# Joint Integrative Computational Biology workshop and CAPRI Meeting

## **Tuesday, 13 February 2024**

<u>Protein conformational flexibility and solution experiments: Chair: Monste Soler-Lopez</u> - IBS seminar room (13:45 - 15:25)

time	[id] title	presenter
13:45	[39] Integrative ensemble modeling that utilizes distance distribution restraints	JESCHKE, Gunnar
14:10	[18] Mechanistic study of MexAB-OprM efflux pump by an integrative approach	BROUTIN, Isabelle
14:35	[21] Challenges in visualizing structural flexibility of the SAGA complex	PAPAI, Gabor
	[16] Deciphering protein conformational dynamics with cryo-EM and MD simulations	VUILLEMOT, Rémi

#### Protein conformational flexibility and solution experiments: Chair: Matin Weik - IBS seminar room (15:55 - 17:10)

time [id] title	presenter
15:55 [47] Mariage of Cryo-EM, Solution Scattering, and Computational Science	SUGIYAMA, Masaaki
16:20 [9] Protein Dynamics at extreme Temperatures	CAVIGLIA, Beatrice
16:45 [32] POU5F1B and GOLPH3, two challenging proteins in structural biology	Dr MARCAIDA, Maria

#### Protein conformational flexibility and solution experiments: Chair: Gunnar Jeschke - IBS seminar room (17:40 - 18:55)

time	[id] title	presenter
17:40	[37] Integrative structural biology of cell extracts : an application to structurally undercharacterized organisms	DESFOSSES, Ambroise
	[10] Ensemble based calculations of spin-spin couplings in proteins: from ordered to disordered peptides	GAFFOUR, Amina
	[23] Hinge disulfides in human IgG2 CD40 antibodies modulate receptor signaling by regulation of conformation and flexibility	FISHER, Hayden

### Wednesday, 14 February 2024

# <u>Protein conformational flexibility and solution experiments: Chair: Martin Blackledge</u> - IBS seminar room (08:30 - 09:45)

time	[id] title	presenter
	[50] Intrinsically disordered regulators of endocytosis - an integrated NMR/single molecule fluorescence approach	MILLES, Sigrid
	[8] The Influence of Globular Domains on an Intrinsically Disordered Region of p53: A Molecular Dynamics Investigation	BAKKER, Michael
	[30] Integrative Biology to tackle mitochondrial respiration in Alzheimer's pathogenesis	SOLER LOPEZ, Montserrat

#### Protein conformational flexibility and solution experiments: Chair: Sigrid Milles - IBS seminar room (10:15 - 11:30)

time	[id] title	presenter	
	[56] NMR Provides Unique Insight into the Functional Dynamics and Interactions of Intrinsically Disordered Proteins involved in Viral Replication	BLACKLEDGE, martin	
10:40	[41] Structure and function relationships in protein homorepeats	BERNADO, Pau	
11:05	[38] Integrative structural biology with atomic force microscopy data	PELLEQUER, Jean-Luc	