Uniting NMR and Computational Approaches to Push the Frontiers of Dynamic Structure and Conformational Transitions Critical to Function and Dysfunction

June 11 - 16, 2017

Chair
Valerie Daggett

Vice Chair
Christian Griesinger

Grand Summit Hotel at Sunday River
97 Summit Road
Newry, ME, US

Conference Description

The Gordon Research Conference on Computational Aspects of Biomolecular NMR provides a unique forum for the presentation and discussion of emerging methods at the intersection of experimental Nuclear Magnetic Resonance (NMR), computational methods and other complementary biophysical techniques.

NMR is one of the most versatile methods for the investigation of biomolecular systems, whether these are proteins, nucleic acids, glycans, membranes, or functioning cellular and *in vivo* systems. Computational approaches have long been a necessary component of NMR applications. In combination with other complementary biophysical methods, NMR and computation contribute to our understanding and diagnosis of function and disease, the development of therapeutics to combat disease, and characterization of increasingly challenging systems due to their size, dynamics, and complicated conformational behavior. The combined use of NMR and computational methods provides unique structural, dynamical and functional information to achieve these goals, and increasingly many other complementary methods and techniques are being integrated for a more comprehensive view. This GRC conference will bring together practitioners in NMR, computational structural biology and other complementary biophysical techniques for the purpose of generating new ideas and promoting collaborations in order to catalyze the next generation of integrative methods that will allow us to tackle ever more challenging systems.

The 2017 meeting will have sessions devoted to advances and applications in computational methods, and as applied in combination with NMR and other biophysical methods to push the frontiers of structural biology particularly in the areas of conformational transitions, intrinsically disordered systems and interactions, dynamics and drug design, conformational variability and challenges in structure determination. The prominent list of speakers, along with the small format of the conference, will provide unique opportunities for graduate students, postdocs, and both those in the field and new to this research area, to discuss their ideas. Extensive poster sessions, along with oral presentations chosen from the submitted poster abstracts, will facilitate this process.

Related Meeting

This GRC will be held in conjunction with the "Computational Aspects of Biomolecular NMR (GRS)" Gordon Research Seminar (GRS). Those interested in attending both meetings must submit an application for the GRS in addition to an application for the GRC. Refer to the associated GRS program page for more information.

Conference Program

Sunday	
2:00 pm - 9:00 pm	Arrival and Check-in
6:00 pm - 7:00 pm	Dinner
7:30 pm - 7:40 pm	Introductory Comments by GRC Site Staff / Welcome from the GRC Chair
7:40 pm - 9:30 pm	**Bringing It All Together: NMR, Computation and Complementary Biophysical Techniques to Map Dynamic Structure and Interactions** Discussion Leader: **Jeffrey Hoch** (University of Connecticut Health Center, USA)
7:40 pm - 7:50 pm	Opening Remarks

7:50 pm - 8:30 pm	**Alexandre Bonvin** (Utrecht University, The Netherlands) "3D Modelling of Biomolecular Complexes from Fuzzy Data"
8:30 pm - 8:40 pm	Discussion
8:40 pm - 9:20 pm	**Angela Gronenborn** (University of Pittsburgh, USA) "Integrative Methods"
9:20 pm - 9:30 pm	Discussion
Monday	
7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	**Computer Simulation Techniques Across Length and Timescales** Discussion Leader: **Heather Carlson** (University of Michigan, Ann Arbor, USA)
9:00 am - 9:30 am	**Kresten Lindorff-Larsen** (University of Copenhagen, Denmark) "Conformational Exchange from Molecular Simulations and NMR: How Well Do They Match?"
9:30 am - 9:40 am	Discussion
9:40 am - 10:10 am	**Tamar Schlick** (New York University, USA) "Probing Higher-Order Chromatin Architecture by Mesoscale Simulations"
10:10 am - 10:20 am	Discussion
10:20 am - 10:50 am	Coffee Break
10:50 am - 11:20 am	**James Prestegard** (University of Georgia, USA) "Resonance Assignment Strategies for Sparsely Labeled Proteins"
11:20 am - 11:30 am	Discussion
11:30 am - 12:00 pm	**Matthias Buck** (Case Western Reserve University, USA) "Dynamic Protein-Protein and Protein-Membrane Complexes: NMR Studies and Molecular Dynamics Simulations"
12:00 pm - 12:10 pm	Discussion

12:10 pm - 12:25 pm	**Joshua Rackers** (Washington University in St. Louis, USA) "AMOEBA 2.0: A Physics-First Approach to Biomolecular Simulations"
12:25 pm - 12:30 pm	Discussion
12:30 pm - 1:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time
4:00 pm - 6:00 pm	**Poster Session**
6:00 pm - 7:00 pm	Dinner
7:30 pm - 9:30 pm	**Data, Signal Processing and Pushing the Limits of NMR** Discussion Leader: **Tatyana Polenova** (University of Delaware, USA)
7:30 pm - 8:00 pm	**Ilya Kuprov** (University of Southampton, United Kingdom) "3D Reconstruction of Lanthanide Tag Densities in Paramagnetic Proteins"
8:00 pm - 8:10 pm	Discussion
8:10 pm - 8:40 pm	**Michael Nilges** (Institut Pasteur, France) "Computational Methods for Integrative Structural Biology"
8:40 pm - 8:50 pm	Discussion
8:50 pm - 9:20 pm	**Chad Rienstra** (University of Illinois at Urbana-Champaign, USA) "Determining Challenging Structures by Solid-State NMR: Methods and Examples"
9:20 pm - 9:30 pm	Discussion
Tuesday	
7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	**Characterizing the Edges of Structure and the Dark Proteome** Discussion Leader: **Arthur Palmer** (Columbia University, USA)

9:00 am - 9:30 am	**Ashok Deniz** (The Scripps Research Institute, USA) "Single Molecule Biophysics of Protein Disorder"
9:30 am - 9:40 am	Discussion
9:40 am - 10:10 am	**Malene Ringkjobing-Jensen** (Institut de Biologie Structurale, France) "Visualizing the Assembly of Highly Dynamic MAPK Cell Signalling Complexes"
10:10 am - 10:20 am	Discussion
10:20 am - 10:50 am	Coffee Break
10:50 am - 11:20 am	**Colin Smith** (Wesleyan University, USA) "Structural Ensembles and Their Kinetics from NOEs and Relaxation Dispersion"
11:20 am - 11:30 am	Discussion
11:30 am - 12:00 pm	**Geerten Vuister** (University of Leicester, United Kingdom) "The NMR Exchange Format"
12:00 pm - 12:10 pm	Discussion
12:10 pm - 12:25 pm	**Aaron Frank** (University of Michigan, USA) "Discriminating Native from Non-Native RNA Structure Using Unassigned Chemical Shift Data: Toward Rapid RNA Structure Elucidation"
12:25 pm - 12:30 pm	Discussion
12:30 pm - 1:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time
4:00 pm - 6:00 pm	**Poster Session**
6:00 pm - 7:00 pm	Dinner

7:30 pm - 9:30 pm	**Protein Interactions Involving Intrinsically Disordered Species** Discussion Leader: **Andrei Alexandrescu** (University of Connecticut, USA)
7:30 pm - 8:00 pm	**Monika Fuxreiter** (University of Debrecen, Hungary) "Dynamic Interactions and Fuzziness in Protein Complexes and Higher-Order Assemblies"
8:00 pm - 8:10 pm	Discussion
8:10 pm - 8:40 pm	**Richard Kriwacki** (St. Jude Children's Research Hospital, USA) "Elucidating the Role of Intrinsically Disordered Proteins in Regulation"
8:40 pm - 8:50 pm	Discussion
8:50 pm - 9:20 pm	**Ivet Bahar** (University of Pittsburgh, USA) "Allosteric Modulation of g-Secretase Complex Dynamics"
9:20 pm - 9:30 pm	Discussion
Wednesday	
7:30 am - 8:30 am	Breakfast
8:30 am - 9:00 am	Group Photo
9:00 am - 12:30 pm	**Molecular Mechanisms of Allostery** Discussion Leader: **James Prestegard** (University of Georgia, USA)
9:00 am - 9:30 am	**Ruth Nussinov** (National Cancer Institute, NIH, USA) "Ras Conformational Ensembles, Allostery, and Signaling"
9:30 am - 9:40 am	Discussion
9:40 am - 10:10 am	**Emanuele Paci** (University of Leeds, United Kingdom) "Modeling Allostery"
10:10 am - 10:20 am	Discussion
10:20 am - 10:50 am	Coffee Break

10:50 am - 11:20 am	**Andrei Alexandrescu** (University of Connecticut, USA) "Intrinsically Dynamic Protein Segments in Phage Assembly and Stability"
11:20 am - 11:30 am	Discussion
11:30 am - 12:00 pm	**Elena Papaleo** (Danish Cancer Society Research Center, Denmark) "Long-Range Structural Communication in Cancer-Related Transcription Factors"
12:00 pm - 12:10 pm	Discussion
12:10 pm - 12:25 pm	**Hans Koss** (Columbia University, USA) "Dynamic Allosteric Communication of Tyr783 Phosphorylation in PLCγ1"
12:25 pm - 12:30 pm	Discussion
12:30 pm - 1:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time
4:00 pm - 6:00 pm	**Poster Session**
6:00 pm - 7:00 pm	Dinner
7:00 pm - 7:30 pm	**Business Meeting** *Nominations for the Next Vice Chair; Fill in Conference Evaluation Forms; Discuss Future Site and Scheduling Preferences; Election of the Next Vice Chair*
7:30 pm - 9:30 pm	**Protein Dynamics and Drug Design** Discussion Leader: **David Case** (Rutgers University, USA)
7:30 pm - 8:00 pm	**Heather Carlson** (University of Michigan, Ann Arbor, USA) "MixMD: Cosolvent Molecular Dynamics for Mapping Protein Hotspots"
8:00 pm - 8:10 pm	Discussion

8:10 pm - 8:40 pm	**Nikolay Dokholyan** (University of North Carolina at Chapel Hill, USA) "Regulation of Cellular Networks by Controlling Protein Structural Disorder"
8:40 pm - 8:50 pm	Discussion
8:50 pm - 9:20 pm	**John Karanicolas** (Fox Chase Cancer Center, USA) "A New Druggable Site to Rescue p53 Folding and Activity"
9:20 pm - 9:30 pm	Discussion
Thursday	
7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	**Fast Protein Dynamics, Combining Computation and NMR to Shed Light on Function** Discussion Leader: **Rafael Bruschweiler** (The Ohio State University, USA)
9:00 am - 9:30 am	**Lucia Banci** (University of Florence, Italy) "Atomic-Level Description of Functional Processes"
9:30 am - 9:40 am	Discussion
9:40 am - 10:10 am	**Teresa Head-Gordon** (University of California, Berkeley, USA) "Computational Methods and Models for Intrinsically Disordered Peptides"
10:10 am - 10:20 am	Discussion
10:20 am - 10:50 am	Coffee Break
10:50 am - 11:20 am	**Lorna Smith** (University of Oxford, United Kingdom) "Proteins at Low pH: Conformational Ensembles from Magnetic Resonance Data"
11:20 am - 11:30 am	Discussion
11:30 am - 12:00 pm	**Josh Wand** (University of Pennsylvania, USA) "Evaluation of Entropy in Molecular Recognition by Proteins"

12:00 pm - 12:10 pm	Discussion
12:10 pm - 12:25 pm	**Simon Olsson** (Free University of Berlin, Germany) "Integrating MD and NMR Data Analysis Though Augmented Markov Models"
12:25 pm - 12:30 pm	Discussion
12:30 pm - 1:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time
4:00 pm - 5:30 pm	**Poster Session**
5:30 pm - 7:30 pm	**Tackling Large-Scale Protein Motions** Discussion Leader: **Angela Gronenborn** (University of Pittsburgh, USA)
5:30 pm - 6:00 pm	**Sophie Sacquin-Mora** (CNRS, France) "Protein Mechanics as a Bridge Between Structure and Function, a Coarse-Grain Approach"
6:00 pm - 6:10 pm	Discussion
6:10 pm - 6:40 pm	**Vincent Hilser** (Johns Hopkins University, USA) "How the Unfolding of Segments of Structures Is Used to Tune Km and Kcat of Enzymes"
6:40 pm - 6:50 pm	Discussion
6:50 pm - 7:05 pm	**Iva Pritisanac** (Goethe University Frankfurt, Germany) "Automatic Assignment of Methyl Resonances of High Molecular Mass Proteins Using MAGMA and FLYA"
7:05 pm - 7:10 pm	Discussion
7:10 pm - 7:25 pm	**Naohiro Kobayashi** (Institute for Protein Research, Osaka University, Japan) "Highly Automated NMR Signal Assignments Using Peak-Noise Recognition Assisted by Deep Neural Networks"
7:25 pm - 7:30 pm	Discussion

8:00 pm - 9:00 pm	Dinner
Friday	
7:30 am - 8:30 am	Breakfast
9:00 am	Departure

Contributors

Gordon Research Conferences	SIGMA-ALDRICH	BRUKER