Program

Monday, 26 April 2021

08:30 – 09:00	**Technical check**	
09:00 – 09:30	Christian Freund Frank Noé	**Welcome**
	Stefan Jorda	**About the Wilhelm and Else-Heraeus Foundation**
Session I:	*NMR methods for probing dynamics*	
09:30 – 10:15	Christian Freund	**Dynamic aspects of antigen presentation by MHC class II molecules**
10:15 – 11:00	Michael Sattler	**Combining NMR and integrative structural biology to study dynamics and allostery in protein complexes**
11:00 – 11:45	Birthe B. Kragelund	**Dynamic complexes of intrinsically disordered proteins by NMR spectroscopy**
11:45 – 12:30	*LUNCH BREAK*	
12:30-13:30	*Cultural Event: Virtual Tour in Museum Barberini*	
13:30-14:00	*COFFEE BREAK*	
14:00 – 16:00	**Poster session I**	
16:00 – 16:30	*COFFEE BREAK*	

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16:30 – 17:15	Nikolaos Sgourakis	**Dynamics of MHC-I molecules in the antigen processing and presentation pathway**
17:15 – 18:00	Lewis E Kay	**The important role of dynamics in the function and misfunction of molecular machines**
18:00 – 18:45	Julie D. Forman-Kay	**NMR insights into phase separation of a CAPRIN1 intrinsically disordered protein region**
18:45 – 19:30	Roundtable discussion I: **Perspectives of NMR**	

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Session II: *Molecular dynamics simulation and free energy landscapes*

09:00 – 09:45	Cecilia Clementi	**Designing molecular models by machine learning and experimental data**
09:45 – 10:30	Carlo Camilloni	**Modelling biomolecules structure and dynamics by combining small-angle X-ray scattering and computer simulations**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	De Fabritiis	**Neural networks potentials for molecular simulations**
11:45 – 12:30	Frank Noé	**Exploring protein dynamics with Markov modeling and deep learning**
12:30 – 13:30	*LUNCH BREAK*	
13:30 – 14:30	*Cultural event: Virtual Musical Performance*	
14:30 – 16:00	**Poster session II**	
16:00 – 16:30	*COFFEE BREAK*	

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16:30 – 17:15	Kresten Lindorff-Larsen	**Biophysical experiments and biomolecular simulations: A perfect match?**
17:15 – 18:00	Bert de Groot	**The molecular dynamics of potassium channel gating**
18:00 – 18:45	Rommie Amaro	**A glycan gate controls the opening of the SARS-CoV-2 spike protein**
18:45 – 19:30	Roundtable discussion II: **Future aspects of theoretical approaches**	

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Wednesday, 28 April 2021

Session III: *Structure and dynamics of macromolecular systems*

09:00 – 09:45	Oliver Daumke	**The mechanism of dynamin in membrane constriction - From static snapshots to a dynamic model**
09:45– 10:30	Christian Spahn	**A cold look at the formation and activation of the bacterial large ribosomal subunit**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Ben Schuler	**Probing the dynamics and interaction mechanisms of disordered proteins with single-molecule spectroscopy**
11:45 – 12:30	Enrica Bordignon	**Probing conformational heterogeneity of ABC transporters in vitro and in cells via EPR**
12:30 –13:30	*LUNCH BREAK*	
13:30 – 14:15	Markus Wahl	**RNA polymerase dynamics during transcription termination and anti-termination**
14:15 – 15:00	Alke Meents	**Fixed target serial crystallography for studying protein dynamics**
15:00 –15:45	**4 best poster presentations**	
15:45 –16:15	*COFFEE BREAK*	

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16:15 – 17:00	Brian Baker	**Dynamic allostery in class I major histocompatibility complex proteins**
17:00 – 17:45	Stefan Raunser	**Bringing life into frozen proteins to elucidate molecular mechanisms**
17:45 – 18:30	Roundtable discussion III: **Towards cellular structural biology**	
18:30	Christian Freund Frank Noé	**Final remarks**

End of the Symposium