

# Tuesday, November 8, 2016

08:00 - 08:45	Registration
08:45 - 09:00	Welcome by Jayant B. Udgaonkar and C. Robert Matthews

#### Session 1 – Functional impact of Protein Folding

Chairpersons: Yvonne Chan and Tyler Harmon

09:00 – 09:05	Patricia Clark Ignite talk — What can protein function tell us about folding mechanisms, and vice versa?
09:05 – 09:25	Kathryn Geiger Trainee talk - Functional instability in Transcription Activator — Like Effectors (TALEs)
09:25 – 09:45	Kapil Dave Trainee talk - Effect of fluorescent tags on an enzyme's (PGK) stability
09:45 – 10:05	Luke Wheeler Trainee talk - Tracing the evolution of peptide bindingspecificity in the S100 protein family using phage display and deep sequencing
10:05 – 10:30	Open discussion
10:30 – 11:00	Tea/Coffee Break

#### <u>Session 2 – Intersecting theory and techniques</u>

Chairpersons: Yvonne Chan and Tyler Harmon

11:00 – 11:20	Rohit Pappu Tutorial talk – Computational methods to studying protein folding
11:20 – 11:25	Lisa Lapidus Ignite talk— Getting to a Predictive Theory of Protein Folding

# Third International Symposium on Protein Folding and Dynamics November 8-11, 2016

11:25 – 11:45	<b>Dipak B. Sanap</b> Trainee talk - Interpretation of hydrogen exchange mass spectrometry data using molecular dynamics simulations
11:45 – 12:05	Emily Guinn  Trainee talk - Using single molecule chemo-mechanical unfolding to probe the effect of environmental conditions on protein folding
12:05 – 12:30	Abani Bhuyan PI talk - Internal friction in protein – what is it?
12:30 – 13:00	Open discussion
13:00 –14:30	Lunch Break

#### Session 3 – Protein Dynamics

Chairpersons: Yvonne Chan and Tyler Harmon

14:30 – 14:35	Cathy Royer Ignite talk – Pressure for Protein Dynamics: How and Why?
14:35 –14:55	Sureshbabu Nagarajan Trainee talk - Dynamics of amyloid beta peptide early aggregation events
14:55 –15:15	Gautam Basu PI talk - Direct observation of concerted backbone – side chain dynamics in short linear peptides
15:15 –15:35	Ishita Sengupta Trainee Talk-Salt-binding induced oligomerization of the mouse prion protein monitored by real time NMR
15:35–16:00	Open Discussion
16:00 –16:30	Tea/Coffee Break
16:00 – 19:00	Poster Session – 1
19:00 –20:30	Dinner

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# Wednesday November 9, 2016

#### Session 4 – Cooperativity

Chairpersons: Emily Guinn and Katie Geiger-Schuller

09:00 - 09:05	<b>Doug Barrick</b> <i>Ignite talk – Ising models and protein folding</i>
09:05 – 09:25	Kelly Jenkins Trainee talk - Exploring folding cooperativity of a repeat protein using high pressure fluorescence and NMR
09:25 – 09:45	Santosh K. Jha PI talk - Alternatively packed, near – native states of a multi – domain protein
09:45 – 10:05	<b>Tyler Harmon</b> Trainee talk - Charge Patterned Sequences Form Helical Structures ThroughCharge Neutralization
10:05 – 10:30	Open discussion
10:30 – 11:00	Tea/Coffee Break

#### Session 5 – Folding Pathways

Chairpersons: Emily Guinn and Katie Geiger-Schuller

11:00– 11:20	Sagar Kathuria Tutorial talk– Microfluidic turbulent mixers, time resolved SAXS and folding intermediates of CheY
11:20 – 11:25	<b>Tobin Sosnick</b> <i>Ignite talk – Alternative methods for characterizing the folding transition state</i>
11:25 – 11:45	Krishnananda Chattopadhyay  PI talk - Subtle changes in the charge distribution at a protein surface can attenuate the competition between early conformational fluctuations and oligomerization

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11:45 – 12:05	Sri Rama Koti Ainavarapu PI talk - Structural and mechanistic insights into the copper – modulated unfolding pathways of azurin
12:05 – 12:30	Ranabir Das  PI talk - Observing a late folding intermediate of ubiquitin at atomic resolution by NMR
12:30 – 13:00	Open discussion
13:00– 14:30	Lunch Break

#### <u>Session 6 – Consequences of Sequence</u>

#### Chairpersons: Emily Guinn and Katie Geiger-Schuller

14:30 – 14:35	Mike Harms Ignite Talk – High order epistasis in protein evolution
14:35 – 14:55	<b>Yvonne Chan</b> Trainee talk - Sequence and structure impose limits on the fitness landscape across three TIM barrel orthologs
14:55–15:15	Josh Riback Trainee talk - Hydrophobicity modulates IDR collapse and stress granule formation
15:15–15:35	Nilesh Aghera Trainee Talk-HomodimericE.coli Toxin CcdB (Controller of Cell Division or Death B Protein) Folds via Parallel Pathways
15:35 – 16:00	Open discussion
16:00 – 16:30	Tea/Coffee Break
16:00– 19:00	Poster Session – 2
19:00- 20:30	Dinner

# Program

# Thursday November 10, 2016

#### <u>Session 7 – The Unfolded State</u>

Chairperson: Gautam Basu

09:00 – 09:30	<b>Rohit Pappu</b> Unfolded states under folding conditions
09:30 – 10:00	Satoshi Takahashi Dynamics of protein folding studied by single molecule fluorescence measurements at microsecond resolution
10:00- 10:30	Govardhan Reddy Protein collapse and folding
10:30– 11:00	Tea/Coffee Break

#### Session 8-Folding Mechanisms- I

Chairperson: Abani K. Bhuyan

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11:00–11:30	<b>Tobin Sosnick</b> The dimensions of the denatured state ensemble (DSE) and the degree to which water is a good solvent
11:30-12:00	Michael Harms Physical origins and evolutionary effects of high-order epistasis in genotype-phenotype maps
12:00– 12:30	Gerhard Hummer Native and nonnative interactions in protein folding
12:30–13:00	Shachi Gosavi Understanding the effect of non-folding factors on the folding landscapes of proteins
13:00 – 14:15	Lunch Break



## Special Sponsor Talk (GE)

14:15-14:25 **DevChandran**Contínuous Chromatography

# Session 9 – Membrane Protein Folding

Chairperson: Ravindra Venkatramani

14:30–15:00	<b>Tae-Young Yoon</b> <i>Mapping the energy landscape for second-stage folding of a single membrane protein</i>
15:00– 15:30	Paula Booth Biological self-assembly – membrane lipids and protein folding
15:30– 16:00	<b>R. Mahalakshmi</b> Balancing protein folding and aggregation by interface residues
16:00 –16:30	Tea/Coffee Break

#### Session 10 – Folding in the Cell

Chairperson: Raghavan Varadarajan

16:30–17:00	Jane Clarke Protein folding –on and off the ribosome
17:00–17:30	Patricia Clark Kinetic effects on protein folding in vivo
17:30 – 18:00	Lila M. Gierasch The allosteric landscape of Hsp70 chaperones—molecular machines that help proteins fold and stay folded
18:00 –18:30	Hideki Taguchi Conversion of a chaperoninGroEL-independent protein into an obligate substrate, and vice versa
19:00 – 20:30	Dinner

# Program

# Friday November 11, 2016

#### Session 11 – Folding Mechanisms II

Chairperson: Santosh K Jha

09:00-09:30	Thomas Kiefhaber The dry molten globule and its role in protein folding and function
09:30–10:00	Catherine Royer Pressure-based mapping of protein conformational landscapes
10:00–10:30	<b>Douglas Barrick</b> Folding of repeat and globular consensus proteins
10:30-11:00	Tea/Coffee Break

#### **Session 12 – Folding and Misfolding**

Chairperson: Krishnananda Chattopadhyay

11:00–11:30	Michael Woodside  Effects of an anti-prion pharmacological chaperone on the folding dynamics of single PrP molecules
11:30-12:00	Sheena Radford The challenges and opportunities of understandingprotein folding and protein misfolding in health and disease
12:00–12:30	<b>Lisa Lapidus</b> <i>Monomer dynamicscontrol the first steps of aggregation and folding</i>
12:30–13:00	Jooyoung Lee Protein structure prediction/determination by global optimization
13:00–14:30	Lunch Break

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#### **Session 13- Misfolding and aggregation**

Chairperson: Kanchan Garai

14:30–15:00	Sudipta Maiti A reaction coordinate for amyloid beta misfolding
15:00–15:30	<b>Yuji Goto</b> Revisiting supersaturation as a factor determining amyloid fibrillation
15:30–16:00	Samrat Mukhopadhyay Water in amyloidogenic intrinsically disordered proteins
16:00 –16:30	Tea/Coffee Break

#### **Session 14 –Native-State Dynamics**

Chairperson: Sri Rama Koti Ainavarapu

16:30–17:00	<b>Tahei Tahara</b> Microsecond protein dynamics revealed by two-dimensional fluorescence lifetime correlation spectroscopy
17:00–17:30	Gilad Haran Every molecule is special: enzyme molecules in action
17:30–18:00	Athi Naganathan A general mechanism for mutation-induced destabilization and modulation of allosteric coupling in proteins
18:00–18:30	<b>Hagen Hofmann</b> Observation of nanometer fluctuations in a multifunctional protein complex
18:30–18:45	Conclusion
19:00 – 20:30	Dinner