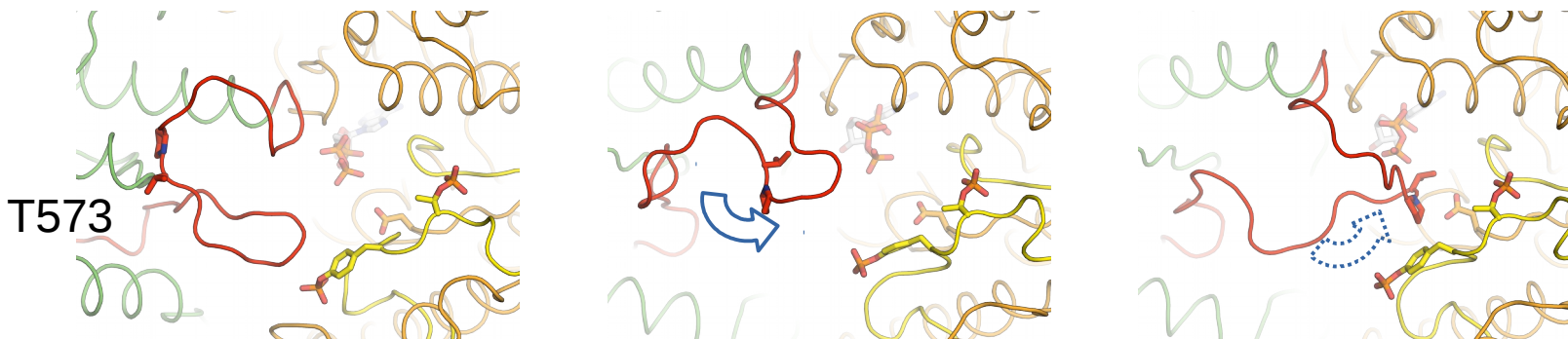
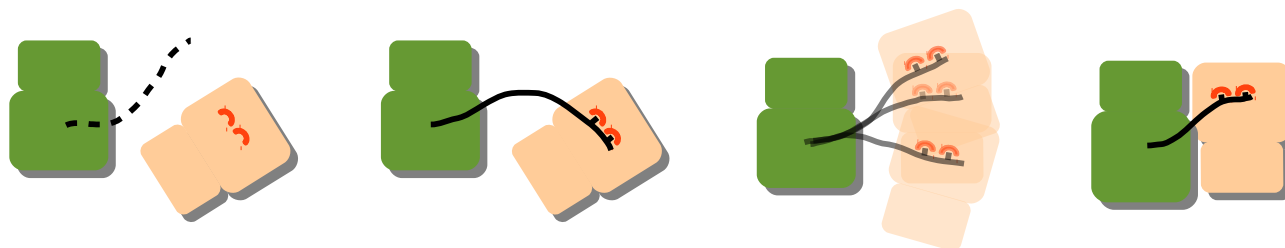
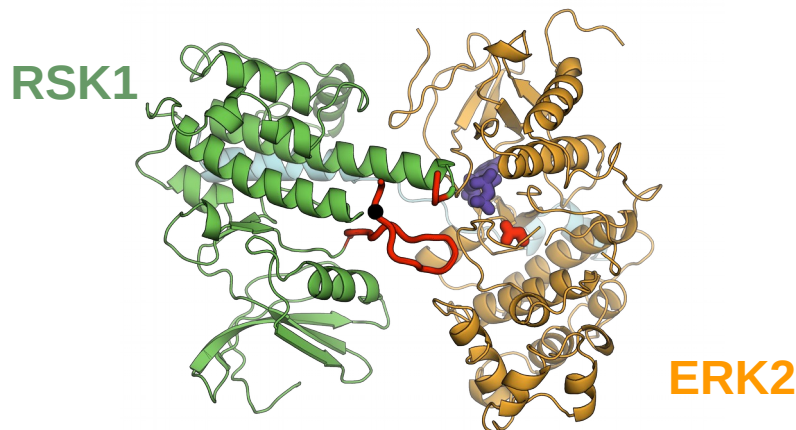
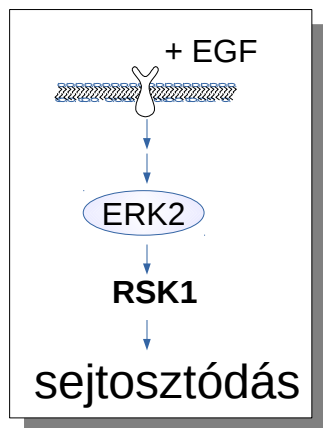
- Hogyan jön létre a katalitikusan aktív ERK2-RSK1 komplex?
- Mi az NDR/LATS kinázok allosztérikus aktivációjának a szerkezeti alapja?

Az ERK2-RSK1 jelátviteli komplex



Structural assembly of the signaling competent ERK2-RSK1 heterodimeric protein kinase complex

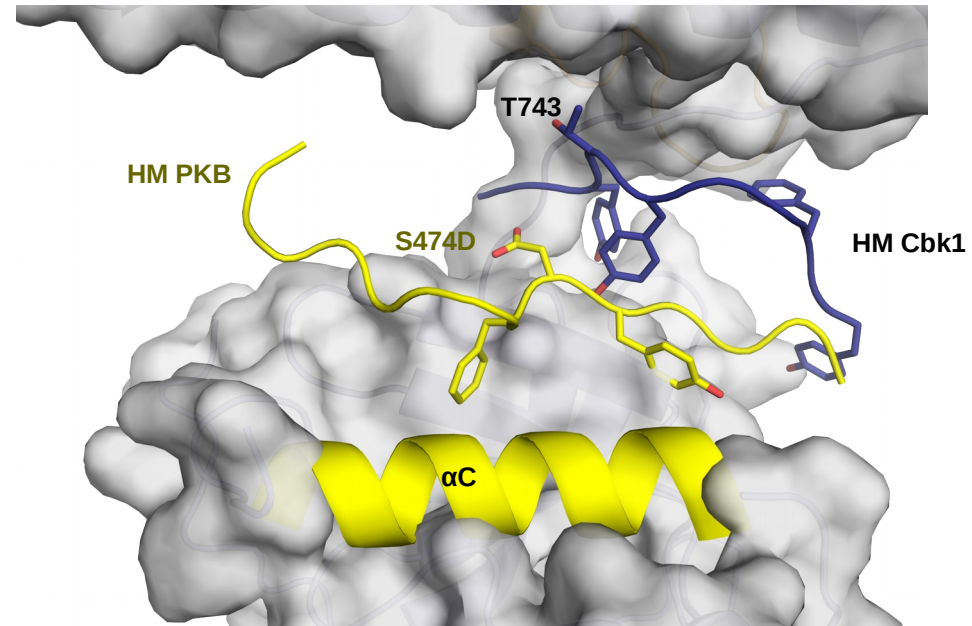
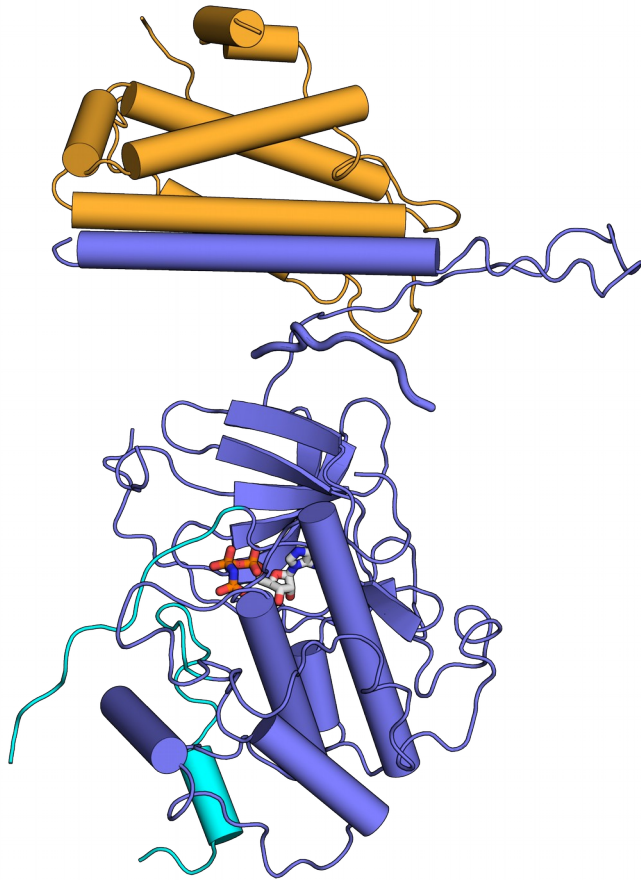
Proc Natl Acad Sci U S A. 2015; 112(9):2711-6



Gógl G, Schneider KD, Yeh BJ, Alam N, Nguyen Ba AN, Moses AM, Hetényi C, Reményi A*, Weiss EL*

The Structure of an NDR/LATS Kinase-Mob Complex Reveals a Novel Kinase-Coactivator System and Substrate Docking Mechanism

PLoS Biol. 2015; 13(5):e1002146



Jeszenői N, Horváth I, Bálint M, van der Spoel D, **Hetényi C***

Mobility-based prediction of hydration structures of protein surfaces

Bioinformatics, 31:1959-65. 2015

MobyWat - SCOPE

mobywat.com

lermann Göring

SCOPE BACKGROUND PROGRAM MODES TECHNICAL HELP ABOUT DOWNLOAD

TARGET

LIGAND

MobyWat calculates the hydration structure of a molecular surface (I) and/or an interface (II)

SCOPE

MobyWat is a program for analysis and prediction of hydration structure of molecular surfaces and interfaces. The program uses a series of frames sampled from molecular simulations performed with explicit water models. It has been thoroughly tested on [protein surfaces](#) and interfaces, and can be recommended for experimental or theoretical investigations dealing with hydration problems. Possible applications may include but are not restricted to the following projects.

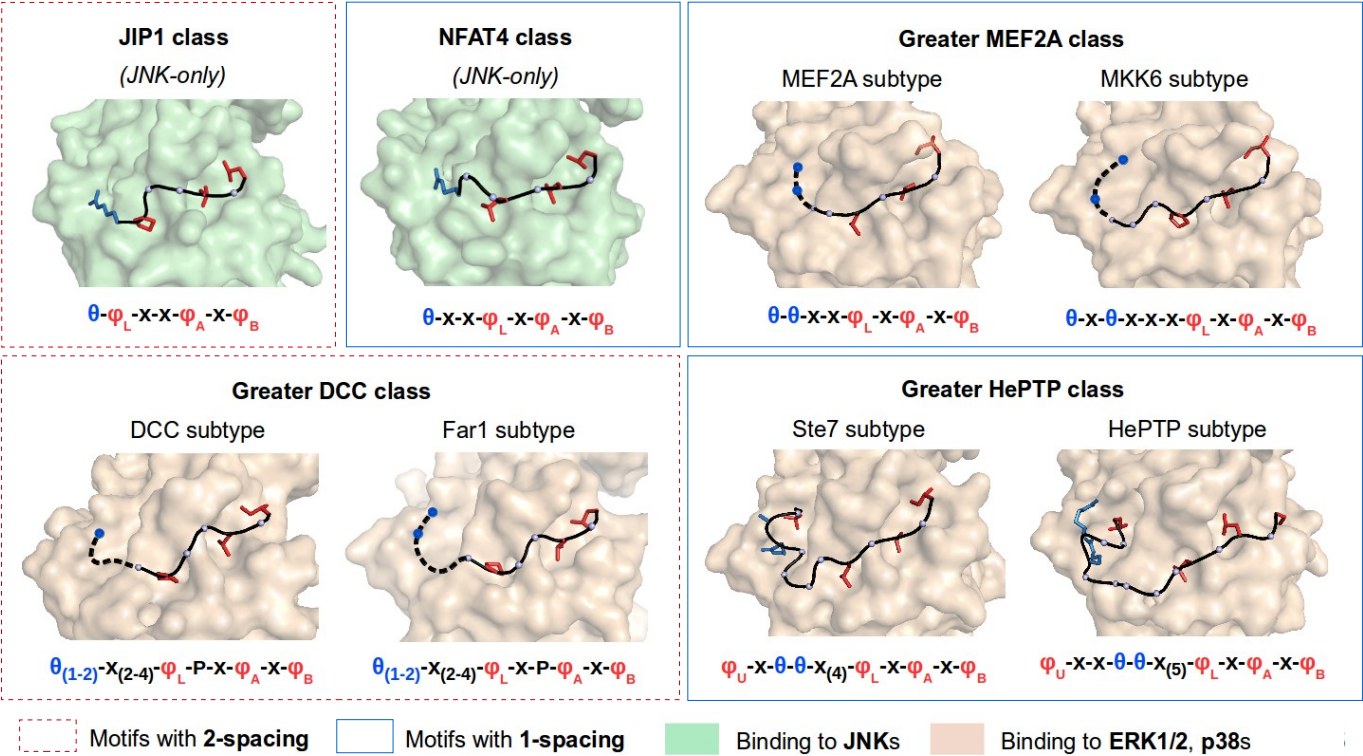
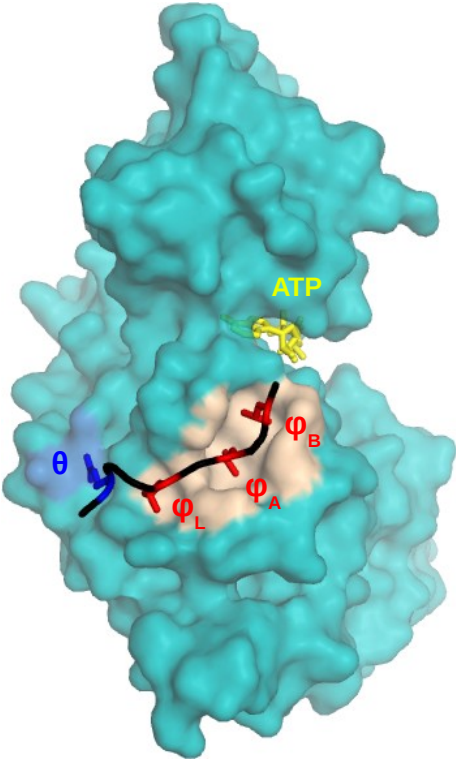
- Refinements and analyses of hydration structure assigned by crystallography.

www.mobywat.com

Zeke A, Bastys T, Alexa A, Garai Á, Mészáros B, Kirsch K, Dosztányi ZS, Kalinina O, Reményi A*

Systematic discovery of linear binding motifs targeting an ancient protein interaction surface on MAP kinases

Molecular Systems Biology, 11(11):837, 2015



Példák Szinergiára

Attila: Hogyan lehetne megbízható módon egyszerű protein-peptid típusú fehérje-fehérje kölcsönhatásokat proteóm szinten feltérképezni?

Csaba: A vizeken keresztül!

Csaba: Hogyan tesztelhetném a vizek jelentőségét a fehérje kölcsönható felszíneken?

Attila: A MAP-kinázokon keresztül!