

A grayscale electron micrograph showing a cell membrane with a prominent vesicle. The membrane is highly textured and folded, with a large, roughly circular vesicle containing a grid-like internal structure. The overall appearance is that of a biological membrane at a high magnification.

18th Annual Gibbs Conference on Biothermodynamics

**Touch of Nature Conference Center
Southern Illinois University
Carbondale, Illinois**

October 9-12, 2004

**Doug Barrick
Kathleen Hall**

18th Annual Gibbs Conference on Biothermodynamics

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Southern Illinois University
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October 9 - October 12, 2004

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18th Annual Gibbs Conference on Biothermodynamics

Saturday, October 9

- 4-7 Check-in at Indian Room
7-10 Reception in Indian Room

Sunday, October 10

7:30 – 8:30 Breakfast, *Freeberg Hall*

SESSION I: WATER & SOLUTION THERMODYNAMICS

Moderator: Kelli Baran (Garcia-Moreno lab, JHU)

- 9:00 **Rohit Pappu** (Wash Univ)
Excluded Volume and Solvation: The Hammer and Chisel for Sculpting Energy Landscapes of Unfolded Proteins
- 9:40 **Daniel Harries** (Parsegian lab, NIH)
Solutes Probe Hydration of Nonpolar Surfaces in Association of Cyclodextrin and Adamantane
- 10:10 Break
- 10:40 **Jorg Rosgen** (Bolen lab, UTMB)
Statistical Thermodynamics of Activity Coefficients: A Structural Perspective
- 11:10 **Ken Dill** (UCSF)
Modeling Water, the Hydrophobic Effect, and Ion Solvation
- 12:00 Lunch, *Freeberg Hall*

SESSION II: STABILITY & DYNAMICS

Moderator: Katie Tripp (Barrick lab, JHU)

- 2:30 **George Makhatadze** (U Penn)
Engineering Proteins for Thermostability
- 3:10 **Brian Chellgren** (Creamer lab, U Kentucky)
Physical Determinants of the P_{II} Helix
- 3:40 Break
- 4:00 **Daniel Isom** (Garcia-Moreno lab, JHU)
Highly Perturbed pK_a Values of Ionizable Residues in Internal Positions of Staphylococcal Nuclease
- 4:25 **David Draper** (JHU)
Why are there ribosomal proteins?
- 5:10 **Keynote address**
Nacho Tinoco (UCB)
Thermodynamics and Kinetics of Unfolding RNA by Force
- 6:30 Dinner, *Freeberg Hall*
- 8:00 - ? **POSTERS & BEER I**

Monday, October 11

7:00 – 8:30 Breakfast, *Freeberg Hall*

SESSION III: PROTEIN-PROTEIN INTERACTIONS

Moderator: Allison Joubert (LiCata lab, LSU)

9:00 **Brian Baker** (U of Notre Dame)
T Cell Receptor – Ligand Interactions: Multiple Solutions to the Protein Docking Problem

9:40 **Zeynep Akyol** (Shea lab, U Iowa)
Calmodulin Recognition of the NMDA (Glutamate) Receptor

10:10 Break

10:40 **Abigail Doura** (Fleming lab, JHU)
Complex Interactions at the Helix-Helix Interface Stabilize the Glycophorin A Transmembrane Dimer

11:10 **Gary Pielak** (U North Carolina)
Impact of Protein Denaturants and Stabilizers on Water Structure

Announcements

12:00 Lunch, *Freeberg Hall*

SESSION IV: NUCLEIC-ACID: PROTEIN INTERACTIONS

Moderator: Kathleen Dori (Beckett lab, U Maryland)

3:00 **Linda Jen-Jacobsen** (U Pittsburgh)
Thermodynamics of DNA Recognition by Restriction Endonucleases

3:40 **Jason Wong** (Lohman lab, Wash Univ)
Effects of Single Stranded DNA Tail Length on the Equilibrium Binding of E. coli RecBC and RecBCD Helicases to Duplex/ ssDNA Junctions

4:10 Break

4:40 **Andy Wowor** (LiCata lab, LSU)
DNA Structure Dependent Heat Capacities of DNA Binding by E. coli and Taq DNA Polymerases

5:10 **Mike Mossing** (U of Mississippi)
Slow Assembly of Cro Dimers: Implications for the lambda Switch

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

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

Tuesday, October 12

7:00 – 8:30 Breakfast

8:30 Announcements

SESSION V: LINKAGE & ALLOSTERY

Moderator: Holland Alday (Correia lab, U Mississippi)

8:40 **Vince Hilser** (UTMB)

Insights into the Protein Ensemble

9:10 **Alka Prasad** (Pedigo lab, U Mississippi)

Effect of Adjoining Linker Segments upon the Stability of Domain 2 of Epithelial Cadherin

9:40 Break.

Be sure to check out before 12:30. Drop keys at main office.

10:00 **Kelly Knee** (Mukerji lab, Wesleyan)

Theoretical and Experimental Evidence for a Sequential Mechanism for the DNA B-A Transition

10:30 **Phil Bevilacqua** (Penn State)

Linkage Between Proton Binding and RNA Folding: A Thermodynamic Framework and its Experimental Application for Investing pK_a Shifting

11:00-12:30 Lunch, *Freeberg Hall*

POSTER INFORMATION:

Posters will be presented in one of two evening sessions in Sledgefoot Hall (next to Freeberg Dining Hall). Session I will be held Sunday and Session II will be held Monday.

Session I: First authors whose last names begin with Z through J. Posters may be mounted starting on Sunday morning.

Session II: First authors whose names begin with K through A. Posters may be mounted starting on Monday morning.

Posters I: Sunday 8-10 pm in Sledgefoot Hall

Thermodynamic and Structural Characterization of the WWE domain from *Drosophila Deltex*

Mark Zweifel and Doug Barrick

Calcium Binding to E-Cadherin Two Domain Construct

Huaying Zhao and Susan Pedigo

Multi-Method Global Analysis of Thermodynamics and Kinetics in Reconstitution of Monellin

Wei-Feng Xue, Jannette Carey and Sara Linse

Time-resolved FRET Studies of Double-labeled Double Strand Oligonucleotides to Define Average Donor and Acceptor Dye Positions

Sarah L. Williams and Lawrence J. Parkhurst

DNA-binding and phenolic recognition by the transcriptional regulator HucR from *Deinococcus radiodurans*

Steven P. Wilkinson and Anne Grove

Do the Thermodynamics of the Denatured States of Proteins Code Unique Information about Native Folds?

Suwei Wang, Jason Vertrees, Scott A. Larson, Tong Liu and Vincent J. Hilser

Modeling interfacial water in biomolecular systems

Jason Wagoner, Artem Melnykov, Nathan A. Baker

Hydrophilic Camptothecin Analogs that Stabilize Cleavable Complexes

Randy M. Wadkins, David Bears, Govindarajan Manikumar, Ansukhlal C. Wani, Monroe E. Wall, and Daniel D. Von Hoff

Development of a Framework to Identify and Quantify thermodynamic Homology Between Protein Folds

Jason Vertrees, Suwei Wang, Scott A. Larson, Tong Liu and Vincent J. Hilser

Characterization of nascent chains dynamics by steady-state fluorescence anisotropy

Krastyu G. Ugrinov, Marc-Andre Frese and Patricia L. Clark

Insertion of Designed Repeats in the Notch Ankyrin Domain: Alteration of Cooperativity, Stability, and Folding Mechanism

Katherine Tripp and Doug Barrick

Intrinsic Versus Extrinsic Conformational Propensities of Amino Acids in the Excluded Volume Limit: Implications for Unfolded Proteins

Hoang T. Tran and Rohit V. Pappu

Differences in the salt dependence of DNA binding by *Thermus aquaticus* and *Escherichia coli* DNA polymerases.

Gregory S. Thompson, Daniel J. Deredge, Carmen R. Ruiz, Kausiki Datta, and Vince J. LiCata

Transmembrane helix interactions in Adenosine A2a Receptor
Damien Thévenin, Matthew Roberts, Tzvetana Lazarova, and Clifford R. Robinson

Neuronal Voltage-Dependent Sodium Channel Lowers Calcium Affinity of the C-domain of Calmodulin
Nathaniel T. Theoharis and Madeline A. Shea

Activation Domain of Human Procarboxypeptidase A2: Cloning, Expression, Purification, and Characterization of the Wild Type and Variants Engineered to have Enhanced Stability
Samantha Strickler, Tracey Reihle and George Makhatadze

Additivity tests for a model of the stability distribution in the Notch ankyrin domain.
Timothy O. Street, Christina M. Bradley, Doug Barrick

Mutational Change in the Cooperativity of Protein Unfolding Caused by Changes in Native State Interactions
Wesley E. Stites and Junmei Chen

Self-association energetics of the OMPLA transmembrane β -barrel
Ann Marie Stanley and Karen G. Fleming

A Global Fitting Program for the Analysis of General Hetero- and Self- Associating Systems by Sedimentation Equilibrium
Walter F. Stafford and Peter J. Sherwood

On Interaction of Divalent Cations with an RNA Pseudoknot
Ana Maria Soto and David E. Draper

Effects of Physiologically Significant Domain-Specific Mutations and Species-Specific Sequence Variations on the Thermostability of Calmodulin
Brenda R. Sorensen, Laurel A. Faga and Madeline A. Shea

The Thermodynamics of DNA Binding and Distortion by the Hyperthermophile Protein SAC7D
John W. Shriver, William B. Peters and Stephen P. Edmondson

Thermodynamics of Intramolecular DNA Triplexes: Contributions from TAT/TAT Base Triplet Stacks and Single TAT -> TTA Substitutions
Ronald Shikiya and Luis A. Marky

The Free-Energy Landscape and Folding of Model Proteins
A.K. Setty and J. Liang

Quantitating cooperativity in L3-L6-rRNA complex in *B. stearothermophilus*
Uttara SenGupta and David E. Draper

Calcium-dependent Stability of E-Cadherin Domain 1 and 2

Alka Prasad, Matt Rutherford and Susan Pedigo

Human and Yeast TATA-Binding Proteins (TBP) have Markedly Different DNA Binding Kinetics Despite Nearly Identical DNA Binding Domains

Lawrence J. Parkhurst, Kristina Masters, Kay M. Parkhurst, and Margaret Daugherty

Characterization of the Spectral Changes Associated with Calcium Binding to the C-domain of Calmodulin and Several of Its Mutants

Shakirat O. Oyetunji, Charles Odonkor, Huaying Zhao and Susan Pedigo

Unfolding of G-Quadruplexes: Thermodynamic Contributions for the Stacking of Two G-Quartets

Chris Olsen and Luis A. Marky

Preliminary Characterization of Self-Association and Activity of *E. coli* MutL.

Anita Niedziela-Majka and Timothy M. Lohman

Insight Into Residues Important for Domain-Specific Interactions of Calmodulin with Melittin, a Model Basic Amphipathic Alpha Helix

Rhonda A. Newman and Madeline A. Shea

Slow Assembly of Cro Dimers: Implications for the lambda Switch

Michael C. Mossing, John Satumba, Gene L. Bidwell, Haifeng Jia, Yong Xiang, Melva James, and Ibrahim Al-Duraibi

Folding of Apaf-1 CARD

Sara L. Milam, Jennifer Rochette, Brett Feeney, Nate Nicely, Carla Mattos, and A. Clay Clark

The Effect of Changing the Detergent Concentration on the Free Energy of Transmembrane Helix-Helix Association: Wyman Linkage or Dilution?

Naveen Michaud-Agrawal, Thomas B. Woolf, and Karen G. Fleming

Structure-thermodynamics correlation of the p53 peptide - HDM2 interaction

Daumantas Matulis, Dianne Maguire, Carsten Schubert, Ingrid Deckman, Bruce Grassberger, Barry Springer, and Matthew J. Todd

Assembly State and Catalytic Activity of a Viral DNA Packaging Machine

N. Karl Maluf, Yang, Q., Bogner, E., and Catalano, C.E.

Behavior of Nascent Chain Folding of HP Model Proteins under Point Mutations

Hsiao-Mei Lu and Jie Liang

The Crystal Structure of a Partial Mouse Notch-1 Ankyrin Domain: Repeats 4 Through 7 Preserve an Ankyrin Fold

Olga Y. Lubman, Raphael Kopan, Gabriel Waksman and Sergey V. Korolev

Reconciling the “Dynamic” and the “Mechanical” Views of Energy Propagation in Allosteric Proteins.

Tong Liu, Steven T. Whitten, and Vincent J. Hilser

Thermodynamic Characterization of the High Temperature Stability of *Thermus aquaticus* DNA polymerase I.

Chin-Chi Liu, Allison M. Joubert, and Vince J. LiCata

What Defines the Specificity of Cyclic Nucleotide in E. coli cyclic AMP Receptor Protein?

Jianquan Li, Shaoning Yu, Rodrigo Maillard and J. Ching Lee

Posters II: Monday 8-10 pm in Sledgefoot Hall

The Native State Ensemble, Energy Landscapes, and Cold Denaturation
Andrew J. Kurtz, Steven T. Whitten, A. Joshua Wand, and Vincent J. Hilser

Equilibrium Binding of yeast (*Sacchromyces cerevisiae*) Replication Protein
A to single-stranded DNA
S.Kumaran and Timothy M. Lohman

Thermodynamics and salt-dependence of unfolding of YopM, a very large leucine-rich-
repeat protein
Ellen Kloss and Doug Barrick

Comparison of the structures in solution of *Saccharomyces Cerevisiae*
TBP and TBPc free and complexed to DNA
Sergei Khrapunov, Huiyong Cheng, Michael Brenowitz

Hemiprotonated CC⁺ Duplex \leftrightarrow I-Motif Equilibrium in the Unfolding of
d[C₃TA₂]₄ and d[C₃TA₂]₃C₃T Below Physiological pH.
Mahima Kaushik, Nathan Suehl and Luis A. Marky

Influence of HIV-1 Nucleocapsid Protein on Stability of DNA Quadruplexes and
Duplexes
Besik I. Kankia and Karin Musier-Forsyth

Structural Thermodynamics of the Hyperthermophile Antiparallel Coiled-coil Protein
Sso10a with a Buried Salt Bridge
Mebrahtu A. Kahsai, Andrew T. Clark, Stephen P. Edmondson, John W. Shriver

Folding Rates and Energy Landscapes of HP Lattice Model Proteins
Sëma Kachalo and Jie Liang

Folding Energetics of Human Serum Albumin
William T. Jones, III and G. Reid Bishop

Resonance Energy Transfer Studies of Equilibrium Dimerization in the Lambda Cro
Repressor
Haifeng Jia and Michael Mossing

Ordered Structure of Monomeric Polyglutamine
Veronique Hermann, Brian Chellgren, Trevor Creamer

Divalent Ion-binding Properties of the Avian β -Parvalbumins
Michael T. Henzl

Characterization of the Human Pancreatic Polypeptide (HPPT) and Effect of
Substitutions on the Ccap Position (THR32) on the Protein Stability
Anzor Gvritishvili, Marimar Lopez and George I. Makhatadze

Mg²⁺-RNA Interactions: Mg²⁺ Stabilization of a 58-Nucleotide RNA Structure.
Dan Grilley and David E. Draper

Mechanism of Thermostabilization of a Designed Cold Shock Protein with Optimized Surface Electrostatic Interactions
Alexey V. Gribenko, Vakhtang Loladze, Marimar Lopez, Jessica L. Wolgemuth, Samantha S. Strickler, and George I. Makhatadze

Unfolding Thermodynamics of DNA Triplexes: A Comparative Investigation of Purine versus Pyrimidine Triplex Motifs
Rajkumar Ganugula, Ana Maria Soto, Ronald Shikiya and Luis A. Marky

DNA Binding Mechanism of O6-Alkylguanine-DNA Alkyltransferase (AGT): Effects of Protein- and DNA-Alkylation on DNA Binding
Michael G. Fried, Sambit R. Kar and Anthony E. Pegg

Stochastic Association of the GxxxG-Containing Transmembrane Helix of the CCK-4 Oncogene
Karen G. Fleming and Felix J. Kobus

The Protein Denatured State: How Organized Is It?
Nicholas C. Fitzkee and George D. Rose

Effects of Translation on Protein Folding *In Vivo*
Michael S. Evans, Mary C. Finn and Patricia L. Clark

Solvation, Stability and Solubility of Halophilic Proteins
Christine Ebel, Lionel Costenaro, Adriana Irimia, Dominique Madern, Frederic Vellieux, Giuseppe Zaccai

Turnip Crinkle Virus Coat Protein Expression and Purification
Kathleen Dori, Anne Colgrove and Dorothy Beckett

Kinase-Interacting FHA Domain from a Transmembrane Phosphatase of Plants: Interactions with Phosphokinase and pThr Peptides, Dynamics, and Folding
Zhaofeng Ding, Xiangyang Liang, Gui-in Lee, and Steven R. Van Doren

Activation of the ATPase Activity of Adenoassociated Virus Rep68 Protein by DNA
John David Dignam, Susan S. Dignam, John J. Correia, James P. Trempe

Time-Resolved Acceptor-Detected FRET for Precise Distance Measurements Beyond 100Å.
Roberto Fabio Delgadillo and Lawrence J. Parkhurst

Some Structural Features of Zymogen and Enzyme Forms of Plasminogen
Vesna S. de Serrano, Joey Buettner, Stefan Franzen, and Clay Clark

Recognition of the Same Peptide/MHC Ligand by Two Different T Cell Receptors:
Multiple Solutions to the Protein-Protein Docking Problem

Rebecca L. Davis-Harrison and Brian M. Baker

A TIRFS Investigation of a High Affinity Ternary Complex of Platelet Osteonectin
with lys-Plasminogen and Collagen V

Margaret A. Daugherty, Daniel Schuler, Dylan Burns and Thomas Orfeo

Mechanism of PKR Activation: Dimerization and Kinase Activation in the
Absence of Double-Stranded RNA

James L. Cole, Peter A. Lemaire and Jeffrey Lary

Testing “functional selection” in TCR recognition of ligand

*John R. Clemens, Rebecca L. Davis-Harrison, Susan J. Gagnon, William E. Biddison,
and Brian M. Baker*

Enzymatic Degradation of Sup35NM, a Prion-like Protein from Yeast

Ching-Ying Chen, Clay Clark and Jason C.H. Shih

Location of Internal Water Molecules in Proteins: Comparison of Structure-based
Calculations with Crystallographic Observations in Staphylococcal Nuclease

Carlos A. Castañeda and Bertrand García-Moreno E.

Substrate Ground State Binding Energy Concentration is Realized as Transition State
Stabilization in Physiological Enzyme Catalysis

Mark Britt

Crystal Structure of HLA-A2 in Complex with Melanoma Related gp100₂₀₉ and gp100<sub>209-
T2M</sub> Peptides at 1.8 Å Resolution

Oleg Ya. Borbulevych, Tiffany Baxter, and Brian M. Baker

Thermodynamic Contributions for the Unfolding of DNA Complexes Containing Joined
Triplex and Hairpin Loop Motifs

Sarah Betzold and Luis A. Marky

Relating Surfactant Properties to Activity and Solubilization of Integral Membrane
Proteins

Bryan W. Berger, Abraham M. Lenhoff, Eric W. Kaler and Clifford R. Robinson

Kinetic Analysis of a Transcriptional Switch

Dorothy Beckett and Emily D. Streaker

Strategic Mutations In The Class I MHC HLA-A2 Independently Affect Both Peptide
Binding and T Cell Receptor Recognition

*Tiffany K. Baxter, Susan J. Gagnon, Rebecca L. Davis, John C. Beck, Anne-Kathrin
Binz, Richard V. Turner, William E. Biddison, and Brian M. Baker*

Domain-Domain Interactions in the *Saccharomyces cerevisiae* HMGB Protein HMO1

Kevin T. Bauerle, Edwin Kamau, and Anne Grove

Molecular Determinants of pKa Values of Surface Residues: Magnitude of Short-Range Interactions in Clusters and Networks, and Contributions by Local Structural Fluctuations

Kelli Baran, Carolyn Fitch, Jamie Schlessman, Bertrand García-Moreno

Quantitative Analysis of Progesterone Receptor Function: Cooperative DNA Binding and Hetero-Protein Interactions.

David L. Bain, Aaron F. Heneghan, Nancy Berton, and Michael T. Miura

Calorimetric Characterization of a TCR-peptide/MHC Interaction

Kathryn M. Armstrong and Brian M. Baker

Interaction of a Stathmin-GFP construct with Tubulin and Tubulin-Fluorescein by Absorbance and Fluorescence Analytical Ultracentrifugation.

P. Holland Alday, Eric George, David Brown, Tom Laue and John J.

Correia

Formation of AA/UU Base Pair Stacks and UAU/UAU Base Triplet Stacks: Energetics, Ion and Water Binding

Sharon Agers, Chris Olsen and Luis A. Marky