Poster Session Tuesday

26	Huan Lan	**Exchange catalysis by tapasin exploits conserved and allele-specific features of MHC-I molecules**
27	Eric Lang	**How can molecular modelling support de novo protein design, and vice versa?**
28	Stefano Leoni	**Advanced molecular dynamics simulations for drug discovery**
29	Stephanie Linker	**Polar/apolar interfaces modulate the conformational and kinetic behavior of cyclic peptides and catalyze their passive membrane permeability**
30	Mohamed Marzouk Sobeh	**Investigating the dissociation process and Binding energy of the DBD-p53/DNA complex by PaCS-MD and MSM**
31	Samuel Musson	**Deep learning protein conformational space with convolutions and latent interpolations**
32	Daniel Nagel	**MSMPathfinder: Finding Pathways of Markov State Models**
33	Rainer Nikolay	**Snapshots of native pre-50S ribosomes reveal a biogenesis factor network and evolutionary specialization**
34	Jeffrey K. Noel	**Quantification and demonstration of the constriction-by-ratchet mechanism in the dynamin molecular motor**
35	Oscar Palomino Hernandez	**On the impact of Tyr-39 for the structural features of α-synuclein and for the interaction with small molecules**
36	Guillermo Pérez Hernández	**mdciao: Analysis of molecular dynamics simulations using residue neighborhoods**

Poster Session Tuesday

37	Matthias Post	**Memory kernel estimation from constrained MD simulations**
38	Victor Principe	**Improving MM/PBSA binding affinity calculations using machine learning**
39	Lluís Raich	**Discovery of a hidden transient state in all bromodomain families**
40	Tatiana Rosales	**Understanding the implication of peptide register shifts in TCR cross-reactivity**
41	Joseph Rudzinski	**Automated identification of collective variables and metastable states from molecular dynamics data**
42	Florian Seufert	**Investigation of different protonation states on ADGRL1 flap dynamics**
43	Jiale Shi	**Novel elastic response in twist-bend nematic models**
44	Kamolrat Somboon	**Computational simulations reveal substrate translocation pathway through hydrophobic transporters**
45	Marija Sorokina	**Structural models of ACE2 with RBD of SARS-CoV-2 Spike protein**
46	Rene Staritzbichler	**SmoothT unbiased construction and visualization of transition pathways, linking monte carlo and molecular dynamics simulations**
47	Matthias Stein	**Accurate receptor-ligand binding free energies from fast QM conformational chemical space sampling**

Poster Session Tuesday

48	Hao Tian	**Deciphering the allosteric process of the phaeodactylum tricornutum aureochrome 1a LOV domain**
49	Felix Wiggers	**Diffusion of the disordered E-cadherin tail on β-catenin**
50	Romina Wild	**Counter transport of potassium ions in the human serotonin transporter**
51	Jayasubba Reddy Yarava	**Probing the site-specific backbone dynamics of YadA autotransporter in microcrystals and native membranes using solid-state NMR spectroscopy**