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The 31st Gibbs Conference on Biothermodynamics

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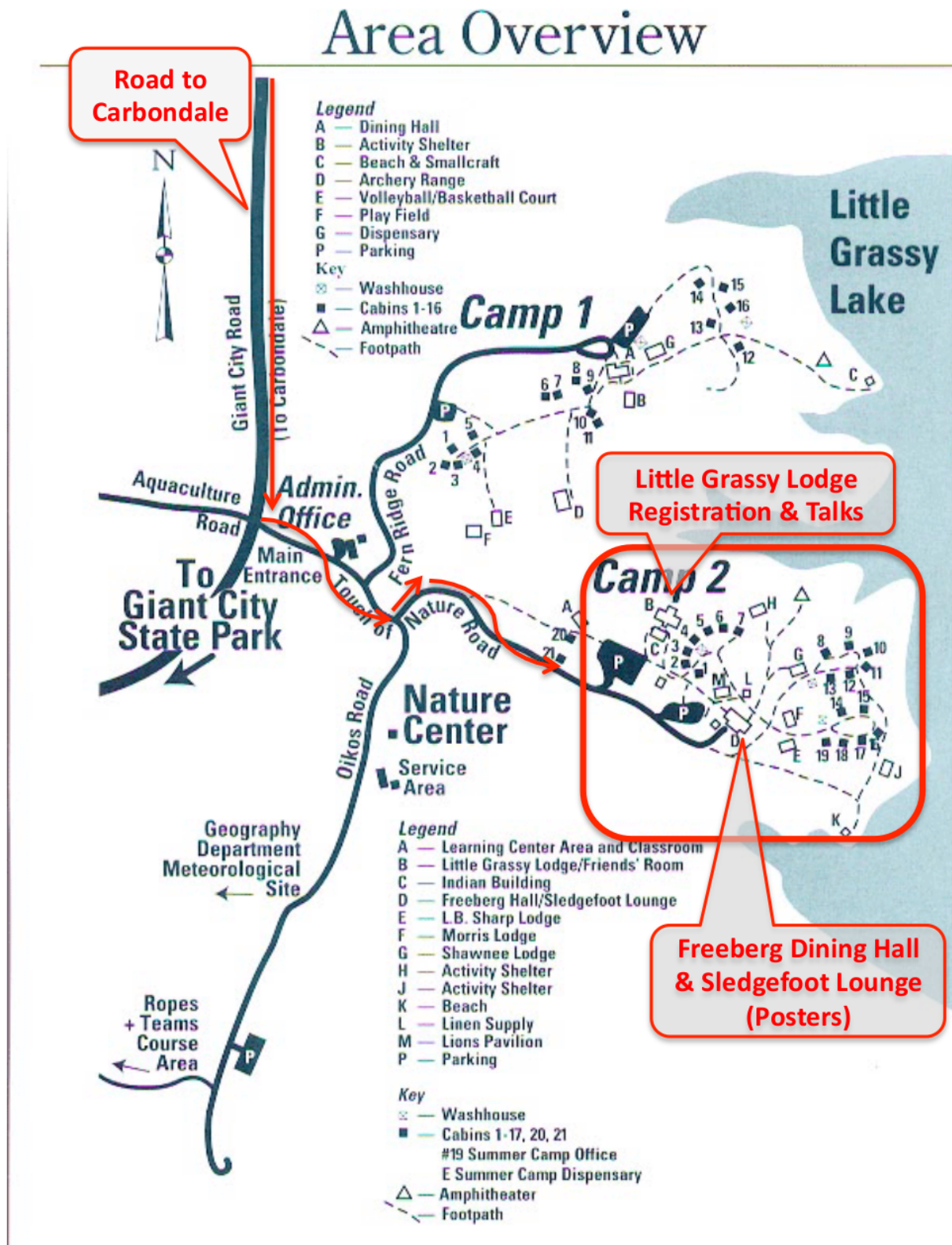
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Map of Touch of Nature Environmental Center

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

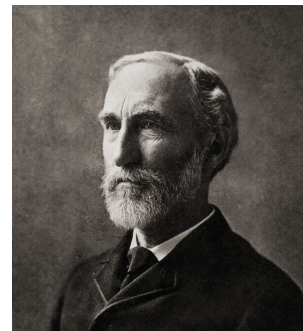
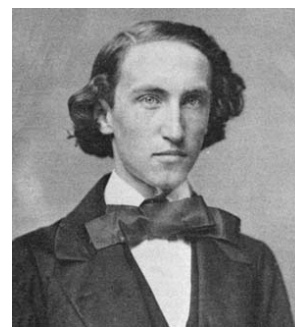
Discussion of the discipline: Thermodynamics in Biological Systems
At the Gill residence in Vail, Colorado
Gary Ackers, Wayne Bolen, Ernesto Freire, Stan Gill, Jim Lee

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 Makhatadze
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
- 2016 Organizers: Sarah Bondos and Nick Fitzkee
Keynote Speaker: Patricia Clark
The Gary K. Ackers Lecture in Biothermodynamics: Ken Dill
- 2017 Organizers: Scott Showalter and Ana-Maria Soto
Keynote Speaker: Enrique de la Cruz
The Gary K. Ackers Lecture in Biothermodynamics: Dorothy Beckett

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. Articles of Incorporation and By Laws are available here: <http://www.jhu.edu/~gibbs>

Current Officers

- ❖ President: James Cole, 2016 – 2017
- ❖ Vice President: Michael L. Johnson, 2010 – 2016
- ❖ President Elect: Clay Clark, 2016-2017
- ❖ Secretary: Liskin Swint-Kruse, 2013 – 2019
- ❖ Treasurer: John J. “Jack” Correia, 2010 – 2017

Board of Directors, listed alphabetically

- ❖ Clay Clark
- ❖ James Cole
- ❖ John J. “Jack” Correia
- ❖ Michael Johnson
- ❖ Vince LiCata
- ❖ Madeline Shea
- ❖ Liskin Swint-Kruse

Past Presidents

2001-2002	Gary K. Ackers	2009-2010	Bertrand Garcia-Moreno E.
2002-2003	J. Jack Correia	2010-2011	Karen G. Fleming
2003-2004	D. Wayne Bolen	2011-2012	Doug Barrick
2004-2005	Madeline A. Shea	2012-2013	David L. Bain
2005-2006	Dorothy Beckett	2013-2014	George I. Makhatadze
2006-2007	J. Brad Chaires	2014-2015	Patricia Clark
2007-2008	Tim M. Lohman	2015-2016	Vince LiCata
2008-2009	Luis A. Marky		

Past Treasurer

2001-2011 Michael L. Johnson

Past Secretary

2004-2013 Margaret A. Daugherty

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

Confidentiality Statement

Please remember that the abstracts for this meeting are confidential material and may contain unpublished results. They will not be posted online. Please ask permission from the authors before taking photos of posters. Please do not record the talks unless a speaker has given you permission.

9th Annual Gary K. Ackers Lecture

2017 Lecturer – Dorothy Beckett, University of Maryland

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.



• Saturday Evening • September 23, 2017

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, Pints and Mugs – pick up at registration

Saturday Night Thermo – Event for trainees only

Faculty Organizers: Vince J. LiCata, Louisiana State University and Susan Pedigo, University of Mississippi

Trainee Moderators: Nitija Tiwari, Fuentes Lab, University of Iowa

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. Effects of Doxorubicin on the Thermodynamic and Hydrodynamic Properties of an ELP-Drug Carrier**
Valeria Zai-Rose, Correia lab, University of Mississippi Medical Center
- 2. Molecular Driving Forces and Kinetics in Large Hairpin Polyamide-DNA Interactions**
Yang Song, Dupureur lab, University of Missouri-St. Louis
- 3. Annexin a5 Cooperatively Interacting with Membrane Cholesterol to Induce a Ca²⁺-Dependent Signal Transduction Termination Event**
Robby Miller, Hinderliter lab, University of Minnesota Duluth
- 4. Modeling Sequence Dependent Peptide Fluctuations in Immunologic Recognition**
Cory Ayres, Baker lab, University of Notre Dame
- 5. Structural Modeling and Molecular Dynamic Simulations of Dystrophin Spectrin Repeats**
Sarah Moe, Cembran lab, University of Minnesota Duluth
- 6. Impact of transient helicity on binding of intrinsically disordered proteins**
Grace Usher, Showalter lab, Pennsylvania State University

7:00 – 7:15 pm

Refreshment break

7:15 – 8:15 pm

Career panel – Session open to all trainees
Michael Bradley, Ph.D., Syros Pharmaceuticals
Austin Elam, Ph.D., C4 Therapeutics
Wyatt Strutz, M.Sc., NanoTemper Technologies

8:15 pm

Adjourn to reception in Indian Lodge



• **Sunday Morning • September 24, 2017**

7:00 – 8:20 am

Breakfast served in Freeberg Hall

Macromolecular Mechanisms and Interactions

8:25 – 8:30 am

President's Welcome by Jim Cole, University of Connecticut

Moderator

Ellie Kolb, Kovall Lab, University of Cincinnati

8:30 – 8:40 am

Introduction to the 31st Annual Gibbs Conference Keynote Speaker

Jack Correia, University of Mississippi Medical Center

8:40 – 9:25 am

Keynote Lecture

How cells use chemistry and physics to break the bones that power their movements

Enrique de la Cruz, Yale University

9:25 – 9:45 am

Accessibility of the histone H3 tail regulates recognition by effector domains

Emma Morrison, Musselman Lab, University of Iowa

9:45 – 10:05 pm

Distinct properties of a novel electron-transferring flavoprotein FixAB underlie flavin-based electron bifurcation that redistributes energy among electrons

Diessel Duan, Miller Lab, University of Kentucky

10:05 – 10:35 am

Break – Refreshments in Indian Lodge

10:35 – 11:05 am

Glutamate promotes SSB protein-protein Interactions via intrinsically disordered regions

Tim Lohman, Washington University in Saint Louis

11:05 – 11:25 am

Mechanism of transcription initiation by E. coli RNA polymerase: Productive initiation and escape from the λ PR promoter

Kate Henderson, Record Lab, University of Wisconsin-Madison

11:25 – 11:55 am

Molecular mechanisms of enzyme catalyzed protein unfolding and translocation by class 1 AAA+ motors

Aaron Lucius, University of Alabama at Birmingham

11:55 – 12:15 pm

Rational design of PDZ specificity based on “Binding Pocket Characteristics”

Young Joo Sun, Fuentes Lab, University of Iowa

12:20 pm

Conference photo near Freeberg Hall

12:25 pm

Lunch in Freeberg Hall

Workshop: Careers in the Biotechnology Industry

This optional workshop will explain how to transition into careers in biotechnology.

1:30 – 2:30 pm

Presenter: Michael Bradley, Syros Pharmaceuticals

Panelists: Michael Bradley, Austin Elam (C4 Therapeutics), Wyatt Strutz (NanoTemper)

Interpretive Nature Hike

The Environmental Education staff will take up to 25 participants for this hike on the trail along the little grassy lake shore . Please contact Alan Teska at the front desk to register.

1:00 – 2:45 pm

Meet at Freeberg patio to start hike

Free Time until Afternoon Session.

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



• Sunday Afternoon • September 24, 2017

Thermodynamics of Folding and Assembly

Moderator

Alexander Yarawsky, Herr Lab, University of Cincinnati

3:00 – 3:30 pm

Phase separation of UBQLN2 is modulated by oligomerization and ubiquitin binding

Carlos Castañeda, Syracuse University

3:30 – 3:50 pm

Sequence order versus composition: How does hydrophobic clustering affect protein disorder?

Micayla Bowman, Clark Lab, University of Notre Dame

3:50 – 4:20 pm

Multiple structure-intrinsic disorder interactions regulate and coordinate Hox protein function

Sarah Bondos, Texas A&M Health Science Center

4:20 – 4:40 pm

Calcium-independent dimerization of N-Cadherin

Samantha Davila, Pedigo Lab, University of Mississippi

4:40 – 5:10 pm

Break – Refreshments in Indian Lodge

5:10 – 5:40 pm

Immunoglobulins, elbow motions, asymmetry and misfolding

Marina Ramirez-Alvarado, Mayo Clinic

5:40 – 6:00 pm

Hyperstability and functional characterization of protein consensus sequences

Matthew Sternke, Barrick Lab, Johns Hopkins University

6:00 – 6:30 pm

Thermodynamic driving forces and fluctuation dynamics in IDPs of the Ct family

Sara Vaiana, Arizona State University

6:35 pm

Dinner in Freeberg Hall



• Sunday Evening • September 24, 2017

8:00 – 10:00 pm

Poster Session I in Sledgefoot (lower level) & Freeberg (upper level)

Presenters with last name A to Mah

Please remove posters before midnight to make room for Monday presenters

Sponsor's displays in Freeberg (upper level) – near beer, wine, and soft drinks



• Monday Morning • September 25, 2017

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

7:00 – 8:20 am **Breakfast served in Freeberg Hall**

Allostery, Binding and Coupled Equilibria

8:25 – 8:30 am **Announcements by Organizers**

Moderator Sukrit Singh, Bowman Lab, Washington University in St. Louis.

8:30 – 8:40 am **Introduction to the Gary K. Ackers Lecture in Biothermodynamics**
Jannette Carey, Princeton University

8:40 – 9:25 am **9th Annual Gary K. Ackers Lecture**
Coupled equilibria in transcription regulation: A multi-level analysis
Dorothy Beckett, University of Maryland

9:25 – 9:45 am **Inter-active site communication mediated by the dimer interface beta-sheet in the half-the-sites enzyme, thymidylate synthase.**
Paul Sapienza, Lee Lab, University of North Carolina Chapel Hill

9:45 – 10:05 am **The basis of an engineered specificity switch reveals the distributed and cooperative nature of T cell receptor specificity**
Nishant Singh, Baker Lab, University of Notre Dame

10:05 – 10:35 am **Break – Refreshments in Indian Lodge**

10:35 – 11:05 am **Calmodulin choreography on voltage-gated sodium channels: Allostery in action**
Madeline Shea, University of Iowa

11:05 – 11:25 am **The thermodynamics of metal and substrate binding to the nonheme iron(II) and α KG dependent metalloenzymes**
Mingjie Li, Emerson Lab, Mississippi State University

11:25 – 11:55 am **How do protein domains talk to each other? Insights from single molecule biophysics**
Rodrigo Maillard, Georgetown University

11:55 – 12:15 pm **Vendor Introduction**

12:20 pm **Lunch in Freeberg Hall**

1:10 – 2:10 pm **Business Meeting of Past and Current Organizers – Indian Building**
Refreshment area will be unavailable to other meeting attendees during this time

Canoeing

Those interested should contact Alan Teska at the front desk.

1:00 – 2:45 pm **Meet at Freeberg patio to walk to the lake.**

Free Time until Afternoon Session.

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



• Monday Afternoon • September 25, 2017

Nucleic Acids Conformation & Interactions with Proteins

Moderator

Robert McDonnell, Elcock Lab, University of Iowa

3:00 – 3:30 pm

Simulating the co-transcriptional folding of RNA in atomistic detail using SHAPE constraints.

Alan Chen, University at Albany SUNY

3:30 – 3:50 pm

Tetrahelical monomolecular architecture of DNA for biotechnological applications

Besik Kankia, The Ohio State University

3:50 – 4:20 pm

Mechanism of action and physiological function of DbpA: a ribosomal RNA chaperone.

Eda Koculi, University of Central Florida

4:20 – 4:40 pm

Quaternary interactions and DNA twist modulate the cooperative binding of AGT

Michael Fried, University of Kentucky

4:40 – 5:10 pm

Break – Refreshments in Indian Lodge

5:10 – 5:40 pm

Two nucleic acid binding modes for HIV-reverse transcriptase: Salt linkages and effects of the antiretroviral drug Nevirapine

Vince LiCata, Louisiana State University

5:40 – 6:00 pm

Studying protein-RNA interactions using contrast variation SAXS

Suzette Pabit, Pollack Lab, Cornell University

6:00 – 6:30 pm

Reaction of DNA intramolecular structures with their partially complementary strands: A thermodynamic and kinetic approach

Luis Marky, University of Nebraska Medical Center

6:35 pm

Dinner in Freeberg Hall



• Monday Evening • September 25, 2017

8:00 – 10:00 pm

Poster Session II in Sledgefoot (lower level) & Freeberg (upper level)

Presenters with last name Mal to Z

Sponsors displays in Freeberg (upper level) – near beer, wine, and soft drinks



• Tuesday Morning • September 26, 2017

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

7:00 – 8:20 am	Breakfast served in Freeberg Hall
	Thermodynamics of Membranes and Aggregation
8:25 – 8:30 am	Closing Announcements by Organizers
<i>Moderator</i>	Brendan Mahoney, Peng Lab, University of Notre Dame
8:30 – 9:00 am	The trimerization process of membrane protein AcrB Yinan Wei, University of Kentucky
9:00 – 9:20 am	Observation of intermolecular interactions and dynamics in the early stages of ELP phase separation Yue Zhang, Fitzkee Lab, Mississippi State University
9:20 – 9:40 am	Analytical ultracentrifuge studies of therapeutic proteins in human serum Robert Wright, Correia Lab, University of Mississippi Medical Center
9:40 – 10:10 am	Break – Refreshments in Indian Lodge
10:10 – 10:30 am	Thermodynamics of amyloid fibrils: effects of the hydrophobicity of the peptide sequence Cristiano Dias, New Jersey Institute of Technology
10:30 – 10:50 am	Calcium and calmodulin regulation of Nav1.4 and Nav1.5 Jesse Yoder, Amzel Lab, Johns Hopkins University
10:50 – 11:10 pm	Kinetic stability of urine derived Bence-Jones proteins from multiple myeloma and light chain amyloidosis patients. Luis Blancas-Mejia, Ramirez-Alvarado Lab, Mayo Clinic
11:10 – 11:40 am	Role of topological defects in integral membrane proteostasis Jonathan Schleich, Indiana University
11:40 – 11:50 am	Closing Remarks by Organizers and President
12:00 pm	Box lunch in Freeberg Hall
Check-out	Please leave your keys at the counter in Little Grassy Lodge