# 10th Annual Gibbs Conference on Biothermodynamics

Little Grassy Lake Conference Center Southern Illinois University Carbondale, Illinois

October 5 - 8, 1996

#### Thanks to the following sponsors:

Calorimetry Sciences Corp.

ISS, Inc.

Microcal, Inc.

On-Line Instrument Systems, Inc.

Department of Biochemistry University of Mississippi Medical Center

> Jonathan B. Chaires Michael L. Doyle *Organizers*

# **Table of Contents**

	Page Number
Schedule and Program	
Poster Session I: List of Posters Presentations	. 19. 19. . 19. 19. 19. 19. 19. 19. 19. 19. 19. 19
Poster Session II: List of Poster Presentations	9
Keynote Address I: Abstract	13
Session I: Nucleic Acids: Folding and Stability (Abstracts)	15
Session II: Protein Folding (Abstracts)	20
Keynote Address II: Abstract	27
Session III: Macromolecule-Macromolecule Interactions (Abstracts)	29
Session IV: Nucleic Acids: Interactions (Abstracts)	34
Session V. Binding and Linkage (Abstracts)	40
Poster Session I (Abstracts)	47
Poster Session II (Abstracts)	86
List of Participants	124

# **Table of Contents**

		Page Number
Schedule and Program		1
Poster Session I: List of Posters Presentations		
Poster Session II: List of Poster Presentations		9
Keynote Address I: Abstract		13
Session I: Nucleic Acids: Folding and Stability (Abstracts		15
Session II: Protein Folding (Abstracts)		20
Keynote Address II: Abstract		27
Session III: Macromolecule-Macromolecule Interactions (	(Abstracts)	29
Session IV: Nucleic Acids: Interactions (Abstracts)		34
Session V. Binding and Linkage (Abstracts)	기기가 해면할 수야됐 그 이번 강동이 있다. 첫	40
Poster Session I (Abstracts)		47
Poster Session II (Abstracts)		86
List of Participants		124

### Saturday, October 5

4:00 - 9:00pm Registration in Little Grassy Lodge

7:00 - 10:00 Beer & Pizza Reception

#### **POSTER INFORMATION:**

Posters for **Poster Session I** (A through Li, by last name of the first author) may be mounted in Sledgefoot Lodge. Posters for **Poster Session II** (Lien - Z) may be mounted **Monday (October 7) morning**. Please remember that poster space is very limited, so mount your poster to conserve as much space as possible.

	Sunday, October 6
7:00	Breakfast, Freeberg Hall
8:30	Gary Ackers
	History of the Gibbs Conference
8:50	Keynote Address I
	J. Michael Schurr
	Long-Range Modulation of DNA Tertiary and Secondary Structure by Protein
	Binding
9:50	Refreshments
SES	SION I: NUCLEIC ACIDS: FOLDING AND STABILITY
	Moderator: Lori McFail-Isom
10:05	A. Steve Benight
	Sequence Dependence of DNA Thermodynamic Stability
10:50	Sarah Woodson
	Alternative pre-rRNA Structures Modulate Self-Splicing of the Tetrahymena
11.00	Group I Intron.
11:20	Roger Wartell
	Relative Stabilities of Duplex RNA with Single Base Pair Changes, Mismatches
11.50	and Bulges Measured by Temperature Gradient Gel Electrophoresis.
11:50	Charlie Spink
12.20 1.20	The Stability of Duplex and Triplex DNA in the Presence of Polyethyleneglycols.
12:30 - 1:30 CECC	Lunch, Freeberg Hall SION II: PROTEIN STABILITY
SESS	Moderators Sulvey Healt !!
2:30	Moderator: Sydney Hoeltzli John Carra
2.50	-
3:00	Energetics of Folding and DNA Binding of the MAT \a2 Homeodomain  Gregory DeKoster
5.00	
	Thermodynamics of Unfolding for Kazal-type Serine Protease Inhibitors: Stabilization of Ovomucoid First Domain by Glycosylation.
3:30	Vincent Hilser
2.20	Site Specific Thermodynamic Mutation Analysis (SSTM): Structural Mapping of
	Cooperative Interactions.
4:00	Refreshments
4:20	Roxana Ionescu
	Global Analysis of the Acid-Induced and Urea-Induced Unfolding of
	Staphylococcal Nuclease and Some of Its Variants.
4:50	Elisar Barbar
	Local Fluctuations and Global Unfolding of Partially Folded BPTI Detected by
	NMR.
5:20	Wayne Bolen
	Thermodynamic Properties of the Denatured Ensemble in Guanidine
	Hydrochloride.
6:30	Dinner, Buffalo Tro at Freeberg Hall
8:00 - 10:00	POSTERS & BEER I

	Monday, October 7
7:00	Breakfast, Freeberg Hall
8:30	Keynote Address II
•	Allen Minton
	Macromolecular Crowding, Confinement, and Stickiness: Three Factors
	Significantly Influencing Chemical Rates and Equilibria in Living Systems.
<u>.</u>	SESSION III: MACROMOLECULE - MACROMOLECULE INTERACTIONS
	Moderator: Harry Guttman
9:30	Tom Laue
	Sedimentation Equilibrium as a Thermodynamic Tool.
10:05	Refreshments
10:20	J. J. Correia
	Sedimentation Velocity Studies of the Vinca Alkaloid Induced Self-Association of
	Tubulin and Tubulin Isotypes.
11:00	Alessandro Vindigni
	Energetics of Thrombin-Thrombomodulin Interaction
11:30	Murad Nayal
	Electrostatic Effects in Thrombin-Hirudin Interaction
12:00-1	00 Lunch, Freeberg Hall
1:15	Round Table Discussion of Biothermodynamics Online (Optional for PI's)
	SESSION IV: NUCLEIC ACIDS: INTERACTIONS
	Moderator: Peter Riccelli
3:30	Loren Williams
	New & Old Methods for Structural Analysis of DNA-Ligands
4:00	Mike Mossing
	Engineering the $\lambda$ Cro Repressor to Study the Coupling between Folding,
	Dimerization and DNA Binding.
4:30	Bianca Scalvi
	Time-resolved Synchrotron X-ray "Footprinting". A New Approach to the Study
	of Nucleic Acid Structure and Function: Application to Protein-DNA Interactions
	and RNA Folding.
4:50	Refreshments
5:05	David Giedroc
	RNA Pseudoknot Structure and Stability: the Autoregulatory Gene 32 mRNA of
	Phages T2, T4 and T6.
5:35	Janid Ali
	E. Coli UvrD (Helicase II) Unwinds Duplex DNA with a Step Size of Five Base
	Pairs.
6:30	Dinner, Freeberg Hall
8:00-10	00 POSTERS & BEER II

# **Tuesday, October 8**

	7:00	Breakfast, Freeberg Hall
	8:00 - 12:30	Check-out. Return all keys to main office by 12:30.
_	SESS	ION IV: BINDING AND LINKAGE
		Moderator: Jim Krantz
	8:30	Enrico Bucci
		Isobaric Temperature Scan as a New Approach to the Thermodynamics of Oxygen Binding
	9:00	Alexandra Klinger
		The Contributions to Cooperativity by Singly and Doubly Oxygenated
		Hemoglobin Intermediates
	9:30	Vince LiCata
		Is Substrate Inhibition a Consequence of Allostery in Aspartate
		Transcarbamylase?
	10:00	Refreshments
	10:20	Enrico Di Cera
	and the state of t	Dissecting Protease Specificity Using Site Specific Thermodynamics
	11:00	Dorothy Beckett
		Binding and Linkage in the Escherichia coli Biotin Repressor System
	11:30	Brian Baker
		Proton Linkage Effects in Ligand Binding Reactions Studied by Isothermal
	•	Titration Calorimetry.
	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 6 8 - 10 pm Sledgefoot Hall

Thermodynamics and Kinetics of Protein Folding from Hydrogen Exchange in Native Protein: Two-State or Not Two-State?

Cammon Arrington and Andrew D. Robertson

Mapping Conformational Transition in a Protein by Iron-EDTA Protein Footprinting Technique: Application to cAMP Interaction with cAMP Receptor Protein (CPR)

Noel Baichoo and Tomasz Heyduk

Does trimethylamine N-oxide counteract the effects of urea on rabbit muscle lactic dehydrogenase: A test of a basic tenet of the biology of adaptation hypothesis

Ilya Baskakov, Aijun Wang and Wayne Bolen

Influence of di- and trivalent cations on the entropic elasticity of single  $\lambda$ -phage DNA molecules

C. G. Baumann S. B. Smith, C. Bustamante and V. A. Bloomfield

Effect of Acid and Salt on the Structure and Stability of Sac7d Jennifer Bedell, Steve Edmonson and John Shriver

ATP Hydrolysis Stimulates Binding and Release of Single Stranded DNA from Alternating Subunits of the Dimeric E. coli Rep Helicase. Implications for ATP-driven Helicase Translocation

Keith P. Bjornson, Isaac Wong and Timothy M. Lohman

Thermodynamic Characterization of the Heptameric Chaperonin GroES
Olga Boudker, Matthew J. Todd and Ernesto Freire

Protein-Protein Interactins on a Membrane Using Surface Plasmon Resonance: The Association of Coagulation Proteins, Factors Va and Xa

Michael Brigham-Burke, Matthew Hawkins, Kenneth Mann, and Preston Hensley

The Conformational Space of Hemoglobin as Revealed by the Enthalpy of the Subsequent Steps of Oxygenation in Normal and Intramolecularly Crosslinked Hemoglobin

Enrico Bucci, Zygmunt Grycrynski, Anna Razynska, Herman Kwansa, and MichaelO'Gern

Interactions of L11-binding region within large subunit ribosomal RNA with ions Yury V. Bukhman and David E. Draper

GroEL-Mediated Folding of Structurally Homologous Dihydrofolate Reductases
A. Clay Clark and Carl Frieden

Thermodynamic Interactions Between the Osmoprotectant Glycine Betaine and Macromolecules in Solution

Elizabeth S. Courtenay, Wentao Zheng, Michael W. Capp, Charles F. Anderson and M. Thomas Record, Jr.

Suppression of Na+ Binding Converts Thrombin into an Anticoagulant Quoc D. Dang, Enriqueta R. Guinto, and Enrico Di Cera

Actinomycin D Binds Single-Strand DNA in a Highly Sequence Specific Manner Numukumda Darboe, Susan Bailey and David Graves

Studies of  $\lambda$  Phage cro Repressor-DNA Interactions Paul J. Darling and Gary K. Ackers

Binding of Turkey Ovomucoid Third Domain to Porcine Pancreatic Elastase Monitored by Differential Scanning Calorimetry Stephen P. Edgcomb, Brian M. Baker and Kenneth P. Murphy

Thermodynamics of Protein Unfolding: Some Questions Pertinent to Testing the Validity of the Two-State Model

Maurice R. Eftink and Roxana M. Ionescu

Measurement of Amino pKa Values in Turkey Ovomucoid Third Domain William R. Forsyth and Andrew D. Robertson

VDSC: Virtual Differential Scanning Calorimetry

Ernesto Freire

Denaturation Dynamics of Horseradish Peroxidase in Presene of Guanidine Hydrochloride: Effects of Long Term Storage

Vladimir G. Frolov, Gediminas A. J. Vidugiris and Catherine A. Royer

Protein Stabilization by Xylose: Evidene for Dehydration as the Rate Limiting Step in Protein Folding

Kelly J. Frye and Catherine A. Royer

Towards a Physical Interpretation of the High Effective Dielectric inside a Protein: Crystallographic Evidence that Water can Penetrate Deep Into the Hydrophobic Core

Bertrand Garcia-Moreno E., Eaton E. Lattman, John J. Dwyer, Apostolos G. Gittis and Wesley E. Stites

### Thermal Stabilities of $\alpha$ Operon mRNA and 16S rRNA in the Presence of Ribosomal Protein S4

Resi B. Gerstner and David E. Draper

#### Osmotic Stress Stabilizes RNA Tertiary Structure

T. C. Gluick and D. E. Draper

#### Assembly State of E. coli Helicase II

Razmic S. Ggregorian Jr. and Timothy M. Lohman

#### Critical role of W60 in thrombin allosterism

Enriqueta R. Guinto and Enrico Di Cera

### Osmotic Balance and Turgor Pressure in *Escherichia coli* K-12 as a Function of External Osmolarity

Harry J. Guttman, Scott Cayley, Mike W. Capp and Thomas Record Jr.

#### Energetics of Calcium Binding to α-Lactalbumin

Tonya M. Hendrix and Peter Privalov

# Real-time Refolding Studies of 6-19F-Tryptophan Labeled E. coli Dihydrofolate Reductase using Stopped-Flow NMR Spectroscopy

Sydney D. Hoeltzli and Carl Frieden

# Do Different Hemoglobin Ligation System Follow A Common Cooperative Mechanism?

Yingwen Huang and Gary K. Ackers

## Uncoupling of Interfacial Interactions in the Allosteric Activation of cAMP Receptor Protein

Lubomir Kovac and J. Ching Lee

# Insights For Structure-Based Drug Design From the High Affinity Streptavidin-Biotin System

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

# Effects of Salt Concentration and Type on the Enthalpy and Heat Capacity Changes for E. coli SSB protein - ssDNA Interactions

Alexander G. Kozlov and Timothy M. Lohman

#### Thermodynamics of RNA-Protein Interactions in an RNA-Binding Domain

James K. Kranz and Kathleen B. Hall

#### Is Trypsin a Good Model for the Slow form of Thrombin?

Maxwell M. Krem and Enrico Di Dera

#### Mechanism of Salt-Induced Folding of Acid-Denatured Apomyoglobin

Frithjof Kuntze and Bertrand Garcia-Moreno E.

#### The Crystal Structure of Recombinant Actophorin

Shonda A. Leonard, Apostolos G. Gittis, Eugene Petrella, Thomas D. Pollard and Eaton E. Lattman

# Water Release Associated with Dna Binding by the Ultrabithorax and Deformed homeodomains of Drosophila melanogaster.

Likun Li, Doris von Kessler, Philip A. Beachy and Kathleen S. Matthews

#### POSTER SESSION II

Monday, October 7 8 - 10 pm Sledgefoot Hall

Thermodynamic Properties of a DNA Threading Agent: Interactions of CI-921 (Enzacrine) with Nucleic Acids

Chin-Yi Lien, David Graves and William Denny

Using the Structural Parameterization of the Energetics to Identify Conformations that Minimize the Gibbs Energy

Irene Luque and Ernesto Freire

Structure-Function Analysis of Avian Myeloblastosis Virus Preintegration Complexes Containing Purified Integrase

Mark McCord, Ajaykumar Vora and Duane Grandgenett

Hyperthermophile Protein Folding Thermodynamics: Differential Scanning Calorimetry and Chemical Denaturation of Sac7d

Bradford S. McCrary, Stephen P. Edmondson and John Shiver

Characterization of the Multiple Modes of Binding by the bis-Intercalator WP631 using Scanning Force Microscopy

Lori McFail-Ison, Fenfei Leng, Joseph Coury, Lisa Holt, Tina Conti, Lawrence Bottomley, Waldemar Preibe, Jonathan Chaires, and Loren Dean Williams

Temperature dependence 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 and Michael Brenowitz

Transcription Control: Simulation and Fitting of Gene Expression.

Peter D. Munro and Gary K. Ackers

Kinetic analysis of a protein antigen-antibody interaction limited by mass transport on an optical biosensor

David G. Myszka and Michael L. Doyle

Salt Ion Distributions around Polyion DNA Calculated with Alternative Description of Long Range Coulombic Interaction

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

What is the best set of published nearest neighbor interactions for predicting Thermodynamic Stability of Duples DNA from Sequence?

Richard Owczarzy, Frank J. Gallo and Albert S. Benight

Concentration-Dependence of Variability in Growth Rates of Microtubules

Susan Pedigo and Robley C. Williams, Jr.

Thermodynamic studies of the interaction of the Saccharomyces cerevisiae TATA Binding Protein (TBP) with Transcription Factor IIB

Victoria Petri and Michael Brenowitz

Calorimetric Characterization of the Folding Energetics of a Cystein-Free Mutant of Dihydrofolate Reductase from *Escherichia Coli* 

Stehania Pucciarelli and Ernesto Ffeire

Structural Characterization of Intermediates in Open Complex Formation by  $E\sigma^{70}$  RNA Polymerase at the  $\lambda PR$  pormoter

Marni Raffaelle, Maria L. Craig and N. Thomas Record, Jr.

Thermodynamic Contribution of Bulges and Mismatches to the Stability of Short DNA Hairpins

Dionision Rentzeperis, James Ho and Luis A. Marky

Thermodynamics investigation of a Protein-rRNA associatrion: The ribosomal protein L11 with a 23S rRNA fragment

Luis P. Reynaldo and David E. Draper

Thermodynamics of Self-Complementary DNA and RNA Oligomers with Sequences from the Chicken Glutamine Syntheatase Gene

Peter V. Riccelli, Jovenico Hilario, Frank J. Gallo and Albert S. Benitht

Kinetic and Thermodynamic Approaches for Distinguishing Regulatory Mechanisms

Paula J. Schlax, M. Thomas Record Jr. and David E. Draper

A Dichroic Revision of the Lifson-Roig Model for Prediction fo Peptide Helicity William Shalongo and Earle Stellwagen

Molecular Recognition at the V<sub>H</sub>/V<sub>L</sub> Interface of Engineered scFv Antibodies Patrick S. Stayton and Philip H. Tan

The Free Solution Mobility of DNA

Nancy C. Stellwagen, Cecilia Gelfi and Pier Giorgio Righetti

Design and Tests of Conformational Change for a Transcription Repressor Protein Liskin Swint-Kruse, Montgomery B. Pettitt and Kathleen Shive Matthews

# Contributions of Nonoperator DNA to Stability of 1:1 and 2:1 Lac Operator: Lac Repressor Complexes

Oleg V. Tsodikov, Sonya E. Melcher, Mark M. Levandoski, Diane E. Frand, Ruth M. Saeker and M. Thomas Record, Jr.

#### Structural Transitions in a Membrane: Generating the Tools

George J. Turner and Lynell Martinez

# Thermodynamics of DNA Hairpins Containing the Universal Base 5-Nitorindole Peter M. Vallone and Albert S. Benight

## Study of Conformational Dynamics of Human Growth Hormone and its Relation to Transport Across Tissue Membranes

Shyam S Vangala and Catherine A. Royer

#### Interactions of Selected Acridine-Based DNA Binding Agents

Luminita M. Velea, David Graves and William Denny

#### High Pressure Denaturation of ApoMb

Gediminas N. A. Vidugiris and Catherine A. Royer

# Thermodynamic and Structural Analysis of Microtubule Assembly: The Role of GTP-Hydrolysis

Bojana Vulevic and John J. Correia

#### Systematic Derivation of Partition Functions for Ligand Binding to Twodimensional Lattices

Luyu Wang and Enrico Di Cera

# Contributions by Electrostatic Interactions to the Thermostability of Thermophilic Proteins

Renjie Wang and Bertrand Garcia-Moreno E.

# A Thermodynamic Comparison of the Salt Dependence of Natural RNA Hairpins and RNA Hairpins with Non-nucleotide Spacers

D. Jermy Williams and Kathleen B. Hall

### Energetics of Target Peptide Recognition by Calmodulin: A Calorimetric Study Patrick L. Wintrode and Peter L. Privalov

### Insights into Purine Repressor Biological Function by Kinetic Studies Han Xu and Kathleen Matthews

# Thermodynamic Evidence for Significant Mutation Effects on the Acid Dena<sub>tured</sub> State of Staphylococcal Nuclease

Mingli Yang and D. W. Bolen

# Effects of Mutation in the C-terminal Tail of Human U1A RBD1 on RNA Binding Affinity and Specificity

Qingyi Zeng and Kathleen B. Hall

Mechanism of Urea Denaturation of Proteins: A Model Compound Study Win Zou, Susan M. Habermann and Kenneth P. Murphy