# 15th Annual Gibbs Conference on Biothermodynamics

Saturday, September 29
4:00 - 7:00 pm Check-in in Indian Room
7:00 - 10:00 pm Reception in Indian Room

	Sunday, September
7:30-8:30	Breakfast
	Keynote
8:30-9:30	George Rose (The Johns Hopkins University)
	"Protein Folding: Questioning the Paradigm"
9:30-10:00	Refreshment break
	Session I: Nucleic Acids I
	(Moderator: Wendy VanScyoc)
10:00-10:40	Eric Kool
	"Noncovalent Interactions in Protein-DNA Recognition"
10:40-11:00	Ana Maria Soto
	"Thermodynamics of DNA Triple Helices: Contributions of TAT/TAT an
	TAT/CGC* Base-Triplet Stacks"
11:00-11:20	Aaron L. Lucius
	"DNA Unwinding Step-size of <i>E. coli</i> RecBCD Helicase Determined from
	Single Turnover Kinetic Studies"
11:20-12:00	Jonathan B. Chaires
	"Structural Selectivity of Drug-Nucleic Acid Interactions"
12:00-1:00	Lunch
1:00-3:00	Free time
	Session II: Proteins I
	(Moderator: Sethe Burgie)
3:00-3:40	Neville Kallenbach
	"The Unfolded State of Polypeptides"
3:40-4:20	Angel E. Garcia
	"Molecular Evidence for Alpha Helix Stabilization by Shielding of the
	Backbone Hydrogen Bonds by Side Chain Atoms"
4:20-4:40	Irene Karantzeni
	"Thermodynamic Basis of Thermal Stability of Tag DNA Polymerase: A
	Comparative Study with E. Coli Pol 1"
4:405:00	Refreshment break
5:00-5:20	Esther A. Strohmeyer
	"Direct Measurement of Local and Global Contributions in the Binding o
	Conformycin to Bovine Adenosine Deaminase"
5:20-6:00	Kenneth P. Murphy
	"Binding and Linkage in Serine Protease Inhibition"
6:00-7:00	Dinner
8:00-10:00	POSTER SESSION I

	Monday, October
7:30-8:30	Breakfast
	Session III: Nucleic Acids II
	(Moderator: Ana Maria Soto)
8:30-9:10	Robert Clegg
	"Looking at Conformational Properties of DNA and DNA/Dye Interactions,
	Using Covalently Attached Cy3, Cy5 and Tetramethylrhodamine"
9:10-9:30	Irina Rouzina
	"DNA Melting by Mechanical Force"
9:30-10:00	Refreshment break
10:00-10:20	Shi-Jie Chen
	"RNA Hairpin Folding Kinetics"
10:20-10:40	Murrell Godfrey
	"Interactions of Selected Anilinoacridines with DNA: Thermodynamic
	Considerations of Acridine Ring Substituents"
10:40-11:20	Tim Lohman
	"DNA Unwinding by the <i>E. coli</i> SF-1 DNA Helicases, Rep and UvrD"
11:20-12:00	Carlos Bustamante
	"Some Issues Regarding the Thermodynamics of Single Molecule
	Experiments"
12:00-1:00	Lunch
1:00-3:30	Free time
	Session IV: Proteins II
	(Moderator: Matthew Auton)
3:30-4:10	Dorothy Beckett
	"Kinetic Mechanism of Cooperative Association of the Biotin Repressor with DNA"
4:10-4:30	Beatrice Huyghues-Despointes
	"pKa Values of Histidine Residues in RNase Sa: Effect of Salt Concentration
	and Net Charge"
4:30-5:00	Refreshment break
5:00-5:20	Eric M. Nicholson
	"Differences Between Prp and Its Homolog Dpi: Implications of a Partially
	Structured State in the Formation of Prpscii
5:20-6:00	George J. Turner
	"Subdomains in the F and G Helices of Bacteriorhodopsin Regulate the
	Conformational Transitions of the Reprotonation Mechanism"
6:00-7:00	Dinner
8:00-10:00	POSTER SESSION II

	Tuesday, October 2
7:30-8:30	Breakfast
	Session V: Interacting Systems
	(Moderator: David Schell)
8:30-9:10	Walter F. Stafford
	"Sedimentation Velocity Analysis of Interacting Systems: Thermodynamic
	Information from Non-linear Curve Fitting to Sedimentation Boundaries
9:10-9:30	James K. Kranz
	"Hydrostatic Pressure as a Probe of Conformational Transitions in the
	Calmodulin:peptide Complex"
9:30-10:00	Refreshment break
10:00-10:20	Daumantas Matulis
	"Determination of Hydrophobic Interactions Between Long Chain Aliphatic
	Hydrocarbons by Titration Calorimetry: Aliphatic Amine Aggregation and
	Protonation pK <sub>a</sub> Shift"
10:20-10:40	Olga Y. Lubman
	"Structural and Thermodynamic Analysis of the Peptide Binding Specificity
	of the SH2 Domain of Src Kinase"
10:40-11:20	John J. Correia
	"The Regulation and Energetics of Receptor-Mediated Smad Trimerization""
11:40-12:30	Lunch

#### POSTER INFORMATION

Posters will be presented in one of two sessions, I and II, to be held Sunday and Monday evenings, respectively, in Sledgefoot Hall (Next to Freeberg, the dining hall).

Session I: First Authors A through Landt. Posters may be mounted starting on Sunday morning.

Session I: First Authors Langsetmo through Z. Posters may be mounted starting on Monday morning.

#### POSTERS I, alphabetical by author Sunday 8-10 pm, Sledgefoot Hall

#### Influence of Pro-21 and Pro-26 on Rat β-Parvalbumin Stability

Sayeh Agah and Michael T. Henzl

# Structural and Thermodynamic Properties of *Parmecium Calmodulin Mutants Defective in K\** Channel Regulation

Zeynep Akyol, Rhonda Newman, Yulia Volokhina, Brenda Sorensen, and Madeline Shea

#### Proline Isomerase Assisted Refolding of Cro Repressor Variants

Ibrahim A. Al-Duraibi and Michael C. Mossing

#### Interaction of Fluoroalcohols with the Peptide Backbone

Matthew Auton and D. W. Bolen

#### T-cell receptor ligand specific oligomerization revisited

Brian M. Baker and Don C. Wiley

# Changes in flexibility upon dissociation of a cytoplasmic dynein light chain and relation to dynein assembly

Elisar Barbar and Michael Hare

### The Temperature Dependence of Denaturant Interactions with Proteins and Effects on Protein Stability Curves

Doug Barrick and Mark E. Zweifel

#### Folding and Stability of Procaspase-3

Kakoli Bose and A. Clay Clark

#### The Symmetry Rule Model of Hemoglobin Cooperativity Predicts the Strong Correlations Observed Between Heats of Oxygen Binding and Bohr Proton Release

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

# Unfolding of Fatty Acid Binding Protein Studied by Fluorescence Correlation Spectroscopy Krishnananda Chattopadhyay and Carl Frieden

# Comparison of ab-initio and molecular dynamics calculated free energies for a predicted arginine-wobble interaction.

Alan Cheng, Stephen P. Edgcomb, and Alan D. Frankel

#### Characterization of Caspase Recruitment Domains of RICK and Procaspase-1

Yun-Ru (Ruby) Chen and Clay A. Clark

#### Thermodynamics of Denaturant-Induced Unfolding of a Protein G B1 Domain Variant

Allan Chris M. Ferreon and D. W. Bolen

### Determinants of Cooperativity: the Doubly ligated structure of human ileal Bile Acid binding protein

Gregory T. DeKoster, Gregory P. Tochtrop, and David P. Cistola

#### Heat Capacity Changes upon Burial of Polar and Non-Polar Groups in Proteins

Dmitri N. Ermolenko, Vakhtang V. Loladze, and George I. Makhatadze

#### **Buried Polar Groups and Protein Stability**

Dmitri N. Ermolenko, Vaktang V. Loladze, and George I. Makhatadze

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

Debra Ferraro, T. Sivaraman, Lynn Teesch, and Andrew D. Robertson

# The Protein-Detergent Interaction Studied by Isothermal Titration Calorimetry and Differential Scanning Calorimetry

Jaime M. Ferreira and Mark Chiu

# Experimental $pK_a$ values of buried groups for calibration of continuum methods for $pK_a$ calculations and for assessment of contributions by buried water to the dielectric response in the protein interior

Carolyn Fitch, D. Karp, A. Gittis, D. Nguyen, E. Lattman, and B. Garcia-Moreno

### Protein electrostatics from the experimental perspective: are we ready to trade in the pH meter for a PC?

Carolyn Fitch, Kelly Lee, and Bertrand Garcia-Moreno

#### Energetics of transmembrane helix-helix interactions

Karen G. Fleming

# Pressure Perturbation Calorimetry: A novel technique to measure volumetric and solvation properties of proteins and biopolymers in solution

Verna Frasca, Valerian Plotnikov, J. Michael Brandts, John F. Brandts and Lung-Nan Lin

#### In vitro Interactions of CAP and lac Repressor

Michael G. Fried and Margaret A. Daugherty

#### In vitro Interactions of RNA Polymerase with CAP

Michael G. Fried and Damian Dyckman

### Interactions of Nucleotide Cofactors with the *Escherichia Coli* Replication Factor DNAC Protein

Roberto Galletto, S. Rajendran and W.M. Bujalowski

#### Conformational and Thermodynamic Propertied of Peptide Binding to S100P

Alexey V. Gribenko, Mercedes Guzmán-Cassado, Maria M. Lopez, and George I. Makhatadze

#### The Coefficient of Thermal Expansion of Ribonuclease T1 in Osmolyte Solutions

Marko Häckel and D. Wayne Bolen

#### Ligand-Linked Stability of Calmodulin

Kenosha F. Hobson, Susan Pedigo, and Maurice R. Eftink

#### Structural Insight into the Energetics of OMTKY3-Subtilisin Carlsberg Binding

James R. Horn and Kenneth P. Murphy

### Energetics of Acridine-based Anticancer Agents with DNA: Influence of Ring Modifications on Binding Thermodynamics

Rachel Hutchins and David Graves

#### Stability of G-Quadraplex DNA

Mack Kennington, Patrick Harkins, and Susan Pedigo

### Kinetic Evidence for Direct Transfer of E.coli SSB Protein between Two Molecules of ssDNA Alexander G. Kozlov and Timothy M. Lohman

# Thermodynamics of Distamycin A and Netropsin Competitive binding to the DNA Duplexes Containing two Binding Sites

Jurij Lah and Gorazd Vesnaver

#### Requirements for 2' OH group in the Salt-dependent binding of Tat peptides to TAR RNA

Stephen G. Landt, Stephen P. Edgcomb, Valerie Calabro, A. Rene Tipton and Alan D. Frankel

#### POSTERS II, alphabetical by author Monday 8–10 pm, Sledgefoot Hall

#### Heterodimer Preference in Myosin Phosphatase Subunit Coiled Coil Interactions

Knut Langsetmo, Walter F. Stafford and Terence Tao

#### Ligand Design for Virus Agglomeration-Coprecipitation

Rex Lovrien, Daumantus Matulis and Vytautas Raulinaitis

### Interactions of cytoplasmic dynein light chains Tctex-1 and LC8 with the intermediate chain IC74

Moses Makokha, Michael Hare, and Elisar Barbar

#### Single Turnover DNA Unwinding Studies of E. coli UvrD-DNA Helicase Activity

N. Karl Maluf and Timothy M. Lohman

### The Relation between Stability and Repeat Number in a Structurally Modular Protein Cecilia C. Mello and Doug Barrick

### Determinants of Ligand Binding Stoichiometry: Intestinal Fatty Acid Binding Protein Benhur Ogbay John Monsey and David P. Cistola

### A Genetic Polymorphism in Human Intestinal fatty acid binding Protein Affects Ligand Release

Jeramia J. Ory, John D. Monsey, Sethe Burgie and David P. Cistola

# Characterization of a procaspase-3 mutant that disrupts the oligomeric state of the native protein

Cristina Pop, Ashutosh Tripathy, Erin Shiver, Brett Feeney, and Clay Clark

#### Molecular Dynamics and Quantum Mechanical Studies of Cytochrome c

Ninand V. Prabhu, Sergio E. Dalosto, Jane M. Vanderkooi and Kim A. Sharp

#### Efficacy of Macromolecular Crowding in Forcing Proteins to Fold

Youxing Qu and D. W. Bolen

### Intestinal Fatty Acid Binding Protein: Structural Perturbations by Single Site Mutations Massy Rajabzadeh and Carl Frieden

# Multiple-step Kinetic Mechanism of DNA-Independent ATP Binding and Hydrolysis by Escherichia Coli Replicative Helicase DnaB Protein: Quantitative analysis using the Rapid Quench-Flow method

S. Rajendran, M. J. Jesewska and W. Bujalowski

#### **Detection of Membrane-Protein Conformations by PWR**

G. Ramsay, Z. Salamon, S. Cowell, V. J. Hruby, G. Tollin

#### Thermodynamics of Helix Unfolding

John Richardson and George Makhatadze

#### Sequence Determinants of the Ubiquitin Fold

Andrew D. Robertson

# Osmolyte Effects on Protein Folding Dynamics: Is How You Get There as Important as Where You're Going?

Andrew T. Russo and Wayne Bolen

### Stability of Cognate and Near Cognate Codon-Anticodon-Ribosome Interactions Involving $tRNA^{Phe}$

Kevin Y Sambomatsu and Simpson Joseph

#### Folding and Assembly Kinetics of Cro Dimers

John Satumba and Michael C. Mossing

#### Design of a Hyperthermostable Variant of RNase Sa

David Schell, Niles Peirce, Travis Waldron, Kenneth Murphy, Stephen Mayo, and Nick Pace

#### First Principles Calculation of Macromolecular Binding Constants

Kim Sharp

### Thermodynamics of the Inclusion of dC Bulges and dC\*dC Mismatches in DNA Hairpin Molecules

Ronald A. Shikiya and Luis A. Marky

### Non-Linear Least Squares Curve Fitting of Sedimentation Velocity Data for Self-Associating Tubulin Heterodimes

Chris A. Sontag, Walter F. Stafford III, and John J. Correia

#### Cooperative Binding of Alkyltrimethylammonium Ions to Natural and Homopolymeric DNA Charles H. Spink and Dominik Mantella

### Addition of a Flexible "Tail" Raises Thermostability and Lowers Calcium Affinity of Calmodulin N-domain

Brenda R. Sorensen, Laurel A. Coffeen, Rainbo Hultman and Madeline A. Shea

#### The Stability Curve of Bovine Adenosine Deaminase is Bimodal

Ester A. Strohmeyer and B. Mark Britt

#### Electrostatic interactions in ubiquitin: Stabilization of carboxylates by lysine amino groups Monica Sundd, Nicole Iverson, Rhonda Newman, Jared Helm and Andrew D. Robertson

### Improving the Lac Repressor: the L148F Mutation Increases Inducibility Liskin Swint-Kruse, Bonnie Fairbanks, Atul Maheshwari and Kathleen Shive Matthews

# Cooperativity in Ligand-Protein Recognition: Human Ileal Bile Acid-Binding Protein Gregory P. Tochtrop, Douglas F. Covey and David P. Cistola

# Asp 79 Makes a Large, Unfavorable Contribution to the Stability of Ribonuclease Sa Saul Trevino, Kevin Shaw, Stephanie Newsom, J. Martin Scholtz and C. Nick Pace

# Domain-Specific Optical Spectroscopy of Calmodulin: Intrinsic Phenylalanine Fluorescence Selectively Reports on Conformational Change of the N-domain as shown by Time-Resolved and Steady-State Studies

Wendy S. Van Scyoc, Brenda Sorensen, Elena Rusinova, William Laws, J.B. Alexander Ross, and Madeline A. Shea

#### **Anion Binding to Protein-Protein Complexes**

Travis T. Waldron, Modestos A. Modestou, Rhonda A. Newman, Keith Bryan, and Kenneth P. Murphy

## Properties of Microtubule synthesized in *Escherichia coli* and Folded *in vitro* by the Chaperonin CCT

Robley Williams, Chirayu Shah, Cathy Xu and Jonathan Vickers

### A Three-Dimensional Statistical Mechanical Model of Folding Double-Stranded Chain Molecules

Wenbing Zhang and Shi-Jie Chen

# Structure, Stability and Modularity of the Ankyrin-Repeat Domain from *Drosohila* Notch Mark Zweifel and Doug Barrick