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*KEMIJSKE ZNANOSTI*

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z naslovom:

# Prediction of protein structure and interactions by GALAXY programs

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*Vljudno vabljeni !*

## *Abstract*

The GALAXY protein modeling program suite consists of protein structure prediction programs (GalaxyTBM for template-based modeling, GalaxyLoop for loop modeling, GalaxyRefine for model refinement, GalaxyGemini for homo-oligomer prediction), protein-ligand docking programs (GalaxyDock and GalaxySite), and a protein-protein docking program (GalaxyPPDock). These programs have been tested in community-wide competitions such as CASP (Critical Assessment of techniques for protein Structure Prediction), CAPRI (Critical Assessment of PRediction of Interactions), CSAR (Community Structure-Activity Resource), and GPCRDock (GPCR Structure-based Homology Modeling and Docking Assessment) with some successes. We believe that the successes are due in part (1) to the carefully optimized GALAXY physical energy functions that combine information from the structure database and (2) to efficient conformational search methods such as conformational space annealing and triaxial loop closure. However, participating in those blind prediction experiments also helped us to identify limitations of the current GALAXY programs. For example, simultaneous modeling and docking combined with softer docking energy would be useful for docking on homology models. In addition, more efficient algorithms are necessary for sampling longer loops such as extracelluar loops of GPCR proteins. In protein-protein docking problems, combining interface information derived from experimental data or prediction would be helpful. Web servers of some of the above programs are available at http://galaxy.seoklab.org, and the GalaxyDock protein-ligand docking program is available at http://galaxy.seoklab.org/softwares/galaxydock.html.