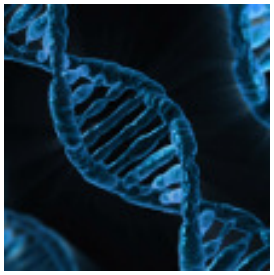

Contribution ID: **68** Type: **Oral presentation**

KEYNOTE 7 - Computer simulations of antibody solutions: from structure to dynamics?

Tuesday 5 June 2018 10:40 (40 minutes)

Concentrated solutions of monoclonal antibodies have attracted considerable attention due to their importance in pharmaceutical formulations, yet their tendency to aggregate and the resulting high solution viscosity has posed considerable problems. It remains a very difficult task to understand and predict the solution behavior and stability of such solutions.
In this talk I will discuss a recent study [1] of the concentration dependence of the structural and dynamic properties of monoclonal antibodies using a combination of different scattering methods and microrheological experiments. The system is also investigated within a simple model of patchy colloids that incorporates the characteristic Y-shape of antibodies. To this aim we perform Monte Carlo simulations which are compared to analytical results, based on Wertheim theory applied to the case of hyperbranched polymers. Thanks to this colloid-inspired approach, we are able to disentangle self-assembly and intermolecular interactions and to describe the concentration dependence of structural and dynamic quantities such as the osmotic compressibility, the collective diffusion coefficient and the zero shear viscosity over the entire range of concentrations investigated.
Perspectives of this work will also be discussed.

[1] N. Skar-Gislinge, M. Ronti, T. Garting, C. Rischel, P. Schurtenberger, E. Zaccarelli and A. Stradner, to be submitted [2018].

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Session Classification: Antibody Dynamics and Internal Motion in Proteins

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