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29th Annual Gibbs Conference on Biothermodynamics

The 29th Gibbs Conference on Biothermodynamics

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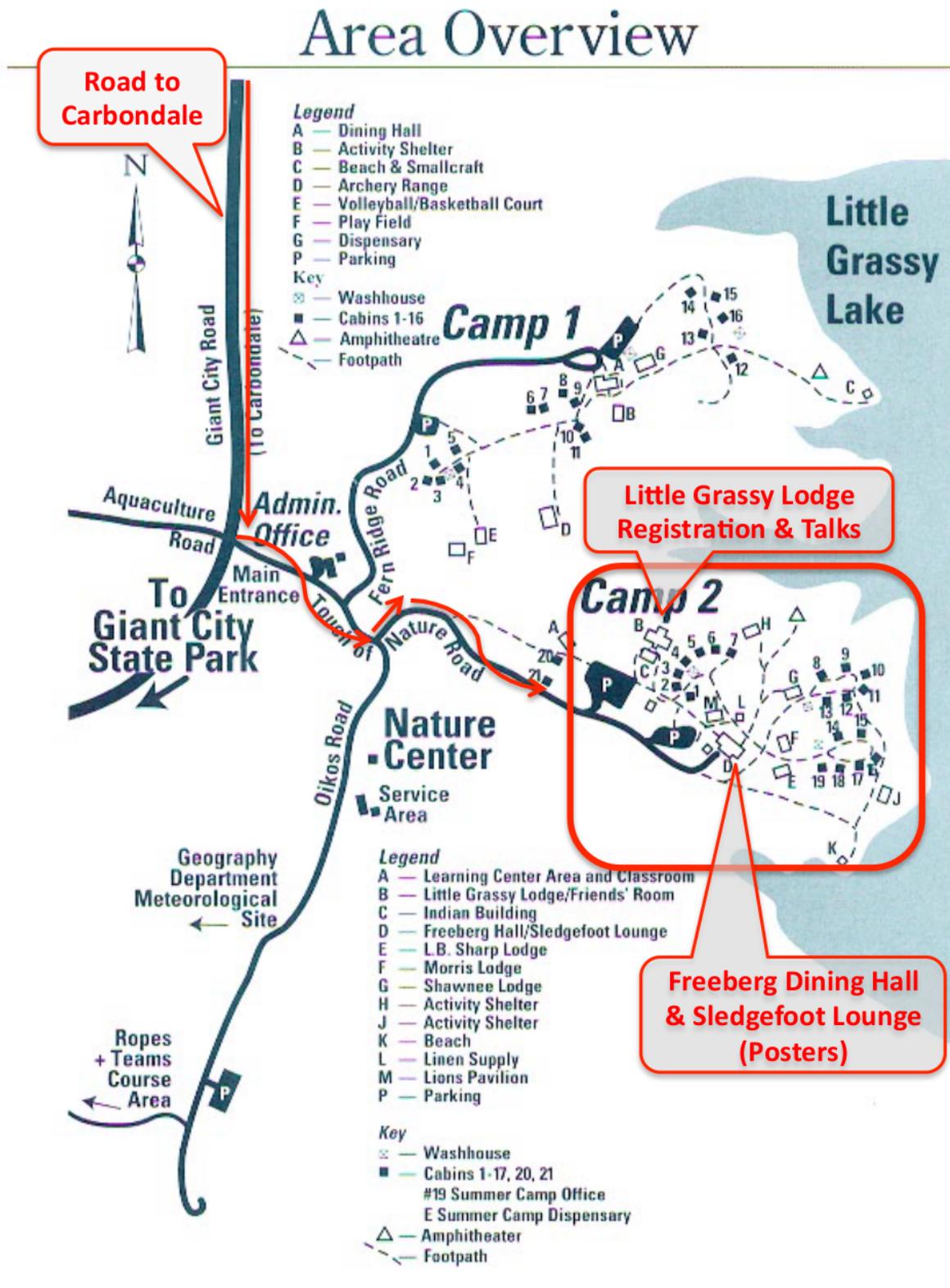
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Map of Touch of Nature Environmental Center

Most of the Gibbs Conference activities will be held in "Camp 2" as shown in the map below. Cell phone reception is extremely limited; parking lots are popular places for making calls.



The Gibbs Conference on Biothermodynamics

History

Fall, 1986

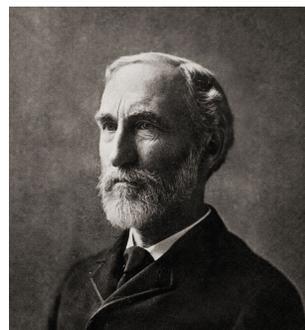
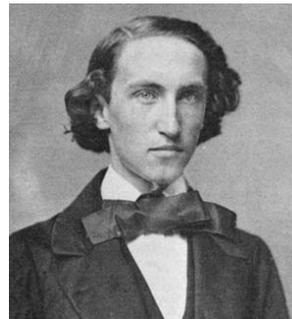
Discussion of the discipline: Thermodynamics in Biological Systems
At the Gill residence in Vail, Colorado
Gary Ackers, Wayne Bolen, Ernesto Freire, Stan Gill, Jim Lee

February, 1987

Discussion of the discipline: Thermodynamics in Biological Systems
The Gumbo Shop, New Orleans, LA during the 31st Annual Biophysical Society Meeting - Gary Ackers, Norma Allewell, Wayne Bolen, Ken Breslauer, Ken Dill, Ernesto Freire, Stan Gill, Jim Lee

A history of the first ten years of the meeting was provided by Ackers GK and Bolen DW in the article entitled "The Gibbs Conference on Biothermodynamics: Origins and Evolution" published in *Biophysical Chemistry* **64** (1997) 3-5 (doi:10.1016/S0301-4622(96)02246-6).

An update is provided by Shea, MA, Correia, JJ, and Brenowitz, MD, entitled "Introduction: Twenty five years of the Gibbs Conference on Biothermodynamics" available in *Biophysical Chemistry* **159** (2011) 1-5 (doi:10.1016/j.bpc.2011.07.002).



Meetings

All meetings have been held at the Touch of Nature Environmental Center associated with Southern Illinois University – Carbondale. From 1987 through 1993, all of the speakers in the scientific sessions were students or postdoctoral fellows.

- 1987 Organizers: Jim Lee and Wayne Bolen
Philosophical Talks: Gary K. Ackers and Ken Dill
- 1988 Organizers: Gary Ackers and Michael Johnson
- 1989 Organizers: Susan G. Frasier and Michael Johnson
- 1990 Organizers: Michael Johnson and Marty Straume
- 1991 Organizers: Gary Ackers and Tim Lohman
Keynote Speaker: Ernesto Freire
- 1992 Organizers: Jim Lee and Tomasz Heyduk
Keynote Speakers: Serge Timasheff and John Schellman
- 1993 Organizers: Maurice Eftink and Glen Ramsay
Keynote Speakers: Peter von Hippel and Julian Sturtevant
- 1994 Organizers: Enrico Di Cera and Madeline Shea
Keynote Speakers: Gary Ackers and Kathleen S. Matthews
- 1995 Organizers: Kenneth P. Murphy and Michael D. Brenowitz
Keynote Speakers: Victor Bloomfield and Mario Amzel
- 1996 Organizers: Jonathan B. Chaires and Michael L. Doyle
Keynote Speakers: J. Michael Schurr and Allen Minton

- 1997 Organizers: Dorothy Beckett and Jack Correia
Keynote Speaker: Adrian Parsegian
- 1998 Organizer: Andy Robertson
Keynote Speaker: David Draper
- 1999 Organizers: Bertrand Garcia-Moreno E. and John Shriver
Keynote Speakers: Wayne Bolen and Gary Ackers
- 2000 Organizers: George Turner and Kim Sharp
Keynote Speaker: Steve White
- 2001 Organizers: Margaret A. Daugherty and Luis A. Marky
Keynote Speaker: George Rose
- 2002 Organizers: Michael Mossing and George Makhataдзе
Keynote Speaker: Rodney Biltonen
- 2003 Organizers: Vince Hilser and Dick Sheardy
Keynote Speaker: Jim Lee
- 2004 Organizers: Doug Barrick and Kathleen Hall
Keynote Speaker: Nacho Tinoco
- 2005 Organizers: Trevor Creamer and Clay Clark
Keynote Speaker: Carl Frieden
- 2006 Organizers: Karen Fleming and Rohit V. Pappu
Keynote Speakers: Madeline A. Shea and Timothy Lohman
- 2007 Organizers: Brian M. Baker and Michael T. Henzl
Keynote Speaker: Jamie Williamson
- 2008 Organizers: Jannette Carey and David Bain
Keynote Speakers: Dorothy Beckett and Ken Dill
- 2009 Organizers: Nathan Baker and Liskin Swint-Kruse
Keynote Speaker: Linda Jen-Jacobson
The Gary K. Ackers Lecture in Biothermodynamics: Michael Brenowitz
- 2010 Organizers: Elisar Barbar and Vince LiCata
Keynote Speaker: C. Nick Pace
The Gary K. Ackers Lecture in Biothermodynamics: Timothy Lohman
- 2011 Organizers: Gibbs Society of Board of Directors
Keynote Speaker: Bertrand Garcia-Moreno E.
The Gary K. Ackers Lecture in Biothermodynamics: Madeline Shea
Editors of Special Issue of *Biophysical Chemistry* – Enrico Di Cera, Tim Lohman, Jack Correia
- 2012 Organizers: Aaron L. Lucius and Patricia L. Clark
Keynote Speaker: Terry G. Oas
The Gary K. Ackers Lecture in Biothermodynamics: Enrico Di Cera
- 2013 Organizers: James L. Cole and Aron W. Fenton
Keynote Speaker: Doug Barrick
The Gary K. Ackers Lecture in Biothermodynamics: Bertrand Garcia-Moreno E.
- 2014 Organizers: Andrew B. Herr and Steven T. Whitten
Keynote Speaker: Karen G. Fleming
The Gary K. Ackers Lecture in Biothermodynamics: David E. Draper
- 2015 Organizers: Ernesto J. Fuentes and James R. Horn
Keynote Speaker: Rohit V. Pappu
The Gary K. Ackers Lecture in Biothermodynamics: Walter S. Englander

Gibbs Society Governance

Incorporation

In 2002, the Gibbs Society of Biological Thermodynamics incorporated in the Commonwealth of Virginia, under the guidance of Michael L. Johnson, then Treasurer of the Society and originator of the Society website. Articles of Incorporation and By Laws are available here: <http://www.jhu.edu/~gibbs>

Current Officers

- ❖ President: Patricia L. Clark, 2014 – 2015
- ❖ Vice President: Michael L. Johnson, 2010 – 2015
- ❖ Secretary: Liskin Swint-Kruse, 2013 – 2016
- ❖ Treasurer: John J. “Jack” Correia, Oct 2010 – Oct 2017

Board of Directors, listed alphabetically

- ❖ George I. Makhatadze, Past President
- ❖ Vince J. LiCata, President Elect
- ❖ John J. Correia, Treasurer
- ❖ Michael L. Johnson, Vice President
- ❖ Patricia L. Clark, President
- ❖ Madeline A. Shea
- ❖ Liskin Swint-Kruse, Secretary

Past Presidents

2001-2002	Gary K. Ackers
2002-2003	J. Jack Correia
2003-2004	D. Wayne Bolen
2004-2005	Madeline A. Shea
2005-2006	Dorothy Beckett
2006-2007	J. Brad Chaires
2007-2008	Tim M. Lohman
2008-2009	Luis A. Marky
2009-2010	Bertrand Garcia-Moreno E.
2010-2011	Karen G. Fleming
2011-2012	Doug Barrick
2012-2013	David L. Bain
2013-2014	George I. Makhatadze

Past Treasurer

2001-2011	Michael L. Johnson
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Past Secretary

2004-2013	Margaret A. Daugherty
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Committees & Other Contributions

Ackers Lecturer Selection Committee – Madeline A. Shea, Chair
Gibbs Society Website Hosting – Karen G. Fleming (2010 – present)
GoogleDocs Application/Registration & PayPal – Nathan A. Baker and J. Jack Correia
Mailing List – Liskin Swint-Kruse
Saturday Night Thermo Organizers – Susan Pedigo and Vincent J. LiCata
With thanks to Alan Teska at the Touch of Nature Conference Center

7th Annual Gary K. Ackers Lecture

2015 Lecturer – S. Walter Englander, University of Pennsylvania

This lecture honors the scientific contributions of Gary K. Ackers (1939-2011) to the field of Biological Thermodynamics. He served on the faculty at the University of Virginia, Johns Hopkins University and the Washington University School of Medicine. He was a Fellow of the Biophysical Society and was one of the founding organizers of the Gibbs Conference.

Gary demonstrated a lifelong commitment to the growth and development of an intellectual community of scholars devoted to furthering the field of biothermodynamics. Gary was an active member of the Biophysical Society throughout his career and served as President of the Society, as well as Organizer of the annual meeting. While on the faculty of the University of Virginia, he was a leader in the graduate biophysics training program. When on the faculty in the Department of Biology at the Johns Hopkins University, he conceived and organized the Institute for Biophysical Studies of Macromolecular Assemblies, a university-wide training program in molecular biophysics that has continued for decades. While at Johns Hopkins, he also played a leading role in the establishment of the Gibbs Conference on Biothermodynamics, an annual meeting organized to promote innovative development of biophysical principles applied to current problems in biology and to train the next generation of molecular biophysicists to tackle hard problems rigorously. After moving to St. Louis to chair the Department of Biochemistry and Molecular Biophysics at Washington University, he spearheaded a new graduate program in biophysics and hired many faculty who have joined the community of regular contributors to the Gibbs Conference.

Gary was a pioneer in the development of methods and application of principles of equilibrium thermodynamics to the study of linkage in complex macromolecular assemblies. Studies from his laboratory on the energetics of self-association and ligand binding in human hemoglobin proved unequivocally that the classic and elegant MWC model of intersubunit allostery was insufficient to explain cooperative oxygen binding: the position, as well as the number, of ligands matters. His contributions in this area greatly enhanced our understanding of the relationship between structure, energy and function in hemoglobin, and in multimeric allosteric systems in general. By probing ever more deeply into the molecular mechanism of cooperativity, he demonstrated a beautiful, useful, and general strategy for dissecting functional energetics in macromolecular assemblies.

His quantitative study of the interactions between proteins and nucleic acids in the bacteriophage lambda system included the development of quantitative DNase footprinting methods for measuring free energies of repressor-operator interactions. The footprinting assay remains an effective tool for measuring the extremely tight binding constants that are often encountered in site-specific interactions between proteins and nucleic acids. Those studies paved the way for similar methods to study protein-nucleic acid interactions in more complex systems, including time-resolved studies of the kinetics of RNA folding. Based on his experimental studies of phage lambda, his group developed statistical thermodynamic models to simulate the lysogenic-to-lytic growth switch: the series of macromolecular events that determine the fate of bacteriophage lambda during infection of *E. coli*. This work demonstrated how a complex biological function could be predicted quantitatively, strictly from the kinetics of transcription and translation, and the Gibbs free energy of interactions between the key macromolecular components in the genetic switch.

During Gary's early career, he developed methods to measure association constants in self-associating systems based on analytical gel permeation chromatography. Those methods have since become standard tools in the field. His group was also responsible for modifications of the cryo-gel electrophoresis methods, moving from applying them to hemoglobin to protein-DNA interactions. These contributions focused on developing the capacity to quantify intermediate states that are only transiently populated during the course of a biochemical process. His more than 200 articles and chapters changed our view of the molecular mechanisms that govern complex biochemical reactions.

△Gibbs₂₉ • Saturday Evening • October 3, 2015

4:00 – 10:00 pm **Check-in at Little Grassy Lodge**

7:30 – 10:00 pm **Open Reception in Indian Lodge – Light refreshments, beer, wine, and soft drinks**
Participants are expected to make dinner arrangements independently

Gibbs T-shirts and Pint glasses – pick up at registration

Saturday Night Thermo – Event for trainees only

Faculty Organizers: Vince J. LiCata, Louisiana State University; Susan Pedigo, University of Mississippi; and Sarah Bondos, Texas A&M Health Science Center

Trainee Moderators: Young-Joo Sun, Fuentes Lab and Amber Rolland, Dunlap Lab

5:30 pm **Freeberg Hall – Dinner for trainees who registered in advance**

6:00 – 7:00 pm **Flash Talks (Poster Introductions) – Session open to all trainees**

- 1. Direct observation of coupling in E. coli adenylate kinase**
Joseph E. Rehfus, Hilser Lab, Johns Hopkins University
- 2. Mechanism AL amyloid fibril formation: Seeding-nucleation and polymerization of in vitro AL amyloid formation and the cross-seeding phenomenon**
Luis Blancas-Mejia, Ramirez-Alvarado Lab, Mayo Clinic
- 3. Developing realistic simulations of cotranslational protein folding**
Ian M. Walsh, Clark Lab, University of Notre Dame
- 4. Polyproline II helix formation by an intrinsically disordered region of the Staphylococcus epidermidis accumulation associated protein**
Andrew E. Yarawsky, Herr Lab, University of Cincinnati
- 5. Simulation of OMP biogenesis elucidates mechanistic behavior and reveals differential pathway flux**
Shawn M. Costello, Fleming Lab, Johns Hopkins University
- 6. Measuring the monomer-dimer equilibrium of CLC-EC1 in membranes by single fluorescent molecule imaging of proteoliposomes**
Rahul Chadda, Robertson Lab, University of Iowa
- 7. Enzyme engineering for the development of a high throughput thermal shift assay of Burkholderia pseudomallei IspF inhibitors**
Joy M. Blain, Horn Lab, Northern Illinois University
- 8. Hydrodynamic radii of intrinsically disordered proteins determined from experimental polyproline II propensities**
Maria E. Tomasso, Whitten Lab, Texas St. University

7:00 – 7:15 pm **Refreshment break**

7:15 – 8:15 pm **Career panel – Session open to all trainees**
Dr. Sherry Hemmingsen, Jasco Inc.
Dr. Ed Lattman, Hauptman-Woodward Medical Research Institute
Dr. Jim Kranz, GlaxoSmithKline

8:15 pm **Adjourn to reception in Indian Lodge**

△Gibbs₂₉ • Sunday Morning • October 4, 2015

7:00 – 8:30 am **Breakfast served in Freeberg Hall**

Computational Thermodynamics of Folded and Unfolded Ensembles

8:30 – 8:35 am **President's Welcome by Patricia L. Clark, University of Notre Dame**

Moderator Stephen LuCore, Schnieders Lab, University of Iowa

8:35 – 8:50 am **Introduction to the 29th Annual Gibbs Conference Keynote Speaker**
Doug Barrick, Johns Hopkins University

8:50 – 9:30 am **Keynote Lecture**
Complexities of simple sequences
Rohit V. Pappu, Washington University

9:30 – 9:50 am **Dissecting cooperativity one hydrogen bond at a time**
Brittany K. Smith, Livesay Lab, University of North Carolina at Charlotte

9:50 – 10:20 am **Loss of conformational entropy in protein folding calculated using realistic ensembles (with implications to NMR-based calculations)**
Tobin R. Sosnick, University of Chicago

10:20 – 10:50 am **Break – Refreshments in Indian Lodge**

10:50 – 11:20 am **Effect of surfaces in modulating protein folding and aggregation mechanisms**
Joan-Emma Shea, University of California at Santa Barbara

11:20 – 11:40 am **ITC and van't Hoff: measuring consistency between van't Hoff and calorimetric enthalpies as a method to validate binding data**
Samuel A. Kantonen, Gilson Lab, University of California at San Diego

11:40 – 12:00 am **FAST conformational searches by balancing exploration/exploitation tradeoffs**
Maxwell I. Zimmerman, Bowman Lab, Washington University

12:05 pm **Conference photo near Freeberg Hall**

12:10 pm **Lunch in Freeberg Hall**

Free Time until Late Afternoon Session.

Information about local parks and attractions is available near the entrance to Little Grassy Lodge.

ΔGibbs₂₉ • Sunday Afternoon • October 4, 2015

Proteins at Membranes and Surfaces

- Moderator* Stephanie Kobany, Hinderliter Lab, University of Minnesota at Duluth
- 3:00 – 3:30 pm **Merging macroscopic and microscopic approaches for measuring the free energy of CLC-ec1 dimerization in lipid membranes**
Janice L. Robertson, University of Iowa
- 3:30 – 3:50 pm **Skp trimer formation is insensitive to ionic strength**
Clifford W. Sandlin, Fleming Lab, Johns Hopkins University
- 3:50 – 4:20 pm **Crowding effects on diffusion of small molecular probes: a temporal scaling perspective**
Erin D. Sheets, University of Minnesota at Duluth
- 4:20 – 4:50 pm **Break – Refreshments in Indian Lodge**
- 4:50 – 5:20 pm **From micelles to bacterial invasion: a biophysical approach to investigating host-pathogen interactions**
Linda Columbus, University of Virginia
- 5:20 – 5:40 pm **Influence of the intracellular environment on ligand-modulated membrane-bound ion channels**
Selcuk Atalay, Kekenos-Huskey Lab, University of Kentucky
- 5:40 – 6:00 pm **The role of conserved variant amino acids in the stability and function of the biofilm protein Aap**
Catie Shelton, Herr Lab, University of Cincinnati
- 6:00 – 6:20 pm **General Discussion**
- 6:25 pm **Dinner in Freeberg Hall**

ΔGibbs₂₉ • Sunday Evening • October 4, 2015

- 8:00 – 10:00 pm **Poster Session I in Sledgefoot (lower level) & Freeberg (upper level)**
Presenters with last name A to Li
- Please remove posters before midnight to make room for Monday presenters
- Sponsor's displays in Freeberg (upper level) – near beer, wine, and soft drinks

△Gibbs₂₉ • Monday Morning • October 5, 2015

Posters to be presented on Monday night may be mounted as soon as space is available on Sunday night. Airport Ride Board will be available in Little Grassy Lodge, near check-in window

7:00 – 8:30 am **Breakfast served in Freeberg Hall**

Macromolecular Folding and Binding

8:30 – 8:35 am **Announcements by Organizers**

Moderator Erik Cook, Creamer Lab, University of Kentucky College of Medicine

8:35 – 8:50 am **Introduction to the Gary K. Ackers Lecture in Biothermodynamics**

A. Joshua Wand, University of Pennsylvania

8:50 – 9:30 am **7th Annual Gary K. Ackers Lecture**

Protein folding: how and why by hydrogen exchange, fragment separation, and mass spectrometry

S. Walter Englander, University of Pennsylvania

9:30 – 9:50 am **Thioredoxin evolution under pressure**

Daniel Vasilchuk, Makhatadze Lab, Rensselaer Polytechnic Institute

9:50 – 10:20 am **Thermodynamic and structural analysis of calmodulin interaction with the skeletal muscle ryanodine receptor**

Adina M. Kilpatrick, Drake University

10:20 – 10:50 am **Break – Refreshments in Indian Lodge**

10:50 – 11:20 am **Sedimentation velocity and equilibrium data for a cytokine, soluble receptor interaction: comparison of simulations and experiments**

John J. Correia, University of Mississippi Medical Center

11:20 – 11:40 am **Transcription activator-like effectors (TALES) significantly populate partially folded states where one repeat is unfolded**

Kathryn Geiger-Schuller, Barrick lab, Johns Hopkins University

11:40 – 12:00 am **An engineered symmetrical protein illuminates the origins of kinetic stability, and why rational improvements in stability are hard**

Aron Broom, Meiering Lab, University of Waterloo

12:00 – 12:05 **Vendor introduction**

12:10 pm **Lunch in Freeberg Hall**

1:00 – 2:00 pm **Meeting of past organizers – Indian Building**

Refreshment area will be unavailable to other meeting attendees during this time

Free Time until Late Afternoon Session.

Information about local parks and attractions is available near the entrance to Little Grassy Lodge.

ΔGibbs₂₉ • Monday Afternoon • October 5, 2015

Allostery, Dynamics and Design

- Moderator* Kelly Churion, Bondos Lab, Texas A&M Health Science Center
- 3:00 – 3:30 pm **Simultaneous tuning of activation and repression in intrinsic disorder-mediated allostery**
Vincent J. Hilser, Johns Hopkins University
- 3:30 – 3:50 pm **The hepatitis B virus capsid has diverse structural responses to ligand-induced thermodynamic trapping**
Balasubramanian Venkatakrishnan, Zlotnick Lab, Indiana University
- 3:50 – 4:20 pm **Hemoprotein design using minimal sequence information**
Ronald L. Koder, The City College of New York
- 4:20 – 4:50 pm **Break – Refreshments in Indian Lodge**
- 4:50 – 5:20 pm **Protein disorder, allostery and heat capacity changes**
Dorothy Beckett, University of Maryland
- 5:20 – 5:40 pm **Revisiting allostery in the lac repressor protein**
Matthew A. Stetz, Wand Lab, University of Pennsylvania
- 5:40 – 6:10 pm **Evolutionary biochemical studies of S100 proteins**
Michael J. Harms, University of Oregon
- 6:10 – 6:30 pm **Site specific dynamics modulate allostery in the zinc metalloregulator CzrA**
Daiana A. Capdevila, Geidroc Lab, Indiana University
- 6:30 – 6:40 pm **General Discussion**
- 6:45 pm **Dinner in Freeberg Hall**

ΔGibbs₂₉ • Monday Evening • October 5, 2015

- 8:00 – 10:00 pm **Poster Session II in Sledgefoot (lower level) & Freeberg (upper level)**
Presenters with last name Lo to Z
- Sponsors displays in Freeberg (upper level) – near beer, wine, and soft drinks

△Gibbs₂₉ • Tuesday Morning • October 6, 2015

Check-out: Please leave your room keys at the counter in the lobby of the Little Grassy Lodge. Airport Ride Board will be available in Little Grassy Lodge, near check-in window.

7:00 – 8:30 am **Breakfast served in Freeberg Hall**

Nucleic Acids

8:40 – 8:45 am **Closing announcements by organizers**

Moderator Kayla McConnell, Lewis Lab, Mississippi State University

8:45 – 9:15 am **Single-molecule studies of FeS-containing DNA helicases: kinetics, conformational dynamics and molecular mechanisms**

Maria Spies, University of Iowa

9:15 – 9:35 am **Quantitative evaluation of the RNA polymerase I nucleotide addition cycle**

Francis D. Appling, Lucius Lab, University of Alabama-Birmingham

9:35 – 9:55 am **RNA pseudoknot folding energy landscape elucidated with T-jump measurements and kinetic modeling**

Jorjetha Roca, Ansari Lab, University of Illinois-Chicago

9:55 – 10:25 am **Break – Refreshments in Indian Lodge**

10:25 – 10:45 am **Monitoring local and global folding in a 60mer RNA with site specific fluorescent labels**

Robb S. Welty, Hall Lab, Washington University

10:45 – 11:15 am **Allostery in Trp-dependent RNA remodeling by TRAP**

Mark P. Foster, Ohio State University

11:15 – 11:20 am **Closing remarks by organizers and President**

11:25 am **Box lunch in Freeberg Hall**

Check-out Please leave your keys at the counter in Little Grassy Lodge