



PROGRAM

Baltimore, Maryland USA July 16-19, 2016





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1986-2016

The Protein Society is a not-for-profit scholarly society with a mission to advance state-of-the-art science through international forums that promote communication, cooperation, and collaboration among scientists involved in the study of proteins.

For 30 years, The Protein Society has served as the intellectual home of investigators across all disciplines -and from around the world- involved in the study of protein structure, function, and design. The Society provides forums for scientific collaboration and communication and supports the professional growth of young investigators through workshops, networking opportunities, and by encouraging junior researchers to participate fully in the annual symposium. As well as the meeting, the Society's prestigious journal Protein Science, edited by Brian Matthews, serves as an ideal platform for furthering the science of proteins in the broadest possible sense.

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WELCOME

WELCOME

Welcome to the 30th Anniversary Symposium of The Protein Society.



This special occasion celebrates thirty years of bringing together scientists interested in protein research at the Annual Symposium of The Protein Society.

The idea for our society was born in 1985 when Ralph Bradshaw, known by some as the "Father of the Protein Society," along with Garry Merry worked to organize an ad hoc meeting of protein chemists in 1985 where the formation of a new Society was discussed. Two years later, in the summer of 1987, the first

Symposium of the newly incorporated Protein Society was held in San Diego. And now with this years' meeting, the symposium has been going strong for thirty years.

The decision was made at the 4th Symposium for the Society to have a journal, and the first issue of Protein Science appeared in 1992. Two of the many leading-edge features of the journal are the support of travel awards for young protein scientists to attend the symposium, and the Annual Best-Paper Awards, which will be presented at this symposium. I also take this opportunity to remind you the journal, along with the symposium, is what makes our Society thrive, and so encourage you to publish in Protein Science.

This 30th Anniversary Symposium promises to be equally stimulating as all the past symposia. The Program Planning Committee has invited a number of outstanding scientists to present their latest results. We also have a number of remarkable young investigators giving talks. Pay attention – these are tomorrow's leaders in protein science! For the next three and a half days, you will have an opportunity to see numerous posters in various sessions, to catch up with old friends and to meet new ones at the mixers and networking dinners. You should also visit the numerous exhibitors helping to support the symposium. You'll find all kinds of information on new products and instrumentation at their booths.

In particular, I'd like to invite you to attend the Members' Reception on the second night. David Eisenberg will speak and you'll have a chance to mingle with some of the founding members of the Society. In 1987, David became the first President of The Protein Society. David, along with Finn Wold (President-elect), Ken Walsh (Secretary/Treasurer), and the Councilors Ralph Bradshaw, Gerald Fasman, Robert Hill, Garry Merry, Hans Neurath and Emil Smith, worked hard to form and build the Society.

We strive to keep the Society symposia enlightening, accessible, and relevant. Because your perspective can only help us to improve, at the conclusion of the meeting you will receive a link to a survey via email. I hope you will take a few minutes to give us some honest feedback.

Thanks for coming to Baltimore and contributing to making this 30th Anniversary Symposium a stimulating conference.

Kind regards,

Cand BPost

Carol B. Post, Ph.D.



COMMITTEES

2016 PROGRAM PLANNING COMMITTEE

Brenda Schulman, Ph.D. (Chair) St. Jude Children's Research Hospital; HHMI; Co-Director, Cancer Genetics, Biochemistry & Cell

Nieng Yan, Ph.D. Professor, School of Medicine, Tsinghua University; HHMI

EXECUTIVE COUNCIL

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Councilor Karyn O'Neil, Ph.D. Johnson & Johnson 2017

Councilor Catherine Royer, Ph.D. Rensselaer Polytechnic Institute 2016

Councilor Charles Sanders, Ph.D. Vanderbilt University 2017

Councilor Gunnar von Heijne, Ph.D Stockholm University 2018

Raluca Cadar, Executive Director

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NOMINATING COMMITTEE

Daniel Bolon, Ph.D. (Chair) University of Massachusetts Medical School

Bil Clemons, Ph.D. California Institute of Technology

Judith Frydman, Ph.D. Stanford University

Jeanne Hardy, Ph.D. University of Michigan

Andrew Mirnaker, Ph.D. Yale University

Heather Pinkett, Ph.D. Northwestern University

MENTORING COMMITTEE

Stephen Fuchs, Ph.D. (Chair) Tufts University

Andrew Vendel, Ph.D. Eili Lilly and Co.

Matthew Cordes, Ph.D University of Arizona

Piero Blanco, Ph.D. University of Buffalo

Blake Hill, Ph.D. Medical College of Wisconsin

Carly Huitema, Ph.D. SIAF institute

Patricia Jennings, Ph.D. University of California, San Diego

Eric Sundberg, Ph.D. University of Maryland School of Medicine

EDUCATION COMMITTEE

Matthew Gage, Ph.D. (Chair) Northern Arizona University

Margaret Cheung, Ph.D. University of Houston

Lisa Gentile, Ph.D. University of Richmond

Peter Kahn, Ph.D. Rutgers University

Betsy Komives, Ph.D. University of California, San Diego

Mary Konkle, Ph.D. Eastern Illinois University

John Osterhout, Ph.D. Angelo State University

Jane Richardson, Ph.D. Duke University

Srebrenka Robic, Ph.D. Agnes Scott College

Frieda Texter, Ph.D. Albright College

Jeff Watson, Ph.D. Gonzaga University



ABSTRACT REVIEW COMMITTEE

John Osterhout, Ph.D. (Chair) Angelo State University

Jie Zheng, Ph.D. David Geffen School of Medicine at UCLA

Emily C. Mundorff, Ph.D. Hofstra University

Azucena Gonzalez Horta, Ph.D. Univesidad Autonoma De Nuevo Leon

Ambarish Kunwar, Ph.D. Indian Institute of Technology Bombay

James M. Lipchock, Ph.D. Washington College

James R. Ketudat Cairns, Ph.D. Suranaree University of Technology

Suresh Kumar Thallapuranam, Ph.D. University of Arkansas

Donald Jacobs, Ph.D.

University of North Carolina at Charlotte

Shahir S. Rizk, PhD Indiana University South Bend

Bin Xu, Ph.D. Virginia Tech

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Jeffrey Urbauer, Ph.D. The University of Georgia

CORPORATE SUPPORT

Thank you for helping us celebrate 30 years of impact.

The Protein Society is extremely grateful to the following sponsor's for their generosity and continued support:

Gold Level





Silver Level

biomedical, inc.





HOTEL FLOOR PLAN





REGISTRATION

The Registration Area will open at 3:00 PM on Tuesday, July 15th (refer to hours below). Registration includes admission to all scientific and poster sessions, exhibits, and one delegate bag. Registration does not include any meals.

HOURS

Friday, July 15:	5:00pm – 7:00pm
Saturday, July 16:	7:30am – 6:30pm
Sunday, July 17:	6:30am – 6:30pm
Monday, July 18:	8:00am – 6:30pm
Tuesday, July 19:	8:00am – 12:00pm

REGISTRATION FEES

FULL MEMBER	\$400
EMERITUS MEMBER	\$150
LAB STAFF MEMBER	\$150
GRADUATE STUDENT MEMBER	\$125
UNDERGRADUATE STUDENT MEMBER	FREE
EARLY CAREER MEMBER	\$225
ONE-DAY MEMBER	\$150
NON-MEMBER	\$750
NON-MEMBER GRADUATE STUDENT	\$275
NON-MEMBER LAB STAFF / EMERITUS	\$275
NON-MEMBER EARLY CAREER	\$325
NON-MEMBER CORPORATE	\$900
NON-MEMBER UNDERGRADUATE STUDENT	FREE
NON-MEMBER EXHIBIT HALL ONLY	\$400
NON-MEMBER ONE-DAY	\$275

BADGE/DELEGATE BAG PICKUP

All registrants must go to the Symposium Registration Desk on the 2nd floor of the venue. All attendees are required to wear their badge at all times. In addition to being a means of identification, the name badge is required for admission to scientific sessions and exhibits. Each registrant will receive one copy of the Symposium Program and one delegate bag.



CAMERAS/VIDEO RECORDING

The unauthorized use of cameras/video recording inside session rooms or among the posters is prohibited.

MOBILE DEVICES

As a courtesy to your fellow attendees, please silence all cell phones and beepers prior to entering a session room.

CERTIFICATES OF ATTENDANCE

Certificates of Attendance may be obtained in person at the Society Registration Desk. Additionally, all attendees will receive a certificate of attendance via email in PDF format.

INTERNET ACCESS

There is complimentary wi-fi internet access for the symposium in the meeting space. Please use the following information to gain access: Network Name: The Protein Society Password: PS30

MOBILE APP

The Protein Society's "PS 30" mobile application is available for download in the Apple App Store, Google Play, and Windows Store. You can view/create schedules; view abstracts, and interact virtually with speakers using the app.

PHOTOGRAPHY

Registration for the meeting implies consent to having photographs taken and to their use by officials of the Protein Society, or their representatives, for editorial and promotional purposes, on the Society website, social media outlets, and publications. Recordings of any kind (audio taping, videotaping, camera, tablets, or cell phones) in the session rooms, Exhibit Hall, and poster areas are strictly prohibited, unless accompanied by a member of the Society staff. Any individual seen taking photographs of any session or presentation will be escorted out by security.

SOCIAL MEDIA

The Society staff will be updating its Facebook page and Twitter feed with Anniversary Meeting information throughout the meeting. Follow us on: Twitter: @ProteinSociety, use hashtag #PS30 Facebook: www.facebook. com/ProteinSociety

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SPEAKER READY ROOM

Located in the Convention Office on the 2nd floor near between the Atrium and Foyer. We highly encourage all presenters in Symposium Sessions and Workshops to visit the Speaker Ready Room one day prior to their scheduled presentation time. This room will be set up for your use. A Protein Society representative will be available during room hours to assist you in setting up your presentation and to answer any questions. A representative will be available during the hours listed below to answer questions.

GENERAL INFORMATION

Friday:	5:00 pm – 7:00 pm
Saturday:	7:30 am - 6:00 pm
Sunday:	7:30 am - 6:00 pm
Monday:	7:30 am - 6:00 pm
Tuosdav	7:30 am - 10:00 am

TRANSPORTATION

The Charm City Circulator: This completely free bus system shuttles through the heart of the city, with stops every 10-15 minutes at all of the major attractions and areas. Hop on Baltimore's Circulator from your hotel to the aquarium, then out to lunch and shopping. If you arrive to Baltimore via train, bus or car, the Charm City Circulator can be used as your connector from various train stations, bus and commuter lots. Bonus points: The Circulator is green (zero emissions 40% of the time!), techie (text alerts keep you updated on the bus schedule) and family-friendly. Visit www.charmcitycirculator.com for schedules, maps and additional details.

Metro/Light Rail: The host hotel is conveniently located only four blocks from the Metro subway system and only three blocks from the Light Rail. The Light Rail runs daily with frequent trips to and from the airport. To see all of the stops and to plan your schedule, please visit: http://mta.maryland. gov/light-rail.

Taxis: Taxis will be available from the Hyatt Regency Baltimore Inner Harbor.

Baltimore City Taxi 410-327-7777

Arrow Cab 443-575-4111

County Cab 443-575-4110

Diamond Cab of Baltimore 410-947-3333

Yellow Cab Cooperative, Inc. 415-333-3333



POSTER SET UP & REMOVAL

Posters can be mounted 2 hours prior to the assigned session time. Poster boards are 4' high by 8' wide, with a usable space of 3'8" high by 7'7" wide. Posters can remain mounted for 30 minutes after the session. Any posters remaining after that point will be discarded.

POSTER VIEWING TIMES

Posters are on display from Saturday morning until Monday afternoon. During the following shifts, exhibitors will be on hand and a Mix & Mingle networking reception taking place:

Saturday, July 16th:	4:30 pm - 6:30 pm
Sunday, July 17th:	11:30 pm - 1:30 pm
Sunday, July 17th:	4:30 pm - 6:30 pm

POSTER SESSION 1

Saturday, July 15, 2016 Saturday July 16th, 2016 Maryland Suites & Harborview Rooms 4:30-6:30pm Last Names A-G

POSTER SESSION 2

Sunday July 17th, 2016 Maryland Suites & Harborview Rooms 11:30am – 1:30pm Last Names H-O

POSTER SESSION 3

Sunday July 17th, 2016 Maryland Suites & Harborview Rooms 4:40pm – 6:30pm Last Names P-Z





BOARD #'S

PA- Amyloid and Aggregation	PA - 002-023
PB – Bioinformatics	PB - 005
PC – Chaperones	PC - 002-003
PD- Chemical Biology	PD - 003-009
PE - Computational Modeling / Simulation	PE - 002-024
PF - Design / Engineering	PF - 004-039
PG- Dynamics and Allostery	PG - 002-023
PH – Enzymology	PH - 002-024
PJ – Folding	PJ - 003-019
PK - Intrinsically Disordered Proteins	PK - 004-007
PL- Membrane Proteins	PL - 001-013
PN- Peptides	PN - 002-009
PO- Protein in Cells	PO - 003-007
PP- Protein Interactions and Assemblies	PP - 001-025
PQ- Proteomics	PQ - 001
PT - Structure (X-Ray / NMR / EM)	PT - 005-031
PU- Synthetic Biology	PU - 001
PV- Therapeutics and Antibodies	PV - 002
PW-Transcription/ Translation/ Post-Translational Modifications	PW - 001-005



PB - BIOINFORMATICS

PB-005 Automating TULIP, a Protein Clustering Method

Nick Biffis¹

1. - University of Richmond

PC - CHAPERONES

PC-002 Design and Characterization of Small Heat Shock Protein Dimers

Caley Butler¹, Hannah Arbach¹, Kathryn A. McMenimen¹

Mount Holyoke College

PC-003 Identification and Characterization of Small Heat Shock Protein Interacting Domains

Elizabeth De Leon¹, Mahima Poreddy¹, Hannah Arbach¹, Kathryn A. McMenimen¹ 1. - Mount Holvoke College

PE - COMPUTATIONAL MODELING / SIMULATION

Generating in silico Mutations to Infer the Effect of Multiple Amino PE-007 Acid Substitutions on Protein Stability

Rebecca Hsieh¹

Western Washington University

PE-013 Mechanism of Improved Doripenem Binding in Several Clinical Mutations in OXA-66 Beta-Lactamase

Zachary Klamer¹, Emma Schroder², Troy Wymore³, David A. Leonard², Agnieszka Szareckal

- 1. Department of Cell and Molecular Biology, Grand Valley State University,
- 2. Department of Chemistry, Grand Valley State University,
- 3. Department of Chemistry, University of Michigan

PE-016 Carbohydrate and protein effects on antibody-receptor binding

Morgan L. Nance^{1.2.} Jason W. Labonte², and Jeffrey J. Gray²

- 1. College of Biological Sciences, University of California, Davis,
- 2. Department of Chemical & Biomolecular Engineering, Johns Hopkins University



PF - DESIGN / ENGINEERING

PF-023 Drug design against trichomoniasis

<u>Vique Sanchez JL¹</u>, Brieba Luis² Rossana Arroyo³, Jaime Ortega⁴, Arturo Rojo⁴, Benítez Cardoza C¹

- 1. Laboratorio de Investigación Bioquímica, ENMyH, Instituto Politécnico Nacional
- 2. LANGEBIO, CINVESTAV-Irapuato;
- Departamento de Infectómica y Patogénesis Molecular; CINVESTAV-Zacatenco, Departamento de Biotecnología, CINVESTAV-Zacatenco;
- 4. UAM-Cuajimalpa. México

PH – ENZYMOLOGY

PH-006 Kinetic characterization of Trypanosoma cruzi His₁₀β-hydroxybutyrate dehydrogenase (βHBDH) and functional exploration of Trypanosoma brucei βHBDH via RNA interference.

William Escboar-Arrillaga¹, Linh Nguyen¹, and Jennifer Palenchar¹

1. - Villanova University

PH-014 Engineering the reversal of Pseudomonas putida β-hydroxybutyrate dehydrogenase cofactor specificity.

Jorna Sojati¹, Connor Ott¹, Nadia Galchak¹, and Jennifer B Palenchar¹

1. - Department of Chemistry, Program in Biochemistry, Villanova University

PH-016 Enzyme Mechanism Influences Macromolecular Crowding Effects

A.E. Wilcox¹

1. - Hobart and William Smith Colleges, New York

PJ - FOLDING

PJ-017 Validation of Native-state Hydrogen Exchange Mass Spectrometry to map protein folding landscapes

Minjee Kim¹, Jacob Witten¹, Sheila Jaswal¹

1. - Amherst College, Biochemistry/Biophysics Program

PJ-019 Investigating residue-specific dynamics with native-state hydrogen exchange mass spectrometry

<u>Nevon Song¹</u>, Jovan Damjanovic¹, Jacob Witten¹, Sheila Jaswal¹

1. - Amherst College Biochemistry and Biophysics Program

POSTERS

PK - INTRINSICALLY DISORDERED PROTEINS

PK-006 Site Specific 1H-13C Phenylalanine in the Study of the Pth1:Peptidyl tRNA Complex

Bhargavi Ramaraju¹, Hana McFeeters¹, Robert McFeeters¹

1. - Department of Chemistry, University of Alabama in Huntsville, AL

PK-007 Characterization of order and disorder in domains of IncC – a plasmid partitioning protein from pRK2

<u>Muhammad Fayyaz ur Rehman¹</u>, Mark Jeeves², Anmol Gautam¹, Scott A White¹, David Scott³, Christopher M. Thomas¹ and Eva I Hyde¹

- 1. School of Biosciences, University of Birmingham
- 2. HWB-NMR, School of Cancer Sciences, University of Birmingham
- School of Biosciences, University of Nottingham, Sutton Bonington Campus Leicestershire LE12 5RD and Research Complex at Harwell, Rutherford Appleton Laboratory

PT - STRUCTURE (X-RAY / NMR / EM)

PT-014 Crystallization by controlled evaporation with acoustic monitoring

<u>Limone Rosa</u>¹, Anna Tsygelnytska¹, Andrea Kocmarek¹, Olivia Wiggins¹, Denise Laspina¹, Alexei Soares¹

1. - Brookhaven National Laboratory





PA- AMYLOID AND AGGREGATION

PA-002 Amyloidogenicity and Cytotoxicity of Bovine Amylin; Implications for Xenobiotic Transplantation and the Design of Non-toxic Amylin Variants

<u>Rehana Akter¹</u>, Andisheh Abedini², Rebekah L. Bower³, Ann Marie Schmidt², Debbie L. Hay³, Daniel P. Raleigh1,⁴

- 1. Department of Chemistry, Stony Brook University
- 2.- Diabetes Research Program, NYU School of Medicine
- 3.- School of Biological Sciences, University of Auckland
- 4.- Graduate Program in Biochemistry and Structural Biology, Stony Brook University

PA-004 Typical and Atypical Prion-like Propagation of Neurotoxic Amyloid-β Oligomers

<u>Dexter N. Dean¹</u>, Kayla M. Pate², Pradipta K. Das¹, Sarah E. Morgan¹, Melissa A. Moss², Vijayaraghavan Rangachari¹

- 1. The University of Southern Mississippi
- 2. The University of South Carolina

PA-005 Lipid interaction and membrane perturbation of different protofibrillar Aβ9-40 trimers: an atomistic simulation study

Xuewei Dong¹, Yunxiang Sun¹, Buyong Ma², Ruth Nussinov^{2,3}, Guanghong Wei¹

- 1. State Key Laboratory of Surface Physics, Key Laboratory for Computational Physical Sciences (MOE), and Department of Physics, Fudan University, Shanghai, P. R. China.
- 2. Basic Science Program, Leidos Biomedical Research, Inc. Cancer and Inflammation Program, National Cancer Institute, Frederick, Maryland 21702, USA.
- Sackler Inst. of Molecular Medicine Department of Human Genetics and Molecular Medicine Sackler School of Medicine, Tel Aviv University, Tel Aviv 69978, Israel.

PA-009 DLPC Liposomes Inhibit Ab Fibrillation and Remodel Preformed Fibrils Through a Detergent-like Mechanism

<u>Kyle Korshavn¹</u>, Cristina Satriano², Rongchun Zhang³, Mark Dulchavsky⁴, Anirban Bhunia⁵, Magdalena Ivanova⁴, Carmelo La Rosa², Mi Hee Lim⁶, Ayyalusamy Ramamoorthy¹,

- 1. Department of Chemistry, University of Michigan, Ann Arbor
- 2. Department of Chemical Sciences, University of Catania
- 3. Biophysics Program, University of Michigan,
- 4. Department of Neurology, University of Michigan
- 5. Department of Biophysics, Bose Institute
- 6. Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST)



PA-010 SUPERMETALLIZATION OF PEPTIDES AND PROTEINS STUDIED BY HIGH RESOLUTION MASS SPECTROMETRY

<u>Eugeny Kukaev^{1.3.4}</u>, Yury Kostyukevich^{1,2}, Alexey Kononikhin^{1,3}, Maria Indeykina^{3,4,6}, Igor Popov^{1,4}, Eugene Nikolaev^{1,2,3,4}

- 1. Moscow Institute of Physics and Technology, Moscow
- 2. Skolkovo Institute of Science and Technology
- 3. Institute for Energy Problems of Chemical Physics
- 4. Emanuel Institute of Biochemical Physics.

PA-014 Predicting Aggregation and Cross-Seeding Activity of Yeast **Prion-Like Proteins**

Jenifer Shattuck¹, Aubrev Waechter¹ and Eric Ross¹

1. - Biochemistry and Molecular Biology Department, Colorado State University

Rosmarinic acid, a catechol-containing natural product, potently PA-017 inhibits amylin amyloidosis.

Paul Velander¹, Ling Wu¹, Anne Brown¹, Keith Ray¹, Rich Helm¹, David Bevan¹. Bin Xu1.₂

- 1. Department of Biochemistry, Virginia Tech
- 2. Center for Drug Discovery 2. Virginia Tech

RNA binding and subcellular localisation of TIA protein in the PA-018 formation of stress granules

Saboora Waris¹, Menachem Gunzburg¹, Kylie Wagstaff¹, Belinda Maher¹,

David Jans¹, Matthew Wilce¹, Jackie Wilce¹

1. - Department of Biochemisty and Molecular biology, School of Biomedical sciences, Monash University, Australia, Victoria, VIC 3800, Australia

PA-020 EGCG binds to different intermediates populated during Human lysozyme fibrillation and modulates them towards less toxic off-pathway aggregates

Fatima Kamal Zaidi¹, Rajiv Bhat¹

1. - Jawaharla Nehr University



PA-022 Understanding the structure and self-assembly of the hydrophobin protein RodA from Aspergillus fumigatus and development of novel nanocarriers

<u>Jennifer I-Chun Lai¹</u>, Victor Lo¹, Ivan Cheung², Matthew Hampsey², Ann H. Kwan², Chi Pham¹, Iñaki Guijarro³, Ariane Pille³, Jake A. Campbell¹, Margaret Sunde¹

- 1. Discipline of Pharmacology, School of Medical Sciences, The University of Sydney
- 2. School of Life and Environmental Sciences, The University of Sydney
- 3. Institut Pasteur

PA-023 The Role of Micelle-like Oligomers in the Aggregation of Human Calcitonin

<u>Kian Kamgar-Parsi</u>1

1. - University of Michigan

PD - CHEMICAL BIOLOGY

PD-003 Design of Modular Switches for Allosteric Control over Protein Kinases and Protein Phosphatases

Matthew Bienick1

1. - University of Arizona

PD-004 Characterization of Novel Pth-like Nucleotide Binding Protein PTRHD1

<u>Geordan Burks¹</u>

1. - University of Alabama

PD-007 Utilizing computational and experimental chemistry to characterize the functions of Structural Genomics proteins.

Caitlyn L. Mills¹, Penny J. Beuning¹, Mary Jo Ondrechen¹

1. - Northeastern University

PD-009 DNA binding and unwinding mechanisms of archaeal and human DNA repair helicase homologues Hel308 and HelQ.

Sarah Northall², Rebecca Lever¹, Nathan Jones¹, Panos Soultanas², Edward Bolt¹

- 1. School of Life Sciences, The University of Nottingham.
- 2. School of Chemistry, The University of Nottingham.

PE- COMPUTATIONAL MODELING/ SIMULATION

PE-002 Coevolutionary analysis and structural prediction of the bacterial divisome

<u>Samson Condon¹</u>, Gladys Diaz-Vazquez¹, Deena-al Mahbuba¹, Alessandro Senes¹ 1. - University of Wisconsin-Madison

PE-004 An Improved Search Algorithm for Protein-Ligand Docking Using FFTs

Xingiang Ding¹, Charles L. Brooks III¹ 1. - University of Michigan

PE-005 Differences on the conformational substates visited by native and mutants versions of the LAOBP obtained by Accelerated Molecular Dynamics.

Diego S. Granados¹, Jesus BandaVazquez¹, Alejandro SosaPeinado¹

1. - Department of Biochemistry, School of Medicine

PE-006 A new definition of inter-residue interaction provides insight into sequence-structure relationships

Jack Holland¹

1. - Dartmouth College

PE-008 Unique allosteric mechanism regulating protein-protein interaction through phosphorylation : a case study of the conformational changes in the Syk tandem SH2 protein

Duy P. Hua¹, Carol Beth Post¹

1.- Department of Medicinal Chemistry and Molecular Pharmacology, Purdue University

PE-010 Atomistic simulations of unfolding and translocation of the Immunoglobulin domain 127 in repetitive cycles of the ClpY Biological Nanomachines

<u>Abdolreza Javidialesaadi¹</u>, George Stan¹

1. - Department of Chemistry, University of Cincinnati

PE-011 The degradation and inhibition mechanism of Alzheimer's Aβ fiber by dihydrochalcone molecules

<u>Yibo Jin¹</u>, Yunxiang Sun¹, Guanghong Wei*

 State Key Laboratory of Surface Physics, Key Laboratory for Computational Physical Sciences (Ministry of Education), Department of Physics, Fudan University

PE-017 On the ability of molecular dynamics force fields to recapitulate NMR derived protein side chain NMR order parameters

Evan S. O'Brien¹, A. Joshua Wand, and Kim A. Sharp

1. - University of Pennsylvania

PE-018 Electrostatic interactions and the multi-layered local structure of active sites: Key features in natural and designed enzymes

<u>Timothy A. Coulther</u>¹, Lisa Ngu¹, Penny J. Beuning¹, and Mary Jo Ondrechen¹ 1. - Department of Chemistry & Chemical Biology, Northeastern University



PE-020 Computational prediction and functional annotation of enzymes in the Haloacid Dehalogenase Superfamily for Bioremediation

<u>Lydia A. Ruffner¹</u>, Mong Mary Touch¹, Penny J. Beuning¹, and Mary Jo Ondrechen¹ 1. - Department of Chemistry & Chemical Biology, Northeastern University

PE-021 Computational Studies of Green Fluorescent Protein Unfolding and Translocation by the ClpY ATPase during Protein Degradation

<u>Yu-Hsuan Shih¹</u>, George Stan¹

1. - Department of Chemistry, University of Cincinnati

PE-024 Studying protein conformational transitions using adaptive biased sampling optimization (ABPO)

<u>Heng Wu¹</u>, Carol B. Post¹ 1. - Purdue University

PF - DESIGN/ ENGINEERING

PF-004 Computational Design of Small Protein Inhibitors Targeting PD-1

Cassie Bryan¹, Gabriel J. Rocklin¹, Nicole Lieberman¹, Courtney Crane¹,

David Baker¹

1. - University of Washington

PF-005 De novo design of protein homo-oligomers with modular hydrogen bond network-mediated specificity

<u>Scott E. Boyken, Zibo Chen¹, Benjamin Groves¹, Robert A. Langan¹,</u> <u>Gustav Oberdorfer¹, Alex Ford¹, Jason M. Gilmore¹, Chunfu Xu¹, Frank DiMaio¹,</u> <u>Jose Henrique Pereira¹, Banumathi Sankaran¹, Georg Seelig¹, Peter H. Zwart¹,</u> <u>David Baker¹</u>

1. - University of Washington

PF-007 De Novo Design of Protein Scaffolds Suited for Ligand-Binding

<u>Tamuka Chidyausiku¹</u>, Enrique Marcos Ph.D. ¹, Benjamin Basanta¹, David Baker¹ 1. - University of Washington, Biological Physics Structure and Design Program

PF-008 Controlling the Phosphoproteome: Ligand Activated Split-Kinases and Split- Phosphatases

<u>Mahsa M.E. Ghaffari</u>¹, Karla Camacho-Soto¹, Javier Castillo- Montoya¹, Indraneel Ghosh¹

1. - University of Arizona



PF-012 Harnessing the Reactivity of Selenocysteine for Expressed Protein Ligation

Jun Liu¹, Qingqing Chen¹, and Sharon Rozovsky¹

1. - Brown lab 138, Department of Chemistry & Biochemistry, University of Delaware

PF-014 Caspase-7 with Reprogrammed Specificity Allows Identification of Exosites for Substrate Recognition

<u>Derek MacPherson</u>¹, Maureen Hill¹, Peng Wu¹, Olivier Julien ², James A. Wells ², Jeanne A. Hardy¹

- 1. Department of Chemistry, University of Massachusetts Amherst
- 2. Department of Pharmaceutical Chemistry and Cellular & Molecular Pharmacology, University of California at San Francisco

PF-025 Nicking Mutagenesis: A Plasmid-Based Single-Pot Saturation Mutagenesis Method

<u>Emily E. Wrenbeck¹</u>, Justin R. Klesmith², James A. Stapleton¹, Timothy A. Whitehead^{1,3}

- 1. Department of Chemical Engineering and Materials Science, Michigan State University, East Lansing, Michigan, 48824
- 2. Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, Michigan, 48824
- 3. Department of Biosystems and Agricultural Engineering, Michigan State University, East Lansing, Michigan, 48824

PF-029 Super WA20 (SUWA), an Ultra-Stabilized Dimeric de Novo Protein for Self-Assembling Protein Nanobuilding Blocks

Naoya Kimura¹, Naoya Kobayashi¹, and Ryoichi Arai¹

1. - Graduate School of Science & Technology, Shinshu University

PF-032 Flipping the Switch: Engineering Alternate Function in the Lactose Repressor

David H. Richards¹, Corey J. Wilson¹

1. - Yale University

PF-033 Resurfacing Proteins Using a Structural Search Engine

Jianfu Zhou¹, Gevorg Grigoryan^{1,2}

- 1. Department of Computer Science, Dartmouth College
- 2. Biological Sciences, Dartmouth College



PF-038 Statistical and combinatorial approaches to designing repeat proteins as recognition elements in microbial sensors

<u>Rachael N. Parker¹</u>, Ana Mercedes¹, Tijana Z. Grove¹ 1. - Department of Chemistry, Virginia Tech

PF-039 Engineering of a modular "Split-enzyme" protein G-based sandwich immunoassay for Ebola-virus Nucleoprotein detection

<u>Tomasz Slezak</u>¹, Mateusz Jaskolowski¹, Lucas J. Bailey¹, Zachary P. Schaefer¹, Elena K. Davydova¹, Anthony A. Kossiakoff¹

1. - Department of Biochemistry and Molecular Biology, The University of Chicago

PG - DYNAMICS AND ALLOSTERY

PG-002 Probing the Domain Architecture and Dynamics of Caspase-6 Reveal Mechanisms for its Regulation

Kevin B. Dagbay¹, Nicolas Bolik-Coulon², and Jeanne A. Hardy¹

- 1. Department of Chemistry, University of Massachusetts Amherst
- 2. Graduate Research Tower, 710 North Pleasant Street
- 2. Department of Chemistry, École Normale Supérieure, 45th rue d'Ulm, Paris, France

PG-003 Direct Measurements of the Long-Range Collective Vibrations of Photoactive Yellow Protein

<u>Yanting Deng</u>¹, Mengyang Xu¹, Katherine A. Niessen², Marius Schimidt¹, Andrea G. Markelz¹

- 1. University at Buffalo
- 2. University of Wisconsin

PG-005 Deciphering the Dual Regulatory Mechanisms of Phosphorylation on Caspase---7

Scott J. Eron¹, Dr. Jeanne A. Hardy¹

1. - University of Massachusetts Amherst

PG-007 Trapping Catalytic Conformations by Crosslinking the Swinging-Arm Domain of Pyruvate Carboxylase

<u>Joshua Hakala¹</u>

1. - Marquette University

PG-009 The swinging arm of pyruvate carboxylase is allosterically regulated by acetyl-coenzyme A

Yumeng Liu, Martin St. Maurice¹

1. - Department of Biological Sciences, Marquette University

PG-010 Tuning Catalytic Activity by Perturbing Amino Acid Networks in a (β/α)8 Barrel Enzyme

Kathleen O'Rourke¹

1. - Penn State University

PG-011 Regulation, activation and deactivation of guanylate cyclase

Olga Petrova¹, Isabelle Lamarre¹, Michel Négrerie¹

1. - Laboratory for optics and biosciences, Ecole Polytechnique, France

PG-014 Soluble Guanylate Cyclase: A Therapeutic Target for Cardiovascular Disease

Jessica Wales¹

1. - University of Arizona

PG- 013 P53-binding Domain of MdmX Undergoes a Conformational Transition Favorable for Ligand Binding

Rong Chen¹ ,Lingyun Qin¹, Jinjin Zhou¹, Fei Yang¹, Huili Liu² and Zhengding Su¹

- 1. Institute of Biomedical and Pharmaceutical Sciences, Hubei University of Technology
- 2. National Center for Magnetic Resonance, State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Chinese Academy of Sciences

PG-015 The Role of Dynamical Transition in Protein Function: Coupling of Protein Collective Vibrations and Water Dynamics

<u>Mengyang Xu¹</u>, Katherine Niessen¹, Yanting Deng¹, Nigel Michki¹, Edward Snell², Andrea Markelz¹

- 1. Department of Physics, University at Buffalo
- 2. Hauptman-Woodward Medical Research Institute & Department of Structural Biology, University at Buffalo

PG-019 Reciprocal allosteric communication in E.coli BirA

Jingheng Wang¹, Dorothy Beckett¹

1. - Department of Chemistry and Biochemistry, University of Maryland



PG-023 Extended Impact of Catalytic Loop Phosphorylation in Human Pin1

<u>Brendan J. Mahoney¹</u>, Meiling Zhang¹, Jeffrey W. Peng¹

1. - Department of Chemistry & Biochemistry, University of Notre Dame

PH - ENZYMOLOGY

PH-002 In crystallo Phosphorylation of Tobramycin by the Antibiotic Kinase APH(2")-la

<u>Shane J. Caldwell¹</u>, Albert M. Berghuis¹ 1. - McGill University

PH-004 IpdAB, a key virulence determinant in Mycobacterium tuberculosis, is a cholesterol ring-opening hydrolase

<u>Adam M. Crowe¹</u>, Nobu Watanabe¹, Israël Casabon¹, Kirstin Brown¹, Jason Rogalski¹, Timothy Hurst¹, Victor Snieckus¹, Leonard Foster¹, Natalie C. Strynadka¹, Lindsay D. Eltis¹

1. - The University of British Columbia, Canada

PH-007 Rapid detection of single-stranded DNA-specific 3' exonucleases in human serum

Simin Fang¹, Meiping Zhao¹

1. - College of Chemistry and Molecular Engineering, Peking University

PH-008 Active Site Binding is not Sufficient for Reductive Deiodination by lodotyrosine Deiodinase

Nattha Ingavat¹, Jennifer M. Kavran², Zuodong Sun¹, Steven E. Rokita¹

- 1. Department of Chemistry, Johns Hopkins University
- 2. Department of Biochemistry and Molecular Biology, Johns Hopkins Bloomberg School of Public Health

PH-009 Analysis of a polyextremophilic galactosidase from an Antarctic Haloarchaeon: Mutagenic analysis of residues important for cold activity

Victoria Laye¹, Priya DasSarma¹, Wolf Pecher¹, Shiladitya DasSarma¹

1. - Department of Microbiology & Immunology, and Institute of Marine and Environmental Technology, University of Maryland



PH-017 Investigation on the specific recognition between lambda exonuclease and DNA substrates with chemical modification and mismatches

<u>Tongbo Wu¹</u>, Meiping Zhao¹

 Beijing National Laboratory for Molecular Sciences, MOE Key Laboratory of Bioorganic Chemistry and Molecular Engineering, College of Chemistry and Molecular Engineering, Peking University

PH-024 The role of the Protein Structural Network (PSN) in the thermostability

<u>Valquiria P. Souza¹</u>, Cecília M. Ikegami¹, Guilherme M. Arantes¹, Sandro R. Marana¹ 1. - Department of Biochemistry, Institute of Chemistry - University of São Paulo

PJ- FOLDING

PJ-003 Effect of Circular Permutations on Transient Partial Unfolding in Proteins

Chen Chen¹, Jung-Hun Yun¹, Jae-Hoon Kim¹, Chiwook Park¹

1. - Purdue University1

PJ-010 Conformational status and activation of peroxidase function of cytochrome c upon glycation: Implications to cytochrome c release and apoptosis

<u>Gurumayum Suraj Sharma¹</u>, Laishram Rajendrakumar Singh¹

1. - Dr. B. R. Ambedkar Center for Biomedical Research, University of Delhi

PJ-013 Measuring the effects of vectorial appearance of the polypeptide chain on protein folding

Micayla A. Bowman¹, Ian M. Walsh¹, Patricia L. Clark¹

1. - Department of Chemistry and Biochemistry, University of Notre Dame

PK - INTRINSICALLY DISORDER PROTEINS

PK-004 DISORDER WITHIN CYSTEINE-RICH PROTEIN AND ITS IMPLICATIONS FOR MULTIFUNCTIONAL ROLES: THE CURIOUS CASE OF GRANULIN-B.

<u>Gaurav Ghag</u>¹, Lauren M. Wolf², Randi G. Reed¹, Nicholas P. van der Munnik³, Claudius Mundoma⁴, Melissa A. Moss^{2,3}, Vijay Rangachari¹.

- 1. Department of Chemistry and Biochemistry, University of Southern Mississippi, Hattiesburg, MS
- 2. Biomedical Engineering Program
- 3. Department of Chemical Engineering, University of South Carolina, Columbia, SC
- 4. Institute of Molecular Biophysics, Florida State University, Tallahassee, FL



PK-006 Site Specific 1H-13C Phenylalanine in the Study of the Pth1:Peptidyl tRNA Complex

Bhargavi Ramaraju¹, Hana McFeeters¹, Robert McFeeters¹

1. - Department of Chemistry, University of Alabama in Huntsville, AL

PL - MEMBRANE PROTEINS

PL-001 Distinct structural elements govern folding, stability and catalysis in the outer membrane enzyme PagP

<u>Bharat Ramasubramanian Iyer¹, Radhakrishnan Mahalakshmi¹</u>

1. - Molecular Biophysics Laboratory, Department of Biological Sciences, Indian Institute of Science Education and Research, Bhopal, India.

PL-009 Molecular explanations for metal selectivity and the conformational change process in Nramp-family divalent metal transporters

<u>Aaron Bozzi¹</u>, Lukas Bane¹, Wilhelm Weihofen¹, Brandon Lee¹, Rachelle Gaudet¹ 1. - Harvard University

PL-011 Solution NMR studies on membrane proteins in lipid bilayers

Philipp Ansorge¹, Oliver Zerbe¹

1. - Department of Chemistry, University of Zurich

PL-013 TRPV4 ion channel regulates normal human lung fibroblast migration

<u>R. Goswami¹</u>, S. Sharma¹, K. Adlerz², M. Merth¹, J. H. Aranda-Espinoza², S. O. Rahaman^{1*}

1. - University of Maryland, Department of Nutrition and Food Science

2. - University of Maryland, Fischell Department of Bioengineering

PN- PEPTIDES

PN-002 Comparison of Solid-Phase Extraction and Size Exclusion Chromatography applied for preparation of urine samples from pregnant women for LC-MSMS

<u>V.A. Shirokova¹</u>, A.E. Bugrova^{1,4}, N.L. Starodubtseva^{1,2}, A.S. Kononikhin^{1,2}, Z.S. Khodzhaeva¹, K. Muminova¹, I.A. Popov^{1,2,3}, V.E. Frankevich¹, E.N. Nikolaev^{2,3,4}, G.T. Sukhikh¹

PN-004 Developing potent and specific inhibitors of the Grb7 breast cancer target using phosphotyrosine mimetics and bicyclic peptides

<u>Gabrielle Watson</u>, Menachem Gunzburg¹, Ketav Kulkarni^{1,3}, Katie Cergol², Richard Payne², Patrick Perlmutter³, Matthew Wilce¹, Jackie Wilce¹.

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- 2. Department of Chemistry, The University of Sydney, NSW
- 3. Department of Chemistry, Monash University VIC



PN-009 Comparison of Solid-Phase Extraction and Size Exclusion Chromatography applied for preparation of urine samples from pregnant women for LC-MSMS

V.A. Shirokova¹, A.E. Bugrova^{1,4}, N.L. Starodubtseva^{1,2}, A.S. Kononikhin^{1,2},

Z.S. Khodzhaeva¹, K. Muminova¹, I.A. Popov^{1,2,3}, V.E. Frankevich¹,

E.N. Nikolaev^{2,3,4}, G.T. Sukhikh¹

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- 3. V.L. Talrose Institute for Energy Problems of Chemical Physics, Russian Academy of Sciences, Moscow, Russia
- 4. Emanuel Institute for Biochemical Physics, Russian Academy of Sciences, Moscow, Russia.

PO - PROTEIN IN CELLS

PO - 003 Importance of protein kinetic stability in extremophiles: A study of thermoacidophilic archaea Sulfolobus acidocaldarius

Javeeta Sen¹, Ke Xia¹, Wilfredo Colón¹

1. - Rensselaer Polytechnic Institute, Center for Biotechnology and Interdisciplinary Studies, Department of Chemistry and Chemical Biology, Trov. NY

PO-005 Effects of macromolecular crowding on protein folding kinetics

Annelise H. Gorensek¹, Austin E. Smith¹, Gerardo M. Perez Goncalves¹, Garv J. Pielak^{1,2,3}

- 1. Department of Chemistry, University of North Carolina at Chapel Hill
- 2. Department of Biochemistry and Biophysics, University of North Carolina at Chapel Hill
- 3. Lineberger Comprehensive Cancer Center

PO-006 ACETYL-COA CARBOXYLASES IN DINOFLAGELLATES: FUELING THE POLYKETIDE SYNTHASE PATHWAYS

Saddef Hag¹, Tsyetan R, Bachvaroff², David R, Goodlett³, Allen R, Place²

- Graduate Program in Life Sciences. University of Maryland
- 2. Institute of Marine and Environmental Technology, University of Maryland Center for

PO-007 Crowding and protein dimerization

Alex J Guseman^{1.2}, Gary J. Pielak²

- 1 Molecular and Cellular Biophysics Training Program
- 2 Department of Chemistry, University of North Carolina-Chapel Hill



PP - PROTEIN INTERACTIONS AND ASSEMBLIES

PP-001 Deciphering the molecular and functional basis of the RhoGAP family proteins: A systematic approach towards selective inactivation of the Rho family proteins

<u>Ehsan Amin¹</u>, Mamta Jaiswal¹, Urszula Derewenda², Katarina Reis³, Kazem Nouri¹, Katja T. Kossemeier¹, Pontus Aspenström³, Avril Somlyo², Radovan Dvorsky¹, Mohammad R. Ahmadian¹

- 1. Institute of Biochemistry and Molecular Biology II, Medical Faculty, Heinrich-Heine-University
- 2. Department of Molecular Physiology and Biological Physics, University of Virginia
- 3. Department of Microbiology, Tumor and Cell Biology, Karolinska Institute

PP-004 Structure Of Serum Amyloid A Suggests A Mechanism For High-Density Lipoprotein Binding And Function As A Protein Hub

Nicholas M. Frame¹, Olga Gursky¹

1. - Department of Physiology & Biophysics, Boston University School of Medicine

PP-007 Novel antimicrobial lectin Myxovirin

Tyler H. Jones¹, Robert L. McFeeters¹

1. - University of Alabama Huntsville

PP-013 Investigating DNA Recognition by the Methyl-CpG Binding Protein ZBTB38

Sven A. Miller¹, Bethany A. Buck-Koehntop¹

1. - Department of Chemistry, University of Utah

PP-017 Analysis of Eukaryotic Heme a Synthase Cox15 and Associated Dysfunctions

<u>Samantha Swenson</u>¹, Andrew Cannon¹, Nicholas Harris², Nicholas Taylor², Jennifer L. Fox², and Oleh Khalimonchuk¹

1. - University of Nebraska-Lincoln, Department of Biochemistry, Redox Biology Center College of Charleston, Department of Chemistry and Biochemistry

PP-20 Mapping Integrin I Domain Binding Sites on Type I Collagen Monomers and Fibrils by microscopy

Jie Zhu¹, Ana Monica Nunes¹, Jean Baum¹

1. - Rutgers University



PP-021 Biochemical Determination of APOBEC3A Interactions with ssDNA

<u>Samantha Ziegler¹</u>, Yong Xiong¹ 1. – Yale University

PP-024 Towards quantitative mapping of protein interactions in vivo

<u>O. Matalon¹</u>, ED. Levy¹

1. - Weizmann Institute of Science, Department of Structural Biology

PP-025 Expression and purification of Arabidopsis phosphatase PP2A-3 catalytic subunit in E.coli and approaches to its activation in trans.

Priyanka Sandal¹, Shweta Shah¹, A. Gururaj Rao¹

1. - Roy J. Carver Dept. of Biochemistry, Biophysics & Molecular Biology, Iowa State University

PQ - PROTEOMICS

PQ-001 Spatial and Temporal control of Lysine Acetyl transferases (KATs): Ligand gated split KATs

C.S. DeSilva¹, Ghosh E. Restituyo¹

1. - Department of Chemistry and Biochemistry, University of Arizona

PT - STRUCTURE (X-RAY/ NMR/ EM)

PT-005 Recognition of diverse NES peptides by the Exportin CRM1

Ho Yee Joyce Fung¹, Yuh Min Chook¹

1. - University of Texas Southwestern Medical Center

PT-007 Structural and functional studies of Mycobacterium tuberculosis MazF-mt6 toxin provide insight into RNA substrate specificity.

Eric Hoffer¹², Stacey J. Miles¹, Samantha Schwartz² and Christine M. Dunham¹

- 1. Department of Biochemistry, Emory University School of Medicine
- 2. Biochemistry, Cell and Developmental Biology program

PT-011 Hydration Dynamics of Hen Egg-White Lysozyme

Bryan S. Marques¹, Nathaniel V. Nucci¹, Matthew A. Stetz¹, A. Joshua Wand¹

1. - Johnson Research Foundation and Department of Biochemistry and Biophysics, University of Pennsylvania Perelman School of Medicine



PT-012 The unique structure of HSV-1 UL21, a multifunctional tegument protein.

Claire M. Metrick¹, Ekaterina E. Heldwein¹

 Department of Molecular Biology and Microbiology and Graduate Program in Biochemistry, Sackler School of Graduate Biomedical Sciences, Tufts University School of Medicine

PT-019 Crystal structure of the D444V disease-causing mutant of human dihydrolipoamide dehydrogenase

<u>Eszter Szabo¹</u>, Reka Mizsei¹, Zsofia Zambo¹, Beata Torocsik¹, Manfred S. Weiss², Vera Adam-Vizi¹, Attila Ambrus¹

- 1. Department of Medical Biochemistry, Semmelweis University, Budapest
- 2. Helmholtz-Zentrum Berlin für Materialien und Energie

PT-021 Detection of Small Molecule Effectors of Pyruvate Carboxylase via the Development of a Novel High-throughput Screen

Brittney N. Wyatt¹, Martin St. Maurice¹

1. - Marquette University

$\label{eq:pt-024} \begin{array}{ll} \mbox{Anatomy}\beta \mbox{ of the -branching enzyme of polyketide biosynthesis and} \\ \mbox{its interaction with an acyl-ACP substrate} \end{array}$

Finn P. Maloney¹², Lena Gerwick³, William H. Gerwick³, David H. Sherman¹⁴,

Janet L. Smith^{1,5}

- 1. Life Sciences Institute, University of Michigan
- 2. Chemical Biology Doctoral Program, University of Michigan
- 3. Center for Marine Biotechnology and Biomedicine, Scripps Institution of Oceanography
- 4. Department of Medicinal Chemistry, University of Michigan
- 5. Department of Biological Chemistry, University of Michigan

PT-031 The Unique Myristoylation Signal of the Feline Immunodeficiency Virus Matrix Protein

Janae L. Baptiste¹, Michael F. Summers¹

1. - Howard Hughes Medical Institute, Department of Chemistry and Biochemistry, University of Maryland



PU - SYNTHETIC BIOLOGY

PU-001 Mutagenesis of Ribonuclease U2 : Rational, Semi-rational and **Random Approaches**

Solivio, Beulah¹ 1. - University of Toronto

PV - THERAPEUTICS AND ANTIBODIES

PV-002 Monoclonal antibodies specifically targeting amyloidogenic forms of transthyretin (TTR) with potential to treat TTR-related cardiomyopathy and polyneuropathy

<u>Natalie J. Galant¹</u>, Jeffrey N. Higaki², Kevin C. Hadley¹, Amy Won³, Stephen J. Tam², Ken Flanagan², Tarlochan Nijjar², Ronald Torres², Jose R. Tapia², Joshua Salmans², Robin Barbour², Wagner Zago², Gene G. Kinney², Christopher M. Yip³, Avi Chakrabartty²

- 1. Princess Margaret Cancer Centre, University Health Network, University of Toronto, Toronto, Ontario M5G 2C1, Canada
- 2. Prothena Biosciences Inc. South San Francisco. California 94080. USA
- 3. Institute of Biomaterials and Biomedical Engineering, University of Toronto. Toronto, Ontario M5S 3E1, Canada

PW - TRANSCRIPTION/ TRANSLATION/ POST- TRANSLATIONAL MODIFICATIONS

PW-001 Caspase-9 is regulated by phosphorylation through diverse mechanisms

Banyuhay P. Serrano¹, Kristen L. Huber¹, Jeanne A. Hardy¹

University of Massachusetts

PW-005 Determining histone deacetylase 8 substrates using non-natural amino acids

Jeffrev Lopez¹

1. - University of Michigan



TRAVEL AWARDS

The following outstanding students and early-career investigators received travel assistance to attend the 30th Anniversary Symposium of The Protein Society from The Finn Wold Travel Awards fund and *The Protein Science* Young Investigator Travel Awards:

UNDERGRADUATE STUDENTS

Nicholas Biffis, University of Richmond Aakash Mehta, Pielak Lab, University of North Carolina at Chapel Hill Ana Romero, University of Texas at Austin Limone Rosa, Dowling College Jorna Sojati, Villanova University Jose Vique, Instituto Politecnico Nacional Allison Wilcox, Hobart and William Smith Colleges

GRADUATE STUDENTS

Mohd Shamoon Asmat, Aligarh Muslim University Javier Castillo, University of Arizona Samson Condon, University of Wisconsin Madison Tim Coulther. Northeastern University Yanting Deng, University at Buffalo Scott Eron, University of Massachusetts Amherst Nicholas Frame, Boston University School of Medicine Florian Heinkel, University of British Columbia Mahsa Ghaffari, University of Arizona Elizabeth Gichana, University of Michigan Annelise Hocevar Gorensek, University of North Carolina at Chapel Hill Hisashi Kobayashi, Nara Institute of Science and Technology Derek MacPherson. University of Massachusetts Amherst Or Matalon, Weizmann Institute Claire Metrick, Tufts University School of Medicine Takaaki Miyamoto, Nara Institute of Technology Jayeeta Sen, Rensselaer Polytechnic Institute Victoriya Shirokova, Moskow Institute of Physics and Technology Eszter, Szabò, Department of Medical Biochemistry, Semmelweis University Saboora Waris, Monash University Gabrielle Watson, Monash University Brittney Wvatt. Marguette University Mengyang Xu, University at Buffalo Fatima Zaidi, Jawaharlal Nehru University Chen Zibo, University of Washington


TRAVEL AWRDS

POST DOCTORATE

Ghader Bashiri, The University of Auckland Shanadeen Begav. Northeastern University Rebecca Cooper, Tufts University School of Medicine Sorin Fedeles, Yale School of Medicine Alex Kintzer. University of California at San Francisco Kamalika Mukherjee, Massachusetts General Hospital/Harvard Medical School Glaucia Melina Squizato Pinheiro, UNICAMP Somavesadat Badievan. University of Michigan

EARLY-CAREER SCIENTIST

Ernesto Andrés Roman, Consejo Nacional de Investigaciones Científicas v Tecnológicas

THANK YOU

Thank you, on behalf of the leadership and Executive Council of the Protein Society, to the recent donors to the Finn Wold Travel Awards Fund. In 2016. greater than 40 students and young investigators will be able to attend and take part in the 30th Anniversary Symposium because they received some form of travel assistance

Additional Travel Award funding is provided by The Protein Science Young Investigator Travel Grants and the Hans Neurath Outstanding Promise Travel Awards (sponsored by the Hans Neurath Foundation).

Congratulations to the winners of the Hans Neurath Outstanding Promise Travel Awards:

Begum Alaybeyoglu, Bogazici University Matthew Bienick, University of Arizona Hoo Yee Joyce Fung, University of Texas Southwestern Medical Center **Neelakshi Gohain.** Institute of Human Virology, University of Maryland, Baltimore David Greening. La Trobe Institute for Molecular Biology Timothy Kurt, University of California, San Diego Jun Lui, University of Delaware Caitlyn Mills, Northeastern University Fabio Parmeggiani, University of Washington Nida Zaidi, Aligarh Muslim University



THE PROTEIN SOCIETY MEMBERSHIP

2016 MEMBERSHIP DUES

FULL MEMBER	\$200
EMERITUS MEMBER	\$25
LAB STAFF MEMBER	\$50
GRADUATE STUDENT MEMBER	\$50
UNDERGRADUATE STUDENT MEMBER	\$25
EARLY CAREER MEMBER	\$100

INDIVIDUAL MEMBERSHIPS

Protein Society members represent an international community of all those who share an interest in the structure, function, design, synthesis and utilization of proteins. The diversity of disciplines and perspectives represented by Society members could be said to be its defining characteristic. They work - or are planning to work- in academia, industry, government, and non-profit labs at leading institutions in more than 50 nations.

Some of the benefits for becoming a member include:

- Members save as much as 50% against the general registration rate
- ONLY members are able to submit or sponsor an abstract for the Best Poster Competition, or to be considered for a Young Investigator Talk
- Complimentary online access to The Premier Journal focused on all aspects of proteins
- \$250 Discount on Publication Fees
- Connect with Society Leaders and have a say in direction of your Society at The Members Business Meeting / New Member Welcome Breakfast
- Get funding for your local Protein-Centered Mini-Symposium, Workshop, or other event with a Member Mini-Grant

Please visit our website for a comprehensive membership benefits list.

CALL FOR NOMINATIONS

2017 AWARDS OF THE PROTEIN SOCIETY

Presented annually to distinguished scientists, the Protein Society Awards recognize excellence and outstanding achievements in the multidisciplinary fields of protein science and honor distinguished contributions in the areas of leadership, education, and service.

The 2017 awards will be presented at the 31st Annual Symposium of The Protein Society on July 24-27, 2017, in Montreal, Canada, The deadline for submitting complete award nomination packages for the 2017 Awards cycle will be noon (EDT) on September 30, 2016.

STEIN AND MOORE AWARD

To recognize eminent leaders in protein science who have made sustained high impact research contributions to the field.

HANS NEURATH AWARD

Seeks to honor individuals who have made a recent contribution of exceptional merit to basic protein research. Sponsored by the Neurath Foundation

DOROTHY CROWFOOT HODGKIN AWARD

Granted in recognition of exceptional contributions in protein science which profoundly influence our understanding of biology. Sponsored by Genentech

EMIL THOMAS KAISER AWARD

Recognizes a recent, highly significant contribution in applying chemistry to the study of proteins. Christian B. Anfinsen Award Recognizes significant technological achievements and/or methodological advancements in protein research.

CARL BRÄNDÉN AWARD

Honors an outstanding protein scientist who has also made exceptional contributions in the areas of education and/or service. Sponsored by Rigaku

PROTEIN SCIENCE YOUNG INVESTIGATOR AWARD

Recognizes a scientist in the first 8 years of an independent career who has made an important contribution to the study of proteins.



MEETING AT A GLANCE

PROTEIN 2016 | SYMPOSIUM SCHEDULE

	Saturda	y, July 16	Sunday	, July 17	Monday	y, July 18	Tuesda	y, July 19
7:00			New Members Welcome Breakfast/ Members Business Meeting					
8:30	Opening Plenary Session		Membrane				Interface	
9:40	Equity and in STEM Ed Rese	l Inclusivity ucation and arch	Protein Folding & Function	Proteins on the Move	Protein Folding & Misfolding	Protein Evolution & Design	Between Proteins & Nucleic Acids	Interdisciplinary Approaches to Protein Science
ц:30			Lunch / Exhibits Open			Closing Ple	nary Session	
Noon		All Lu	nch Worksh	ops Noon - 1	:00 pm		(10:50 am - 12:00 pm)	
1:30	Birth, Life & Death of Proteins	Emerging Methods for Protein Research	Applied Protein Research	Dynamic Modulation of Protein Function	Denary Awards Session			
4:30	Poster Displa Oj	ays & Exhibits pen	Poster Displays & Exhibits Open					
5:30	Mix & Ming	le Reception	Mix & Mingle Reception					
6:30								
	Education & Mixer (9:0 at Geppi's	& Mentoring o - u:oo pm s Museum)	2016 Membe (8:00 - 1	er's Reception 0:00 pm)				

Program Key		
Constellation Ballroom		
Constellation AB		
Constellation CDEF		
Constellation Foyer		
President		
Maryland Suites / Harbor View		

PROGRAM



PROGRAM

DAY 1 - SATURDAY, JULY 16, 2016

OPENING PLENARY SESSION 8:30 AM - 9:45 AM | CONSTELLATION BALLROOM

8:30 am - 8:35 am	Introduction & Welcome from Protein Society President Carol B. Post, Purdue University, West Lafayette, IN, U.S.
8:35 am – 8:40 am	Presentation of the Hans Neurath Award to H. Eric Xu
8:40 am - 9:10 am	<i>X-Ray laser structure of rhodopsin-arrestin complex</i> H. Eric Xu , Van Andel Research Institute, Grand Rapids, MI, U.S.
9:10 am - 9:15 am	Presentation of the Dorothy Crowfoot Hodgkin award Carol B. Post, Purdue University, West Lafayette, IN, United States
9:15 am - 9:45 am	From BRCA1 to Parkin and Back Again Rachel Klevit, University of Washington, Seattle, WA, United States

COFFEE BREAK | 9:45 AM - 10:15 AM

EQUITY AND INCLUSIVITY IN STEM EDUCATION AND RESEARCH SESSION 10:15 AM – 11:30 AM | CONSTELLATION BALLROOM

10:15 am - 10:20 am	Session Introduction Jacquelyn Fetrow, University of Richmond, Richmond, VA, U.S.
10:20 am - 10:50 am	The Meyerhoff Model: Successful Strategies for Developing an Inclusive STEM Workforce Michael Summers, UMBC, Baltimore, MD, United States
10:50 am – 11:25 am	Moving from Surviving to Thriving: Transforming the First Year STEM Experience April Hill , University of Richmond, Richmond, VA, United States

LUNCH 11:30 AM - 1:30 PM

EXHIBITS OPEN | 11:30 AM - 1:30 PM

EDUCATOR LUNCHEON HOSTED BY THE EDUCATION COMMITTEE: *"TRANSLATING PROTEIN SCIENCE FOR THE CLASSROOM AND BEYOND"* 12:00 PM - 1:00 PM | CHESAPEAKE AB



12:00pm - 1:00pm	Career Panel I Hosted by the Mentoring Committee - Constellation AB
	CONCURRENT AFTERNOON SESSION 1 BIRTH, LIFE, & DEATH OF PROTEINS 1:30 PM – 4:30PM CONSTELLATION AB
1:30 pm – 1:35 pm	Introduction from Chair Dan Bolon , University of Massachusetts Medical School, Worcester, MA, United States
1:35 pm – 2:05 pm	Substrate Recognition by the Proteasome Kylie Walters, NIH, Bethesda, MD, United States
2:05 pm – 2:20 pm	Molecular mechanism of protein kinase recognition and sorting by the Hsp90 kinome-specific cochaperone Cdc37 Ioannis Gelis *, University of South Florida, Tampa, FL, United States
2:20 pm - 2:50 pm	<i>Multiple selection filters ensure accurate protein targeting</i> Shou-ou Shan , California Institute of Technology, Pasadena, CA, U.S.
	COFFEE BREAK 2:50 PM – 3:15 PM
3:15 pm – 3:45 pm	GsdmD pore formation permeabilizes membranes in pyroptotic cell death Erin Dueber , Genentech, San Francisco, CA, United States
3:45 pm – 4:00 pm	Mechanism of a cytosolic O-glycosyltransferase essential for the synthesis of a bacterial adhesion protein Yu Chen *, Harvard Medical School/HHMI, Boston, MA, United States
4:00 pm - 4:30 pm	In Silico to In-Cell Folding of Metastable Serpins Anne Gershenson, University of Massachusetts Amherst, Amherst, MA, United States
I	CONCURRENT AFTERNOON SESSION 2 MERGING METHODS FOR PROTEIN RESEARCH 1:30 PM – 4:30 PM CONSTELLATION CDEF
1:30 pm – 1:35 pm	<i>Introduction from Chair</i> Daniel Deredge , University of Maryland School of Pharmacy, Baltimore, MD, United States
1:35 pm – 2:05 pm	Atomic-Level Structure and Dynamics of HIV-1 Capsid Assemblies: Insights from an Integrated MAS NMR, MD, and Density Functional Theory Approach Tatayana Polenova , University of Delaware, Newark, DE, United States
2:05 pm – 2:20 pm	Rapid Bioorthogonal Protein Conjugation Reactions via ortho- Formylphenylboronic Acid-Based Coupling Chemistry Kamalika Mukherjee* , Massachusetts General Hospital/Harvard Medical School, Boston, MA, United States



2:20 pm - 2:50 pm	<i>MicroED : Three dimensional electron crystallography</i> Tamir Gonen, Howard Hughes Medical Institute, Ashburn, VA, U.S.
	COFFEE BREAK 2:50 PM – 3:15 PM
3:15 pm – 3:45 pm	New single molecule methods to study transcription and chromosome dynamics Sunney Xie , Harvard University, Cambridge, MA, U.S.
3:45 pm - 4:00 pm	Spatially targeted optical microproteomics (STOMP): Isolation and proteomic analysis of micron-scale features in pathological specimens Kevin Hadley , University of Toronto, Toronto, Canada
4:00 pm - 4:30 pm	NSLS-II macromolecular crystallography beamlines: opportunities for advanced data collection Alexei Soares, Brookhaven National Laboratory, Upton, NY, U.S.
POSTER DISPLAYS & I	EXHIBITS OPEN, MIX & MINGLE RECEPTION 4:30 PM – 6:30 PM

PIZZA NETWORKING DINNER

7:00 PM - 9:00 PM | PISCES ROOM

EDUCATION & MENTORING MIXER 9:00 PM - 11:00 PM | GEPPI'S ENTERTAINMENT MUSEUM

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DAY2 - SUNDAY, JULY 17, 2016

NEW MEMBER WELCOME BREAKFAST/ MEMBER BUSINESS MEETING 7:30 AM - 8:30 AM | PRESIDENT ROOM

	CONCURRENT MORNING SESSION 1 MEMBRANE PROTEIN FOLDING & FUNCTION 8:30 AM - 11:30 AM CONSTELLATION AB
8:30 am - 8:35 am	Introduction from Chair Chiwook Park, Purdue University, West Lafayette, IN, United States
8:35 am – 9:05 am	<i>Structural studies of purinergic receptor P2Y1R</i> Beili Wu, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai, China
9:05 am - 9:35 am	The intrinsically disordered membrane enzymes selenoprotein S and Selenoprotein K Sharon Rozovsky, University of Delaware, Newark, DE, United States
9:35 am – 9:50 am	Structure, inhibition, and regulation of a two-pore channel TPC1 Alexander Kintzer*, University of California at San Francisco, San Francisco, CA, United States
	COFFEE BREAK 9:50 AM – 10:15 AM
10:15 am - 10:45 am	Membrane Protein Studies in nano discs using NMR and electron microscopy Gerhard Wagner , Harvard Medical School, Cambridge, MA, U.S.
10:45 am - 11:00 am	A Plaque by Any Other Name: Mechanistic Insights into Functional and Dysfunctional Amyloidogenesis Abhinav Nath, University of Washington, Seattle, WA, United States
* 11:00 am - 11:30 am	The versatile beta-barrel gives up secrets of the membrane Karen Fleming, Johns Hopkins University, Baltimore, MD, United States
	CONCURRENT MORNING SESSION 2 PROTEINS ON THE MOVE 8:30 AM - 11:30 AM CONSTELLATION CDEF
8:30 am - 8:35 am	Introduction from Chair Amitava Roy, NIH, United States
8:35 am - 9:05 am	Targeting of tail-anchored membrane proteins by the GET pathway Bil Clemons , CalTech, Pasadena, CA, United States
9:05 am - 9:35 am	Bacterial Warfare: A new role for Type IV Secretion Systems Latin American Protein Society Exchange Speaker Chuck Farah, Department of Biochemistry, University of São Paulo, São Paulo, Brazil



SUNDAY, JULY 17, 2016

9:35 am – 9:50 am	Mechanisms and Applications of R bodies, Membrane-Breaking Protein Needles Jessica Polka*, Harvard Medical School, Boston, MA, United States
	COFFEE BREAK 9:50 AM – 10:15 AM
10:15 am – 10:45 am	<i>Isomerization in real time: the structural basis of signaling</i> Keith Moffat, University of Chicago, Chicago, IL, United States
10:45 am - 11:00 am	Subunit exchange and activation of human CaMKII variants Margaret Stratton*, University of Massachusetts, Amherst, MA, U.S.
11:00 am - 11:30 am	Signals and blockers in Nuclear-Cytoplasmic Transport Yuh-Min Chook, UT Southwestern, Dallas, TX, United States
	LUNCH 11:30 AM - 1:30 PM
	EXHIBITS OPEN 11:30 AM - 1:30 PM
12:00 pm – 1:00 pm	Career Panel II Hosted by the Mentoring Committee - Constellation AB
	CONCURRENT AFTERNOON SESSION 1 APPLIED PROTEIN RESEARCH 1:30 PM – 4:30 PM CONSTELLATION AB
1:30 pm – 1:35 pm	Introduction from Chair Chris Snow, Colorado State University, Fort Collins, CO, United States
1:35 pm - 2:05 pm	Cell Free Methods for Producing Protein Microarrays Joshua LaBaer, Arizona State University, Tempe, AZ, United States
2:05 pm – 2:20 pm	Design and characterization of ebolavirus GP prehairpin intermediate mimics as drug targets. 2016 Protein Science Best Paper Award Winner Tracy R. Clinton, US Air Force, United States
2:20 pm - 2:50 pm	Engineering Phytochelatin-Based Heavy Metal Tolerance Joseph Jez, Washington University in St. Louis, St. Louis, MO, U.S.
	COFFEE BREAK 2:50 PM - 3:15 PM
3:15 pm – 3:45 pm	Designing Robust Bispecific Antibodies to Treat Cancer and Autoimmunity Stephen Demarest, Eli Lilly, San Diego, CA, United States
3:45 pm – 4:00 pm	Antigen clasping: novel antibody-antigen recognition mechanism enabling extraordinarily high specificity Takamitsu Hattori* , Tohoku University, Sendai, Miyagi, Japan
4:00 pm - 4:30 pm	Directed Evolution of a LOV-Trap for Deciphering Intracellular Signaling Pathways Rihe Liu, University of North Carolina at Chapel Hill, Chapel Hill, NC, U.S.

CONCURRENT AFTERNOON SESSION 2 DYNAMIC MODULATION OF PROTEIN FUNCTION 1:30 PM – 4:30 PM | CONSTELLATION CDEF

1:30 pm – 1:35 pm	Introduction from Chair Jeffrey Urbauer, University of Georgia, Athens, GA, United States	
1:35 pm – 2:05 pm	Single molecule study of protein-nucleic acid interaction Sua Myong, University of Illinois, Urbana, IL, United States	
2:05 pm – 2:20 pm	Breaking the fourth wall: Quaternary organizations forge a link to the novel non-enzymatic function of RNR-a Yimon Aye*, Cornell University and Weill Medicine, New York, NY, U.S.	
2:20 pm – 2:50 pm	Measuring the Intracellular Dew Point: Phase Transitions in Cells Cliff Brangwynne, Princeton University, Princeton, NJ, United States	
	COFFEE BREAK 2:50 PM – 3:15 PM	
3:15 pm – 3:45 pm	The molecular toolbox for building axonemal microtubules Masa Kikkawa, University of Toyko, Graduate School of Medicine, Tokyo, Japan	
3:45 pm – 4:00 pm	An allosteric model for control of pore opening by substrate binding in the EutL microcompartment shell protein. 2016 Best Paper Protein Science Award Winner Michael C. Thompson, University of California, San Francisco, CA, U.S.	
4:00 pm - 4:30 pm	Inhibitor peptide design – improving affinity without losing specificity Lorne Exchange Speaker Jacqueline Wilce, Department of Biochemistry & Molecular Biology, Monash University, Melbourne, Australia	
POSTER DISPLAYS & EXHIBITS OPEN, MIX & MINGLE RECEPTION 4:30 PM – 6:30 PM		

MEMBER'S RECEPTION 8:00 PM - 10:00 PM | CONSTELLATION BALLROOM

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DAY3 - MONDAY, JULY 18, 2016

CONCURRENT MORNING SESSION 1 PROTEIN FOLDING & MISFOLDING 8:30 AM – 11:30 AM | CONSTELLATION AB

8:30 am - 8:35 am	Introduction from Chair Kathyrn McMenimen , Mount Holyoke College, South Hadley, MA, U.S.
8:35 am – 9:05 am	Mapping the multi-state pathways for native folding and misfolding of SOD1 at the single-molecule level Michael Woodside, University of Alberta, Edmonton, Canada
9:05 am - 9:35 am	Internal Motion and Conformational Entropy in Protein Function Josh Wand, University of Pennsylvania, Philadelphia, PA, United States
9:35 am - 9:50 am	Key Asn and Gln residues promote cross-species prion conversion Timothy D. Kurt *, University of California, Los Angeles, CA, U.S.
	COFFEE BREAK 9:50 AM – 10:15 AM
10:15 am - 10:45 am	Prion Biology: At the Intersection of Protein Misfolding and Cellular Proteostasis Tricia Serio, University of Arizona, Tucson, AZ, U.S.
10:45 am - 11:00 am	<i>Structural details of RNA-binding protein disordered domain phase separation in ALS and cancers</i> Nicolas Fawzi *, Brown University, Providence, RI, United States
11:00 am - 11:30 am	Complexities of huntingtin aggregation and phase behavior Rohit Pappu, Washington University in St. Louis, St. Louis, MO, U.S.
	CONCURRENT MORNING SESSION 2 PROTEIN EVOLUTION & DESIGN 8:30 AM – 11:30 AM CONSTELLATION CDEF
8:30 am - 8:35 am	Introduction from Chair Elif Ozkirimli, Bogazici University, Istanbul, Turkey
8:35 am - 9:05 am	Computational design of new protein function using homologous backbone fragments Sarel Fleishman, Weizmann Institute of Science, Rehovot, Israel
9:05 am - 9:35 am	Novel Proteins Provide Life Sustaining Activities in vivo Michael Hecht, Princeton University, Princeton, NJ, United States
9:35 am - 9:50 am	De Novo Design of Multi-nuclear Clusters in Helical Bundles Shao-Qing Zhang*, University of California at San Francisco, San Francisco, CA, United States
	COFFEE BREAK 9:50 AM – 10:15 AM
10:15 am - 10:45 am	How do proteins evolve? Dan Tawfik, Weizmann Institute of Science, Rehovot, Israel



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10:45 am - 11:00 am	Designing highly specific protein-based small molecule biosensors Srivatsan Raman*, University of Wisconsin-Madison, Madison, WI, U.S.			
11:00 am - 11:30 am	Enzyme Engineering of a Transaminase for the Synthesis of Pregabalin Michael Karmilowicz, Pfizer, Groton, CT, United States			
	LUNCH 11:30 AM - 1:30 PM			
	EXHIBITS OPEN 11:30 AM - 1:30 PM			
EXHIBITOR WORKSHOP: NEXT GENERATION RESINS AND PLATFORMS FOR HIGHER THROUGHPUT AND AUTOMATION IN PROTEIN PURIFICATION 12:00PM - 1:00 PM CHESAPEAKE AB				
UNDERGRADUATE RESEARCH SESSION, CHAIR - DR. GAGE 12:00PM - 1:00PM PRESIDENT ROOM				
1:30	PLENARY AWARDS SESSION PM - 5:10 PM CONSTELLATION BALLROOM			
1:30 pm – 1:35 pm	Introduction from Chair: Protein Society President Carol B. Post, Purdue University, West Lafayette, IN, U.S.			
1:35 pm – 1:40 pm	Presentation of the Carl Brändén Award			
1:40 pm – 2:10 pm	A New Role for Protein Surfaces 2016 Carl Branden Award Winner Talk Gary Pielak, University of North Carolina, NC, United States			
2:10 pm – 2:15 pm	Presentation of The Christian B. Anfinsen Award			
2:15 pm – 2:45 pm	Combinatorial and Evolutionary Protein Engineering applied to GPCRs 2016 The Anfinsen Award Winner Talk Andreas Plückthun, University of Zürich, Zürich, Switzerland			
2:45 pm – 2:50 pm	Presentation of The Emil T. Kaiser Award			
2:50 pm – 3:20 pm	<i>Global Analysis of Post-translational Modifying Enzymes in Disease</i> 2016 Kaiser Award Winner Talk Charles Craik, University of California, San Francisco, San Francisco, CA, United States			
COFFEE BREAK 3:20 PM – 3:40 PM				
3:40 pm - 3:45 pm	Presentation of The Protein Science Young Investigator Award			
3:45 pm – 4:15 pm	Quantitative Proteomics for Understanding the Histone Code 2016 Young Investigator Award Winner Talk Benjamin A. Garcia, UPenn Perelman School of Medicine, Philadelphia, PA, United States			
4:15 pm - 4:20 pm	Presentation of the Protein Society Service Awards			
4:50 pm – 5:10 pm	Presentation of the Best Poster Awards			



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DAY4 - TUESDAY, JULY 19, 2016

CONCURRENT MORNING SESSION 1 INTERFACE BETWEEN PROTEINS & NUCLEIC ACIDS 8:30 AM – 10:20 AM | CONSTELLATION AB

8:30 am - 8:35 am	Introduction from Chair Bethany Buck-Koehntop, University of Utah, Salt Lake City, UT, U.S.
8:35 am - 9:05 am	The higher-order structure of chromatin fiber revealed by electron microscopy Ping Zhu, Institute of Biophysics, CAS, Beijing, China
9:05 am – 9:20 am	<i>Tet3 CXXC domain is an epigenetic reader for 5-carboxylcytosine</i> Jikui Song*, University of California, Riverside, Riverside, CA, U.S.
9:20 am – 9:50 am	RNA recognition by the RIG-I innate immune receptor: a pathway to therapeutics Anna Marie Pyle, Yale University, New Haven, CT, U.S.
9:50 am – 10:20 am	Structural insights into H2B deubiquitination by the SAGA DUB module Cynthia Wolberger, John Hopkins University School of Medicine, Baltimore, MD, United States
INTERDI 8:	CONCURRENT MORNING SESSION 2 SCIPLINARY APPROACHES TO PROTEIN SCIENCE 30 AM – 10:20 AM CONSTELLATION CDEF
8:30 am – 8:35 am	<i>Introduction from Chair</i> David Greening, La Trobe University, Victoria, Australia
8:35 am - 9:05 am	<i>Towards the Animated Cell</i> Graham Johnson, Allen Institute for Cell Science, San Francisco, CA, United States
9:05 am – 9:20 am	A new mechanism of pancreatic <i>B</i> -cell toxicity in type 2 diabetes Andisheh Abedini*, New York University School of Medicine, New York, NY, United States
9:20 am – 9:50 am	A general synthetic gateway to study the function of protein phosphorylation Jesse Rinehart, Yale University, West Haven, CT, U.S.
9:50 am - 10:20 am	Structural Biology Using Light Sources - Combating Microbial Antibiotic Resistance Andrzej Joachimiak, Argonne National Laboratory, Argonne, IL, U.S.
	COFFEE BREAK 10:20 AM - 10:50 AM
CLOSING PL	ENARY SESSION FOR STEIN & MOORE AWARD TALK
10:50 am - 10:55 am	Introduction from Protein Society President Carol B. Post
10:55 am – 11:25 am	Protein Folding On and Off the Ribosome

Jane Clark, University of Cambridge, United Kingdom



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PROGRAM PLANNING COMMITTEE

BRENDA SHULMAN, PH.D. (CHAIR)

St. Jude Children's Research Hospital; HHMI; Co-Director, Cancer Genetics, Biochemistry & Cell Biology Program



Science took hold of Brenda Schulman early. She credits outstanding high school math, biology, and chemistry teachers with stimulating her interests in molecular mechanisms underlying biological regulation. While still in high school, Schulman also had a chance to work in a university lab that was exploring how genes are turned on. It was an exciting time in the field, because high-resolution views of regulatory proteins bound to DNA were just becoming available. This gave Schulman an appreciation for how molecular structure and function are linked to achieve biological regulation.

Schulman is still curious about biological structure, and she integrates knowledge of structural biology, biochemistry, cellular biology, and genetics to address a central question in biology: How can cells respond quickly to the changing demands and cues of their environments?

Often, a cell can react most rapidly by tweaking an existing protein, rather than by taking the time to make a new one. In the case of regulatory proteins, this can mean attachment or removal of entire other molecules that in some way change the appearance, and thus function, of the original protein.

She is currently studying how cells employ a protein "accessory" system to reassign, redeploy, or disintegrate other proteins. The set of accessories, called ubiquitin-like proteins (UBLs), carry out vital signaling for immune responses and cell division. Schulman points out, "Just as eyeglasses improve vision, a coat provides warmth, or an umbrella wards off rain, cells use this set of UBLs as accessories that adapt the functions of their 'wearers' as needed in the cell." Several of the UBLs are deregulated in cancer, neurodegenerative diseases, and viral infections.

Schulman studies how the different UBLs are chosen for their specific jobs, and how attachment of a UBL changes a protein's structure and function. Figuring out those differences will help define the roles of various family members and the molecular basis of recognition, and make it easier to develop therapeutic agents.

Schulman has largely solved a central and long-standing question of how UBLs can work in specific ways. A complex series of reactions is catalyzed by a cascade of enzymes called E1, E2, and E3. The enzymes find, prepare, escort, and attach a UBL



to its assigned target molecule. The UBL tag triggers a specific cellular activity, such as one of the steps of cell division.

One focus of the Schulman lab has been to follow a UBL, called NEDD8, through the entire process, from being prepared by E1, escorted by E2, and attached to targets by E3. The lab also wanted to know how NEDD8 serves as an accessory to alter function when it is worn by a protein called cullin-RING.

The lab found that cullin-RING's shape changes into an active form when it wears NEDD8. The attachment of NEDD8 transforms cullin-RING into a kind of molecular "valet" that can then attach a different accessory (ubiquitin) onto other proteins to foster a myriad of biochemical reactions. Among its effects, NEDD8 ultimately sets off a cascade of biochemical reactions to eliminate a molecular brake on cell replication. In the absence of this brake, cell replication could get out of control, and if left unchecked, could be associated with cancer. Schulman plans to study how a family of UBLs is directed to a wide range of molecules, how they perform their own functions as accessories, and how the ubiquitin family regulates the timing of cell division.

ANDREAS PLÜCKTHUN, PH.D.

Director of the Dept. of Biochemistry University of Zürich



Andreas Plückthun studied chemistry at the University of Heidelberg and received his graduate education at the University of California at San Diego, where he obtained a Ph.D. in 1982 with Prof. Edward Dennis. He was a postdoctoral fellow at the Chemistry Department of Harvard University (1982-85) where he worked with Prof. Jeremy Knowles. From 1985 until 1993, he was group leader at the Genzentrum and Max-Planck-Institut for Biochemistry in Martinsried, Germany. He was appointed to the faculty of the University of Zurich as a Full Professor of Biochemistry in 1993.

He received the Young Investigator's Award of the German Chemical Industry Trust and was elected member of EMBO. In 2000, he received the Karl-Heinz-Beckurts Award (Munich, Germany) and in 2001 he became a finalist in the World Technology Awardin the Biotechnology category (London, UK). In 2002 he received the J. P. Morgan Chase Health Award (San Jose, CA, USA), the Wilhelm-Exner Medal (Vienna, Austria) and The Jury's Grand Prix (European Grand Prix for Innovation, Monaco). In 2003 he became an elected member of the German National Academy of Science. In 2011 he received a Senior Investigator Grant of the European Research Council and in 2016, he received the Christian B. Anfinsen award of the Protein Society Org. (Baltimore, MA, USA)



In 1992, he co-founded the Munich biotech company MorphoSys AG (listed on the Frankfurt TecDAX) and he served as a member of the supervisory board and as Chief Scientific Advisor until 2007.

In 2004 he co-founded the Biotech Company Molecular Partners AG which is located in Zurich-Schlieren, where he serves on the Supervisory board. Together with the other founders he was awarded the Swiss Technology Award and the De Vigier Awardin 2005.

His research achievements include fundamental contributions enabling the emergence of antibody engineering, notably by the use of E. coli as an engineering platform, studies on synthetic antibodies which lead to the first fully synthetic antibody library, the development of ribosome display — a true in vitro protein evolution technology—, and the development of the Designed Ankyrin Repeat Protein (DARPin) technology. More recently his laboratory developed technologies for evolving stable G-protein coupled receptors for advancing their detailed study.

His current research is centered on protein engineering, combining protein design, directed evolution and applications. While protein engineering is always in the center, his research is very interdisciplinary.

NIENG YAN, PH.D.

Professor, School of Medicine, Tsinghua University; HHMI



Nieng Yan dreams of becoming a movie producer. Not a red-carpet, Hollywood star, but a creator of movies that reveal the intricate motion of molecules inside living cells. Yan finds beauty in the tiniest details of biology and wants to share that with others. She has already created static images of pumps on the cellular membrane that use energy to move molecules in and out of cells. Next, she wants to show the world the pumps' movements. The pumps that Yan studies, and ones related to them, are mutated in a number of diseases and understanding their fluid motion could help design drugs to fix them.

As Yan began her undergraduate studies in biology at Tsinghua University in Beijing, science was emerging as a leading industry in China. Believing their daughter could make important contributions in this growing field, Yan's parents urged her to pursue a career as either a doctor or a scientist.

"I wasn't sure what I wanted to do myself until one summer as an undergraduate I worked in a structural biology lab," she says. "As soon as I saw the beautiful crystals and the elegant structures of molecules, I was hooked."



In that lab, Yan learned how to use X-ray crystallography to determine the arrangement of atoms within a molecule. The technique relies on the fact that when light shines through a crystal, it scatters in different patterns depending on the arrangement of molecules inside. Biological molecules can be turned into crystals by purifying them and letting the surrounding liquid slowly evaporate.

As a graduate student at Princeton University, Yan used X-ray crystallography to see the structure of a handful of proteins involved in cell death in the nematode Caenorhabditis elegans. Those structures revealed how one protein, EGL-1, binds to another, CED-9, to activate a linear pathway that eventually causes cells to self-destruct.

After Yan completed her Ph.D., her Princeton advisor, Yigong Shi, convinced her to stay on for a postdoctoral fellowship by presenting her with a new task—solving the structure of a protein embedded inside the plasma membrane of a cell. "For structural biologists, membrane proteins represent the most challenging targets," Yan says. "I couldn't turn down the challenge."

Yan spent two years studying the structure, learning how to work with finicky membrane proteins. But before she could finish the project, she was offered a position at Tsinghua University in Beijing. At the age of 30, she became the youngest professor at her alma mater. She turned the research over to her Princeton labmates and returned to China.

Her work with membrane proteins was far from finished, however. Once settled in her new lab at Tsinghua, Yan set out to study the structures of transporters and channels—proteins that move molecules in and out of cells through the plasma membrane. That was in 2007. Yan has since found the crystal structures of three key transport proteins involved in moving nutrient molecules.

"These transport proteins are the customs officers for the cells," she says. "They can very specifically select what they want to bring across in each direction." Working with an interdisciplinary team of scientists, Yan is attempting to figure out the structures of glucose transporters, information vital to the study of diabetes and some cancers. "Most cells rely on glucose as their major nutrient. The uptake of glucose is absolutely essential for life," Yan says. Ultimately, she wants to create not just static images of the transporters but a series of images that illustrate changes that occur as transporters pump materials through the membrane.

"These transporters are very dynamic," Yan notes. "It'd be great if we could capture many different structures of a transporter and make a continuous movie of how it moves through cycles." Such a documentary, she adds, would offer a three-dimensional view of a protein's structure, information that could help in the development of drugs designed to block or activate a particular protein.



RALPH LANGEN, PH.D.

Professor, Dept. of Biochemistry & Molecular Biology Keck School of Medicine of USC



Dr. Ralph Langen's main interests lie in the basic areas of protein folding and misfolding, and particular emphasis is placed on these processes when they occur on or around membranes. The interaction of proteins with membranes underlies many important biological processes. Proteins can regulate the structure and function of biological membranes by controlling the composition, fluidity, permeability and curvature of cellular membranes. Membranes, in turn, can have a pronounced effect on the structure and function of proteins and help to promote physiologically important

structural reorganizations of proteins. In addition, membrane interaction can also result in protein misfolding which could ultimately cause disease. Dr. Langen investigates the interaction between proteins and membranes in two biological contexts: recognition and stabilization of membrane curvature and protein misfolding and amyloid fibril formation in disease.

BEST PAPER AWARD WINNERS

Protein Science Best Paper awards to Tracy Clinton and Michael Thompson

Warmest congratulations to Tracy Clinton and Michael Thompson, the recipients of the Protein Society's Year 2016 "Best Paper" awards.

At the beginning of each year, two "best papers" are selected from articles published in Protein Science during the preceding 12 months. A junior author (typically the first author) is designated as the award winner and invited to give a talk at the following Annual Protein Society Symposium.

TRACY CLINTON

Tracy Clinton is an Air Force biochemist who earned her Ph.D. at the University of Utah through the Air Force graduate education civilian institute program. As Tracy puts it, "I am passionate about science and earning my Ph.D. was a wonderful way to further my scientific education while working in an area of biological relevance to my career. The research I had the privilege to take part in was both exciting and challenging and allowed me to bring many new skills and knowledge back to my professional life. I am very thankful for the opportunity to be a small part of the great things that Dr. Kay's lab has and will continue to achieve.

Michael Kay comments on Tracy's somewhat non-traditional career path as follows. "Interestingly, I first met Tracy at the 2009 Protein Society Symposium in Boston, where I presented our work on developing D-peptide inhibitors of HIV entry. Tracy was then an Air Force chemist serving as an instructor at the Air Force Academy



in Colorado. She was applying for a special Air Force program that provided a three-year leave to pursue Ph.D. training at a civilian university. Tracy was selected for this competitive program and thankfully decided to pursue her Ph.D. work in my lab at the University of Utah starting in late 2010. Tracy's strong interest in translational research problems in biodefense was a perfect fit with our embryonic efforts to apply D-peptide design to block Ebola entry. Working closely with Dr. Debra Eckert, Tracy launched the Ebola project in our lab, developing and validating the Ebola drug target mimics described in the Protein Science paper. These mimics provide the

foundation for our lab's active D-peptide discovery program, which has generated over \$3 million in NIH funding (in collaboration with a local startup company, Navigen). Tracy's accelerated Ph.D. is unprecedented in my experience. From day one, you could say that she was "on a mission", operating with a sense of urgency, focus, and intensity that would have destroyed most students. A key factor in Tracy's success on this challenging project was her ability to train and manage a large collaborative team, as evidenced by the paper's long author list."

MICHAEL THOMPSON

Michael Thompson grew up in the San Fernando Valley area, outside of Los Angeles, and was an undergraduate at UC-Berkeley (degree 2007), in the Department

of Molecular and Cell Biology. While at Berkeley, he worked as a research assistant in Tom Alber's lab, where he developed interests in protein crystallography and in understanding how conformational changes control the functions of proteins. He then attended graduate school at UCLA (degree 2014), under the mentorship of Todd Yeates.

Todd says "Mike was a terrific graduate student (now a postdoc with Jamie Fraser at UCSF). In terms of technical interests, Mike stands out among other students in the degree to which he insisted on getting at the heart of many of the crystallography problems he faced while



working on the structures of bacterial microcompartment shell proteins in my lab. They tend to form flat sheets (which is their function), and crystals often showed lattice translocations or other kinds of disorders. Mike worked through such cases rather than abandoning them, and as a result became one of the most deeply knowledgeable students in crystallography that I have had.

On the biology side, Mike was determined to dissect the mechanisms of molecular

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transport through a dynamic shell protein, and this turned out to be a tough problem. He got partial answers early on, but the story was incomplete (and faced unfavorable publishing decisions) until he finally figured out the allostery component: the interior substrate holds the large pore in the closed conformation so that the toxic aldehyde intermediate doesn't escape into the cytosol while the microcompartment is actively metabolizing. It took a lot of perseverance to get to the finish line.

Mike is dedicated to mechanism at the fine scale. He came out of Tom Alber's lab as an undergraduate where he had some exposure to the early work on dissecting alternate conformations in proteins. He continued his technical and mechanistic interests in my group, and now with Jamie Fraser where he continues along that path.

As a senior student, Mike was an intellectual leader in my lab and really for other structure labs at UCLA as well. He's an academic at heart, with very high scientific standards. It's nice to see him recognized."



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MARK YOUR CALENDARS

The 2017 Program Planning Committee:

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Yibing Shan Senior Scientist Chemistry And Biology D E Shaw Research

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Jane Clarke

Professor Of Molecular Biophysics Senior Wellcome Trust Research Fellow Department Of Chemistry University Of Cambridge

Dan S. Tawfik

Principal Investigator Department Of Biomolecular Sciences Weizmann Institute Of Science

Volker Dötsch

Professor, Institute Of Biophysical Chemistry Goethe University

Travel Awards ను

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Contributed Talks র্জ

Young Investigator Talks

SESSIONS:

- Transient Protein-protein Interactions
- Approaches To Therapeutics
- Chaperones And Amyloid
- Synthetic Biology
- Protein Evolution
- Protein Dynamics And Allostery
- Intrinsically Disordered Proteins And Phase Transitions
- Structural Insights Into Ion-transporting Membrane Proteins

Please visit our registration desk for further information during the 2016 event. Inquires can be sent to staff@proteinsociety.org.

- Ubiquitin-proteasome System
- Protein Folding
- Advances In Membrane Proteins
- Analysis Of Large Complexes



EXHIBITOR WORKSHOPS

Workshop – GE Monday, July 18th. 11:30am - 1:30pm. Chesapeake AB Next generation resins and platforms for higher throughput and automation in protein purification Dan Plaska, GE Healthcare Life Sciences, Field Application Specialist

The needs of protein purification have evolved over the past two decades, driven by the needs of biopharma as well as researchers who require high purity and activity to study protein structure and function. Today's modern resins (media) can provide higher throughput, better capacity and recovery while new generation instrumentation provides more automation for less hands-on time during the chromatography steps required.

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AMYLOID AND AGGREGATION	PA
BIOINFORMATICS	PB
CHAPERONES	PC
CHEMICAL BIOLOGY	PD
COMPUTATIONAL MODELING / SIMULATION	PE
DESIGN / ENGINEERING	PF
DYNAMICS AND ALLOSTERY	PG
ENZYMOLOGY	РН
EVOLUTION	PI
FOLDING	PJ
INTRINSICALLY DISORDERED PROTEINS	РК
MEMBRANE PROTEINS	PL
MOTORS AND MACHINES	РМ
PEPTIDES	PN
PROTEIN IN CELLS	РО
PROTEIN INTERACTIONS AND ASSEMBLIES	РР
PROTEOMICS	PQ
PROTEOSTASIS AND QUALITY CONTROL	PR
SINGLE MOLECULE STUDIES	PS
STRUCTURE (X-RAY / NMR / EM	PT
SYNTHETIC BIOLOGY	PU
THERAPEUTICS AND ANTIBODIES	PV
TRANSCRIPTION / TRANSLATION / POST-TRANSLATIONAL MODIFICATIONS	PW
METABOLIC ENGINEERING / ENERGY APPLICATIONS	РХ
SYSTEMS BIOLOGY	РҮ



PA - AMYLOID AND AGGREGATION

PA-001 A new mechanism of pancreatic β-cell toxicity in type 2 diabetes

<u>Andisheh Abedini ¹</u>, Annette Plesner, Ping Cao, Jinghua Zhang, Chris T. Middleton, Daniel Sartori, Julia Derk, Rosa Rosario, Fei Song, Jacqueline Lonier, Martin T. Zanni, Daniel P. Raleigh, Ann Marie Schmidt

1. - NYU School of Medicine

PA-002 Amyloidogenicity and Cytotoxicity of Bovine Amylin; Implications for Xenobiotic Transplantation and the Design of Non-toxic Amylin Variants

<u>Rehana Akter¹,</u> Andisheh Abedini², Rebekah L. Bower³, Ann Marie Schmidt², Debbie L. Hay³, Daniel P. Raleigh^{1,4}

- 1. Department of Chemistry, Stony Brook University
- 2. Diabetes Research Program, NYU School of Medicine
- 3. School of Biological Sciences, University of Auckland
- 4. Graduate Program in Biochemistry and Structural Biology, Stony Brook University

PA-003 Toward the molecular mechanism by which vitamin C inhibits amyloid formation and remodels mature amyloid fibrils: possible therapeutic interventions

<u>Parvez Alam¹</u>, Sumit Kumar Chaturvedi¹, Mohammad Khursheed Siddiqi¹, Rizwan Hasan Khan¹

1. - Molecular Biophysics and Biophysical Chemistry group, Interdisciplinary Biotechnology Unit, Aligarh Muslim University

PA-004 Typical and Atypical Prion-like Propagation of Neurotoxic Amyloid-β Oligomers

<u>Dexter N. Dean¹</u>, Kayla M. Pate², Pradipta K. Das¹, Sarah E. Morgan¹, Melissa A. Moss², Vijayaraghavan Rangachari¹

- 1. The University of Southern Mississippi
- 2.- The University of South Carolina



PA-005 Lipid interaction and membrane perturbation of different protofibrillar Aβ9-40 trimers: an atomistic simulation study

<u>Xuewei Dong¹</u>, Yunxiang Sun¹, Buyong Ma², Ruth Nussinov^{2,3}, Guanghong Wei¹

- 1.-State Key Laboratory of Surface Physics, Key Laboratory for Computational Physical Sciences (MOE), and Department of Physics, Fudan University, Shanghai, P. R. China.
- 2.-Basic Science Program, Leidos Biomedical Research, Inc. Cancer and Inflammation Program, National Cancer Institute, Frederick, Maryland 21702, USA.
- Sackler Inst. of Molecular Medicine Department of Human Genetics and Molecular Medicine Sackler School of Medicine, Tel Aviv University, Tel Aviv 69978, Israel.

PA-006 Decreasing amyloidogenicity of immunogloublin light chain variable domain by mutation of surface exposed residues and peptide inhibitor targeting partially unfolded state

<u>Daizo Hamada</u> Graduate School of Engineering and Center for Applied Structural Science (CASS)

1. - Kobe University

PA-007 Mechanism of Amyloidogenesis of an AAA+ Chaperone

Walid A. Houry¹

1. - Department of Biochemistry, University of Toronto

PA-008 Sialylation of the prion protein controls prion infectivity.

Elizaveta Katorcha¹

1. - University of Maryland Baltimore

PA-009 DLPC Liposomes Inhibit Ab Fibrillation and Remodel Preformed Fibrils Through a Detergent-like Mechanism

<u>Kyle Korshavn¹</u>, Cristina Satriano², Rongchun Zhang³, Mark Dulchavsky⁴, Anirban Bhunia⁵, Magdalena Ivanova⁴, Carmelo La Rosa², Mi Hee Lim⁶, Ayyalusamy Ramamoorthy¹,

- 1. Department of Chemistry, University of Michigan, Ann Arbor
- 2. Department of Chemical Sciences, University of Catania
- 3. Biophysics Program, University of Michigan,
- 4. Department of Neurology, University of Michigan
- 5. Department of Biophysics, Bose Institute
- 6. Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST)



PA-010 Supermetallization Of Peptides And Proteins Studied By High **Resolution Mass Spectrometry**

<u>Eugeny Kukaev^{1.3.4}</u>, Yury Kostyukevich^{1,2}, Alexey Kononikhin^{1,3}, Maria Indeykina^{3,4,6}, Igor Popov^{1,4}, Eugene Nikolaev^{1,2,3,4}

- 1. Moscow Institute of Physics and Technology, Moscow
- 2. Skolkovo Institute of Science and Technology
- 3. Institute for Energy Problems of Chemical Physics
- 4. Emanuel Institute of Biochemical Physics.

PA-011 Key asparagine and glutamine residues promote cross-species prion conversion

Timothy D. Kurt¹, Lin Jiang², Nazilla Alderson¹, Jun Liu1, David Eisenberg², Christina J. Sigurdson^{1,3}

- 1. Departments of Pathology and Medicine
- 2. UCLA-DOE Institute, Howard Hughes Medical Institute, and Molecular Biology Institute. UCLA
- 3. Department of Pathology, Immunology, and Microbiology, UC Davis

PA-012 The 99-residue C-terminal transmembrane domain (C99) of the amyloid precursor protein

Loren M. LaPointe¹

1. - Vanderbilt University

PA-013 Mapping the Functional Amyloid Landscape in S. aureus Biofilms

Abhinav Nath¹

1. - Medicinal Chemistry University of Washington

PA-014 Predicting Aggregation and Cross-Seeding Activity of Yeast **Prion-Like Proteins**

Jenifer Shattuck¹. Aubrev Waechter¹. Eric Ross¹

1. - Biochemistry and Molecular Biology Department, Colorado State University

Macromolecular crowding induces holo α-lactalbumin aggregation PA-015 by converting to its apo form

Shruti Mittal¹, Laishram R, Singh¹

1. - Dr. B.R. Ambedkar Center for Biomedical Research, University of Delhi



PA-016 Disulfide Bond Scrambling at Acidic pH is Key to Insulin Aggregation and Toxicity

Ashutosh Tiwari¹, Colina Dutta¹

1. - Department of Chemistry, Michigan Technological University

PA-017 Rosmarinic acid, a catechol-containing natural product, potently inhibits amylin amyloidosis.

<u>Paul Velander</u>¹, Ling Wu1, Anne Brown¹, Keith Ray¹, Rich Helm¹, David Bevan¹, Bin Xu1²

1. - Department of Biochemistry, Virginia Tech

2. - Center for Drug Discovery 2 , Virginia Tech

PA-018 RNA binding and subcellular localisation of TIA protein in the formation of stress granules

<u>Saboora Waris</u>¹, Menachem Gunzburg¹, Kylie Wagstaff¹, Belinda Maher¹, David Jans¹, Matthew Wilce¹, Jackie Wilce¹

1. - Department of Biochemisty and Molecular biology, School of Biomedical sciences, Monash University, Australia, Victoria, VIC 3800, Australia

PA-019 Discovery and Mechanisms of Small Molecule Inhibitors against Amylin Amyloidosis in the pancreas and the brain

Ling Wu¹, Paul Velander¹, Keith Ray¹, Anne Brown¹, Rich Helm¹, David Bevan¹, Bin Xu¹²

- 1. Department of Biochemistry
- 2. Center for Drug Discovery

PA-020 EGCG binds to different intermediates populated during Human lysozyme fibrillation and modulates them towards less toxic off-pathway aggregates

Fatima Kamal Zaidi¹, Rajiv Bhat1

1. - Jawaharla Nehr University

PA-021 Unveiling the inhibitory behavior of n-acetylneuraminic acid against fibrillation of amyloidogenic proteins-a biophysical insight

<u>Nida Zaidi¹</u>, Rizwan Hasan Khan¹

1. - Aligarh Muslim University



Understanding the structure and self-assembly of the hydrophobin PA-022 protein RodA from Aspergillus fumigatus and development of novel nanocarriers

<u>Jennifer I-Chun Lai¹</u>, Victor Lo¹, Ivan Cheung², Matthew Hampsey², Ann H. Kwan², Chi Pham¹, Iñaki Guijarro³, Ariane Pille³, Jake A. Campbell¹, Margaret Sunde¹

- 1. Discipline of Pharmacology, School of Medical Sciences, The University of Sydney
- School of Life and Environmental Sciences. The University of Sydney.
- 3. Institut Pasteur

The Role of Micelle-like Oligomers in the Aggregation of Human PA-023 Calcitonin

Kian Kamgar-Parsi¹

1. - University of Michigan

PA-024 Prion Propagation and Curing by AAA+ Chaperone Proteins in the Saccharomyces cerevisiae model system PSI+

Shannon May¹, Jodi L. Camberg^{1,2}

- 1. Interdisciplinary Neurosciences Program, University of Rhode Island
- 2. Department of Cell and Molecular Biology, University of Rhode Island

PB - BIOINFORMATICS

A proteome view of structural, functional, and taxonomic PB-001 characteristics of major protein domain clusters

Chia-Tsen Sun¹, Austin W.T. Chiang¹, and Ming-Jing Hwang¹

Institute of Biomedical Sciences

PB-002 Functional Clustering of the Amidohydrolase

Julia Havden¹

1. - University of Richmond

PB-003 Mapping side chain interactions at protein helix termini

Nicholas Newell¹

1. - Newell, NE, BMC Bioinformatics 2015 16:231

PB-004 Manual Curation in the Conserved Domain Database

Gonzales NR¹, Chitsaz F¹, Derbyshire MK¹, Geer L¹, Gwadz M¹, Han L1, He J¹, Hurwitz DI¹, Lanczycki CJ¹, Lu F¹, Marchler GH¹, Song JS¹, Thanki N¹, Wang Z¹, Yamashita RA¹, Zheng C¹, Bryant SH¹, Marchler-Bauer A¹ 1. - NCBI



PB-005 Automating TULIP, a Protein Clustering Method

Nick Biffis1

1. - University of Richmond

PB-006 Functional Labeling of Protein Domain Architectures with SPARCLE

<u>Thanki N¹</u>, Han L¹, Lanczycki CJ¹, He J¹, Lu S¹, Chitsaz F¹, Derbyshire MK¹, Gonzales NR¹, Gwadz M¹, Lu F¹, Marchler GH¹, Song JS¹, Yamashita RA¹, Zheng C¹, Bryant SH¹, Geer L¹, Marchler-Bauer A¹

1. - National Center for Biotechnology Information, National Library of Medicine, National Institutes of Health

PC – CHAPERONES

PC-001 A novel GroEL to DnaK sequential chaperone network to modulate the stability and activity of E. coli heat-shock transcription factor σ 32 at physiological temperature

Monobesh Patra¹, Tarakdas Basu¹

1. - University of Kalyani

PC-002 Design and Characterization of Small Heat Shock Protein Dimers

Caley Butler¹, Hannah Arbach¹, Kathryn A. McMenimen¹

1. - Mount Holyoke College

PC-003 Identification and Characterization of Small Heat Shock Protein Interacting Domains

<u>Elizabeth De Leon¹</u>, Mahima Poreddy¹, Hannah Arbach¹, Kathryn A. McMenimen¹ 1. - Mount Holyoke College

PC-004 Molecular mechanism of protein kinase recognition and sorting by the Hsp90 kinome-specific cochaperone Cdc37

<u>Dimitra Keramisanou</u>¹, Adam Aboalroub¹, Ziming Zhang¹, Ralf Landgraf¹, Ioannis Gelis¹

1. - University of South Florida

PC-005 Design and Characterization of the Chaperone Activity of "Artificial" Small Heat Shock Proteins

Elizabeth De Leon¹, Mahima Poreddy¹, Pei Liu¹, Kathryn A. McMenimen¹

1. - Mount Holyoke College



PD - CHEMICAL BIOLOGY

PD-001 The oxidation of hydroxilamines with H2O2 mediated by Myoglobin.

Lucía Álvarez¹, Sebastián Suarez¹, Fabio Doctorovich¹, Marcela Martí²

- Departamento de Química Inorgánica
- 2. Departamento de Química Biológica, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Ciudad Universitaria, Pabellón

PD-002 The Influence of Distal Residues on Catalysis through Alpha-helical Motion

Shanadeen C. Begay¹, Penny J. Beuning¹, Mary Jo Ondrechen¹

1. - Northeastern University

PD-003 Design of Modular Switches for Allosteric Control over Protein Kinases and Protein Phosphatases

Matthew Bienick¹

1. - University of Arizona

PD-004 Characterization of Novel Pth-like Nucleotide Binding Protein PTRHD1

Geordan Burks¹

1. - University of Alabama

PD-005 Controlling The Phosphoproteome: Ligand-Gated Split-Kinases and Split-Phosphatases

Javier Castillo-Montova¹, Karla Camacho-Soto¹, Blake Tve¹, Luca Ogunleve¹, Indraneel Ghosh¹

1. - University of Arizona

PD-006 Enzymatic degradation of chitin by chitinase from dried seed plant

Wichuda Jankangram¹

Faculty of Science and Social Sciences

Utilizing computational and experimental chemistry to characterize PD-007 sthe functions of Structural Genomics proteins.

Caitlyn L. Mills¹, Penny J. Beuning¹, Mary Jo Ondrechen¹

1. - Northeastern University



PD-008 Rapid Bioorthogonal Protein Conjugation Reactions via ortho-Formylphenylboronic Acid-Based Coupling Chemistry

<u>Kamalika Mukherjee¹</u>, Tak Ian Chio², Saptarshi Ghosh², Han Gu², Zhen Lei², Samantha L. Grieco², Susan Bane²

1. - Massachusetts General Hospital/Harvard Medical School

2. - State University of New York

PD-009 DNA binding and unwinding mechanisms of archaeal and human DNA repair helicase homologues Hel308 and HelQ.

<u>Sarah Northall²</u>, Rebecca Lever¹, Nathan Jones¹, Panos Soultanas², Edward Bolt¹ 1. - School of Life Sciences, The University of Nottingham.

2. - School of Chemistry, The University of Nottingham.

PD-010 Next-generation assays to define and manipulate lysine acetyltransferase function

Jonathan Shrimp¹

1. - National Cancer Institute/NIH

PD-011 Probing cation-pi interactions of Heterochromatin Protein 1 using in vivo unnatural amino acid mutagenesis

<u>Baril, Stefanie A¹</u>, Koenig, Amber L¹, Krone, Mackenzie W¹, Brustad, Eric M¹, Waters, Marcey L¹

1. - `The University of North Carolina at Chapel Hill

PE - COMPUTATIONAL MODELING / SIMULATION

PE-001 Characterization of honey proteins with immunomodulatory activities.

<u>M. Kamran Azim¹</u>, Nida Dastagir¹, M. Ahmed Mesaik¹, Bushra Bilal¹, Atia Gohar¹ 1. - Nanyang Technologies University

PE-002 Coevolutionary analysis and structural prediction of the bacterial divisome

<u>Samson Condon¹</u>, Gladys Diaz-Vazquez¹, Deena-al Mahbuba¹, Alessandro Senes¹ 1. - University of Wisconsin-Madison

PE-003 An Improved Search Algorithm for Protein-Ligand Docking Using FFTs

Xingiang Ding¹, Charles L. Brooks III¹

1. - University of Michigan

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POSTER

PE-004 Differences on the conformational substates visited by native and mutants versions of the LAOBP obtained by Accelerated Molecular Dynamics.

Diego S. Granados¹, Jesus BandaVazquez¹, Alejandro SosaPeinado¹

1. - Department of Biochemistry, School of Medicine

PE-005 A new definition of inter-residue interaction provides insight into sequence-structure relationships

Jack Holland¹

1. - Dartmouth College

PE-006 Generating in silico Mutations to Infer the Effect of Multiple Amino Acid Substitutions on Protein Stability

Rebecca Hsieh¹

1. - Western Washington University

PE-007 Unique allosteric mechanism regulating protein-protein interaction through phosphorylation : a case study of the conformational changes in the Syk tandem SH2 protein

Duy P. Hua¹, Carol Beth Post¹

1. - Department of Medicinal Chemistry and Molecular Pharmacology, Purdue University

PE-008 The Slow To Fast Transition In Cytochrome C Oxidase Catalysis Is Facilitated By A Loop Flip In Subunit Ii Of The Enzyme

<u>Trevor Alleyne¹</u>, Diane N. Ignacio¹, Damian Ashe¹, Valerie B. Sampson²

- 1. Faculty of Medical Sciences, The University of the West Indies, St. Augustine Campus
- 2. Nemours Center for Cancer and Blood Disorders, Alfred I. duPont Hospital for Children

PE-009 Atomistic simulations of unfolding and translocation of the Immunoglobulin domain 127 in repetitive cycles of the ClpY Biological Nanomachines

Abdolreza Javidialesaadi¹, George Stan¹

1. - Department of Chemistry, University of Cincinnati



PE-010 The degradation and inhibition mechanism of Alzheimer's A β fiber by dihydrochalcone molecules

<u>Yibo Jin¹</u>, Yunxiang Sun¹, Guanghong Wei*

 State Key Laboratory of Surface Physics, Key Laboratory for Computational Physical Sciences (Ministry of Education), Department of Physics, Fudan University

PE-011 A COMPUTATIONAL STUDY ON AQUAPORIN-EMBEDDED WATER PURIFICATION SYSTEM

Youngjin Kim¹, Sangjae Seo¹, Eugene Ham², Jong Sung Kim², Moon Ki Kim¹

- 1. School of Mechanical Engineering, Sungkyunkwan University,
- 2. Stevenson High School

PE-012 Mechanism of Improved Doripenem Binding in Several Clinical Mutations in OXA-66 Beta-Lactamase

Zachary Klamer¹, Emma Schroder², Troy Wymore³, David A. Leonard², Agnieszka Szarecka¹

- 1. Department of Cell and Molecular Biology, Grand Valley State University
- 2. Department of Chemistry, Grand Valley State University
- 3. Department of Chemistry, University of Michigan

PE-013 Carbohydrate and protein effects on antibody-receptor binding

Morgan L. Nance^{1,2}, Jason W. Labonte², and Jeffrey J. Gray²

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PE-014 On the ability of molecular dynamics force fields to recapitulate NMR derived protein side chain NMR order parameters

Evan S. O'Brien¹, A. Joshua Wand, Kim A. Sharp

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PE-015 Electrostatic interactions and the multi-layered local structure of active sites: Key features in natural and designed enzymes

<u>Timothy A. Coulther</u>¹, Lisa Ngu¹, Penny J. Beuning¹, Mary Jo Ondrechen¹ 1. - Department of Chemistry & Chemical Biology, Northeastern University

PE-016 Analysis of Multi-domain Protein Dynamics

Amitava Roy¹

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PE-017 Computational prediction and functional annotation of enzymes in the Haloacid Dehalogenase Superfamily for Bioremediation

<u>Lydia A. Ruffner¹</u>, Mong Mary Touch¹, Penny J. Beuning¹, Mary Jo Ondrechen¹ 1. - Department of Chemistry & Chemical Biology, Northeastern University

PE-018 Computational Studies of Green Fluorescent Protein Unfolding and Translocation by the CIpY ATPase during Protein Degradation

<u>Yu-Hsuan Shih¹</u>, George Stan¹

1. - Department of Chemistry, University of Cincinnati

PE-019 Predicting allosteric interactions with rigidity theory

<u>Adnan Sljoka¹</u>

1. - Crest Japan Science and Technology Agency

PE-020 Modeling Protein Folding/aggregation on Nanoparticle-based Biosensors in Complex Solvent Environments by a Coarse-grained Simulation System.

Shuai Wei¹, Charles L. Brooks III¹

1. - Department of Chemistry and Biophysics, University of Michigan

PE-021 Studying protein conformational transitions using adaptive biased sampling optimization (ABPO)

Heng Wu¹, Carol B. Post¹

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PE-022 An Investigation of the Thermostability of DNA Polymerase using Molecular Dynamics Simulations

Erica Modeste¹, Lily Mawby¹, Bill Miller III¹, Eugene Wu¹, Carol Parish¹

1. - Department of Chemistry, University of Richmond

PE-023 Disordered tail of linker histone H1 in chromatin compaction dynamics studied by coarse-grained simulations

Nobu C. Shirai¹

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PF - DESIGN / ENGINEERING

PF-001 Self-Assembling Nano-Architectures Created From A Protein Nano-Building Block Using An Intermolecularly Folded Dimeric De Novo Protein

<u>Naoya Kobayashi¹</u>, Keiichi Yanase¹, Takaaki Sato¹, Satoru Unzai², Michael H. Hecht³, and Ryoichi Arai¹

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3.- Department of Chemistry, Princeton University

PF-002 A General, Symmetry-Based Methodology in Protein Cage Assembly

<u>Aaron Sciore</u>¹, Somayesadat Badieyan¹, Min Su1, Philipp Koldewey¹, Kelsey A. Diffley¹, Brian M. Linhares¹, James C. A. Bardwell¹, Georgios Skiniotis¹, E. Neil G. Marsh¹

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PF-003 Enzymatic synthesis of size controlled, water soluble quantum dots

Bryan Berger¹

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PF-004 Computational Design of Small Protein Inhibitors Targeting PD-1

<u>Cassie Bryan</u>¹, Gabriel J. Rocklin¹, Nicole Lieberman¹, Courtney Crane¹, David Baker¹

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PF-005 De novo design of protein homo-oligomers with modular hydrogen bond network-mediated specificity

<u>Scott E. Boyken</u>, Zibo Chen¹, Benjamin Groves¹, Robert A. Langan¹, Gustav Oberdorfer¹, Alex Ford¹, Jason M. Gilmore¹, Chunfu Xu¹, Frank DiMaio¹, Jose Henrique Pereira¹, Banumathi Sankaran¹, Georg Seelig¹, Peter H. Zwart¹, David Baker¹

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PF-006 Computational Design of Dynamics into a Stable Globular Protein

<u>James A. Davey¹</u>, Adam M. Damry¹, Natalie K. Goto¹, Roberto A. Chica¹ 1. - Department of Chemistry and Biomolecular Sciences, University of Ottawa



De Novo Design of Protein Scaffolds Suited for Ligand-Binding PF-007

Tamuka Chidvausiku¹, Enrique Marcos Ph.D.¹, Beniamin Basanta¹, David Baker¹ 1. - University of Washington, Biological Physics Structure and Design Program

PF-008 Controlling the Phosphoproteome: Ligand Activated Split-Kinases and Split-Phosphatases

Mahsa M.E. Ghaffari¹, Karla Camacho-Soto¹, Javier Castillo- Montoya¹, Indraneel Ghosh¹

1. - University of Arizona

PF-009 Developing a soluble bifunctional receptor/co-receptor mimetic for structural characterization of the HIV envelope glycoprotein

Agnes Haiduczki¹

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Antigen clasping: novel antibody-antigen recognition mechanism PF-010 enabling extraordinarily high specificity

Takamitsu Hattori1², Darson Lai², Irina Dementieva², Sherwin Montano², Kohei Kurosawa², Akiko Koide², Alexander J. Ruthenburg^{2,3} and Shohei Koide²

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PF-011 Novel Proteins Provide Life Sustaining Activities In Vivo

Michael Hecht¹

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PF-012 Harnessing the Reactivity of Selenocysteine for Expressed Protein Ligation

Jun Liu, Qingging Chen, Sharon Rozovsky

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Induced domain swapping (INDOS): a modular design for controlling **PF-013** protein function with a small molecule

Jeung-Hoi Ha¹, Joshua M, Karchin¹, Stewart N, Loh¹

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PF-014 Caspase-7 with Reprogrammed Specificity Allows Identification of Exosites for Substrate Recognition

<u>Derek MacPherson</u>¹, Maureen Hill¹, Peng Wu¹, Olivier Julien², James A. Wells ², Jeanne A. Hardy¹

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PF-015 Construction of Zn-SO4 Cluster-encapsulating Protein Nanocage by Domain Swapping

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- 4. RIKEN SPring-8 Center

PF-016 Computational design of novel repeat protein families with atomic level accuracy

<u>Fabio Parmeggiani¹</u>, TJ Brunette1, Po-Ssu Huang¹, Damian Ekiert², Gira Bhabha², Susan Tsutakawa³, Greg L. Hura³, John A. Tainer³, David Baker¹

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PF-017 Protein engineering of Caf1 from the plague bacterium Yersinia pestis for tissue engineering applications.

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PF-018 Designing highly specific protein-based small molecule biosensors

<u>Srivatsan Raman¹</u>

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PF-019 Controlling protein structure and function using engineered allosteric effectors

<u>Matthew Krusen¹</u>, Akiko Koide², Shohei Koide², Anthony A. Kossiakoff², Kasturi Haldar¹, Rovert V. Stahelin^{1,3}, Shahir S. Rizk⁴

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PF-020 Engineering the FabA and FabZ fatty acid dehydratase domains from Escherichia coli into dimeric artificial constructs

Carlos Rullán¹

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PF-021 A Residue Code to Mapping Protein Structure

<u>Hyun Joo¹</u>, Keith Fraga¹, Jerry Tsai¹

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PF-022 Drug design against trichomoniasis

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PF-023 Comprehensive evaluation of protein sequence-function landscapes using deep sequencing

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PF-024 Nicking Mutagenesis: A Plasmid-Based Single-Pot Saturation Mutagenesis Method

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PF-025 De Novo Design of Multi-nuclear Clusters in Helical Bundles

<u>Shao-Qing Zhang¹</u>, Lijun Liu¹, Youzhi Tang¹, Yibing Wu¹, William F. DeGrado¹ 1. - UCSF

PF-026 Structure Relationships

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PF-027 A Directed Evolution Approach to Engineer Caspase Specificity

<u>Maureen E. Hill¹</u>, Derek J. MacPherson¹, Peng Wu, Ph.D.¹, Olivier Julien, Ph.D.¹, James A. Wells, Ph.D.¹, Jeanne A. Hardy, Ph.D.¹

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PF-028 Super WA20 (SUWA), an Ultra-Stabilized Dimeric de Novo Protein for Self-Assembling Protein Nanobuilding Blocks

<u>Naoya Kimura¹</u>, Naoya Kobayashi¹, Ryoichi Arai¹

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PF-029 Experimental Characterization of Computationally Predicted "Metamorphic" Proteins

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PF-030 Artificially designed peptides that degrade amyloid fibrils

Yoshihiro Iida¹

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PF-031 Flipping the Switch: Engineering Alternate Function in the Lactose Repressor

David H. Richards¹, Corey J. Wilson¹

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PF-032 Resurfacing Proteins Using a Structural Search Engine

Jianfu Zhou¹, Gevorg Grigoryan^{1,2}

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PF-033 Engineering a Surface Immobilized Enzyme to Obtain High Levels of Water-free Activity

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PF-034 Computational design and screening of leave-one-out green fluorescent protein biosensors for viral targets.

<u>Keith Fraser</u>¹, Shounak Banerjee¹, Danielle Chan¹, Julia Reimertz¹, Nailah Wade¹, Emily Crone¹, Monica Miles¹, Mason Gentner¹, Alex Stevens¹, Megan Jenkins¹, Eric Carlin¹, Lauren Paul¹, Angela Choi¹, Rachel Atschul¹, Casey Thornton¹, Colleen Lamberson¹, Christian D. Schenkelberg¹, Yao-ming Huang¹, Derek J. Pitman¹, Donna E. Crone¹, Jonathan S. Dordick¹, Scott Michael¹, Christopher Bystroff¹

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PF-035 Mispacking and the fitness landscape of green fluorescent protein (GFP).

<u>Shounak Banerjee</u>¹, Keith Fraser¹, Danielle Chan¹, Julia Reimertz¹, Emily Crone¹, Mason Gentner¹, Robert Langan¹, Priscilla Hempel¹, Oluwadamilola Lawal¹, Kangning Zhang¹, Colleen Lamberson¹, Angela Choi¹, Rachel Alschul¹, Christian D. Schenkelberg¹, Yao-ming Huang¹, David Rosenman¹, Benjamin Walcott¹, Derek J. Pitman¹, Donna E. Crone¹, John Karanicolas¹, Jonathan S. Dordick¹, Christopher Bystroff¹

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PF-036 Self-Assembling Supramolecular Nanostructures Created by de Novo Extender Protein Nanobuilding Blocks

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PF-037 Statistical and combinatorial approaches to designing repeat proteins as recognition elements in microbial sensors

Rachael N. Parker¹, Ana Mercedes¹, Tijana Z. Grove¹

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PF-038 Engineering of a modular "Split-enzyme" protein G-based sandwich immunoassay for Ebola-virus Nucleoprotein detection

<u>Tomasz Slezak</u>¹, Mateusz Jaskolowski¹, Lucas J. Bailey¹, Zachary P. Schaefer¹, Elena K. Davydova¹, Anthony A. Kossiakoff¹

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PF-039 Engineering a Universal Dengue Vaccine Using a Virus-Like Particle Scaffold

Danielle Basore¹², Thomas Jordan^{1,2}, Carolyn Barcellona³, Eric Carlin³, Emilie Mausser¹, Kanthi Bommareddy¹, Donna Crone¹, Sharon Isern³, Scott Michael³, Chris Bystroff^{1,2,4}

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PF-040 Dynamic combinatorial libraries from designed armadillo repeat protein fragments

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PF-041 Characterization and single chain Fv construction of neutralizing antibody to measles virus

<u>Takashi Tadokoro</u>¹, Lubna Mst Jahan¹, Atsutoshi Imai¹, Natsumi Sugimura¹, Koki Yoshida¹, Mizuki Saito¹, Yuri Ito¹, Surui Chen¹,Takao Hashiguchi², Yusuke Yanagi², Maino Tahara³, Makoto Takeda³, Hideo Fukuhara¹, Katsumi Maneaka¹

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PF-042 Lessons in Protein Electrostatics from Natural Enzymes Applied to Enzyme Design

<u>Tim Coulther</u>¹, Penny Beuning¹, Mary Jo Ondrechen¹

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PF-043 Computational design of allosteric antibody

Olga Khersonsky¹, Sarel J. Fleishman¹

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PF-044 Substitutions affecting the flexibility of the N-terminus of the cold adapted subtilase, VPR, are important for its temperature adaptive properties.

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PF-045 An Engineered High Affinity Fbs1 Carbohydrate Binding Protein for Selective Capture of N-glycans and N-glycopeptides

<u>Minyong Chen¹</u>, Xiaofeng Shi¹, Rebecca Duke¹, Cristian Ruse¹, Nan Dai¹, Christopher H. Taron¹, James C. Samuelson¹

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PG - DYNAMICS AND ALLOSTERY

PG-001 Entropy Redistribution Drives Allostery in a Metalloregulatory Protein

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PG-002 Probing the Domain Architecture and Dynamics of Caspase-6 Reveal Mechanisms for its Regulation

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PG-003 Direct Measurements of the Long-Range Collective Vibrations of Photoactive Yellow Protein

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PG-004 Heme Induced Allostery Drives The Interaction Of Pseudomonas Aeruginosa Cytoplasmic Heme Binding Protein (Phus) With Heme Oxygenase.

<u>Daniel Deredge</u>¹, Weiliang Huang¹, Colleen Hui², Hirotoshi Matsumura², Pierre Moenne-Locoz², Patrick Wintrode¹, Angela Wilks¹

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PG-005 Deciphering the Dual Regulatory Mechanisms of Phosphorylation on Caspase---7

Scott J. Eron¹, Dr. Jeanne A. Hardy¹

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PG-006 Allostery in Trp-Dependent RNA Remodeling by TRAP

<u>Elihu C. Ihms¹</u>, Ian R. Kleckner¹, Craig A. McElroy¹, Melody L. Holmquist¹, Aparna Unnikrishnan¹, Vicki Wysocki¹, Paul Gollnick¹, Mark P. Foster¹

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PG-007 Trapping Catalytic Conformations by Crosslinking the Swinging-Arm Domain of Pyruvate Carboxylase

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PG-008 First Structure of Full-Length Mammalian Phenylalanine Hydroxylase Reveals the Architecture of the Resting-state Tetramer

<u>Emilia C. Arturo¹²</u>, Kushol Gupta³, Annie Heroux⁴, Linda Stith¹, Penelope J. Cross⁵, Emily J. Parker⁵, Patrick J. Loll², Eileen K. Jaffe¹

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- 3. Perelman School of Medicine, University of Pennsylvania
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PG-009 The swinging arm of pyruvate carboxylase is allosterically regulated by acetyl-coenzyme A

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PG-010 Tuning Catalytic Activity by Perturbing Amino Acid Networks in a (β/α) 8 Barrel Enzyme

Kathleen O'Rourke¹

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PG-011 Regulation, activation and deactivation of guanylate cyclase

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PG-012 Subunit Exchange and activation of human CaMKII variants

Ana Pamela Torres Ocampo¹, Brendan Page¹, Margaret M. Stratton¹

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PG- 013 P53-binding Domain of MdmX Undergoes a Conformational Transition Favorable for Ligand Binding

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PG-014 Soluble Guanylate Cyclase: A Therapeutic Target for Cardiovascular Disease

Jessica Wales¹

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PG-015 The Role of Dynamical Transition in Protein Function: Coupling of Protein Collective Vibrations and Water Dynamics

<u>Mengyang Xu¹</u>, Katherine Niessen¹, Yanting Deng¹, Nigel Michki¹, Edward Snell², Andrea Markelz¹

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PG-016 Effector-linked high-frequency thermal fluctuations of hemoglobin regulate its O2-affinity, cooperativity, and Bohr effects

<u>Takashi Yonetani¹, Kenji Kanaori²</u>

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PG-017 Studying protein-protein binding through T-jump induced dissociation: Transient 2D IR spectroscopy of insulin dimer

Xin-Xing Zhang¹, Kevin C. Jones¹, Andrei Tokmakoff¹

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PG-018 Insights into protein flexibility in ligand recognition from a NMR chemical shift perturbation analysis

Xinxin Zhang¹, Jie J Zheng^{1,2}

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PG-019 Reciprocal allosteric communication in E.coli BirA

Jingheng Wang¹, Dorothy Beckett¹

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PG-020 Hemi-methylated DNA regulates DNA methylation inheritance through allosteric activation of H3 ubiquitylation by UHRF1

<u>Joseph S. Harrison^{1,2}</u>, Evan M. Cornett^{3*}, Dennis Goldfarb^{4*}, Paul A. DaRosa^{5*}, Zimeng M. Li⁶, Feng Yan⁷, Bradley M. Dickson³, Angela H. Guo¹, Daniel V. Cantu¹, Lilia Kaustov⁸, Peter J. Brown⁸, Cheryl H. Arrowsmith⁸, Rachel E. Klevit⁵, Dorothy A. Erie⁹, Michael B. Major^{4,7}, Krzysztof Krajewski¹, Brian Kuhlman^{1,2}, Brian D. Strahl^{1,2}, Scott B. Rothbart³

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PG-021 Single Molecule Analysis of Allosteric Interactions in Protein Kinase A

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15N Direct-Detect NMR Spectroscopy Experiments to Examine PG-022 Determinants of Anomalous pKa Values of Lvs Residues in **Hvdrophobic Environments**

Christos M. Kougentakis¹, Emily M. Grasso¹, Ananya Majumdar², Bertrand García-Moreno¹

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PG-023 Extended Impact of Catalytic Loop Phosphorylation in Human Pin1

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PG-024 Understanding the role of distal residues in the activity of ornithine transcarbamovlase using small angle x-ray solution scattering

Jenifer N. Winters¹, Lisa Ngu¹, Lee Makowski¹, Penny J. Beuning¹, Marv Jo Ondrechen¹

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PH - ENZYMOLOGY

PH-001 Structure-based mutational studies of AcvI Carrier Protein of Leishmania maior **Reveals a Novel Phosphopantetheinyl Transferase Binding Interface**

Richa Arya¹, Ambrish Kumar², Monica Sundd², Suman Kundu¹

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- 2. National Institute of Immunology, Aruna Asaf Ali Marg



PH-002 In crystallo Phosphorylation of Tobramycin by the Antibiotic Kinase APH(2")-la

<u>Shane J. Caldwell¹</u>, Albert M. Berghuis¹ 1. - McGill University

PH-003 Mechanism of a cytosolic O-glycosyltransferase essential for the synthesis of a bacterial adhesion protein

<u>Yu Chen¹</u>, Ravin Seepersaud², Barbara A. Bensing², Paul M. Sullam², Tom A. Rapoport¹

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- 2. San Francisco Veteran Affairs Medical Center and University of California

PH-004 IpdAB, a key virulence determinant in Mycobacterium tuberculosis, is a cholesterol ring-opening hydrolase

<u>Adam M. Crowe¹</u>, Nobu Watanabe¹, Israël Casabon¹, Kirstin Brown¹, Jason Rogalski¹, Timothy Hurst¹, Victor Snieckus¹, Leonard Foster¹, Natalie C. Strynadka¹, Lindsay D. Eltis¹

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PH-005 Non-Specific Interactions of Dihydrofolate Reductase Ligands in Crowded Environments

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PH-006 Kinetic characterization of Trypanosoma cruzi His₁₀-bhydroxybutyrate dehydrogenase (βHBDH) and functional exploration of Trypanosoma brucei βHBDH via RNA interference.

William Escboar-Arrillaga¹, Linh Nguyen¹, Jennifer Palenchar¹

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PH-007 Rapid detection of single-stranded DNA-specific 3' exonucleases in human serum

Simin Fang¹, Meiping Zhao¹

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PH-008 Active Site Binding is not Sufficient for Reductive Deiodination by lodotyrosine Deiodinase

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PH-009 Analysis of a polyextremophilic b-galactosidase from an Antarctic Haloarchaeon: Mutagenic analysis of residues important for cold activity

Victoria Laye¹, Priya DasSarma¹, Wolf Pecher¹, Shiladitya DasSarma¹

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PH-010 Characterization of PTP1B function and inhibition

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PH-011 Molecular basis of substrate recognition and catalysis in Phosphatidylinositol 3-kinase

<u>Sweta Maheshwari¹, Michelle M. Miller¹, Robert O'Meally¹, Robert Cole¹, Kenneth W. Kinzler¹, L. Mario Amzel¹, Bert Vogelstein¹, Sandra B. Gabelli¹</u>

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PH-012 Biochemical characterization of two haloalkane dehalogenases: DccA from Caulobacter crescentus and DsaA from Saccharomonospora azurea

Emily C. Mundorff¹

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PH-013 Cadmium Inhibits MutLα within the Human Mismatch Repair System

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- 2.- Howard Hughes Medical Institute Duke University Medical Center



PH-014 Engineering the reversal of Pseudomonas putida β-hydroxybutyrate dehydrogenase cofactor specificity.

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PH-015 Kinetic and mutational studies of the adenosine diphosphate ribose hydrolase from Mycobacterium tuberculosis

Puchong Thirawatananod¹

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PH-016 Enzyme promiscuity and Evolution of Enzyme Kinetic Mechanisms

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PH-017 Enzyme Mechanism Influences Macromolecular Crowding Effects

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PH-018 Investigation on the specific recognition between lambda exonuclease and DNA substrates with chemical modification and mismatches

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PH-019 The intrinsically disordered selenoprotein K has autoproteolytic activity

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PH-020 Oxyanions as Inhibitors of Protein Tyrosine Phosphatase Isolated from Roots of Germinating Seedlings of Cicer arietinum

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PH-021 The Crystal Structure Of Sdre From S. Aureus

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PH-022 Promiscuous hydrolysis of p-nitrophenyl sulfate by Vibrio alkaline phosphatase coincides with loss of active-site magnesium ions and loss of phosphatase activity.

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PH-023 Calpain/calpastatin proteolytic system as a target of geomagnetic field disturbances

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PH-024 Determination of Kinetic Parameters of Trypsin I from Pyloric Caeca of Monterey Sardine (Sardinops sagax caerulea) Using Isothermal Titration Calorimetry

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PH-025 The role of the Protein Structural Network (PSN) in the thermostability

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PI - EVOLUTION

PI-001 A covariance-based model to estimate antimicrobial drug resistance

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PI-002 Biophysical Mechanisms Driving The Evolution Of Androgen Specificity.

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PI-003 Experimental evidence for the existence of thermally stable proteins in early life

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PJ - FOLDING

PJ-002 Structural Studies of Protein Folding on the Ribosome

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PJ-003 Effect of Circular Permutations on Transient Partial Unfolding in Proteins

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PJ-004 In Silico to In-Cell Folding of Metastable Serpins

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PJ-005 Biophysical studies on 4-Hydroxynonenal modified Human Serum Albumin: A Possible Role in Rheumatoid Arthritis

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PJ-007 Proxy analysis of the structural and functional impact of a pathogenic mutation in a human protein chaperone using an archaeal model

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PJ-008 Modulating protein folding kinetics with and without non-natural amino acids

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PJ-009 Conformational status and activation of peroxidase function of cytochrome c upon glycation: Implications to cytochrome c release and apoptosis

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PJ-010 Cooperative folding of a low sequence complexity, PP2 protein lacking a hydrophobic core

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PJ-011 Complex lassos: new entangled motifs in proteins

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PJ-012 Measuring the effects of vectorial appearance of the polypeptide chain on protein folding

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PJ-013 Modulation of Proteins Unfolding under Exposure to High Frequency Electromagnetic Field following Proteins Dipole Moment

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PJ-014 Amide A Band Decreases in a Tetrameric Hemeprotein under Exposure to Static or 50 Hz Electromagnetic Fields

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PJ-015 ACPro: A curated database of verified protein folding kinetics

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PJ-016 Validation of Native-state Hydrogen Exchange Mass Spectrometry to map protein folding landscapes

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PJ-017 Characterization of Truncated Hemoglobins from Chlamydomonas reinhardtii.

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PJ-018 Investigating residue-specific dynamics with native-state hydrogen exchange mass spectrometry

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PJ-019 Investigation of Confinement Effects on Protein Stability Using Reverse Micelles and Chemical Denaturation

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PJ-020 Investigating the relationship between enzyme function, native-state dynamics and kinetic stability in trypsin

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PJ-021 Cotranslational folding studies of spectrin and Ig-like domains show folding occurs close to the ribosome

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PJ-022 Folding of Metastable Serpin at Atomic Resolution

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PK - INTRINSICALLY DISORDERED PROTEINS

PK-001 Functional Protein Disorder In Coupled Binding-Folding And Liquid-Liquid Demixing

<u>Priya R. Banerjee¹</u>, Diana M. Mitrea¹, Richard W. Kriwacki¹, Ashok A. Deniz¹

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PK-002 A bacterial antitoxin's conformational ensemble provides insight into distinct functional roles of its distinct disordered states

<u>Virginia M. Burger¹</u>, Alexandra Vandervelde¹, Albert Konijnenberg¹, Jelle Hendrix¹, Frank Sobott¹, Remy Loris¹, Collin M. Stultz¹

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PK-003 Structural details of RNA-binding protein disordered domain phase separation in ALS and cancers

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PK-004 Disorder Within Cysteine-Rich Protein And Its Implications For Multifunctional Roles: The Curious Case Of Granulin-B.

<u>Gaurav Ghag</u>¹, Lauren M. Wolf², Randi G. Reed¹, Nicholas P. van der Munnik³, Claudius Mundoma⁴, Melissa A. Moss^{2,3}, Vijay Rangachari¹

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PK-005 Understanding dengue virus capsid protein disordered N-terminal biological activity – playing Lego with proteins to develop peptide inhibitors

<u>André F. Faustino¹</u>, Filomena A. Carvalho¹, Fábio Almeida², Andrea T. Da Poian², Nuno C. Santos¹, Ivo C. Martins¹

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PK-006 Site Specific 1H-13C Phenylalanine in the Study of the Pth1:Peptidyl tRNA Complex

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PK-007 Characterization of order and disorder in domains of IncC – a plasmid partitioning protein from pRK2

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PK-008 Nucleophosmin-mediated molecular networks reveal insights into the structural organization of the granular component of the nucleolus

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PK-009 Localized assembly of RNA granules by intrinsically-disordered proteins that bind RNA.

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PK-010 Autoregulation of the p53 Binding Activity of Mdm2 by Intrinsically Disordered Regions

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PK-011 Stabilization of a globular protein by a disordered tardigrade protein

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PL - MEMBRANE PROTEINS

PL-001 Distinct structural elements govern folding, stability and catalysis in the outer membrane enzyme PagP

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PL-002 Characterization of the interaction between cyt c and cardiolipin-incorporated bicelles by solution NMR.

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PL-003 A new Rosetta refinement algorithm to improve membrane protein structures

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PL-004 Application of the dual split protein reporter to a high throughput screening of potential fusion inhibitors of HIV-1 envelope protein

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PL-005 Essential Oil Antifungals: The Search for Novel Targets

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PL-006 The intrinsically disordered membrane enzymes selenoprotein S and Selenoprotein K

Jun Liu1, Zhenqui Zhang¹, Sharon Rozovsky¹

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PL-007 Using thermodynamics to cure disease -- nucleotide analogs provide significant correction of the temperature-dependent defect in F508del-CFTR

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PL-008 Enhanced resolution in size exclusion chromatography for separation of proteins with Mr 3000-70 000

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PL-009 Molecular explanations for metal selectivity and the conformational change process in Nramp-family divalent metal transporters

<u>Aaron Bozzi¹</u>, Lukas Bane¹, Wilhelm Weihofen¹, Brandon Lee¹, Rachelle Gaudet¹ 1. - Harvard University

PL-010 Role of Transmembrane Domain of Arabidopsis CRINKLY4 Receptor-like Kinase (ACR4) in a Membrane-like Environment

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PL-011 Solution NMR studies on membrane proteins in lipid bilayers

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PL-012 Heterologous expression of teleost trace amine-associated receptor fused with N-terminal sequence of rod opsin

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PL-013 TRPV4 ion channel regulates normal human lung fibroblast migration

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PL-014 An efficient microbial system for the preparation of GLP-1 receptor

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PL-015 **Cell-Free Protein Expression for Soluble Expression of Functional Class A G Protein Coupled Receptors**

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PM - MOTORS AND MACHINES

PM-001 Mechanisms and Applications of R bodies, Membrane-Breaking **Protein Needles**

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PN - PEPTIDES

PN-001 Uptake Mechanism of the Cell-penetrating Peptide pVEC: How Does the Hydrophobic N-terminus Contribute?

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PN-002 Comparison of Solid-Phase Extraction and Size Exclusion Chromatography applied for preparation of urine samples from pregnant women for LC-MSMS

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PN-003 The Relationship Between Urine Peptidome And Protein Misfolding During Preeclamsia

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PN-004 Developing potent and specific inhibitors of the Grb7 breast cancer target using phosphotyrosine mimetics and bicyclic peptides

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PN-005 Developing Novel Peptide Scaffold for Protein-Protein Interactions (PPIs) Inhibition

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PN-006 Uptake Mechanism of the Cell-penetrating Peptide pVEC: How Does the Hydrophobic N-terminus Contribute?

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PN-007 Leucine And Isoleucine Contribute Differently To The Binding Of Amphipathic Peptides To Membranes

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PN-008 Comparison of Solid-Phase Extraction and Size Exclusion Chromatography applied for preparation of urine samples from pregnant women for LC-MSMS

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PN-009 Creating Of A Non-Invasive Method For The Diagnosis Of Cervical Neoplasia Degree Using Cvf Proteomic Analysis

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PO - PROTEIN IN CELLS

PO-001 Breaking the fourth wall: Quaternary organization forge a link to the novel non-enzymatic function of RNR-a

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PO-002 Creative destruction of DNA builds CRISPR immunity: Identification of E. coli host helicase, nuclease and polymerase enzymes that target replication forks to promote Cas1-Cas2 CRISPR adaptation.

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PO - 003 Importance of protein kinetic stability in extremophiles: A study of thermoacidophilic archaea Sulfolobus acidocaldarius

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PO -004 Protein stability in cells after hyperosmotic shock

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PO-005 Effects of macromolecular crowding on protein folding kinetics

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PO-006 Acetyl-Coa Carboxylases In Dinoflagellates: Fueling The Polyketide Synthase Pathways

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PO-007 Crowding and protein dimerization

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PP - PROTEIN INTERACTIONS AND ASSEMBLIES

PP-001 Deciphering the molecular and functional basis of the RhoGAP family proteins: A systematic approach towards selective inactivation of the Rho family proteins

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PP-002 Biomolecular interaction determination and quantification by MicroScale Thermophoresis

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PP-003 The Role of Dimerization in the Methylation Activity of EcoP151 DNA Methyltransferase

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PP-004 Structure Of Serum Amyloid A Suggests A Mechanism For High-Density Lipoprotein Binding And Function As A Protein Hub

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PP-005 An Autoinhibited Dimeric Form of Pro-apoptotic BAX Regulates Apoptosis'

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PP-006 Domain Swapping in c-Type Cytochromes and Myoglobin

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PP-007 Novel antimicrobial lectin Myxovirin

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POSTERS

PP-008 Canonical Mapping of bZip Protein-DNA Recognition

<u>Hyun Joo¹, Jerry Tsai1</u> 1. - University of the Pacific

PP-009 Improving the affinity of the phosphoepitope-binding FHA1 domain

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PP-010 Gene Ontology in Comparative Protein Docking

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PP-11 Silk Fibroin/Sericin Interaction at the Biomimetic Interface

Hyo Won Kwak¹, Ki Hoon Lee¹

1. - Department of Biosystems & Biomaterials Science and Engineering, Seoul National University, Republic of Korea

PP-012 Versatile Nucleotide Recognition with the Peptidyl-tRNA Hydrolase Fold

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PP-013 Investigating DNA Recognition by the Methyl-CpG Binding Protein ZBTB38

Sven A. Miller¹, Bethany A. Buck-Koehntop¹

1. - Department of Chemistry, University of Utah

PP-014 Site Specific 1H-13C Phenylalanine in the Study of the Pth1:Peptidyl tRNA Complex

Bhargavi Ramaraju¹, Hana McFeeters¹, Robert McFeeters¹

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PP-015 A New Dimension of Detection in Analytical Ultracentrifugation with Fluorescence Detection System Using Photoswitchable GFPs as Time Domain Probes

<u>Huaying Zhao¹</u>, Yan Fu², Carla Glasser³, Eric Andrade², Mark L. Mayer³, George Patterson², Peter Schuck¹

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- 2. Section on Biophotonics, National Institute of Biomedical Imaging and Bioengineering
- 3. Laboratory of Cellular and Molecular Neurophysiology, Porter Neuroscience Research Center National Institute of Child Health and Human Development National Institutes of Health

PP-016 Signaling by assembly: how the host innate immune system responds to pathogen dsDNA.

<u>Seamus R. Morrone¹</u>, Sarah Stratmann², Mariusz Matyszewski¹, Xiong Yu³, Edward H. Egelman³, Antoine van Oijen^{2,4}, and Jungsan Sohn¹

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PP-017 Analysis of Eukaryotic Heme a Synthase Cox15 and Associated Dysfunctions

<u>Samantha Swenson</u>¹, Andrew Cannon¹, Nicholas Harris², Nicholas Taylor², Jennifer L. Fox², Oleh Khalimonchuk¹

- 1. University of Nebraska-Lincoln, Department of Biochemistry, Redox Biology Center
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PP-18 Peptide binders based on complementary Armadillo Repeat Protein Fragments

Erich Michel¹, Randall Watson¹, Andreas Plückthun², Oliver Zerbe¹

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- 2. Department of Biochemistry, University of Zurich

PP-19 Global Analysis of Data from Multiple Biophysical Methods for Studying Protein Complex Stoichiometry and Affinity

Huaying Zhao¹, Peter Schuck¹

 Dynamics of Macromolecular Assembly Section, Laboratory of Cellular Imaging and Macromolecular Biophysics, National Institute of Biomedical Imaging and Bioengineering, National Institutes of Health

PP-20 Mapping Integrin I Domain Binding Sites on Type I Collagen Monomers and Fibrils by microscopy

Jie Zhu¹, Ana Monica Nunes¹, Jean Baum¹

1. - Rutgers University

PP-021 Biochemical Determination of APOBEC3A Interactions with ssDNA

Samantha Ziegler¹, Yong Xiong¹

1. - Yale University

PP-022 Expression, Purification, and Characterization of Human M6PR Extra Cellular Domain

<u>Brian Dwyer¹</u>, Andrea Iskenderian¹, Dianna Lundberg¹, Muthu Meiyappan¹, Bohong Zhang¹

1. - Shire/University of Massachusetts Lowell

PP-023 Subunit interaction and asymmetry of cold-active alkaline phosphatase studied using bimane fluorescence label at dimer interface.

- Jens G. Hjörleifsson¹, Bjarni Ásgeirsson¹
- 1. Science Institute, Department of Biochemistry, University of Iceland, Dunhaga 3, 107 Reykjavik, Iceland

PP-024 Towards quantitative mapping of protein interactions in vivo

O. Matalon¹, ED. Levy¹

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PP-025 Expression and purification of Arabidopsis phosphatase PP2A-3 catalytic subunit in E.coli and approaches to its activation in trans.

Priyanka Sandal¹, Shweta Shah¹, A. Gururaj Rao¹

1. - Roy J. Carver Dept. of Biochemistry, Biophysics & Molecular Biology, Iowa State University

PP-026 On the role of C-Terminal tail helical domain of anabaena sensory rhodopsin transducer in unusual high stability, ligand and receptor interaction.

<u>Vishwa Trivedi¹</u>, Tashmay Jones¹ and Rene Walker¹, Rory Henderson² and TK S Kumar²

- 1. Department of Natural Science, College of Science, Engineering and Mathematics
- 2. Department of Chemistry and Biochemistry, University of Arkansas



PP-027 The Determining Factors of the Self-assembly of a Collagen Mimetic Triple Helix

Fangfang Chen¹, Sam Wong1, Parminder Jeet Kaur1

1- Department of Biochemistry, Hunter College, The Graduate Center of The City University of New York, NY

PP-028 Characterisation of Non-Histone Lysine Acetyltransferases and Deacetylases in Probiotics

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- 1. Enzyme and Protein Chemistry, Department of Systems Biology, Technical University of Denmark
- 2-Protein and Immune Systems Biology, Department of Systems Biology, Technical University of Denmark

PQ - PROTEOMICS

PQ-001 Spatial and Temporal control of Lysine Acetyl transferases (KATs): Ligand gated split KATs

C.S. DeSilva¹, Ghosh E. Restituyo¹

1. - Department of Chemistry and Biochemistry, University of Arizona

PQ-002 Oncogenic epithelial cell-derived exosomes containing Rac1 and PAK2 induce angiogenesis in recipient endothelial cells

David Greening¹

1. - La Trobe Institute for Molecular Biology

PQ-003 Spatially targeted optical microproteomics (STOMP): Isolation and proteomic analysis of micron-scale features in pathological specimens

<u>Hadley, K.C.¹²</u>, Rakhit R.³, Guo, H.⁴, Sun, Y.¹², Jonkman, J.E.⁵, McLaurin, J.⁶, Hazrati, L.N.⁷, Emili, A.⁴, Chakrabartty, A.^{12,8}

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- 5. Advanced Optical Microscopy Facility, Princess Margaret Cancer Centre, University Health Network
- 6. Biological Sciences, Sunnybrook Research Institute
- 7. Department of Paediatric Laboratory Medicine, The Hospital for Sick Children
- 8. Department of Biochemistry, University of Toronto

POSTERS

PQ-004 Comparative Study Of Urine Proteome Of Preterm Newborns With Respiratory Disorders

<u>A.S. Kononikhin^{1,2*}</u>, N.L. Starodubtseva^{1,2}, A.E. Bugrova¹, K.N. Krokhina¹, I.V. Nikitina¹, I.A. Popov^{1,2}, V.E. Frankevich¹, O.V. Ionov¹, E.N. Nikolaev², G.T. Sukhikh¹

- 1. V.I. Kulakov Research Center for Obstetrics, Gynecology and Perinatology, Ministry of Healthcare of the Russian Federation
- 2. -Moscow Institute of Physics and Technology

PQ-006 Creating Of A Non-Invasive Method For The Diagnosis Of Cervical Neoplasia Degree Using Cvf Proteomic Analysis

<u>Starodubtseva N.L.¹</u>, Zardiashvili M.D.¹, Bugrova A.E.¹, Kononikhin A.S¹, Chagovets V.V.¹, Nazarova N.M.¹, Frankevich V.E.¹

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PQ-007 Mass spectrometry analysis of NXS/T glycosylation sites in recombinant glycoproteins.

<u>Izabela Sokolowska¹</u>, Armand G. Ngounou Wetie¹, Alisa G. Woods¹, Costel C. Darie¹

1. - Clarkson University

PR - PROTEOSTASIS AND QUALITY CONTROL

PR-001 Dynamic Periplasmic Chaperone Reservoir Facilitates Biogenesis of Outer Membrane Proteins

Shawn Costello¹

1. - Johns Hopkins University

PR-002 Substrate Ubiquitination Controls the Unfolding Ability of the Proteasome

Eden L. Reichard¹, Giavanna G. Chirico¹, William J. Dewey¹, Nicholas D. Nassif¹, Katelyn E. Bard¹, Nickolas E. Millas¹, Daniel A. Kraut¹

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PR-003 Assembly and dysregulation of the M. tuberculosis Clp protease

Karl R Schmitz¹, Alvaro J Amor¹, Jason K Sello², Robert T Sauer¹

1. - Department of Biology, Massachusetts Institute of Technology

2. - Department of Chemistry, Brown University

PR-004 Calpain- and proteasome-dependent proteolysis regulates growth rate in salmonid fish

Lysenko L.A¹, Kantserova N.P¹, Efremov D.A¹, and Nemova N.N.¹

1. - Institute of Biology, Karelian Research Centre of RAS



PS - SINGLE MOLECULE STUDIES

PS-001 Single-protein free-solution optical trap for studying their dynamics, structure, and behavior

Ryan M Gelfand¹

1. - CREOL The College of Optics and Photonics, UCF

PS-002 Identification of the Molecular Origin of Disease with Single Molecular Optical Tweezers

Jeneffer England¹, Yuxin Hao¹, Susan S. Taylor², Rodrigo A Maillard¹

1. - Department of Chemistry, Georgetown University

2. - Department of Pharmacology, University of California, San Diego

PT - Structure (X-Ray / NMR / EM)

PT-001 Catalytic cycle of MenD (SEPHCHC synthase) from the menaquinone biosynthesis pathway revealed by X-ray crystallography

<u>Ghader Bashiri</u>¹, Ehab N. M. Jirgis¹, Jodie M. Johnston¹, Esther M. M. Bulloch¹, Laura Nigon¹, Edward N. Baker¹

1. - The University of Auckland

PT-002 Investigating zinc finger recognition of epigenetically modified DNA

Bethany Buck-Koehntop1

1. - University of Utah

PT-003 Structural Characterization of the Membrane Associated Regions of HSV-1 gB

Rebecca Cooper¹

1. - Tufts University School of Medicine

PT-004 Structural studies of class C G-protein coupled receptors

Qing Fan¹

1. - Columbia University

PT-005 Recognition of diverse NES peptides by the Exportin CRM1

Ho Yee Joyce Fung¹, Yuh Min Chook¹

1. - University of Texas Southwestern Medical Center



PT-006 Isolating the inner domain of the HIV-1 envelope as an independent molecule exposing the C1-C2 gp120 region involved in potent Fc mediated effector function to HIV-1

<u>Neelakshi Gohain¹</u>, William D. Tolbert¹, Maxime Veillette¹, Jean-Philippe Chapleau¹, Chiara Orlandi¹, Andrés Finzi¹, George Lewis¹, Marzena Pazgier¹

1. - University of Maryland

PT-007 Structural and functional studies of Mycobacterium tuberculosis MazF-mt6 toxin provide insight into RNA substrate specificity.

Eric Hoffer¹², Stacey J. Miles¹, Samantha Schwartz² and Christine M. Dunham¹

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PT-008 Structural basis of protein kinase Cα auto-inhibition by the C-terminal tail

Yuan Yang¹, Julia A. Callender², Alexandra C. Newton², Tatyana I. Igumenova²

1. - Department of Biochemistry and Biophysics, Texas A&M University

2. - Department of Pharmacology, University of California at San Diego

PT-009 Structure, inhibition, and regulation of a two-pore channel TPC1

Alexander Kintzer¹

1. - University of California at San Francisco

PT-010 Structural and Functional Studies of the Mycobacterium Tuberculosis VapBC30 Toxin-Antitoxin System

<u>In-Gyun Lee¹</u>, Sang Jae Lee¹, Susanna Chae¹, Ki-Young Lee¹, Ji-Hun Kim¹, Bong-Jin Lee^{1*}

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PT-011 Hydration Dynamics of Hen Egg-White Lysozyme

Bryan S. Marques¹, Nathaniel V. Nucci¹, Matthew A. Stetz¹, and A. Joshua Wand¹

1.- Johnson Research Foundation and Department of Biochemistry and Biophysics, University of Pennsylvania Perelman School of Medicine

PT-012 The unique structure of HSV-1 UL21, a multifunctional tegument protein.

Claire M. Metrick¹, Ekaterina E. Heldwein¹

 Department of Molecular Biology and Microbiology and Graduate Program in Biochemistry, Sackler School of Graduate Biomedical Sciences, Tufts University School of Medicine



PT-013 Structural characterization of protein Sis1 by Nuclear Magnetic Resonance

<u>Pinheiro, Glaucia M.S.¹</u>, Almeida, Fabio C.L.², Amorim, Gisele C. Ramos, C.H.I.¹

- 1. Institute of Chemistry, University of Campinas UNICAMP, Campinas SP. Brazil.
- 2. Institute of Medical Biochemistry and Nucleus for Structural Biology and Bioimaging (CENABIO) - Federal University of Rio de Janeiro

PT-014 Crystallization by controlled evaporation with acoustic monitoring

<u>Limone Rosa¹</u>, Anna Tsygelnytska¹, Andrea Kocmarek¹, Olivia Wiggins¹, Denise Laspina¹, Alexei Soares¹

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PT- 015 Structural studies of a recently characterised family of bacterial chemosensors: first insight into the mechanism of sensing attractants and repellents

Machuca M.¹², Liu Y.^{1,2}, Roujeinikova Anna^{1,2,3}

- 1. Monash Biomedicine Discovery Institute, Infection and Immunity Program
- 2. Monash University, Department of Microbiology
- 3. Monash University, Department of Biochemistry and Molecular Biology

PT- 016 NSLS-II macromolecular crystallography beamlines: opportunities for advanced data collection

<u>Jean Jakoncic</u>¹, Martin R. Fuchs¹, Wuxian Shi¹, Edwin Lazo¹, Alexei Soares¹, Dileep K. Bhogadi¹, Herbert Bernstein¹, Stuart Myers¹, Robert M. Sweet¹, Lonny E. Berman¹, John Skinner¹, Dieter K. Schneider¹, Sean McSweeney¹

1. - Brookhaven National Lab

PT- 017 Tet3 CXXC domain is an epigenetic reader for 5-carboxylcytosine

<u>Jikui Song</u>¹, Seung-Gi Jin^{2,3}, Zhi-Min Zhang¹, Thomas L. Dunwell³, Matthew R. Harter¹, Xiwei Wu⁴, Jennifer Johnson², Zheng Li⁵, Jiancheng Liu⁶, Piroska E. Szabó^{2,4}, Qiang Lu⁶, Guo-liang Xu⁵, Gerd P. Pfeifer^{2,3}

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PT-018 Structural characterization of non-active site, TrkA selective kinase inhibitors.

<u>Hua Su1, Keith Rickert¹, Kartik Narayan¹, Christine Burlein¹, Marina Bukhtiyarova¹, Danielle Hurzy¹, Craig Stump¹, Xufang Zhang¹, John Reid¹, Srivanya Tummala¹, Jennifer M. Shipman¹, Maria Kornienko¹, Abdelghani Achab¹, Chad Chamberlin¹, Peter Saradjian¹, Berengere Sauvagnat¹, Xianshu Yang¹, Michael Ziebell¹, Nickbarg Elliott¹, John Sanders¹, Steve Carroll¹, Darrell Henze¹, Andy Cooke¹</u>

1. - Merck & Co.

PT-019 Crystal structure of the D444V disease-causing mutant of human dihydrolipoamide dehydrogenase

<u>Eszter Szabo¹</u>, Reka Mizsei¹, Zsofia Zambo¹, Beata Torocsik¹, Manfred S. Weiss², Vera Adam-Vizi¹, Attila Ambrus¹

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PT-020 New labware for high throughput screening of crystallization conditions and chemical libraries

<u>Ella Teplitsky</u>¹, Karan Joshi², Lauren Zipper³, Anthony Borelli⁴, Alexander Scalia⁵, Daniel Ericson⁶, Denise Laspina⁷, Alexei Soares⁸

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- 8. Energy Sciences Directorate, NSLS-II, Brookhaven National Laboratory

PT-021 Detection of Small Molecule Effectors of Pyruvate Carboxylase via the Development of a Novel High-throughput Screen

Brittney N. Wyatt¹, Martin St. Maurice¹

1. - Marquette University

PT-022 The structure basis of ceramide transfer protein functional regulation

<u>Xiaolan Yao¹</u>, Jennifer Prashek¹

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PT-023 Uncovering Stimulator Binding Mechanism to Soluble Guanylyl Cyclase by Solution NMR

<u>Cheng-Yu Chen¹</u>, Jessica A. Wales¹, Andrzej Weichsel¹, James E. Sheppeck², Joon Jung², Paul A. Renhowe², William R. Montfort¹

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- 4. Department of Medicinal Chemistry, University of Michigan
- 5. Department of Biological Chemistry, University of Michigan

PT-025 Crystal structure of a novel Ca2+-dependent lectin GJL-I from the sea anemone Gyractis japonica and its carbohydrate-recognition mechanism

<u>Azusa Nakamura¹</u>, Hideaki Unno¹, Shuichiro Goda¹, Tomomitsu Hatakeyama¹

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PT-026 Molecular Understanding of USP7 Substrate Recognition and C-Terminal Activation

<u>Lionel Rougé¹</u>, Travis W. Bainbridge, Paola Di Lello, Ingrid E. Wertz, Till Maurer, James A. Ernst, Jeremy Murray

1. - Genentech

PT-027 Structure and Physical Studies of the AlgH protein from Pseudomonas aeruginosa and the AlgH Protein Family

<u>Jeffrey L. Urbauer</u>¹, Aaron B. Cowley¹, Henry T. Niedermaier¹, Hayley E. Broussard¹, Ramona J. Bieber Urbauer¹

1. - Department of Chemistry, and Department of Biochemistry and Molecular Biology, The University of Georgia

PT-028 The crystal structure of SdrE from S. aureus

Jun Zhang¹², Xuefei Cai¹, Ke Chen¹, Wang Deqiang¹

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- 2. College of Basic Medicine, Chongqing Medical University

PT-029 Structure and carbohydrate-binding properties of a C-type lectin SPL with novel carbohydrate-recognition motifs

<u>Shuhei Itakura¹, Hideaki Unno¹, Shuichiro Tatyana¹, Tomomitsu Hatakeyama¹</u> 1. - Graduate School of Engineering, Nagasaki University

PT-030 Structural basis for effective nitric oxide decomposition in microbial denitrification

<u>Tosha, Takehiko¹</u>, Terasaka, Erina^{1,2}, Matsumoto, Kimil², Sugimoto, Hiroshi¹, Shiro, Yoshitsugu^{1,2}

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PT-031 The Unique Myristoylation Signal of the Feline Immunodeficiency Virus Matrix Protein

Janae L. Baptiste¹, Michael F. Summers¹

1. - Howard Hughes Medical Institute, Department of Chemistry and Biochemistry, University of Maryland

PU - SYNTHETIC BIOLOGY

PU-001 Mutagenesis of Ribonuclease U2 : Rational, Semi-rational and Random Approaches

Solivio, Beulah¹

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PU-002 Producing Membrane Bound Proteins as Countermeasures to Infectious Diseases

<u>Wei He¹, Angela C. Evans¹</u>, Martina Felderman², Delia F. Tifrea³, Amy Rasley¹, David Homan¹, Kurt Kamrud², Nathaniel Wang², Sukumar Pal³, Luis M. de la Maza³, Bolyn Hubby², Todd Peterson², Nicholas O. Fischer¹, Matthew A. Coleman^{1,4}

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PU-003 A novel strategy for constructing the topological network of protein-protein interactions

Jun Zhang¹, Wang Deqiang²

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- 2. Key Laboratory of Molecular Biology on Infectious Disease (Ministry of Education)





PV - THERAPEUTICS AND ANTIBODIES

PV-001 Characterization of honey proteins with immunomodulatory activities.

M. Kamran Azim¹, Nida Dastagir¹, M. Ahmed Mesaik¹, Bushra Bilal¹, Atia Gohar¹

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PV-002 Monoclonal antibodies specifically targeting amyloidogenic forms of transthyretin (TTR) with potential to treat TTR-related cardiomyopathy and polyneuropathy

<u>Natalie J. Galant¹</u>, Jeffrey N. Higaki², Kevin C. Hadley¹, Amy Won³, Stephen J. Tam², Ken Flanagan², Tarlochan Nijjar², Ronald Torres², Jose R. Tapia², Joshua Salmans², Robin Barbour², Wagner Zago², Gene G. Kinney², Christopher M. Yip³, Avi Chakrabartty²

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- 3. Institute of Biomaterials and Biomedical Engineering, University of Toronto, Toronto, Ontario M5S 3E1, Canada

PV-003 How insulin binds: structure of a micro-receptor complex and implications for analog design

<u>Nischay Rege¹</u>, Michael Glidden¹, Nelson Phillips¹, Yanwu Yang¹, Faramarz Ismail-Beigi¹, Michael A. Weiss¹

1. - Departments of Biochemistry and Medicine, Case Western Reserve University School of Medicine

PV-004 Effects of rearranging the domain order of a diabody-based IgG-like bispecific antibody on antitumor activity, degradation resistance, and pharmacokinetics

<u>Ryutaro Asano^{1,2}</u>, Ippei Shimomura¹, Shozo Furumoto³, Mitsuo Umetsu¹, Izumi Kumagai¹

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- 3. Department of Radiopharmaceutical Chemistry, Graduate School of Pharmaceutical Sciences, Tohoku University



PV-005 Contributions of loop histidine residues for Zinc ion binding and its stability of an anti-ZnO VHH antibody

<u>Ryosuke Sasaki</u>¹, Hikaru Nakazawa¹, Izumi Kumagai¹, Mitsuo Umetsu¹, Koki Makabe¹

1. - Yamagata University

PV-006 An antibody discovery platform of KBIO and its application to developing antibody therapeutics and diagnostics

<u>Kyungjae Kang¹</u>, Hyung-Kyung Choi¹, Keunwan Park¹, Sungjin Kim¹, Kiweon Cha¹, Daeyoung Kim¹

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PV-007 Energetic Basis for Optimization of Cysteine Protease Inhibitors.

<u>Conceição A. Minetti¹, Igor M. Prokopczyk², Erika V.M. Orozco², Fabiana Rosini², David P. Remeta¹, Carlos A. Montanari²</u>

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2. - Institute of Chemistry, University of São Paulo

PW - TRANSCRIPTION / TRANSLATION / POST - TRANSLATIONAL MODIFICATIONS

PW-001 Caspase-9 is regulated by phosphorylation through diverse mechanisms

Banyuhay P. Serrano¹, Kristen L. Huber¹ Jeanne A. Hardy¹

1. - University of Massachusetts

PW-002 Refolding and Purification of Unmodified Human Elongation Factor 2

Nirja B. Patel¹, Joshua R. Ostovitz², Nathaniel Donahue1, John E. Weldon^{1,2}

- 1. Molecular Biology, Biochemistry and Bioinformatics Program &
- 2. Department of Biological Sciences, Towson University

PW-003 Protein targets of tyrosine nitration in human astrocytomas

Dr. Xianquan Zhan¹

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PW-004 Determining histone deacetylase 8 substrates using non-natural amino acids

Jeffrey Lopez¹

1. - University of Michigan

PW-005 Phosphopeptide mapping and mass spectrometry analysis of human tristetraprolin

Heping Cao¹, Leesa J. Deterding², Perry J. Blackshear³

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- 2. Laboratory of Structural Biology, National Institute of Environmental Health Sciences, National Institutes of Health
- 3. Laboratory of Signal Transduction, National Institute of Environmental Health Sciences, National Institutes of Health, and Departments of Biochemistry and Medicine, Duke University Medical Center

PX - Metabolic Engineering / Energy Applications

PX-001 Characterization of protein compositions of glanded and glandless cotton seeds

Heping Cao¹, Kandan Sethumadhavan₁

1. - U.S. Department of Agriculture, Agricultural Research Service, Southern Regional Research Center, New Orleans, LA

PY – SYSTEMS BIOLOGY

PY-001 A novel strategy for constructing the topological network of protein-protein interactions

Jun Zhang¹, Wang Deqiang²

- 1. The Department of Cell Biology & Genetics, Chongqing Medical University
- 2. Key Laboratory of Molecular Biology on Infectious Disease (Ministry of Education







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Jane Clarke

Professor Of Molecular Biophysics Senior Wellcome Trust Research Fellow Department Of Chemistry University Of Cambridge

Dan S. Tawfik Principal Investigator Department Of Biomolecular Sciences Weizmann Institute Of Science

Volker Dötsch Professor, Institute Of Biophysical Chemistry Goethe University

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- Approaches To Therapeutics
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- Structural Insights Into Ion-transporting Membrane Proteins

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