

POSTERS

22. **Yulia Pustovalova, Alexandra Pozhidaeva, Dmitry Korzhnev**
University of CT Health Center
NMR studies of interactions between mutagenic translesion synthesis DNA polymerases REV1, pol η and pol ζ .
23. **Justin Radolf**
University of CT Health Center
Structural and functional characterization of the major sheath protein in treponema denticola, the parental ortholog for the Tpr family of outer membrane proteins in treponema pallidum, the syphilis spirochete.
24. **Amit Luthra, Anna Allard, Justin D. Radolf and Melissa Caimano**
University of CT Health Center
Functional and partial structural characterization of Hk1, a Borrelia burgdorferi histidine kinase required for survival during tick feeding environmental.
25. **Sarah Sheftic**
University of CT
NMR structure and dynamics of the unusual response regulator SMA0114.
26. **Latasha Fraser**
University of CT
Insights into the structural dynamics of the P22 coat protein telokin-like domain.
27. **Bushra Husain, James L. Cole**
University of CT
Bringing PKR monomers together.
28. **Katherine Lauer-Felty, James L. Cole**
University of CT
To be or psuedoknot to be: Tertiary Interactions in adenovirus VAI.
29. **Jeffrey Lary, Bushra Husain, James L. Cole**
University of CT
Are fluorescence-detected sedimentation velocity data reliable?
30. **Ala M. Shaqra¹, Alicia E. Every¹, Megan A. deLivron¹, Danny N. Ho², Joachim Frank², Moorthy S. Balakrishnan³, Ganesh S. Anand³, Victoria L. Robinson¹**
¹University of CT, ²Columbia Univ., ³National University of Singapore
An allosteric pathway controls differential binding of translational factor BipA to the 70S and 30S ribosomal species.
31. **Alessandro A. Rizzo, LaTasha C.R. Fraser, Sarah R. Sheftic, Margaret M. Suhanovsky, Andrei T. Alexandrescu, Carolyn M. Teschke**
University of CT
NMR structure of the telokin-like domain from bacteriophage P22 coat protein.

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32. **Nadia G. D'Lima, Carolyn M. Teschke**
University of CT
Not all SecA proteins are created equal: biochemical insights into the SecA proteins of Mycobacterium tuberculosis.
33. **Margaret Suhanovsky, Carolyn M. Teschke**
University of CT
Parting is such sweet sorrow: teasing apart the contributions of the telokin-like domain and the HK97-like core to the stability and function of bacteriophage P22 coat protein.
34. **Molly Siegel, Carolyn M. Teschke**
University of CT
The tail of the coat: Investigating the C-terminus of bacteriophage P22 coat protein.
35. **Markus-Frederik Bohn, Shivender M. Shandilya, Celia A. Schiffer**
UMASS Medical School
Homology modeling of APOBEC3A based on the crystal structure of APOBEC3G C-terminal domain reveals a putative DNA binding groove and intermolecular interfaces
36. **Shivender M. Shandilya, Markus-Frederik Bohn, Celia A. Schiffer**
UMASS Medical School
HIV-1 Restricting Human Proteins APOBEC3G/3F: A structural perspective

DIRECTIONS TO STANLEY-WHITMAN HOUSE *

From UCHC
263 Farmington Ave
Farmington, CT 06032
Take left onto **CT-4 W/Farmington Ave** heading **southwest** (1.1 mi)
Turn right onto **CT-4 W** (0.8 mi)
Turn left onto **High St** (0.3 mi)
Destination will be on the left
Stanley-Whitman House
37 High Street, Farmington, CT

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UNIVERSITY OF CONNECTICUT
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STRUCTURAL BIOLOGY

The 9th Annual North Eastern Structure
Symposium

NESS 2012

Protein Dynamics: From Folding to Function

Keller Auditorium

University of Connecticut Health Center
Farmington, CT

Friday, October 26th, 2012

8.00 am - 6.00 pm

Chair: **Dmitry Korzhnev**
Co-Chair: **Oлга Vinogradova**

<http://www.sb.uconn.edu/ness.html>

NESS 2012 PROGRAM

- 08:00 – 09:00** Registration, Breakfast, Poster Setup
- 09:00 – 09:15** Welcome by the organizers
Introduction by **Frank Torti**
- Session A:**
- Plenary Lecture I:**
- 09:15 – 10:00** **Peter Wright**
The Scripps Research Institute
The evolution of protein dynamics
- 10:00 – 10:30** Coffee Break / Poster Viewing
- Session B:**
- 10:30 – 11:15** **Rieko Ishima**
University of Pittsburgh School of Medicine
Uncertainty of NMR-derived parameters to characterize protein dynamic equilibrium systems
- 11:15 – 12:00** **Patrick Loria**
Yale University
Conformational exchange motions and chemistry in related protein tyrosine phosphatases
- 12:00 – 12:45** Lunch
- 12:45 – 01:30** Poster Session
- Session C:**
- Plenary Lecture II:**
- 01:30 – 02:15** **Peter Moore**
Yale University
What can be learned about macromolecular dynamics using X-ray Crystallography?
- 02:15 – 03:00** **Andrei Alexandrescu**
University of Connecticut
Hydrogen exchange dynamics in protein folding and misfolding
- 03:00 – 03:30** Coffee Break / Poster Viewing
- Session D:**
- 03:30 – 04:15** **Dorothee Kern**
Brandeis University
Choreographing an enzyme 's dance - dynamics during catalysis
- 04:15 – 05:00** **Arthur Palmer**
Columbia University
Protein dynamics from NMR spectroscopy and MD simulations
- 05:00 – 05:15** Poster Prize & Closing Remarks, **Victoria Robinson**
- 05:15 – 06:00** Reception
- 06:30 – 10:00** Dinner (Stanley-Whitman House)*

POSTERS

- Yufeng Cai¹, Nese Kurt Yilmaz¹, Wazo Myint², Rieko Ishima², Celia A. Schiffer¹**
¹UMASS Med. School, ²Univ. of Pittsburgh
Energetic and dynamic study on drug resistant HIV-1 protease.
- Eileen Troconis, Sheila Jaswa**
Amherst College
Interrogating myoglobin while adding to the denaturant arsenal to facilitate mass spectrometry studies of protein folding.
- Tim Poterba, Alex Jaramillo, Andrew Miranker, Sheila Jaswal**
Amherst College
Mapping folding landscapes of native proteins at equilibrium using hydrogen exchange mass spectrometry.
- Bowu Luan, Bing Shan, Daniel P. Raleigh**
Stony Brook University
Are unfolded proteins random coils? Studies of the unfolded state of the C-terminal domain of the ribosomal protein L9 (CTL9)
- Vanessa C. Ducas, Elizabeth Rhoades**
Yale University
Understanding the role of intrachain diffusion in protein self-association.
- Abhinav Nath, Elizabeth Rhoades, Andrew D. Miranker**
Yale University
Conformational ensembles of intrinsically disordered proteins: Combining single-molecule FRET and simulations
- Lauren Ann Metskas, Elizabeth Rhoades**
Yale University
Conformation and dynamics of the troponin I C-terminal domain.
- David C. DeWitt, Elizabeth Rhoades**
Yale University
Alpha-synuclein inhibits SNARE-mediated vesicle fusion.
- Aysegul Ozen, Celia A. Schiffer**
UMASS Med. School
Parallels in the in the molecular basis of drug resistance against HIV-1 and HCV NS3/4A protease inhibitors.
- Ivan Peran, Osman Bilsel, C. Robert Matthews, Daniel P. Raleigh**
Stony Brook University
Time-resolved p-cyanophenylalanine fluorescence as a probe of protein folding.
- Yi Shang, Carlos Simmerling**
SUNYSB
Simulations of spin-labeled HIV-1 protease exhibit diverse flap dynamics due to sequence polymorphism.

POSTERS

- A. Yang, R. Camarda, E. Novikova, M. Carriere, L. Nunez, D. Dilts, X. Qiu, G. Zlotnick, J. Withka**
Pfizer
Structural characterization of LP2086 subfamily A and its Interactions with human factor H using NMR Spectroscopy: insights into the role of a virulence factor and meningococcal vaccine candidate.
- Konstantin Zeldovich**
UMass Medical School
Thermodynamic origins of amino acid usage in prokaryotes.
- Adam Wespiser, Konstantin Zeldovich**
UMass Medical School
Hands-free manipulations in molecular graphics with Microsoft Kinect (TM).
- Sergey Venev, Konstantin Zeldovich**
UMass Medical School
Evolutionary connectivity of model protein sequence space under folding constraints.
- Matthew Fenwick, R.J. Nowling, Jay Vyas, Gerard Weatherby, Heidi Ellis, Michael Gryk**
University of CT Health Center
Extension of CONNJUR-ST to support non-uniform spectral data.
- Yunfeng Li, Kai Jin, Xuan Y. Butzin, Andrew Davis, Barbara Setlow, Peter Setlow, Bing Hao**
University of CT Health Center
Crystal structure of the catalytic domain of the bacillus cereus SleB protein important in cortex peptidoglycan degradation during spore germination.
- Yunfeng Li, Andrew Davis, George Korza, Pengfei Zhang, Yongqing Li, Barbara Setlow, Peter Setlow, Bing Hao**
University of CT Health Center
Role of a SpoVA protein in dipicolinic acid uptake into developing spores of Bacillus subtilis.
- Alexandra Pozhidaeva, Irina Bezsonova**
University of CT Health Center
USP7 C-terminal region is a potential drug target in pediatric neuroblastoma
- Luciana ESF Machado¹, Yulia Pustovalova¹, Fabio Almeida², Irina Bezsonova¹, Dmitry Korzhnev¹**
¹University of CT Health Center, ²University Federal of Rio de Janeiro
Solution structure of PHD domain from human SHPRH and its interaction with methylated histones.
- Alexandra Pozhidaeva, Yulia Pustovalova, Irina Bezsonova, Dmitry Korzhnev**
University of CT Health Center
Solution NMR structure of REV1 C-terminal domain and its complex with pol η peptide.