

*11th Annual Gibbs Conference on Biothermodynamics*  
**SCHEDULE**

**Saturday, October 4**

4:00 pm Registration in Little Grassy Lodge

7:00 - 10:00 Beer, Wine & Sandwich Reception

**POSTER INFORMATION:**

Posters for **Poster Session I** (A through Jana, by last name of the first author) may be mounted in Sledgefoot Lodge or Freeberg Hall any time **Sunday (October 5)**. Posters for **Poster Session II** (Kankia - Z) may be mounted any time **Monday (October 6)**. Please remember that poster space is very limited, so mount your poster to conserve as much space as possible.

**Sunday, October 5**

7:00 Breakfast, *Freeberg Hall*

8:30 **Keynote Address**  
**Adrian Parsegian**  
*Collapse of a Single Protein Cavity Under Osmotic Stress: Thermodynamics in a VERY Small System.*

9:30 Refreshments

**SESSION I: Systems Coupled to Nucleotide Hydrolysis**

**Moderator: Cam Arrington**

10:00 **Robley Williams, Jr.**  
*Microtubules: Equilibria and Dynamics in the Presence of GTP.*

10:20 **Susan Pedigo**  
*Variability in Growth Rates of Microtubules is Independent of Growth Rate.*

10:50 **Tim Lohman**  
*Helicase-Catalyzed DNA Unwinding.*

11:30 **Wlodzimierz Bujalowski**  
*Thermodynamics and Structure of the E. Coli Primary Replicative Helicase DnaB Protein - DNA Complexes.*

12:30 - 1:30 Lunch, *Freeberg Hall*

**SESSION II: Protein Folding**

**Moderator: Laura Ann Sealy**

2:30 **Andy Robertson**  
*Microsecond Protein Folding Kinetics from Native-State Hydrogen Exchange.*

3:05 **Kelly Frye**  
*The Role of Cavities in the Pressure Denaturation of Staphylococcal Nuclease.*

3:35 **Iliia Baskakov**  
*How to Fold a Thermodynamically Unstable Protein.*

4:05 Refreshments

4:30 **Shi-Jie Chen**  
*Predicting the Conformational Changes of Biomolecules - a Graphic Theoretic Approach.*

5:00 **Clay Clark**  
*The Presence of Non-native Conformations in the "Native" Protein Allows the Binding of E. Coli and Murine Dihydrofolate Reductases to the Chaperonin GroEL.*

6:30 Dinner, **Buffalo Tro at Freeberg Hall**

8:00 - 10:00 **POSTERS & BEER I**

7:00 Breakfast, *Freeberg Hall*

**SESSION III: Nucleic Acids**

*Moderator: Harry Guttman*

8:30 **Brad Chaires**  
*Energetics of Drug-DNA Interactions.*

9:05 **Tina Davis**  
*UV Fails to Detect a DNA Hairpin to Coil Transition.*

9:35 Refreshments

10:00 **T. J. Wilson**  
*Characterization of Macromolecular Charge in Solution by Membrane-Confined Analytical Electrophoresis.*

10:30 **Lori McFail-Isom**  
*Change in DNA Binding Mode of Ethidium Homodimer Detected using Scanning Force Microscopy and Fluorescence Measurements.*

11:00 **Dick Sheardy**  
Assessing the Sequence Specificity in the Binding of Co(III) to DNA via a Thermodynamic Approach.

(Meeting of previous organizers after Session III & before lunch)

12:00-1:00 Lunch, *Freeberg Hall*

**SESSION IV: Binding & Linkage**

*Moderator: Alexandra Klinger*

2:30 **Madeline Shea**  
*Calmodulin Cooperativity: The Pluses and Minuses.*

3:05 **Bradford S. McCrary**  
Linkage of Protonation and Anion Binding to the Folding of Sac7d.

3:35 **Doug Barrick**  
*The Binding of Structural Isomers to Myoglobin: Structural and Energetic Consequences of Hydrogen Bond Deletion and Evolutionary Implications.*

4:05 Refreshments

4:30 **Yingwen Huang**  
*The Oxygen-Binding Intermediates of Human Hemoglobin: Evaluation of Their Contribution to Cooperativity Using Zinc-Containing Hybrids.*

5:00 **Jennifer Jewett VanAntwerp**  
Thermodynamic Characterization of Affinity Maturation: The D1.3 Antibody and a Higher Affinity Mutant.

5:30 **Kip Murphy**  
*Prediction of Structural Changes from Thermodynamic Measurements: Uses and Pitfalls.*

6:30 Dinner, *Freeberg Hall*

8:00-10:00 **POSTERS & BEER II**

**Tuesday, October 7**

7:00 Breakfast, *Freeberg Hall*

8:00 - 12:30 Check-out. Return all keys to main office by 12:30.

**SESSION IV: Protein-Nucleic Acid (Macromolecular) Interactions.**

*Moderator: Vince Hilser*

8:30 **Michael Fried**  
*Role of Water in CAP-DNA Interactions.*

9:05 **James K. Kranz**  
*Investigating Local Cooperativity in RNA-Protein Association.*

9:35 Refreshments

10:00 **Karen G. Fleming**  
The Effect of Point Mutations on the Free Energy of Glycophorin A  
Transmembrane  $\alpha$ -Helix Dimerization

10:30 **Vince LiCata**  
*Variability of the Structural Magnitude of the Allosteric Conformational Change  
of Aspartate Transcarbamylase.*

11:00 **Kim Sharp**  
*The Hydrophobic Effect. Water Structure, and Heat Capacity Changes.*

12:00 - 1:00 Lunch, *Freeberg Hall*

***Please be sure to check-out before 12:30. Drop keys off at the main office between 8:00 am and 12:30 pm.***

# POSTER SESSION I

*Sunday, October 5*

*8-10 pm*

**Sledgefood Hall**

## **Effect of Non-Uniform Base Sequence on the Electrostatic Potential of Dissolved DNA**

*Scott V. Adams, Katrina Wagner, Thomas W. Kephart, and Glenn Edwards*

## **Kinetic Measurement of the Step Size of DNA Unwinding by *Escherichia coli* UvrD Helicase**

*Janid A. Ali and Timothy M. Lohman*

## **Microsecond Protein Folding Kinetics from Native-State Hydrogen Exchange**

*Cammon B. Arrington and Andrew D. Robertson*

## **Interaction of Thrombin with Its Receptor 1**

*Youhna M. Ayala and Enrico Di Cera*

## **Molecular Origin of Na<sup>+</sup> Specificity in Thrombin**

*Dolly Banerjee and Enrico Di Cera*

## **Nature's strategy for stabilizing proteins: the denatured state as a target of solutes**

*Ilya Baskakov and Wayne Bolen*

## **Affinity Maturation of an Anti-Hapten scFv by Yeast Surface Display**

*Eric T. Border and K. Dane Wittrup*

## **Specificity of Src SH2 domain - tyrosyl phosphopeptide interactions: thermodynamic and structural studies.**

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

## **Stability Curves of Bovine Adenosine Deaminase as Function of Reaction Coordinate**

*Billy Mark Britt*

## **The Response of the trp-Repressor-DNA Binding Interaction to solvent stress**

*Martha P. Brown and Catherine A. Royer*

## **Interactions of L11 Binding Region within 23S Ribosomal RNA with Ions**

*Y. V. Bukhman and D. E. Draper*

## **Analysis of Protein-DNA Interactions in Crowded Solutions by Fluorescence Recovery After Photobleaching and Dynamic Light Scattering.**

*Nathan A. Busch and Victor A. Bloomfield*

## **Role of the P2 site in substrate recognition by thrombin**

*Wei Cheng and Enrico Di Cera*

## **Human Ileal Lipid-Binding Protein Binds Two Bile Salts with Apparent Positive Cooperativity**

*D. P. Cistola, T. C. Lee, E. Westover, J. Monsey, P. Dawson and J. J. Toner*

**Phage *cro* Repressor-DNA Interactions**

*Paul J. Darling and Gary K. Ackers*

**Analytical Ultracentrifugation Studies on the Self-Association of Yeast TBP**

*Margaret A. Daugherty, Michael Brenowitz and Michael G. Fried*

**Engineered Variants of I-FABP with Increased Affinity for Bile Salts**

*G. T. DeKoster, K. Richter, K. R. Miller, J. J. Toner, D. P. Cistola*

**Protein Unfolding Pathway for Pressure Denatured APOTRP-Repressor(TR-WT)**

*Gayatri V. Desai and Catherine A. Royer*

**Role of Cl<sup>-</sup> in fibrin polymerization**

*Enrico Di Stasio and Enrico Di Cera*

**Low pH Proton Linkage of OMTKY3 Binding to Porcine Pancreatic Elastase**

*Stephen P. Edgcomb, Brian M. Baker and Kenneth P. Murphy*

**Disassembly of Microtubules with IR Lasers**

*Daniel Eng, Glenn Edwards and Robley Williams*

**Protons and Salts Regulate Conformational Transitions in an Icosahedral RNA Virus**

*Carolyn Fitch, David Hacker, Abelardo Silva, Bertrand Garcia-Moreno*

**Experimentally Testing Computational Models for Ionization Equilibria in Turkey Ovomuroid Third Domain**

*William R. Forsyth, Michael K. Gilson, Jane Anotosiewicz, Olav R. Jaren and Andrew D. Robertson*

**Electrostatic and Structural Contributions to Heat Capacities of Binding and Solvation.**

*Kelly Gallagher and Kim Sharp*

**Effects of Ions on Pseudoknot Energetics.**

*T. C. Gluick, N. Wills, R. Gesteland and D. E. Draper*

**Influence of Chemical Substituents of Drug-DNA Binding Energies**

*David Graves*

**Salt Dependence of TRP Repressor-Operator Interactions**

*Adeola O. Grillo, Martha P. Brown and Catherine A. Royer*

**Evidence for a Conformational Change in the Tandem SH2 Domain of the Syk Tyrosine Kinase: Linkage to Temperature and Ligand Binding.**

*Richard A. Grucza, Klaus Fhtterer and Gabriel Waksman*

**The structures of thrombin W60dS and D221A/D222K reveal the important role of the R187:D222 ion pair in NA<sup>+</sup> binding to thrombin.**

*E. R. Guinto, E. Zhang, A. Tulinsky, M. M. Krem, and E. Di Cera*

**The Physical Biochemistry of Osmotic Adaptation in *E. coli* K-12: Assessing the Free Concentrations of Ions in the Cytoplasm**

*Harry J. Guttman, Li Man, and M. Thomas Record, Jr.*

**Biophysical Studies on the Interaction of Fibroblast Growth Factor-2 with Heparan Sulfate**

*Andrew B. Herr, Jingsong Xu, David M. Oznitz, and Gabriel Waksman*

**Refolding of 6-<sup>19</sup>F-Tryptophan Labeled *E. coli* Dihydrofolate Reductase in the Presence of Ligand: a Stopped-Flow NMR Spectroscopy Study**

*S. D. Hoeltzli and C. Frieden*

**Evaluation of the Relationship between Different Structural Environments to Binding Energetics**

*James R. Horn and Kenneth P. Murphy*

**Preferential Interaction of Calf Thymus DNA with Sugars, Polyols and Amino Acids**

*Xiaoqun Huang and Victor A. Bloomfield*

**Global Analysis of the Temperature and Urea Induced Unfolding of Staphylococcal Nuclease**

*Roxana Ionescu and Maurice R. Eftink*

**Uncoupling DNA binding from dimerization in lambda Cro**

*Rinka Jana, Jeffery Fields and Mike Mossing*

## POSTER SESSION II

Monday, October 6

8-10 pm

Sledgefood Hall

**Hydration Changes Accompanying the Ni<sup>2+</sup>-Induced B-Z Transition of Poly{d(GC)} Poly{d(GC)}: Ultrasonic Velocity and Density Measurements.**

*Besik I. Kankia and Thomas M. Jovin*

**The Contributions to Cooperativity by Singly and Doubly Oxygenated Hemoglobin Intermediates**

*Alexandra L. Klinger and Gary K. Ackers*

**Minimum Substrate Requirements in *E. Coli* Biotin Ligase-Catalyzed Biotinylation**

*Elena Kovaleva, Peter Schatz and Dorothy Beckett*

**Anion and Cation Effects on the Thermodynamics of *E. coli* SSB protein-oligo(dT) Binding Studied by Isothermal Titration Calorimetry**

*Alexander G. Kozlov and Timothy M. Lohman*

**Characterization of the interactions between the endothelial cell protein C/activated protein C receptor, protein C, activated protein C and thrombomodulin. Analysis by Ultracentrifugation.**

*Rachel R. Kroe, Lisa M. Regan and Thomas M. Laue*

**Changes in the Electrostatic Potential Surface and the Solvent Accessible Surface in Adipocyte Lipid Binding Protein Upon Lipid Binding. Comparison with Intestinal Fatty Acid Binding Protein.**

*Vince J. Licata and David A. Bernlohr*

**Thermodynamics of Vinca Alkaloid-Induced Tubulin Self-Association: An Energetic Structure-Function Study.**

*Sharon Lobert, Bridget T. Hill and John J. Correia*

**Contribution of Surface Residues to the Stability and RNA Binding Properties of Two RBDs of the Human U1A Protein**

*Jirong Lu and Kathleen Hall*

**Urea Induced Unfolding of Tubulin**

*Vivek Malipatil, Susan Pedigo and Robley C. Williams, Jr.*

**Hydration of dA dT Base Pairs of B-DNA: Enthalpy-Entropy Correlation with Differential Hydration and Average Compression of Electrostricted Water**

*Luis A. Marky and Donald W. Kupke*

**Resolving the linkage of Protonation and Anion Binding to the Folding of the Native Hyperthermophile Protein Sac7d**

*Bradford S. McCrary, Jennifer Bedell, Stephen P. Edmondson and John W. Shriver*



**Thermodynamic Studies of the *Lac* Operator:*Lac* Repressor Complex; Effects of DNA length and Small Solutes**

*Sonya E. Melcher, Oleg V. Txodikov, Ruth M. Saecker and M. Thomas Record, Jr.*

**Thermodynamic Study of Higher Affinity Binding Single Chain Fv Antibody Fragments Isolated by Molecular Evolution**

*Katarina S. Midelfort, James D. Marks and K. Dane Wittrup*

**Thermodynamic and Kinetic Analysis of the binding of the TATA Binding Protein (TBP) to the *adenovirus* major late promoter and single base mutants**

*A.K.M.M.(Shopon)Mollah, Brad Gilden, Elizabeth Jamison, Victoria Petri, Georgia Patikoglou, Stephen K. Burly, and Michael Brenowitz*

**Structure and Interactions of Homeodomain Heterodimers: The *Drosophila* Extradenticle and Ultrabithorax Proteins**

*Mike Mossing, Tony Hazbun and Florence Lebreton Stahura*

**Polyelectrolyte Behavior of DNA in Mixed ( $Mg^{2+}$ ,  $Na^+$ ,  $Cl^-$ ) Salt Solutions: Monte Carlo Simulations and Experiment**

*Haihong Ni, Arun Yethiraj, Charles F. Anderson, and M. Thomas Record, Jr.*

**Predictions of the Melting Stability of Short Duplex DNA Oligomers From their Base Pair Sequence**

*Richard Owczarzy, Peter M. Vallone, Frank J. Gallo and Albert S. Benight*

**Modulation of the Association Reaction Between Hemoglobin and Carbon Monoxide by Proton and Chloride**

*M. Perrella, M. Ripamonti and S. Caccia*

**Proline: an inert compatible osmolyte**

*Youzing Qu and Wayne Bolen*

**Nonlinear temperature dependence of  $C_p$ , assoc between an r-protein and cognate RNA.**

*Luis P. Reynaldo and David E. Draper*

**Calculating the energetics of thrombin-substrate interactions**

*Thierry Rose and Enrico Di Cera*

**Purification and Initial Characterization of Single-Site Mutants of the *Escherichia Coli* Biotin Repressor that Hypothetically Define the Protein Monomer-Monomer Interface**

*Shreyesh Ruparelia and Dorothy Beckett*

**Energetics of  $Na^+$  binding to serine protease**

*Michela Sabetta and Enrico Di Cera*

**Use of Capillary Electrophoresis to Study the Unfolding of *Staphylococcal* Nuclease and Its V66W Mutant**

*Laura Ann Sealy and Maurice R. Eftink*

**A Model of Membrane-Confined Free Solution Electrophoresis.**

*Harvey K. Shepard*

**The Melting Behavior of Triplex poly(dT)poly(dA)poly(dT) DNA in the Presence of Osmotic Stressors.**

*Charles Spink and J. B. Chaires*

**Time Difference Sedimentation Velocity Analysis of Rapidly Reversible Interacting Systems: determination of equilibrium constants by non-linear curve fitting procedures.**

*Walter F. Stafford, III*

**The Three-Dimensional Structure of a Helix-Less Variant of Intestinal Fatty Acid-Binding Protein**

*R. A. Steele, D. A. Emmert, J. Kao, M. E. Hodsdon, C. Frieden and D. P. Cistola*

**A Map of the Biotin Repressor-Biotin Operator Interface: Binding of a Winged Helix-Turn-Helix Protein Dimer to a Forty Basepair Site**

*Emily D. Streaker and Dorothy Beckett*

**A Mutational Analysis of BR Containing Asparagine at Amino Acid 85.**

*George J. Turner, Ann Winter-Vann and Lynell Martinez*

**Sequence Dependent Melting Stability and Structure of Flanking DNA Regions Modulate Equilibrium Site-Specific Binding of BamHI Restriction Endonuclease**

*Peter M. Vallone, Peter V. Riccelli, Michael J. Lane and Albert S. Benight*

**Engineering Na<sup>+</sup> binding in serine proteases**

*Alessandro Vindigni and Enrico Di Cera*

**Ising Lattices with Strong Coupling Define General Rules for Cooperativity**

*Luyu Wang and Enrico Di Cera*

**Unfolding of Human Interlekin 1 Induced by Guanidine-HCl and pH**

*Yujin Wang, Roxana Ionescu, Joykrishna Dey and Maurice R. Eftink*

**NMR and Thermodynamic Studies of Duplex-Hairpin Equilibria in RNA**

*D. Jeremy Williams and Kathleen B. Hall*

**Folding of Self-Splicing RNA by Multiple Pathways with non-Native Intermediates.**

*Sarah A. Woodson, Jie Pan and D. Thirumalai*