

# DEPARTMENTS OF CHEMISTRY AND BIOCHEMISTRY/BIOPHYSICS CHEMICAL BIOPHYSICS MINI-SYMPOSIA SERIES

## PAST SYMPOSIUM



UPCOMING  
SYMPOSIA

EXECUTIVE  
COMMITTEE

DEPARTMENT OF  
BIOCHEMISTRY  
& BIOPHYSICS

DEPARTMENT OF  
CHEMISTRY

PAST  
SYMPOSIA

2009:

[Third Annual Chemistry-Biology Interface Picnic](#)

July 24, 2009  
Swarthmore College

[Lasers in Chemistry, Biochemistry, and Medicine](#)

March 19, 2009

2008:

[Oxidation and Reduction](#)

November 18, 2008

[Second Annual Chemistry-Biology Interface Scientific Picnic](#)

July 25, 2008  
Sponsor: NIH Chemistry-Biology Interface Fellowship

[Membrane Structure, Assembly, and Traffic](#)

May 6, 2008  
Financial Sponsor: [Avanti Polar Lipids](#)

2007:

[Chemical Genomics](#)

December 13, 2007  
Financial Sponsors: [PerkinElmer](#) and [ThermoFisher Scientific](#)

[Chemistry/BMB/Wistar Trainee Retreat](#)

July 13, 2007

[Influenza Symposium](#)

February 22, 2007  
Financial Sponsor: [Influmedix](#)

2006:

[The Nature and Role of Water as a Biological Solvent Symposium](#)

October 12, 2006

[Amyloid: Structure & Biology](#)

April 27, 2006  
Financial sponsors: [OLIS, Inc.](#)

[Computational Analysis of Protein Structure and Function](#)

March 9, 2006  
Financial sponsors: [Greater Philadelphia Bioinformatics Alliance](#)

2005:

Metallomolecules

November 17, 2005

Financial Sponsors: Bruker Biospin, GSAC

Trainee Symposium: Membranes and Molecular Recognition

October 25, 2005

Financial Sponsors: Optical Apparatus and GSAC

Single Molecule Studies

April 21, 2005

Financial Sponsors: Optical Apparatus, GSAC

On-Campus Co-Organizer\*: [Nano-Bio Interface Center \(NBIC\)](#)

Protein Design

March 10, 2005

Financial Sponsors: SynPep

2004:

Structure-Based Drug Design

November 18, 2004

Financial Sponsor: Merck Research Labs

Bioinorganic Chemistry: Metalloenzymes

April 22, 2004

Financial Sponsor: Polymedix

Protein Folding

February 26, 2004

Financial Sponsors: Proterion, GSAC

2003:

Inhibitors of Protein-Protein Interactions

November 20, 2003

Financial Sponsors: Biacore

\*Organizer in addition to the Department of Chemistry and the Department of Biochemistry & Biophysics.

All symposia from Fall 2003 - Spring 2006 received partial funding from the Provost's Interdisciplinary Seminar Fund.

## Third Annual Chemistry-Biology Interface Picnic

Friday, July 24, 2009  
Swarthmore College

10:00 a.m. - 12:00 p.m. / **Morning Speakers** / Science Center 101

Julia Richards, Department of Chemistry

"Photoregulation of the 10-23 DNAzyme"

**Bryan Gibb, BMB**

"Breaking down the active site of Cre recombinase: understanding the mechanism of cleavage and ligation"

**Geronda Montalvo, BMB**

"Infrared spectroscopy and folding kinetics of a  $\beta$ -peptide helix

**Ning Shangguan, Department of Chemistry**

Roquefortine C and related biological activities

1:00 p.m. - 2:00 p.m. / **Poster Session**

**Two hydrolase whodunits: on the trail of the yeast histone H4S1 phosphatase and the ant H3 tail clipping protease**

Ed Ballister, Berger Lab, BMB

**Bio-inorganic interface: Ferritin-nanoparticle systems**

Jasmina Cheung-Lau, Dmochowski Lab, Department of Chemistry

**Harnessing Hsp104 to eliminate AB42 fibers implicated in Alzheimer's Disease**

Mimi Cushman, Shorter Lab, Neuroscience Graduate Group

**Structure based drug design of human papillomavirus E7 inhibitors**

Daniela Fera, Marmorstein Lab, Department of Chemistry/Wistar

**Photoregulating gene expression with light activated oligonucleotides**

Julie Griepenber, Dmochowski Lab, Department of Chemistry

**Molecular mechanism and specificity of substrate binding by the E3 Ubiquitin Ligase Pellino**

Yu-San Huoh, Ferguson Lab, BMB

**A mechanism of calcium binding for the regulation of myosin Ib in its role as a tension sensor**

John Lewis, Goldman Lab, CAMB

**The x-ray crystal structure of Acetylpolyamine Amidohydrolase (APAH) from Mycoplasma ramosa**

Pat Lombardi, Christianson Lab, Department of Chemistry

**Characterization of novel PtdIns (4,5)P2 effector domains**

Katarina Moravcevic, Lemmon Lab, BMB

**Motor number controls cargo switching at actin-microtubule intersections in vitro**

Trey Schroeder, Goldman Lab, BMB

**Dynamics of tRNA motions during protein synthesis: Single molecule studies of ribosomes in the pre- and post-translocation states**

Ben Stevens, Goldman Lab, Muscle Institute

**Conformational changes of Hsp104 seen by Small Angle X-ray Scattering (SAXS)**

Elizabeth Sweeny, Shorter Lab, BMB

**The crystal structure of the Rtt109-Vps75 HAT-histone chaperone complex**

Yong Tang & Katie Meeth, Marmorstein Lab, Wista

**Development of novel methods for the synthesis and control of protein structure**

Mark Fagley & Anne Wagner, Petersson Lab, Department of Chemistry

**Validation of 1-aminoanthracene as a fluorescent general anesthetic**  
Zhengzheng (Katie) Liao, Dmochowski Lab, Department of Chemistry

**Mapping foldome changes in cell lysates with cysteine labeling kinetics**  
Brian Chase, Discher Lab, Bioengineering

2:00 p.m. - 4:00 p.m. / **Afternoon Speakers** / Science Center 101

**Brandon Kelley**, Department of Chemistry  
"Nucleophilic ring-opening of trisubstituted aziridines"

**Jasna Maksimoska**, Department of Chemistry/Wistar  
"Structure-based design of organometallic PAK1 inhibitors"

**Kathryn Smith**, BMB  
"Probing the mechanism of action of antimicrobial peptides through lipid diffusion"

**Daniel Dowling**, Department of Chemistry  
"An unexpected protein superfamily: Arginase, Histone Deacetylase, and Acetylpolyamine Amidohydrolase"

**Organizers:**

Julie Aaron  
Daniela Fera  
Brittani Ruble  
Trey Schroeder  
Kate Thorn

**LASERS IN CHEMISTRY, BIOCHEMISTRY, AND MEDICINE**

**Thursday, March 19, 2009**

**1:30 p.m. - 6:45 p.m.**

**Lynch Room, Chemistry Building**

1:30 - 2:10 p.m.

**Bruce Tromberg**, University of California, Irvine  
Spectroscopy and imaging in medicine: moving benchtop optical technologies to the bedside

2:10 - 2:25 p.m.

**Patrick Mayes**, El-Deiry Lab, Department of Pharmacology  
Noninvasive vascular imaging in fluorescent tumors using multispectral unmixing

2:25 - 2:40 p.m.

**XinJing Tang**, Dmochowski Lab, Department of Chemistry  
Using confocal laser scanning microscopy to probe the mechanism of anesthesia in animal models

2:40 - 2:55 p.m.

**Louise Sinks**, Vinogradov Lab, Department of Biochemistry and Biophysics  
Oxygen microscopy with two-photon enhanced phosphorescence nanoprobes

2:55 - 3:35 p.m.

**Charles Shank**, Howard Hughes Medical Institute, Janelia Farm  
Sculpting light for bioimaging and more

3:35 - 3:55 p.m. Coffee Break

3:55 - 4:35 p.m.

**William Eaton**, National Institute of Health

Single molecule FRET trajectories and protein folding transition path times

4:35 - 4:50 p.m.

**Matthias Waegle**, Gai Lab, Department of Chemistry

Folding rates of protein secondary and supersecondary structures in crowded environments

4:50 - 5:05 p.m.

**Dmitriy Vorobyev**, Hochstrasser Lab, Department of Chemistry

Ultrafast dynamics of small ions

5:05 - 4:20 p.m.

**Tim Sechler**, Lester Lab, Department of Chemistry

The role of conical intersections in the quenching of excited electronic states

5:20 - 6:00 p.m.

**Mostafa A. El-Sayed**, Georgia Institute of Technology

Gold nanoparticles, properties and some applications in nano-biology and nano-medicine

6:00 - 6:45 p.m.

Reception in Nobel Hall, Chemistry Building (basement)

**ORGANIZING COMMITTEE:**

Smita Mukherjee, Graduate Student, Chemistry

Julie Glasscock Rogers, Graduate Student, BMB

Amanda Remorino, Graduate Student, Chemistry

Matt Tucker, Post-doctoral fellow, Chemistry

**FACULTY ADVISORS:**

Feng Gai, Professor, Departments of Chemistry and BMB

Robin Hochstrasser, Department of Chemistry and Director of the Regional Laser and Biomedical Technology Laboratories

**SPONSORS:**

Graduate and Professional Student Assembly (GAPSA)

Biomedical Graduate Student Association (BGSA)

The Regional Laser and Biomedical Technology Laboratories (RLBL)

The Department of Chemistry

The Department of Biochemistry & Biophysics

**OXIDATION AND REDUCTION**

**Tuesday, November 18, 2008**

**1:15 p.m. - 6:00 p.m.**

**Grossman Auditorium, The Wistar Institute**

1:15 p.m. - 2:00 p.m.

**John Caradonna**, Boston University

Using synthetic models to re-evaluate the mechanisms of binuclear non-heme iron monooxygenases: do diamonds last forever?

2:00 p.m. - 2:20 p.m.

**Jong-Heum Park**, Penning Lab, Department of Pharmacology

Benzo[a]pyrene-7,8-dihydrodiol produces reactive oxygen species via the Aldo-Keto Reductase (AKR) pathway

in A549 cells: Involvement of B[a]P-mediated redox cycling and alteration in redox status

2:20 p.m. - 2:40 p.m.

**Luigi Di Costanzo**, Christianson and Penning Labs, Department of Chemistry  
Structure and catalytic mechanism of human steroid 5 $\beta$ -reductase (AKR1D1)

2:40 p.m. - 3:25 p.m.

**Anne Jones**, Arizona State University  
Exploring and exploiting redox enzymes

3:45 p.m. - 4:00 p.m.

**Bruce Lichtenstein**, Dutton Lab, Department of Biochemistry and Biophysics  
Addressing biological quinone control in *de novo* proteins

4:00 p.m. - 4:20 p.m.

**Ivan Korendovych**, DeGrado Lab, Department of Biochemistry and Biophysics  
Computational design and experimental characterization of an electron transfer membrane protein

4:20 p.m. - 5:05 p.m.

**Gary Brudvig**, Yale University  
Water oxidation chemistry of photosystem II and artificial systems

5:05 p.m. - 6:00 p.m.

Reception in Wistar Atrium

**SPONSORS:**



Graduate and Professional Student Assembly (GAPSA)  
Biomedical Graduate Student Association (BGSA)  
The Department of Chemistry  
The Department of Biochemistry & Biophysics

**SECOND ANNUAL CHEMISTRY-BIOLOGY INTERFACE**

**July 25, 2008**

**Scientific Picnic at Swarthmore College**

9:20 a.m. - 10:00 a.m.

**Check-in and Breakfast**, Science Center 101

10:00 a.m. - 12:00 p.m.

**Morning Speakers**, Science Center 101

**Peng Xie**, Department of Chemistry/Wistar Institute  
Structure-based design of a potent and specific organoruthenium PI3K inhibitor

**Christopher Butts**, Department of Chemistry  
Fluorescence screening assay for apoferritin binders: A tool for gabaergic anesthetic discovery?

**Julie Aaron**, Department of Chemistry  
Structure of a <sup>129</sup>Xe-cryptophane biosensor complexed with human carbonic anhydrase II

**Julie Glasscock**, BMB  
Using an amino-acid FRET pair to probe protein unfolding

12:00 p.m. - 1:00 p.m.

**Picnic Lunch**

Upper Tarble, Clothier Hall

1:00 p.m. - 2:00 p.m.

**Poster Session**

Upper Tarble, Clothier Hall

**Kim Malecka**, Marmorstein Lab, Department of Chemistry/Wistar  
Crystal structure of a p53 core tetramer bound to DNA

**Julia Richards & Julie Gripenburg**, Dmochowski Lab, Department of Chemistry  
Photoactivatable oligonucleotides for controlling gene expression

**Yong Tang**, Marmorstein Lab, Department of Chemistry/Wistar  
Structure/function studies on the H3K56-acetylating HAT Complex Rtt109-Vps75

**Joe Swift & Jasmina C. Cheung-Lau**, Dmochowski Lab, Department of Chemistry  
Functionalization of colloidal gold using self-assembled ferritin-like systems

**Seth Hayik**, University of Florida and Fox Chase Cancer Center  
Calculating binding affinities of zinc proteins using QM/MM methods

**Smita Mukherjee**, Gai Lab, Department of Chemistry  
Folding kinetics of naturally occurring helical peptides

**Lin Guo**, Gai Lab, Department of Chemistry  
Probing the role of hydration in the unfolding transitions of carbonmonoxy myoglobin and apomyoglobin

**Jose Manuel Perez Aguilar**, Saven Lab, Department of Chemistry  
Computational design of single-chain four-helix bundle proteins that bind non-biological cofactors

**Christopher MacDermaid**, Saven Lab, Department of Chemistry  
Bundle builder: An efficient method for generating large ensembles of helical bundle structures for directed protein design

**Aru Hill & Gary Seward**, Dmochowski Lab, Department of Chemistry  
Towards the development of Xenon-129 magnetic resonance biosensors

**Carol Schultz**, Penning Lab, BMB  
Human AKRs display quinone reductase activity with PAH *o*-quinones

**Michael Harbut**, Greenbaum Lab, Department of Pharmacology  
Development of bestatin-based activity-based probes

2:00 p.m. - 4:00 p.m.

**Afternoon Speakers**, Science Center 101

**Andre Isaacs**, Department of Chemistry  
Synthesis of novel steroidal analogs of cyclopamine

**Yao Zhang**, Department of Chemistry  
Molecular design of TM helical bundle as a tool for probing the feature that drives folding in membrane

**Claude Warzecha**, Cell and Molecular Biology  
Epithelial Splicing Regulatory Proteins 1 & 2 are novel cell type-specific splicing regulatory

proteins identified through a genome-scale functional screen in mammalian cells

**Venkata Krishnan**, Department of Chemistry  
Functional biomolecular materials incorporating non-biological cofactors into amphiphilic 4-helix bundle peptides

4:00 p.m. - 5:00 p.m.  
Reception, Outdoor games, Parish Lawn

5:00 p.m. - 6:00 p.m.  
Buffet Dinner, Upper Table, Clothier Hall

**ORGANIZING COMMITTEE:**

Julie Aaron, Department of Chemistry  
Diana Cabral, Department of Chemistry  
Sarah Chobot, BMB  
Daniela Fera, Department of Chemistry  
Andre Isaacs, Department of Chemistry

**MEMBRANE STRUCTURE, ASSEMBLY, AND TRAFFIC**

**Tuesday, May 6, 2008**  
**Lynch Auditorium, Chemistry Building**  
**1:00 - 6:00 p.m.**

1:00 p.m. - 1:45 p.m.  
**Ken Jacobson**, University of North Carolina, Chapel Hill  
Post-raft era nano- and microdomains

1:45 p.m. - 2:05 p.m.  
**Aiwei Tian**, Baumgart group, Department of Chemistry  
Curvature and composition coupling in lipid bilayer membrane tubes

2:05 p.m. - 2:25 p.m.  
**Julie Glasscock**, Gai group, Department of Chemistry  
Single-molecule study of M2 proton channel conformational dynamics

2:25 p.m. - 3:10 p.m.  
**Wonhwa Cho**, University of Illinois, Chicago  
Spatiotemporal regulation of cellular processes by lipids and lipid-binding proteins: Proteomics and single molecule studies

3:30 p.m. - 4:15 p.m.  
**Frank Brown**, University of California, Santa Barbara  
Elastic and coarse-grained models for biomembranes

4:15 p.m. - 4:35 p.m.  
**Bryan Berger**, DeGrado group, Department of Biochemistry and Molecular Biophysics  
Transmembrane domain interactions in regulation of beta 1 integrins

4:35 p.m. - 5:20 p.m.  
**Randy Schekman**, University of California, Berkeley  
Developmental lesions associated with protein sorting defects in the secretory pathway



5:20 p.m. - 6:00 p.m.  
Reception, Nobel Hall, Chemistry Building

**CHAIR:**

Julie Aaron

**FACULTY ADVISORS:**

Feng Gai, Department of Chemistry  
Tobias Baumgart, Department of Chemistry  
Bill DeGrado, Department of Biochemistry & Biophysics

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Biomedical Graduate Student Association (BGSA)  
The Department of Biochemistry & Biophysics  
The Department of Chemistry

**CHEMICAL GENOMICS**

**Thursday, December 13, 2007**  
**Grossman Auditorium, The Wistar Institute**  
**12:45 P.M. - 6:00 P.M.**

12:45 p.m. - 1:30 p.m.  
**Scott Diamond**, University of Pennsylvania  
The Penn Center for Molecular Discovery: lessons from the first million wells

1:30 p.m. - 1:50 p.m.  
**Peng Xie**, Marmorstein Lab, The Wistar Institute  
In search of potent and specific BRAF inhibitors through *in vitro* high-throughput screening

1:50 p.m. - 2:10 p.m.  
**Nancy Carillo**, Bode Lab, Department of Chemistry  
Aqueous synthesis of  $\beta^3$ -oligopeptides

2:10 p.m. - 2:55 p.m.  
**Jon Ellman**, University of California, Berkeley  
Substrate activity screening - a powerful new method for inhibitor discovery

3:10 p.m. - 3:55 p.m.  
**Jun Liu**, Johns Hopkins University  
Forward and reverse chemical genetic approaches toward angiogenesis

3:55 p.m. - 4:15 p.m.  
**Ryan Coleman**, Sharp Lab, Department of Genomics and Computational Biology  
Two computational tools to analyze small molecule binding sites in proteins: Travel Depth and Geometric Patch Generation

4:15 p.m. - 4:35 p.m.  
**XinJing Tang**, Dmochowski Lab, Department of Chemistry  
Controlling gene silencing with caged oligonucleotides in K562 and zebrafish

4:35 p.m. - 5:20 p.m.

Suzanne Walker, Harvard University  
Glycosyltransferase inhibitors

5:20 p.m. - 6:00 p.m.  
Reception in the Wistar Atrium

**CHAIR:**

Julia Richards

**FACULTY ADVISORS:**

Amos Smith, Chemistry  
Ronen Marmorstein, Wistar/Chemistry/BMB  
Doron Greenbaum, Pharmacology  
Donna Hurny, Penn Center for Molecular Discovery

**SPONSORS:**



Graduate and Professional Student Assembly (GAPSA)  
The Department of Chemistry  
The Department of Biochemistry & Biophysics

**CHEMISTRY/BMB/WISTAR TRAINEE RETREAT**

**Friday, July 13, 2007**

**Location: Swarthmore College**

**SCHEDULE OF EVENTS**

9:20 - 10:00 a.m. Check-in and Breakfast, Science Center 101

10:00 - 12:00 p.m. **MORNING SPEAKERS**, Science Center 101

Michelle Bunagan, Department of Chemistry  
XinJing Tang, Department of Chemistry  
Kay Perry, Biochemistry and Molecular Biophysics (BMB)  
Brandi Sanders, Chemistry/Wistar Institute  
Lin Guo, Department of Chemistry  
Doug Metcalf, BMB

12:00 - 12:30 p.m. **PICNIC LUNCH**  
Box Lunch pickup at Upper Tarble, Clothier Hall

12:30 - 2:00 p.m. **POSTER SESSION**  
Upper Tarble, Clothier Hall

Mike Brent, Marmorstein Lab (Wistar/Chemistry)  
Sarah Chobot, Dutton Lab (BMB)  
Erin Forbeck, Joullie Lab (Chemistry)  
Heather Gennadios, Christianson Lab (Chemistry)  
Bryan Gibb, Van Duyne Lab (BMB)  
David Hokanson, Ostap Lab (BMB)  
Manqing Hong, Marmorstein Lab (Wistar/Chemistry)  
Daryl E. Klein, Lemmon Lab (BMB)  
Ken Lassen, Joullie Lab (Chemistry)  
Dongli Pan, Cooperman Lab (Chemistry)

Haiou Qin, Cooperman Lab (Chemistry)  
Julia Richards, Dmochowski Lab (Chemistry)  
Ning Shangguan, Joullie Lab (Chemistry)  
Katya Shishova, Christianson Lab (Chemistry)  
Lee Solomon, Dutton Lab (BMB)  
Joe Swift, Dmochowski Lab (Chemistry)  
Gai Tang, Gai Lab (Chemistry)  
Xiaobo Wan, Joullie Lab (Chemistry)  
Yongzhong Wu, Joullie Lab (Chemistry)  
Peng Xie, Marmorstein Lab (Wistar/Chemistry)

2:00 - 4:00 p.m. **Afternoon Speakers**  
Science Center 101

Smita Mukherjee, Department of Chemistry  
Gregory Caputo, BMB  
John Lee, Wistar Institute  
Xin Liu, Department of Chemistry/Wistar Institute  
Seung-gu Kang, Department of Chemistry  
Luigi Di Costanzo, Department of Chemistry

4:00 - 4:30 p.m. **Reception, Outdoor games**  
Parish Lawn

4:30 - 6:00 p.m. **Buffet Dinner**  
Upper Tarble, Clothier Hall

## INFLUENZA SYMPOSIUM

**February 22, 2007, 12:50 p.m. - 6:00 p.m.**  
**Location: Grossman Auditorium, The Wistar Institute**

12:50 p.m. - 1:40 p.m.  
**Michael Silverman and Farhad Abtahian**  
University of Pennsylvania MD/PhD Program  
Dissecting a deadly virus: lessons from Avian Influenza and the Pandemic of 1918

1:40 p.m. - 1:55 p.m.  
**Sarah Abdulla**  
Ertl Group, The Wistar Institute  
A flu vaccine for the elderly

1:55 p.m. - 2:10 p.m.  
**Vilma Decman (Post-Doctoral Fellow)**  
Wherry Group, The Wistar Institute  
Influenza infection in aged and young mice

2:10 p.m. - 2:55 p.m.  
**Larry Pinto, Northwestern University**  
Influenza proton channels: their role in infection and mechanism for transport

2:55 p.m. - 3:10 p.m.  
**Amanda Stouffer (Post-Doctoral Fellow)**  
DeGrado Group, Department of Biochemistry and Biophysics  
Amantadine binding to the M2 proton channel and the new wild type

3:25 p.m. - 3:40 p.m.  
**Matteo Dal Peraro (Post-Doctoral Fellow)**  
Klein Group, Department of Chemistry  
Blocking and resistance mechanisms of M2 channel explored by molecular dynamics simulations

3:40 p.m. - 4:25 p.m.

**Ted Jardetzky**, Northwestern University

Structural insights into the membrane fusion mechanism of parainfluenza viruses

4:25 p.m. - 4:40 p.m.

**Darya Zharikova** (Post-Doctoral Fellow)

Gerhard Group, The Wistar Institute

Potential of Influenza A virus to escape protection mediated by antibodies to the matrix protein 2

4:40 p.m. - 5:25 p.m.

**Judith White**, University of Virginia

The fusion proteins of Influenza and Ebola Viruses

5:25 p.m. - 6:00 p.m. Reception

**ORGANIZERS:**

Alexei Polishchuk, Chair, BMB graduate student

**FACULTY ADVISORS:**

Bill DeGrado, Faculty Advisor, Biochemistry/Biophysics Faculty

Jeff Saven, Faculty Advisor, Chemistry Faculty

Robert Doms, Faculty Advisor, Microbiology Faculty

**ORGANIZING DEPARTMENTS:**

Department of Biochemistry and Biophysics

Department of Chemistry

Department of Microbiology

The Wistar Institute

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[Influmeditx](#)

The departments listed above

**THE NATURE AND ROLE OF WATER AS A BIOLOGICAL SOLVENT SYMPOSIUM**

**Thursday, October 12, 2006**

**Location: Carolyn Hoff Lynch Room, First Floor, Cret Wing, Chemistry Complex**

**1 p.m. - 6 p.m.**

1:00 p.m. - 1:45 p.m.

**Dongping Zhong**, Ohio State University

Surface hydration dynamics and protein-water interactions

1:45 p.m. - 2:00 p.m.

**Jennifer Dashnau** (Graduate Student)

Vanderkooi Group, BMB Graduate Group

Small molecule effects on H-bonding in water: polyalcohol case studies

2:00 p.m. - 2:15 p.m.

**Yung Sam Kim** (Post-Doctoral Fellow)

Hochstrasser Group, Department of Chemistry

Ultrafast dynamics of water-peptide interactions

2:15 p.m. - 2:30 p.m.

**Walter Witschey** (Graduate Student)

Reddy Group, Radiology, BMB Graduate Group

Structural and functional characteristics of biological water: Lessons from MRI

2:30 p.m. - 3:15 p.m.

**Theresa Head-Gordon**, University of California, Berkeley  
Theoretical and experimental studies of bulk water and aqueous solutions

3:30 p.m. - 4:15 p.m.

**Steve Granick**, University of Illinois at Urbana-Champaign  
Studies of interfacial water

4:15 p.m. - 4:30 p.m.

**Marco De Vivo** (Post-Doctoral Fellow)  
Klein Group, Department of Chemistry  
The role of water in phosphatase activity in soluble epoxide hydrolase

4:30 p.m. - 4:45 p.m.

**Maxim Pometun** (Post-Doctoral Fellow)  
Wand Group, Department of Biochemistry and Biophysics  
Cold-induced unfolding of encapsulated proteins

4:45 p.m. - 5:30 p.m.

**Ken Dill**, University of California, San Francisco  
Modeling water, the hydrophobic effect, and ion solvation

5:30 p.m. - 6:00 p.m. Reception

**CHAIR:**

Nathaniel Nucci, Chair, BMB graduate student

**FACULTY ADVISORS:**

Jeff Saven, Department of Chemistry  
Jane Vanderkooi, Department of Biochemistry and Biophysics

**SPONSORS:**

The Graduate and Professional Student Assembly (GAPSA)

**AMYLOID: STRUCTURE & BIOLOGY**

**Thursday, April 27, 2006**

**Class of '62 Auditorium, Ground Floor, John Morgan Bldg.**

**1 p.m. - 6 p.m.**

1:00 p.m. - 1:35 p.m.

**Jeffery Kelly**, The Scripps Research Institute  
Understanding and ameliorating misfolding diseases

1:40 p.m. - 1:52 p.m.

**Eric Greenbaum**, Department of Pharmacology  
Advisor: Walter Englander  
The structure and folding of alpha synuclein amyloid: insights from hydrogen exchange and electron microscopy

1:55 p.m. - 2:07 p.m.

**Pramit Chowdhury**, Department of Chemistry  
Advisor: Feng Gai  
Computer aided design of small peptides for serpin depolymerization

2:10 p.m. - 2:45 p.m.

**Peter Lansbury**, Harvard Medical School

Therapeutic approaches to disease-modifying drugs for Parkinson's Disease

2:50 p.m. - 3:02 p.m.

**Casey H. Londergan**, Department of Chemistry

Advisor: R.M. Hochstrasser

The onset of peptide aggregation monitored by two-dimensional infrared spectroscopy

3:25 p.m. - 4:00 p.m.

**Ron Wetzel**, University of Tennessee

Energetics of amyloid assembly

4:05 p.m. - 4:17 p.m.

**Sheldon Park**, Department of Chemistry

Advisor: Jeff Saven

Simulation of pH-dependent edge strand rearrangement in human b-2 microglobulin

4:20 p.m. - 4:32 p.m.

**Jun Han**, Department of Chemistry

Advisor: Hai-Lung Dai

Detection of b-Amyloid peptide oligomers in Alzheimer's Disease through single-pair FRET microscopy

4:35 p.m. - 5:10 p.m.

**Robert Tycko**, National Institutes of Health

Molecular structures of fibrils associated with amyloid diseases and yeast prions

5:15 p.m. - 6:00 p.m. Reception

**CHAIR:**

Kesav Kumar, Chair, Chemistry Graduate Student

**FACULTY ADVISORS:**

Walter Englander, Department of Biochemistry and Biophysics

Robin Hochstrasser, Department of Chemistry

Virginia Lee, Center for Neurodegenerative Research

**SPONSORS:**

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Graduate Student Associations Council (GSAC)

**COMPUTATIONAL ANALYSIS OF PROTEIN STRUCTURE AND FUNCTION**

**Thursday, March 9, 2006**

**Austrian Auditorium, Clinical Research Building**

**1 p.m. - 6 p.m.**

1:00 - 1:35 p.m.

**Eugene Koonin**, NCBI-NIH

Unifying measures of protein function and evolution

1:40 - 1:55 p.m.

**Feng Chen**, Advisor: Jeff Saven/David Roos

Department of Chemistry

A quantitative comparative analysis of ortholog identification methods

2:00 - 2:15 p.m.

**Tammer Farid**, Advisor: Les Dutton/Chris Moser  
Department of Biochemistry and Biophysics  
Electron tunneling simulations in the mitochondrial respiratory chain

2:20 - 2:55 p.m.

**Roland Dunbrack**, Fox Chase Cancer Center  
Predicting the structure of proteins and protein complexes

3:20 - 3:55 p.m.

**Olivier Lichtarge**, Baylor University  
Annotation and re-design of proteins"

4:00 - 4:15 p.m.

**Ravindra Venkatramani**, Advisor: Ravi Radhakrishnan  
Department of Bioengineering  
Studying the DNA replication cycle in a high fidelity polymerase by molecular dynamics simulations

4:20 - 4:35 p.m.

**John Skinner**, Advisor: Kim Sharp  
Department of Biochemistry and Biophysicss  
Pump probe MD: locating allosteric pathways

4:40 - 5:15 p.m.

**Mark Gerstein**, Yale University  
Understanding protein function on a genome-scale using networks

5:20 - 6:00 p.m. Reception

**CHAIR:**

Thomas Petty, Chair  
Genomics and Computational Biology (GCB) Graduate Student

**FACULTY ADVISORS:**

Jeff Saven, Chemistry Faculty  
Kim Sharp, Biochemistry/Biophysics Faculty  
Lyle Unger, Computer and Informations Sciences Faculty  
David Roos, Biology Faculty  
Junhyong Kim, Biology Faculty  
Sridhar Hannenhalli, Genetics Faculty



This event is sponsored by the  
**Greater Philadelphia Bioinformatics Alliance**  
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**METALLOMOLECULES IN CHEMICAL TECHNOLOGY, DYNAMICS AND DISEASE**

**NOVEMBER 17, 2005**

**Auditorium, Biomedical Research Building II/III**

**1 p.m. - 6 p.m.**

1:00 - 1:40 p.m.

**David Bocian**, University of California Riverside  
Hybrid semiconductor/molecular memories

1:40 - 2:00 p.m.

**H. Chris Fry**, Department of Chemistry  
*De novo* designed proteins binding non-biological cofactors

2:00 - 2:20 p.m.

**Hongling Zou** (Graduate Student)  
Department of Chemistry  
Molecular dynamics study of heme cofactor binding to amphiphilic 4-helix bundle peptides at soft interfaces

2:20 - 3:00 p.m.

**Joan Valentine**, University of California, Los Angeles  
Copper-zinc superoxide dismutase and amyotrophic lateral sclerosis (ALS)

3:20 - 4:00 p.m.

**John Shelnett**, Sandia National Laboratories & University of New Mexico  
Ionic self-assembly of porphyrin nanostructures for artificial photosynthesis

4:00 - 4:20 p.m.

**Olga Finikova** (Postdoctoral Fellow), Department of Biochemistry and Biophysics  
Symmetrically  $\pi$ -extended porphyrins: versatile near-infrared chromophores for biomedical applications

4:20 - 4:40 p.m.

**Gretchen Bender** (Graduate Student), Department of Biochemistry and Biophysics  
Correlating structure and function of *de novo* designed metalloporphyrin proteins

4:40 - 5:20 p.m.

**Joel Friedman**, Albert Einstein College of Medicine  
Probing the functional role of equilibrium & non-equilibrium protein dynamics in hemeproteins using sol-gel encapsulation protocols

5:25 - 6:00 p.m. Reception

**CHAIR:**

David Finkelstein, BMB Graduate Student

**FACULTY ADVISORS:**

Michael Therien, Department of Chemistry  
Jane Vanderkooi, Department of Biochemistry and Biophysics

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**Trainee Symposium:**

**MEMBRANES AND MOLECULAR RECOGNITION**

**OCTOBER 25, 2005**

**Grossman Auditorium, Wistar Institute, 36 & Spruce Streets  
1 p.m. - 6 p.m.**

**Novel Membrane Studies:**



1:00 - 1:30 p.m.

**Ian Murray** (Postdoctoral Fellow)

Advisor: Paul Axelsen, Pharmacology

Membrane-mediated amyloidogenesis

1:30 - 2:00 p.m.

**Jia Zeng** (Graduate Student)

Advisor: Hai-Lung Dai, Chemistry

Real-time, nonlinear optical probe of molecular transport across Living *E. coli* cell membranes

2:00 - 2:30 p.m.

**Matthew J. Tucker** (Graduate Student)

Advisor: Feng Gai, Chemistry

A new FRET technique to probe the folding dynamics of membrane binding peptides

2:30 - 3:00 p.m.

**Qing Luo** (Postdoctoral Fellow)

Advisor: Britton Chance, BMB

Non-invasive optical probing of prefrontal cortex function in students

#### **Mechanisms of Molecular Recognition:**

3:15 - 3:45 p.m.

**Joe Swift** (Graduate Student)

Advisor: Ivan Dmochowski, Chemistry

"Application and optimization of ferritin: nature's template for inorganic nanoparticle synthesis"

3:45 - 4:15 p.m.

**Troy Messick** (Postdoctoral Fellow)

Advisor: Ronen Marmorstein, Wistar

"Structure of the OTU deubiquitinating enzyme bound to ubiquitin"

4:15 - 4:45 p.m.

**Sung-wook Choi** (Graduate Student)

Advisors: Bill DeGrado and Jeffrey Winkler, Chemistry

"Bioactive arylamide foldamer"

4:45 - 5:15 p.m.

**Sheldon Park** (Postdoctoral Fellow)

Advisor: J.G. Saven, Chemistry

Biophysical studies and computational design of a DNA binding protein

5:15-6:00 Reception

#### **CHAIR:**

Daniel Dowling, Chair, Department of Chemistry

#### **FACULTY ADVISORS:**

Dewey McCafferty, Department of Biochemistry and Biophysics

Bill DeGrado, Department of Biochemistry and Biophysics

Feng Gai, Department of Chemistry

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### **SINGLE MOLECULE STUDIES**

**Thursday, April 21, 2005**

**Carolyn Hoff Lynch Room, First Floor, Cret Wing, Chemistry Complex**

**1:00 p.m. - 6:00 p.m.**

1:00 - 1:40 p.m.

**Enrico Gratton**, University of Illinois at Urbana-Champaign  
Tracking molecules in cells using a two-photon microscope

1:40 - 1:55 p.m.

**Jia Tang** (Graduate Student)  
Advisor: Feng Gai, Department of Chemistry  
Single molecule study of protein polymerization

2:00 - 2:15 p.m.

**Jennifer Ross** (Postdoctoral Fellow)  
Advisor: Yale Goldman, Dept. of Biochemistry and Biophysics  
Direct observation of single dynein-dynactin complexes walking along microtubules *in vitro*

2:20 - 2:55 p.m.

**Julio Fernandez**, Columbia University  
Force-quench studies of protein folding

3:20 - 3:55 p.m.

**Sunney Xie**, Harvard University  
From *in vitro* to *in vivo* single molecule studies

4:00 - 4:15 p.m.

**Alexey Sharonov** (Postdoctoral Fellow)  
Advisor: Robin Hochstrasser, Department of Chemistry  
Real time imaging of protein interactions with living cells

4:20 - 4:35 p.m.

**Nishant Bhasin** (Graduate Student)  
Advisor: Dennis Discher, Dept. of Chemical Engineering  
Chemistry on a single protein, VCAM-1, during forced unfolding

4:40 - 5:15 p.m.

**Justin Molloy**, National Institute for Medical Research, London  
Single molecule mechanical and optical studies: *in vitro* and inside live mammalian cells

5:20 - 6:00 p.m. Reception

**CHAIR:**

Joe Laakso

**FACULTY ADVISORS:**

Yale Goldman, Department of Physiology  
Feng Gai, Department of Chemistry

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**PROTEIN DESIGN**

**Thursday, March 10, 2005**  
**Austrian Auditorium, Clinical Research Building**  
**1:00 p.m. - 6:00 p.m.**

1:00 - 1:40 p.m.

**Lynne Regan**, Yale University  
Structure, function, and folding of designed repeat proteins

1:40 - 1:55 p.m.

**Jing He** (Graduate Student)  
Advisor: Jeff Saven, Department of Chemistry  
Computational design of anesthetic binding ion channel model

2:00 - 2:15 p.m.

**Michelle DeRitter** (Graduate Student)  
Advisor: Feng Gai, Department of Chemistry  
Fast folding of Trp-cage mini-proteins

2:20 - 3:00 p.m.

**Themis Lazaridis**, City College of New York  
Energy functions for membrane proteins

3:20-4:00

**Karyn O'Neil**, Centocor, Inc  
Epitope directed panning for selection of an anti-tissue factor surrogate antibody

4:00 - 4:15 p.m.

**Vikas Nanda** (Postdoctoral Fellow)  
Advisor: Bill DeGrado, Dept. of Biochemistry & Biophysics  
Doubling the design alphabet - varying backbone and sidechain stereochemistry

4:20 - 4:35 p.m.

**Ting Xu** (Postdoctoral Fellow)  
Advisor: Kent Blasie, Department of Chemistry  
Design, synthesis & characterization of novel electronic biomolecular materials

4:40 - 5:20 p.m.

**Michael Hecht**, Princeton University  
Protein design unplugged: novel proteins from combinatorial libraries

5:20 - 6:00 p.m. Reception

**CHAIR:**

Scott Shandler

**FACULTY ADVISOR:**

Bill DeGrado, Department of Biochemistry and Biophysics  
Jeff Saven, Department of Chemistry

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**STRUCTURE-BASED DRUG DESIGN**

**Thursday, November 18, 2004**  
**JMB Reunion Hall, John Morgan Building**

**1:00 p.m. - 6:00 p.m.**

1:00 - 1:40 p.m.

**Eddy Arnold**, Rutgers University

Aiming at a rapidly evolving target: drug and vaccine design against HIV/AIDS

1:40 - 1:55 p.m.

**Brandi Sanders** (Graduate Student)

Advisor: Ronen Marmorstein, The Wistar Institute

Structure-based activation of Sir2 proteins

2:00 - 2:15 p.m.

**Klara Stefflova** (Graduate Student)

Advisor: Gang Zheng, Department of Radiology, UPHS

Photodynamic therapy agent with built-in apoptosis sensor (PDT-BIAS)

2:20 - 3:00 p.m.

**William Jorgensen**, Yale University

Protein-ligand binding and structure-based drug design

3:20 - 4:00 p.m.

**William Moore Jr**, Locus Pharmaceuticals

4:00 - 4:15 p.m.

**Howard Bregman** (Graduate Student)

Advisor: Eric Meggers, Department of Chemistry

A new avenue to highly potent protein kinase inhibitors

4:20 - 4:35 p.m.

**Seth Snyder** (Postdoctoral Fellow)

Advisor: Bill DeGrado, Department of Biochemistry and Biophysics

4:40 - 5:20 p.m.

**Chris Walsh**, Harvard Medical School

Glycosyltransferases dedicated to the maturation of antibiotics

5:20 - 6:00 p.m. Reception

**CHAIR:**

Michael Brent

**FACULTY ADVISORS:**

Dewey McCafferty, Department of Biochemistry and Biophysics

Ronen Marmorstein, Department of Chemistry

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**BIOINORGANIC CHEMISTRY: METALLOENZYMES**

**Thursday, April 22, 2004**

**Carolyn Hoff Lynch Seminar Room, Cret Chemistry Building**

**1:00 p.m. - 6:00 p.m.**

1:00 - 1:45 p.m.

**Paul A. Lindahl**, Texas A&M University, College Station, TX

Acetyl-coenzyme A synthase: the case for a Ni(0)-based mechanism of catalysis

1:50 - 2:05 p.m.

**Frank V. Cochran** (Postdoctoral Fellow)

Department of Biochemistry and Biophysics

*de novo* design and characterization of a four-helix bundle protein that selectively binds a non-biological cofactor

2:10 - 2:55 p.m.

**Carol A. Fierke**, University of Michigan, Ann Arbor, MI

Function of Zn(II) and Mg(II) in protein prenyltransferases

3:20 - 4:05 p.m.

**Tom L. Poulos**, University of California, Irvine, CA

Transfer in heme enzymes: intermediates, radicals, and electron transfer in heme enzymes: peroxidases as a model system"

4:10 - 4:25 p.m.

**German Gomez** (Graduate Student)

Department of Chemistry

Phosphatase activity in human epoxide hydrolase

4:30 - 5:15 p.m.

**John D. Lipscomb**, University of Minnesota, MN

Keys to the castle gate: the basis for specificity in methane oxidation by methane monooxygenase

5:20 - 6:00 p.m. Reception

**CHAIR:**

Herschel Wade

**FACULTY ADVISORS:**

Joe Jarrett, Department of Biochemistry and Biophysics

Ivan Dmochowski, Department of Chemistry

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**PROTEIN FOLDING**

**Thursday, February 26, 2004**

**Austrian Auditorium, Clinical Research Building**

**1:00 p.m. - 6:00 p.m.**

1:00 - 1:40 p.m.

**Donald M. Engelman**, Yale University

Membrane protein folding and evolution

1:50 - 2:05 p.m.

**Ronald Peterson** (Postdoctoral Fellow)

Department of Biochemistry and Biophysics

Induced folding of metastable proteins

2:10 - 2:25 p.m.

**Mallela M. G. Krishna** (Postdoctoral Fellow)

Department of Biochemistry and Biophysics

Residue resolved structure, stability, folding and unfolding rates of a kinetic protein folding intermediate

2:30 - 3:10 p.m.

**George Rose**, Johns Hopkins University  
Proteins: the unfolding story

3:40 - 3:55 p.m.

**Ting Wang** (Postdoctoral Fellow)  
Department of Chemistry  
Ultrafast folding of a three-helix bundle: 1prb

4:00 - 4:15 p.m.

**Chong Fang** (Graduate Student)  
Department of Chemistry  
Dynamics and interactions within alpha-helices by 2D IR

4:20 - 5:00 p.m.

**Martin Gruebele**, University of Illinois at Urbana-Champaign  
Folding kinetics and dynamics of proteins on rough energy landscapes

5:15 - 6:00 p.m. Reception

**CHAIR:**

Sabrina Bédard

**FACULTY ADVISORS:**

Walter Englander, Department of Biochemistry and Biophysics  
Feng Gai, Department of Chemistry

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**INHIBITORS OF PROTEIN-PROTEIN INTERACTIONS**

**Thursday, November 20, 2003**

**Carolyn Hoff Lynch Room, Chemistry Building, Cret Wing**

**1:00 p.m. - 5:15 p.m.**

1:00 - 1:40 p.m.

**Phil Cole**, Johns Hopkins University  
Bisubstrate analogs for probing structure and function of protein kinases and HATs

1:50 - 2:05 p.m.

**Jason Chruma** (Postdoctoral Fellow)  
Department of Chemistry  
Inhibition of the protein-protein interaction that occurs when the AIDS virus attacks T-cells

2:10 - 2:25 p.m.

**Jaskiran Kaur** (Postdoctoral Fellow)  
Department of Chemistry  
Design and testing of peptides as inhibitors of ribonucleotide reductase

2:30 - 3:10 p.m.

**Zhiping Weng**, Boston University  
An integrated approach to protein-protein docking

3:40 - 3:55 p.m.

**Kendra Frederick** (Graduate Student)

Department of Biochemistry and Biophysics

Comparison of the dynamics of complex formation between calmodulin and different calmodulin binding domain peptides

4:00 - 4:15 p.m.

**Lumelle Schneeweis** (Graduate Student)

Department of Biochemistry and Biophysics

Elucidation of the stoichiometry of binding of RANKL to its receptor, RANK, and to its decoy receptor, osteoprotegerin

4:20 - 5:00 p.m.

**Craig Crews**, Yale University

Chemical genetics: probing protein function with small molecules

**CHAIR:**

Lumelle Schneeweis

**FACULTY ADVISORS:**

Jeff Saven, Department of Chemistry

Marcos Milla, Department of Biochemistry and Biophysics

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