BITC

Biomolecular Interaction Technologies Center

2017 BITC WORKSHOP – "Predicting the properties of pharmaceutical protein solutions: from molecular to phenomenological approaches"

Location: Embassy Suites, Newark DE

Dates: 21 and 22 March, 2017

Registration and Attendance: ***Attendance is by invitation only.*** Registration fees for all attendees are paid for by BITC, and attendees are expected to be present for the full workshop. Contact Kristi Halberg for registration, **khalberg@udel.edu**.

Overview: This workshop focuses on bringing together leading industrial and academic scientists to discuss the state-of-the art in measuring and predicting interactions between proteins and their "environment" (other proteins, solvent, interfaces, etc.) from low- to high-protein concentrations, with an overarching goal of understanding how these impact the properties of protein solutions that are important for the delivery, stability, and manufacture of pharmaceutical proteins. Examples of key properties include solution viscosity; solubility; solution structure / aggregation state and network formation; and multi-body protein interactions. It is structured similar to a Gordon conference, with a small number of focused oral presentations, combined with poster sessions and time for formal and informal extended discussions. A main thrust of the conference is to identify future avenues for industrial and academic partners to develop collaborative research projects to bridge between existing models and prediction of experimental behavior for pharmaceutical proteins.

Tuesday, 21 March

8:45 – 9:00 Welcome and opening remarks, **Chris Roberts** (University of Delaware)

Session 1: Why are the properties of protein solutions difficult to predict?

9:00 – 9:45 *Can Protein Viscosity be Predicted from Two-Body Interactions?* **Jeremy Schmit** (Kansas State University)

10:00 – 10:45 *Notes in Biopharmaceutical Informatics: Aggregation of Therapeutic Antibodies*, **Sandeep Kumar** (Pfizer)

11:00 – 11:45 *Occam's Razor in Modeling Protein-Protein Interactions,* **Abraham Lenhoff** (University of Delaware)

12:00 – 1:00 ***Lunch***

1:00 – 4:00 ***Posters and small group discussions***

Session 2: Advanced experimental techniques & approaches

4:00 – 4:45 *Applications of AU-FDS to Interactions in High Concentration Systems,*
Tom Laue (University of New Hampshire)

5:00 – 5:45 *Rheology of Antibody/Protein Solutions: Advances & Next Frontiers*,
Jai Pathak (National Institutes of Health)

5:45 – 6:00 *Molecular Dynamics and Machine Learning to Predict Chemical Stability*,
Lydia Beasley & Tom Patapoff (Genentech)

7:00 – 8:30 ***Dinner***

8:30 – 10:00 ***Posters and small group discussions***

Wednesday, 22 March

Session 3: From atomistic to phenomenological modeling approaches

9:00 – 9:45 *Molecular Simulations of Cosolvent Effects on Protein Stability,*
Angel Garcia (Los Alamos National Laboratory)

10:00 – 10:45 *Systematic Methods to Generate Coarse-Grained Models of Peptides and Aqueous Solvation,* **M. Scott Shell** (UC-Santa Barbara)

11:00 – 11:45 *The Impact of Arginine-Lysine Mutations on Aggregation Properties of Proteins*,
Robin Curtis (University of Manchester)

12:00 – 1:00 ***Lunch***

1:00 – 2:30 ***Posters and small group discussions***

Session 4: Industrial Feedback and Future Opportunities

2:30 – 4:00 *Panel discussion and roundtable Q&A*

4:00 ***Close of Workshop***