

**Little Grassy Lake  
Conference Center  
Southern Illinois  
University  
Carbondale, Illinois**

**Organized by**

**Kenneth P. Murphy  
University of Iowa  
College of Medicine**

**and**

**Michael D. Brenowitz  
Albert Einstein  
College of Medicine**

**October 7 -10, 1995**



**Gibbs'95**

**Ninth Annual Gibbs Conference  
on Biothermodynamics**

# Poster Information Saturday, October 7

- ◆ 4:00 pm Registration at Main Desk,  
Little Grassy Lodge
- ◆ 7:00 pm Wine and Cheese Reception

*No dinner will be served.*

Posters for Session I (A - La by last name of the first author) may be set up in the *Sledgefoot Lodge* (adjacent to the dining room, *Freeberg Hall*) Saturday night and Sunday morning.

Posters for Session II (Li - Z by last name of the first author) may be set up in the *Sledgefoot Lodge* (adjacent to the dining room, *Freeberg Hall*) Monday morning.



**October 8  
Sunday**

◆ 7:00 am Breakfast, Freeberg Hall

◆ 8:30 am **Keynote Address I**

Victor Bloomfield

*University of Minnesota*

**DNA Condensation and Intermolecular Forces**

***Session I: Electrostatics***

◆ 9:30 am Refreshments

◆ 9:50 am **Kim Sharp**

*University of Pennsylvania*

**Determination of the Heat Capacities of Polar and Apolar Aqueous Solutions Using the Random Network Model (RNM)**

◆ 10:35 am **Bertrand Garcia-Moreno**

*The Johns Hopkins University*

**Experimental Studies of Electrostatic Interactions in Proteins**

◆ 11:20 am **Katrina Wagner**

*Vanderbilt University*

**Structure in the Electric Potential of DNA**

◆ 11:45 am **M. Thomas Record, Jr.**

*University of Wisconsin, Madison*

**Ion Effects on Interactions of Two Charged Ligands KWK<sub>6</sub>NH<sub>2</sub> (+8) and Eo<sup>70</sup> RNA Polymerase) with DNA**

◆ 12:30 pm Lunch, Freeberg Hall

***Session II: Nucleic Acids***

◆ 3:00 pm **David Draper**

*The Johns Hopkins University*

**Protein, Antibiotic and Ion Binding to a Conserved Ribosomal RNA Fragment**

◆ 3:45 pm **Girija Krishnamurthy**

*Wyeth Ayerst Research*

**Recent Biophysical and Biological Studies on the Mechanism of Action of Calicheamicin**

◆ 4:10 pm Refreshments

◆ 4:30 pm **Vitaly Buckin**

*New York University*

**Hydration Effects Upon Substituting Na<sup>+</sup> for Cs<sup>+</sup> or Mg<sup>2+</sup> in the Ionic Atmosphere of poly (rA)<sub>2</sub>poly (rU) and poly (rA)<sub>2</sub>poly (rU) Helices**

◆ 4:55 pm **Keith Bjornson**

*Washington University School of Medicine*

**Kinetic Mechanism of DNA Binding and DNA-Induced Dimerization of the *Escherichia coli* Rep Helicase**

◆ 5:20 pm **Kathleen Hall**

*Washington University School of Medicine*

**Thermodynamics of the Association of the UIA RNA Binding Domain and RNA Hairpins**

◆ 6:35 pm Dinner, Buffalo Tro at Freeberg Hall

**October 9**  
**Monday**

◆ 7:00 am Breakfast, *Freeberg Hall*

◆ 8:30 am **Keynote Address II**

**Mario Amzel**

*The Johns Hopkins University*

**Binding of Flexible Peptides: Structure and Thermodynamics. Calculation of Entropy Changes**

### ***Session III: Linkage & Allostery***

◆ 9:30 am Refreshments

◆ 9:50 am **Donald Senear**

*The University of California, Irvine*

**Coordinate Gene Regulation in *E. coli*: Competitive and Inducer Controlled Cooperative Interactions between CAP and CytR at the deoP2 Promoter.**

◆ 10:35 am **Michael Doyle**

*Smith-Kline Beechem Pharmaceuticals*

**Inhibition Mechanism of Beta Trypsin by Ecotin**

◆ 11:20 am **Yingwen Huang**

*Washington University School of Medicine*

**Transformation of Cooperative Free Energies ( $^{\dagger}\Delta G_c$ ) between Ligation Systems of Hemoglobin: An Exact Resolution of the Carbon Monoxide Binding System**

◆ 11:45 am **J. Ching Lee**

*Univ. Texas Medical Center, GalvEston*

***The Modus Operandi of E.Coli CRP***

◆ 12:30 pm Lunch, *Freeberg Hall*

### ***Session IV: Proteins***

◆ 3:00 pm **Ernesto Freire**

*The Johns Hopkins University*

**Thermodynamics of Protein Stability and Molecular Recognition**

◆ 3:45 pm **Sydney D. Hoeltzli**

*Washington Univ. School of Medicine*

**Stopped-Flow Spectroscopy: Real-time Unfolding Studies of 6-<sup>19</sup>F-Tryptophan labeled *E. coli* Dihydrofolate Reductase**

◆ 4:10 pm Refreshments

◆ 4:30 pm **Nadine C. Gassner**

*University of Oregon*

**Generic Core Replacement in T4 Lysozyme Preserves Protein Activity, Folding Cooperativity & Shape**

◆ 5:15 pm **Peter L. Privalov**

*The Johns Hopkins University*

**On the Entropy of Protein Folding**

◆ 6:30 pm Dinner, *Freeberg Hall*

**October 10  
Tuesday**

◆ 7:00 am Breakfast, Freeberg Hall

***Session V: Molecular Recognition***

◆ 8:20 am **Ruth Saecker Spolar**  
*University of Wisconsin, Madison*

**Thermodynamic Signatures of Conformational Changes in Protein-Nucleic Acid Interactions**

◆ 9:05 am **Javier Gómez**  
*The Johns Hopkins University*

**Thermodynamic Mapping of the Inhibitor Site of the Aspartic Proteinase Endothiapepsin**

◆ 9:30 am Refreshments

◆ 9:50 am **Patrick S. Stayton**  
*University of Washington*

**Molecular Origins of High-Affinity and Slow Dissociation Kinetics in Protein-Ligand Interactions**

◆ 10:15 am **Patrick Connelly**  
*Groton School*

**Immunosuppressive Drug Design and Inosine Monophosphate Dehydrogenase: A Proposed Solution to a Problem in *Differential Molecular Recognition***

◆ 11:00 am Lunch, Freeberg Hall



# Lectures

## **DNA Condensation and Intermolecular Forces**

*Victor Bloomfield*

## **Determination of the Heat Capacities of Polar and Apolar Aqueous Solutions Using the Random Network Model (RNM)**

*Kim Sharp & Bhupinder Madan*

## **Experimental Characterization of Electrostatic Forces in Proteins**

*Bertrand García-Moreno E.*

## **Structure in the Electric Potential of DNA**

*Katrina Wagner, Thomas Kephart, David Hochberg and Glenn Edwards*

## **Ion Effects on Interactions of Two Charged Ligands (KWK6NH<sub>2</sub>(+8) and E $\sigma$ 70 RNA Polymerase) with DNA**

*M. Thomas Record, Jr.*

## **Protein, Antibiotic and Ion Binding to a Conserved Ribosomal RNA Fragment**

*D.E. Draper, S. Huang & Y. Xing*

## **Recent Biophysical and Biological Studies on the Mechanism of Action of Calicheamicin**

*Girija Krishnamurthy and George A. Ellestad*

## **Hydration Effects Upon Substituting Na<sup>+</sup> for Cs<sup>+</sup> or Mg<sup>2+</sup> in the Ionic Atmosphere of poly (rA) $\cdot$ 2poly (rU) and poly (rA) $\cdot$ poly (rU) Helices**

*Vitaly Buckin & Luis A. Marky*

## **Kinetic Mechanism of DNA Binding and DNA-Induced Dimerization of the *Escherichia coli* Rep Helicase**

*Keith P. Bjornson, Keith J.M. Moore and Timothy M. Lohman*

## **Thermodynamics of the Association of the UIA RNA Binding Domain and RNA Hairpins**

*Kathleen B. Hall*

## **Binding of Flexible Peptides: Structure and Thermodynamics. Calculation of Entropy Changes**

*K.H. Lee, Y. Pan, A. D'Aquino, K. Murphy, D. Xie, E. Freire and M. Amzel*

**Coordinate Gene Regulation in *E. coli*: Competitive and Inducer Controlled Cooperative Interactions between CAP and CytR at the deoP2 Promoter**

*L.T. Perini, L.A. Doherty, E. Werner and D.F. Senear*

**Binding Affinity of B-Trypsin and Ecotin Measured by Differential Scanning Calorimetry**

*Michael L. Doyle, Cherice Lee, Mary McGrath, and Robert Fletterick*

**Transformation of Cooperative Free Energies( $^{\ddagger}\Delta G_c$ ) between Ligation Systems of Hemoglobin: An Exact Resolution of the Carbon Monoxide Binding System**

*Yingwen Huang and Gary K. Ackers*

**The Modus Operandi of *E. coli* CRP**

*J. Ching Lee*

**Thermodynamics of Protein Stability and Molecular Recognition**

*Ernesto Freire*

**Stopped-Flow NMR Spectroscopy: Real-time Unfolding Studies of 6-19F-Tryptophan labeled *E. coli* Dihydrofolate Reductase**

*Sydney D. Hoeltzli and Carl Frieden*

**Generic Core Replacement in T4 Lysozyme Preserves Protein Activity, Folding Cooperativity and Shape**

*Nadine C. Gassner, Walter A. Baase and Brian W. Matthews*

**On the Entropy of Protein Folding**

*Peter L. Privalov*

**Thermodynamic Signatures of Conformational Changes in Protein-Nucleic Acid Interactions**

*R. Saecker Spolar and M. Thomas Record, Jr.*

**Thermodynamic Mapping of the Inhibitor Site of the Aspartic Proteinase Endothiapepsin**

*Javier Gómez and Ernesto Freire*

**Molecular Origins of High-Affinity and Slow Dissociation Kinetics in Protein-Ligand Interactions**

*Patrick S. Stayton, Ashutosh Chilkoti, Lisa Klumb and Vano Chu*

**Immunosuppressive Drug Design and Inosine Monophosphate Dehydrogenase: A Proposed Solution to a Problem in Differential Molecular Recognition**

*Patrick Connelly*

# Posters

## **E. coli Helicase II Unwinds DNA by an Active Mechanism**

*Janid A. Ali and Timothy M. Lohman*

## **Folding transitions coupled to hirudin binding to thrombin**

*Youhna M. Ayala, Alessandro Vindigni, Murad Nayal, Ruth S. Spolar, M. Thomas Record, Jr., and Enrico Di Cera*

## **Thermodynamics of Protein-Protein Interactions: Binding of Turkey ovomucoid third domain to porcine pancreatic elastase**

*Brian M. Baker and Kenneth P. Murphy*

## **Structural Characterization of Multiple Partially Folded States of a BPTI Analogue**

*Elisar Barbar, George Barany and Clare Woodward*

## **Fluorescence Derivative of E. coli RNA Polymerase Sigma Subunit in the -10 Recognition Domain of the Protein**

*Sandhya Callaci and Tomasz Heyduk*

## **A Hidden Contribution to van't Hoff Enthalpy Estimates from Small Heat Capacity Changes**

*Jonathan B. Chaires*

## **Effects of Conserved Residues on the REgulation of Rabbit Muscle Pyruvate Kinase**

*Xiaodong Cheng, Robert H.E. Friesen and J. Ching Lee*

## **Mutagenesis studies of the slow and fast forms of thrombin**

*Quoc D. Dang, Enriqueta R. Guinto, Thalia Farazi, Alessandro Vindigni, Youhna M. Ayala, and Enrico DiCera*

## **The Magnitude of the Backbone Conformational Entropy Change in Protein Folding**

*Jose Alejandro D'Aquino, Javier Gómez, Vincent J. Hilser, Kon Ho Lee, L. Mario Amzel and Ernesto Freire*

## **Comparing Stability in Structurally Homologous Proteins with Little Sequence Identity**

*G.T. DeKoster & A.D. Robertson*

## **Equilibrium DNA Binding of the Sac7d Protein from the Hyperthermophile Sulfolobus acidocaldarius: Fluorescence and Circular Dichroism Studies**

*Stephen P. Edmondson, James McAfee and John W. Shriver*

## **Multi-Dimensional Thermodynamic Study of the Unfolding of Staphylococcal Nuclease A and Its V66W Mutant**

*Maurice R. Eftink*

## **Microtubule Assembly Dynamics with Pressure and IR Vibrational Perturbations**

*Daniel Engh, Bruce Johnson, Glenn Edwards and Robley Williams*



**Intramolecular Electrostatic Interactions Accelerate Hydrogen Exchange in Diketopiperazine Relative to 2-Piperidone**

*William R. Forsyth and Andrew D. Robertson*

**Stability And Calcium Binding of Recombinant Fragments of Troponin C**

*R.S. Fredricksen and C. Swenson*

**Thermodynamic Identification of Binding Hot Spots in Protein/Protein Recognition**

*Ernesto Freire, Javier Gómez, Vincent J. Hilser, Craig R. Johnson, and Dong Xie*

**Pressure-Induced Protein Denaturation of *Staphylococcal* Nuclease**

*Kelly J. Frye and Catherine A. Royer*

**An RNA Conformational Switch**

*T.C. Gluick & D.E. Draper*

**The Heat Capacity of Proteins**

*Javier Gómez, Vincent J. Hilser, Dong Xie and Ernesto Freire*

**Heme-Protein Interaction and Hemoglobin Stability Under High Hydrostatic Pressure Probed By Fluorescence Spectroscopy**

*Zygmunt Gryczynski, Jacek Lubkowski, Sabrina Beretta and Enrico Bucci*

**Energetics of Hydrogen Bonding in Proteins: A Model Compound Study**

*Susan M. Habermann and Kenneth P. Murphy*

**The Binding of an Fab to Dimeric Human Interleukin-5: A Solution Interaction Analysis Using the Time Derivative Method to Interpret Sedimentation Velocity Data**

*Preston Hensley, Carol C. Silverman, Dean E. McNulty, Michael L. Doyle, David G. Myszka, Terence G. Porter and Walter F. Stafford III*

**Protein Footprinting: Mapping Domains of *E. coli* RNA Polymerase  $\alpha$  Subunit Involved in Enzyme Assembly**

*Ewa Heyduk, Tomasz Heyduk, Konstantin Severinov, Hong Tang and Richard H. Ebright*

**The Contribution of van der Waals Interactions to the Enthalpy of Folding and Binding**

*Vincent J. Hilser, Javier Gómez and Ernesto Freire*

**Global Analysis Of The Urea And Acid-Induced Unfolding Of *Staphylococcal* Nuclease**

*Roxana M. Ionescu and Maurice R. Eftink*

**Fatty Acids Abolish High-Affinity Binding of Glyburide to Human Serum Albumin: Implications for Type II Diabetes**

*Michael G. Jakoby IV, David Song, Douglas F. Covey and David P. Cistola*

**Biochemical and Biophysical Characterizations of a Temperature Sensitive Mutant of *Escherichia coli* trp Repressor, L75F TrpR**

*Lihua Jin, June Fukayama & Jannette Carey*

**Structural Stability of Small Oligomeric Proteins**

*Craig R. Johnson and Ernesto Freire*

**Visualizing DNA Electric Fields: An Easy-to-Implement Standard**

*Edward Keyes, Thomas Kephart and Glenn Edwards*

**Heterotropic effects of a strong allosteric effector (IHP) on the O<sub>2</sub> and CO binding properties of the hemoglobin partially liganded species**

*Laurent Kiger, Claude Poyart and Michael C. Marden*

**Oxygen Binding Studies of Fell/Coll Hybrid Hemoglobins**

*Alexandra Klinger and Gary K. Ackers*

**The Role of Tyrosines in RBD Stability and RNA-binding**

*James K. Kranz and Kathleen B. Hall*

**Solvents interactions in hemoglobin: role of associated water on the enthalpy of a series of crosslinked hemoglobins**

*Herman Kwansa, Anna Razynska, Zygmunt Gryczynski, Enrico Bucci*

**mRNA Iron Responsive Element Thermodynamic Stability and NMR Structure Study**

*Lance G. Laing and Kathleen B. Hall*

**K<sup>+</sup>-Ribosome Interactions Determine the Large Enhancements of 39K NMR Transverse Relaxation Rates in Viable Cells**

*M. Li, H.J. Guttman, S. Cayley, C.F. Anderson and M. Thomas Record, Jr.*

**CD and Stability Studies of Two Parallel B-Helix Proteins: Pectate Lyases C and E**

*Renhao Li, Frances Jurnak and Clare Woodward*

**Crystal Structure of the Hemopexin-like C-terminal Domain of Gelatinase A**

*Andrew W. Libson, Apostolos G. Gittis, Ivan E. Collier, Barry L. Marmor, Gregory I. Goldberg and Eaton E. Lattman*

**Interactions of CI-921, An Anilinoacridine Threading Agent with Nucleic Acids**

*Ching-Yi Lien and David E. Graves*

**Characterization on Structure and Thermodynamic Stability of the C-terminal RBD2 of Human U1A Protein**

*Jirong Lu and Kathleen Hall*

**Site-Directed Mutagenesis Studies of the Stability of the Sac7d DNA-binding Protein from the Hyperthermophile *Sulfolobus acidocaldarius***

*Branford S. McCrary, Stephen P. Edmondson and John W. Shriver*

**Thermodynamic Studies of Lac Repressor-Operator Interactions**

*Sonya E. Melcher, Diane E. Frank, Mark M. Levandoski, Oleg V. Tsodikov, Ruth S. Spolar and M. Thomas Record, Jr.*

**Core packing defects in an engineered Cro monomer corrected by combinatorial mutagenesis**

*A.K.M.M. Mollah and Michael C. Mossing*

**Fluorescence Studies of the Ligand Induce Conformational Changes in the *E. coli* Hsp70, DnaK**

*Diana Montgomery & Richard Morimoto*

**Determination of Rate Constants using HPLC Affinity Chromatography**

*Peter D. Munro and Gary K. Ackers*

**Proton Linkage In Isothermal Titration Calorimetry**

*Kenneth P. Murphy and Brian M. Baker*

**Valence screening of water in protein crystals reveals potential Na<sup>+</sup> binding sites**

*Murad Nayal and Enrico DiCera*

**Purification and Characterization of Intact and Truncated Forms of the Biotin Accepting Subunit of the Escherichia coli Acetyl-CoA Carboxylase**

*E. Nenortas and Dorothy Beckett*

**Non-random Structure in Reduced and Unfolded Bovine Pancreatic Trypsin Inhibitor**

*Hong Pan, Elisar Barbar, George Barany and Clare Woodward*

**Crystallographic, Molecular Modeling and Biophysical Characterization of the Valine B67 (E11)-Threonine Variant of Hemoglobin**

*Igor Pechik, Xinhua Ji, Krzysztof Fidelis, Michael Karavitis, John Moutt, William Brinigar, Clara Fronticelli and Gary L. Gilliland*

**DNA Sequence-Specific Differences in the TBP-Promoter Interaction**

*Victoria Petri, Elizabeth Jamison and Michael Brenowitz*

**The trp Repressor of E. coli: Further Physical Investigations of Super-Repressor Mutants**

*Ross J. Reedstrom, Shyam Vangala, Kathleen S. Martin, Erik W. Wilker & Catherine A. Royer*

**Interaction of Netropsin and Distamycin with the Grooves of an Intramolecular DNA Triplex**

*Dionisios Rentzeperis & Luis A. Marky*

**Solvent Exchange of the Tyr 31 Hydroxyl Proton in Ovomuroid Third Domain: A Sensitive Measure of the Effect of Protein Structure on Hydroxyl Acid/Base Character**

*Andrew D. Robertson and Junmin Peng*

**Allosteric Modulation by Tertiary Structure in Mammalian Hemoglobins. Introduction of the functional characteristics of bovine hemoglobin into human hemoglobin by five amino acid substitutions.**

*Maria Teresa Sanna, Michael Karavitis, William S. Brinigar and Clara Fronticelli*

**The application of synchrotron x-ray radiation to the development of time resolved methods for the study of RNA folding**

*Bianca Sclavi, Sarah Woodson, Mike Sullivan, Mark Chance and Michael Brenowitz*

**Calcium-Induced Differences in the Hydrodynamic Behavior of Calmodulin Mutants Explored by Gel Permeation Chromatography**

*Brenda R. Sorensen and Madeline A. Shea*

**Excluded Volume Effects on the Melting of DNA Duplexes and Triplexes**

*C.H. Spink and J.B. Chaires*

**Temperature and pH Dependences of Hydrogen Exchange and Global Stability for Ovomuroid Third Domain**

*Liskin Swint-Kruse and Andrew D. Robertson*

**RNA Polymerase-Promoter Kinetics and Thermodynamics: Results of an Analytical Method**

*Oleg V. Tsodikov, Peter E. Schlax Jr., Kristi L. McQuade and M. Thomas Record, Jr.*

**Investigation of Protein-Protein interactions of trp super-repressor mutants**

*Shyam S. Vangala, Kathleen S. Martin, Ross J. Reedstrom and Catherine A. Royer*

**Proline Isomerization and the High-Pressure Denaturation of Staphylococcal Nuclease**

*Gediminas A.J. Vidugiris, Dagmar M. Truckses, John L. Markley and Catherine A. Royer*

**Role of the Peptide Backbone in Stabilization of Proteins by the Counteracting Osmolyte, Trimethylamine-N-Oxide**

*Aijun Wang and D. W. Bolen*

**Effects Of A Naturally Occurring Compatible Osmolyte On The Internal Dynamics of Ribonuclease A**

*Aijun Wang, Andrew D. Robertson, D. W. Bolen*

**Physicochemical Characterization of RNA Stem Loops with Non-nucleotide Spacers**

*D. Jeremy Williams & Kathleen B. Hall*

**Construction And Characterization of the ATPase Activity of a Covalently Cross-Linked Rep-DNA Complex**

*Isaac Wong and Timothy M. Lohman*

**Evidence for Inter-Domain Interaction in the Escherichia coli Repressor of Biotin Biosynthesis from Studies of an N-terminal Deletion Mutant**

*Yan Xu and Dorothy Beckett*

**Thermodynamic Analysis of Binding of the Escherichia coli Repressor of Biotin Biosynthesis to Small Ligands**

*Yan Xu and Dorothy Beckett*

**A Proton Binding Study of Thermodynamic Characteristics of the Denatured States of Staphylococcal Nuclease Proteins**

*Mingli Yang and Wayne Bolen*