

8th Annual Gibbs Conference on Biothermodynamics

Organizers: Enrico DiCera & Madeline A. Shea
October 1 - 4, 1994

Schedule of Events

Unless noted otherwise, all events will be held in Little Grassy Lodge Friends Room
Touch of Nature Conference Center, Carbondale, IL

Saturday, October 1

4:00 p.m. **Registration at Main Desk, Little Grassy Lodge**
Posters for Session I may be set up in Indian Bldg.
No dinner will be served this evening.

7:00 p.m. **Wine and Cheese Reception**

Sunday, October 2

7:00 a.m. ☯ Breakfast, Freeberg Hall

8:15 a.m. Opening Remarks by Conference Organizers

Keynote Address

8:30 a.m. **Gary K. Ackers**, Washington Univ. School of Medicine
*Thermodynamics as a Logic Tool:
Deciphering the Molecular Mechanism of Hemoglobin's Cooperativity*

9:30 a.m. Refreshments

Allosteric Regulation

Moderator: Vince Li Cata

9:45 a.m. **Cathy Royer**, Univ. of Wisconsin
Energetics and Structural Dynamics of the Glucocorticoid Receptor

10:25 a.m. **Isaac Wong**, Washington Univ. School of Medicine
*Mutation of Conserved Lysine in the ATP-Binding Site of E. coli Rep helicase
Disrupts Allosteric Regulation*

10:45 a.m. 7 Refreshments

11:00 a.m. **Quoc Dang**, Washington Univ. School of Medicine
Allosteric Transitions of Thrombin

11:20 a.m. **Tom Gluick**, The Johns Hopkins University
An mRNA Conformational Switch Mediating Translational Regulation: Is There Allostery?

12:30 p.m. ☯ Lunch, Freeberg Hall

☀ Free Time ☀

Posters will be available in the Indian Bldg.

Molecular Recognition

Moderator: *Bertrand García-Moreno E.*

- 3:00 p.m. **Wayne Bolen**, U. of Texas Medical Branch at Galveston
Energy Management by an Enzyme During Catalysis
- 3:40 p.m. **Susan Green**, The Johns Hopkins School of Medicine
A dimeric form of staphylococcal nuclease resulting from deletion of six amino acids
- 4:00 p.m. 7 Refreshments
- 4:15 p.m. **Clare Woodward**, Univ. of Minnesota
Partially Folded and Compact Denatured States of BPTI
- 4:55 p.m. **Ross Reedstrom**, Univ. of Wisconsin
*In vitro differences between wild-type Trp repressor & super-repressor AV77:
Linkage of protein folding & repressor action*
- 5:15 p.m. **Ed Lattman**, The Johns Hopkins School of Medicine
Unfolding studies of an N-terminal fragment of staphylococcal nuclease
- 6:30 p.m. 🍴 Dinner, Freeberg Hall **(BUFFALO TRO)**
- 8:00 p.m. Meeting of the Nominating Committee

Poster Session I Indian Building
8:00 - 10:00 p.m. Refreshments Served

Monday, October 3

- 7:00 a.m. 🍴 Breakfast, Freeberg Hall
Posters for Session II may be set up in Indian Bldg.

Keynote Address

- 8:30 a.m. **Kathleen S. Matthews**, Rice University
Allostery & Subunit Assembly in the Lactose Repressor

9:30 a.m. Refreshments

Nucleic Acid Interactions

Moderator: *Marilyn Ferrari*

- 9:45 a.m. **Tim Lohman**, Washington Univ. School of Medicine
Thermodynamics of E. coli SSB - ssDNA Interactions
- 10:25 a.m. **Brad Chaires**, Univ. of Mississippi Medical Center
Analysis of drug-DNA binding isotherms: Reconsidering neighbor exclusion models
- 10:55 a.m. Refreshments
- 11:10 a.m. **Diane Frank**, Univ. of Wisconsin
Context dependence of interactions in lac repressor-operator complexes
- 11:30 a.m. **Michael D. Brenowitz**, Albert Einstein College of Medicine
Quantitative Footprinting of Protein-DNA Interactions
- 12:30 p.m. 🍴 Lunch, Freeberg Hall

 Free Time 
Posters will be available in the Indian Bldg.

Experimental Design & Analysis

Moderator: Marty Straume

- 3:00 p.m. **Susan Pedigo**, Univ. of Iowa College of Medicine
Energetics of Ca²⁺ Binding to Calmodulin
- 3:20 p.m. **Cing-Yuen Wong**, Univ. of Mississippi
Biosynthetic Incorporation of Tryptophan Analogs into Staphylococcal Nuclease A
- 3:40 p.m. 7 Refreshments
- 4:00 p.m. **Martin Straume**, Univ. of Virginia
Estimating Uncertainty in Model Descriptions of Experimental Data
- 4:30 p.m. **Michael L. Johnson**, Univ. of Virginia
Analysis of Experimental Data That DO NOT Meet Least-Squares Criteria
- 5:00 p.m. **Group Discussion of Nonlinear Least Squares Analysis**
- 6:00 p.m. ¶ Dinner, Freeburg Hall
- 7:30 p.m. Business Meeting

Poster Session II Indian Building
8:00 - 10:00 p.m. Refreshments Served

Tuesday, October 4

7:00 a.m. ¶ Breakfast, Freeburg Hall

Protein Folding

Moderator: Mike Hodsdon

- 9:00 a.m. **Ken Dill**, Univ. of Calif. San Francisco
Conformational Searching and the Kinetics of Protein Folding
- 9:40 a.m. **Liskin Swint**, Univ. of Iowa College of Medicine
Hydrogen Bonds and the pH Dependence of Ovomuroid Third Domain Stability
- 10:00 a.m. 7 Refreshments
- 10:20 a.m. **Neville Kallenbach**, New York University
α-Helix Stabilizing and Capping Interactions Studies in Synthetic Model Peptides
- 11:00 a.m. **Hue Sun Chan**, Univ. of California - San Francisco
Solvation: Effects of Molecular Size and Shape
- 11:20 a.m. **George Rose**, The Johns Hopkins School of Medicine
Helix Capping Motifs and Their Role in Helix Formation
- 12:00 p.m. Closing Remarks
- 12:30 p.m. Check out at Little Grassy Lodge by this time. Baggage may be stored in Indian Building.
- 12:30 p.m. ¶ Lunch, Freeburg Hall

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Poster Presentations on Sunday, Oct. 2

Protein Folding

Thermophilic proteins, protein stability and evolution.

W. J. Becktel.

Temperature and pressure induced unfolding of a mutant of staphylococcal nuclease A.

M. R. Eftink & G. D. Ramsay.

Intestinal fatty-acid binding protein: Effect of bound ligand on backbone amide exchange rates.

M. E. Hodsdon, J. J. Toner & D. P. Cistola.

Entropy of hydrogen bonding in proteins.

K. P. Murphy.

Hydrogen bonding in proteins: A model compound study.

S. Habermann & K. Murphy.

The effect of chloride ions on protein stability: Implications for GuHCl denaturation studies.

P. L. Wintrobe, G. I. Makhatadze & P. L. Privalov.

CheY thermostability and self-association.

G. T. DeKoster, A. D. Robertson, A. M. Stock, J. B. Stock & J. C. Hansen.

Hydrogen bonding and the pH dependence of protein stability.

A. D. Robertson, L. Swint, W. Schaller & P. M. Bowers.

The pressure denatured state of staphylococcal nuclease.

K. J. Frye & C. A. Royer.

Kinetics of pressure unfolding of staphylococcal nuclease.

G. J. A. Vidugiris & C. A. Royer.

Stability and interactions of recombinant fragments of troponin C.

R. S. Fredricksen & C. A. Swenson.

Development of a multi-dimensional CD-fluorescence spectrophotometer with a titration accessory: Application to the guanidinium induced unfolding of apomyoglobin and mutants of staphylococcal nuclease.

G. D. Ramsay, R. Ionescu, & M. R. Eftink.

What makes protein folding cooperative?

S. Bromberg & K. A. Dill

NMR structural characterization of partially folded species of BPTI analogs.

E. Barbar & C. Woodward.

Effects of Sucrose on the Internal Dynamics of Ribonuclease A.

A. Wang, A. Robertson, and W. Bolen.

Calorimetric Study of Denaturation Thermodynamics of Staphylococcal Nuclease in Guanidine Hydrochloride.

D. Liu, M. Yang, and W. Bolen.

An intermediate state in the denaturation of staphylococcal nuclease mutants.

J. H. Carra, E. A. Anderson & P. L. Privalov.

Contribution of hydrogen bonding to protein stability.

G. I. Makhatadze & P. L. Privalov.

From local secondary interaction to non-local tertiary interaction in a protein.

H. Qian & S. I. Chan

Structural Characterization of a Single Disulfide Derivative of Bovine α -Lactalbumin.

V. Hilser and E. Freire.

Thermodynamic Characterization of a Folding Intermediate of Staphylococcal Nuclease P117G Variant.

D. Xie, R. Fox, and E. Freire.

Packing density profiles of protein molecules.

G. Privalov and E. Freire.

Thermodynamic Characterization of the Thermal Stability and Ligand Interactions of the Aspartic Proteinase Endothiapepsin.

J. Gómez and E. Freire.

Molecular Recognition

Tight binding affinity of a monoclonal antibody for the T-cell receptor CD4 determined from the thermodynamic linkage to protons.

M. L. Doyle, T. D. Sokoloski, P. R. Dal Monte, & G. Louie.

Molecular recognition of Mg^{2+} by proteins and nucleic acids.

D. J. Williams, M. Nayal & E. Di Cera.

Studies of the pH dependence of ligand binding to TRP aporepressor from *Escherichia coli*.

M. Kavanoor, D. Hu, & M. R. Eftink.

Investigation of the requirements for a general base-catalyzed mechanism.

T. Baird, Jr., S. McGee, & C. A. Fierke.

Model of lactose repressor core based on alignment with sugar binding proteins is concordant with genetic and chemical data.

J. C. Nichols, N. K. Vyas, F. A. Quiocho & K. S. Matthews.

Structural Energetics of Molecular Recognition: Endothiapepsin/Pepstatin A Binding.

J. Gómez and E. Freire.

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Poster Presentations on Monday, Oct. 3

Nucleic Acid Interactions

The interaction of Δ and Λ Tris(phen)₂DPPZ]⁺ with DNA: A calorimetric and equilibrium binding studies.

I. Haq, B. Norden, B. Z. Cowdhry & J. B. Chaires.

Thermodynamic profile of daunorubicin binding to natural and synthetic DNA.

D. Suh & J. B. Chaires.

Thermal denaturation studies of the T4 gene 32 protein autoregulatory RNA.

D. P. Giedroc, K. Kaluarachchi, & H. Qiu.

Unexpected behavior of bacteriophage T4 gene 32 N-terminal domain mutants in cooperative binding to single-stranded nucleic acids.

J. L. Villemain & D. P. Giedroc.

Binding and bending of DNA by CRP is sequence dependent.

E. A. Pyles & J. C. Lee.

Functional roles of the subunit and domain interfaces in cAMP receptor protein activation.

X. Cheng & J. C. Lee.

Single-turnover kinetics of helicase-catalyzed DNA unwinding monitored continuously by fluorescence energy transfer.

K. P. Bjornson, M. Amaratunga, K. J. M. Moore, T. M. Lohman.

Apparent heat capacity change accompanying a non-specific protein-DNA interaction. *E. coli* SSB tetramer binding to oligodeoxyadenylates.

M. E. Ferrari & T. M. Lohman.

Biophysical Characterization of Native and Recombinant Sac7, a DNA-Binding Protein from the Extreme Thermophile *Sulfolobus acidocaldarius*.

S. Edmondson, J. McAfee, R. Gupta, J. Shriver.

Escherichia coli primary replicative helicase DnaB protein. Structure and interactions with ATP and ssDNA.

W. Bujalowski, U-S. Kim, & M. J. Jezewska.

GCMC thermodynamic analysis of effects of salt concentration on the binding of a model oligocation (L⁸⁺) to model polymeric DNA.

J. P. Bond, M. C. Olmsted, C. F. Anderson, & M. T. Record, Jr.

Studies of the binding of model peptides to double-stranded DNA using fluorescence and circular dichroism spectroscopies.

W. Zhang, S. Padmanabhan & M. T. Record, Jr.

Dependence of *Lac* repressor-operator binding on the length of operator-containing DNA fragment.

S. E. Melcher, D. E. Frank, M. M. Levandoski & M. T. Record

Structural probing of (E σ^{70})- λ P_R complexes.

M. L. Craig & M. T. Record, Jr.

Assessing the Energetic Consequences of Operator Mutations in the *Lac* Repressor System: Statistical Analysis.

D. E. Frank, J. P. Bond, S. Ross & M. T. Record, Jr.

Allosteric Regulation

Definition of carboxyl-terminal region critical for function in *lac* repressor Protein.

L. Li & K. Matthews.

Effects of Cl⁻ on the enthalpies associated with the intermediates of oxygenation of human and bovine hemoglobin.

M. Karavitis & C. Fronticelli.

Pairwise coupling: Deciphering cooperativity codes in biological macromolecules.

E. Di Cera

Structural and energetic components of Na⁺ binding to thrombin.

Y. Ayala, Q. Dang, M. Nayal and E. Di Cera.

Allosteric disruption of *Paramecium* calmodulin.

S. Harmon & M. A. Shea.

Mutational perturbation of calmodulin structure and function.

B. R. Sorensen, M. Hutchins, & M. A. Shea

Computational Studies of Cation Binding to Thrombin.

F. Kuntze and B. García-Moreno E.

Temperature Effects on Electrostatic Interactions in Proteins.

J. Dwyer, R. Wang, and B. García-Moreno E.

Oxygen Binding to Fallow-Deer (Dama Dama) Hemoglobin: Stepwise Enthalpies at pH 7. 4.

C. R. Johnson, M. Angeletti, S. Pucciarelli, and E. Freire.

Effects of osmolytes on the activity of aspartate transcarbamylase.

V. J. Licata, J. Trikha, & N. M. Allewell.

Thermodynamic Stabilities of Co(II)-complexes formed by wild-type and metal-ligand substitution mutants of T4 Gene 32 Protein

J. Guo, H. Qiu, and D. P. Giedroc

Intramolecular crosslink of human hemoglobin with long chain dicarboxylic acids.

E. Bucci, A. Razynska, H. Kwansa, C. Fronticelli, B. K. Urbaitis, J. H. Collins, R. Unger, J. Mout, X. Ji & G. Gilliland.

New Insights Into the Energetics of Cooperative Ligand Binding in Hemoglobin from Mutagenic Analysis

G. K. Ackers, J. M. Holt, V. J. LiCata, P. M. Dalessio & G. Lew