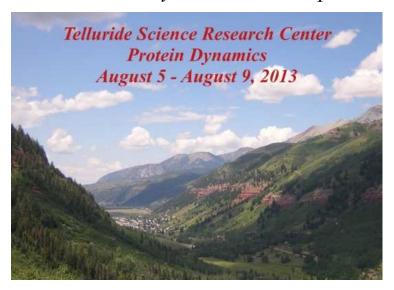
# TSRC Protein Dynamics workshop 2013



### Organisers:

Jasper van Thor – Imperial College London (j.vanthor@imperial.ac.uk) Susan Marqusee – Berkeley University (marqusee@berkeley.edu) Vincent J. Hilser – Johns Hopkins University (hilser@jhu.edu) Kitao Akio- Tokyo University (kitao@iam.u-tokyo.ac.jp)

#### TSRC hosts:

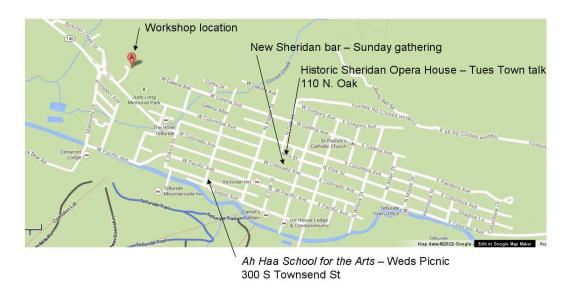
Nana Naisbitt (970-708-0004), Rory Sullivan (970-708-4542, 4)

Location of the meeting – Telluride Intermediate School 725 W. Colorado Ave, Telluride

Sunday, 04 Aug 2013

18:00 – 21:00 Meet & Greet Reception New Sheridan Bar, 231 W Colorado Ave

The New Sheridan offers TSRC scientists and their family & guests drink discounts and free games of pool. This is a place to gather to find friends and talk. Most people eat before or after arriving at the bar. There is not food at the bar, but there are many restaurants nearby.



Anfinrud, Philip - National Institutes of Health

Blackledge, Martin - Institut de biologie structurale

Champion, Paul - Northeastern University

Dror, Ron - D.E.Shaw Research

Fenimore, Paul - Los Alamos National Laboratory

Havenith, Martina - Bochum University

Hayashi, Shigehiko - Kyoto University

Hilser, Vincent - Johns Hopkins University

Jimenez, Ralph - JILA

Kataoka, Mikio - Nara Institute of Science and Technology

Kitao, Akio - The University of Tokyo

Lang, Matthew - Vanderbilt University

Loria, Joseph - Yale University

McDermott, Ann - Columbia University

Mizutani, Yasuhisa - Osaka University

Mulder, Frans - Aarhus University

Nishizaka, Takayuki - Gakushuin University

Palmer, Arthur - Columbia University

Sage, J Timothy - Northeastern University

van Thor, Jasper - Imperial College London

Taraphder, Srabani - Indian Institute of Technology

Tobias, Douglas - UC Irvine

Wand, Josh - University of Pennsylvania

Weik, Martin - Institut de Biologie Structurale

Yamato, Takahisha - Nagoya University

Yano, Junko - Lawrence Berkeley National Lab

Zanni, Martin - University of Wisconsin-Madison

Zhao, Yang - Nanyang Technological University

Zuiderweg, Erik - University of Michigan

#### **Programme**

Monday 05 Aug 1013

- 08:30 09:00 Breakfast at the TSRC meeting site for participants
- 09:00 09:10 *Welcome* and *TSRC* info
- 09:10 09:55 Josh Wand University of Pennsylvania. "The dark energy of proteins comes to light and other stories..."
- 09:55 10:40 Fenimore, Paul Los Alamos National Laboratory "Mossbauer effect, neutron scattering, and protein dynamics: Where do we stand?"
- *10:40 − 11:10 Coffee break*
- 11:10 11:55 Matthew Lang Vanderbilt University "Unfolding and translocation machinery of ClpXP"
- 11:55 12:40 Ron Dror D.E. Shaw Research "Revealing structural dynamics of GPCR signaling through atomic -level simulation"
- 12:40 13:25 Takahisha Yamato Nagoya University "Role of reorganizable interactions between native residue contacts in the allosteric communication in proteins: A computational study by the inter-residue energy conductivity analysis"
- 13:25 19:00 Lunch break and free time
- 19:00 19:45 Vincent Hilser Johns Hopkins University "Intrinsic Disorder, Conformational Fluctuations and Allostery"
- 19:45 20:30 Ralph Jimenez JILA "Excited state dynamics of red fluorescent proteins"
- 20:30 21:15 Frans Mulder Aarhus University "NMR spectroscopic investigation of pH-dependent PYP photocycle dynamics."

- 08:30 09:00 Breakfast at the TSRC meeting site for participants
- 09:00 09:45 Junko Yano Lawrence Berkeley National Lab "Taking Snapshots of Photosynthetic Water Oxidation: Towards Time-Resolved X-ray Spectroscopy and Crystallography"
- 09:45 10:30 Martina Havenith Ruhr-Universität Bochum "Some like it cool"
- 10:30 11:15 Blackledge, Martin Institut de biologie structurale "NMR studies of protein free energy landscapes in their free and bound forms"
- 11:15 11:45 Coffee break
- 11:45 12:30 Jasper van Thor Imperial College London "Ultrafast spectroscopy approaches to interrogate structural dynamics of fluorescent proteins and the photoactive yellow protein"
- 12:30 13:15 J. Patrick Loria Yale University "Millisecond motions in enzymecatalyzed phosphoryl transfer and substrate selectivity"
- 13:15 18:00 Lunch break and free time
- 18:00 Town Talk: Tuesday Nights 6pm at the Historic Sheridan Opera House at 110 N. Oak

Weds 07 Aug 2013

08:30 – 13:00 Free time including lunch break

13:00 – 13:45 Anfinrud, Philip - National Institutes of Health "Picosecond Photobiology: Watching a Signaling Protein Function in Real Time via 150 Picosecond Time-Resolved X-ray Diffraction and Solution Scattering"

13:45 – 14:30 Kataoka, Mikio - Nara Institute of Science and Technology "The mechanism of induced folding of Staphylococcal nuclease"

14:30 – 15:00 Coffee Break

15:00 – 15:45 Paul Champion – Northeastern University "Measurement and theory of proton transport in Green Fluorescent Protein."

15:45 – 16:30 Arthur G Palmer III - Columbia University "Protein dynamics from NMR spectroscopy and MD simulations"

16:30 – 17:15 Martin Weik - Institut de Biologie Structurale "Proteins need it wet. Don't they?"

18:00 - 21:00 TSRC Picnic at the Ah Haa School for the Arts at 300 S. Townsend

Thurs Aug 8

08:30 – 09:00 Breakfast at the TSRC meeting site for participants

09:00 – 09:45 J. Timothy Sage – Northeastern University "Modeling Bioenergetic Processes at the Atomic Scale"

09:45 – 10:30 Yang Zhao - Nanyang Technological University "Energy transfer dynamics in light-harvesting complexes of purple bacteria"

10:30 - 11:00 Coffee Break

11:00-11:45 Martin Zanni - University of Wisconsin-Madison "Kinetic barrier to amyloid fibril formation caused by an intermediate with a transient  $\beta$ -sheet"

11:45 – 12:30 Srabani Taraphder - Indian Institute of Technology "Dynamics of Conformational Fluctuation and Proton Transfer in Human Carbonic Anhydrase II"

12:30 - 14:00 Lunch break

14:00 – 14:45 Ann McDermott - Columbia University "Conformational Exchange Coupled to Ion Binding in the Ion Channel KcsA"

14:45 – 15:30 Akio Kitao - The University of Tokyo "Exploring protein conformational transition pathways with efficient molecular simulation m ethod"

15:30 – 16:00 Coffee break

16:00 – 16:45 Doug Tobias - UC Irvine "Advances in the understanding of transmembrane voltage sensing from concerted scattering and molecular dynamics simulation studies"

16:45 – 17:30 Shigehiko Hayashi - Kyoto University" Crucial Role of Protein Flexibility in Enzymatic Catalysis"

17:30 – 18:15 Takayuki Nishizaka - Gakushuin University" Single-Molecule Imaging of Protein Conformations under Advanced Optical Microscopes"

18:15 - Free time & dinner break

## Fri Aug 9

08:30 – 09:00 Breakfast at the TSRC meeting site for participants

09:00 – 09:45 Erik Zuiderweg - University of Michigan "Protein Dynamics from NMR assignment data?"

09:45-10:30 Yasuhisa Mizutani - Osaka University "Propagations of displacement and energy in proteins"

10:30 – 11:00 Coffee break

11:00 – 11:30 Selection Organisers Protein Dynamics 2015

12:00 – Meeting adjourns