

Joint Integrative Computational Biology workshop and CAPRI Meeting

Monday, 12 February 2024

Computational Methods and Deep Learning: Chair: Sergei Grudin - IBS seminar room (13:40 - 15:20)

time	[id] title	presenter
13:40	[45] Integrative modeling meets deep learning: applications to crosslinking mass spectrometry	Dr SCHNEIDMAN, Dina
14:05	[28] Analysis of protein-nucleic acid interactions in the PPI3D web server	DAPKUNAS, Justas
14:30	[17] Studying specificity in protein–glycosaminoglycan recognition with umbrella sampling	Dr SEBASTIAN, Anila
14:55	[11] VTX: High-performance molecular structure and dynamics visualization	MONTES, Matthieu

Computational Methods and Deep Learning: Chair: Dina Schneidman - IBS seminar room (15:50 - 17:55)

time	[id] title	presenter
15:50	[46] Generating backbone conformational changes with seven league boots	CAZALS, Frederic
16:15	[4] Analysis of interfaces in protein complexes using Voronoi tessellations and graph neural networks	Dr OLECHNOVIC, Kliment
16:40	[52] Complementarity based peptide docking and design	KHRAMUSHIN, Alisa
17:05	[54] Protein structure evolution and convergence	CARPENTIER, Mathilde
17:30	[3] Hybrid methods for analyzing conformational variability in cryo-EM and cryo-ET data	Dr JONIC, Slavica

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Computational Methods and Deep Learning: Chair: Frédéric Cazals - IBS seminar room (08:10 - 09:50)

time	[id] title	presenter
08:10	[40] Generative models and analysis tools for the study of highly-flexible (intrinsically disordered) proteins	CORTÉS, Juan
08:35	[44] Dissecting peripheral protein-membrane interfaces	Prof. REUTER, Nathalie
09:00	[27] Spectral partitioning into protein structural domains	SARTI, Edoardo
09:25	[61] Integrative structure of a histone chaperone-histone complex	VAN INGEN, Hugo

Computational Methods and Deep Learning: Chair: Juan Cortès - IBS seminar room (10:20 - 12:00)

time	[id] title	presenter
10:20	[42] Exploring the conformational space of proteins by enumeration in the frame of the Distance Geometry Problem	MALLIAVIN, Therese
10:45	[48] Integrative spatiotemporal map of nucleocytoplasmic transport	RAVEH, Barak
11:10	[62] Integrative modeling of protein oligomers using Heligeom	PRÉVOST, Chantal
11:35	[24] Asymmetric hydrophobic mismatch in assembly of ATP synthase rotor ring	GUSHCHIN, Ivan