Posters Session Monday

1	Esam Abualrous	**Natural polymorphism modulates the susceptibility of MHC class II proteins to HLA-DM**
2	Reid Alderson	**Structural basis for the dysregulation of HSP27 in Charcot-Marie-Tooth disease**
3	Robert Arbon	**Assessing the generalizability of adaptive sampling policies**
4	Ernest Awoonor-Williams	**Modelling the binding free energy of peptidomimetic inhibitors to SARS-CoV-2 M^{pro}**
5	Cory Ayres	**Force pull quasiequilibrium: investigating the impact of force on tcr/peptide-mhc stability and immunological recognition**
6	Hossein Batebi	**Formation of a β2AR*-Gs^{GDP} intermediate complex**
7	Miriam Bertazzon	**Investigation of the functional role of CD2BP2**
8	Johann Biedermann	**Investigation of cation permeation through AMPA receptors by molecular dynamics simulations**
9	Yasemin Bozkurt Varolgünes	**Allostery in proteins as point-to-point telecommunication in a network: frequency decomposed signal-to-noise-ratio and channel capacity analysis**
10	Matteo Castelli	**Exploring the effects of post-translational modifications through computational approaches**
11	Liwei Chang	**Inferring protein folding pathways from accelerated molecular dynamics**

Posters Session Monday

12	Yaoyi Chen	**Machine learning implicit solvent method for molecular dynamics**
13	Moumita Dasgupta	**Biophysical characterization of interactions of T cell receptor with viral antigens derived from lymphocytic choriomeningitis virus**
14	Andrea Di Luca	**How global motions are involved in the deactivation of complex I**
15	Kathrin Funck	**Structural and functional explorations of the MICOS complex**
16	Toni Giorgino	**Nanobody interaction unveils structure, dynamics and proteotoxicity of the Finnish-type amyloidogenic gelsolin variant**
17	Giulia Glorani	**An unusual aspartic acid cluster in the reovirus attachment fiber σ1 mediates stability at low pH**
18	Sebastian Günther	**Temperature jump X-ray crystallography to analyze protein dynamics in macromolecular crystals**
19	Shozeb Haider	**Allosteric communication in Class A β-lactamases**
20	Nandan Haloi	**Role of the internal loops in gating of outer membrane porins**
21	Tim Hempel	**Molecular mechanism of inhibiting the SARS-CoV-2 cell entry facilitator TMPRSS2 with camostat and nafamostat**
22	Miriam Jäger	**Predicting ion channel conductance from dissipation-corrected TMD and LE simulations**

Posters Session Monday

23	Eoin Kearney	**Molecular dynamics simulations of uranyl adsorption on montmorillonite clay with desferrioxamine-B**
24	Grant Keller	**Determinants of antigenicity in tumor neoepitopes for the development of personalized/multiple peptide vaccines**
25	Christopher Kolloff	**NOE spin diffusion in large biomolecules**