



## 16th Annual Gibbs Conference on Biothermodynamics

Touch of Nature Conference Center  
Southern Illinois University  
Carbondale, Illinois  
*Sept 28 - Oct 1, 2002*

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Michael Mossing

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# 16th Annual Gibbs Conference on Biothermodynamics

	Saturday, September 28
4:00 -7:00 pm	Check-in in Indian Room
7:00 -10:00 pm	Reception in Indian Room
	Sunday, September 29
7:30 -8:30 am	BREAKFAST
8:30 -8:40 am <b>Introduction</b>	Gary Ackers
8:40 -9:40 am <b>Keynote</b>	<b>Rodney Biltonen:</b> Lipid-Lipid Interactions and Protein-Lipid Clustering
9:30 -10:00 am	REFRESHMENT BREAK
10:00 -12:00	<b>SESSION I: THERMODYNAMICS OF NUCLEIC ACIDS</b> Moderator: John Richardson
10:00-10:40 am	<b>Luis A. Marky:</b> Folding and Ligand Binding to DNA Oligonucleotides with Single and Double Hairpin Loops
10:40-11:00 am	<b>Anthony Paiva:</b> The Biophysical Basis of Triplet-Repeat DNA Expansion in Genetic Diseases
11:00-11:20 am	<b>Besik Kankia:</b> Inner-sphere Complexes of Mg <sup>2+</sup> with Poly(rA) and Delocalized Binding to Poly(dA)
11:20-12:00 noon	<b>Tom Gluick:</b> Trimethylamine Oxide (TMAO) Counteracts Urea Induced Denaturation of RNA tertiary Structure
12:00-1:00 pm	LUNCH
1:00-3:00 pm	FREE TIME
3:00 - 6:00	<b>SESSION II: MACROMOLECULAR COMPLEXES</b> Moderator: Abigail Doura
3:00-3:40 pm	<b>Adrian Elcock:</b> Atomistic Simulation of Multi-Macromolecular Systems
3:40-4:00 pm	<b>John Satumba:</b> Folding and Assembly of lambda Cro Repressor Dimers is Kinetically Limited by Proline Isomerization
4:00-4:20 pm	<b>Jo Holt:</b> Human Hemoglobin as a Dimer of Dimers
4:20-4:40 pm	REFRESHMENT BREAK
4:40-5:20 pm	<b>Clay Clark:</b> Engineering the Procaspase-3 Dimer Interface
5:20-6:00 pm	<b>Elisar Barbar:</b> Structural Studies of a Highly Conserved Dynein Light Chain and its Role in Dynein Assembly and Cargo Recruitment
6:00-7:00 pm	DINNER
8:00-10:00 pm	<b>POSTER SESSION I</b>

	Monday, September 30
7:30 – 8:30 am	BREAKFAST
8:30 – 12:00	<b>SESSION III: STABILITY OF MACROMOLECULES</b>
	<b>Session III: Stability of Macromolecules</b> Moderator: Brian Chellgren
8:30-9:10 am	<b>Ed Lattman:</b> X-ray and Thermodynamic Studies of SNase Mutants I92E and I92K: Insights Into Polarity of the Protein Interior
9:10-9:50 am	<b>Marty Scholtz:</b> The Role of Electrostatic Interactions in Protein Stability and Folding
9:50-10:20 am	Refreshment Break
10:20-10:40 am	<b>Monica Sundd:</b> Investigation of Electrostatic Interactions on the Surface of Ubiquitin by Double-Mutant Analysis and NMR
10:40-11:00 am	<b>Dmitri Ermolenko:</b> Thermodynamic Consequences of Burial of Polar & Non-Polar Amino Acid Residues in the Protein Interior
11:00-11:20 am	<b>Josephine Ferreon:</b> Role of Conformational Fluctuations on Binding
11:20-12:00 noon	<b>Doug Barrick:</b> Energetics of Folding of a Modular Protein Domain: Origin of Long-range Cooperativity in the Notch Ankyrin Domain
12:00 – 1:00 pm	LUNCH
1:00 – 3:00 pm	FREE TIME
3:00 – 6:00	<b>SESSION IV: FOLDING AND LIGAND BINDING</b>
	Moderator: Travis Waldron
3:00 – 3:40 pm	<b>Michael Brenowitz:</b> Monovalent Cations Mediate Formation of Native Tertiary Structure of the <i>Tetrahymena</i> Ribozyme: Implications for the Kinetics of Folding
3:40 – 4:00 pm	<b>Roberto Galletto:</b> Kinetic Mechanism of Nucleotide Binding to the <i>E.coli</i> DNAC Protein and Allosteric Regulation of the Pre-Equilibrium Conformational Transition of the Protein
4:00 – 4:30 pm	<b>Patricia Clark:</b> Hysteresis in the Folding/Unfolding of a Monomeric Single-Domain Protein
4:30 – 5:00 pm	REFRESHMENT BREAK
5:00 – 5:20 pm	<b>Wendy Van Scyoc:</b> The Molecular Basis for Defective Ion Channel Regulation by Mutants of Calmodulin
5:20 – 6:00 pm	<b>Michael Henzl:</b> Tertiary Interactions in Rat and -Parvalbumins: Preliminary Data
6:00 – 7:00 pm	DINNER
8:00 – 10:00 pm	<b>POSTER SESSION II</b>

	Tuesday, October 1
7:30 – 8:30 am	BREAKFAST
<b>8:30 – 12:00</b>	<b>SESSION V: PROTEIN-NUCLEIC ACID INTERACTIONS</b> Moderator: Patrick Brown
8:30 – 9:10 am	<b>Janette Carey:</b> Allosteric Activation of DNA Binding
9:10 – 9:30 am	<b>Sergei Khrapunov:</b> Structural Peculiarities of the N- and C-domains of <i>Saccharomyces Cerevisiae</i> “TATA Binding Protein” (TBP) upon Interaction with DNA
9:30 - 9:50 am	<b>Kausiki Datta:</b> Temperature Dependence of DNA Binding by <i>Thermus aquaticus</i> and <i>Escherichia coli</i> DNA Polymerases
9:50 – 10:20 am	REFRESHMENT BREAK
10:20 -10:40 am	<b>Nasib Maluf:</b> Self Association Equilibria of <i>E. coli</i> UvrD Helicase Studied by Analytical Ultracentrifugation
10:40 – 11:20 am	<b>Kathleen Hall:</b> A Single Conserved Glycine in U1A RBD1 Modulates Protein Dynamics and RNA Binding Affinity
11:40 – 12:30 pm	LUNCH

## POSTER INFORMATION:

Posters will be presented in one of two evening sessions in Sledgefoot Hall (next to Freeberg Dining Hall). Session I will be held Sunday and Session II will be held Monday.

Session I: First authors whose last names begin A through H. Posters may be mounted starting on Sunday morning.

Session II: First authors whose last names begin I through Z. Posters may be mounted starting on Monday morning.

Posters I: Sunday 8-10 pm in Sledgefoot Hall

The Energetics of Parvalbumin AB and CD-EF Domain Interactions and the Implications on Metal-ion Affinity

*Sayeh Agah and Michael T. Henzl*

NMDA (Glutamate) Receptor Recognition by Calmodulin

*Zeynep Akyol, Johannes Hell, Madeline A. Shea*

Catalysis of Trp – Pro Peptide Bond Isomerization by SlyD and Trigger Factor in Folding Intermediates of the Lambda Cro Repressor

*Ibrahim A. Al-Duraibi\* and Michael C. Mossing.*

Interaction of Fluoroalcohols with the Peptide Backbone

*Matthew Auton and D.W. Bolen*

The “Osmophobic Effect”: Improving the Gibbs Transfer Model

*Matthew Auton and D.W. Bolen*

Evidence for a kinetic trap in the assembly of class I MHC/peptide antigen presenting complexes

*Brian M. Baker and Anne-Kathrin Binz*

Computational evaluation of electrostatics for large biomolecular assemblages

*Nathan A. Baker, David Sept, Simpson Joseph, Michael Holst, J. Andrew McCammon*

Effects of HLA-A2 mutations on peptide binding studied by fluorescence anisotropy

*Anne-Kathrin Binz, William E. Biddison, and Brian M. Baker*

Structure and Stability of the Archaeal Protein Sso10b-2

*Kalpesh Biyani, Mebrahtu Kahsai, Andrew Clark, William Peters, Stephen P. Edmondson, & John W. Shriver*

Characterization of the Active Site Conformation of Procaspase-3

*Kakoli Bose, Brett Feeney, Cristina Pop and A. Clay Clark*

Ligand Binding and Homodimerization of an *E. coli* BirA-bio-5'-AMP Analog Complex

*Patrick H. Brown & Dorothy Beckett*

Rapid and Facile Thermodynamic Analysis of Hemoglobin Intermediates Using Isoelectric Focusing

*E. Sethe Burgie, Jo M. Holt, and Gary K. Ackers*

Computational Design of a Protein Binding Site

*Brian W. Chellgren and Trevor P. Creamer*

Folding of Caspase Recruitment Domains (CARD) of RICK and Procaspase- 1: Members of -Greek Key Fold Protein Family

*Yun-Ru (Ruby) Chen, A. Clay Clark*

Molecular Basis for <sup>15</sup>N Chemical Shifts in Ubiquitin

*Michael S. Chimenti, Nicole Iverson, Monica Sundd, William R. Kearney, and Andrew D. Robertson*

Assessing the Accuracy of Thermodynamic Parameters Obtained from a Global Linkage Model Describing the Folding of Sac7d and Sso7d

*Andrew Clark, Stephen Edmondson, and John Shriver*

Solution Structure and Thermodynamics of a Luteoviral Frameshifting RNA Pseudoknot

*Peter V. Cornish and David P. Giedroc*

Physical Determinants of the Polyproline II Helical Conformation.

*Trevor P. Creamer, Adam L. Rucker, Brian W. Chellgren, Mark Wurth, Margeret N. Campbell and Cara L. Payer.*

A Density Functional Theory Study of Conformers with Distinct Fe-C-O Configuration in the Ferrous CO Complex of Horseradish Peroxidase.

*Sergio D. Dalosto, Ninad V. Prabhu, Jane M. Vanderkooi and Kim A. Sharp*

Species-Specific Domain Interactions Control TBP Self-Association

*Margaret A. Daugherty, Michael G. Fried, Song Tan, Jon Ramsey & Benjamin Chandler*

Comparative Studies Of Different T Cell Receptors That Bind The Same Ligand In A Topologically, Thermodynamically, And Kinetically Similar Manner

*Rebecca L. Davis, Rene C. Rodriguez, and Brian M. Baker*

Thermodynamics of Nucleotide Binding to Glycyl-tRNA Synthetase

*John David Dignam and Jonathan B. Chaires*

Molecular Determinants of pKa Values of Internal Ionizable Groups

*Michael A. Dolan, Dan Isom, and Bertrand Garcia-Moreno*

Empirical Structure-Based Parameterization of the Effect of Mutations on the Free Energy of GpA Transmembrane Dimerization

*Abigail K. Doura, Felix Kobus, Leonid Dubrosky, Ellen Hibbard, Karen G. Fleming*

Is Partial Folding of Human Cyclin T1 Linked to Binding of Tat-TAR from Human Immunodeficiency Virus?

*Stephen P. Edgcomb, Chandreyee Das, and Alan D. Frankel*

Antibody-Assisted Refolding of Horseradish Peroxidase

*Ermolenko D.N., Zherdev A.V., Popov V.O. and Dzantiev B.B.*

Assessing the Role of the Ribosome in Structure Formation During *In Vitro* Tailspike Refolding

*Michael S. Evans, Mary C. Finn & Patricia L. Clark*

A Salt Bridge Affects the Environments of Two Tryptophanyl Residues in Procaspase-3

*Brett Feeney, Kakoli Bose and A. Clay Clark*

Determining the Cooperativity of Hydrogen Exchange and Unfolding in Ubiquitin via Mass Spectrometry

*Debra M. Ferraro and Andrew D. Robertson*

Calorimetric Enthalpies of Bacteriorhodopsin Intermediate State Transitions

*Jaime M. Ferreira, George J. Turner, and Richard D. Sheardy*

Thermodynamics of Denaturant-Induced Unfolding of a Protein G B1 Domain Variant Implications on the Limitations of the Linear Extrapolation Method in Assessing the Stability of Proteins that Exhibit Variable Two-State Denaturation



*Allan Chris M. Ferreon and D.W. Bolen*

Towards Standardizing the Free Energy Change of Transmembrane Helix-Helix Interactions

*Karen G. Fleming*

Role of Hydration in the Binding of *lac* Repressor to DNA

*Michael G. Fried , Douglas F. Stickle, Karen V. Smirnakis, Claire Adams, Douglas MacDonald, and Ponzy Lu*

Interactions of the DNA-Alkyl Transferase, AGT

*Michael G. Fried, Anthony Pegg and Joseph J. Rasimas*

Atomic Simulation of Protein Folding/Unfolding Thermodynamics

*Angel E. Garcia*

Design of Triplex Forming Molecules Barry Gold

*Barry Gold, Jian-Sen Li, Yun-Hua Fan, Yi Zhang,*

Cloning, Expression, Purification, and Preliminary Characterization of p75-NTR-Associated Cell Death Executor (NADE) – A Putative Target of Human Calcium Binding Proteins S100P and S100Z

*Alexey V. Gribenko, Jessica Wolgemuth, James E. Hopper, and George I. Makhatadze*

An Ensemble View of the Energetic Differences Between Mesophilic Proteins and Their Thermophilic Analogs

*James B. Hamburger and Vincent J. Hilser*

Proteins modulate proton titration through redistribution of the conformational ensemble.

*Steven T. Whitten, Bertrand García-Moreno E., and Vincent J. Hilser*

Ligand-Linked Stability of the C-domain of Calmodulin

*Kenosha F. Hobson\*, Susan Pedigo, Maurice R. Eftink*

Is  $\bar{\Delta V}$  independent of the means used to unfold the protein?

*Nicole Housley\*, Susan Pedigo, Maurice R. Eftink*

Posters II: Monday 8-10 pm in Sledgefoot Hall

Structural Basis for Noncovalent Interactions at the Surface of Ubiquitin

*Nicole Iverson, S. Ramaswamy, and Andrew D. Robertson*

Equilibrium Dimerization and Subunit Exchange Kinetics of Cro Repressor Variants by Fluorescence Resonance Energy Transfer

*Haifeng Jia, Gene L. Bidwell and Michael C. Mossing*

Hydrodynamic and X-ray Scattering Properties of Type I DNA Polymerases from *Escherichia coli* and *Thermus aquaticus*

*Allison M. Joubert, Angela Byrd, and Vince J. LiCata*

Thermodynamics and Kinetics of the Binding of *E. coli* SSB tetramer to (dT)<sub>70</sub> in its (SSB)<sub>35</sub> Binding Mode

*Alexander G. Kozlov and Timothy M. Lohman*

The Tandem SH2 Domain of the Syk Kinase; A Molecular Device to Measure Inter-phosphotyrosine Distances

*S. Kumaran and G. Waksman*

Thermodynamic Descriptors Deconvolute Codon Library Degeneracy

*Scott A. Larson and Vincent J. Hilser*

An Improved Computational Method for Predicting Ligand-Protein Interactions

*Hao-Yang Liu, Irwin D. Kuntz, and Xiaoqin Zou*

Structural and Thermodynamic Basis for the Interaction of the Src SH2 Domain with the Activated Form of the PDGF  $\alpha$ -Receptor

*Olga Y. Lubman and Gabriel Waksman*

Kinetic mechanism for *E. coli* RecBCD-catalyzed DNA Unwinding Determined from Single Turnover Stopped-flow Fluorescence

*Aaron L. Lucius, Andrew F. Taylor, Gerald R. Smith and Timothy M. Lohman*

Structural Analysis of LCB, a Light Chain Subunit of *Drosophila* Cytoplasmic Dynein

*Moses Makokha and Elisar Barbar*

Application of ThermoFluor, a High-Throughput Method to Measure Protein-Ligand Binding Constants, to Obtain Carbonic Anhydrase Inhibitor Structure-Potency Relationships

*Daumantas Matulis and Matthew Todd*

Multiparticle, Atomic Resolution, Macromolecular Crowding Simulations

*Sean McGuffee and Adrian Elcock*

Domain-Specific Interactions of Calmodulin with Ryanodine Receptor I

*Rhonda A. Newman , Liang-Wen Xiong, Susan L. Hamilton, Madeline A. Shea*

Interactions of LC8 with Domains of the Intermediate Chain of Cytoplasmic Dynein

*Afua Nyarko, Michael Hare and Elisar Barbar*

A Simple Model for Poly-Proline II Structure in Peptide Unfolded States

*Rohit V. Pappu*

Characterization of the Metalloregulatory Transcriptional Repressor S. aureus CzrA

*Mario A. Pennella, Christoph Eicken, James C. Sacchettini, and David P. Giedroc*

What Causes Sac7d to Bend DNA?

*William B. Peters, Stephen P. Edmondson, John W. Shriver*

Mutations in the Interface of Procaspase-3 Affect Dimer Formation and Enzymatic Activity

*Cristina Pop, K. Bose, B. Feeney, A. Tripathy and A. C. Clark*

Molecular Dynamics Simulations Predict a pH Dependant Regulation of Access to the Catalytic center of Horseradish Peroxidase C

*N. V. Prabhu, S. D. Dalosto, J. M. Vanderkooi and K. A. Sharp*

Comparisons of Hyperthermophilic and Mesophilic HPr Proteins

*Ali A. Razvi, Jeremiah D. Magers, and J. Martin Scholtz*

Contribution of Helical Propensity to the Thermodynamic Stability of Proteins

*John M. Richardson, Dmitri N. Ermolenko, Vakhtang Loladze and George Makhatadze,*

Intramolecular Interactions at Protein Surfaces and Their Impact on Protein Function

*Andrew D. Robertson*

Progress Toward Virtual Screening for Drug Side Effects

*Bill Rockey and Adrian Elcock*

Activity coefficients can be described by a small number of parameters

*Jörg Rösger & David Wayne Bolen*

Osmolyte and Prolyl Isomerization Effects on the Two-State Folding Kinetics of FKBP12

*Andrew T. Russo, Jörg Rösger and D.W. Bolen*

Analysis of the contribution of van der Waals and electrostatic forces on the change in free energy of RNase Sa variants.

*David Schell, Jerry Tsai, C Nick Pace, J Martin Scholtz.*

Salt effects on the stability of adipocyte lipid binding protein

*Allyn J. Schoeffler, Allison M. Joubert, Lauren Solhjo, Xuemei Yang, and Vince J. LiCata*

Explicit Counterions in Biomolecular Simulations

*David Sept*

Angular structuring of water explains the hydrophobic effect

*Kim A. Sharp and Kelly Gallagher*

Thermodynamic Contributions For The Incorporation Of Cationic 3-Aminopropyl Chains Into DNA

*Ronald A. Shikiya, Jian-Sen Li, Barry Gold, and Luis A. Marky*

Linking Thermodynamic Linkage and Correlated Motion in U1A RBD1

*Scott A. Showalter & Kathleen B. Hall*

Native-State Hydrogen Exchange in Ubiquitin

*Navdeep Sidhu and Andrew D. Robertson*

Abundance and Distributions of Protein Simple Sequences

*Kim Lan. Sim and Trevor P. Creamer*

Stathmin Competes with Vinca Alkaloid-Induced Tubulin Spiral Formation  
*C. A. Sontag, W. F. Stafford, S. Lobert, J. J. Correia*

Exposing the Role of the Domain Boundary in Allosteric Regulation of Calmodulin  
*Brenda R. Sorensen, Laurel A. Faga and Madeline A. Shea*

Coupled denaturation and dimer dissociation reactions of the lambda Cro repressor analyzed over a thousand-fold range in protein concentration  
*Rhonda L. Stennis\* and Michael C. Mossing.*

Improving the *Lac* Repressor: Mutations that Increase DNA Binding and Inducibility in a Commercially Utilized Transcription Repressor  
*Liskin Swint-Kruse, Hongli Zhan, Bonnie Fairbanks, Jan Kemnade, Atul Maheshwari, and Kathleen Shive Matthews.*

Calcium-Dependent Binding of Calmodulin to the Voltage-Dependent Sodium Channel  
*Nathaniel Theoharis and Madeline A. Shea*

Hydrogen Bond Contributions to the Conformational Stability of Ribonuclease T1  
*Richard L. Thurlkill, Geoffrey Horn and C. Nick Pace*

Insertion and Duplication in a Modular Protein: Stability Enhancements, Cooperativity, and Evolutionary Implications in the *Drosophila* Notch Ankyrin Domain  
*Katherine Tripp and Doug Barrick*

Stabilization of Proteins by Ligand Binding: Cautions for Drug Screening  
*Travis T. Waldron and Kenneth P. Murphy*

Stabilization of the Coiled-Coil Region of Swallow, a Double Stranded RNA Binding Protein by Dynein Light Chain LC8  
*Lei Wang, Mike Hare, and Elisar Barbar*

Determination of the koff for the doubly-ligated hemoglobin intermediate Species 21 supports the Symmetry Rule Model  
*Connie Yarian, Jo M. Holt and Gary K. Ackers*

Identifying the Rate-Limiting Steps in Biopolymer Folding  
*Wenbing Zhang and Shi-Jie Chen*