

## Posters - Main-Neckar Martini User Meeting, 13-14 February 2025

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|----|--------------------------------|--|
| 01 | Sanjoy Paul                    | Computational investigations of the interactions between nanoparticles and plant cell walls  |
| 02 | Maziar Heidari                 | Refined Protein–Sugar Interactions in the Martini Force Field  |
| 03 | Christina Goss                 | Parameterizing the O-Linked Glycans of the Intrinsically Disordered Glycoprotein Lubricin for the Martini 3 Coarse-Grained Force Field |
| 04 | Paulius Greicius               | Coarse-grained model of chondroitin sulfate A  |
| 05 | Francesco Carnovale            | Molecular Dynamics Polymerization Study of Orthosilicic Acid in Solution Using a Reactive MARTINI 3 Force Field                        |
| 06 | Thilo Duve                     | Parameterization of Molecular Photoswitches for Martini 3 and their Application in Photoswitchable Kinase Inhibitors                   |
| 07 | Johanna Buck                   | Coarse-Graining With Martini 3 For Studying Crosslinked Collagen Fibrils Under Force   |
| 08 | Gabriel Hella                  | Role of low-complexity and amphipathic regions of Ede1 on ENDS formation   |
| 09 | Lucia Baltz                    | Hierarchical Interaction in Biomolecular Condensates   |
| 10 | Elena Spinetti                 | Coarse-grained simulations of intrinsically disordered regions   |
| 11 | Sergia Alejandro Poveda Cuevas | Modeling autophagic processes using the MARTINI force field  |
| 12 | Ana Marija Knez                | The Role of Sphingomyelin in FGF2 Membrane Translocation   |
| 13 | Kateryna Lohachova             | Quantifying membrane perturbation induced by membrane-remodeling proteins  |
| 14 | Jose Guadalupe Rosas Jimenez   | Modeling lipid binding to tafazzin and the effect of membrane curvature in cardiolipin remodeling                                      |
| 15 | Melanie König                  | Investigating Membrane Curvature Effects on Lipid Distribution and Protein Function Using Coarse-Grained Simulations                   |

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- 16 Cyrille Ngueldjou Tahabo      Designing Novel DNA-Based Transmembrane Receptors through Molecular Dynamics Simulations
- 17 Matthias Post                      AI-Guided Transition Path Sampling of Lipid Flip-Flop in Atomistic and Coarse-Grained Simulations
- 18 Giovanni Settani                    Investigations of the Fusion Process of Lipid-Based Nanoparticles with Model Endosomal Membranes Using Coarse-Grained Molecular Dynamics Simulations
- 19 Jonas Lehnen                        Polyplex formation process investigated by coarse-grained simulations
- 20 Kristyna Pluhackova                Molecular determinants of solvent nanoseparation by amorphous carbon materials