

Computer-Aided Drug Design Symposium

University of Maryland, Baltimore
School of Pharmacy
May 23, 2018
Room 349, SMC Campus Center
University of Maryland, Baltimore, MD

8:00 to 8:50: Breakfast and set up posters

8:50: Introduction from Dean Natalie Eddington

9:00 to 9:30: Drug discovery at UMB (CBT/CADD):

David Weber: UMB Center for Biomolecular Therapeutics Activities

Alex MacKerell: UMB Computer-Aided Drug Design Center Activities

9:30 to 10:00: Jana Shen (UMB, School of Pharmacy): Incorporating pH in Structure-based Drug Design

10:00 to 10:30: Jeff Grey (Johns Hopkins University): Structure Prediction and Docking of Therapeutic Antibodies

10:30 to 10:45: Coffee Break

10:45 to 11:15: Sandeep Somani (Janssen): Molecular Dynamics Studies of Antibodies

11:15 to 11:45: Bruce Yu (UMB, School of Pharmacy): Water Proton NMR for Noninvasive Chemical Analysis and Drug product Inspection

11:45 to 12:15: Joe Curtis (National Institute of Science and Technology): Elucidating Protein-Protein Interactions Using Scattering and Molecular Simulations

12:15 to 1:15 Lunch and poster session

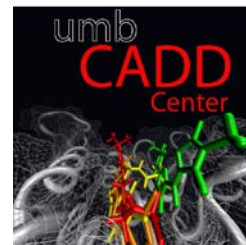
1:15 to 1:20: Overview of the Department of Pharmaceutical Sciences: Paul Shapiro

1:20 to 1:30: Technology Transfer at UMB

1:30 to 2:00: Steve Hoag (UMB, School of Pharmacy): The formulation of therapeutic antibodies for colonic delivery



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2:00 to 2:30: Lisa Jones (UMB, School of Pharmacy): Probing Protein Structure In Vivo

2:30 to 3:00: Luke Arbogast (National Institute of Science and Technology): Chemometric Processing of Monoclonal Antibody Therapeutic NMR Spectra for Rapid and High Resolution Structural Analysis

3:00 to 3:30: Coffee Break

3:30 to 4:00: Eric Sundberg (Institute of Human Virology, UMB School of Medicine): Teaching an old dog new tricks: Developing FosA inhibitors to potentiate the antibiotic fosfomycin

4:00 to 4:30: Alex Drohot (UMB School of Medicine): Inhibiting DNA Repair through Fragment-Based Methods

4:30 to 5:00: Suresh Singh (HotSpot Therapeutics): Drug Design and Discovery: A Small Pharma Perspective

5:00 to 6:30: Poster session with Beer, Wine and Cheese. Note that the posters will be available throughout the day.

