Joint Integrative Computational Biology workshop and CAPRI Meeting

Wednesday, 14 February 2024

CAPRI - IBS seminar room (14:15 - 15:30)

time	[id] title	presenter
14:15	[57] CAPRI 2024: Pre- and post-Alphafold protein docking	LENSINK, Marc
15:00	[55] Integrated pipeline for protein docking with extended and enhanced Alphafold-based modeling methods	KIHARA, Daisuke

CAPRI - IBS seminar room (16:15 - 18:15)

time	[id] title	presenter
16:15	[36] Towards integrative use of pyDock and AI-based modeling in 8th CAPRI	FERNANDEZ-RECIO, Juan
16:45	[35] Prediction and refinement of protein assemblies with ClusPro, Alphafold and Molecular Dynamics.	KOZAKOV, Dima
17:15	[19] MassiveFold: optimized massive sampling with AlphaFold2	BRYSBAERT, Guillaume
17:45	[63] From Interaction Prediction to Sequence Design: Unveiling PeSTo's Potential in Structural Biology	KRAPP, Lucien

Thursday, 15 February 2024

<u>CAPRI</u> - IBS seminar room (09:00 - 10:30)

time	[id] title	presenter
09:00	[12] Impact of AI-Based Modeling on the Accuracy of Protein Assembly Prediction: The CASP Perspective	KARACA, Ezgi
09:30	[51] What have we learned (and memorized) about peptide-mediated interactions in CAPRI and beyond?	SCHUELER-FURMAN, Ora
10:00	[31] HADDOCK in latest CAPRI rounds	Dr GIULINI, Marco Dr REYS, Victor

<u>CAPRI</u> - IBS seminar room (11:00 - 12:15)

time	[id] title	presenter
11:00	[53] Assessing the impact of single-point mutations and alternative splicing-induced variations on protein-protein interactions	LAINE, Elodie
11:30	[58] The Expanding Horizon of Protein Interactions	WODAK, Shoshana

<u>CAPRI</u> - IBS seminar room (14:00 - 15:30)

time	[id] title	presenter
14:00	[20] Multistage Docking Approach for Protein-RNA Interactions Prediction in CAPRI and CASP	CHANG, Shan
14:30	[26] An Iteratively Derived Knowledge-based Scoring Function at Atomic Level for Protein-DNA Complexes Evaluations	ZOU, XIaoqin
15:00	[29] FTDMP: a framework for protein-protein, protein-DNA and protein-RNA docking and scoring	BANCIUL, Rita DAPKUNAS, Justas

<u>CAPRI</u> - IBS seminar room (16:15 - 17:30)

time	[id] title	presenter
16:15	[49] Interpretable Affinity Prediction and Generative Design for Protein-Ligand Interactions	SHEN, Yang
16:45	[59] Automated protein-to-Structure pipelines for new structures and X-ray based ligand screening at EMBL Grenoble. Experience from our first collaboration with CAPRI	MÁRQUEZ, José

Friday, 16 February 2024

<u>CAPRI</u> - IBS seminar room (09:00 - 10:00)

time	[id] title	presenter
09:00	[13] Shape retrieval methods for the classification of protein surfaces	DIAZ LEINES, Grisell
09:30	[25] High-throughput prediction of ATP synthase rotor ring stoichiometries	GUSHCHIN, Ivan

<u>CAPRI</u> - IBS seminar room (10:30 - 11:30)

time	[id] title	presenter
10:30	[5] Unsupervised Machine Learning and Phase Space Reduction: A Robust and Generalisable Approach for Concurrently Solving the Protein Complex Conformation Classification and Quantification Problems.	Dr CELIS GARZA, Daniel
11:00	[34] Modeling of immune recognition and protein complexes with deep learning and physics-based docking	PIERCE, Brian