

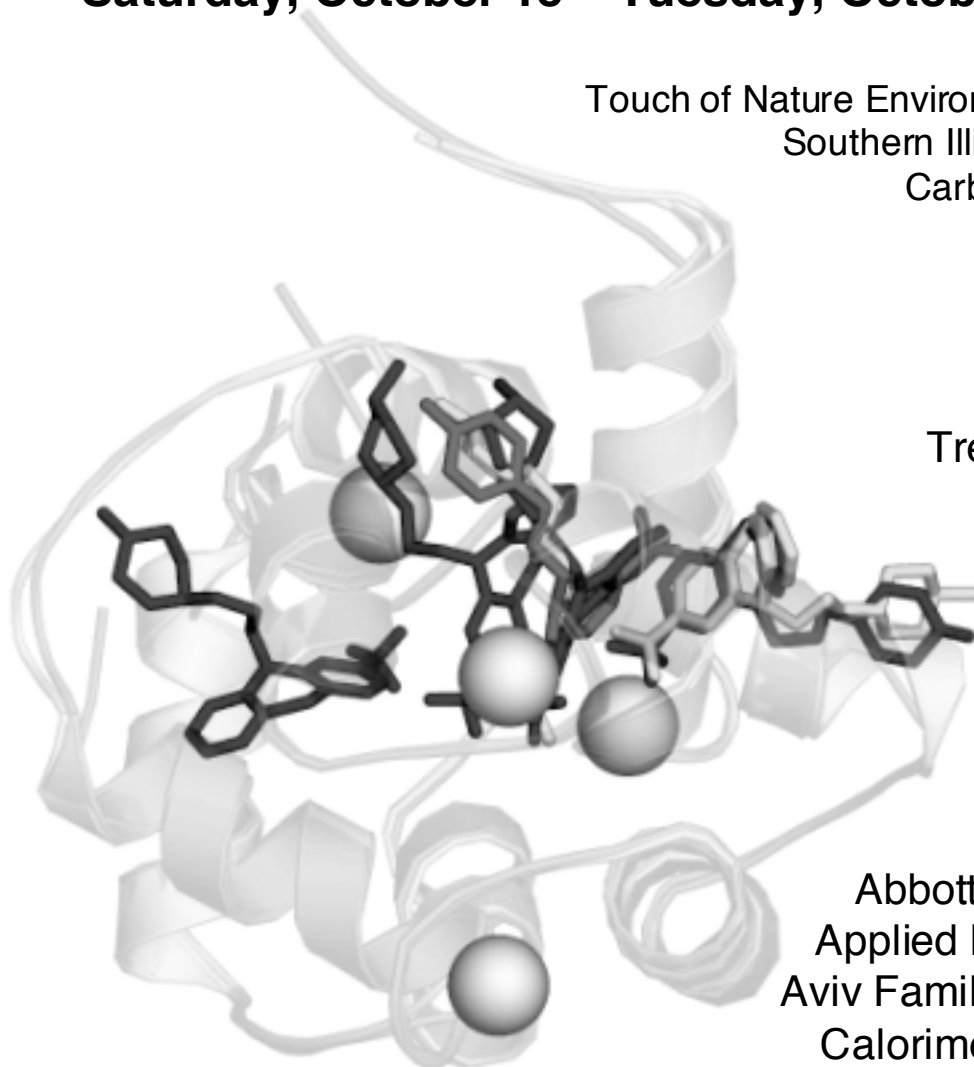
# 19<sup>th</sup> Annual Gibbs Conference on Biothermodynamics

Saturday, October 15 – Tuesday, October 18, 2005

Touch of Nature Environmental Center  
Southern Illinois University  
Carbondale, Illinois

## Organizers

Clay Clark  
Trevor Creamer



## Sponsors

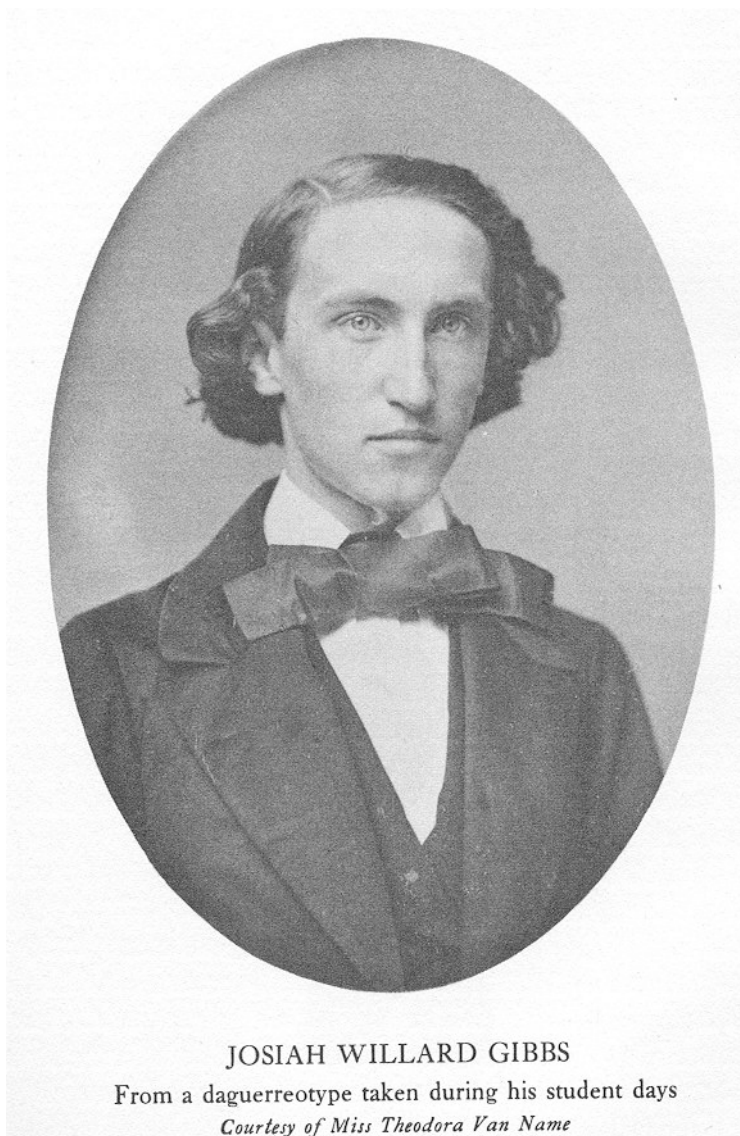
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**Cover figure:** Structural alignment of complexes of Calmodulin (CaM) with Trifluoperazine (TFP) in 1:1, 1:2, and 1:4 CaM:TFP ratios, RMSD = 0.59Å. Alignment and graphics created with Pymol™. Kindly provided by **Michael Feldkamp** (U. Iowa).

**1. The Gibbs Conference on Biothermodynamics  
is only possible because of:**



**Let's face it, without Mr. Gibbs we'd all be doing something else, like genetics, or (gasp!) kinetics...**

## **History of the Gibbs Conference on Biothermodynamics**

### **Touch of Nature Environmental Center, Carbondale, Illinois**

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Fall, 1986      1<sup>st</sup> discussion of the discipline of Thermodynamics in Biological Systems.  
held in Vail, Colorado: Gary Ackers, Wayne Bolen, Ernesto Freire, Stan  
Gill, Jim Lee

Feb, 1987      2<sup>nd</sup> discussion of the discipline of Thermodynamics in Biological Systems.  
held in New Orleans: Gary Ackers, Norma Allewell, Wayne Bolen, Ken  
Breslauer, Ken Dill, Ernesto Freire, Stan Gill, Jim Lee

### **Annual Gibbs Conference on Biothermodynamics**

1<sup>st</sup> – 1987      Organizers: Jim Lee & Wayne Bolen

2<sup>nd</sup> – 1988      Organizers: Gary Ackers & Michael Johnson

3<sup>rd</sup> – 1989      Organizers: Susan G, Frasier & Michael Johnson

4<sup>th</sup> - 1990      Organizers: Michael Johnson & Marty Straume

5<sup>th</sup> - 1991      Organizers: Gary Ackers & Tim Lohman  
Keynote: Ernesto Freire

6<sup>th</sup> - 1992      Organizers: Jim Lee & Tomasz Heyduk  
Keynotes: Serge Timasheff & John Schellman

7<sup>th</sup> - 1993:      Organizers: Maurice Eftink & Glen Ramsay  
Keynotes: Peter von Hippel & Julian Sturtevant

8<sup>th</sup> - 1994:      Organizers: Enrico Di Cera & Madeline Shea  
Keynotes: Gary Ackers & Kathleen S. Matthews

9<sup>th</sup> - 1995:      Organizers: Kenneth P. Murphy & Michael D. Brenowitz  
Keynotes: Victor Bloomfield & Mario Amzel

10<sup>th</sup> - 1996:      Organizers: Jonathan B. Chaires & Michael L. Doyle  
Keynotes: J. Michael Schurr & Allen Minton

11<sup>th</sup> - 1997:      Organizers: Dorothy Beckett & Jack Correia  
Keynote: Adrian Parsegian

- 12<sup>th</sup> - 1998: Organizer: Andy Robertson  
Keynote: David Draper
- 13<sup>th</sup> - 1999: Organizers: Bertrand Garcia-Moreno & John Shriver  
Keynotes: Wayne Bolen & Gary Ackers
- 14<sup>th</sup> – 2000: Organizers: George Turner & Kim Sharp  
Keynotes: Steve White (replaced Rodney Biltonen)
- 15<sup>th</sup> - 2001: Organizers: Margaret A. Daugherty & Luis A. Marky  
Keynote: George Rose
- 16<sup>th</sup> - 2002: Organizers: Michael Mossing & George Makhatadze  
Keynote: Rodney Biltonin
- 17<sup>th</sup> - 2003: Organizers: Vince Hilser & Dick Sheardy  
Keynote: Jim Lee
- 18<sup>th</sup> – 2004: Organizers: Doug Barrick & Kathleen Hall  
Keynote: Ignacio Tinoco
- 19<sup>th</sup> – 2005: Organizers: Clay Clark & Trevor Creamer  
Keynote: Carl Frieden

In 2002 The Gibbs Conference on Biothermodynamics incorporated as a mechanism of preserving the philosophy and spirit of the meeting. For a published 10 year history see Ackers and Bolen, "The Gibbs Conference on Biothermodynamics: Origins and evolution." *Biophys. Chem.* **64**, p 3-5, 1997.

**President:** Madeline Shea, Oct, 2004 – Oct, 2005.

**President Elect:** Dorothy Beckett.

**Secretary:** Margaret A. Daugherty, Oct, 2002 – Oct, 2008.

**Treasurer:** Michael Johnson, Oct, 2002 – Oct, 2007.

**Past Presidents:**

Gary Ackers, Oct, 2001 – Oct, 2002.

Jack Correia, Oct, 2002 – Oct, 2003.

Wayne Bolen, Oct, 2003 – Oct, 2004.

## 2. Meeting Schedule

### Saturday, October 15

4:00-7:00 Check-in

7:00-10:00 Reception in Indian Room

### Sunday, October 16

7:30 – 8:30 Breakfast in Freeberg Hall

#### Session I: Nucleic Acids

**Moderator: Melanie Bozza** (Seton Hall U., R. Sheardy lab)

9:00 Welcome (Clay Clark, Trevor Creamer and Madeline Shea)

9:10 Brad Chaires (U. Louisville)

*Uncovering the energetic basis of G-quadruplex stability.*

9:50 Mikhail Karymov (U. Nebraska, Y. Lyubchenko lab)

*Single molecule analysis of Holliday junction dynamics and branch migration.*

10:20 Break

10:45 Matt Freyer (Northern Arizona U., E. Lewis lab)

*Thermodynamic studies of the binding of netropsin and DAPI to several  $A_2T_2$  containing DNA hairpins.*

11:15 Kathleen Hall (Washington U.)

*Thermodynamics of the conformational change of a  $Mg^{2+}$ -sensing Riboswitch.*

12:00 Lunch in Freeberg Hall

## Session II: Stability & Evolution

**Moderator: Brian Cannon** (Johns Hopkins U., B. García-Moreno lab)

- 2:30 Matt Cordes (U. Arizona)  
*Mutationally induced changes in protein structure during evolution.*
- 3:10 Chris Olsen (U. Nebraska, L. Marky lab)  
*Unfolding of G-quadruplexes: Thermodynamic contributions for the stacking of two G-quartets with T→U substitutions.*
- 3:40 Break
- 4:00 Mirco Junker (U. Notre Dame, P. Clark lab)  
*The pertactin  $\beta$ -helix folding mechanism suggests common themes for the secretion and folding of autotransporter proteins.*
- 4:30 Sarah Woodson (Johns Hopkins U.)  
*How RNA gets in shape.*
- 5:15 **Keynote Address** – Carl Frieden (Washington U.)  
*Protein folding: Are we there yet?*  
Introduction by George Rose
- 6:30 Dinner in Freeberg Hall
- 8:00 Posters & Beer/Wine I in Sledgefoot Hall

## Monday, October 17

7:00 – 8:30 Breakfast in Freeberg Hall

### Session III: Denatured States

**Moderator: Veronique Chellgren** (U. Kentucky, T. Creamer lab)

- 9:00 Dan Raleigh (Stony Brook U.)  
*The role of the unfolded state in protein folding and stability.*
- 9:40 Nick Fitzkee (Johns Hopkins U., G. Rose lab)  
*How sterics and solvation reduce the size of protein conformational space.*
- 10:10 Break
- 10:40 Hoang Tran (Washington U., R. Pappu lab)  
*Towards an accurate model for protein denatured states.*
- 11:10 Neville Kallenbach (New York U.)  
*Structure in peptide models of unfolded proteins.*
- 12:00 Lunch in Freeberg Hall
- 12:00 Gibbs business meeting: All previous organizers please attend.



## Session IV: Macromolecular Interactions

**Moderator: Daniel Deredge** (LSU, V. LiCata lab)

- 2:30 Elizabeth Komives (U. California, San Diego)  
*Biophysics of the NF- $\kappa$ B/I $\kappa$ B $\alpha$  interaction.*
- 3:10 Olga Lubman (Johns Hopkins U., D. Barrick lab)  
*In vitro dissection of Notch/RBPjk interaction: Insights into the mechanism of Notch mediated transcriptional switch.*
- 3:40 Rhonda Newman (U. Iowa, M. Shea lab)  
*Interactions of calmodulin with regulatory regions of the ryanodine receptor type 1: Distinct roles of domains in protein allostery.*
- 4:10 Break
- 4:40 Aaron Lucius (UTMB Galveston, W. Bujalowski lab)  
*Allosteric interactions between the nucleotide-binding sites and the ssDNA-binding site in the PriA helicase-ssDNA complex.*
- 5:10 Jack Correia (U. Mississippi)  
*The use of multi-wavelength and fluorescence AUC: Case studies of tubulin regulatory factors and antimetabolic drugs.*
- 6:30 Dinner in Freeberg Hall – Buffalo Tro
- 8:00 Posters & Beer/Wine II in Sledgefoot Hall

## Tuesday, October 18

7:00 – 8:30 Breakfast in Freeberg Hall

### Session V: Membranes

**Moderator: Horia Petrache** (NIH, A. Parsegian lab)

8:30 Announcements

8:40 Lukas Tamm (U. Virginia)  
*Structural dynamics and thermodynamics of the gating of the OmpA ion channel.*

9:20 Yuhua Song (Washington U., N. Baker lab)  
*Molecular dynamics simulations of salicylate effects on the micro- and mesoscopic properties of a dipalmitoylphosphatidylcholine bilayer.*

9:50 Break

10:10 Damien Thevenin (U. Delaware, C. Robinson lab)  
*Folding and assembly of adenosine receptors.*

10:40 AnnMarie Stanley (Johns Hopkins U., K. Fleming lab)  
*Thermodynamics of dimerization of the outer membrane phospholipase A transmembrane  $\beta$ -barrel.*

11:10 Stephen White (U. California, Irvine)  
*Translocons, membranes, and the folding of membrane proteins.*

11:50 Wrap Up & Lunch

### 3. Posters

#### 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 evening and Session II on Monday evening. Both sessions will start at 8:00pm.

**Session I:** First authors\* whose last names begin with A through I. Posters may be mounted starting on Sunday morning. Please take your poster down by the break on Monday morning.

**Session II:** First authors\* whose last names begin with J through Z. Posters may be mounted starting on Monday morning. Please take your poster down before the talks start on Tuesday morning.



*"Look! The bar is open!"*

*"Yesss!"*

\* Note that we are using the last name of the first author listed on the poster. If you are presenting a poster but are not first author, please present in the session appropriate for the last name of the first author.

## Poster Session I: List of Presentations (A - I)

Oxygenation of normal human hemoglobin contains both cooperative and noncooperative binding steps. Why?

*Gary K. Ackers, Alexandra Klinger, Connie Yarian, Varsha Keelara and Jo M. Holt*

Domain interactions of yeast TBP.

*Claire A. Adams and Michael G. Fried*

Structure and mechanism of calmodulin binding to a cell surface targeting region of the N-methyl-D-aspartate receptor.

*Zeynep Akyol, Johannes W. Hell and Madeline A. Shea*

A method for jointly fitting fluorescence and absorbance AUC data.

*P. Holland Alday, Eric George, David Brown, Tom Laue, Walter Stafford, Peter Sherwood and John J. Correia*

5' coding region cis-acting determinants of bop-gene expression: secondary structure.

*Michael Arent and George J. Turner*

Calorimetric characterization of a TCR-peptide/MHC interaction.

*Kathryn M. Armstrong and Brian M. Baker*

UV resonance Raman studies of polyproline II structure in isotope edited alanine peptides.

*Wendy Barber-Armstrong, Sean Decatur and Ishita Mukerji*

Increased immunogenicity of an anchor-modified tumor-associated antigen is due to the enhanced stability of the peptide/MHC complex: implications for vaccine design.

*Tiffany K. Baxter, Oleg Y. Borbulevych, Jeffrey M. Carney, Paul Helquist, Nicholas P. Restifo and Brian M. Baker*

Thermodynamics and kinetics of the  $\text{NH-}\kappa\text{B}/\text{I}\kappa\text{B}\alpha$  and  $\text{NF-}\kappa\text{B}/\text{DNA}$  interactions.

*Simon Bergqvist, Carries Hughes, Thomas Huxford, Gourisankar Ghosh and Elizabeth Komives*

Effect of surfactant properties on the stability of the solubilized outer membrane protein ompX.

*C. L. Bianco, E. W. Kaler, A. M. Lenhoff and C. R. Robinson*

Transition state thermodynamics of the low- to physiological-temperature nondenaturational conformational change of bovine adenosine deaminase by slow scan rate differential scanning calorimetry.

*Melissa A. Bodnar and B. Mark Britt*

Unfolding dynamics of lima bean trypsin inhibitor by differential scanning calorimetry.  
*Melissa A. Bodnar and B. Mark Britt*

Synthetic porphyrazines: a new class of DNA binding molecules.  
*Melanie Bozza, Carlos Ramirez and Richard D. Sheardy*

Determining the mechanism of allosteric regulation of NikR binding to DNA activated by Ni<sup>2+</sup> binding.  
*Michael Bradley, Peter Chivers and Nathan Baker*

Outer membrane protein F demonstrates strong self-association.  
*Nancy K. Burgess and Karen Fleming*

Nonlinear regression fitting algorithm for multiple independent binding equilibria, Monte Carlo error analysis, and Saroff distributions.  
*R. Buscaglia, M. W. Freyer and E. A. Lewis*

pKa values of internal ionizable residues in ribonuclease H.  
*Brian Cannon and Bertrand García-Moreno*

Oligoproline effects on the structural properties of polyglutamine.  
*Veronique Chellgren, Brian Chellgren, Ronald Wetzal and Trevor Creamer*

SNF: a bifunctional RNA binding protein.  
*Alan Chen and Kathleen Hall*

Molecular determinants of pKa values: role of backbone flexibility and of short-range interactions in networks of polar and ionizable residues.  
*Michael S. Chimenti, Kelli Baran, Carolyn Fitch, Jamie Schlessman, Katie Herbst and Bertrand García-Moreno*

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*

A computational analysis of progesterone receptor-DNA binding isotherms: insight into transcriptional regulation.  
*K. D. Connaghan-Jones, A. F. Heneghan, M. T. Miura and D. L. Bain*

Biophysical investigation of the TCR-peptide/MHC interaction: a comparative study of two receptors that bind a common ligand.  
*Rebecca L. Davis-Harrison and Brian M. Baker*

Structural, thermodynamic, and kinetic comparisons of the binding of full-length  $\gamma$ TBP and C-terminal core TBP with DNA.

*Roberto Delgadillo, JoDell Whittington, Michael Brenowitz and Larry Parkhurst*

Dissimilar “glutamate effects” on DNA binding by the type I DNA polymerases from *E. coli* and *T. aquaticus*.

*Daniel J. Deredge, Gregory S. Thompson, Carmen R. Ruiz, Ke Jiang, Clayton F. Runfalo and Vince J. LiCata*

DNA binding properties and activation of the ATPase activity of adenoassociated virus Rep40 helicase.

*John David Dignam, Susan S. Dignam, Roy F. Collaco, Patrick Needham and James P. Trempe*

Lanthanide spectroscopic studies of Mg(II)-dependent *PvuII* restriction endonuclease.

*Cynthia M. Dupureur, Lori M. Bowen, Gilles Muller and James P. Riehl*

Transmembrane domain interactions contribute to Erythropoietin Receptor activation.

*Alex Ebie and Karen G. Fleming*

Structure and stability of Sso10b2, a hyperthermophile RNA and DNA binding protein.

*Stephen P. Edmondson, Andrew T. Clark, Tracy L. Armstrong and John W. Shriver*

Chain length dependence of *de novo* tailspike folding.

*Michael S. Evans, Mary C. Finn and Patricia L. Clark*

Molecular basis of CaMKII regulation by calmodulin: calcium-dependence of kinase binding.

*T. Idil Apak Evans and Madeline A. Shea*

Interactions of the anti-psychotic drug trifluoperazine with calmodulin and its effects on  $\text{Ca}^{2+}$  binding affinity.

*Michael D. Feldkamp, Susan E. O'Donnell and Madeline A. Shea*

Differentiating the ligand's chemical requirements for allosteric interactions from those for protein binding; phenylalanine inhibition of pyruvate kinase.

*Aron W. Fenton and Gissel McDonald*

Thermodynamics of paperclip DNA triplexes.

*Daniel P. Flaherty and Luis A. Marky*

Investigating the heat capacity effect associated with RNA processes.

*Leslie Frank, Brian Doctrow and David Draper*

Unfolding thermodynamics of a DNA decamer duplex containing dG→deaza-dG substitutions.

*Manjori Ganguly, Luis A. Marky and Barry I. Gold*

Predicting interactions between cytoskeletal proteins.

*Shatadal Ghosh and David Sept*

Increasing protein stability through rational redesign of surface charge-charge interactions.

*Alexey V. Gribenko, Samantha S. Strickler, Alexander V. Gribenko, Timothy R. Keiffer and George I Makhatadze*

Evidence for an evolutionary conserved DNA-recognition code at work in the Cro protein family of transcription factors.

*Branwen M. Hall, Kelly R. LeFevre and Matthew H. J. Cordes*

Osmotic pressure probes interactions in lipid-DNA complexes.

*Daniel Harries, Horia I. Petrache, V. Adrian Parsegian, Dganit Danino and Ellina Kesselman*

Quantitative analysis of progesterone receptor function: role of salt and salt-type in regulating self-association.

*Aaron F. Heneghan, Keith Connaghan-Jones, Michael T. Miura and David L. Bain*

Site-specific mutagenesis of the rat  $\beta$ -parvalbumin CD site.

*Michael T. Henzl and Kelly Ndubuka*

Protein stabilization and the effect of mixed osmolyte solutions: an analysis of the intrinsic stabilizing ability of osmolytes.

*Luis Marcelo F. Holthauzen and D. W. Bolen*

Electrostatic side-chain couplings in the gating of the OmpA ion channel suggest a mechanism for pore opening.

*Heedeok Hong, Gabor Szabo and Lukas K. Tamm*

A general and efficient way of expressing peptide for NMR studies of class I MHC/peptide complexes.

*Francis K. Insaadoo and Brian M. Baker*

## Poster Session II: List of Presentations (J – Z)

Dynamics of *E. coli* RecA filament formation on ssDNA tail of a ssDNA-dsDNA junction.  
*C. Joo, M. Nakamura, S. A. McKinney, I. Rasnik and T. Ha*

Effects of DNA structure DNA binding of  $O^6$ -alkylguanine-DNA alkyltransferase (AGT).  
*Sambit R. Kat, Anthony E. Pegg and Michael G. Fried*

Molecular dynamics simulations of mixed lipid bilayers.  
*Stephen P. Kelty, Roger McMullen and George Turner*

Unfolding of intramolecular triplexes with exclusive TAT base-triplets.  
*Irine Khutsishvili, Ronald Shikiya and Luis A. Marky*

Electrostatic effects in repeat proteins: salt dependence of unfolding of YopM, a leucine-rich-repeat protein.  
*Ellen Kloss and Doug Barrick*

Spectroscopic and molecular dynamics evidence for a sequential mechanism for the DNA A→B transition.  
*Kelly M. Knee, Colin E. Aitken, Sergei Y. Ponomarev, Surjit Dixit, David L. Beveridge and Ishita Mukerji*

Effects of monovalent salt on the observed enthalpy and heat capacity change for *E. coli* SSB binding to ssDNA.  
*Alexander G. Kozlov and Timothy M. Lohman*

Study of DNA-Sfi I complex stability using AFM force spectroscopy.  
*Alexey V. Krasnoslobodtsev, Luda S. Shlyakhtenko, Egor V. Ukraintsev and Yuri L. Lyubchenko*

Thermodynamics of yeast (*Saccharomyces cerevisiae*) replication protein A binding to single-stranded DNA.  
*S. Kumaran, Alexander G. Kozlov and Timothy M. Lohman*

*In vitro* targeting of DNA triplexes with oligonucleotides.  
*Hui-Ting Lee, Ronald Shikiya and Luis A. Marky*

Structure of the SfiI-DNA complexes analyzed by atomic force microscopy.  
*Alexander Y. Lushnikov, Vladimir N. Potaman, Elena A. Oussatcheva, Richard R. Sinden and Yuri L. Lyubchenko*



Communications between distant sites in envelope protein domain III of neutralization-resistant mutants of West Nile virus.

*Rodrigo Maillard, Matthew Jordan and J. Ching Lee*

Assembly of  $\lambda$  terminase protomers into a viral DNA processing and packaging machine.

*N. Karl Maluf, H. Gaussier, M. Feiss and C. E. Catalano*

Predicting the binding location of phospholipids on capping protein.

*Michelle McCully and David Sept*

The effect of cations on the structure and function of NikR proteins.

*Alyssa A. Meheen, Erin L. Benanti and Peter T. Chivers*

Allosterism in the binding of AGT to short single-stranded DNAs.

*Manana Melikishvili and Michael G. Fried*

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*

The effect of dinitroanilines on parasitic protozoan tubulin dynamics.

*Arpita Mitra and David Sept*

The biotin repressor: complexibility in the function of a flexible loop in an allosteric response.

*Saranga Naganathan and Dorothy Beckett*

Pulse proteolysis: a simple method for quantitative determination of protein stability and ligand binding.

*Chiwook Park and Susan Marqusee*

Measured depletion of ions at the biomembrane interface: implications on intermembrane interactions.

*Horia I. Petrache, Daniel Harries and V. Adrian Parsegian*

Unfolding thermodynamics of DNA duplex-hairpin motifs.

*Karim P. Ramos, Ronald Shikiya and Luis A. Marky*

Thermal stability landscape for Klenow DNA polymerase as a function of pH and salt concentration.

*Allison J. Richard, Alexandra L. Klinger, Matthew J. Todd and Vince J. LiCata*

Pressure-modulation temperature-scanning calorimetry.

*Jörg Rösgen, Kristian Boehm and Hans-Jürgen Hinz*

Osmolyte dependence of biochemical reactions quantified by the phase diagram method.

*Jörg Rösgen, Allan C. Ferreon, Josephine Ferreon and David Wayne Bolen*

Allosteric mechanism of the EPD mutation in BK<sub>Ca</sub> channel gating.

*Akansha Saxena and David Sept*

A multiscale model for actin filaments.

*David Sept and Aravind Rammohan*

Thermal unfolding of the  $\beta$ -hairpin peptide trpzip-4.

*Werner W. Streicher and George I. Makhatadze*

Determination of the ATP coupling stoichiometry during *E. coli* UvrD monomer ssDNA translocation.

*Eric J. Tomko, Christopher J. Fischer and Timothy Lohman*

RNA-binding domain of human U1A: expression, purification and characterization of the wild type and engineered variant.

*Jessica M. Tomlinson, Samantha S. Strickler and George I. Makhatadze*

5' coding region cis-acting determinants of *bop* gene expression: primary structure.

*George J. Turner and Michael Arent*

Evaluating the conformational flexibility of stalled nascent chains by fluorescence anisotropy.

*Krastyu G. Ugrinov, David A. Johnson and Patricia L. Clark*

Conformation-dependent interprotein interactions studied by AFM force spectroscopy.

*Egor V. Ukraintsev, Tatiana O. Zaikova, John F. W. Keana and Yuri L. Lyubchenko*

Characterization of HU-cruciform DNA interaction.

*Iulia Vitoc and Ishita Mukerji.*

The importance of solvent detail in modeling biomolecular solvation.

*Jason A. Wagoner and Nathan A. Baker*

What role does the denatured sub-ensemble play in determining the native fold of a protein?

*Suwei Wang, Steven T. Whitten, Tong Liu and Vincent J. Hilser*