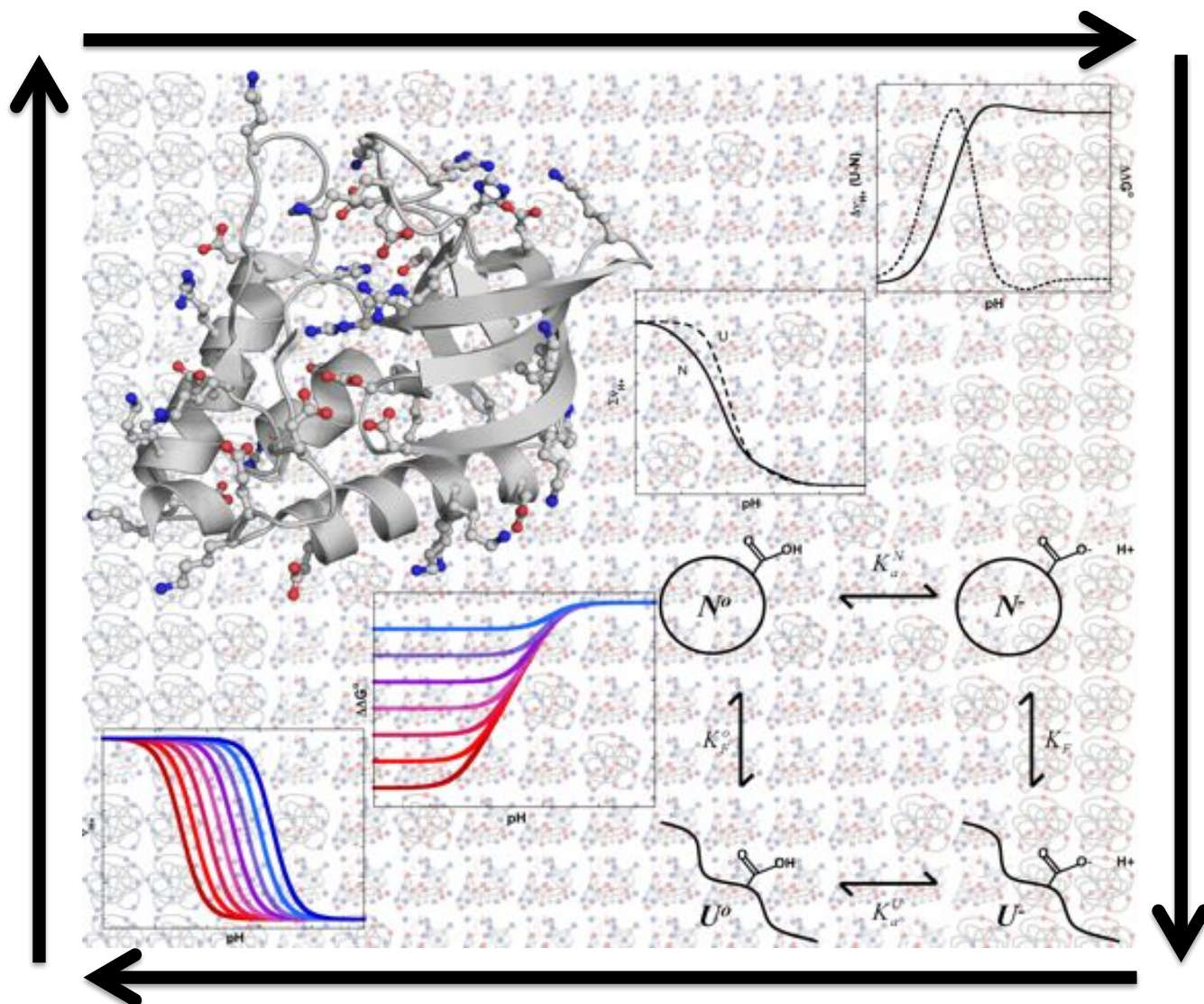


$\Delta G_{\text{ibbs}}_{25}$

25th Annual Gibbs Conference on Biothermodynamics
Touch of Nature Environmental Center • Carbondale • Illinois
September 17-20, 2011



Organized by the Board of Directors
Gibbs Society of Biological Thermodynamics
*Sponsored by Avanti Polar Lipids, Aviv Family Foundation,
Beckman Coulter, GE Healthcare/Microcal, Horiba Scientific,
ISS, Jasco, Micromath, OLIS, and UMMC*

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The 25th Gibbs Conference on Biothermodynamics



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Sponsors

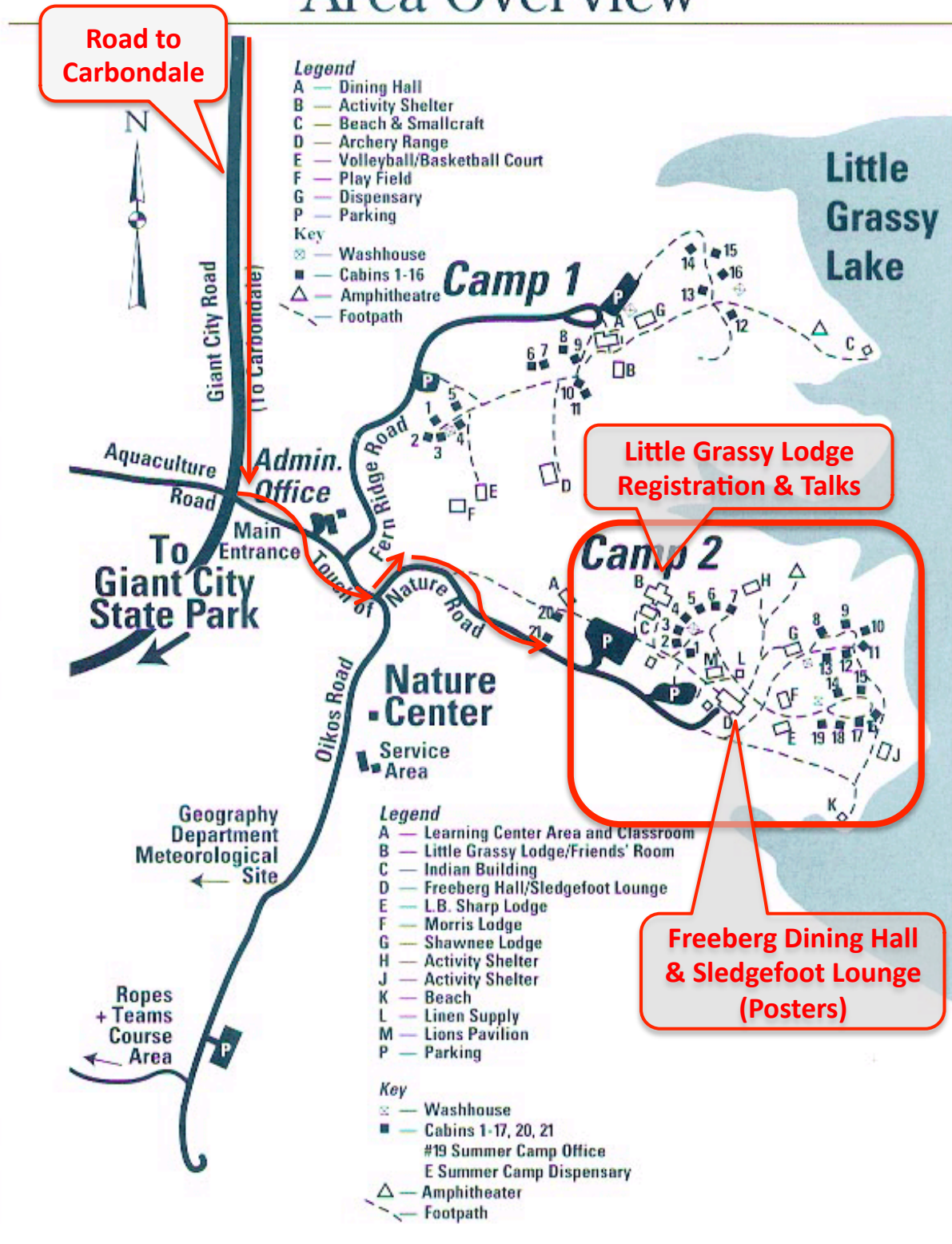
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Cover figure provided by Bertrand Garcia-Moreno E., Gibbs25 Keynote Speaker

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.

Area Overview



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

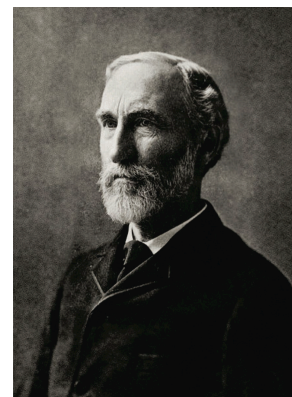
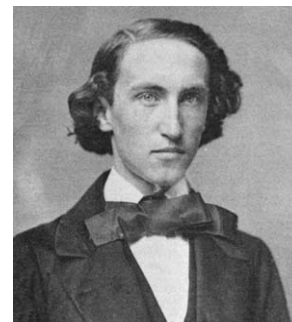
February, 1987

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 *The Gibbs Conference on Biothermodynamics: Origins and Evolution. 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
Introduction: Twenty five years of the Gibbs Conference on Biothermodynamics
Biophysical Chemistry **159** (2011) 1-5 (doi:10.1016/j.bpc.2011.07.002)

A complete list of scientific contributions by past organizers to a special issue of *Biophysical Chemistry* commemorating the 25th Gibbs Conference follows the list of meetings.



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 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 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
Saturday Night Thermo Organizers – Liskin Swint-Kruse and Vincent J. LiCata
Editors of Special Issue of *Biophysical Chemistry* – Enrico Di Cera, Tim Lohman, Jack Correia

Δ Gibbs₂₅ Special Issue of *Biophysical Chemistry*

Edited by Enrico Di Cera, Jack Correia and Tim Lohman

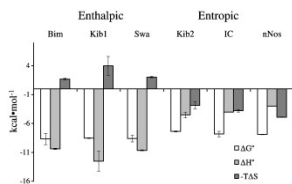
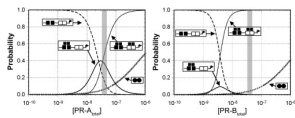
<http://www.sciencedirect.com/science/journal/03014622>

Scientific Contributions

Bain

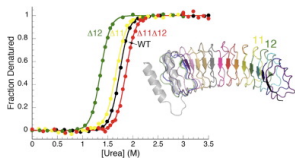
From Steroid Receptors to Cytokines:
The Thermodynamics of Self-Associating Systems

Keith D Connaghan, Ph.D., Amie D Moody, BA, James P Robblee, Ph.D.,
James R Lambert, Ph.D., David L Bain, Ph.D.



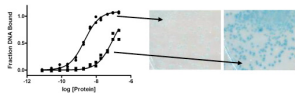
Barbar

Conformational Dynamics Promote Binding Diversity of Dynein Light Chain LC8
Afua Nyarko Justin Hall, Andrea Hall, Michael Hare, Elisar Barbar, Ph.D.



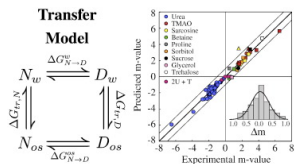
Barrick

Deletion of internal structured repeats increases the stability
of a leucine-rich repeat protein, YopM
Ellen F Vieux, Ph.D., Doug Barrick, Ph.D.



Beckett, Swint-Kruse

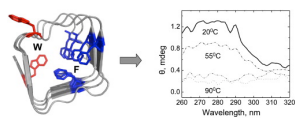
In vivo tests of thermodynamic models of transcription repressor function
Sudheer Tungtur, Harlyn Skinner, Hongli Zhan, Ph.D., Liskin Swint-Kruse, Ph.D.,
Dorothy Beckett, Ph.D.



Bolen

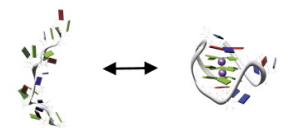
Osmolyte effects on protein stability and solubility:
a balancing act between backbone and sidechains

Matthew Auton, Ph.D., Jörg Rösigen, Ph.D., Mikhail Sinev, Luis Marcelo F
Holthausen, David W Bolen, Ph.D.



Brenowitz

Stability, denaturation and refolding of Mycobacterium tuberculosis MfpA,
a DNA mimicking protein that confers antibiotic resistance
Sergei Khrapunov, Ph.D, Michael Brenowitz, Ph.D



Chaires

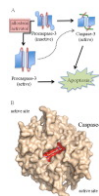
Linkage of cation binding and folding in human telomeric quadruplex DNA
Robert D Gray, Ph.D., Jonathan B. Chaires, Ph.D.

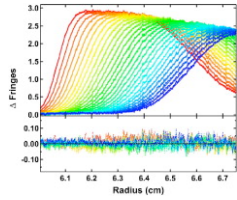
$$\Delta G_{\text{overall}} = 2.5 + (-4.9) = -2.4 \text{ kcal mol}^{-1}$$

Clark

A bifunctional allosteric site in the dimer interface of procaspase-3

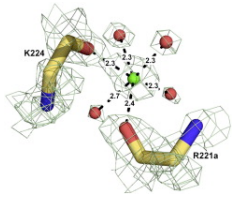
Joshua L Schipper, Sarah H MacKenzie, Ph.D., Anil Sharma, Ph.D., Clay Clark,
Ph.D.





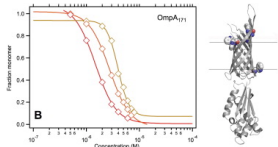
Correia

The use of analytical sedimentation velocity to extract thermodynamic linkage
 James L Cole, Ph.D., John J Correia, Ph.D., Walter F Stafford, Ph.D.



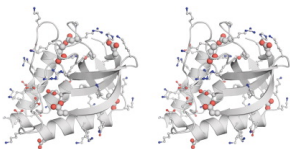
Di Cera

Rigidification of the autolysis loop enhances Na⁺ binding to thrombin
 Nicola Pozzi Raymond Chen, Zhiwei Chen, Alaji Bah, Enrico Di Cera



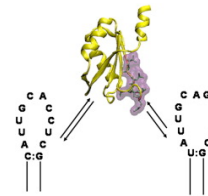
Fleming

The soluble, periplasmic domain of OmpA folds as an independent unit and displays chaperone activity by reducing the self-association propensity of the unfolded OmpA transmembrane β-barrel
 Emily J Danoff, BS, Karen G Fleming, Ph.D.



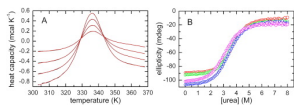
García-Moreno E.

Thermodynamic principles for the engineering of pH-driven conformational switches and acid insensitive proteins
 Peregrine Bell-Upp, Aaron C Robinson, Steven Whitten, Erika L Wheeler, Janine Lin, Wesley E. Stites, Bertrand García-Moreno E



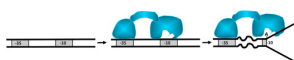
Hall

Human U2B^{''} Protein Binding to snRNA Stemloops
 Sandra G Williams, Kathleen B Hall



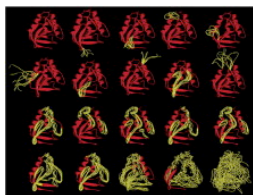
Henzl

Heightened Stability of Polcalcine Phl p 7 Is Correlated with Strategic Placement of Apolar Residues
 Michael T Henzl, Ph.D., Mark A Reed, Anmin Tan, Ph.D.



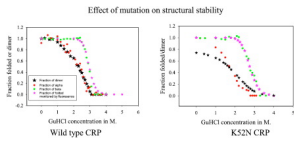
Heyduk

Promoter spacer DNA plays an active role in integrating the functional consequences of RNA polymerase contacts with -10 and -35 promoter elements
 Malgorzata Sztiller-Sikorska, Ewa Heyduk, Tomasz Heyduk



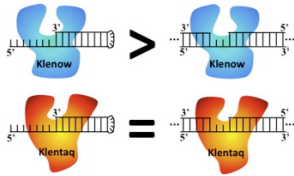
Hilser

The Role of Protein Conformational Fluctuations in Allostery, Function, and Evolution
 James O Wrabl, Ph.D., Jenny Gu, Ph.D., Tong Liu, Ph.D., Travis P Schrank, Ph.D., Steven T Whitten, Ph.D., Vincent J Hilser, Ph.D.



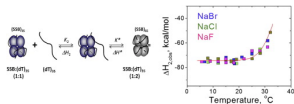
Lee

Modulation of Allosteric Behavior Through Adjustment of the Differential Stability of the Two Interacting Domains in *E. coli* cAMP Receptor Protein
 Jianquan Li, Ph.D. and James Ching Lee, Ph.D.



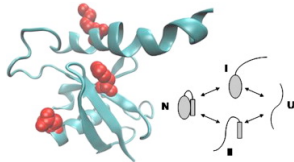
LiCata

Interactions of replication versus repair DNA substrates with the Pol I DNA polymerases from *E. coli* and *T. aquaticus*
 Yanling Yang, Vince J LiCata



Lohman

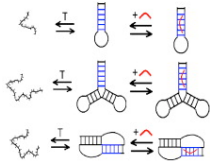
E. coli SSB tetramer binds the first and second molecules of (dT)₃₅ with heat capacities of opposite sign
 Alexander G Kozlov, Timothy Lohman



Makhatadze

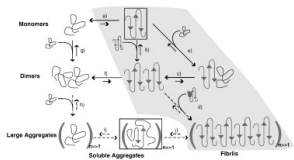
Equilibrium and Kinetic Studies of Protein Cooperativity using Urea-Induced Folding/Unfolding of a Ubq-UIM Fusion Protein
 Mayank M Patel, Franco Tzul, George Makhatadze

Graphics



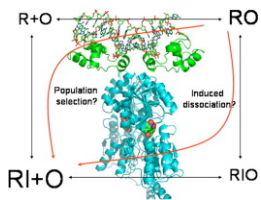
Marky

Melting Behavior and Ligand Binding of DNA Intramolecular Secondary Structures
 Souvik Maiti Ph.D., Besik Kankia, Ph.D., Irine Khutsishvili, Ph.D., Luis A Marky, Ph.D.



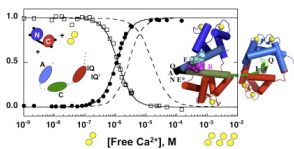
Pappu

Assessing the contribution of heterogeneous distributions of oligomers to aggregation mechanisms for polyglutamine peptides
 Andreas Vitalis, Ph.D., Rohit V Pappu, Ph.D.



Sharp

Allostery in the Lac Operon: Population Selection or Induced Dissociation?
 Kim A Sharp, Ph.D



Shea

Thermodynamic Linkage Between Calmodulin Domains Binding Calcium and Contiguous Sites in the C-Terminal Tail of Ca_v1.2
 T. Idil Apak Evans, Ph.D., Johannes W Hell, Ph.D., Madeline A Shea, Ph.D.

Gibbs Society Governance

Incorporation

In 2002, the *Gibbs Society on 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: Karen G. Fleming, 2010-2011
- ❖ Vice President: Michael L. Johnson, 2011 - 2013
- ❖ Secretary: Margaret A. Daugherty, 2004 – 2013
- ❖ Treasurer: John J. Correia, March 2011 – October, 2016

Board of Directors

- ❖ Karen Fleming, President
- ❖ Douglas Barrick, President Elect
- ❖ Bertrand Garcia-Moreno, Past President
- ❖ Michael L. Johnson, Vice President
- ❖ John J. Correia, Treasurer
- ❖ Margaret Daugherty, Secretary
- ❖ Madeline Shea

Past Presidents

2001-2002	Gary Ackers
2002-2003	Jack Correia
2003-2004	D. Wayne Bolen
2004-2005	Madeline Shea
2005-2006	Dorothy Beckett
2006-2007	Jonathan (Brad) Chaires
2007-2008	Tim Lohman
2008-2009	Luis Marky
2009-2010	Bertrand Garcia-Moreno E.

Past Treasurer

2001-2011	Michael L. Johnson
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Committees & Other Contributions

Ackers Lecturer Selection Committee – James Ching Lee, Chair
Gibbs Society Website Hosting – Karen Fleming (2010 -)

GoogleDocs Application/Registration & PayPal – Nathan Baker and Jack Correia

Mailing List – Madeline Shea

Fundraising – Madeline Shea and Jack Correia

Gibbs25 Website Hosting – Karen Fleming

Catering, Wine and Meal Contract – Jack Correia and Liskin Swint-Kruse

With thanks to Alan Teska and Mike Scott at the Touch of Nature Conference Center!

3rd Annual Gary K. Ackers Lecture in Biological Thermodynamics

2011 Lecturer – Madeline A. Shea, Carver College of Medicine, University of Iowa

This lecture honors the scientific contributions of Gary K. Ackers (1939-2011) to the field of Biological Thermodynamics and co-founding the Gibbs Conference. He served on the faculty of the University of Virginia, and the 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.

ΔGibbs₂₅ • Saturday Evening • September 17, 2011

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-shirt Bazaar – please pay for the shirts ordered during registration.

9:00 pm **Screening of the new PHD Movie** – Friends Room, Little Grassy Lodge
Created by Jorge Cham - <http://www.phdcomics.com/movie/index.php>

Posters to be presented on Sunday night may be mounted any time prior to 8 pm Sunday.

Saturday Night Thermo – Events For Trainees Only

Faculty Organizers

Vince LiCata, Louisiana State University & Liskin Swint-Kruse, Kansas University Medical Center

Trainee Moderators

Sarah MacKenzie, Laboratory of Clay Clark, NCSU

Andy Wowor, Laboratory of Jim Cole, U. Conn.

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

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

1. **Hao Ching Hsiao, Bondos Laboratory, Texas A&M Health Science Center**
Ultrabithorax, An Intrinsically Disordered Protein, Selects Protein Interactions by Topology
2. **Je Ko, Heyduk Laboratory, St. Louis University**
Determinants of the rate of promoter escape by bacterial RNA polymerase
3. **Jaycob Warfel, LiCata Laboratory, Louisiana State University**
Thermodynamic Studies of Deinococcus radiodurans Type I DNA polymerase
Thermodynamic Studies of Deinococcus radiodurans Type I DNA polymerase
4. **Hesam N. Motlagh, Hilser Laboratory, John Hopkins University**
How can a ligand be an agonist and antagonist for the same protein?
5. **Anne Rice, Hinderliter Laboratory, University of Minnesota - Duluth**
A Modeling System for the Deconvolution of the Coupling Energy of Synaptotagmin C2AB
Domains using DSC
6. **Lei Wang, Mossing Laboratory, University of Mississippi**
Cro Variants to Distinguish Kinetic and Equilibrium Control of Gene Circuits
7. **James Campell, Whitten Laboratory, Texas State University – San Marcos**
Correlation of m-value effects to cold-resistant substructures of the protein ensemble.
8. **Megan Murtaugh, Horn Laboratory, Northern Illinois University**
Characterization of an engineered pH-dependent single domain (VHH) antibody to explore the role of individual histidines in the observed pH sensitivity

7:00 - 7:15 pm **Refreshment Break**

7:15 pm **Career Panel – session open to all trainees**
Margaret Daugherty, Colorado College, Colorado Springs, CO
Michael Doyle, Bristol-Myers-Squibb, New Jersey
Glen Ramsay, Aviv Biomedical, Inc., Lakewood, NJ

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

ΔGibbs₂₅ • Sunday Morning • September 18, 2011

7:00 - 8:15 am Breakfast served in Freeberg Hall

Structural Origins of Thermodynamic Potentials

8:30 am Welcome by Karen Fleming, Gibbs Society President

Moderator: **John Froehlig, Wade Laboratory, John Hopkins University**

**8:35 am Introduction to the 25th Annual Gibbs Conference Keynote Speaker
D. Wayne Bolen, University of Texas Medical Branch**
Founding Co-Organizer of the 1987 Conference

**8:50 am Keynote Lecture
Bertrand Garcia-Moreno E.
Johns Hopkins University School of Arts and Sciences**
Protein electrostatics: have we made progress in 25 years?

9:30 – 9:45 am Andrew Hagarman, Oas Laboratory, Duke University
Thermodynamic investigation of protein A antibody binding domain folding

9:45 – 10:00 am Emma Morrison, Henzler-Wildman Laboratory, Washington University
A Protein Dynamics Investigation into Broad Ligand Specificity in the
Multi-Drug Resistance Transporter, EmrE.

10:00 – 10:20 am Break – Refreshments in Indian Lodge

10:20 – 10:50 am Vince Hilser, Johns Hopkins University, School of Arts and Sciences
Allostery in an Ensemble

10:50 – 11:15 am Rodrigo Maillard, Bustamante Laboratory, University of California - Berkeley
Force-Induced Mechanical Unfolding of Protein Substrates by the AAA+ Protease ClpXP

11:15 – 11:45 Mario Amzel, Johns Hopkins University School of Medicine
Computation of free energies by Multi-Step Trajectory Combinations

Panel Leader: **Nathan Baker, Pacific Northwest National Laboratory**

11:45 – 12:00 Panel Discussion by All Speakers

12:05 pm Conference photo near Freeberg Hall

12:15 pm Lunch in Freeberg Hall

Free Time until Late Afternoon Session.

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

ΔGibbs₂₅ • Sunday Afternoon • September 18, 2011

Solvent and Solute Interactions with Macromolecules

Moderator: Ann Murray, Fuentes Laboratory, University of Iowa Carver College of Medicine

3:00 – 3:15 Luis Marky, University of Nebraska Medical Center
Introduction to the Field

3:15 – 3:45 pm David Draper, Johns Hopkins University School of Arts and Sciences
Thermodynamic “crosstalk” in the conversation between RNAs, ions, and osmolytes

3:45 – 4:00 pm Esther Braselmann, Clark Laboratory, University of Notre Dame
Investigating the conformation of an autotransporter protein in the bacterial periplasm

4:00 – 4:30 pm D. Wayne Bolen, University of Texas Medical Branch
Osmolyte effects on protein stability and solubility:
a balancing act between backbone and side-chains

4:30 – 4:45 pm **Break – Refreshments in Indian Lodge**

4:45 – 5:00 pm Joseph Kasper, Park Laboratory, Purdue University
Transient partial unfolding in E. coli DHFR

5:00 – 5:15 pm Ronald Toth, Laue Laboratory, University of New Hampshire
Nonideality in High Concentration Solutions

5:15 – 5:45 pm Karen Fleming, Johns Hopkins University School of Arts and Sciences
Membrane protein stability

Panel Leader: Vince LiCata, Louisiana State University

5:45 – 6 pm Panel Discussion by All Speakers

6:15 Dinner in Freeberg Hall

ΔGibbs₂₅ • Sunday Evening • September 18, 2011

8 – 10 pm Poster Session I in Sledgefoot (lower level) & Freeberg (upper level)
Presenters with last names from Adams to Ma
Please remove posters before midnight to make room for Monday presenters.

Sponsors Displays in Freeberg (upper level) - near Beer, Wine and Soda

ΔGibbs₂₅ • Monday Morning • September 19, 2011

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 – 8:15 am Breakfast in Freeberg Hall

Cooperativity, Allostery and Ensembles of Macromolecular States

8:30 am Announcements by Organizers

Moderator: **Dan Parente, Swint-Kruse Laboratory, KUMC University**

8:35 Introduction to the Gary K. Ackers Lecture in Biothermodynamics
James Ching Lee, University of Texas Medical Branch
Founding Co-Organizer of the 1987 Conference

8:50 – 9:30 am 3rd Annual Gary K. Ackers Lecture in Biothermodynamics
Madeline A. Shea, Carver College of Medicine, University of Iowa
Calcium-Triggered EF-Hands Grasp and Remodel Ion Channels

9:30 – 9:45 am Brian Doctrow, Garcia-Moreno Laboratory, John Hopkins University
Cooperativity in a cluster of carboxylic groups in the active site of a protein

9:45 – 10:00 am Nicola Pozzi, Di Cera Laboratory, Saint Louis University
Conformational Plasticity in Trypsin-like Zymogens: The case of Prethrombin-2

10:00 – 10:20 am Break – Refreshments in Indian Lodge

10:20 – 10:50 am J. Brad Chaires, University of Louisville
Folding and Energy Landscape of Telomeric G-quadruplex DNA

10:50 – 11:05 am Katherine Launer-Felty, Cole Laboratory, University of Connecticut
Inhibition of Protein Kinase R by Adenovirus virus-associated RNA I

11:05 – 11:35 James Ching Lee, University of Texas Medical Branch
Mechanisms in modulating allostery in E. coli cAMP receptor protein, CRP

Panel Leader: **Dorothy Beckett, University of Maryland College Park**

11:35 – 12:00 Panel Discussion by All Speakers

12:10 pm Lunch in Freeberg Hall

1 – 2 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 & attractions is available near the entrance to Little Grassy Lodge.

Airport Ride Board will be available in Little Grassy Lodge, near the check-in window

ΔGibbs₂₅ • Monday Afternoon • September 19, 2011

Biothermodynamics and Disease: Free Energy in the Clinic

Moderator: **Mani Vunnam, Pedigo Laboratory, University of Mississippi**

3:00 – 3:15 pm **Jack Correia, University of Mississippi Medical Center**
Introduction to the Field

3:15 – 3:45 pm **David Bain, University of Colorado Health Sciences Center**
Toward a Quantitative Understanding of the Human Steroid Receptors:
The Role of Energetics

3:45 – 4:00 pm **Josh Schipper, Clark Laboratory, North Carolina State University**
Allosteric Activation of Procaspase-3 as a Novel Cancer Therapeutic

4:00 – 4:30 pm **Jim Cole, University of Connecticut**
Analysis of macromolecular interactions in drug discovery research

4:30 – 4:45 pm **Break – Refreshments in Indian Lodge**

4:45 – 5:00 pm **Daniel Lyons, Correia Laboratory, University Mississippi Medical Center**
Structural and Hydrodynamic Analysis of a
Novel Drug Delivery Vector: ELP[V5G3A2-150]

5:00 – 5:15 pm **William Hawse, Baker Laboratory, Notre Dame University**
Physical Basis of Antigen Recognition and Signaling by T Cell Receptors

5:15 – 5:45 pm **Enrico Di Cera, St. Louis University**
Allostery in trypsin-like proteases suggests new therapeutic strategies

Panel Leader: **A. Clay Clark, North Carolina State University**

5:45 – 6 pm **Panel Discussion by All Speakers**

6:15 pm **Dinner in Freeberg Hall**

ΔGibbs₂₅ • Monday Evening • September 19, 2011

8 – 10 pm **Poster Session I in Sledgefoot (lower level) & Freeberg (upper level)**
Poster Presenters with last name starting from Machha to Yu
(please remove posters before midnight)

Sponsor Displays in Freeberg (upper level) near Beer, Wine and Soda

ΔGibbs₂₅ • Tuesday Morning • September 20, 2011

Checkout - please leave your room keys at the counter in the lobby of Little Grassy Lodge

Airport Ride Board will be available in Little Grassy Lodge, near the check-in window

7:30 – 8:30 am Breakfast in Freeberg Hall

Thermostability and its Pressure on Evolution of Macromolecules

8:40 am Closing Announcements by Organizers

Moderator: **Catherine Carney, Perez-Alvarado Laboratory, SIUC**

8:45 – 9:00 am Patricia Clark, Notre Dame University
Introduction to the Field

9:00 - 9:30 am Doug Barrick, Johns Hopkins University School of Arts and Sciences
Origins of Cooperativity in Protein Folding

9:30 – 9:45 am Katie Hart, Marqusee Laboratory, University of California - Berkeley
Evolution of the Energy Landscape: Using ancestral protein resurrection to investigate changes in RNase H over evolutionary time

9:45 – 10:00 am Sean Fanning, Horn Laboratory, Northern Illinois University
Structural and Biophysical Investigations of an Engineered Dual-Function Camelid Antibody Reveal the Mechanism of Metalloregulation

10:00 – 10:20 am Break – Refreshments in Indian Lodge

10:20 – 10:50 am Kathleen Hall, Washington University
Thermodynamics of U1A/U2B binding to RNA Stemloops

10:50 – 11:05 am Michal Szymanski, Bujalowski Laboratory, University of Texas Medical Branch
Initiation of Primosome Assembly

11:05 – 11:35 am Terry Oas, Duke University
The role of thermodynamic stability in Staphylococcal protein A function

Panel Leader: **Trevor Creamer, University of Kentucky**

11:35 – 11:50 am Panel Discussion by All Speakers

noon Box lunch available in Freeberg Hall

Checkout Please leave your room keys at the counter in Little Grassy Lodge