Contribution ID: **8** Type: **Lecture**

Molecular Modelling Approaches for the Prediction of Nanobody Biophysical Properties

Thursday 25 September 2025 11:00 (1h 30m)

Nanobodies (VHHs) have proved to be valid substitutes of conventional IgG antibodies in basic research and diagnostics, and they are actively tested to confirm their therapeutic potential. Because of their size (~125 amino acids), significantly smaller than that of ordinary antibodies, VHHs can be modelled in silico in relatively short time with the current computational resources.
In this context, a number of computational modelling approaches, i.e. homology modelling, molecular docking, and molecular dynamics, will be reviewed in this session as useful tools able to predict and optimize the biophysical features of nanobodies.
Finally, we will address the problem of predicting how VHHs sequences can tolerate mutations by employing a simulation protocol based on all-atom molecular dynamics and whole-molecule docking.

Presenter: SOLER, Miguel A. (University of Udine, Italy)

Track Classification: Biophysics and Optimization