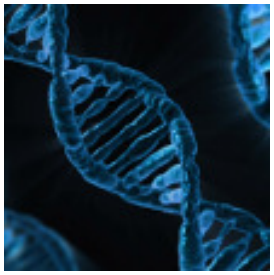

Contribution ID : **48** Type : **Oral presentation**

KEYNOTE 6 - Combining scattering and coarse-grained molecular models to quantify and predict thermodynamic and dynamic contributions to antibody self-interactions and solution properties

Tuesday, 5 June 2018 09:10 (40)

Protein-protein interactions can influence a range of material properties and dynamic/kinetic behaviors, from aggregation kinetics to solution viscosity, self-association, and solubility. This presentation focuses on dilute and concentrated solutions of monoclonal antibodies and synthetic antibodies, from the perspective of predicting the physical properties and/or behavior of these systems as a function of typical formulation variables (e.g., pH, ionic strength). The results illustrate a range of behavior, some of which can be predicted quantitatively or semi-quantitatively with molecular simulations, while others pose a challenge to capture at more than a qualitative level. Comparing a series of different coarse-grained models provides insight into the importance of domain structure, and balances between computational cost and the types of CG models that are used. In the case of single-chain antibodies, the results illustrate examples where the flexibility and dynamics of “linker” peptides can dominate the behavior, and pose a challenge for predicting the behavior and “developability” of candidate molecules.

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Session Classification : Antibody Dynamics and Internal Motion in Proteins

Track Classification : Antibody dynamics and internal motion in proteins