

# 13<sup>th</sup> Annual Gibbs Conference on Biothermodynamics

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Southern Illinois University  
Carbondale, Illinois

October 2 - 5, 1999

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# 13th Annual Gibbs Conference on Biothermodynamics

**Saturday, October 2**

4:00 - 7:00 Registration

7:00 - 10:00 Reception

## POSTER INFORMATION

Posters will be presented in one of two sessions, I and II, to be held on Sunday and Monday evenings, respectively, in Sledgefoot Hall (next to Freeberg, the dining hall). Posters for Session I (first authors Alston - Klinger) may be mounted starting on Sunday morning and posters for Session II (first authors Kozlov - Yu) may be mounted starting Monday morning.

**Sunday, October 3**

7:00 - 8:30 Breakfast

## KEYNOTE ADDRESS I

8:30 - 9:30 **Wayne Bolen** (U. Texas Medical Branch)

*The osmophobic effect: A fundamental force in protein folding*

9:30 - 10:00 Refreshments

## SESSION I: SOLVENT EFFECTS

Moderator: Brian Baker

10:00 - 10:35 **V. Adrian Parsegian** (NIH)

*Stabilization of macromolecules by controlled osmotic stress*

10:35 - 10:55 **Elizabeth Courtenay** (U. Wisconsin-Madison)

*Vapor pressure osmometry studies of osmolyte-protein interactions:*

*Implications for the action of osmoprotectants in vivo and for the interpretation of osmotic stress experiments in vitro*

- 10:55 - 11:30 **Kim Collins** (U. Maryland)  
*Ion-Protein interactions*
- 11:30 - 11:50 **Qin Zou** (U. Iowa)  
*Thermodynamics of the cosolvent effects of TMAO on protein functional groups:  
Model compound studies*
- 12:00 - 1:00 **Lunch**

## SESSION II: NUCLEIC ACIDS

Moderator: Sarae Bausch

- 3:00 - 3:35 **Anna Marie Pyle** (Columbia U.)  
*Antagonistic binding of a ribozyme substrate and thermodynamic control of  
cleavage site selection*
- 3:35 - 3:55 **Corie Ralston** (Albert Einstein)  
*Probing the energetics of the individual tertiary contacts that stabilize the  
Tetrahymena thermophila group I intron*
- 4:00 - 4:25 **Refreshments**
- 4:25 - 5:00 **Loren Williams** (Georgia Tech)  
*Nucleic acid structure: Cations in control?*
- 5:00 - 5:20 **Ioulia Rouzina** (U. Minnesota)  
*Heat capacity effects in DNA melting and the possibility of DNA cold  
denaturation*
- 5:20 - 5:55 **David Giedroc** (Texas A & M)  
*Thermodynamics of folding of translational regulatory RNA pseudoknots*
- 6:30 **Dinner**
- 8:00 - 10:00 **POSTER SESSION I**

**Monday, October 4**

- 7:00 - 8:30 **Breakfast**

## KEYNOTE ADDRESS II

- 8:30 - 9:30 **Gary K. Ackers** (Washington U.)  
*Is there a molecular code for hemoglobin cooperativity?*
- 9:30 - 10:00 **Refreshments**

### SESSION III: COOPERATIVITY & ALLOSTERY

Moderator: Kelly Ghallager

- 10:00 - 10:35 **Ernesto Freire** (Johns Hopkins)  
*From structure to function through energetics*
- 10:35 - 10:55 **Lynell Martinez** (U. Miami)  
*Thermodynamic analysis of conformational changes in bacteriorhodopsin*
- 10:55 - 11:30 **J. Ching Lee** (U. Texas Medical Branch)  
*Diversity and specificity in DNA recognition by E. Coli cAMP receptor protein*
- 11:30 - 11:50 **Margaret Daugherty** (Pennsylvania State U. College of Medicine)  
*Solution-composition dependence of eukaryotic species dependence of TBP self assembly*
- 12:00 - 1:00 Lunch

### SESSION IV: PROTEINS

Moderator: Kelly Lee

- 2:30 - 3:05 **Susan Marqusee** (U. California-Berkeley)  
*An experimental tour of the energy landscape*
- 3:05 - 3:25 **Kevin Shaw** (Texas A & M)  
*Reversing the net charge of RNase Sa: The role of general electrostatics in protein conformational stability*
- 3:25 - 3:45 Refreshments
- 3:45 - 4:20 **Mario Amzel** (Johns Hopkins)  
*Calculation of entropy changes in biological processes: Folding, binding and oligomerization*
- 4:20 - 4:40 **Chris Sontag** (U. Mississippi)  
*The interaction of dimeric kinesin K420 with tubulin heterodimers by analytical ultracentrifugation*
- 4:40 - 5:15 **Josh Wand** (U. Pennsylvania)  
*Stability, dynamics and divisibility of a metastable protein: Apocytochrome b562*
- 5:15 - 5:30 Refreshments
- 5:30 - 6:30 **Ernesto Freire (organizer & moderator), Gary Ackers, Maurice Eftink, Susan Marqusee and Bruce Tidor**  
*Round table discussion: Thermodynamics in the post-genomic era*
- 6:30 Dinner
- 8:00 - 10:00 **POSTER SESSION II**

**Tuesday, October 5**

7:00 - 8:30 Breakfast

**SESSION V: BINDING, LINKAGE & RECOGNITION**

Moderator: William Forsyth

8:30 - 9:05 **Charles Spink** (SUNY Cortland)

*Direct measurement of the release of sodium ions from DNA upon the binding of cationic ligands*

9:05 - 9:25 **Vinod Misra** (Johns Hopkins)

*Magnesium binding to nucleic acids: The nonlinear Poisson-Boltzmann model*

9:30 - 9:50 Refreshments

9:50 - 10:10 **Michael Bradshaw** (Washington U.)

*Mutational investigation of Src SH2 domain recognition*

10:10 - 10:30 **Besik Kankia** (U. Nebraska)

*Thermodynamic investigation of the hydration effects accompanying the binding of  $Mg^{2+}$  to nucleic acids*

10:30 - 11:05 **Bruce Tidor** (MIT)

*Solvation effects on protein folding, binding, and design: Exploring the electrostatic balance*

11:30 - 12:30 Lunch

12:30 Check-out and departure

## POSTER SESSION I

*Sunday October 3, 1999*

*8-10 pm*

*Sledgefoot Hall*

### **Characterization of Four Single-Site Tryptophan Variants of Ribonuclease Sa**

*Roy W. Alston and C. Nick Pace*

### **Hemoglobin Hydration in the Presence and Absence of Osmolites**

*Daniele Arosio, Herman E. Kwansa, Grzegorz Piszczek, and Enrico Bucci*

### **Correlated Motions in Native Proteins from MS Analysis of NH Exchange Between the EX2 and EX1 Kinetic Limits**

*Cammon B. Arrington and Andrew D. Robertson*

### **Cavities and Water in T-cell Receptor Specificity**

*Brian M. Baker, Yuan-Hua Ding, William E. Biddison, and Don C. Wiley*

### **Insights into the Initiation and Process of Protein Folding from NMR Relaxation Measurements**

*Elisar Barbar, Brian Kleinman and Moses Makokha*

### **Strong Energetic Coupling Between the Proximal Protein Matrix and Distal Ligand Binding in Myoglobin**

*Doug Barrick*

### **Functional Analyses of AmpC $\beta$ -lactamase by Differential Stability**

*Beth M. Beadle, Susan L. McGovern, Alexandra Patera, and Brian K. Shoichet*

### **A Disordered Loop that Functions in Ligand Binding and Allostery**

*Dorothy Beckett and Kee Hwan Kwon*

### **Reversible Thermal Denaturation of Human FGF-1 Induced by Low Concentrations of Guanidine HCl**

*Sachiko I. Blaber, Juan F. Culajay, Archana Khurana and Michael Blaber*

### **Binding of a Cationic Graft Copolymer to Poly[d(AT)]•poly[d(AT)]**

*Tatiana K. Bronich, Alexander V. Kabanov and Luis A. Marky*

### **Recognition of DNA Topology in Reactions Between Plasmid DNA and Cationic Copolymers**

*T.K. Bronich, H.-K. Nguyen, A. Eisenberg, and A.V. Kabanov*

### **Evidences of Polymeric Intermediates During the Subsequent Steps of Oxygenation of Hemoglobin**

*Enrico Bucci, Herman E. Kwansa and Daniele Arosio*

**Binding Thermodynamics of the Transition State Analogue Coformycin and of the Ground State Analogue 1-Deazaadenosine to Bovine Adenosine Deaminase**

*Christian Castro and B. Mark Britt*

**RNA Folding Energy Landscapes**

*Shi-Jie Chen and Ken Dill*

**The Role of Hydrophobic Core Packing in Enhancing the Stability of a Hyperthermophile Protein**

*Andrew Clark, Bradford McCrary, Stephen P. Edmondson, and John W. Shriver*

**Quantitative Proteolytic Footprinting Titrations Detect Site Heterogeneity and Map Pathways of Ligand-Linked Conformational Change**

*Laurel A. Coffeen, Olav R. Jaren and Madeline A. Shea*

**Structural Parameterization of the Conformational Entropy of Small Organic Molecules**

*Jose Alejandro D'Aquino, Mario Amzel and Ernesto Freire*

**Comparing the Kinetics of Unfolding and Folding of *Staphylococcal* Nuclease, Its V66W Mutant and V66W' Fragment**

*Numukunda Darboe and Maurice R. Eftink*

**Functional Energetics of the Bacteriophage  $\lambda$  *cro* Repressor**

*Paul J. Darling and Gary K. Ackers*

**Entropic Stabilization of a Protein by an Unstructured Region**

*Stephen P. Edgcomb, Travis T. Waldron, Sandhya Jain, and Kenneth P. Murphy*

**Proton Linkage of Protein-Protein Interactions Associated with the Removal of Histidine Residues from Solvent**

*Stephen P. Edgcomb, William R. Kearney, and Kenneth P. Murphy*

**Domain-Specific Interactions between *Paramecium* Calmodulin Mutants & Melittin**

*Jason-Thomas Eppel and Madeline A. Shea*

**Specificity in Transmembrane Helix-Helix Association Defines a Hierarchy of Stabilities that is Independent of the Hydrophobic Environment**

*Karen G. Fleming and Donald M. Engelman*

**Testing the Role of Basic Groups in Perturbing Carboxyl  $pK_a$  Values of Ovomuroid Third Domain**

*William R. Forsyth, Michael K. Gilson, Jan Antosiewicz, and Andrew D. Robertson*

**Conformational and Functional Relevance of the COO<sup>-</sup> Terminal Residues in Sperm Whale Myoglobin**

*Clara Fronticelli, Cristina Piro, Daniele Arosio, Fred Friedman and William Brinigar*

**Structural Analysis of the Water Hydrogen Bonding Network Around Antifreeze Proteins**

*Kelly Gallagher, Bhupinder Madan, and Kim Sharp*

**Effects of Polyethylene Glycols on RNA Secondary and Tertiary Structure**

*Thomas C. Gluick and David E. Draper*

**A Versatile, Statistical Mechanics-Based, Two-State Analysis of DSC Data Implemented on the Windows Platform**

*Sasha Grek, John Davis and Michael Blaber*

**Oligomerization and Divalent Cation Binding Properties of the S100P Protein: a Ca<sup>2+</sup>/Mg<sup>2+</sup> Switch Model**

*Alexey V. Gribenko and George I. Makhatadze*

**The Role of Electrostatics in SH2 Domain / Phosphopeptide Recognition Probed by the Salt Dependence of Equilibrium and Kinetics**

*Richard A. Grucza, J. Michael Bradshaw, Vesselin Mitakov and Gabriel Waksman*

**Characterizing the Structure-Function Relationship of Cyanovirin, a Potent Anti-HIV Protein**

*Paul Grulich, Toshiyuki Mori, Michael Boyd, John Erickson and Dong Xie*

**Monovalent Cation-Binding Properties of the Mammalian  $\alpha$ - and  $\beta$ -Parvalbumins**

*Michael T. Henzl and Sayeh Agah*

**Molecular Basis for Activation of FGF Signaling by Heparin**

*Andrew B. Herr, Jingson Xu, Irina A. Libova, David M. Ornitz and Gabriel Waksman*

**Thermodynamic and Folding Kinetic Comparisons Between Thermophilic and Mesophilic RNases H**

*Julie Hollien and Susan Marqusee*

**Analysis of Structure-Energetic Correlations for the Prediction of Protein-Protein Binding Energetics**

*James R. Horn and Kenneth P. Murphy*

**Protein Conformational Stabilities can be Determined from Hydrogen Exchange Rates**

*Beatrice M.P. Huyghues-Despointes, Ulrike Langhorst, Jan Steyaert, J. Martin Scholtz, and C. Nick Pace*

**Anticooperative Interdomain Interactions Are Necessary for Calmodulin-Dependent Sodium Channel Activation *In Vivo***

*Olav Jaren and Madeline A. Shea*

**Experimental Measurement and Structural Interpretation of the Apparent Dielectric Constant in the Interior of Staphylococcal Nuclease**

*Daniel Karp, Kelly Lee, Carolyn Fitch, Apostolos Gittis, Eaton Lattman, Wesley Stites, and Bertrand García-Moreno*

**Calculation of Binding Curves for Hemoglobin Constrained in "T": Do Existing Measurements Disprove the Symmetry Rule?**

*Alexandra L. Klinger, Jo M. Holt, and Gary K. Ackers*

**Non-Cooperative Pathways in the Hemoglobin O<sub>2</sub> Binding Cascade**

*Alexandra L. Klinger, Jo M. Holt, and Gary K. Ackers*

## POSTER SESSION II

Monday October 4, 1999

8-10 pm

Sledgefoot Hall

### **Coupling of Protonation to *E. coli* SSB-ssDNA Binding and Its Contribution to Observed Enthalpy and Heat Capacity Changes**

*Alexander G. Kozlov and Timothy M. Lohman*

### **Structural Investigations of Calmodulin:myr4 Interactions**

*James K. Kranz and A. Joshua Wand*

### **Enthalpy-Entropy Compensation in a Calmodulin•Peptide Complex**

*Andrew L. Lee, Sandra A. Kinnear, and A. Joshua Wand*

### **Thermodynamics of Microtubule Inhibition Applied to Combination Chemotherapy with Antimitotic Agents**

*Sharon Lobert, Jeff Ingram, Jeremy Ferris and John J. Correia*

### **Solvent Exposed Amino Acid Residues and Protein Stability**

*Vakhtang V. Loladze and George I. Makhatadze*

### **Interactions of the Major Cold Shock Protein of *Bacillus subtilis* CspB with Single Stranded DNA Templates of Different Base Composition**

*Marimar Lopez and George I. Makhatadze*

### **Structure-Based Thermodynamic Analysis of Binding Sites in Proteins**

*Irene Luque and Ernesto Freire*

### **The Heat Capacity of Hydration of Nucleic Acid Bases and the Ribose Molecule Using Random Network Model Calculations**

*Bhupinder Madan and Kim Sharp*

### **Equilibrium Unfolding of Lambda Cro (F58W) Repressor and the Effect of Added Salts**

*Haripada Maity, Michael C. Mossing and Maurice R. Eftink*

### **A Quantitative Study of the Effect of a Base Substitution in the -10 Region of Promoter DNA on Binding *E. coli* RNA Polymerase Holoenzyme (RNAP)**

*Dennis L. Matlock and Tomasz Heyduk*

### **Thermodynamics of Cobalt (III) Hexamine and Spermidine Binding to DNA, and DNA Condensation by Isothermal Titration Calorimetry**

*Daumantas Matulis, Ioulia Rouzina and Victor A. Bloomfield*

### **Dissecting the Pathway of Affinity Maturation of a Femtomolar Anti-Fluorescein Single Chain Antibody Fragment**

*Katarina S. Midelfort, Eric T. Boder, and K. Diane Wittrup*

**Sedimentation Equilibrium Analysis of the  $\gamma A/\gamma'$  Fibrinogen-Factor XIII Complex**

*Maia Moaddel, David H. Farrell, and Michael G. Fried*

**Membrane-Confined Electrophoresis in an Ionic Strength Gradient**

*Thomas P. Moody*

**Structure-Based Thermodynamic Characterization of Binding Reactions Between Stable Proteins**

*Azin Nezami and Ernesto Freire*

**Detection of Partially Unfolded Forms of the Prion Protein: Implications for Scrapie Formation**

*Eric M. Nicholson and Susan Marqusee*

**Circular Dichroism Studies of Triplet Repeat DNA Oligomers of Sequence (CNG)<sub>x</sub>, Where N = A, C, G or T and x = 4, 10 or 15**

*Anthony M. Paiva and Richard D. Sheardy*

**Two State or not Two State? That is the Question**

*Martin J. Parker and Susan Marqusee*

**Linkage of Sac7d Protein Folding to DNA Binding**

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

**Hydrogen Exchange *m* Values are Larger Than Global in Wild-Type *E. coli* Hpr**

*Ronald W. Peterson and J. Martin Scholtz*

**Thermodynamic and Structural Characterization of the MEARA Sequence Repeat from the Human CstF-64 Polyadenylation Factor**

*John M. Richardson, K. Wyatt McMahon, Clinton C. MacDonald, and George I. Makhatadze*

**Investigating the Contributions of Folding Cores to Thermostability of RNase H**

*Srebrenka Robic and Susan Marqusee*

**Helix Formation in Designed Repeating-Sequence Polypeptides**

*Carol A. Rohl, Yuri Griko and Robert L. Baldwin*

**Folding and Assembly Kinetics of Lambda Cro Dimers**

*John W. Satumba and Michael C. Mossing*

**Entropy-Enthalpy Compensation: Fact or Artifact?**

*Kim Sharp*

**Thermodynamic Contributions of the Inclusion of a dG•dC Base Pair and dG or dC Bulges in the Middle of Four dA•dT Base Pairs of DNA**

*Ronald Shikiya and Luis A. Marky*

**Folding and Stability of s SH3 Domain Regulated by an Intramolecular Association**

*Amy L. Siegling, Kristine Brazin, Amy Hamilton Andreotti, and  
Kenneth P. Murphy*

**Physical Effects Resulting From the Incorporation of 5-Aminopropyl-Uridine in a Small DNA Hairpin**

*Ana Maria Soto, Prasad Dande, Barry Gold and Luis A. Marky*

**Functional Cooperativity in the Src Tyrosine Kinase**

*Jonathon Stillman and Ernesto Freire*

**Thermodynamic Criteria for Discovering Binding Sites in Co-Regulated Promoters**

*Gary D. Stormo*

**Unfolding Thermodynamics of Free and Coformycin-Complexed Bovine Adenosine Deaminase from Physiological Conditions**

*Esther A. Strohmeyer, Janel R. Beckley and B. Mark Britt*

**A Novel Ubx Interacting Protein**

*Xin-Xing Tan, Sarah E. Bondos, and Kathleen S. Matthews*

**Calcium Binding to Low Affinity Sites I and II of Mutant *Paramecium* Calmodulin Studied by Phenylalanine Fluorescence and NMR**

*Wendy Van Scyoc and Madeline A. Shea*

**HIV-1 Protease Inhibitors: Enthalpic versus Entropic Optimization of the Binding Affinity**

*A. Velázquez-Campoy, M. Todd and E. Freire*

**Influence of Substituent Modification on the Energetics of Ligand-DNA Interactions**

*Luminita M. Velea and David E. Graves*

**Non-Additive Effects of Osmolytes on Protein Stability**

*J. P. Villa, M. A. Daugherty, and M. G. Fried*

**Influence of DNA Sequence on the Energetics of Actinomycin D-DNA Interactions**

*Yujin Wang and David E. Graves*

**The Protein Binding Behavior of Staphylococcal Nuclease Measured by H-NMR and by Potentiometric Methods is Strikingly Different from the Behavior Reflected in the pH Dependence of Stability Measured by Thermal and Chemical Denaturation**

*Steven Whitten, Carolyn A. Fitch, and Bertrand García-Moreno*

**The Measure of Interior Disorder in a Folded Protein and Its Contribution to Stability**

*Y. Bruce Yu, Pierre Lavigne, Peter Privalov, and Robert S. Hodges*