



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 33 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 professional growth of young investigators through workshops, networking opportunities, and by encouraging junior researchers to participate fully in the Annual Symposium. In addition to our Symposium, the Society's prestigious journal, *Protein Science*, serves as an ideal platform to further the science of proteins in the broadest sense possible.





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### Program Planning Committee Seattle | June 30 - July 3, 2019

Sheena Radford,

University of Leeds



Welcome to Seattle and to the 2019 33rd Annual Symposium of the Protein Society!

We are excited to bring you this year's Annual Symposium comprising 12 exceptional scientific sessions that cover a wide range of scientific achievement in the field of protein science, as well as a Nobel Laureate Lecture from 2017 Chemistry Nobel Laureate Richard Henderson. Our program committee, chaired by Robert C. Matthews, Ph.D, has convened a host of stimulating speakers and topical areas of current research. This year's Symposium continues our

commitment to open participation with a number of Symposium talks coming from contributed sessions and speakers across a broad range of topics. We are proud of the amazing line-up of poster presentations, and our ability to recognize outstanding young scientists through specially-designated sessions and awards. Protein Society Award-winners will also present their work throughout the Symposium, which is not to be missed! However, if you cannot make it to all talks, you can read about their work in a future special issue of Protein Science, the Society journal. Finally, I personally encourage you to participate in the numerous activities we've planned for Seattle – from mixers and social events, including a Seattle Sounders game, to mentoring and education panels, and our Members' Reception (which is open to all).

While we celebrate more than 3 decades of impact in the field of protein science, future challenges drive us to advocate for the importance of scientific research in the United States and throughout the world, and to continue to strive for diversity, equity and inclusivity in all of our endeavors. I urge you to engage in important dialogues within our community and, of growing importance, with the public, on the critical need for scientific research.

Thank you for joining us in our 33rd Annual Symposium in Seattle. We hope you will take advantage of everything our event has to offer. Finally, we would appreciate it greatly if you will take a few moments to give us your feedback and suggestions for improvement in the survey you'll receive at the end of the conference. We are committed to strengthening our events to meet the needs of members and constituents, and your honest feedback will directly shape future events.

Wishing you all a fruitful and engaging Symposium. Please take a moment to introduce yourselves to me during the meeting; I would love to meet you.

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Kind Regards,

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Charles L. Brooks III, Ph.D. President





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Karen Fleming, John Hopkins University



Gerhard Wagner, Harvard University



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\* 20 AUG 2016 \* CHICAGO

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Sanela Martic, Ph.D. Oakland University

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**Carrie Partch, Ph.D.** University of California Santa Cruz

Sebastian Pechmann, Ph.D. University of Montreal

Kay Perry, Ph.D. Argonne National Laboratory





The Protein Society is extremely grateful to the following sponsors for their generosity and continued support.



Thank you for helping us celebrate 33 years of impact.



Cesar Ramirez-Sarmiento, Ph.D.

Philipp Schmidpeter, Ph.D.

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Jeffrey L Urbauer, Ph.D.

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Pontifical Catholic University of Chile



The Registration Area will be open from 5 to 8 p.m. on Saturday, June 29 (refer to hours below). Registration includes admission to all scientific and poster sessions, exhibits, and one t-shirt. Registration does not include any , meals.

Register early to be eligible to win an Amazon Fire TV!

#### Hours

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5:00 p.m 8:00 p.m. 7:00 a.m 6:30 p.m. 7:30 a.m 7:00 p.m. 8:30 a.m 7:00 p.m. 8:30 a.m 12:00 p.m.
8:30 a.m 12:00 p.m.

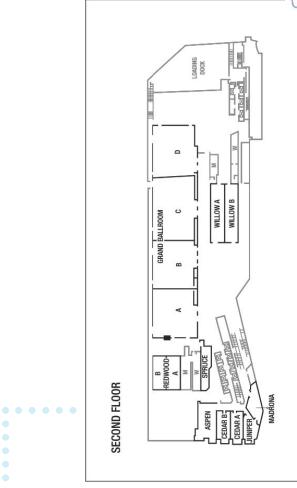
#### Badge/Delegate Pickup

All registrants must go to the Symposium Registration Desk on the Second Floor. 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 all Symposium-related events.



Hotel Floor Plan





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# **Diversity**

#### Protein Society DEI Statement:

Protein science is an integrative and inclusive endeavor that utilizes concepts and methods from a diverse array of disciplines to strive for a more complete understanding of the role that proteins play in biological structure and function across many levels. As a membership-based society and leader in its field, The Protein Society values and is committed to diversity, equity, and inclusion in all aspects of its societal endeavors. We, therefore, strive to provide a safe and supportive environment for all of our constituents, where everyone is treated with respect and is encouraged to contribute their unique strengths and abilities to our shared mission. We are committed to acting on these principles for the betterment of the field of protein science and all activities with which The Protein Society is engaged.

#### The Protein Society Diversity Committee

Chair Charles L. Brooks The Protein Society President

Elizabeth Komives

Elizabeth Meiering The Protein Society Councilor

Charney Robinson-Williams

Director of Events and Communications for The Protein Society

#### We Care About Your Pronouns!

Stop by The Protein Society's booth outside of the Exhibit Hall and grab a pronoun sticker for your name badge!

These let us all know how to address one another, and help everyone feel more comfortable.

When you meet someone, look for their pronoun sticker!

## Posters

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DEPARTED SYDNEY

20 AUG 2016

#### Poster Set Up & Removal

All posters will be displayed in Grand Ballroom CD of the Sheraton Grand Seattle and will be available for viewing during lunch hours and for presentations on the following days:

 Sunday, June 30, 2019:
 4:30 - 6:30 p.m.

 Monday, July 1, 2019:
 4:30 - 6:30 p.m.

 Tuesday, July 2, 2019:
 5:30 - 7:30 p.m.

#### Instructions for Preparing Posters

Posters are displayed on a standard poster board with the dimensions of 90 inches (2.3 meters) wide by 42 inches (1.1 meters) high of usable space.

This year, due to the number of posters received, each poster will be up for 1 day only. It is important that you install it at least 30 minutes prior to the time of presentation and remove it after the end of the entire session. If it is not removed by the end of the day, we will discard in order to install other posters.





#### Social Media

The Society staff will be updating its Facebook page, Instagram, and Twitter feed with Annual Meeting information throughout the meeting. Follow us on: Facebook: www.facebook. com/ProteinSociety; www.instagram/proteinsociety; Twitter: @ProteinSociety, use hashtag #PS33.

#### Public Transportation Light Rail

Sound Transit's Link light rail makes trips from Angle Lake Station to the University of Washington through downtown Seattle making 14 stops along the way, including downtown Seattle and Sea-Tac Airport. Trains arrive every 6 to 15 minutes, depending on the time of day, and take about 40 minutes to travel between Sea-Tac International Airport and Westlake Station in downtown Seattle. One-way fare for adults ranges from \$2.25 to \$3.25. Schedules and sta- 🔴 tion maps are available on the Sound Transit website.

#### King County Metro Transit

King County Metro Transit provides bus service in downtown Seattle and outlying neighborhoods in King county. Time-tables and route maps are available at the Transit Information Center in the tunnel under Westlake Center at 4th Avenue & Pine Street, or can be found on the King County Metro Transit website. King County Metro also has a mobile app available for iPhone and Android.

#### All Day Regional Transit Pass

An all-day regional transit pass is available for visitors to Seattle. These \$8 all-day passes are loaded onto regional transit cards (\$5 each) at all ORCA vending machines and are used for unlimited riding on all local public transit (excluding the Seattle Monorail and Washington State Ferries). Transit pass value covers \$3.50 per ride.

#### Seattle Center Streetcars

The South Lake Union Streetcar makes 11 stops through the South Lake Union area. Streetcars arrive every 10-15 minutes and run from 6am to 9pm (Monday-Thursday), 6am to 11pm (Friday & Saturday), and 10am to 7pm (Sunday & holidays). Adult fare is \$2.50. Schedules and maps are available on their website

The First Hill Streetcar makes 10 stops from the Chinatown-International District through Capitol Hill. Departures are every 10-25 minutes and operate from 5am to 1am (Monday-Thursday), 6am to 1am (Friday & Saturday), 10am to 7pm (Sunday) and 10am to 8pm (holidays). Adult fare is \$2.50. Route maps and schedules are available on their website. - - -

General Info

#### Live Mobile App

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The NEW PS33 Mobile App (search Protein Society Symposium) provides on-the-go Symposium information including a program planner, poster presentations info, exhibitor list, social media updates, #PS33 alerts, and maps. The Protein Society's "PS 33" mobile application is available for download in the Apple App Store and Google Play. You can view/create schedules; view abstracts, and interact virtually with speakers using the app. Use the QR code at right to dowload, for both iPhone and Android.



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 prior to entering a session room.

#### Certificates of Attendance

All attendees will receive a certificate of attendance via email in PDF format after the Symposium.

#### 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: P\$33 Password: Proteins

#### 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.



## @#PS33 **TPS Membership**

	1 Year Price/	2 Year Price/	5 Year Price/
	Discount Code	Discount Code	Discount Code
Undergraduate	Regular Rate: \$25 <i>Early-Bird Rate: \$20</i> Code: kxuesyfv	Regular Rate: \$50 <i>Early-Bird Rate: \$40</i> Code: hzapbec9	
Graduate	Regular Rate: \$50 <i>Early-Bird Rate: \$40</i> Code: vt8bupqd	Regular Rate: \$90 <i>Early-Bird Rate: \$75</i> Code: xdhsxha4	
Early-Career	Regular Rate: \$100	Regular Rate: \$180	Regular Rate: \$475
	<i>Early-Bird Rate: \$80</i>	<i>Early-Bird Rate: \$150</i>	<i>Early-Bird Rate: \$375</i>
	Code: ppb3r6vt	Code: vhncnmwn	Code: ujnucurf
Lab Staff	Regular Rate: \$50	Regular Rate: \$90	Regular Rate: \$230
	<i>Early-Bird Rate: \$40</i>	<i>Early-Bird Rate: \$75</i>	<i>Early-Bird Rate: \$180</i>
	Code: axkbqrhu	Code: azsjdkhf	Code: gjkfzsfb
Full	Regular Rate: \$200	Regular Rate: \$380	Regular Rate: \$950
	<i>Early-Bird Rate: \$150</i>	<i>Early-Bird Rate: \$285</i>	<i>Early-Bird Rate: \$700</i>
	Code: zkmbg6wx	Code: 7sj9cxrk	Code: kzxgwn99
Emeritus	Regular Rate: \$25	Regular Rate: \$50	Regular Rate: \$115
	<i>Early-Bird Rate: \$20</i>	<i>Early-Bird Rate: \$40</i>	<i>Early-Bird Rate: \$90</i>
	Code: 7d4dmat9	Code: wurmkky	Code: 6c6wveax

#### Individual Memberships

TPS members represent an international community of all those who share an interest in the structure, function, design, synthesis, and utilization of proteins. In fact, it is this diversity of disciplines and perspectives represented by TPS members that is the group's defining characteristic.

Members include chemists, biologists, physicists, and mathematicians researchers of all stripes, whose collaboration and communication comprise the Society's core mission. They represent academia, industry, government, non-profits, and leading institutions in more than 50 nations.



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## Benefits Include:

### Annual Symposium and Awards

- Members save as much as 50% for the Annual Symposium
   Get funding for your local protein-centered mini-symposium, workshop, or other event with a Member Mini-Grant
- Connect with TPS leaders and have a say in the direction of your Society
- Only members can submit or sponsor an abstract for the Best Poster Competition
- Nominate your colleagues for one of seven prestigious TPS awards
- Eligibility to submit a contributed talk or be considered for a Young Investigator Talk
- Design your own session at an upcoming Symposium

#### **Protein Science Benefits**

- Complimentary online access to the premier Journal focused on all aspects of protein science
- \$250 discount on publication fees
  Pain-Free Publishing: Fast turnaround under the guidance of Edi-
- tor-in-Chief Brian Matthews
  Reduced open-access fees from publisher Wiley Blackwell

#### Networking and Leadership

- Connect and collaborate privately with other members through the Member Directory or the members-only LinkedIn group
- Be eligible to vote or stand yourself for TPS Executive Council, Nominating Committee, and other leadership roles
- Stay informed with the monthly member e-news

#### Legislative Action

Public affairs representation through FASEB



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## 御#PS33 2019 Protein Society Award Winners Dave Thirumalai, Ph.D., University of Texas at Austin

2019 Hans Neurath Award Winner - Sponsored by the Hans Neurath Foundation



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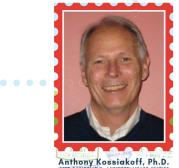
In 2019, the Hans Neurath Awardee is Professor Dave Thirumalai (University of Texas at Austin), Professor Thirumalai has been a pioneer in advancing our understanding of biomolecular actions, particularly protein and RNA folding, and the basis for how molecular motors convert energy to motion. Professor Thirumalai, one of the top theorists in delineating the principles of protein and RNA folding, is unique in driving and interpreting experiments, and collaborating with experimentalist colleagues. He was the first to quantify the heterogeneity and bumpiness of protein folding landscapes, through the definition of a glass temperature and its ratio with the folding temperature.

Dame Carol Robinson, Ph.D., University of Oxford 2019 Stein & Moore Award Winner



The 2019 recipient is Professor Dame Carol Robinson (University of Oxford). Professor Robinson's research focuses on applications of mass spectrometry to the study of proteins and their interactions. Early in her career she modified instrumentation to transmit folded proteins, molecular chaperones and other dynamic macromolecular assemblies. Subsequently, she has concentrated on membrane protein complexes, their modulation through lipid and drug binding, and their study from native membrane environments. Overall, Professor Robinson's sustained and focused effort has resulted not only in new insights into protein structure and function but has also established a new field - that of structural biology in the gas phase.

Anthony Kossiakoff, Ph. D., University of Chicago 2019 Christian B. Anfinsen Award Winner



Anthony Kossiakoff, Ph.D.

Hao Wu, Ph.D., Harvard University 2019 Dorothy Crowfoot Hodgkin Award Winner - Sponsored by Genentech

biomolecules.



Hao Wu, Ph.D. 2010 LOV # LONDON WWARD WINNER

The 2019 recipient is Professor Hao Wu (Harvard University). The selection of Professor Wu was driven by two interconnecting threads: the remarkable achievements she has made in changing how we view the molecular mechanism of signal transduction and recent work from her laboratory that has illuminated inflammasome assembly and the resulting pyroptotic cell death. The signalosome concept that Professor Wu pioneered established the importance of oligomeric, cooperatively assembled protein complexes for immune receptor signaling and by extension, for intracellular signaling more generally.

The recipient of this award in 2019 is Professor Anthony Kossiakoff (University of Chicago).

Professor Kossiakoff's achievements have had broad and sustained impact through

the development of innovative technol-

ogies and major discoveries in the field of protein structure and function. Areas in

which he has made significant advances in

protein science include: pioneering the use

chemistry; determination of the first cytokine-

receptor complex: a structural paradigm for

the cytokine family and signaling; allostery in

protein-protein interfaces; and development

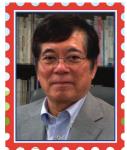
of crystallization chaperones for challenging

of neutron-crystallography to understand protein structure, dynamics, catalysis and



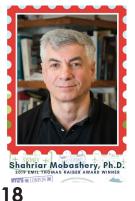
## #PS33 2019 Protein Society Award Winners

Minoru Kanehisa, Ph.D., Kyoto University 2019 Carl Brändén Award Winner - Sponsored by Rigaku Corp.



Minoru Kanehisa, Ph.D. 2019 CARL BRANDEN AWARD WINNER

and Asia Pacific Protein Association (APPA). Shahriar Mobasherry, Ph.D., University of Notre Dame 2019 Emil Thomas Kaiser Award Winner



The 2019 recipient is Professor Shahriar Mobashery (University of Notre Dame). Professor Mobashery has made numerous contributions to the discovery of new antibiotics, antibiotic mechanisms of action, mechanisms of antibiotic resistance, and studies of cell-wall biosynthesis, recycling and regulation. He has authored >370 scientific publications and his work has been cited >19,000 times to date. Professor Mobashery is recognized with the Emil Thomas Kaiser Award for his applications of outstanding creative chemistry to the understanding of protein science, specifically his recent, seminal work on cell-wall biosynthesis, recycling and regulation is noted.

The 2019 recipient of this award is Professor

Minoru Kanehisa (Kyoto University). Profes-

sor Kanehisa is one of the world leaders in

the bioinformatics field. The KEGG (Kyoto

and continues to develop, provides a very

original and useful data resource not only in the protein science field, but also in much wider fields of general biology and medicine.

KEGG integrates information on biological

both for understanding biological systems

sor Kanehisa will receive his award and be

recognized at the 2020 World Conference

on Protein Science in Sapporo, Japan, a joint

symposium organized by The Protein Society, the PSSJ (Protein Science Society of Japan),

and practical applications in society. Profes-

systems from the organismal-level, to the cell-level, to the molecular level and includes genomic, chemical, and human health data

Encyclopedia of Genes and Genomes)

database, which he established in 1995





Gabriel Lander, Ph.D., Scripps Research Institute 2019 Protein Science Young Investigator Award Winner - Sponsored by Wiley



The 2019 recipient is Professor Gabriel Lander (Scripps Research Institute). Professor Lander is recognized as one of the most prolific scientists of his generation in developing and applying methods of cryo-electron microscopy (cryo-EM), to provide groundbreaking structural and mechanistic insights into a variety of complex macromolecular machines. His outstanding body of work as an independent faculty, combined with his unparalleled expertise and enthusiasm for tackling difficult biological questions have propelled him to the forefront of structural biology.

David Baker, Ph.D., University of Washington 2018 Hans Neurath Award Winner - Sponsored by the Hans Neurath Foundation



DAVID BAKER, PH.D. 2018 HANS NEURATH AWARD

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In 2018 the Hans Neurath Awardee was Professor David Baker. Dr. Baker's scientific achievements put him at the forefront of many disciplines in computational pro-tein science over the past decade. Some of these achievements have included: Advances in de novo protein design and protein structure prediction of thousands of proteins of unknown structure using Rosetta atomistic modeling and evolutionary couplings; atomistic refinement of x-ray crystallographic structures, which has been packaged in the most popular software suite for x-ray crystallography, PHENIX; and reproducible design of stable, atomically accurate, small proteins, which may be used as binders and inhibitors. These breakthroughs required many additional technical advances in modeling and experimental characterization, and they reduce to practice what was for many decades the holy grail of protein science: fundamental understandina of the determinants of protein structure and stability that leads to consistent predictive capabilities, including the ability to desian protein shapes and functions as desired.

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Yu-ming "Mindy" Huang, Ph.D., University of California, San Diego 2018 Best Paper Award Winner

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Yu-ming Huang, Ph.D UNIVERSITY OF CALIFORNIA SAN DIEGO



Mindy Huang completed her undergraduate education in both chemistry and physics at the National Taiwan University. Her Ph.D. in computational chemistry was at UC-Riverside under the guidance of Chia-en Chang. She is currently a postdoctoral fellow with Andrew McCammon at UC-San Diego where her work focuses on the development and application of advanced simulation tools to better understand biomolecular diffusion.

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As noted by Dr. McCammon, "Mindy is a remarkably versatile young theoretician of pro-tein science. She has successfully developed new computer simulation methods and applied these in studies of protein dynamics and of biomolecular diffusion. The work recognized here is in an important area of cell biology, namely, how co-localization of enzymes and other macromolecules lead to efficiency in metabolism, signaling and other processes. The importance of diffusional channeling of intermediates from one enzyme to another is increasingly recognized in such processes. Beyond its fundamental significance, targeting channeling in signaling or metabolic arrays rep-resents a novel opportunity for drug discovery. In addition to her outstanding research, Mindy has been active in mentorship of students in the aroups she has been associated with, and she brims with enthusiasm for all her projects. She is on her way to a productive career as a professor of molecular biophysics!"

Abhay Thakur, Pall Corporation 2018 Best Paper Award Winner



Abhay Thakur, Ph.D.



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Abhay Thakur received his initial training in India, including his Ph.D. with Mohan Rao at the Center for Cellular and Molecular Biology in Hyderabad. The work for which he received the Best Paper Award was carried out as a postdoctoral associate in the group of Lila Gierasch at the University of Massachusetts. He is currently a Senior Scientist with Pall Corporation.

Abhay summarizes his career path in the following way. "When I started my career I was fascinated with protein folding, misfolding and aggregation. I joined Dr. Mohan Rao's Lab at the Centre for Cellular and Molecular Biology (CCMB, India) to investigate the conformational changes of prion protein in the presence of copper. I was fortunate to explore multiple biophysical techniques in his lab. Utilizing multiple techniques we proposed a novel long-range interaction between N- and C-terminal of prion protein in the presence of copper. During my graduate tenure, I attended Lila's seminar on protein folding. Her research work on folding of the beta-barrel protein, CRABP1 is inspiring and extensive. I felt it was a logical route for me to understand the folding of the complex protein. In her lab, I learned a lot about protein folding and used NMR to understand the denatured ensemble of CRABP1. Her mentoring has significantly helped in refining my thoughts and approaches to tackle scientific problems."

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## @#PS33 Travel Awards



Congratulations to the following outstanding students and early-career investigators for receiving travel assistance to attend The 33rd Annual Symposium of The Protein Society.

Under the strong belief that our Symposia presents an invaluable opportunity for future protein scientists, The Protein Society is committed to making it possible for young scientists to participate and benefit from our Annual Meeting by awarding the **Finn Wold Travel Awards**. The leadership and Executive Council of The Protein Society also **THANKS** the recent donors to the **Finn Wold Travel Awards Fund**. The Protein Society would also like to recognize the **Hans Neurath Foundation** for supporting the generous **Hans Neurath Outstanding Promise Travel** awards and **Wiley**, for supporting the **Protein Science** travel awards.

## 2019 Finn Wold Fravel Award Recipients

Chunfu Xu, University of Washington Stephanie Zimmerman, University of Washington Elizabeth Speltz, University of Washington Satchal Erramilli, The University of Chicago Rylee Simons, Clark University Young Sun Lee, Clark University Kayla Rich, Clark University Christopher Lim, Yale University Aurelio Dregni, Massachusetts Institute of Technology Xiaozhe Ding. California Institute of Technology Heather Forsythe, Oregon State University Aidan Estelle, Oregon State University Venkata S. Mandala, Massachusetts Institute of Technology Martin Gelenter, Massachusetts Institute of Technology Acacia Dishman, Medical College of Wisconsin Therese Herling, University of Cambridge I-Jin Lin, University, Hsinchu, Taiwan Riley D. Metcalfe, University of Melbourne Sandesh Deshpande, University of Verona Giuditta Dal Cortivo, University of Verona



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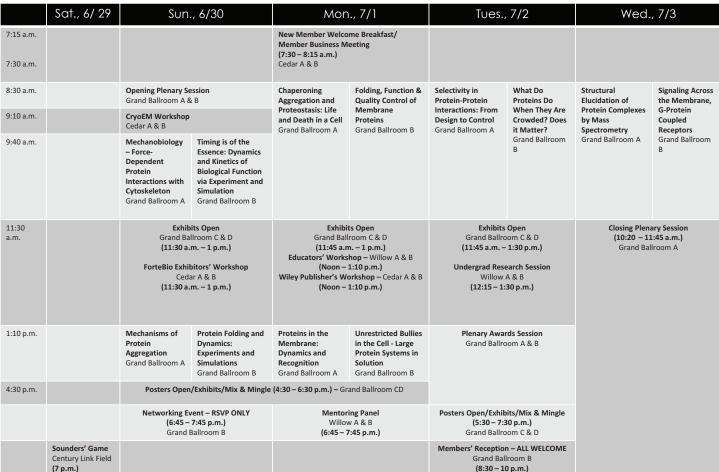
- 2019 Protein Science Young Investigator Travel Award
- Recipients
   Jun Liu, University of California, San Francisco
- Jun Liu, University of California, San Francisco
   Megan Shelby, Lawrence Livermore National Lab
- Megan Shelby, Lawrence Livermore National Lab
   Jacob Parres Gold, California State University, Los Angeles
- Anshika Jain, NIH
- Jeanmarie W. Loss, Clark University
- Diana Argiles Castillo, Clark University
- Aaron Bogle, Clark University
- Mikaela Rosen, University of Richmond
- Emily Ladda, Clark University
- Mike Thorsen, Tufts Sackler School
- Patrick DePaolo, Stevens Institute of Technology
  - Misa Mai, Clark University Jillian Baker, Towson University
- Abigail Ward, Colorado State University
- Samantha Cohen, San Diego State University

Rezaul Karim, University of South Florida Justine Bohl, Clark University Hao Shen, University of Washington Dennis Özcelik, University of Copenhagen Magdalena Zamora Corona, Universidad Nacional Autónoma de México Arti Kataria, Kusuma School of Biological Sciences Geetika Verma, Jawaharlal Nehru University Irvinder Wason, University of British Columbia Yu Seby Chen, McGill University Wei He, Lawrence Livermore National Laboratory Sashank Agrawal, Institute of Molecular Biology, Academia Sinica Shalini Verma, National Institute of Immunology

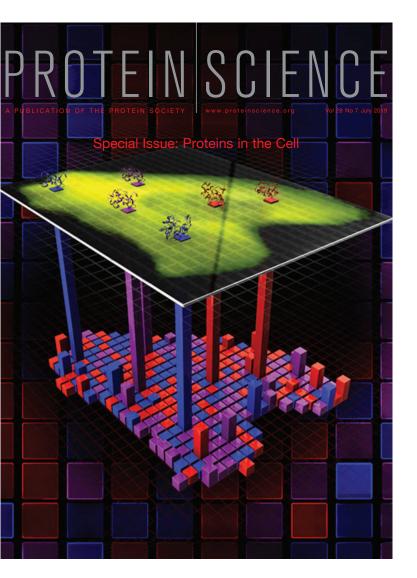
#### 2019 Hans Neurath Dutstanding Promise Travel Awards

Sean Cascarina, Colorado State University Archana G. Chavan, University of California, Merced Zibo Chen, University of Washington Ryan Hayes, University of Michigan Jens Hjörleifsson, Science Institute University of Iceland Sunhee Hwang, Stanford University Mingyue Li, Department of Structural Biology, University of Pittsburgh Valerio Marino, University of Verona Bikash Sahoo, Biophysics Program, Department of Chemistry, University of Michigan, Ann Arbor Prerna Sharma, Arizona State University Jonathan Williams, Rutgers University





ARRIVED 20 AUG 2016 PEHI Int. AIRPORT



# NETWORKING EVENT

## June 30, 2019 6:45 to 7:45 P.M. Grand Ballroom

**RSVP ONLY** 

Join us to network with fellow TPS members and leadership. #PS33

## @#PS33 **P**royram

#### Day 1 - Sunday, June 30, 2019 Opening Plenary Session 8:30 - 9:10 a.m. | Grand Ballroom A & B 8:30 - 8:35 a.m. Intro & Welcome From The Protein Society President Charles L. Brooks III, University of Michigan 8:35 - 8:40 a.m. Introduction of Nobel Laureate Lecturer Richard Henderson\* 8:40 - 9:10 a.m. Nobel Laureate Lecture Impact of Electron Cryomicroscopy in Macromolecular Structural Biology

#### Richard Henderson, 2017 Nobel Prize in Chemistry MRC Lab, Cambridge, England; United Kingdom Coffee Break | 9:10 - 9:40 a.m. | Grand Ballroom D Cryo-EM Workshop, Presenter: Salvatore Sechi; NIH/NIDDK | 9:10 - 9:40 a.m. | Cedar A & B

#### **CONCURRENT MORNING SESSION 1**

Mechanobiology	Force-Dependent Protein Interactions with Cytoskeleton 9:40 - 11:30 a.m.   Grand Ballroom A
9:40 - 9:45 a.m.	Introduction From Chair <b>Eva-Maria Strauch</b> , University of Georgia; Athens,Georgia; United States
9:45 - 10:15 a.m.	Dissecting Structural Mechanisms of Force-sensitive Actin Binding <b>Greg Alushin</b> , The Rockefeller University New York, New York; United States
10:15 - 10:45 a.m.	The Stability of Mechanosensing Force-transmission Supramolecular Linkages Jie Yan, National University of Singapore; Malaysia
10:45 - 11:00 a.m.	The Role of Conformational Dynamics in Shear- Enhanced FimH-mediated Bacterial Adhesion <b>Pearl Magala</b> , University of Washington; Seattle, Washington; United States
11:00 - 11:30 a.m.	Orthogonal Biophysical Techniques on Proteins and Intact Cells Reveal the Secrets of Integrin Activation <b>Timothy Springer</b> , Harvard University; Cambridge,

Massachusetts; United States

\* travel support provided by Fred Hutchinson Cancer Research Center

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#### Day 1 - Sunday, June 30, 2019 - (cont.) **CONCURRENT MORNING SESSION 2** Timing is of the Essence: Dynamics and Kinetics of Biological Function via Experiment and Simulation 9:40 - 11:30 a.m. | Grand Ballroom B Introduction From Chair 9:40 - 9:45 a.m. Ying Li, University of Louisville; Louisville, Kentucky; United States 9:45 - 10:15 a.m. Optical Tweezers: Watching a Riboswitch Switch Steven Block, Stanford University; Palo Alto, California; United States 10:15 - 10:45 a.m. Phase Transitions and Timing Mechanisms Governing Signaling at the Membrane Jay Groves, University of California, Berkeley; Berkeley, California; United States

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10:45 - 11:00 a.m. Real-time Monitoring of Clock Controlled Signal Transduction Pathway Archana Chavan; University of California Merced; Merced, California; United States

11:00 - 11:30 a.m. Molecular Mechanisms of RNA Polymerase II Transcription Elongation Elucidated by Kinetic Network Models **Xuhui Huang**, Hong Kong University of Science and Technology; Hong Kong; China

Box Lunch Pickup | 11:30 a.m. - 1:10 p.m. | Grand Ballroom D

ForteBio Exhibitor's Workshop | 11:30 a.m. - 1 p.m. | Cedar A & B

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Program Day 1 - Sunday, June 30, 2019 CONCURRENT AFTERNOON SESSION 1 • Mechanisms of Protein Aggregation • 1:10 - 4:30 p.m. | Grand Ballroom A • 1:10 - 1:15 p.m. Introduction From Chair • Jonathan Pruneda, Oregon Health & Science University; Portland, Oregon; United States Amyloid Fibrils: Structure, Energetics, and Function David Eisenberg, University of California, Los Angeles; 1:15 - 1:45 p.m. Los Angeles, California; United States • 1:45 - 2:15 p.m. The Division of Amyloid Fibrils – Stability, Toxicity and Infectious Potential Wei-Feng Xue, University of Kent; Kent, England; United Kingdom • 2:15 - 2:30 p.m. Oxidized Dopamine Causes Neuronal Cell Death by Impairing Protein Function and Folding Dennis Ozcelik, University of Copenhagen; • Copenhagen; Denmark Coffee Break | 2:30 - 3:15 p.m. | Grand Ballroom C & D • 3:15 - 3:45 p.m. Proteins at the Centre of Neurodegeneration in Alzheimer's Disease Louise Serpell, University of Sussex; Sussex, England; United Kingdom Dynamics of Amyloid Fibrils Play a Role in Seeding and 3:45 - 4:00 p.m. Propagating the Aggregation of a-Synuclein •

New Jersey; United States 4:00 - 4:30 p.m. Modulation of Interactome by Protein Self-assembly: the Case of Alpha-synuclein **Emma Sierecki**; The University of New South Wales, Kensington Campus; Sydney; Australia

Jonathan Williams, Rutgers University; New Brunswick,

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#### Day 1 - Sunday, June 30, 2019 (cont.)

CONCURRENT AFTERNOON SESSION 2 Protein Folding and Dynamics: Experiments and Simulations 1:10 - 4:30 p.m.   Grand Ballroom B			
1:10 - 1:15 p.m.	Introduction From Chair <b>Karin Crowhurst</b> , California State University, Northridge; Los Angeles, California; United States		
1:15 - 1:45 p.m.	Rational Enhancement of Protein Conformational Switching Kinetics: Weighted Ensembles of Folding Trajectories Lillian Chong, University of Pittsburgh; Pittsburgh, Pennsylvania; United States		
1:45 - 2:15 p.m.	Deciphering Protein Dynamics and Function by Combining HDX-Mass Spectrometry with MD Simulations Lars Konermann, Western University; London, Ontario; Canada		
2.15 - 2.30 p.m.	Local and Non-local Topological Information in the Denatured State Ensemble of a Beta-barrel Protein 2018 Protein Science Best Paper Award Winner <b>Abhay Thakur</b> ; Pall Corporation; Port Washington, New York; United States		
Coffee	Break   2:30 - 3:15 p.m.   Grand Ballroom C & D		
3:15 - 3:45 p.m.	Folding, Frustration and Function <b>Shachi Gosavi</b> , National Center for Biological Sciences; Bangalore, Karnataka; India		
3:45 - 4:00 p.m.	Exploring Sequence-Space in TIM Barrel Proteins Gloria Saab Rincón; UNAM; Mexico City, Mexico		
4:00 - 4:30 p.m.	Measuring Weak Protein-protein and Protein-RNA Interactions Inside the Cell <b>Martin Gruebele</b> , University of Illinois; Urbana-Champaign, Illinois; United States	(	
Poster Presentation and Mix & Mingle Reception, 4:30 - 6:30 p.m.   Grand Ballroom C & D			
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Networking Event | 6:45 - 7:45 p.m. | Grand Ballroom B



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## @#PS33 **Prog**ram

#### Day 2 - Monday, July 1, 2019 New Member Welcome Breakfast/Member Business Meeting 7:30 - 8:15 a.m. | Cedar A & B

#### CONCURRENT MORNING SESSION 1 Chaperoning Aggregation and Proteostasis: Life and Death in a Cell 8:30 - 11:45 a.m. | Grand Ballroom A

8:30 - 8:35 a.m.	Introduction From Chair <b>Mark Herzik</b> ; University of California, San Diego; San Diego, California; United States	
8:35 - 9:05 a.m.	Chaperone Functions in Protein Folding and Proteome Maintenance <b>Ulrich Hartl</b> , Max Planck Institute of Biochemistry; Munich; Germany	
9:05 - 9:35 a.m.	Factors Modulating Hsp70 Substrate Recognition and Mediation of the Stress Response Sarah Perrett, Institute of Biophysics Chinese Academy of Sciences; Beijing, China	
9:35 - 9:50 a.m.	Distinct Pathways of Activation of Human Small Heat Shock Protein HSPB5 by Different Stress Factors Maria Janowska; University of Washington; Seattle, Washington; United States	
Coffee Break   9:50 - 10:15 a.m.   Grand Ballroom C & D		
10:15 - 10:45 a.m.	High Throughput Methods for Discovering Protein Fold Correctors Jason Gestwicki, University of California, San Francisco; San Francisco, California; United States	
10:45 - 11:15 a.m.	Molecular Details of Protein Misfolding in Myocilin- associated Glaucoma Raquel Lieberman, Georgia Institute of Technology; Atlanta, Georaia: United States	

The Impact of Diverse Triggers of Proteostasis Stress on
Proteome Aggregation-State
Danny Hatters; The University of Melbourne;
Melbourne, Australia

#### Day 2 - Monday, July 1, 2019 (cont.) CONCURRENT MORNING SESSION 2 . . . . . . . . Folding, Function & Quality Control of Membrane Proteins 8:30 - 11:45 a.m. | Grand Ballroom B 8:30 - 8:35 a.m. Introduction From Chair Donald Spratt, Clarke University; Worcester, Massachusetts; United States 8:35 - 9:05 a.m. Probing Sequence Constraints Associated with the Cotranslational Folding and Misfolding of Integral Membrane Proteins Jonathan Schlebach, Indiana University; Bloomington, Indiana; United States 9:05 - 9:35 a.m. Unfolding and Refolding of Individual Bacteriorhodopsin Molecules Probed with 1-µs Resolution Thomas Perkins, University of Colorado Boulder; Boulder, Colorado; United States 9:35 - 9:50 a.m. Computational Design of Multipass Transmembrane Proteins Peilong Lu, University of Washington; Seattle, Washington; United States Coffee Break | 9:50 - 10:15 a.m. | Grand Ballroom C & D

10:15 - 10:45 a.m.	Weak Hydrogen Bonds and Packing Modulate the Stability of Transmembrane Dimers Alessandro Senes, University of Wisconsin; Madison, Wisconsin; United States
10:45 - 11:15 a.m.	Guiding Membrane Proteins to the ER in a Chaperone Cascade

Shu-ou Shan, California Institute of Technology; Pasadena, California; United States

11:15 - 11:45 a.m. Structural and Functional Characterization of p13ll Protein from Human T-cell Leukemia Virus Type 1 **Elka Georgieva**, Cornell University; Ithaca, New York; United States

#### Box Lunch Pickup | 11:45 a.m. - 1:10 p.m. | Grand Ballroom C & D

#### Wiley Publisher's Workshop | Noon - 1:10 p.m. | Cedar A & B

Educators' Workshop | Noon - 1:10 p.m. | Willow A & B 33

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# **Phogstam** Day 2 - Monday, July 1, 2019

## CONCURRENT AFTERNOON SESSION 1 Proteins in the Membrane: Dynamics and Recognition 1:10 - 4:30 p.m. | Grand Ballroom A

1:10 - 1:15 p.m.	Introduction From Chair Amanda Duran, Cyrus Biotechnology; Seattle, Washington; United States	
1:15 - 1:45 p.m.	Dynamics of GPCR Signal Transmission and Allosteric Regulation Detected by NMR <b>Stephan Grzesiek</b> , University of Basel; Basel, Switzerland	
1:45 - 2:15 p.m.	How Do Membrane Protein Extracellular Domains Regulate Intracellular Catalytic Function? Adam Smith, University of Akron; Akron, Ohio; United States	
2:15 - 2:30 p.m.	Directed Evolution of Sensor Proteins for GPCR Signaling Mechanisms Andre Berndt, University of Washington; Seattle, Washington; United States	
Coffee Break   2:30 - 3:15 p.m.   Grand Ballroom C & D		
Coffee B	oreak   2:30 - 3:15 p.m.   Grana Ballroom C & D	
3:15 - 3:45 p.m.	Receptor Clustering and Activation Driven by its Transmembrane Anchor James Chou, Harvard Medical School; Cambridge, Massachusetts; United States	
	Receptor Clustering and Activation Driven by its Transmembrane Anchor James Chou, Harvard Medical School;	
3:15 - 3:45 p.m.	Receptor Clustering and Activation Driven by its Transmembrane Anchor James Chou, Harvard Medical School; Cambridge, Massachusetts; United States Native-state Prolyl Isomerization is Involved in the Activation of a CNG Channel Phillip Schmidpeter; Weill Cornell Medical College;	

Unrestricted	CONCURRENT AFTERNOON SESSION 2 I Bullies in the Cell - Large Protein Systems in Solution 1:10 - 4:30 p.m.   Grand Ballroom B
1:10 - 1:15 p.m.	Introduction From Chair <b>Mikaela Stewart</b> , Texas Christian University; Fort Worth, Texas; United States
1:15 - 1:45 p.m.	Structural Basis for the Binding of Non-native Proteins Molecular Chaperones <b>Charalampos Kalodimos</b> , St. Jude Children's Researc Hospital; Memphis, Tennessee; United States
1:45 - 2:15 p.m.	Targeting KRAS Oncoprotein at Biological Membrane <b>Mitsu Ikura</b> , University of Toronto; Toronto, Canada
2:15 - 2:30 p.m.	Turning Up the Heat on Dynamic Proteins: Observing Molecular Motion in Real Time with Temperature-jum, X-ray Crystallography and Solution Scattering <b>Michael Thompson</b> , University of California, San Francisco; San Francisco, California; United States
Coffee	Break   2:30 - 3:15 p.m.   Grand Ballroom C & D
3:15 - 3:45 p.m.	Structural Biology of Pmhc Receptors Functioning as Mechanosensors in the Ab T-Cell Lineage Ellis Reinherz, Dana-Farber Cancer Institute; Boston, Massachusetts; United States
3:45 - 4:00 p.m.	The Structure of Discoidal High-density Lipoprotein Particles <b>Stefan Bibow;</b> University of Basel; Basel, Switzerland
4:00 - 4:30 p.m.	Activation of the Exocyst Tethering Complex for Snar Complex Regulation and Membrane Fusion <b>Mary Munson</b> ; University of Massachusetts Medical School; Worcester, Massachusetts; United States
Pos	ter Presentation and Mix & Mingle Reception 4:30 - 6:30 p.m.   Grand Ballroom C & D

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## Day 3 - Tuesday, July 2, 2019 (cont.)

CONCURRENT MORNING SESSION 2

Day 3 - Tuesday, July 2, 2019		What do Proteins do When They Are Crowded? Does it Matter? 8:30 - 11:45 a.m.   Grand Ballroom B	
Selectivity	CONCURRENT MORNING SESSION 1 in Protein-Protein Interactions: From Design to Control 8:30 - 11:45 a.m.   Grand Ballroom A	8:30 - 8:35 a.m.	Introduction From Chair David Ban, Merck; Kenilworth, New Jersey; United States
8:30 - 8:35 a.m.	Introduction From Chair Jeanine Amacher, Western Washington University; Bellingham, Washington; United States	8:35 - 9:05 a.m.	Exploring the Determinants of Protein Crowding Effects by Molecular Simulation <b>Rebecca Wade</b> , Heidelberg Institute for Theoretical Studies gGmbH; Heidleberg; Germany
8:35 - 9:05 a.m.	Engineered Circular Tandem Repeat Proteins: Structure, Behavior and Function Barry Stoddard, Fred Hutchinson Cancer Research Center; Seattle, Washington; United States	9:05 - 9:35 a.m.	Solution NMR Approaches to 3D Structure Determination of Proteins In Living Eukaryotic Cells Yutaka Ito, Tokyo Metropolitan University; Tokyo; Japan
9:05 - 9:35 a.m.	Engineering Linkage-Specific Polyubiquitin Antibodies: Tools for Elucidation of Novel Signaling Pathways <b>Marissa Matsumoto</b> , Genentech; San Francisco, California; United States	9:35 - 9:50 a.m.	Brownian Dynamic Study of an Enzyme Metabolon in the TCA Cycle: Substrate Kinetics And Channeling 2018 Protein Science Best Paper Award Winner <b>Yu-ming "Mindy" Huang</b> ; University of California San Diego; San Diego, California; United States
9:35 - 9:50 a.m.	Microfluidic Methods Reveal the Thermodynamics of Chaperone Binding Therese Herling; University of Cambridge; Cambridge, England; United Kingdom	<b>Coffee I</b> 10:15 - 10:45 a.m.	Break   9:50 - 10:15 a.m.   Grand Ballroom C & D
Coffee I	Break   9:50 - 10:15 a.m.   Grand Ballroom C & D	10.10 10.10 4.11.	Cell Simon Ebbinghaus, Ruhr-Universität Bochum; Bochum; Germany
10:15 - 10:45 a.m.	From Systems Biology to Systems Biologics <b>Dev Sidhu</b> , University of Toronto; Toronto, Canada	10:45 - 11:15 a.m.	
10:45 - 11:15 a.m.	Cellular Consequences of Systematic Perturbations of a Highly Conserved Biological Switch Tanja Kortemme, University of California, San Francisco; San Francisco, California; United States	11:15 - 11:45 a.m.	Austin, Texas; United States
11:15 - 11:45 a.m.	A Molecular View of the Liquid to Gel Phase Transition of Heterochromatin Protein HP1a Galia Debelouchina; University of California, San Diego;	Day Lunch Di	Margaret Cheung; University of Houston; Houston, Texas; United States
	San Diego, California; University of California, san Diego, San Diego, California; United States	BOX LUNCH PI	ckup   11:45 a.m 1:30 p.m.   Grand Ballroom C & D
		Undergra	d Research Session   12:15 - 1:30 p.m.   Willow A & B

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#### @#**P**S**3**3 Program Day 3 - Tuesday, July 2, 2019 PLENARY AWARDS SESSION 1:30 - 5:30 p.m. | Grand Ballroom A & B 1:30 - 1:35 p.m. Introduction from The Protein Society President Charles L. Brooks III, University of Michigan 1:35 - 1:40 p.m. Presentation - Hans Neurath Award GroEL and RNA Chaperones as Stochastic Machines 1:40 - 2:10 p.m. 2019 Hans Neurath Award Winner Dave Thirumalai, University of Texas at Austin; Austin, Texas, United States 2:10 - 2:15 p.m. 2:15 - 2:45 p.m. Presentation - Dorothy Crowfoot Hodgkin Award Higher-order Supramolecular Assemblies for Immune Signaling and Beyond 2019 Dorothy Crowfoot Hodgkin Award Winner Hao Wu, Harvard University; Cambridge, Massachusetts; United States 2:45 - 2:50 p.m. 2:50 - 3:20 p.m. Presentation - Christian B. Anfinsen Award Chaperone-Assisted Structure Determination: Bringing High Hanging Fruit to Ground Level 2019 Christian B. Anfinsen Award Winner Anthony Kossiakoff, University of Chicago; Chicago, Illinois; United States Coffee Break | 3:20 - 3:45 p.m. | Grand Ballroom 3:45 - 3:50 p.m. Presentation - Emil Thomas Kaiser Award 3:50 - 4:20 p.m. Cell-wall Recycling in Pseudomonas aeruginosa and the Nexus to Antibiotic Resistance 2019 Emil Thomas Kaiser Award Winner Shahriar Mobashery, University of Notre Dame; Notre Dame, Indiana; United States 4:20 - 4:25 p.m. Presentation -Protein Science Young Investigator Award 4:25 - 4:55 p.m. Using Cryo-EM to Understand the Mechanisms of Mitochondrial Machines of Mass Destruction Protein Science Young Investigator Award Winner Gabriel Lander, Scripps Research Institute; La Jolla, California; United States 4:55 - 5:00 p.m. HNOPTA and Society Service Awards Charles L. Brooks III, University of Michigan Poster Presentations/Mix & Mingle Reception | 5:30 - 7:30 p.m. | Grand Ballroom C & D Members' Reception (All Welcome) | 8:30 - 10 p.m. | 38 Grand Ballroom B

#### Day 4 - Wednesday, July 3, 2019

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CONCURRENT MORNING SESSION 1 Structural Elucidation of Protein Complexes by Mass Spectrometry 8:30 - 10:20 a.m.   Grand Ballroom A		
8:30 - 8:35 a.m.	Introduction From Chair <b>Benjamin Garcia</b> , University of Pennsylvania; Philadelphia, Pennsylvania; United States	
8:35 - 9:05 a.m.	Elucidation of Protein Complexes in Heart James Bruce, University of Washington; Seattle, Washington; United States	
9:05 - 9:35 a.m.	Ultraviolet Photodissociation Mass Spectrometry for Characterization of Proteins and Protein Complexes Jennifer Brodbelt, University of Texas at Austin; Austin, Texas; United States	
9:35 - 9:50 a.m.	Measuring the Functional Effect of Amino Acid Substitutions Proteome-wide using Mistranslation <b>Stephanie Zimmerman</b> ; University of Washington; Seattle, Washington; United States	
9:50 - 10:20 a.m.	Native Mass Spectrometry for a Top-Down View of Protein Structures Joseph Loo, University of California, Los Angeles; Los Angeles, California; United States	
Coffee Break   10:20 - 10:45 p.m.   Grand Ballroom		
CONCURRENT MORNING SESSION 2 Signaling Across the Membrane, G-protein Coupled Receptors 8:30 - 10:20 a.m.   Grand Ballroom		
8:30 - 8:35 a.m.	Introduction From Chair Anna Groat-Carmona; University of Washington, Tacoma; Tacoma, Washington; United States	
8:35 - 9:05 a.m.	Single-molecule Analysis of Ligand Efficacy in β2AR-G Protein Activation Scott Blanchard, Weill Cornell Medical College; New York, New York; United States	
9:05 - 9:35 a.m.	Snapshots of G Protein-Coupled Receptors at Work Georgios Skiniotis, Stanford University; Palo Alto, California; United States	

## #PS33 Program Day 4 - Wednesday, July 3, 2019

9:35 - 9:50 a.m.	Elucidating Relayed Proton Transfer Through a His-Trp- His Triad of a Transmembrane Proton Channel by Solid-State NMR
	Byongsu Kwon, Massachusetts Institute of Technology Cambridge, Massachusetts; United States
9:50 - 10:20 a.m.	Structural Insights into G Protein-coupled Receptor Signaling Andy Kruse, Harvard University; Cambridge, Massachusetts; United States
	PLENARY AWARDS SESSION 10:20 - 11:45 a.m.   Grand Ballroom A
10:20 - 10:25 a.m.	Introduction from The Protein Society President Charles L. Brooks III, University of Michigan
10:25 - 10:55 a.m.	Mass Spectrometry: From Plasma Proteins to Mitochondrial Membranes 2019 Stein & Moore Award Winner
	Dame Carol Robinson; University of Oxford; Oxford, England; United Kingdom
11:00 - 11:30 a.m.	The Coming of Age of de novo Protein Design 2018 Hans Neurath Award Winner <b>David Baker</b> , University of Washington; Seattle, Washington; United States
11:30 - 11:45 a.m.	Closing Charles L. Brooks III, University of Michigan



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# educator's workshop



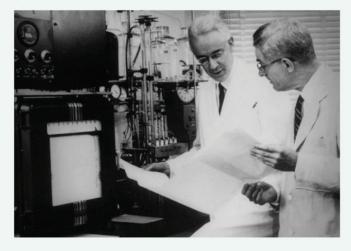
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JULY 1, 2019 12 - 1:10 P.M.



WILLOW ROOM

## @#**PS33** Exhibitor List

Beckman Coulter	Booth 8
Bon Opus Biosciences	Booth 5
Cell Free Sciences	Booth 10
Fluidic Analytics	Booth 4
ForteBio LLC	Booth 1
Malvern Panalytical	Booth 9
Nicoya Lifesciences	Booth 7
Pacific Northwest Center for Cryo-EM	Booth 11
PerkinElmer	Booth 2
Refeyn	Booth 12
St. Jude Children's Research Hospital	Booth 3
TA Instruments	Booth 22
Trialtus Bioscience	Booth 13
UniProt	Booth 6
The Protein Society/Wiley	Outside Exhibit Hall

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6:45 - 7:45 p.m.





BOOTH 8

**BOOTH 5** 

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BOOTH 7

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#### BOOTH 11

**BOOTH 2** 



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**BOOTH 22** 

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Since 1985, TPS 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. TPS provides forums for scientific collaboration and communication and supports 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.

BOOTH 6



## The Protein Society ....

...presents seven awards annually to distinguished scientists. They recognize excellence and outstanding achievements in the multidisciplinary fields of protein science, and honor contributions in the areas of leadership, education & service.

We will present the 2020 awards at our 34th Annual Symposium - The World Conference on Protein Science - in Sapporo, Japan, July 7 - 10, 2020. Deadline to submit complete award nomination packages is noon EDT on November 15, 2019.

## Awards

Carl Brändén Award Christian B. Anfinsen Award Dorothy Crowfoot Hodgkin Award Emil Thomas Kaiser Award Hans Neurath Award Stein & Moore Award Protein Science Young Investigator Award

Poster/Abstract

June 30, 2019

	Board		
AbS	(BOD)	Track	Date
ABS008		1. Amyloid and aggregation	6/30/201
ABS145	2	1. Amyloid and aggregation	6/30/201
ABS019	3	1. Amyloid and aggregation	6/30/201
ABS147	4	1. Amyloid and aggregation	6/30/201
ABS041	5	1. Amyloid and aggregation	6/30/201
ABS062		1. Amyloid and aggregation	6/30/201
ABS053		1. Amyloid and aggregation	6/30/201
ABS057	8	1. Amyloid and aggregation	6/30/201
ABS134	9	1. Amyloid and aggregation	6/30/201
ABS040	10	<ol> <li>Amyloid and aggregation</li> </ol>	6/30/201
ABS044	11	1. Amyloid and aggregation	6/30/201
ABS434	12	10. Folding	6/30/201
ABS226	13	10. Folding	6/30/201
ABS276	14	10. Folding	6/30/201
ABS443	15	10. Folding	6/30/201
ABS274	16	10. Folding	6/30/201
ABS034	17	11. Intrinsically disordered proteins	6/30/201
ABS138	18	11. Intrinsically disordered proteins	6/30/201
ABS150	19	11. Intrinsically disordered proteins	6/30/201
ABS087	20	12. Membrane proteins	6/30/201
ABS020	21	12. Membrane proteins	6/30/201
ABS092	22	12. Membrane proteins	6/30/201
ABS029	23	12. Membrane proteins	6/30/201
ABS143	24	12. Membrane proteins	6/30/201
ABS037	25	12. Membrane proteins	6/30/201
ABS211	26	12. Membrane proteins	6/30/201
ABS214	27	14. Motors & machines	6/30/201
ABS424	28	14. Motors & machines	6/30/201
ABS102	29	15. Peptides	6/30/201
ABS295	30	15. Peptides	6/30/201
ABS202	31	15. Peptides	6/30/201
ABS017	32	16. Protein interactions and assemblies	6/30/201
ABS009	33	16. Protein interactions and assemblies	6/30/201
ABS011	34	16. Protein interactions and assemblies	6/30/201
ABS099	35	16. Protein interactions and assemblies	6/30/201
ABS038	36	16. Protein interactions and assemblies	6/30/201
ABS016	37	16. Protein interactions and assemblies	6/30/201
ABS035	38	16. Protein interactions and assemblies	6/30/201
ABS108	39	16. Protein interactions and assemblies	6/30/201
ABS071	40	16. Protein interactions and assemblies	6/30/201
ABS049	41	16. Protein interactions and assemblies	6/30/201
ABS068	42	16. Protein interactions and assemblies	6/30/201
ABS055	43	17. Proteins in cells	6/30/201
ABS144	44	16. Protein interactions and assemblies	6/30/201
ABS082	45	16. Protein interactions and assemblies	6/30/201

	Board		
AbS	(BOD)	Track	Date
ABS086	46	16. Protein interactions and assemblies	6/30/2019
ABS097	48	16. Protein interactions and assemblies	6/30/2019
ABS104	49	16. Protein interactions and assemblies	6/30/2019
ABS027	50	16. Protein interactions and assemblies	6/30/2019
ABS117	51	16. Protein interactions and assemblies	6/30/2019
ABS039	52	16. Protein interactions and assemblies	6/30/2019
ABS187	53	16. Protein interactions and assemblies	6/30/2019
ABS160	54	16. Protein interactions and assemblies	6/30/2019
ABS080	55	16. Protein interactions and assemblies	6/30/2019
ABS066	56	17. Proteins in cells	6/30/2019
ABS148	57	18. Proteomics	6/30/2019
ABS354	58	18. Proteomics	6/30/2019
ABS242	59	18. Proteomics	6/30/2019
ABS069	60	19. Proteostasis and quality control	6/30/2019
ABS132	61	19. Proteostasis and quality control	6/30/2019
ABS154	62	19. Proteostasis and quality control	6/30/2019
ABS251	63	19. Proteostasis and quality control	6/30/2019
ABS115	64	2. Bioinformatics	6/30/2019
ABS333	65	2. Bioinformatics	6/30/2019
ABS033	66	20. Single molecule studies	6/30/2019
ABS091	67	20. Single molecule studies	6/30/2019
ABS423	68	20. Single molecule studies	6/30/2019
ABS024	69	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS002	70	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS265	71	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS013		21. Structure (x-ray/NMR/EM)	6/30/2019
ABS065	73	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS014	74	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS047		21. Structure (x-ray/NMR/EM)	6/30/2019
ABS304	77	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS258	78	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS054	79	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS141	80	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS284	81	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS177	82	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS220	83	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS300		21. Structure (x-ray/NMR/EM)	6/30/2019
ABS249	85	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS331		21. Structure (x-ray/NMR/EM)	6/30/2019
ABS061	87	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS287	88	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS302	89	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS118	90	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS328	91	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS350	92	21. Structure (x-ray/NMR/EM)	6/30/2019

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Poster/Abstract

ALC	Board	Tee els	Data
AbS	(BOD)	Track	Date
ABS351		21. Structure (x-ray/NMR/EM)	6/30/201
ABS028		24. Therapeutics and antibodies	6/30/201
ABS070		24. Therapeutics and antibodies	6/30/201
ABS077		24. Therapeutics and antibodies	6/30/201
ABS113		24. Therapeutics and antibodies	6/30/201
ABS194	98	24. Therapeutics and antibodies	6/30/201
ABS253	99	24. Therapeutics and antibodies	6/30/201
ABS271	100	24. Therapeutics and antibodies	6/30/201
ABS272	101	24. Therapeutics and antibodies	6/30/201
ABS186	102	25. Transcription/translation/post-translational modifications	6/30/201
ABS275	104	25. Transcription/translation/post-translational modifications	6/30/201
ABS204	105	3. Chaperones	6/30/201
ABS207	106	3. Chaperones	6/30/201
ABS030	107	4. Chemical biology	6/30/201
ABS021	108	4. Chemical biology	6/30/201
ABS110	109	4. Chemical biology	6/30/201
ABS184	110	4. Chemical biology	6/30/201
ABS454	111	12. Membrane proteins	6/30/201
ABS310		4. Chemical biology	6/30/201
ABS369		4. Chemical biology	6/30/201
ABS374		4. Chemical biology	6/30/201
ABS025		5. Computational modeling/simulation	6/30/201
ABS048		5. Computational modeling/simulation	6/30/201
ABS237		5. Computational modeling/simulation	6/30/201
ABS122		5. Computational modeling/simulation	6/30/201
AB\$321		5. Computational modeling/simulation	6/30/201
ABS322		5. Computational modeling/simulation	6/30/201
ABS0322		6. Design/engineering	6/30/201
ABS052		6. Design/engineering	6/30/201
ABS043		6. Design/engineering	6/30/201
ABS256		6. Design/engineering	6/30/201
ABS084		6. Design/engineering	6/30/201
ABS094		6. Design/engineering	6/30/201
ABS166		6. Design/engineering 6. Design/engineering	6/30/201
ABS100			6/30/201
		6. Design/engineering	
ABS107 ABS180		6. Design/engineering	6/30/202
		6. Design/engineering	6/30/201
ABS212		6. Design/engineering	6/30/201
ABS223		6. Design/engineering	6/30/201
ABS072		6. Design/engineering	6/30/201
ABS262		6. Design/engineering	6/30/201
ABS171		6. Design/engineering	6/30/201
ABS146		6. Design/engineering	6/30/201
ABS063		7. Dynamics and allostery	6/30/20:
ABS174	139	7. Dynamics and allostery	6/30/201

	Board		
AbS	(BOD)	Track	Date
ABS067	140	7. Dynamics and allostery	6/30/2019
ABS175	141	7. Dynamics and allostery	6/30/2019
ABS085	142	7. Dynamics and allostery	6/30/2019
ABS225	143	7. Dynamics and allostery	6/30/2019
ABS169	144	8. Enzymology	6/30/2019
ABS010	145	8. Enzymology	6/30/2019
ABS116	146	8. Enzymology	6/30/2019
ABS208	147	8. Enzymology	6/30/2019
ABS124	148	8. Enzymology	6/30/2019
ABS200	149	8. Enzymology	6/30/2019
ABS229	150	8. Enzymology	6/30/2019
ABS203	151	8. Enzymology	6/30/2019
ABS239	152	8. Enzymology	6/30/2019
ABS149	153	9. Evolution	6/30/2019
ABS268	154	9. Evolution	6/30/2019
ABS347	155	9. Evolution	6/30/2019

Poster/Abstract

July 1, 2019

	Board		
AbS	(BOD)	Track	Date
ABS073		1. Amyloid and aggregation	7/1/2019
ABS078		1. Amyloid and aggregation	7/1/2019
ABS196		1. Amyloid and aggregation	7/1/2019
ABS213		1. Amyloid and aggregation	7/1/2019
ABS290		1. Amyloid and aggregation	7/1/2019
ABS230		1. Amyloid and aggregation	7/1/2019
ABS389		1. Amyloid and aggregation	7/1/2019
ABS254		1. Amyloid and aggregation	7/1/2019
ABS294		1. Amyloid and aggregation	7/1/2019
ABS363		1. Amyloid and aggregation	7/1/2019
ABS292		1. Amyloid and aggregation	7/1/2019
ABS450		1. Amyloid and aggregation	7/1/2019
ABS198		1. Amyloid and aggregation	7/1/2019
ABS337		10. Folding	7/1/2019
ABS340		10. Folding	7/1/2019
ABS329	16	8. Enzymology	7/1/2019
ABS152	17	11. Intrinsically disordered proteins	7/1/2019
ABS156		11. Intrinsically disordered proteins	7/1/2019
ABS388	19	11. Intrinsically disordered proteins	7/1/2019
ABS158	20	11. Intrinsically disordered proteins	7/1/2019
ABS181		11. Intrinsically disordered proteins	7/1/2019
ABS089	22	12. Membrane proteins	7/1/2019
ABS224	23	12. Membrane proteins	7/1/2019
ABS312	24	12. Membrane proteins	7/1/2019
ABS112	25	12. Membrane proteins	7/1/2019
ABS407	26	12. Membrane proteins	7/1/2019
ABS130		12. Membrane proteins	7/1/2019
ABS411	28	12. Membrane proteins	7/1/2019
ABS081	29	6. Design/engineering	7/1/2019
ABS083	30	16. Protein interactions and assemblies	7/1/2019
ABS197	31	16. Protein interactions and assemblies	7/1/2019
ABS283	32	16. Protein interactions and assemblies	7/1/2019
ABS098	33	16. Protein interactions and assemblies	7/1/2019
ABS285	34	16. Protein interactions and assemblies	7/1/2019
ABS296	35	16. Protein interactions and assemblies	7/1/2019
ABS100	36	16. Protein interactions and assemblies	7/1/2019
ABS325	37	16. Protein interactions and assemblies	7/1/2019
ABS348	38	16. Protein interactions and assemblies	7/1/2019
ABS413	39	16. Protein interactions and assemblies	7/1/2019
ABS125	40	16. Protein interactions and assemblies	7/1/2019
ABS436	41	16. Protein interactions and assemblies	7/1/2019
ABS458	42	16. Protein interactions and assemblies	7/1/2019
ABS111	43	16. Protein interactions and assemblies	7/1/2019
ABS462	44	16. Protein interactions and assemblies	7/1/2019
ABS463	45	16. Protein interactions and assemblies	7/1/2019

	Board		
AbS	(BOD)	Track	Date
ABS119	47	16. Protein interactions and assemblies	7/1/2019
ABS241	48	16. Protein interactions and assemblies	7/1/2019
ABS135	49	16. Protein interactions and assemblies	7/1/2019
ABS293	50	16. Protein interactions and assemblies	7/1/2019
ABS326	51	16. Protein interactions and assemblies	7/1/2019
ABS137	52	16. Protein interactions and assemblies	7/1/2019
ABS336	53	16. Protein interactions and assemblies	7/1/2019
ABS344	54	16. Protein interactions and assemblies	7/1/2019
ABS486	55	16. Protein interactions and assemblies	7/1/2019
ABS172		17. Proteins in cells	7/1/2019
ABS341		17. Proteins in cells	7/1/2019
ABS367	58	18. Proteomics	7/1/2019
ABS375		18. Proteomics	7/1/2019
ABS165	60	19. Proteostasis and quality control	7/1/2019
ABS403		19. Proteostasis and quality control	7/1/2019
ABS478	62	19. Proteostasis and quality control	7/1/2019
ABS045	63	2. Bioinformatics	7/1/2019
ABS046	64	2. Bioinformatics	7/1/2019
ABS060	65	2. Bioinformatics	7/1/2019
ABS120		2. Bioinformatics	7/1/2019
ABS051	67	2. Bioinformatics	7/1/2019
ABS018	68	20. Single molecule studies	7/1/2019
ABS022	69	20. Single molecule studies	7/1/2019
ABS031	70	20. Single molecule studies	7/1/2019
ABS352	71	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS129	72	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS353		21. Structure (x-ray/NMR/EM)	7/1/2019
ABS359		21. Structure (x-ray/NMR/EM)	7/1/2019
ABS136		21. Structure (x-ray/NMR/EM)	7/1/2019
ABS364		21. Structure (x-ray/NMR/EM)	7/1/2019
ABS151		21. Structure (x-ray/NMR/EM)	7/1/2019
ABS370		21. Structure (x-ray/NMR/EM)	7/1/2019
ABS378		21. Structure (x-ray/NMR/EM)	7/1/2019
ABS162		21. Structure (x-ray/NMR/EM)	7/1/2019
ABS420		21. Structure (x-ray/NMR/EM)	7/1/2019
ABS433		21. Structure (x-ray/NMR/EM)	7/1/2019
ABS182		21. Structure (x-ray/NMR/EM)	7/1/2019
ABS435		21. Structure (x-ray/NMR/EM)	7/1/2019
ABS479		21. Structure (x-ray/NMR/EM)	7/1/2019
ABS218		21. Structure (x-ray/NMR/EM)	7/1/2019
ABS481		21. Structure (x-ray/NMR/EM)	7/1/2019
ABS076		21. Structure (x-ray/NMR/EM)	7/1/2019
ABS221	89	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS288		21. Structure (x-ray/NMR/EM)	7/1/2019
ABS289	91	21. Structure (x-ray/NMR/EM)	7/1/2019

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	Board		
AbS	(BOD)	Track	Date
ABS227	92	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS442	93	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS233	94	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS247	95	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS349	96	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS297	97	22. Synthetic biology	7/1/2019
ABS476	98	22. Synthetic biology	7/1/2019
ABS185	99	23. Systems biology	7/1/2019
ABS164	100	24. Therapeutics and antibodies	7/1/2019
ABS261	101	24. Therapeutics and antibodies	7/1/2019
ABS255	102	24. Therapeutics and antibodies	7/1/2019
ABS273	103	24. Therapeutics and antibodies	7/1/2019
ABS222	104	24. Therapeutics and antibodies	7/1/2019
ABS270	105	24. Therapeutics and antibodies	7/1/2019
ABS324	106	25. Transcription/translation/post-translational modifications	7/1/2019
ABS023	107	3. Chaperones	7/1/2019
ABS042	108	3. Chaperones	7/1/2019
ABS250	109	3. Chaperones	7/1/2019
ABS064	110	3. Chaperones	7/1/2019
ABS252	111	3. Chaperones	7/1/2019
ABS248	112	4. Chemical biology	7/1/2019
ABS376	113	4. Chemical biology	7/1/2019
ABS381	114	4. Chemical biology	7/1/2019
ABS106	115	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS392	116	4. Chemical biology	7/1/2019
ABS410	117	4. Chemical biology	7/1/2019
ABS128	118	5. Computational modeling/simulation	7/1/2019
ABS345	119	5. Computational modeling/simulation	7/1/2019
ABS371	120	5. Computational modeling/simulation	7/1/2019
ABS139	121	5. Computational modeling/simulation	7/1/2019
ABS475	122	5. Computational modeling/simulation	7/1/2019
ABS075	123	6. Design/engineering	7/1/2019
ABS384	124	6. Design/engineering	7/1/2019
ABS399	125	6. Design/engineering	7/1/2019
ABS088	126	6. Design/engineering	7/1/2019
ABS428	127	6. Design/engineering	7/1/2019
ABS155	128	6. Design/engineering	7/1/2019
ABS466	129	6. Design/engineering	7/1/2019
ABS105	130	6. Design/engineering	7/1/2019
ABS469	131	6. Design/engineering	7/1/2019
ABS127	132	6. Design/engineering	7/1/2019
ABS474		6. Design/engineering	7/1/2019
ABS142	134	6. Design/engineering	7/1/2019
ABS282		7. Dynamics and allostery	7/1/2019
ABS406	136	7. Dynamics and allostery	7/1/2019

	Board		
AbS	(BOD)	Track	Date
ABS385	137	7. Dynamics and allostery	7/1/2019
ABS427	138	7. Dynamics and allostery	7/1/2019
ABS444	139	7. Dynamics and allostery	7/1/2019
ABS445	140	7. Dynamics and allostery	7/1/2019
ABS263	141	8. Enzymology	7/1/2019
ABS365	142	8. Enzymology	7/1/2019
ABS036	143	8. Enzymology	7/1/2019
ABS402	144	8. Enzymology	7/1/2019
ABS052	145	8. Enzymology	7/1/2019
ABS416	146	8. Enzymology	7/1/2019
ABS314	147	25. Transcription/translation/post-translational modifications	7/1/2019
ABS303	148	8. Enzymology	7/1/2019
ABS167	149	8. Enzymology	7/1/2019
ABS306	150	8. Enzymology	7/1/2019
ABS431	151	8. Enzymology	7/1/2019
ABS245	152	8. Enzymology	7/1/2019
ABS419	153	0	7/1/2019
ABS395	154	16. Protein interactions and assemblies	7/1/2019
ABS472	155	0	7/1/2019

Poster/Abstract

AbS	Board (BOD)	Track	Date
ABS299		1. Amyloid and aggregation	7/2/2019
ABS315		1. Amyloid and aggregation	7/2/2019
ABS429		1. Amyloid and aggregation	7/2/201
ABS432		1. Amyloid and aggregation	7/2/2019
ABS457		1. Amyloid and aggregation	7/2/201
ABS004		10. Folding	7/2/2019
ABS311		10. Folding	7/2/2019
ABS357		10. Folding	7/2/2019
ABS277		11. Intrinsically disordered proteins	7/2/2019
ABS320		11. Intrinsically disordered proteins	7/2/2019
ABS334		11. Intrinsically disordered proteins	7/2/2019
ABS397	12	11. Intrinsically disordered proteins	7/2/2019
ABS484	13	11. Intrinsically disordered proteins	7/2/2019
ABS131		12. Membrane proteins	7/2/2019
ABS168	15	12. Membrane proteins	7/2/2019
ABS199		12. Membrane proteins	7/2/2019
ABS216		12. Membrane proteins	7/2/2019
ABS217		12. Membrane proteins	7/2/2019
ABS234		12. Membrane proteins	7/2/2019
ABS269	20	12. Membrane proteins	7/2/2019
ABS286		12. Membrane proteins	7/2/2019
ABS313	22	12. Membrane proteins	7/2/2019
ABS438		12. Membrane proteins	7/2/2019
ABS459	24	12. Membrane proteins	7/2/2019
ABS465	25	12. Membrane proteins	7/2/2019
ABS015		13. Metabolic engineering/energy applications	7/2/2019
ABS338	27	15. Peptides	7/2/2019
ABS393	28	15. Peptides	7/2/201
ABS398	29	15. Peptides	7/2/2019
ABS189	30	16. Protein interactions and assemblies	7/2/2019
ABS190	31	16. Protein interactions and assemblies	7/2/2019
ABS191	32	16. Protein interactions and assemblies	7/2/2019
ABS210	33	16. Protein interactions and assemblies	7/2/2019
ABS228	34	16. Protein interactions and assemblies	7/2/2019
ABS232	35	16. Protein interactions and assemblies	7/2/2019
ABS238	36	16. Protein interactions and assemblies	7/2/2019
ABS246	37	16. Protein interactions and assemblies	7/2/201
ABS259	38	16. Protein interactions and assemblies	7/2/2019
ABS291	39	16. Protein interactions and assemblies	7/2/2019
ABS309	40	16. Protein interactions and assemblies	7/2/2019
ABS339	41	16. Protein interactions and assemblies	7/2/2019
ABS346	42	16. Protein interactions and assemblies	7/2/2019
ABS415	43	16. Protein interactions and assemblies	7/2/2019
ABS240	44	17. Proteins in cells	7/2/2019
ABS267	45	17. Proteins in cells	7/2/2019

	Board		
AbS	(BOD)	Track	Date
ABS437		17. Proteins in cells	7/2/2019
ABS059		18. Proteomics	7/2/2019
ABS093	48	18. Proteomics	7/2/2019
ABS455		18. Proteomics	7/2/2019
ABS026		19. Proteostasis and quality control	7/2/2019
ABS079		19. Proteostasis and quality control	7/2/2019
ABS153		19. Proteostasis and quality control	7/2/2019
ABS330		19. Proteostasis and quality control	7/2/2019
ABS163		2. Bioinformatics	7/2/2019
ABS179		2. Bioinformatics	7/2/2019
ABS307		2. Bioinformatics	7/2/2019
ABS318		2. Bioinformatics	7/2/2019
ABS449		2. Bioinformatics	7/2/2019
ABS473		2. Bioinformatics	7/2/2019
ABS219		20. Single molecule studies	7/2/2019
ABS298	62	20. Single molecule studies	7/2/2019
ABS446		20. Single molecule studies	7/2/2019
ABS335	64	21. Structure (x-ray/NMR/EM)	7/2/2019
ABS342	65	21. Structure (x-ray/NMR/EM)	7/2/2019
ABS356	66	21. Structure (x-ray/NMR/EM)	7/2/2019
ABS372		21. Structure (x-ray/NMR/EM)	7/2/2019
ABS383	68	21. Structure (x-ray/NMR/EM)	7/2/2019
ABS390		21. Structure (x-ray/NMR/EM)	7/2/2019
ABS401	70	21. Structure (x-ray/NMR/EM)	7/2/2019
ABS409	71	21. Structure (x-ray/NMR/EM)	7/2/2019
ABS421	72	21. Structure (x-ray/NMR/EM)	7/2/2019
ABS422	73	21. Structure (x-ray/NMR/EM)	7/2/2019
ABS430	74	21. Structure (x-ray/NMR/EM)	7/2/2019
ABS448	75	21. Structure (x-ray/NMR/EM)	7/2/2019
ABS461	76	21. Structure (x-ray/NMR/EM)	7/2/2019
ABS464	77	21. Structure (x-ray/NMR/EM)	7/2/2019
ABS482	78	21. Structure (x-ray/NMR/EM)	7/2/2019
ABS308	79	24. Therapeutics and antibodies	7/2/2019
ABS379	80	24. Therapeutics and antibodies	7/2/2019
ABS387	81	24. Therapeutics and antibodies	7/2/2019
ABS408	82	24. Therapeutics and antibodies	7/2/2019
ABS441	83	24. Therapeutics and antibodies	7/2/2019
ABS453	84	24. Therapeutics and antibodies	7/2/2019
ABS456		24. Therapeutics and antibodies	7/2/2019
ABS468	86	24. Therapeutics and antibodies	7/2/2019
ABS485		24. Therapeutics and antibodies	7/2/2019
ABS417	88	25. Transcription/translation/post-translational modifications	7/2/2019
ABS451	89	25. Transcription/translation/post-translational modifications	7/2/2019
ABS114	90	26. Other	7/2/2019
ABS074	91	3. Chaperones	7/2/2019

Poster/Abstract

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AbS	(BOD)	Track	Date
ABS095	92	3. Chaperones	7/2/2019
ABS109	93	3. Chaperones	7/2/2019
ABS192	94	3. Chaperones	7/2/2019
ABS323	95	3. Chaperones	7/2/2019
ABS425	96	3. Chaperones	7/2/2019
ABS467	97	3. Chaperones	7/2/2019
ABS368	98	4. Chemical biology	7/2/2019
ABS380	99	4. Chemical biology	7/2/2019
ABS382	100	4. Chemical biology	7/2/2019
ABS386	101	4. Chemical biology	7/2/2019
ABS396	102	4. Chemical biology	7/2/2019
ABS404	103	4. Chemical biology	7/2/2019
ABS480	104	4. Chemical biology	7/2/2019
ABS140	105	<ol><li>Computational modeling/simulation</li></ol>	7/2/2019
ABS193	107	5. Computational modeling/simulation	7/2/2019
ABS319	108	<ol><li>Computational modeling/simulation</li></ol>	7/2/2019
ABS362	109	5. Computational modeling/simulation	7/2/2019
ABS366	110	5. Computational modeling/simulation	7/2/2019
ABS405	111	<ol><li>Computational modeling/simulation</li></ol>	7/2/2019
ABS418		<ol><li>Computational modeling/simulation</li></ol>	7/2/2019
ABS426	113	5. Computational modeling/simulation	7/2/2019
ABS440	114	<ol><li>Computational modeling/simulation</li></ol>	7/2/2019
ABS183	115	6. Design/engineering	7/2/2019
ABS188	116	6. Design/engineering	7/2/2019
ABS201	117	6. Design/engineering	7/2/2019
ABS206	118	6. Design/engineering	7/2/2019
ABS231	119	6. Design/engineering	7/2/2019
ABS243		6. Design/engineering	7/2/2019
ABS257		6. Design/engineering	7/2/2019
ABS260		6. Design/engineering	7/2/2019
ABS327		6. Design/engineering	7/2/2019
ABS343		6. Design/engineering	7/2/2019
ABS355		6. Design/engineering	7/2/2019
ABS360		6. Design/engineering	7/2/2019
ABS373		6. Design/engineering	7/2/2019
ABS447		6. Design/engineering	7/2/2019
ABS470		6. Design/engineering	7/2/2019
ABS483		6. Design/engineering	7/2/2019
ABS123		7. Dynamics and allostery	7/2/2019
ABS173		7. Dynamics and allostery	7/2/2019
ABS205		7. Dynamics and allostery	7/2/2019
ABS209		7. Dynamics and allostery	7/2/2019
ABS235		7. Dynamics and allostery	7/2/2019
ABS279		7. Dynamics and allostery	7/2/2019
ABS280	138	<ol><li>Dynamics and allostery</li></ol>	7/2/2019

	Board		
AbS	(BOD)	Track	Date
ABS377	139	7. Dynamics and allostery	7/2/2019
ABS264	140	8. Enzymology	7/2/2019
ABS281	141	8. Enzymology	7/2/2019
ABS301	142	8. Enzymology	7/2/2019
ABS305	143	8. Enzymology	7/2/2019
ABS358	145	8. Enzymology	7/2/2019
ABS361	146	8. Enzymology	7/2/2019
ABS391	147	8. Enzymology	7/2/2019
ABS394	148	8. Enzymology	7/2/2019
ABS414	149	8. Enzymology	7/2/2019
ABS439	150	8. Enzymology	7/2/2019
ABS452	151	8. Enzymology	7/2/2019
ABS400	152	0	7/2/2019
ABS412	153	0	7/2/2019
ABS460	154	0	7/2/2019
ABS471	155	0	7/2/2019

# undergrad research session

TUESDAY, JULY 2. 12:15 - 1:30 P.M. WILLOW ROOM

Learn about groundbreaking research from undergraduate scholars TUESDAY, JULY 2 8:30 - 10:00 P.M. GRAND BALLROOM B

THE PROTEIN SOCIETY

> Members' RECEPTION all welcome

> > PROTEIN

## Abstracts

### TPS Award Winners & Speakers

GROEL AND RNA CHAPERONES AS STOCHASTIC MACHINES Dave Thirumalai - 2019 Hans Neurath Award Winner University of Texas at Austin

Protein and RNA chaperones are involved in rescuing proteins and ribozymes that have a high propensity to misfold. The functions of these stochastic machines require ATP, especially for stringent substrates. I will show that a unifying theory based on the Iterative Annealing Mechanism (IAM) quantitatively predicts the experimental outcomes and efficiencies of assisted folding. For the bacterial chaperonin GroEL, assisted folding is intimately coupled to the spectacular allostery that the GroEL particle undergoes in response to GroES and substrate binding. I will show that GroEL and RNA chaperones maximize the yields of the folded states of proteins and RNA by driving them out of equilibrium.

#### CHAPERONE-ASSISTED STRUCTURE DETERMINATION: BRINGING HIGH HANGING FRUIT TO GROUND LEVEL Anthony Kossiakoff - 2019 Christian B. Anfinsen Award Winner

University of Chicago

Determining how proteins utilize conformational transitions to regulate their function has been a long standing Grand Challenge Problem. Despite great effort and resources, the path towards a fundamental understanding of the interconnections between function and dynamics has been frustrated by a set of daunting technical obstacles. To overcome these barriers, we have developed the Chaperone-Assisted Structure Determination (CASD) pipeline, a multi-faceted technology platform that generates novel, high performance antibody-based reagents that can be exquisitely conformation-specific, making them unique probes for studying protein conformation dynamics. We have demonstrated that these reagents can effectively "lock" a protein in a desired conformational state providing for unequivocal annotation of each functional state through biophysical analyses and structure determination. These reagents are produced by phage display mutagenesis employing fully synthetic libraries and thus, are termed "synthetic antibodies" or sABs. They are based on well-characterized Fab scaffolds and have proven very useful as crystallization chaperones and fiducial markers for single-particle (SP) cryo-EM. To further increase the utility of these sABbased modules, we have engineered a series of constructs to serve as prefabricated modules of assembly. In some cases they can be universally employed as structural chaperones irrespective of the system they are applied to. The power of this approach is that they can be added to the molecule of interest in a "plug and play" fashion allowing any investigator access to the powerful technology without requiring generating target specific sABs. As an example of this utility, its application to determining the cryo-EM structures of GPCR signaling complexes will be presented.



#### HIGHER-ORDER SUPRAMOLECULAR ASSEMBLIES IN IMMUNE SIGNALING AND BEYOND Hao Wu - 2019 Dorothy Crowfoot Hodgkin Award Winner Harvard University

My laboratory has been interested in using structural biology to address fundamental questions in immunological processes. In innate immunity, which offers the first line of defense against infections and other types of danger, studies from my lab and other labs have established a new paradigm that involves formation of large oligomeric intracellular signaling complexes, or "signalosomes". In this presentation, I will recount briefly how we encountered these supramolecular complexes in our structural studies, and will elaborate our recent cryo-EM studies on some of these complexes in the context of inflammasomes, which are cytosolic caspase-1 activating machines.

#### CELL-WALL RECYCLING IN PSEUDOMONAS AERUGINOSA AND THE NEXUS TO ANTIBIOTIC RESISTANCE Shahriar Mobashery - 2019 Carl Brand Award Winners

## University of Notre Dame

Pseudomonas aeruginosa has the ability to sense damage inflicted to its cell wall by B-lactam antibiotics. The process involves chemical signaling, which will be a subject of my presentation. A primary mechanism for this sensing and signalling involves the events of cell-wall recycling. The cell wall is degraded for recycling and then it is resynthesized de novo for the repair function. The recycling events get initiated by the functions of a family of 11 lytic transglycosylases in P. aeruginosa, which generate the signalling factors that influence transcriptional events in the cytoplasm. The mechanisms of these enzymes and those of the early cytoplasmic steps of recycling have been the subject of study in my lab, which I will disclose in my presentation.

#### MASS SPECTROMETRY: FROM PLASMA PROTEINS TO MITOCHONDRIAL MEMBRANES Dame Carol Robinson - 2019 Stein & Moore Award Winner University of Oxford

Beginning with the preservation of the first soluble complexes from plasma, in the gas phase of a mass spectrometer, I will describe our early experiments that capitalize on the heterogeneity of subunit composition during assembly and exchange reactions. To assess the overall topology of these complexes we then adapted ion mobility and soft-landing methodologies to show how ring-shaped complexes could survive the phase transition. The next logical progression from soluble complexes was to membrane protein assemblies but this was not straightforward. We encountered many pitfalls along the way, largely due to the use of detergent micelles to protect and stabilize these complexes. Further obstacles presented when we attempted to distinguish lipids that co-purify from those that are important for function. Developing new experimental protocols, we have subsequently defined lipids that

## **Abstracts** TPS Award Winners & Speakers

change protein conformation, mediate oligomeric states, and facilitate downstream coupling of G protein-coupled receptors. Very recently, using a new method—ejecting protein complexes directly from native membranes into mass spectrometers—we provided insights into associations within membranes and mitochondria. In my lecture I will trace the history of these developments and look towards future innovations and discoveries.

#### BROWNIAN DYNAMIC STUDY OF AN ENZYME METABOLON IN THE TCA CY-CLE: SUBSTRATE KINETICS AND CHANNELING Yu-ming "Mindy" Huang - 2019 Protein Science Best Paper Award Winner

University of California, San Diego Gary A. Huber2, Nuo Wang3, Shelley D. Minteer4, and J. Andrew McCam-

Gary A. Huber2, Nuo Wang3, Shelley D. Minteer4, and J. Andrew McCammon1,2,3

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- San Diego
- 4 Department of Chemistry, The University of Utah, Salt Lake City

Abstract Malate dehydrogenase (MDH) and citrate synthase (CS) are two pacemaking enzymes involved in the tricarboxylic acid OCA) cycle. Oxaloacetate (OAA) molecules are the intermediate substrates that are transferred from the MDH to CS to carry out sequential catalysis. It is known that, to achieve a high flux of intermediate transport and reduce the probability of substrate leaking, a MDH-GS metabolon forms to enhance the OAA substrate channeling. In this study, we aim to understand the OAA channeling within possible MDH-GS metabolons that have different structural orientations in their complexes. Three MDH-GS metabolons from native bovine, wild-type porcine, and recombinant sources, published in recent work, were selected to calculate OAA transfer efficiency by Brownian dynamics (BD) simulations and to study, through electrostatic potential calculations, a possible role of charges that drive the substrate channeling. Our results show that an electrostatic channel is formed in the metabolons of native bovine and recombinant porcine enzymes, which guides the oppositely charged OAA molecules passing through the channel and enhances the transfer efficiency. However, the channeling probability in a suggested wildtype porcine metabolon conformation is reduced due to an extended diffusion length between the MDH and CS active sites, implying that the corresponding arrangements of MDH and CS result in the decrease of electrostatic steering between substrates and protein surface and then reduce the substrate transfer efficiency from one active site to another.



## LOCAL AND NON-LOCAL TOPOLOGICAL INFORMATION IN THE DENATURED STATE ENSEMBLE OF A BETA-BARREL PROTEIN

Abhay Thakur - 2019 Protein Science Best Paper Award Winner Departments of Biochemistry & Molecular Biology and Chemistry, University of Massachusetts Amherst

Wenli Meng, and Lila M. Gierasch

The folding of predominantly  $\beta$ -sheet proteins is complicated by the presence of a large number of non-local interactions in their native states, which increase the ruggedness of their folding energy landscapes. However, forming non-local contacts early in folding or even in the unfolded state can smooth the energy landscape and facilitate productive folding. We report that several sequence regions of a p-barrel protein, cellular retinoic acid-binding protein 1 (CRABPI), populate native-like secondary structure to a significant extent in the denatured state in 8 M urea. In addition' we provide evidence for both local and non-tocal interactions in the denatured state of CRABP1. NMR chemical shift perturbations (CSPs) under denaturing conditions upon substitution of single residues by mutation support the presence of several non-local interactions in topologically key sites, arguing that the denatured state is conformationally restricted and contains topological information for the native fold.

Among the most striking non-local interactions are those between the N- and C-tefminal regions, which are involved in closure of the native p-barrel. In addition, CSPs support the presence of two features in the denatured state: a major hydrophobic cluster involving residues from various pans of the sequence and a native-like interaction similar to one identified in previous studies as forming early in folding (Budyak et al., Structure 2'1,476 [20130. Taken together, our data support a model in which transient structures involving nonlocal interactions prime early folding interactions in CRABP1, determine its barrel topology, and may protect this predominantly β-sheet protein against aggregation.

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### **TPS Award Winners & Speakers**

Following is the list of invited speakers, denoted by (1), listed alphabetically.

# DISSECTING STRUCTURAL MECHANISMS OF FORCE-SENSITIVE ACTIN BINDING Greg Alushin (1)

(1) The Rockerfeller University

Mechanical regulation ("mechanoregulation") of the interactions between filamentous actin (F-actin), the main load-bearing element of the cytoskeleton, and its dozens of binding partners (ABPs) is postulated to play an important role in cellular force sensing. To test this hypothesis, we have developed a medium-throughput platform for directly probing the sensitivity of ABP-F-actin binding interactions to force, utilizing a modified gliding-filament assay wherein surface immobilized myosin motor protein apply stress to filaments while ABP binding is monitored with Total Internal Reflection Fluorescence (TIRF) microscopy. We have focused our initial studies on groups of homologous ABPs, hypothesizing they might have differential force-sensitivity which could readily be dissected through structure-function studies. I will describe one mechanosensitive / insensitive pair of ABPs we have identified using this approach. Simultaneous optical trapping / fluorescence microscopy studies confirm the mechanosensitive binder is directly regulated by force. High-resolution (~3 Å) cryo-electron microscopy (cryo-EM) structures of both ABPs bound to F-actin reveal differential folding and actin engagement by flexible "tail" elements, which TIRF assays of chimeric proteins establish to be responsible for differential force sensitivity. In addition to providing mechanistic insights in this particular case, our approach should be broadly applicable for dissecting structural mechanisms of force-sensitive actin binders.

#### SINGLE-MOLECULE ANALYSIS OF LIGAND EFFICACY IN B2AR-G PROTEIN ACTIVATION Scott C. Blanchard1(1)

(1) Weill Cornell Medical College

G. Glenn Gregorio1\*, Matthieu Masureel2\*, Daniel Hilger2\*, Daniel S. Terry1, Manuel Juette1, Hong Zhao1, Zhou Zhou1, Jose Manuel Perez-Aguilar1,9, Maria Hauge3,5,7,8, Signe Mathiasen3,5, Jonathan A. Javitch3,4,5, Harel Weinstein1,6, Brian K. Kobilka2‡,

G protein-coupled receptor (GPCR)-mediated signal transduction is central to human physiology and disease intervention, yet the molecular mechanisms responsible for ligand-dependent signaling responses remain poorly

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understood. In Class A GPCRs, receptor activation and G protein coupling entail outward movements of transmembrane segment 6 (TM6). Using single-molecule Fluorescence Resonance Energy Transfer (smFRET) imaging, we examine TM6 motions in the  $\beta$ 2 adrenergic receptor ( $\beta$ 2AR) upon exposure to orthosteric ligands with different efficacies, in the absence and presence of the Gs heterotrimer. We show that partial and full agonists affect TM6 motions in a manner that differentially regulates the rate at which GDP-bound  $\beta$ 2AR-Gs complexes are formed and the efficiency of nucleotide exchange leading to Gs activation. These data also reveal transient nucleotide-bound  $\beta$ 2AR-Gs species distinct from known structures and single-molecule perspectives on the allosteric link between ligand and nucleotide binding pockets that shed new light on the G protein activation mechanism.

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- 6 The HRH Prince Alwaleed Bin Talal Bin Abdulaziz Alsaud Institute for Computational Biomedicine, Weill Cornell Medical College of Cornell University, New York, New York, USA
- 7 Laboratory for Molecular Pharmacology, Department of Neuroscience and Pharmacology, University of Copenhagen,
- 8 NNF Center for Basic Metabolic Research, University of Copenhagen
- 9 Present address: IBM Thomas J. Watson Research Center, Yorktown Heights, New York, USA

### ULTRAVIOLET PHOTODISSOCIATION MASS SPECTROMETRY FOR CHARACTER-IZATION OF PROTEINS AND PROTEIN COMPLEXES

Jennifer Brodbelt (1) (1) The University of Texas at Austin

Advances in mass spectrometry instrumentation and experimental design have led to significant inroads in the characterization of intact proteins and protein complexes, thus translating to new applications in the field of proteomics and structural biology. Ultraviolet photodissociation (UVPD) results in broad sequence coverage of intact proteins via more extensive backbone fragmentation than obtained from other ion activation methods,

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### **TPS Award Winners & Speakers**

and ion activation/dissociation can be accomplished using a single 5 ns laser pulse. UVPD offers a frontier MS/MS technology for characterization of intact proteins, including mapping post-translational modifications and ligand binding sites. There has been growing interest in employing topdown approaches to examine native-like protein structures by using MS/ MS to disassemble the complexes and sequence the constituent proteins. In the context of protein-ligand complexes, the relative abundances of fragment ions generated by UVPD correlate with variations in the intramolecular and intermolecular interactions that stabilize particular regions of the proteins. Owing to the fast, high energy deposition of UV photoactivation, products retaining non-covalently bound ligands are formed and afford binding site information. For multimeric protein complexes, UVPD disassembles the complexes to reflect sub-unit architecture as well as sequence ions that identify the proteins.

### ELUCIDATION OF PROTEIN COMPLEXES IN HEART

James E. Bruce (1) (1) University of Washington

Juan D. Chavez, Andrew Keller, Xiaoting Tang, Jared P. Mohr, Martin Mathay, Arianne Caudal, Matthew Walker, Bo Zhou, Rong Tian University of Washington

Over countless generations, natural selection processes have finely tuned protein complexes to fulfill most functional roles within the crowded and complex environment inside cells. Despite exciting recent advances in structural techniques for isolated complex analyses, many proteins are shaped by and even require their native interacting environment to maintain conformations and interactions. For these, new technologies and approaches are required to achieve improved understanding of their function inside cells. Our lab has pursued development of novel chemical cross-linking, mass spectrometry technologies and informatics to enable insight on protein complex structures as they exist inside cells, tissues and organs. One particular area of focus includes the elucidation of the mitochondrial interactome to gain understanding of normal function and dysfunction in heart. This presentation will highlight our technical advances and applications to reveal greater insight on mitochondrial complex structures that exist in respiring mitochondria and heart tissues.

#### RATIONAL ENHANCEMENT OF PROTEIN CONFORMATIONAL SWITCHING KINETICS: WEIGHTED ENSEMBLES OF FOLDING TRAJECTORIES Lillian Chong (1)

(1) University of Pittsburgh

The design of protein conformational switches has great potential for developing novel biosensors, diagnostic tools, and therapeutic agents. Among the defining properties of such switches, the response time has been the most challenging to optimize. Here we apply a computational design strategy to rationally improve the response time of an engineered protein-based Ca2+-sensor in which the switching process occurs via mutually exclusive folding of two alternate frames. Our strategy involves the use of molecular simulations and the weighted ensemble approach, which enhances the sampling of rare events (e.g. protein folding) without biasing the dynamics. Notably, the strategy identified mutations that increase switching rates by as much as 32-fold, achieving response times on the order of fast physiological Ca2+ fluctuations. Our computational design strategy is general and may aid in optimizing the kinetics of other protein conformational switches.

# PROTEIN FOLDING, AGGREGATION AND PHASE SEPARATION IN THE CELL Simon Ebbinhaus (1)

(1) Ruhr-Universität Bochum

Proteins fold and function in the densely crowded and highly heterogeneous cell, which is filled up to a volume of 40% with macromolecules. That under such conditions cells can keep their proteome folded and organized without uncontrollable aggregation is a remarkable aspect of biology. In this talk, I will first discuss how the different cosolutes in the cellular milieu such as ions, crowders and osmolytes govern the protein folding equilibrium. I will thereby present a novel classification scheme of cosolute effects based on their thermodynamic fingerprints. This model is of fundamental importance to understand how the proteome stability is modulated by cellular processes, e.g. to understand how osmolytes or chaperones protect the proteome or how most destabilized proteins aggregate under different cell stresses. I will further present spectroscopic probes that explore the different cosolute effects directly in cells and show that cell stress can significantly modulate the folding equilibrium. Remarkably, protective cellular mechanisms such as the heat shock response or the regulatory volume increase are highly adapted to minimize the impact on the proteome.

Enduring stress leads to protein aggregation and liquid-liquid phase separation. In-cell protein unfolding experiments in different subcellular compartments show how these processes are coupled inside cells. I will

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### **TPS Award Winners & Speakers**

conclude by presenting potential inhibitors to modulate protein aggregation as a new therapeutic approach for neurodegenerative diseases.

#### PATHOGENIC VS. REVERSIBLE AMYLOID; STERIC ZIPPERS VS. LARKS

David S. Eisenberg (1)

(1) University of California, Los Angeles

Michael Sawaya, Lorena Saelices, Michael Hughes, Sarah Griner, Qin Cao, Paul Seidler, David Boyer, Jeannette Bowler, Kevin Murray, Shruti Sahay, Melinda Balbirnie, Gregory Rosenberg, Jaihui Lu, Duilio Cascio

Pathogenic amyloid fibrils are not evolved structures, whereas natural selection must have honed the structures of functional amyloid-like fibrils found in subcellular assemblies. Yet both types of fibrils share architectural features, including protein chains folded in two-dimensional layers, which are then stacked via hydrogen bonds into elongated fibrils. Near atomic-resolution structures are now known for more than 20 such fibrils, permitting quantitative structural and energetic comparisons. We have studied the structural and energetic features that account for the reversibility of functional fibrils and the irreversibility of pathogenic fibrils, and for the propensity for polymorphism of pathogenic fibrils and its consequences for disease and treatment.

# HIGH THROUGHPUT METHODS FOR DISCOVERING PROTEIN FOLD CORRECTORS Jason E. Gestwicki (1)

(1) University of California, San Francisco

Abstract: Many inherited protein misfolding diseases, such as cataract and cystic fibrosis, are caused by mutations that destabilize the target protein. One approach to potentially treat these diseases is to identify "correctors" that bind to the mutant and restore its lost stability. In addition, such molecules can be useful probes for understanding the molecular origins of the folding defect. Our group is working to create high throughput differential scanning fluorimetry (HT-DSF) methods to rapidly identify potential correctors. In our first model, we screened a cataract-associated mutation in alpha-crystallin by HT-DSF to identify molecules that limit misfolding and aggregation. After a medicinal chemistry campaign, we found that the best molecules bound to the native, dimeric state of the alpha-crystallin and that it did not bind to the misfolded or amyloid structures. In turn, this compound partially reversed aggregation of this

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target in vitro and in multiple animal models. From a mechanistic perspective, we used these compounds revealed the reversible aggregation of alpha-crystallin, which is unusual amongst the amyloid-prone proteins. Inspired by this concept, we have been building next-generation HT-DSF approaches that improve sensitivity, scope and scale.

# PHASE TRANSITIONS AND TIMING MECHANISMS GOVERNING SIGNALING AT THE MEMBRANE

Jay Groves (1) (1) University of California, Berkeley

The proximal signaling molecules that transduce the signal from T cell receptors to Ras undergo a phase transition into a two-dimensional gel or liquid during signaling activity. Recent single molecule studies on the activation of the Ras GEF, SOS, in these molecular assemblies reveal the physical mechanism by which the phase transition governs Ras activation involves a molecular timing mechanism and kinetic proof reading. I will discuss our experimental evidence for this mechanism as well as the potential for this type of process to be more widespread in biology.

# MEASURING WEAK PROTEIN-PROTEIN AND PROTEIN-RNA INTERACTIONS INSIDE THE CELL

Martin Gruebele (1) (1) University of Illinois

Protein-protein and protein-RNA interactions range widely in strength, from string picomolar binding to weak micromolar binding. There are likely to be very many such weak but functional interactions in cells. Transient functional interactions, or 'quinary structure,' are highly susceptible to the in-cell environment. After discussing the perturbative effect of cell type and organelle type on protein folding, I will discuss two examples of protein-protein and protein-RNA interactions modulated by their native environment in the cell.

# Dynamics of GPCR Signal Transmission and Allosteric Regulation Detected by NMR

Stephan Grzesiek (1) (1) University of Basel

Anne Grahl1, Layara Abiko1, Shin Isogai1, Rajesh Sonti1, Johannes Schlotte1, Christian Opitz1, Xavier Deupi2, Gebhard Schertler2, Dmitry Veprintsev2, Oliver Hantschel3

- 1 Biozentrum, University of Basel
- 2 Paul Scherrer Institute
- 3 École Polytechnique Federale de Lausanne

## **Abstracts** TPS Award Winners & Speakers

The function of G protein-coupled receptors (GPCRs) as that of many other proteins is regulated via intricate, allosteric interactions. These are not visible in static structures, but can only be derived from additional dynamical information. In recent years, we have sought to obtain such dynamical information on allosteric regulation by solution NMR methods. GPCRs are particularly challenging for NMR due to their large size and since they are difficult to express in functional isotope-labeled form in E. coli.

The  $\beta$ 1-adrenergic GPCR ( $\beta$ 1AR) is one of the targets of beta-blockers in the heart muscle. We could recently show that allosteric receptor motions in response to different agonist and antagonist ligands and a G protein mimetic nanobody can be followed at virtually any backbone site via 1H-15N chemical shifts in a detergent-solubilized thermostabilized mutant of the turkey  $\beta$ 1AR [1], which was produced in insect cells using isotope-labeled amino acids [2]. The response to the various ligands is heterogeneous in the vicinity of the binding pocket, but gets transformed into a homogeneous readout at the intracellular side of helix 5 (TM5), which correlates linearly with ligand efficacy for the G protein pathway.

We have now obtained highly detailed, quantitative information on the dynamics of B1AR in various complexed forms from precise measurements of four types of 15N NMR relaxation rates at 14 backbone amide sites. Significant micro- to millisecond motions are observed throughout the receptor. Particularly pronounced ligand-dependent motions occur for TM6 residue V314 at the extracellular ligand entry tunnel. The dynamical equilibrium at this site is strongly shifted by the binding of the G protein mimetic nanobody (Nb80) at the cytoplasmic side. This phenomenon can be explained by a pivoting motion of TM6, which couples the effector site to the orthosteric ligand supon G protein/Nb80 binding, which results from a compression of the binding pocket by the TM6 motion, (ii) the ingher affinity and (iii) antagonistic function of larger antagonist ligands, which fill the apparent void in the binding pocket by hydrophobic substitutions in their head group and impede pivoting.

Time permitting we will also discuss NMR detection of allosteric regulation of Abelson (Abl) kinase, which is a prime drug target in the treatment of chronic myelogenous leukemia [3,4] as well as technical advances of isotope-labeling in higher eukaryotic cells [2] and the effect of growth under deuteration on the E. coli proteome [5].

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# CHAPERONE FUNCTIONS IN PROTEIN FOLDING AND PROTEOME MAINTENANCE F. Ulrich Hartl (1)

(1) Max Planck Institute of Biochemistry

The past two decades have witnessed a paradigm shift in our understanding of cellular protein folding. While the three-dimensional structures of functional proteins are determined by their amino acid sequences, it is now firmly established that in the cell many proteins depend on molecular chaperones to reach their folded states efficiently and on a biologically relevant time scale. Assistance of protein folding is provided by different types of chaperone which act to prevent misfolding and aggregation, often in an ATP-dependent mechanism. Molecular chaperones also cooperate with the degradation machinery (ubiquitin-proteasome system and autophagy) in the removal of terminally misfolded proteins.

Once folded, many proteins continue to require chaperones to retain their functional states, especially under conditions of proteotoxic stress. Failure of the chaperone network to maintain proteostasis, i.e. the conformational integrity of the cellular proteome, facilitates the manifestation of diseases in which proteins misfold and are deposited as aggregates, such as Parkinson's and Huntington's disease.

I will discuss recent insights into the role of chaperone networks in preventing or reversing toxic protein aggregation in different cellular compartments.

#### MOLECULAR MECHANISMS OF RNA POLYMERASE II TRANSCRIPTION ELONGA-TION ELUCIDATED BY KINETIC NETWORK MODELS Xuhui Huang (1)

(1) Department of Chemistry, The Hong Kong University of Science and Technology

Transcription, the synthesis of RNA from a complementary DNA template, plays a crucial role in cellular regulation, including differentiation, development, and other fundamental processes. In this talk, I will discuss our results on modeling the RNA polymerase II (Pol II, a system with ~400K atoms) Translocation and other functional conformational changes of this enzyme at

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sub-millisecond timescales. We have developed a novel algorithm, Hierarchical Nystrom Extension Graph method, to construct kinetic network models to extract long timescale dynamics from short simulations. For example, we reveal that RNA polymerase II translocation is driven purely by thermal energy and does not require the input of any additional chemical energy. Our model shows an important role for the bridge helix: Large thermal oscillations of this structural element facilitate the translocation by specific interactions that lower the free-energy barriers between four metastable states. The dynamic view of translocation presented in our study represents a substantial advance over the current understanding based on the static snapshots provided by X-ray structures of transcribing complexes. At the end of my talk, I will briefly discuss our recent progress on extending our kinetic network model to include sequence-dependent molecular dynamics of Pol II elonaation to predict transcriptional accuracy in the genome-wide transcriptomic datasets. This model creates a critical link between the structural-mechanics understanding of Pol II fidelity and the genome-wide transcriptional accuracy.

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#### TARGETING SMALL GTPASE K-RAS4B ON BIOLOGICAL MEMBRANES Mitsu Ikura (1)

(1) Princess Margaret Cancer Centre, University Health Network and Department of Medical Biophysics, University of Toronto,

RAS proteins are frequently mutated in cancer (~30% of all human tumours) and an estimated world-wide death pole of RAS-associated cancers exceeds 2 million/yr. Despite of enormous efforts in the RAS research over three decades, there is no clinically approved RAS inhibitor and the RAS protein remains to be a challenging target for cancer therapy development. In order to overcome this challenge, we ought to better understand how RAS functions under physiological conditions and alters related signaling pathways in the mutant RAS-driven tumours. Fully-matured protein K-RAS4B, the major target for cancer therapeutics, is prenylated and methylated at the carboxy-terminus, which enables K-RAS4B to anchor to the plasma membrane where it receives an upstream signal and transmits the signal to a number of downsteam pathways. There is, however, a large gap in our understanding of how the matured K-RAS4B protein functions at the surface of the plasma membrane. In order to tackle this challenge in RAS-driven cancer research, we have been extensively employing isotope-aided NMR spectroscopy and have developed new conformational and functional assays for the RAS protein on lipid bilayers using the nanodisc platform developed by Sligar et al. We elucidated how the membrane environment dictates the conformation of K-RAS4B and how oncogenic mutations influences the membrane-dependent conformational states of the protein (Mazhab-Jafari et al. PNAS 2015). More recently, we have been investigating multiple aspects of K-RAS4B functions and I will discuss (i) how the biological membrane influences K-RAS4B interaction with a binding domain of RAF kinases and (ii) how we could inhibit K-RAS4B at the membrane surface by small molecules (Fang et al. Cell Chem Biol 2018) and an engineered protein. Supported by CCS, CIHR, CFI & PMCF.

#### SOLUTION NMR APPROACHES TO 3D STRUCTURE DETERMINATION OF PROTEINS IN LIVING EUKARYOTIC CELLS Yutaka Ito (1)

(1) Department of Chemistry, Tokyo Metropolitan University, Japan

### Teppei Ikeya

In vivo observations of 3D structures, folding stability, dynamics or interactions of proteins are essential for the explicit understanding of the structural basis of their functions inside cells. Solution NMR of biomacromolecules in live cell samples (in-cell NMR) is currently the only approach that can provide structural information of proteins inside cells at atomic resolution. In 2009 we reported the first 3D protein structure calculated exclusively based on the information obtained in living *E.coli* cells. Currently in-cell NMR studies in various eukaryotic cells have become possible by either expressing target proteins inside cells or by introducing stable isotope-enriched proteins.

We will report our recent methodological developments which enabled the first high-resolution protein structure determinations in eukaryotes using the Sf9 insect cell line with the baculovirus protein expression system. The method was applied to five proteins, rat calmodulin, human HRas, human ubiquitin, *T. thermophilus* HB8 TTHA1718, and Streptococcus protein G B1 domain. In all cases, we could observe well-resolved 3D NMR spectra and obtain structural information from in-cell NOESY data, suggesting that our method can be a

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standard tool for protein structure determinations in living eukaryotic cells. For three proteins, we achieved well-converged 3D structures. Among these, the in-cell structure of protein G B1 domain was most accurately determined, demonstrating that a helix-loop region is tilted away from a beta-sheet compared to the conformation in diluted solution presumably due to molecular crowding or other intracellular effects.

#### DECIPHERING PROTEIN DYNAMICS AND FUNCTION BY COMBINING HDX-MASS SPECTROMETRY WITH MD SIMULATIONS Lars Konermann (1)

(1) Department of Chemistry, The University of Western Ontario

HDX methods probe protein dynamics by reporting on short-lived opening/closing events of backbone H-bonds. This presentation summarizes some of our studies in this area, with emphasis on recent efforts to complement HDX with MD simulations. F1-ATPase uses ATP hydrolysis to drive rotation of the gamma subunit. The gamma C-terminal helix constitutes the rotor tip that is seated in an apical bearing. It remains uncertain to what extent the gamma conformation during rotation differs from that seen in rigid crystal structures. Existing models assume that the entire gamma subunit participates in every rotation. We found that rotation causes enhanced HDX in the gamma C-terminal helix, implying that the rotor tip is prone to unfolding. An MD strategy was developed to model the off-axis forces acting on gamma. The simulations showed stalling of the rotor tip and unfolding of the gamma C-terminal helix. MD-predicted H-bond opening events coincided with experimental HDX patterns. Our data suggest that in vitro operation of F1-ATPase is associated with significant rotational resistance in the apical bearing. These conditions cause the gamma C-terminal helix to get "stuck" (and unfold) sporadically while the remainder of gamma continues to rotate. This scenario contrasts the traditional "greasy bearing" model that envisions smooth rotation of the gamma C-terminal helix. Time permitting, we will also discuss our recent efforts to uncover the mechanism of calcium-regulated allosteric substrate recognition in \$100 proteins. Overall, MD/HDX strategies appear well suited for interrogating the intricate relationships between protein structure, dynamics, and function.

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#### CELLULAR CONSEQUENCES OF SYSTEMATIC PERTURBATIONS OF A HIGHLY CONSERVED BIOLOGICAL SWITCH Tanja Kortemme (1)

(1) University of California, San Francisco

Cellular protein-protein interactions can be highly interconnected. Because of this complexity, it is often difficult to extract quantitative information on how each interaction contributes to distinct or overlapping cellular functions, and, moreover, how changes to individual interactions result in altered function or disease. We are developing an experimental platform for studying perturbations to multi-functional network "hub" proteins by combining high-throughput in vivo genetic interaction screening technology (Epistatic MiniArray Profile (E-MAP)) with mass-spectrometry and biophysical assays. Our case study protein is the highly-conserved multi-functional Gsp1/Ran GTPase switch that controls key eukaryotic processes. The approach first engineers defined perturbations to Gsp1/Ran protein-protein interactions by amino acid point mutations. The second step determines the functional effects of these perturbations at the cellular level in the model S. cerevisiae. We find that E-MAPs have a resolution that enables us to identify quantitative functional differences in vivo between individual point mutations, even those between different amino acid substitutions of the same residue. Our analysis reveals several classes of observed phenotypes that are explained by the underlying biophysical perturbations of the on/off balance of the fundamental GTPase switch and considerable allosteric effects in the system.

#### MOLECULAR DETAILS OF PROTEIN MISFOLDING IN MYOCILIN-ASSOCIATED GLAUCOMA Raguel L. Lieberman (1)

(1) Georgia Institute of Technology

Missense mutations in myocilin are causative for the early-onset, hereditary form of open angle glaucoma. Using biophysical and structural methods, we have assembled a molecular picture of myocilin, including its wild-type supramolecular arrangement as defined by its coiled coil and olfactomedin domains, as well as its pathogenic misfolding. Annotated glaucoma-causing variants within each structural domain exhibit different protein defects. The olfactomedin domain, which harbors 90% of annotated variants, is exquisitely sensitive to mutation. Most olfactomedin-resident mutations are destabilizing

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and promote templated amyloid-like aggregation within the endoplasmic reticulum (ER). This misfolding includes an aberrant interaction with the ER-resident chaperone Grp94, resulting in cytotoxicity that compromises the function of the trabecular meshwork, a key ocular tissue diseased in most forms of glaucoma. Taken together, our work has elaborated atomic-level details of myocilin misfolding relevant to glaucoma pathogenesis and offers a new, disease-modifying therapeutic strategy to treat myocilin-associated glaucoma.

# NATIVE MASS SPECTROMETRY FOR A TOP-DOWN VIEW OF PROTEIN STRUCTURES Joseph A. Loo (1)

(1) Department of Chemistry and Biochemistry; Department of Biological Chemistry, David Geffen School of Medicine

Native mass spectrometry (MS) of proteins and protein assemblies reveals size and binding stoichiometry. But elucidating their structures to understand their function is more challenging. Using electrospray ionization (ESI), relative charging by native ESI-MS appears to give some information on protein folding. We show that native MS and native top-down MS, i.e., fragmentation of the gas-phase protein, can be effective for deriving structural information for soluble and membrane protein complexes, and much of this information can be correlated to the solution-phase structure. Native top-down MS generates information on the surface topology, ligand binding sites, and post-translational modifications (PTMs) of protein complexes. We use native MS/MS to investigate the molecular action of compounds that prevent amyloid fibril formation in neurodegenerative diseases such as Alzheimer's and Parkinson's disease. The importance of salt bridges, those that are suggested to be present in the solution-phase structure, in the dissociation behavior of gas-phase proteins will be discussed.

Acknowledgments: Support from the US National Institutes of Health (GM103479, AG054000), US National Science Foundation (1808492), and the US Department of Energy (DE-FC-02-02ER63421) is acknowledged.

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ENGINEERING LINKAGE-SPECIFIC POLYUBIQUITIN ANTIBODIES: TOOLS FOR ELUCIDATION OF NOVEL SIGNALING PATHWAYS Marissa L. Matsumoto (1) (1) Genentech. Inc.

Ubiquitin is a post-translational modification involved in nearly every signaling pathway. Ubiquitination occurs when the carboxy-terminus of ubiquitin is linked through an isopeptide bond to a lysine residue on a substrate protein. Ubiquitin itself contains seven lysines and a free amino-terminus through which additional ubiquitin subunits can be linked, resulting in polyubiquitin chains of different topologies. Determination of polyubiquitin chain linkages historically required the use of ubiquitin mutants or complex mass spectrometry experiments. We have engineered antibodies with exquisite specificity to the M1, K11, K48, and K63 linkages. These antibodies work in a variety of applications, allow rapid determination of polyubiquitin linkages and have been widely used in the ubiquitin field to elucidate ubiquitin-dependent signaling mechanisms. Recently the polyubiquitin code has been demonstrated to be more complex than initially anticipated with the identification of heterotypic polyubiquitin chains containing more than one linkage. Using the knobs-into-holes technology we engineered a bispecific antibody that can detect K11/K48-branched polyubiquitin chains. This antibody helped reveal that these branched chains modify nascent, misfolded, aggregation-proteins targeting them for priority degradation at the proteasome. By uncovering a novel role for K11/K48-branched chains in protein quality control, the K11/K48-bispecific underscores the utility of linkage-specific antibodies in ubiquitin research and highlights the need to expand the toolkit to help elucidate functions of newly identified ubiquitin post-translational modifications.

#### UNFOLDING AND REFOLDING OF INDIVIDUAL BACTERIORHODOPSIN MOLE-CULES PROBED WITH 1-MS RESOLUTION Thomas T. Perkins (1)

(1) JILA, NIST & CU-Boulder

High-precision single-molecule force spectroscopy studies can yield kinetic rate constants, energetics, intermediate states, unfolding pathways, and even a projection of the underlying free-energy landscape. However, such studies of membrane proteins have lagged analogous studies of nucleic acids and globular proteins due to instrumental limitations. We developed a set of technical advances to atomic force microscopy (AFM) that enabled us to reexamine the unfolding of individual bacteriorhodopsin (bR) molecules embedded in their native lipid bilayer with a 100-fold improvement in time resolution and a 10-fold improvement in force precision. The resulting data revealed the unfolding pathway in unprecedented detail. Numerous newly detected intermediates—many

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separated by as few as 2-3 amino acids—exhibited complex dynamics, including frequent refolding and state occupancies of <10 µs. We next integrated these technical advances with site-specific covalent coupling of bR to an AFM tip to quantify the initial unfolding of bR. The resulting records revealed rapid near-equilibrium dynamics between three states spanning a mere 8 amino acids. The third of these states corresponded to Lys216, where bR's retinal is covalently attached; dynamic force spectroscopy revealed this previously unobserved state was retinal-stabilized and, indeed, the most mechanically robust state in bR's extensively characterized unfolding pathway. Toward the broader goal of measuring quantitative energetics, we leveraged these rapid and reversible dynamics to reconstruct the 1D free-energy landscape of bR's initial unfolding and to determine  $\Delta\Delta$ GO for select point mutants. Hence, we have established a platform for precisely quantifying membrane-protein energetics under native-like conditions.

#### FACTORS MODULATING HSP70 SUBSTRATE RECOGNITION AND MEDIATION OF THE STRESS RESPONSE Sarah Perrett (1)

(1) Institute of Biophysics, Chinese Academy of Sciences

Hsp70 is a conserved molecular chaperone which plays an indispensable role in regulating protein folding, translocation and degradation. The conformational dynamics of Hsp70 and its regulation by cochaperones is vital to its function. We are using fluorescence resonance energy transfer (FRET) techniques to study the conformational distribution of Hsp70 and the kinetics of conformational changes induced by nucleotides and the Hsp40 cochaperone during the functional cycle. The results indicate the importance of the dynamic and heterogeneous nature of Hsp70 for its function. We are also investigating the role of other factors that modulate Hsp70 substrate recognition and the stress response, using a combination of cellular, biochemical and biophysical techniques. We have found that post-translational modification of cysteine residues in Hsp70 enters its interaction with substrates, thus potentially acting as a redox sensor. Further, we have investigated the role of the intrinsically disordered C-terminal tail of Hsp70 in mediating substrate recognition and the stress response.

# STRUCTURAL BIOLOGY OF PMHC RECEPTORS FUNCTIONING AS MECHANO-SENSORS IN THE $\alpha\beta$ T CELL LINEAGE Ellis Reinherz (1)

(1) Dana Farber Cancer Institute

Robert J. Mallis 1,2,3, Kristine N. Brazin 3,4, Jonathan S. Duke-Cohan 3,4, Wonmuk Hwang 5,6,7, Jia-huai Wang 1,3,8, Gerhard Wagner 1, Haribabu Arthanari 1,9\*, Matthew J. Lang 10, 11\*, Ellis L. Reinherz 3,4

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- Astronomy, Texas A&M University
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- 8 Department of Pediatrics, Harvard Medical School
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aß T cells are key components of vertebrate adaptive immunity, being responsible for self vs non-self discrimination and essential for protection against a myriad of viruses, other infectious pathogens and cancers. Recent studies reveal that physical bioforces consequent to cell motility and/or cytoskeletal rearrangements play a central role in aß T-lineage cell biology by impacting thymocyte development and repertoire selection as well as antigen recognition and activation of mature T cells. The T cell receptor (TCR) and its early thymic precursor, the preTCR, function as mechanosensors to recognize their ligands, peptides bound to self-MHC molecules (pMHC) on the surface of antigen presenting cells.

Bioforces place piconewton load on single receptor-pMHC bonds to effect structural change and impact cellular fate including peptide discrimination, cellular activation and developmental progress. Force is linked to induction of different receptor conformers associated with energized and non-energized states that drives a digital output. Here we discuss how the convergence of NMR, real-time single molecule optical tweezers and molecular dynamics studies is advancing our understanding of these multi-subunit receptor complexes.

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#### TPS Award Winners & Speakers PROBING SEQUENCE CONSTRAINTS ASSOCIATED WITH THE COTRANSLA-TIONAL FOLDING AND MISFOLDING OF INTEGRAL MEMBRANE PROTEINS Jonathan P. Schlebach (1) (1) Indiana University

Francis J. Roushar, 1 Laura M. Chamness, 1 Charles P. Kuntz, 1 Wesley D. Penn, 1 Bian Li, 2 Hope Woods, 2 Beata Jastrzebska, 3 Jens Meiler 2 1 Department of Chemistry, Indiana University, Bloomington, IN USA 47405 2 Department of Chemistry, Vanderbilt University, Nashville, TN USA 37235 3 Department of Pharmacology, Case Western Reserve University, Cleve-Iand, OH USA 44106

Many integral membrane proteins contain semi-polar transmembrane (TM) domains that are essential for their native structure and function. However, these domains generate topological frustration that potentially compromises cotranslational folding of the nascent chain. This physicochemical conflict between the sequence constraints of folding and function occurs within TM7 of rhodopsin, which contains a functional lysine (K296) along with several other polar residues. We recently found that TM7 fails to achieve its native topology in at least ~30% of nascent rhodopsin molecules. Moreover, we find that the cellular expression of rhodopsin is exquisitely sensitive to the topological energetics of TM7, which suggests the proteostasis network is capable of recognizing and degrading this aberrant topomer. Certain mutations that stabilize the native topology of TM7 improve the efficiency of rhodopsin biosynthesis without compromising its function. This observation implies the cotranslational folding efficiency of rhodopsin may be highly tunable. To gain insights into how the polarity of TM7 may constrain the evolution of rhodopsin, we employed deep mutational scanning to survey the effects of thousands of mutations on the expression of mature rhodopsin at the plasma membrane. Our results reveal that a wide variety of mutations within TM7 are capable of increasing or decreasing rhodopsin levels at the plasma membrane. In contrast to mutations within a hydrophobic TM domain (TM2), we find that most mutagenic effects within TM7 persist in the presence of excess concentrations of rhodopsin's stabilizing retinal cofactor. Together, these findings highlight the evolutionary constraints associated semi-polar TM domains, and suggest new ways in which they may shape the evolutionary trajectories of integral membrane proteins.

#### PROTEINS AT THE CENTRE OF NEURODEGENERATION IN ALZHEIMER'S DISEASE Louise Serpell (1)

(1) Sussex Neuroscience, School of Life Sciences, University of Sussex

Protein misfolding is central to many diseases including Alzheimer's disease. However, the mechanism by which conformational change is initiated remains elusive. Alzheimer's disease is characterised by key proteins including Tau, Amyloid-beta and by the risk factor isoform Apolipoprotein E4. However, the role of each of these in the neurodegenerative disease cascade is unclear. Our work aims to explore the initiation events that lead to misfolding and the downstream effects on neuronal function, whilst clarifying the potentially toxic species. In this talk, I will describe work that aims to uncover fundamental mechanisms at the heart of the structural changes in Amyloid-beta, tau and ApoE4.

ApoE is the major genetic risk factor for developing AD. Despite decades of research, the way in which ApoE exerts its effect remains elusive. We have recently compared and characterised the three isoforms of ApoE and show that ApoE4 is able to self-assemble into non-amyloid-like filaments. Tau is a natively unfolded protein which, unlike Amyloid-beta, does not readily self-assemble. We have developed a model fragment which self-assembles to form paired helical filaments in vitro which we have used to examine cellular mechanisms of transmission and toxicity. Amyloid beta rapidly self-assembles and oligomeric species have been previously shown to affect neuronal health. We have studied the uptake and effects on organelles including lysosomes, synaptic vesicles and mitochondria to dissect mechanisms that lead to neuronal dysfunction and cell death. We reveal damage to specific organelles of the cell which are accompanied by impaired synaptic vesicle release and reuptake. We consider the underlying mechanisms that may consolidate these findings.

This work has involved significant contributions from Karen Marshall, Mahmoud Bukar Maina, Youssra Al-Hilaly, Saskia Pollack, Luca Biasetti, Kevin Staras.

#### HOW DO MEMBRANE PROTEIN EXTRACELLULAR DOMAINS REGULATE INTRA-CELLULAR CATALYTIC FUNCTION? Adam Smith (1)

(1) University of Akron

Receptor tyrosine kinases (RTKs) are transmembrane proteins that regulate cell growth, proliferation, and differentiation. Aberrant RTK signaling is at the heart of many diseases connected to development and growth. Lateral contacts between RTK extracellular domains have a direct effect on their phosphorylation state and enzymatic activity. This spatial regu-

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lation is linked to cellular function, but it is challenging to resolve in the complex environment of the plasma membrane. In my lab we develop fluorescence assays to measure membrane protein interactions in situ. Pulsed interleaved excitation fluorescence cross-correlation spectroscopy (PIE-FCCS) has been especially powerful because it is sensitive to protein mobility, concentration, and monomer/dimer/oligomer distributions. In this talk, I will describe ongoing work in my group to investigate the spatial regulation of two RTKS, EGFR and EphA2.

#### EXPLORING THE DETERMINANTS OF PROTEIN CROWDING EFFECTS BY MO-LECULAR SIMULATION Rebecca C. Wade (1), (2)

(1) Molecular and Cellular Modeling Group, Heidelberg Institute for Theo-

retical Studies (HITS), Schloss-Wolfsbrunnenweg (2) Zentrum für Molekulare Biologie (ZMBH), DKFZ-ZMBH Alliance and Interdisciplinary Center for Scientific Computing (IWR)

Cellular environments are highly crowded by a heterogeneous mixture of diverse macromolecules and small molecules and they are confined by membranes and structural proteins. To understand the effects of macro-molecular crowding, we focus on the simulation of highly concentrated protein solutions. The oligomerization properties of such protein solutions are important for the formulation of protein therapeutics. Concentrated protein solutions also provide model systems for understanding cellular crowding. I will describe the application of Brownian dynamics and molecular dynamics simulation methods to investigate the effects of protein crowding on protein diffusion and protein-protein interactions, on protein-surface interactions, and on the diffusion of enzyme substrates and drug molecules.

# THE DIVISION OF AMYLOID FIBRILS – STABILITY, TOXICITY AND INFECTIOUS POTENTIAL

Wei-Feng Xue (1) (1) University of Kent

The division of amyloid protein fibrils is required for the propagation of the amyloid state, and is an important contributor to their stability, pathogenicity and normal function. Here, I will present our recent experimental and theoretical work on the division of amyloid fibrils and biological impact of their size distributions. Our new theoretical results show that the division of any type of

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filament is uniquely described by a set of three characteristic properties, resulting in self-similar length distributions distinct to each fibril type and conditions applied. By applying these results to profile the dynamical stability towards breakage for different amyloid types, we reveal particular differences in the division properties of disease- and non- disease related amyloid, the former showing lowered intrinsic stability towards breakage and increased likelihood of shedding smaller particles. Our results enable the comparison of protein filaments' intrinsic dynamic stabilities, which are key to unravelling their toxic and infectious potentials.

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#### THE STABILITY OF MECHANOSENSING FORCE-TRANSMISSION SUPRAMOLEC-ULAR LINKAGES

#### Jie Yan (1), (2)

Mechanobiology Institute, National University of Singapore
 Department of Physics, Faculty of Science, National University of Singapore

The task of mechanosensing of cells involves dynamic assembly of various supramolecular force-transmission linkages, which allow the cells to properly sense and respond to the level of mechanical force in the linkages. While sufficient mechanical stability is a necessity for the mechanosensing function of the force-transmission linkages, the mechanical stability for most crucial force-transmission linkages remains poorly understood. As a force-transmission linkage typically consists of a few non-covalently linked proteins, we reason that the stability of the force-bearing interfaces between neighboring proteins in a force-transmission linkage is the most critical determinant of the linkage mechanical stability. In this talk, I will introduce a novel single-molecular interfaces, and its applications to the investigation of several inter-molecular interfaces that play crucial mechanosensing functions at cell-matrix and cell-cell adhesion sites.

# Posters

#### BOD = Board Number

#### ABS002/BOD70

#### Structural and Biophysical characterization of Acyl-Co-A binding proteins of Leishmania major Shalini Verma, 1,

(1) National Institute of Immunology

#### ABS004/BOD6

- Fast pressure jump all-atom simulations and experiments reveal site-specific protein dehydration-folding dynamics Taras Pogorelov, 1, Maxim Prigozhin, Yi Zhang, Klaus Schulten,
- Martin Gruebele (1) University of Illinois at Urbana-Champaign

#### ABS008/BOD1

- Transthyretin Disassembly Mechanism and Metal-Induced Oxidation Degradation Pathway Studied via Native Mass Spectrometry and Surface-Induced Dissociation Mehdi Shirzadeh.1
- (1) Texas A&M University

#### ABS009/BOD9

- Unlocking the mechanism of HIV-1 viral assembly nucleation with native mass spectrometry
- Samantha Sarni, 1, Erik Olson, Shuohui Liu, Karin Musier-Forsyth, Vicki Wysocki
- Ohio State Biochemistry Program, The Ohio State University

#### ABS010/BOD145

(1)

Structural and Functional Analysis of Neuroserpin Cysteine Mutants Suggests Functional Role of F helix for Polymerization and Inhibition Mechanism Shoyab Ansari, 1

(1) Jamia Millia Islamia University, New Delhi, INDIA

#### ABS011/BOD34

#### Rotenone Interactions Remodel Protein in-to Cytotoxic Conformers

Shweta Devi, 1, Tulika Srivastava, Minal Chaturvedi, Smriti Priya
 Academy of Scientific & Innovative Research (AcSIR), India

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#### ABS013/BOD72

### Snapshots of irreversible FGFR1 inhibition

- Maria Kalyukina, 1, Yuliana Yosaatmadja, Adam Patterson, Jeff Smaill, Christopher Squire
- (1) School of Biological Science, The University of Auckland; Maurice Wilkins Centre for Molecular Biodiscovery

#### ABS014/BOD74

#### Structure of the Influenza B Virus M2 Proton Channel in Lipid Bilayers From Solid-State NMR Venkata S. Mandala, 1, Martin D. Gelenter, Shu-Yu Liao, Alex R. Loftis, Alexander A. Shcherbakov, Bradley L. Pentelute,

- Mei Hong (1) Massachusetts Institute of Technology

### ABS015/BOD26

Uncovering the important enzymes involved in the biosynthetic pathway of bioactive polyacetylenes in Bidens pilosa using integrative omics approaches

- Lie-Fen Shyur, 1, Hieng-Ming Ting, Hsiao-Hang Chung, Wei-Hsi Wang, Ya-Ting Chao, Yi-Chang Sung, Shih-Shun Lin
- (1) Agricultural Biotechnology Research Center, Academia Sinica

#### ABS016/BOD37

(1)

(1)

Kinetic Trapping and Robustness in Proteasome Assembly

Anupama Kante, 1, Pushpa Itagi, Eric Deeds University of Kansas

#### ABS017/BOD32

Oscillatory Mechanism of a Circadian Clock System

- Andy LiWang, 1, Archana Chavan, Joel Heisler
- 1) University of California, Merced

#### ABS018/BOD68

NSF-mediated disassembly of on- and off pathway SNARE complexes and inhibition by complexin

- Ucheor Choi, 1, Minglei Zhao, Ian White, Axel Brunger Stanford University
- . ,

### ABS019/BOD3

### A Novel Amyloid Fibril Structure Formed by the Peptide Hormone Glucagon

Martin Gelenter, 1, Katelyn Smith, Shu-Yu Liao, Venkata Mandala, Aurelio Dregni, Matthew Lamm, Yu Tian, Wei Xu, Darrin Pochan, Thomas Tucker, Yongchao Su, Mei Hong

(1) Massachusetts Institute of Technology

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#### ABS020/BOD21

# Native-state prolyl isomerization is involved in the activation of a CNG channel

Philipp Schmidpeter,1, Crina Nimigean

(1) Weill Cornell Medicine

#### ABS021/BOD108

- Identification of Novel Small Molecule Ras Modulators: A New Path in Cancer Drug Discovery
- Patrick DePaolo, 1, Michael Sabio, William Windsor, Peter Tolias
- Stevens Institute of Technology

#### ABS022BOD69

### Micro-second X-ray Single Molecule Dynamics of Functional Proteins using SR and Lab X-ray Source

Yuji Sasaki, 1, Masahiro Kuramochi, Masaki Ishihara, Shoko Fujimura, Kazuhiro Mio The University of Tokyo

### ABS023/BOD107

(1)

#### Transient splitting of Hsp104 hexameric ring and its implication in protein disaggregation

Masafumi Yohda,1, Yosuke Inoue, Yuya Hanazono, Kentaro Noi, Akihiro Kawamoto, Kazuki Takeda, Keiichi Noguchi, Keiichi Namba, Teru Ogura, Kunio Miki, Kyosuke Shinohara

(1) Tokyo University of Agriculture & Technology

#### ABS024/BOD69

### Structure, Mechanism, and Functional Relevance of Filament Formation by a Non-Cytoskeletal Enzyme

- N.C. Horton, 1, Smarajit Polley, Dmitry Lyumkis
- (1) University of Arizona

#### ABS025/BOD115

Advanced clustering, machine learning and conformational
change: new methods and some applications
Freddie Salsbury,1, Ryan Melvin, Jiajie Xiao

(1) Wake Forest University

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#### ABS026/BOD51

- Spontaneous isomerization in long-lived proteins is the key to understanding why Alzheimer's disease could be a lysosomal storage disorder Ryan Julian,1
- (1) UC Riverside

#### ABS027/BOD50

### An Analytical Revolution: Introducing the Next Generation Optima AUC

Chad Schwartz, 1 ) Ex Beckman Coulter Employee

### ABS028/BOD94

#### High throughput glycan profiling for improved quality control of therapeutic glycoproteins

- Baolin Zhang, 1, Lei Zhang, Shen Luo
- (1) Food and Drug Administration

#### ABS029/BOD23

A Comprehensive Study on a Monotopic Membrane Protein (S)-Mandelate Dehydrogenase and its Chimeras Narayanasami Sukumar, 1, Bharati Mitra, Sahana Sukumar, Scott Mathews Cornell University

#### AB\$030/BOD107

(1)

#### Genetically Encoded Photocaged Quinone Methide for Photo-controlled Chemical Crosslinking Jun Liu, 1, Shanshan Li, Nayyar A. Aslam, Feng Zheng, Bing Yang, Rujin Cheng, Nanxi Wang, Sharon Rozovsky, Peng G. Wang, Qian Wang, Lei Wang

(1) University of California, San Francisco

#### ABS031/BOD70

- Protein Synthesis Studies on Single Molecule Level
  - Joerg Fitter, 1, Henning Hoefig, Alexandros Katranidis
- (1) Research Centre Juelich

### ABS032/BOD121

(1)

QTY Designed Heat Resistant Soluble Transmembrane Proteins Receptor with Tunable Ligand Affinity Rui Qing, 1, Qiuyi Han, Myriam Badr, Haeyoon Chung, Michael Skuhersky, Thomas Schubert, Shuguang Zhang Massachusetts Institute of Technology

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#### ABS033/BOD66

#### Molecular Origin of Disease Mutations in cAMP-Dependent Protein Kinase A

- Amy Chau, 1, Yuxin Hao, Clare Canavan, Susan Taylor, Rodrigo Maillard
- (1) Department of Chemistry, Georgetown University

#### ABS034/BOD17

#### Recruitment of Amyloid-B Oligomers by the Prion Protein

- Priyanka Madhu, 1, Samrat Mukhopadhyay
   Indian Institute of Science Education and Research, Mohali

#### ABS035/BOD38

Targeting FtsZ along with LamA is an effective Antibacterial Strategy against Mycobacterium Species Rishu Tiwari, 1, Dulal Panda

- Indian Institute Of Technology Bombay
- (-)

### ABS036/BOD143

- Intersubunit interactions involving a large surface loop shape the catalytic properties and stability of an alkaline phosphatase Jens Hjörleifsson, 1, Elena Papaleo, Bjarni Ásgeirsson
- (1) Science Institute University of Iceland

#### ABS037/BOD25

#### Elucidating Relayed Proton Transfer Through a His-Trp-His Triad of a Transmembrane Proton Channel by Solid-State NMR Byungsu Kwon, 1, Matthias Roos, Venkata Mandala,

- Alexander Shcherbakov
- (1) MIT

#### ABS038/BOD36

#### The Critical Role of Tyrosine Kinase Sequence Specificity in T Cell Activation

- Neel Shah, 1, Wan-Lin Lo, Arthur Weiss, John Kuriyan
- (1) Columbia University, Department of Chemistry

#### ABS039/BOD52

#### Emerging Roles for the Actin Binding Protein Palladin in Regulation of Highly Motile Cells Moriah Beck, 1, Ritu Gurung, Sharifah Albariki, Aaron Dhanda,

- Carol Otey, Wayne Vogl, Julian Guttman
- (1) Wichita State University

#### ABS040/BOD10

#### Real-Time Monitoring of a-Synuclein-Induced Cell Membrane Disruption in Parkinson's Disease Jacob Parres-Gold, 1, Stephanie Wong Su, Andy Chieng,

Yixian Wang

(1) California State University, Los Angeles

#### ABS041/BOD5

#### Rutin Interacts Weakly with a-Synuclein and Suppresses its Aggregation by Modulating its Fibrillation Pathway Geetika Verma, 1, Rajiv Bhat

1) Jawaharlal Nehru University

#### ABS042/BOD108

#### Generation of Recombinant Ligand-Binding Fragments of Low-Density Lipoprotein Receptor-Related Protein 1 Using Co-Expression with its Chaperone Receptor-Associated Protein Ekaterina Marakasova, 1, Gabriela Uceda-Cortez, Svetlana Shestopal, Timothy K Lee, Andrey Sarafanov

 Division of Plasma Protein Therapeutics; Office of Tissues and Advanced Therapies; Center for Biologics Evaluation and Research; U. S. Food and Drug Administration

#### ABS043/BOD124

#### Construction of Protein Supramolecules Based on Domain-Swapping Mechanism

Masaru Yamanaka, 1, Satoshi Nagao, Chunguang Ren, Mohan Zhang, Akiya Oda, Yoshiki Higuchi

 Graduate School of Science and Technology Division of Materials Science, Nara Institute of Science and Technology

### ABS044/BOD11

(1)

#### Molecular Mechanisms of Peptide Self-Assembly in Hydrogel Formation

Gabriel Braun, 1, Sara Linse, Karin Åkerfeldt, Department of Chemistry, Haverford College

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#### ABS045/BOD63

- UniProt: A universal hub of protein knowledge
- Alex Bateman, 1,
- (1) EMBL-EBI

#### ABS046/BOD64

- **Evolutionary Analysis of Rossmann-like Fold Proteins**
- Kirill Medvedev, 1, Lisa Kinch, Nick Grishin, Department of Biophysics, University of Texas Southwestern
- Medical Center, Dallas, Texas, United States of America

#### ABS047/BOD76

- Cryo-EM structure of the apo form of human PRMT5:MEP50 complex
- Wei Zhou, 1, Gaya Yadav, Qiu-Xing Jiang, Chenglong Li, Department of Biochemistry and Molecular Biology, College of
- (1) Medicine, University of Florida, USA

### ABS048/BOD116

Optimized Molecular Dynamics Force Field Reveals Atomistic Pathways of Spontaneous Disorder-to-Order Peptide-Protein Binding

Lei Yu,1, Da-Wei Li, Rafael Brüschweiler,

Department of Chemistry and Biochemistry, The Ohio State University

#### ABS049/BOD41

- Effect of Ethanol and Protein Content on the Gelation of Almond, Lentil , and Pea Proteins
- Nahla kreidly, 1, Graciela Padua, Hakime Yavuz,
- (1) University of illinois at urbana champaign

#### ABS051/BOD67

#### **Bioinformatics for Sperm Capacitation**

Nailis Syifa', 1, Jiahn-Haur Liao, Tzu-Hua Wu\*,

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Taipei Medical University
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#### AB\$052/BOD145

#### Functional Analysis of Thermostable PQQ-Dependent Glucose Dehydrogenase

Tsutomu Mikawa, 1, Ako Kagawa, Kayo Kitaura, Takanori Kigawa, **RIKEN** Center for Biosystems Dynamics Research

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### ABS053/BOD7

#### Tandem Domain Swapping and the Link to Protein Aggregation Aleix Lafita, 1, Pengfei Tian, Robert Best, Alex Bateman,

European Bioinformatics Institute EMBL-EBI, Wellcome Genome Campus, Hinxton, Cambridge, UK

### ABS054/BOD79

Two-Step BAK Activation Initiates Mitochondrial Apoptosis Geetika Singh, 1, Siva Vaithiyalingam, Jaeki Min, Brett Waddell, Cristina Guibao, Dan McNamara, Zoran Rankovic, Seetharaman Jayaraman,

St. Jude Children's Research Hospital (1)

#### ABS055/BOD43

Binding and Molecular Dynamics Simulation Studies of Bryostatin 1 and Munc13-1 C1 Domain Interaction in the Presence of Phospholipid

Youngki You, 1, Francisco Blanco, Agnes Czikora, Noemi Kedei, Peter Blumberg, Joydip Das,

(1) College of Pharmacy, University of Houston

#### ABS056/BOD122

Observations of an Unfolding Intermediate during the Thermal Unfolding of the Proteinase K like Serine Proteinase VPR Kristinn Ragnar Óskarsson, 1, Magnús Már Kristjánsson,

(1) University of Iceland

#### ABS057/BOD8

#### Characterization and Inhibition of Insulin Amyloid Formation at Physiological pH

Sinem Apaydin, 1, Chris D. Tran, Anne Kokel, Béla Török, Marianna Török,

University of Massachusetts Boston, College of Science and (1) Mathematics, Department of Chemistry and Integrative Biosciences (IB) Program

#### ABS059/BOD47

Expression and characterization of a lipid peroxidase from Nitrosomonas europeae structurally related to prostaglandin H2 synthase

Alecia Cunniff, 1, Rebecca Skaf, Virginia Butchy, Villanova University

(1)



#### Mapping Structure and Interaction in Beta Turns

Nicholas Newell, 1,

(1)Newell

### ABS061/BOD87

#### NorthEastern Collaborative Access Team (NE-CAT) Crystallography Beam Lines for Challenging Structural Biology Research

Igor Kourinov, 1, Malcolm Capel, Surajit Banerjee, Ed Lynch, Frank Murphy, David Neau, Kay Perry, Kanagalaghatta Rajashankar, Cynthia Salbego, Jonathan Schuermann, Narayanasami Sukumar, James Withrow, Steven E Ealick, Cornell University

### ABS062/BOD6

(1)

Kinetic Barriers to Protein Self-Assembly In Vivo Randal Halfmann, 1, Tejbir Kandola, Shriram Venkatesan,

- Jianzheng Wang, Alejandro Rodriguez Gama,
- Stowers Institute for Medical Research (1)

#### ABS063/BOD138

Investigation of structural factors controlling loop dynamics in acyl protein thioesterases

R. Jeremy Johnson, 1, Asif Hossain, (1) **Butler University** 

#### ABS064/BOD110

Distinct chaperone activities in nascent protein folding

Christian Kaiser, 1, Kaixian Liu, Kevin Maciuba, Johns Hopkins University

#### ABS065/BOD73

(1)

Inner workings of a COMPASS: Crystal structure of the COMPASS H3K4 methyltransferase catalytic module Peter Hsu, 1, Heng Li, Ho-Tak Lau, Calvin Leonen, Abhinav Dhall,

Shao-en Ong, Champak Chatterjee, Ning Zheng,

(1) University of Washington

#### ABS066/BOD56

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	Vasoinhibin Inhibits Thrombin-Induced Angiogenesis,
	Vasopermeability, Platelet Aggregation, and Cancer Invasion
	Juan Pablo Robles, 1, Magdalena Zamora,
	Gonzalo Martínez de la Escalera, Carmen Clapp,
1)	Instituto de Neurobiología, UNAM (Universidad Nacional

(1) Autónoma de México)

#### ABS067/BOD140

Structural and Dynamic Mechanisms by which 1918 Spanish Flu Virus Antagonizes Host Antiviral Immune Responses Qingliang Shen, 1, Baoyu Zhao, Nowlan Savage, James Byrnes, Lin Yang, Pingwei Li,

(1) Department of Biochemistry and Biophysics, Texas A&M University

#### ABS068/BOD42

#### Physiologically-relevant crowding effects on the SH3-Son of Sevenless interaction

Samantha Stadmiller, 1, Jhoan Sebastian Aguilar, Gary Pielak, University of North Carolina at Chapel Hill Chemistry Department

### ABS069/BOD60

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(1)

The Role of KLHDC2 in Recognizing Diglycine C-end Degron and its Therapeutic Potential Domnita Valeria Rusnac, 1, Daniele Canzani, Hsiu-Chuan Lin, Karena Tien, Thomas R. Hinds, Ashley F. Tsue, Hsueh-Chi S. Yen, Matthew F. Bush, Jie Fan, Ning Zheng, University of Washington

#### ABS070/BOD95

Translesion Synthesis Pathway as Target for Anti-Cancer Drug Desian Dmitry Korzhnev, 1,

- (1) Department of Molecular Biology & Biophysics, University of Connecticut Health Center

#### ABS071/BOD40

Inhibition of transcriptional activator-coactivator protein-protein interactions with natural products Meghan Breen, 1, Stephen Joy, Matthew Beyersdorf, Matthew Henley, Samantha De Salle, Anna Mapp,

(1) University of Michigan

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### ABS072/BOD134

#### Harnessing new and emerging computational technologies to advance design of folding protein-like heteropolymers Vikram Mulligan, 1,

1) Center for Computational Biology, Flatiron Institute

#### ABS073/BOD1

#### Influence of Porous Materials on Amyloid-Beta Protein Aggregation

Michael Lucas, 1, Benjamin Keitz,

(1) University of Texas at Austin

#### ABS074/BOD91

#### The chaperonin TRIC/CCT associates with Prefoldin through a conserved electrostatic interface essential for cellular proteostasis

Daniel Gestaut, 1, Soung Hun Roh, Boxue Ma, Grigore Pintile, Lukasz Joachimiak, Alexander Leitner, Thomas Walzotheini, Ruedi Aebersold, Wah Chiu, Judith Frydman, Stanford University

(1)

(1)

#### ABS075/BOD123 Engineering halogen bonds to affect protein stability, activity, and recognition

P. Shing Ho, 1, Rhianon Kay Hartje, Anna-Carin Carlsson,
 Colorado State University

- ABS076/BOD88 Structural and Mechanistic Studies of the Immune Response to the Blood Coagulation Factor VIII C1 Domain Shaun Peters,1, Steven Reese, Cris Mitchell, Joseph Gish,
  - Western Washington University

#### ABS077/BOD96

Coupling of Stability and Self-Association of a Therapeutic Protein Natalia Markova, 1, Matthew McGann, Erik Noprdling, Vilhelm Ek,

Sergi Kuprin, (1) Malvern Panalytical

### ABS078/BOD2

The Structure of alpha-synuclein secondary nuclei is dominated by the solution conditions rather than the seed fibril strain Alessia Peduzzo, 1, Sara Linse, Alexander Büll,

(1) Institute of Physical Biology, Heinrich Heine Universität Düsseldorf

#### ABS079/BOD52

Conformational changes responsible for activation of parkin, an E3 ubiquitin ligase involved in Parkinson's disease Kalle Gehring, 1,

McGill University

#### ABS080/BOD55

(1)

**Cellular signaling through cysteine phosphorylation** Kalle Gehring, 1,

1) McGill University

#### ABS081/BOD123

#### De Novo Design of Bioactive Protein Switches

Robert Langan, 1, Scott Boyken, Andrew Ng, Jennifer Samson, Galen Dods, Taylor Nguyen, Alexandra Westbrook, Marc Lajoie, Zibo Chen, Stephanie Berger, Vikram Mulligan, John Dueber, Walter Novak, Hana El-Samad, David Baker,

(1) University of Washington

#### ABS082/BOD45

Wanted: Small molecules to inhibit PNT domain-mediated polymerization of ETV6 chimeric oncoproteins Chloe Gerak, 1, Sophia Cho, Mark Okon, Richard Sessions, Michel Roberge, Lawrence McIntosh,

(1) University of British Columbia

#### ABS083/BOD30

Modulation of ligand and receptor state in DDR-collagen interactions

(1) Gunjan Agarwal, 1, Ohio State University

#### ABS084/BOD126

Elucidating a code for RNA sequence recognition Wei Zhou, 1, Daniel Melamed,

(1) University of Washington

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### Activation dynamics of USP7 deubiquitinase

- Irina Bezsonova, 1, Gabrielle Valles, Dmitry Korzhnev,
- (1) UCONN Health

#### ABS086/BOD46

- Select Ionic Residues in the C-terminal Domain of Human Apolipoprotein A-I Regulate Self-association John Burdick,1, Rohin Basi, Kaitlyn Burns, Paul Weers,
- (1) California State University Long Beach

### ABS087/BOD20

- Structure meets function: agonist action at AChR neurotransmitter binding sites (structural correlates of affinity, efficacy, and efficiency) Sushree Tripathy, 1, Wenjun Zheng, Anthony Auerbach,
- State University of New York at Buffalo
- ABS088/BOD126

(1)

- Computational Design and Functionalization of Porous Proteins Chunfu Xu, 1, Peilong Lu, Tamer Gamal El-Din, Xue-Yuan Pei, Matthew Johnson, Atsuko Uyeda, Matt Bick, Michael Luciano, Venu Bandi, Martin Schnermann, Tomoaki Matsuura, Ben Luisi, William Catterall, David Baker,
- (1) University of Washington

#### ABS089/BOD22

### Expression of Band 3, a Membrane Protein

- Chun-Fu Chen, 1, Chia-Rui Shen,
- (1) Ming Chi University of Technology

#### ABS091/BOD67

#### Functional Analysis of ACA – 01, a Novel Chemokine-Binding Tick Evasin

- Sayeeda Chowdhury,1, Ram Bhusal,
- Monash University

#### ABS092/BOD22

#### Discovering Novel Antibodies Against Peptidisc Stabilized Membrane Proteins

- James Saville, 1, Franck Duong, Katherine Zhao,
- (1) University of British Columbia



### ABS093/BOD48

	Coincidence Maps of Proteolytic Cleavage, Secondary
	Structure, and Exon Origins for the Soluble Human Protein Hormone Proteome: Functional Associations?
	Kenneth L Campbell, 1, Nurit Haspel, Naomi Stuffers,
(1)	Univ. of Mass. Boston

### ABS094/BOD127

#### De novo design of self-assembling helical protein filaments Hao Shen.1.

(1) Institute for Protein Design, University of Washington

#### ABS095/BOD92

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(1)

Distinct pathways of activation of human small heat shock protein HSPB5 by different stress factors Maria Janowska, 1, Rachel Klevit,

University of Washington

#### ABS097/BOD48

Determining the Mechanism of Action of the Antibiotic Argyrin B Chris Swanson, 1, Riley Roberts, Jessica Mantchev, Catie Shelton, Justin Walter, Bassam Haddad, P. Clint Spiegel, Western Washington University

### ABS098/BOD33

- A Molecular View of the Liquid to Gel Phase Transition of Heterochromatin Protein HP1a Bryce Ackermann,1,
- University of California, San Diego

### ABS099/BOD35

Impact of Oxidative Stress on the Structural Conformation and Chemical Integrity of Soluble CLIC1 Olga Faerch, 1, Stoyan Stoychev, Heini Dirr,

(1) PSFRU, School of Molecular and Cell Biology, Faculty of Science, University of the Witwatersrand, Johannesburg

#### ABS100/BOD36

Structural Basis for -35 Element Recognition by Sigma 4-Chimera Proteins and Their Interactions with PmrA Response Regulator Chinpan Chen, 1, Yuan-Chao Lou,

(1) Institute of Biomedical Sciences, Academia Sinica

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### ABS102/BOD29

### Novel hevein-like defense peptides from wild cereals

Eugene Rogozhin, 1, Dmitry Ryazantsev, Sergey Zavriev, Shemyakin And Ovchinnikov Institute Of Bioorganic Chemistry

Russian Academy Of Sciences

### ABS104/BOD49

(1)

The Structure of the interleukin 11 signalling complex Riley D. Metcalfe, I, Kahenia Aizel, Courtney O. Zlatic, Paul M. Nguyen, Paul R. Gooley, Tracy L. Putoczki, Michael D.W. Griffin,

- Department of Biochemistry and Molecular Biology, Bio2 (1)Molecular Science and Biotechnology Institute, University of
  - Melbourne, Parkville, Victoria 3010, Australia

### AB\$105/BOD130

### Directed Evolution of sensor proteins for GPCR signaling mechanisms

Andre Berndt.1.

(1) University of Washington

#### ABS106/BOD75

#### Cryo-EM of the malaria parasite PA28/20S proteasome complex reveals an unusual activation mechanism with implications for artemisinin sensitivity

Stanley Xie, 1, Riley Metcalfe, Eric Hanssen, Tuo Yang, David Gilley, Andrew Leis, Craig Morton, Michael Kuiper, Michael Parker, Natalie Spillman, Wilson Wong, Christopher Tsu, Lawrence Dick, Leann Tilley,

(1) University of Melbourne

#### ABS107/BOD130

#### Testing Protein Design in Massive Throughput Using High-Density Peptide Arrays

Oana-Nicoleta Antonescu, 1, Kristoffer Enøe Johansson, Jakob Rahr Winther,

Linderstrøm-Lang Centre for Protein Science, University of (1) Copenhagen

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#### ABS108/BOD39

The Interaction of IAA-94 with the Soluble Conformation of the CLIC1 Protein and its Structural Homolog hGSTP1-1 Roland Worth, 1, Heinrich Dirr,

University of the Witwatersrand

### ABS109/BOD93

Microfluidic methods reveal the thermodynamics of chaperone binding

University of Cambridge

#### ABS110/BOD109

Discovery and Characterization of Small Molecule Inhibitors of
the Bromodomain Containing Proteins BRD9 and BRD7—the
Targetable Subunits of SWI/SNF Chromatin Remodeling
Complexes

Rezaul Karim, 1, Alice Chan, Ernst Sch?nbrunn, USF Health Morsani College of Medicine, University of South (1) Florida; Department of Drug Discovery, Moffitt Cancer Center

#### AB\$111/BOD43

Calcium Binding Proteins and the Regulation of the Visual Sensory System: from Molecules to Networks Daniele Dell'Orco,1,

University of Verona

#### ABS112/BOD25

Is Wza the Only Bacterial Outer-Membrane Protein with Helical Transmembrane Segments?

- Sajith Jayasinghe, 1, Simon Keng, Ekta Priyam,
- California State University San Marcos

#### ABS113/BOD97

The Use of small-angle scattering for studying excipient modulated physical stability and viscosity of monoclonal antibody formulations

Joseph Curtis, 1, Amy Xu, Monica Castellanos, Kevin Mattison,

(1) NIST

#### ABS114/BOD90

Taking a Magic Leap into Augmented Reality Protein Structure Visualization

- Sajith Jayasinghe, 1, Byron Dehlavi, Lei Tang, (1)
  - California State University San Marcos

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Therese Herling, 1, Anais Cassaignau, John Christodoulou, Tuomas Knowles



#### ABS115/BOD64

#### Evaluating the Molecular Function Families of Phosducins Using Multi-iterative Sequence Searching Technique Sarah Hosler, 1, Jacquelyn Fetrow,

Albright College

#### ABS116/BOD146

(1)

A Novel and Promising Multi-Enzyme Co-Embedded Organic–In organic Hybrid Nanoflower with Enhanced Stability and Catalytic Activity

Duygu Aydemir, 1, Firdevs Gecili , Nalan Ozdemir, Nuriye Nuray Ulusu,

(1) Koc University School of Medicine Department of Medical Biochemistry

#### ABS117/BOD51

Comparison of Calorimetry Measurements of Binding of a Streptomyces Trypsin Inhibitor to the Thermostable Subtilase Aqualysin I and its Cold Adapted Homologue, VPR Sveinn Bjarnason, 1, Kristinn Ragnar Óskarsson,

Magnús Már Kristjánsson,

(1) University of Iceland

#### ABS118/BOD90

Structure of a complete talin head module in complex with integrin beta3 tail reveals new insights into domain configuration and specific interaction Jinhua Wu,1, Yijuan Sun,

Fox Chase Cancer Center

#### ABS119/BOD47

#### A Human Acidic Fibroblast Variant with Increased Stability and Enhanced Cell Proliferation Activity

- Chynna Denham, 1, Shilpi Agrawal, T.K.S. Kumar,
- (1) University of Arkansas

#### ABS120/BOD66

#### Properties for predicting protein function

- Caitlyn L. Mills, 1, Lydia A. Ruffner, Penny J. Beuning,
- (1) Northeastern University

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#### AB\$122/BOD118

Network-Level Analysis of Molecular Dynamics Simulations Reveals Allosteric Properties of Calcium Sensor proteins Valerio Marino, 1, Daniele Dell'Orco,

(1) University of Verona

#### AB\$124/BOD148

A Single Mutation Asp98Ser, which Improves the Catalytic Properties of the Thermostable Subtilase Aqualysin I, Increases Flexibility at its Active Site Arnor Saevarsson, 1, Brynjar Ellertsson,

(1) University of Iceland

#### AB\$125/BOD40

Generation of 13 full length proteins of the cGAS-STING Pathway for drug tractability assessment Yong Jiang, 1,

(1) GSK

#### ABS126/BOD46

Bid as a novel interacting partner of IRE1: A differential modulator determining diverse outputs of its RNAse activity Samirul Bashir, 1, Maryam Banday, Ozaira Qadri, Arif Bashir, Nazia Hilal,

Department of Blotechnology, University of Kashmir

#### AB\$127/BOD132

#### A Generative Algorithm For Proteins From The Ntf2-Like Superfamily

Benjamin Basanta, 1, Mathew Bick, Ted Baughman, Philip Leung, Eric Nalefski, David Baker,

(1) Institute for Protein Design

#### ABS128/BOD118

Influence of pulling geometry on mechanical stability of protein-peptide complexes

Maksim Kouza, 1, Andrzej Kolinski, Irina Buhimschi,

- Andrzej Kloczkowski,
- (1) Nationwide Childrens Hospital

#### AB\$129/BOD72

Crystal structures of the complex of a kallikrein inhibitor from Bauhinia bauhinioides with trypsin and modeling of kallikrein complexes Mi Li.1.

(1) Leidos Biomedical Research, Inc

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#### ABS130/BOD27

### DNA-Corralled nanodiscs for the structural and functional characterization of membrane protein and viral entry

Gerhard Wagner, 1, William Shih, Meng Zhang, Krishna Das,

(1) Harvard Medical School

#### AB\$131/BOD14

- The Structure of Discoidal High-density Lipoprotein Particles Stefan Bibow, 1, Yevhen Polyhach, Cédric Eichmann, Celestine Chi, Henning Stahlberg, Gunnar Jeschke, Roland Riek,
- (1) University of Basel

#### AB\$132/BOD61

5112 isolated from Aquilegia nivalis, provokes dual inhibition of Ire1a and perk arms of Unfolded Protein Response signaling Nazia Hilal, 1, Aarif Bashir, Samirul Bashir,

(1) University of Kashmir

#### AB\$133/BOD49

Measuring the functional effect of amino acid substitutions proteome-wide using mistranslation

Stephanie Zimmerman, 1, Ricard Rodriguez-Mias, Kyle Hess, Judit Villen, Stanley Fields,

(1) University of Washington Department of Genome Sciences

#### ABS134/BOD9

- Dynamics of Amyloid Fibrils Play a Role in Seeding and Propagating the Aggregation of a-Synuclein Jonathan Williams, 1, Xue Yang, Jean Baum,
- (1) Rutgers University

#### ABS135/BOD49

### The mechanism of CaMKII regulation: from fertilization to encoding long-term memory

(1) Margaret Stratton, 1, (1) University of Massachusetts, Amherst

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#### AB\$136/BOD75

#### Visualizing Conformational Changes of the Magnesium Channel CorA using Synthetic Antibodies

Satchal Erramilli, 1, Piotr Tokarz, Kamil Nosol, Przemysław Dutka, Blazej Skrobek, Pawel Dominik, Somnath Mukherjee, Anthony Kossiakoff, The University of Chicago

### ABS137/BOD52

(1)

#### High-throughput identification of dominant negative polypeptides in yeast Michael Dorrity, 1, Michael Dorrity, Christine Queitsch, Stanley Fields,

(1) University of Washington

#### AB\$138/BOD18

EPR reveals different conformations of LcrG
Pallavi Guha Biswas, 1, Pavanjeet Kaur, Andrew McShan,
Kawaljit Kaur, Likai Song, Roberto De Guzman,
University of Kansas

(1) University of Kansas

#### AB\$139/BOD121

### Better together: 20+ years of scientific software development in the Rosetta macromolecular modeling suite

Julia Koehler Leman, 1, Brian Weitzner, Douglas Renfrew, Richard Bonneau.

) Simons Foundation / NYU

#### ABS140/BOD105

#### Mechanical properties of designed protein fibers

- Neville Bethel, 1, Matt Bick, David Baker,
- (1) Institute for Protein Design, University of Washington

#### ABS141/BOD80

#### Biophysical Studies of Minor Translocon IpaC of the Type III Secretion System in Shigella

Amritangshu Chakravarty, 1, Helen Peng,

- Dr Roberto N De Guzman,
- (1) University of Kansas

#### AB\$142/BOD134

Computational Protein Design with Multisite lambda Dynamics Ryan Hayes, 1, Jonah Vilseck, Charles Brooks III,

(1) University of Michigan

Pastens

### ABS143/BOD24

Profiling the E. coli Membrane Interactome Captured in Peptidisc Libraries

Irvinder Wason, 1, Irvinder S. Wason, Greg Stacey, John Young, Michael Carlson, Zhiyu Zhao, David G. Rattray, Nichollas Scott, Craig Kerr, Mohan Babu, Leonard J. Foster, Franck Duong, University of British Columbia

#### ABS144/BOD44

(1)

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- Systems Structural Biology of the Heart: Impact of Lysine Acetylation on Protein Conformations and Interactions Juan Chavez, 1, Matthew Walker, Arianne Caudal, Bo Zhou, Andrew Keller, Rong Tian, James Bruce,
- University of Washington

### ABS145/BOD2

Novel a-sheet secondary structure in amyloid ß-peptide drives aggregation and toxicity in Alzheimer's Disease Valerie Daggett, 1,

(1) University of Washington

#### AB\$146/BOD137

Generation of Polymeric Recombinant Hemoglobin Using PEG-azide Dendrimers and DBCO-modified Hemoglobin Dedeepya Gudipati, 1, Johann Sigurjonsson, Leah Huey, Spencer Anthony-Cahill,

(1) Western Washington University

#### ABS147/BOD4

#### In Search for potential Small Molecule Inhibitors for Super Oxide Dismutase fibril formation

Shashank Deep, 1, Nidhi Bhatia, Priya Modi, Shilpa Sharma,

Indian Institute of Technology Delhi

#### AB\$148/BOD57

(1)

Multidimensional Cross-linking with a Tetra-reactive Cross-linker

Jared Mohr, 1, Juan Chavez, James Bruce,

(1) University of Washington

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#### AB\$149/BOD153

#### Indirect Sexual Selection Drives Rapid Evolution of an Intrinsically Disordered Sperm Protein

- Damien Wilburn, 1, Lisa Tuttle, Rachel Klevit, Willie Swanson,
- University of Washington

### ABS150/BOD19

Structural Basis for Binding of AmotL1 to the WW domain proteins, Yes-associated Protein and Kibra Amber Vogel, 1, Ethiene Kwok, Diego Rodriguez, Afua Nyarko,

Oreaon State University

### AB\$151/BOD77

(1)

Examination of Substrate Binding and Specificity in a PEPX from L. helveticus Deanna Dahlke Ojennus, (1), Nicholas Bratt, Tersa Almaw,

- Kent Jones, Douglas Juers, (1) Whitworth University
- (1) Whitworth University

#### AB\$152/BOD17

Mutual communication between the Kibra WW domains modulates interactions with LATS1

- Kasie Baker, 1, Ethiene Kwok, Diego Rodriguez, Afua Nyarko,
- (1) Oregon State University

#### ABS153/BOD53

#### Evaluating Biophysical Constraints on the Sequence of Rhodopsin by Deep Mutational Scanning Wesley Penn, 1, Andrew McKee, Veronica Nash, Charles Kuntz, Timmothy Gruenhagan, Hope Hicks, Francis Roushar, Mahesh Chandak, Christopher Hemmermich, Douglas Rusch, Jens Meiler,

Jonathan Schlebach,

(1) Indiana University

#### ABS154/BOD62

Rapid Pharmacological Profiling of Genetic Variants by Deep Mutational Scanning

Francis Roushar, 1, Wesley Penn, Jonathan Schlebach, Indiana University

#### ABS155/BOD128

(1)

**Biotin binder design using de novo protein scaffolds** Gyu Rie Lee, 1, Anastassia Vorobieva, Brian Weitzner, Benjamin Basanta, David Baker, University of Washington

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### AB\$156/BOD18

#### An examination of the surface of the intrinsically disordered protein alpha synuclein

María Rocío Rial Hawila, 1, Gabriela Elena Gómez, University of Buenos Aires

### AB\$158/BOD20

(1)

(1)

### Combining smFRET and DEER Distance Measurements to Characterize Disordered Proteins

Tatyana Smirnova,1, Keith Weninger, Hugo Sanabria, North Carolina State University

#### ABS160/BOD54

- Maintenance of Alpha-helices in Non-ideal Dimeric Plasminogen-binding Group A Streptococcal M-proteins Determines Their Tight Bindings to Human Plasminogen Cunjia Qiu, 1, Yue Yuan, Zhong Liang, Shaun Lee, Victoria Ploplis, Francis Castellino, Department of Chemistry and Biochemistry, University of
- (1) Department of Chemistry and Biochemistry, University of Notre Dame

#### ABS162/BOD80

- The Role of Conformational Dynamics in Shear-Enhance FimH-mediated Bacterial Adhesion
  - Pearl Magala, 1, Dagmara Kisiela, Angelo Ramos,
- Wendy Thomas, Evgeni Sokurenko, Rachel Klevit,
- (1) University of Washington

#### ABS163/BOD55

Engaging the Protein Science Community to Expand Protein
Literature Representation and Annotations in UniProt
Cecilia Arighi, 1, Hongzhan Huang, Yongxing Chen,
Qinghua Wang, Peter McGarvey, Cathy Wu, UniProt Consortium,
UniProt Consortium, UniProt Consortium,
Protein Information Resource, University of Delaware

#### AB\$164/BOD100

Discovery of a Novel Small-Molecule Activator that Corrects G6PD Deficiency

Sunhee Hwang,1, Stanford University



### AB\$165/BOD60

#### Molecular Basis for the Evolved Instability of a Human G-Protein Coupled Receptor

Laura Chamness, 1, Charles Kuntz, Wesley Penn, Jens Meiler, Jonathan Schlebach,

(1) Indiana University

#### ABS166/BOD128

#### Programmable Design of Orthogonal Protein Heterodimer Zibo Chen, 1, Scott Boyken, Mengxuan Jia, Florian Busch, David

Flores-Solis, Matthew Bick, Peilong Lu, Zachary VanAernum, Aniruddha Sahasrabuddhe, Robert Langan, Sherry Bermeo, T.J. Brunette, Vikram Mulligan, Vicki Wysocki, Frank DiMaio, David Baker

(1) University of Washington

#### AB\$167/BOD149

	Design of catalytic de novo proteins
	Shane Caldwell, 1, Susana Vazquez Torres, Cathleen Zeymer,
	Ian Haydon, Don Hilvert, David Baker,
(1)	University of Washington

#### AB\$168/BOD15

#### Nanopore-confined lipid bilayers for oriented sample EPR and NMR studies of membrane proteins Sergey Milikisiyants,1, Melanie Chestnut, Morteza Jafarabadi,

Antonin Marek, Maxim Voinov, Alexander Nevzorov, NCSU

(1) NCSU

#### AB\$169/BOD144

High Pressure Optical Spectroscopy (HiPOS) and Real-Time Analysis of Enzymes Kinetics at Elevated Hydrostatic Pressure Gary Smejkal, 1, Alana Murphy, Vera Smejkal, Nicole Cutri, Ed Ting, Alexander Lazarev,

(1) Pressure Biosciences

#### ABS171/BOD136

Design of Novel Lectins by Computer-Aided Directed Evolution Prema Sharma, 1, Ismail C Kazan, Sefika B Ozkan, Giovanna Ghirlanda,

(1) Arizona State University

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#### AB\$172/BOD56

#### Determining the concentration of a recombinant protein in Escherichia coli cells

Shannon Speer, 1, Alex Guseman, Gary Pielak,

Department of Chemistry, University of North Carolina at (1) Chapel Hill

#### ABS173/BOD133

Staphylococcus aureus IsdH: the chemical and dynamic basis of heme extraction from human hemoglobin Ken Ellis-Guardiola, 1, Joseph Clayton, Brendan Mahoney, Clarissa Pham, Sinan Sabuncu, Jeff Wereszczynski, Pierre Moenne-Loccoz, Robert Clubb,

UCLA (1)

#### AB\$174/BOD139

Altered Dynamics of Cataracts-Associated ?S-crystallin Mutants Measured by NMR

Heather Forsythe, 1, Kayla Jara, Calvin Vetter, Patrick Reardon, Elisar Barbar, Kirsten Lampi, Oregon State University

### AB\$175/BOD141

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Force-dependent allosteric enhancement of aE-catenin binding to F-actin by vinculin Nicolas Bax, 1, Derek Huang, Sabine Pokutta, Alexander Dunn, William Weis,

(1) Structural Biology, Stanford University

#### AB\$177/B0D82

The cyclic nucleotide-binding homology domain of the integral membrane protein CNNM mediates dimerization and is required for Mg2+ efflux activity

Yu Seby Chen, 1, Guennadi Kozlov, Rayan Fakih, Yosuke Funato, Hiroaki Miki, Kalle Gehring,

(1) McGill University

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#### ABS179/BOD56

#### Analyzing DIA-only Proteomics Datasets with Deep Neural Network MS2 Modeling Outperforms Sample-specific DDA Libraries

Brian Searle, 1, Tobias Schmidt, Siegfried Gessulat, Bernhard Kuster, Mathias Wilhelm,

Institute for Systems Biology (1)

#### AB\$180/BOD131

Computational design of multipass transmembrane proteins Peilong Lu, 1, Chunfu Xu, Duyoung Min, Frank Dimaio Tamer El-Din, Lance Stewart, Justin Kollman, Tomoaki Matsuura, William A. Catterall, James U. Bowie, David Baker,

University of Washington (1)

#### ABS181/BOD21

Coming Together in the DNA Damage Response: Interactions with the Intrinsically Disordered Region of BRCA1 Christine Hurd, 1, Brian Morote-Costas, Texas Christian University

(1)

(1)

### AB\$182/BOD83

Five reasons to pay attention to CASP-SAXS Susan Tsutakawa, 1, Greg Hura, Andry Kryshtafovych,

- Krzysztof Fidelis, John Tainer,
- Lawrence Berkeley National Laboratory

### AB\$183/BOD115

The Limits of Tethering in Kinase Signaling Reactions Elizabeth Speltz, 1, TJ Brunette, Fabio Parmeggiani, David Baker, Jesse Zalatan,

University of Washington

#### AB\$184/BOD110

Molecular Basis of GPCR Biased Agonist Recognition John McCorvy,1,

Medical College of Wisconsin

#### ABS185/BOD99

Systematic Identification of Recognition Motifs for the Hub Protein LC8

Aidan Estelle, 1, Nathan Jespersen, David Hendrix, Ylva Ivarsson, Norman Davey, Department of Biochemistry and Biophysics, Oregon State

(1) University 115



#### AB\$186/BOD102

#### The Structural and Functional Organization of Ribosomal Compartment in the Cell: The new model with highly ordered network of ribosomes Elizaveta Karpova, 1,

 Department of Chemistry, College of Arts and Sciences, University of Alabama at Birmingham

#### ABS187/BOD53

- Mapping the cellular exchange of Fe-S cluster mediated by NFU1
- Anshika Jain,1, Tracey Rouault, nih
- (.)

### AB\$188/BOD116

Protein shape sculpting using rigid helical junctions

- TJ Brunette, 1, Matthew Bick, Jesse Hansen, David Baker,
- (1) University of Washington

#### ABS189/BOD30

- Ordered 2D multi-component protein materials design: from local molecular interactions to biologically active materials Ariel J Ben-Sasson, 1, Matthew C Johnson, Joseph Watson, Logesh Somasundaram, Hannele Ruohola-Bake, Emmanuel Derivery, David Baker,
- Institute for Protein Design, University of Washington, Seattle, WA, USA

#### ABS190/BOD31

#### Analysis of Computationally Designed Cooperative Protein-Protein Interactions by Native Mass Spectrometry Florian Busch, 1, Zachary VanAerum, Mengxuan Jia, Zibo Chen, David Baker, Vicki Wysocki,

(1) The Ohio State University

### ABS191/BOD32

# Real-time monitoring of clock controlled signal transduction pathway

- Archana G. Chavan, 1, Andy LiWang, Joel Heisler,
- Yonggang Chang,
- University of California, Merced

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#### ABS192/BOD94

# Structural Analysis of DnaJ Protein ERdj6 and Non-Native Proinsulin

- Lindsay Hammack, 1, Mary Clay, Charalampos Kalodimos,
- St. Jude Children's Research Hospital

#### AB\$193/BOD107

- Predicting protein function from experimental and predicted structures using Graph Convolutional Neural Networks Vladimir Gligorijevic, 1, Douglas Renfrew, Richard Bonneau,
- ) Flatiron Institute, Simons Foundation

#### ABS194/BOD98

- Exploring Composition of Peptide Linker to Enhance Stability of Antibody Fragments for Cancer Therapeutics Jeong Min Han, 1, Thomas Magliery,
- (1) Department of Chemistry and Biochemistry, The Ohio State University

#### ABS196/BOD3

The Bacterial Curli Accessory Protein CsgF Influences the Aggregation of Human Islet Amyloid Polypeptide Sajith Jayasinghe, 1, Allison Newel, Ashwag Binmahfooz, California State University San Marcos

#### ABS197/BOD31

#### Comparison of Strategies for the Enrichment of Cross-Linked Peptides

- Andrew Norris, 1, Florian Busch, Vicki Wysocki,
- The Ohio State University

#### ABS198/BOD13

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Computational Study on Aggregation and Disruption of Amyloid Fibrils

Seokmin Shin, 1, Kyunghee Lee, MinJun Lee, Jeseong Yoon, Seoul National University

#### ABS199/BOD16

Mapping accessibility in the bacterial mechanosensitive channel MscS to a small photoreactive probe Gabriela Elena Gómez, 1, Yan Wang, Andriy Anishkin, Sergei Sukharev, University of Rucease Airos

(1) University of Buenos Aires



#### ABS200/BOD149

#### Ionic Strength Modulates Dimerization and Enzyme Activity of a ß-Glycosidase

Felipe Akihiro Otsuka,1, Rafael Chagas, Vitor Almeida, Maiara Frutoso, Sandro Roberto Marana,

(1) University of São Paulo

### ABS201/BOD117

- Design of Light Harvesting Proteins for Photosynthesis Nathan Ennist, 1, Adam Moyer, Derrick Hicks, Chunfu Xu,
- TJ Brunette, David Baker,
- (1) University of Washington

#### ABS202/BOD31

- Thrombin Cleaves Prolactin into Novel Vasoinhibin Isoforms Magdalena Zamora Corona, 1, Juan Pablo Robles, Manuel Benigno Aguilar, Livia Lenke, Thomas Bertsch, Gonzalo Martínez de la Escalera, Jakob Triebel, Carmen Clapp,
- Instituto de Neurobiología, Universidad Nacional Autónoma de México (UNAM)

#### ABS203/BOD151

- Structural and biochemical studies of Mtb L-asparaginase reveal survival mechanism of Mycobacterium tuberculosis inside macrophages Arti Kataria, 1, Bishwajit Kundu,
- (1) Kusuma School of Biological Sciences, IIT D, India

#### ABS204/BOD105

Removal of Zinc Gives Insights into the Effect of this Metal on the Stability and Function of the Zinc-binding Co-chaperone Ydj1 Jemmyson Jesus,1, Annelize Aragão, Marco Arruda, Carlos Ramos,

(1) University of Campinas

#### ABS205/BOD134

Selective Inhibition of Calcineurin Activity in Pathogenic Fungi Ronald Venters,1, Sophie Gobeil, Leonard Spicer, Benjamin Bobay,

(1) Duke University NMR Center

#### ABS206/BOD118

### Tuning Zinc Binding Ability of Calprotectin

Aslin Rodriguez Nassif, 1, Walter Chazin,

Vanderbilt University

#### AB\$207/BOD106

#### Alternative Forms of Energy Modulate Group II Chaperonin Activity

Kevin Goncalves, 1, Tom Lopez, Judith Frydman,

Stanford University

#### ABS208/BOD147

(1)

Molecular mechanism of Ubiquitin E2 enzyme activation in ERAD Tobias Ritterhoff, 1, Christian Lips, Thomas Sommer, Rachel Klevit,

(1) University of Washington

#### ABS209/BOD135

Profiling Latent and Engineerable Allostery in Ion Channels through Systematic Domain Insertion Daniel Schmidt, 1, Willow Coyote-Maestas, David Nedrud, Yungui He, Chad Myers, University of Minnesota

#### ABS210/BOD33

#### Applications Of Ultracentrifugation In Purification And Characterization Of Biomolecules Akash Bhattacharya, 1, Ross Verheul, Eric Von Seggern, Stephen Otts.

(1) Beckman Coulter Life Sciences

#### ABS211/BOD26

Cellular Abundance Measurements of Thousands of Variants of Vitamin K Epoxide Reductase (VKOR) Resolves Topology and Mechanisms of Drug Resistance Melissa Chiasson, 1, Katherine Sitko, Jason Stephany, Allan Rettie, Douglas Fowler,

(1) Department of Genome Sciences, University of Washington

#### ABS212/BOD132

Modular and Expandable Protein-DNA Co-crystal Scaffolds to Assist in X-ray Diffraction of DNA-Binding Macromolecules Abigail Ward, 1, Christopher Snow,

(1) Colorado State University



#### ABS213/BOD4

#### Amyloid Formation by the RNA Recognition Motifs of Disease-linked RNA-binding Proteins

Sashank Agrawal, 1, Woei-Chyn Chu, Hanna S. Yuan, (1) 1Institute of Molecular Biology, Academia Sinica, Taipei, Taiwan 11529, ROC, 2Molecular and Cell Biology Program, Taiwan International Graduate Program, Academia Sinica, Taipei, Taiwan 11529, ROC. 3Graduate Institute of Life Sciences, National Defense Medical Center, Taipei, Taiwan

#### ABS214/BOD27

#### Molecular mechanisms of the interhead coordination by interhead tension in cytoplasmic dyneins Qian Wang, 1, Biman Jana, Michael Diehl, Margaret Cheung, Anatoly Kolomeisky, José Onuchic,

Rice University, Center for Theoretical Biological Physics

#### ABS216/BOD17

#### Function/Structure in OPA1-mediated mitochondrial innermembrane fusion

Luke Chao, 1, Yifan Ge, Sivakumar Boopathy, Julie McDonald, MGH (1)

### ABS217/BOD18

#### Structural Modeling and In Silico Screening of Potential Small Molecule Allosteric Agonists of GLP-1 Receptor

Zhijun Li, 1, Tejashree Redij, Rajan Chaudhari, Zhiyu Li, Xianxin Hua, University of the Sciences in Philadelphia

#### ABS218/BOD86

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Protein, Ligand and Water Characterization by Multiple Solvent **Crystal Structures** 

Sorabh Agarwal, 1, Mychal Smith, Miriam Segura-Totten, Carla Mattos,

Northeastern University (1)

#### ABS219/BOD61

#### Direct observation of target site bypassing during rotationcoupled protein diffusion on DNA

Emil Marklund, 1, Bradly van Oosten, Mao Guanzhong, Elias Amselem, Kalle Kipper, Anton Sabantsev, Daniel Globisch,

- Xuan Zhen, Otto Berg, Magnus Johansson, Johan Elf,
- Uppsala University (1)

#### ABS220/BOD83

#### Histamine Dehydrogenase from Rhizobium sp. 4-9: 2.1 Å Resolution Crystal Structure and Evidence for a Substrate Access Channel

Priyanka Goyal, 1, Steve Seibold, Mark Richter, George Wilson, Scott Lovell,

(1)University of Kansas

#### ABS221/BOD89

A Structural and Functional Analysis of BshA: Insights into the Catalytic Mechanism and Feedback Inhibition by Bacillithiol Paul Cook, 1, Christopher Royer, Kelsey Winchell,

Grand Valley State University (1)

#### ABS222/BOD104

#### A Two-prong approach to developing an inhibitor screening method for compounds against Cryptosporidium parvum N-Myristoyltransferase

Alexandra Reers, 1, Yi Liu, Matt Hulverson, Alexis Kaushansky, Peter Myler, Wesley Van Voorhis, Erkang Fan, Bart Staker, Seattle Children's Research Institute

(1)

#### AB\$223/BOD133

Engineering Sortase A; Activity and Selectivity of New Hybrid and Ancestral Variants of Sortase A Sarah Struyvenberg, 1, Jordan Valgardson, Nick Horvath, John Antos, Jeanine Amacher, (1) Western Washington University

#### ABS224/BOD23

Use of Spin-Labeled Nanodiscs to Improve Structural **Determination of Membrane Proteins by ESR** Chieh-Chin Li,1, Yun-Wei Chiang,

(1) Department of Chemistry, National Tsing Hua University



### AB\$225/BOD143

### Protein Local Dynamics and Its Coupling to Solvent

- Yun-Hsuan Kuo,1, Yun-Wei Chiang,
- National Tsing Hua University

#### ABS226/BOD13

#### Unfolding Events of Bid Protein During Thermal Denaturation by ESR Absorption-mode Spectroscopy

- Chien-Lun Hung, 1, Yun-Wei Chiang,
- (1) Department of Chemistry, National Tsing Hua University

#### ABS227/BOD92

- Structural Insights into Chloramphenicol-metabolizing Enzyme from Metagenome Sang-Hoon Kim,1,
- 1) Seoul National University

#### ABS228/BOD34

- Biochemical Analysis of PriA Helicases from Gram-positive Bacteria Reveals Distinct DNA Unwinding Activity in DNA Replication Restart
- Chwan-Deng Hsiao, 1, Min-Guan Lin, Yi-Ching Li,
- Institute of Molecular Biology, Academia Sinica

#### ABS229/BOD150

Effects of Reactive Glutamines and a Binding Site Region on the Factor XIII Substrate Specificity for Fibrinogen aC (233-425) Muriel Maurer, 1, Mohammed Hindi, Francis D.O. Ablan, Chad Stephens, Kelly Mouapi

(1) University of Louisville

### ABS230/BOD6

#### Identify the amyloidogenic peptides and create photocontrollable probes for neurodegenerative disease Jen-Tse Huang, 1,

(1) Institute of Chemistry, Academia Sinica

#### ABS231/BOD119

Thermal Reconstruction of Protein Nano-Building Block Complexes Using an Ultra-Stable de Novo Protein Domain Ryoichi Arai, 1, Naoya Kimura, Naoya Kobayashi,



(1) Shinshu University

#### ABS232/BOD35

**Reversible and Orthogonal Four Helix Bundle Heterodimers** Ajasja Ljubetic, 1, Ryan Kibler, Zibo Chen, Sherry Bermeo, Roman Jerala, David Baker,

 Department of Biochemistry, UW; Institute for Protein Design, UW; Department of Synthetic Biology and Immunology, National Institute of Chemistry, Ljubljana, SI

#### ABS233/BOD94

Crystal Structure of the UDP-Glucose Pyrophosphorylase from Yersinia Pestis, An Anti-Plague Drug Target George Lountos, 1, Morgan Gibbs, Rajesh Gumpena,

- David Waugh, Basic Science Program, Frederick National Laboratory for
- (1) Basic Science Program, Frederick National Laboratory fo Cancer Research

### ABS234/BOD19

Structural and Functional Characterization of p13II Protein from Human T-cell Leukemia Virus Type 1 Elka R Georgieva, 1, Peter P Borbat, Christine Fanourakis,

- Jack H Freed,
- (1) Cornell University

#### ABS235/BOD136

Population Shifts from Allosteric Coupling of RNA and Tryptophan in the Gene-Regulating Ring-Shaped Protein TRAP Melody Holmquist, 1, Elihu Ihms, Weicheng Li, Cameron Jamshidi, Vicki Wysocki, Paul Gollnick,

(1) The Ohio State University

#### AB\$237/BOD117

The Structural and Functional Roles of Disulphide Bridges in the Solanum tuberosum Plant Specific Insert, a Saposin-Like Protein John H. Dupuis, 1, Rickey Y. Yada,

 Food, Nutrition, and Health Program, Faculty of Land and Food Systems, The University of British Columbia

### ABS238/BOD36

Novel Way to Study the Function of Native Proteins in Solution Gabriella Kiss, 1, Matthias Langhorst, Gavin Young, Daniel Cole, Phillipp Kukura,

(1) Refeyn Ltd, 33 George St, Oxford OX1 2AY, UK



#### ABS239/BOD152

Hysteresis and Allostery in Human UDP-Glucose Dehydrogenase Require a Flexible Protein Core Nathaniel Beattie, 1, Brittany Pioso, Andrew Sidlo, Nicholas Keul,

Zachary Wood,

(1) University of Georgia

#### ABS240/BOD44

The Polydispersity Problem: Investigating The Effect Of Crowding Agent Polydispersity On Protein Stability

Alan van Giessen, I, Anastasia Osti, (1) Mount Holyoke College

### ABS241/BOD48

The Role of Non-Motif Selectivity Determinants in PDZ

Domain-Binding Interactions Melody Gao, 1, Nick Pederson, Sarah Struyvenberg, Iain Mackley, Jeanine Amacher,

Western Washington University

#### ABS242/BOD59

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#### Proteome Comparison of Different Honeys Using Electrophoresis and Mass Spectrometry

Tyler Thornton, 1, Taylor Anderson, Casey Harding, Rawlings Lyle, Clayton Rawson, Austin Sherwin, Craig Thulin,

(1) Utah Valley University

### AB\$243/BOD120

### An Efficient, generalizable method for creating highly specific chemically induced protein dimerization systems

Liangcai Gu, 1, Shoukai Kang, Luis Gomez-Castillo, Huayi Jiang, University of Washington

#### AB\$245/BOD152

Novel Insights into Substrate Specificity and Structure of Non-Ribosomal Peptide Synthetases

Sandesh Deshpande, 1, Shayhan Chunkath, J. Shaun Lott,

- T. Verne Lee,
- (1) University of Auckland

### ABS246/BOD37

#### Activation of the exocyst tethering complex for SNARE complex regulation and membrane fusion Mary Munson, 1, Dante Lepore, Michael Feyder, Lillian Kenner,

Leonora Martinez-Nunez, Adam Frost,

(1) University of Massachusetts Med School

#### ABS247/BOD95

#### Fixed target delivery for serial femtosecond crystallography of weakly-diffracting objects

Megan Shelby, 1, Deepshika Gilbile, Thomas Grant, Carolin Seuring, Brent Segelke, Wei He, Angela Evans, Tim Pakendorf, Pontus Fischer, Mark Hunter, Alex Batyuk, Miriam Bathelmess, Alke Meents, Tonya Kuhl, Matthew Coleman, Matthias Frank

(1) Lawrence Livermore National Lab

#### ABS248/BOD112

 
 Oxidized dopamine causes neuronal cell death by impairing protein function and folding

 Dennis Özcelik, 1, Eduardo Felipe Alves Fernandes, Dominik Johann Essig,

 (1)
 University of Copenhagen

#### ABS249/BOD85

Structural elucidation of a novel, tandem deubiquitinase/ biquitin-binding domain from the pathogenic bacterium, Orientia tsutsugamushi Christopher Lim, 1, Jason Berk, Yong Xiong, Mark Hochstrasser,

(1) Yale University

#### ABS250/BOD109

 Transient Interactions Involving a Disordered Region of HspB1

 Drive Chaperone Activity toward Tau

 Hannah Baughman, 1, Amanda Clouser, Rachel Klevit,

 Abhinav Nath,

 (1)

#### ABS251/BOD63

Examining the effects of mutation on the aggregation and degradation of an ALS-associated protein Mikaela Elder, 1, Sean Cascarina, Lindsey Brookbank, Eric Ross, (1) Colorado State University



#### AB\$252/BOD111

#### Small molecule modulation of HSP60/10 chaperonin systems: More common than previously thought?

Mckayla Stevens, 1, Sanofar Abdeen, Nilshad Salim, Anne-Marie Ray, Alex Washburn, Siddhi Chitre, Jared Sivinski, Yangshin Park, Quyen Hoang, Eli Chapman, Steven Johnson,

(1) Indiana University School of Medicine

#### ABS253/BOD99

Influence of the Endoplasmic Reticulum Localization Sequence on the Cytotoxicity of Pseudomonas Exotoxin A-based Recombinant Immunotoxins Jillian Baker, 1, John Weldon,

(1) Towson University

### ABS254/BOD8

Natural and Pathogenic Protein Sequence Variation Affecting Prion-Like Domains Within and Across Human Proteomes Sean Cascarina, 1, Eric Ross,

1) Colorado State University

#### ABS255/BOD102

High Throughput sialylation measurement on Octet label free instrument for cell line development Sunny Song,1,

(1) Molecular Devices

#### ABS256/BOD125

Development of LOCKR-Activating Logic Circuits Ryan Kibler, 1, Zibo Chen, Marc Lajoie, Bobby Langan, David Baker, University of Washington

#### ABS257/BOD121

#### Engineering Protein Assemblies with Allosteric Control via Monomer Fold-Switching

Victor Munoz, 1, Luis Campos, Rajendra Sharma, Sara Alvira, Federico Ruiz, Beatriz Ibarra-Molero, Mourad Sadqi, Carlos Alfonso, German Rivas, Jose-Manuel Sanchez-Ruiz, Antonio Romero, Jose-Maria Valpuesta, University of California Merced

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#### ABS258/BOD78

Accelerating Infectious Disease Research Through Structural Genomics - the Seattle Structural Genomics Center for Infectious Diseases (SSGCID)

Garry W. Buchko, İ, Thomas E. Edwards, Donald Lorimer, Bart L. Staker, Robin Stacy, David Veesler, Gabriele Varani, Lance J. Stewart, Wesley C. Myler, Peter J. Myler, Pacific Northwest National Laboratory

#### ABS259/BOD38

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#### Amelogenin - A Multi-Pronged Approach to Identify Structural Features Guiding Enamel Formation Garry W. Buchko, 1, Jinhui Tao, Rajith J. Arachchige,

Sarah D. Burton, Yongsoon Shin, Bojana Ginovska, Barbara J. Tarasevich, Wendy J. Shaw,

Pacific Northwest National Laboratory

### ABS260/BOD122

Harnessing backbone strain to design beta-barrel proteins de novo: from first principles to application Anastassia Vorobieva, 1, Jiayi Dou, William Sheffler, Binchen Mao, Matthew Bick, Lindsey Doyle, Jason Klima, Lauren Gagnon, Yakov Kipnis, Barry Stoddard, David Baker, University of Washington

#### ABS261/BOD101

Non-ideality of Protein-based Therapeutics in Biological Environments Hayli Larsen,1,

University of Washington Department of Medicinal Chemistry

#### ABS262/BOD135

Structural Studies of Engineered Adeno-Associated Virus Capsids that Cross Blood-Brain Barrier Efficiently Xiaozhe Ding, 1, Sripriya Kumar, Andrey Malyutin, Viviana Gradinaru, California Institute of Technology

### ABS263/BOD141

Os9BGlu31 transglucosidase variants with high and promiscuous activity James R Ketudat Cairns, 1, Linh Tran, Sunaree Choknud, Vincent Blay Roger, Robert C. Robinson,

(1) Suranaree University of Technology

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#### AB\$264/BOD140

Genetic selections for the discovery of new reductases and oxidases of methionine Bruno Manta, 1, Mehmet Berkmen, (1)

New England Biolabs

#### ABS265/BOD71

### Structure and Dynamics of Tau Amyloid Fibrils Investigated by Solid-State NMR Spectroscopy

Aurelio Dregni, 1, Venkata S. Mandala, Haifan Wu, Matthew R. Elkins, William F. DeGrado, Mei Hong,

- Department of Chemistry, Massachusetts Institute of Technology, (1)
- ABS267/BOD45

#### Critical phenomena in the temperature-pressure-crowding phase diagram of a protein

Margaret Cheung, 1, Andrei Gasic, Mayank Boob, Maxim Prigozhin, Dirar Homouz, Anna Wirth, Caleb Daugherty, Martin Gruebele, University of Houston

#### ABS268/BOD154

(1)

Report from the Ribosome: The Origins of Protein Folding Loren Williams, 1, (1) Georgia Tech

- ABS269/BOD20 Modulation of rod opsin stability, function and membrane supramolecular organization by flavonoids Joseph T Ortega, 1, Tanu Parmar, Beata Jastrzebska, (1)
  - Case Western Reserve University

#### AB\$270/BOD105

Modulation of IgG blood-brain barrier permeability via Fab glycan sialylation John Finke, 1, Emily Swanson, Lewis Samantha, Ayres Kari,

Emily Wing, William Banks, (1) University of Washington

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#### ABS271/BOD100

Mass Spectrometry Profiling of N-linked Glycans That Modulate IgG Blood-Brain Barrier Permeability John Finke, 1, Samantha Lewis, Abigail Deleon, Emily Wing, William Banks,

University of Washington (1)

#### ABS272/BOD101

HPLC Profiling of N-linked Glycans That Modulate IgG Blood-Brain Barrier Permeability John Finke, 1, Emily Swanson, Abigail Deleon, Emily Wing, William Banks,

(1) University of Washington

#### ABS273/BOD103

	New regulatory drugs of the cholecystokinin hormones for the
	treatment of overweight and obesity
	Jose Vique-Sanchez, 1, Ana Galíndez-Fuentes,
	Claudia Benítez-Cardoza ,
(1)	Instituto Politecnico Nacional

### ABS274/BOD16

Knock-out mutations in a knotted protein improve the success of folding John Finke,1,

University of Washington Tacoma

#### AB\$275/BOD104

Biophysical and Structural Analysis of Abdominal A and Abdominal B Homeodomain Transcription Factors Rylee Simons, 1, Donald Spratt, Rachel Orlomoski, Jaqueline Dresch, Robert Drewell,

(1) Clark University

#### ABS276/BOD14

Differences in structural dynamics of bacterial NusG and RfaH transcription factors upon binding to transcription elongation complexes

Jose Alejandro Molina Ramirez, 1, Steve Silletti, Irina Artsimovitch, Elizabeth A. Komives, Cesar A. Ramirez-Sarmiento,

(1) Institute for Biological and Medical Engineering, Schools of Engineering, Medicine and Biological Sciences, Pontificia Universidad Católica De Chile



#### ABS277/BOD9

Exploiting Autoinhibition Mechanism for Screening of Small Molecules that Modulate DNA Binding to ETS Transcription Factors Jennifer Bui, 1, Cecilia Borajero, Lawrence McIntosh,

Joerg Gsponer,

(1) University of British Columbia

#### ABS278/BOD129

- Designing buttressed loops to diversify the functionality of de novo protein scaffolds Hanlun Jiana 1.
- (1) University of Washington

#### ABS279/BOD137

Understanding the Interface: Exploring Malate Dehydrogenase using Computational and Experimental Approaches Ellis Bell, 1, James Burnett, Michael Schwabe, Jessica Bell,

(1) University of San Diego

#### ABS280/BOD138

- Turning Up the Heat on Dynamic Proteins: Observing molecular motion in real time with temperature-jump X-ray crystallography Michael Thompson, 1, Alexander Wolff, Eriko Nango, Minoru Kubo, Iris Young, Takanori Nakane, Michihiro Sugahara, Rie Tanaka, Kazutaka Ito, Aaron Brewster, Shigeki Owada, Fumiaki Yumoto, Nicholas Sauter, Kensuke Tono, So Iwata, James Fraser
- (1) University of California, San Francisco

### AB\$281/BOD141

### A Community Based CURE Project to Explore Structure-Function Relationships in Malate Dehydrogenase

- Jessica Bell, 1, Joseph Provost, Ellis Bell,
- University of San Diego

#### AB\$282/BOD135

#### The Role of dynamics in transcription factor DNA-binding specificity

Karlton Scheu, 1, Soymya De, Lawrence McIntosh, University of British Columbia

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#### ABS283/BOD32

- Electrostatics Govern Membrane Interactions of the HSV-1 Nuclear Egress Complex Mike Thorsen, 1, David Hoogerheide, Janna Bigalke, Elizabeth Draganova, Ekaterina Heldwein,
- (1) Tufts Sackler School

#### ABS284/BOD81

#### Structure of trp repressor and its complexes from Francisella tularensis shows preservation of key water molecule Youngchang Kim, 1, Natalia Maltseva, Argonne National Laboratory

#### ABS285/BOD34

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Designing FRET Based Assays To Study The Binding of Fibroblast Growth Factor To Its Receptor Mamello Mohale, I, Ashley Howard, Musaab Habeeb Ali Al-Ammeer, Ravi Kumar Gundampati, T.k.s Kumar, Colin Heyes, University of Arkansas

ABS286/BOD21

The Unique amino acid composition of the chromophorebinding pocket contributes to the retinal binding specificity in human cone opsins Beata Jastrzebska, 1, Joseph Ortega, Kota Katayama, Sahil Gulati, Krzysztof Pakczewski, Case Western Reserve University

#### ABS287/BOD88

The Structure of a highly conserved picocyanobacterial protein reveals a Tudor domain with a novel tRNA binding function Katherine Bauer, 1, Rose Dicovitsky, Maria Pellegrini, Olga Zhaxybayeva, Michael Ragusa,

(1) Department of Biochemistry & Cell Biology

#### ABS288/BOD90

 
 Structural Characterization of Acinetobacter-Derived Cephalosporinase-7 in Complex With Ceftazidime and its Transition State Analog

 Brandy Curtis, 1, Emilia Caselli, Magdalena Taracila, Robert Bonomo, Fabio Prati, Rachel Powers, Brad Wallar,

 (1)
 Department of Chemistry, Grand Valley State University

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#### ABS289/BOD91

- Characterization of Novel Triazole-Containing Boronic Acid Transition State Inhibitors (BATSIs) of Acinetobacter-derived Cephalosporinase (ADC-7)
- Erin Fish, 1, Emilia Caselli, Magdalena Taracila, Robert Bonomo, Fabio Prati, Rachel Powers, Brad Wallar,
- (1) Department of Chemistry at Grand Valley State University

#### ABS290/BOD5

- Discovery and Characterization of a PAP248-286/Lipid Co-Assembly: The Messicle Story Eleanor W Vane, 1, Abhinav Nath,
- University of Washington Department of Medicinal Chemistry

#### ABS291/BOD39

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#### Two calcium sensors, one target: Prp40 interactions with both calmodulin and centrin

Adalberto Diaz-Casas, 1, Walter Chazin, Vanderbilt University

### ABS292/BOD11

### Design of Dual-Action Lipid-Nanodiscs in Controlling Amylin Aggregation Involved in Type-2 Diabetes

Bikash Sahoo, 1, Takuya Genjo, Takahiro Watanabe-Nakayama, Toshio Ando, Ayyalusamy Ramamoorthy,

Biophysics Program, Department of Chemistry, University of Michigan

#### ABS293/BOD50

### Functional and Structural Study on HERC4

- Young Sun Lee, 1, Donald Spratt,
- (1) Clark University

#### ABS294/BOD9

SUMO-derived Peptides as Inhibitors of a-Synuclein Aggregation Zhaohui Liang, 1, Junqing Yang, Ho Yin Edwin Chan, Ming Ming Marianne Lee, Michael Kenneth Chan

(1) The Chinese University of Hong Kong

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#### ABS295/BOD30

Novel pore-forming peptides assembling in liposome membranes selected by combining cDNA display method with cell sorter system

Naoto Nemoto, 1, Toshiki Miyajima, Takeru Yoshinobu, Yusuke

- Sekiya, Ryuji Kawano,
- Saitama University (1)

#### ABS296/BOD35

#### Expression and Characterization of the Drosophila melanogaster (Dm)IKKß:? complex

- Samantha Cohen, 1, Sheri Wu, Tom Huxford,
- (1) San Diego State University

#### ABS297/BOD97

High-density lipoprotein-based nanoparticles support functional
assessment of chlamydial membrane bound proteins and
induce protection in mice against a C. muridarum respiratory
challenge
Wei He 1. Matthew Coleman

- Lawrence Livermore National Laboratory
- (1)

#### ABS298/BOD62

Enteropathogenic E. coli hijacks programmed host-cell death pathways by interfering with the higher order oligomerization of immune system proteins Yann Gambin, 1, Ana Monserrat-Martinez, Emma Sierecki,

(1) EMBL Australia

#### ABS299/BOD1

#### Modulation of interactome by protein self-assembly: the case of alpha-synuclein

Emma Sierecki, 1, Andre Leitao, James Brown, Alex Chappard, Yann Gambin,

(1) UNSW

#### ABS300/BOD84

Crystal Structures Of Snx11 Reveal The Membrane Binding Mechanism

- Xu Tingting, 1, Liu Jinsong, Guangzhou Institutes of Biomedicine and Health, CAS
- (1)



#### AB\$301/BOD142

#### Catalytic Mechanism of TiaS5 in Tiacumicin B Biosynthesis Pathway

- Yongzhi Lu, 1, Yan Dong, Mingze Sun, Jinsong Liu,
- (1) Guangzhou Institutes of Biomedicine and Health,
  - Chinese Academy Sciences

#### ABS302/BOD89

- Structure of the Trimethylamine Methyltransferase Reveals a Distinct Environment for Methylamine Activation by Pyrrolysine Jiaxin Li, 1, Patrick T. Kang, Jodie Y. Lee, Ruisheng Jiang, Jitesh A. Soares, Joseph A. Krzycki, Michael K. Chan,
- School of Life Science and Center of Novel Biomaterials, The Chinese University of Hong Kong

#### AB\$303/BOD148

#### Structural and Biochemical Analysis of the HECT E3 Ubiquitin Ligase HECW2

- Justine Bohl, 1, Donald Spratt,
- Clark University

#### ABS304/BOD77

Crystal Structure of the Redß C-terminal Domain in Complex with ? Exonuclease Reveals an Unexpected Homology with ? Orf and an Interaction with Escherichia coli Single Stranded DNA Binding Protein

- Brian Caldwell, 1, Ekaterina Zakharova, Gabriel Filsinger, Timothy Wannier, Jordan Hempfling, Lee Chun-Der, Dehua Pei, George Church, Charles Bell,
- (1) Ohio State Biochemistry Program

#### ABS305/BOD143

#### The Neglected High Molecular Weight Enzymes of Snake Venom: Candidate Targets for Treating Tissue Necrosis by Snakebite Envenoming

- I-Jin Lin, 1, Chun-Lin Long, Yue-Hu Wang, Wen-guey Wu,
   Institute of Bioinformatics and Structural Biology, National Tsing Hua University, Hsinchu, Taiwan
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#### ABS306/BOD150

#### Structural and Mechanistic Characterization of HERC2 E3 Ubiquitin Ligase with Implications in Cancer, Prader-Willi Syndrome, and Eye Color

- Kayla Rich, 1, Noah Schwaegerle, Donald Spratt,
- Clark University

#### ABS307/BOD57

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- Prediction of deleterious protein mutants
- Andrzej Kloczkowski, 1, Robert Jernigan, Eshel Faraggi,
- Maksim Kouza,
- (1) Nationwide Children's Hospital

#### ABS308/BOD79

- Trimeric Immune Traps for Blockade of PD-1 and LPS Signaling in Combination Cancer Immunotherapy Rihe Liu, 1, Jingjing Li, Leaf Huang, Karthik Tiruthani,
- University of North Carolina at Chapel Hill

#### ABS309/BOD40

#### Characterization of Zn2+ Binding Properties of Postsynaptic Protein SAP102

Yonghong Zhang, 1, Angela Gonzalez, Mario Villarreal, The University of Texas Rio Grande Valley

#### ABS310/BOD112

#### Biophysical and Structural Analysis of Drosophila Transcription Factors

Aaron Bogle, 1, Rachel Orlomoski, Robert Drewell, Jacqueline Dresch, Donald Spratt, Clark University

### ABS311/BOD7

The Measurement of Volume Change by Capillary Dilatometry

- Peter Kahn,1, Rutgers University
- ABS312/BOD24

Oligomerization of lipid membrane bound Cytochrome P450 Nirupama Sumangala, 1, Thirupathi Ravula, Ayyalusamy Ramamoorthy,

(1) Biophysics, University of Michigan

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#### ABS313/BOD22

Cardiolipin Triggers Cytochrome-C Peroxidase Activity via Dynamic Changes to Mediate Mitochondrial Apoptosis Mingyue Li, 1, Abhishek Mandal, Vladimir Tyurin, Maria DeLucia, Jinwoo Ahn, Valerian Kagan, Patrick van der Wel,

Department of Structural Biology, University of Pittsburgh

#### ABS314/BOD103

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### iPTMnet: An Integrated Resource for Protein Post-Translational Modification Network Discovery

Cecilia Arighi, 1, Hongzhan Huang, Karen Ross, Jla Ren, Julie Cowart, Sachin Gavali, Qinghua Wang, K Vijay-Shanker, Cathy Wu,

(1) CBCB, University of Delaware

#### ABS315/BOD2

#### Fibril Formation, Phase Transition, and Interactors of Orb2, a Protein Important in Long-Term Memory

Connor Hurd, 1, Connor Hurd, Silvia Cervantes, Alexander Falk, Maria Soria, Samridhi Garg, Ansgar Siemer, University of Southern California

#### ABS317/BOD123

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Generative Modeling for Protein Structures

- Possu Huang, 1, Namrata Anand, Raphael Eguchi,
- (1) Department of Bioengineering, Stanford University

#### AB\$318/BOD58

- Using Deep Learning Neural Networks for Inverse Protein Folding Predictions
  - Alyssa La Fleur, 1, Tersa Almaw, Deanna Ojennus, Kent Jones, Whitworth University

#### ABS319/BOD108

#### Novel perspectives on olfactory receptor-odorant dynamics simulations

Chiquito Crasto,1, Peter Lai,

(1) Texas Tech University

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#### ABS320/BOD10

The Human Zinc- and Iron-regulated Transport Protein 4 Intracellular Loop Remains Disordered upon High-affinity Zinc Binding

Elizabeth Bafaro, 1, Mark Maciejewski, Jeffrey Hoch,

- Robert Dempski,
- (1) Worcester Polytechnic Institute

#### AB\$321/BOD119

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The Rational Discovery and Design of Disordered Protein Ligands David Baggett, 1, Abhinav Nath, University of Washington

### AB\$322/BOD120

Analysis of Loop Motions in 1 µs Simulations of OXA-66 Reveals Striking Differences in Flexibility between Mutants Joshua Grey, 1, David Leonard, Agnieszka Szarecka,

Grand Valley State University

#### ABS323/BOD95

Measuring the unfolding and ligand-binding of CusF, a copper chaperone

Isabel Zecua, 1, Blake Gillespie, CSU Channel Islands

#### ABS324/BOD106

Biophysical and Structural Analysis of Antennapedia and Ultrabithorax Homeodomain Transcription Factor-DNA Binding Affinities

Jeanmarie W. Loss, 1, Rachel J. Orlomoski, Jacqueline M. Dresch, Robert A. Drewell, Donald E. Spratt, Clark University

#### ABS325/BOD37

Biophysical Examination of Ubiquitin E3 ligase, HECTD1: An Important Regulator in Neurological Development Misa Mai,1, Donald Spratt,

(1) Clark University

#### AB\$326/BOD51

Structural Examination of the HECT E3 Ligase Arel1 and its Implications in Apoptosis Emily Ladda, 1, Donald Spratt,

(1) Clark University



#### AB\$327/BOD124

#### Computational Design of a hyper-stable avb6 Integrin Binding Protein with High Affinity and Specificity

Anindya Roy, 1, Lei Shi, Xianchi Dong, Alexander I Salter, Maxwell Cherf, Jing Li, Jennifer Cochran, Timothy Springer, Stanley Riddel, David Baker,

University of Washington (1)

#### AB\$328/BOD91

Structure and Intrinsic Hydrolysis of NRas Q61 Mutants

- Derion Reid, 1, Spiro Pavlopoulos, Carla Mattos,
- Northeastern University

### AB\$329/BOD144

#### Reversible Inactivation Of Alkaline Phosphatase At High Pressure: Insights Into Pressure-Mediated Protein Refolding Gary Smejkal, 1, Vera Gross, Nicole Cutri, Edmund Ting,

- Alexander Lazarev,
- Pressure Biosciences (1)

#### AB\$330/BOD54

Molecular Basis of ClpP Protease Activation by Small Molecules Walid Houry,1,

University of Toronto (1)

### ABS331/BOD86

#### Structure-Activity Relationships In The Metamorphic, Antimicrobial Protein Xcl1

Acacia Dishman, 1, Michelle Lee, Gerard Wong, Brian Volkman, (1) Medical College of Wisconsin

#### ABS333/BOD65

### Functionally Relevant Clustering of the Arsenate Reductase (ArsC) Superfamily

Mikaela Rosen, 1, Jacquelyn Fetrow, Carol Parish, Janelle Leuthaeuser,

(1)University of Richmond

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#### AB\$334/BOD11

### Defining GP41-1 Extein Splice Junction

- Carla Madrid, 1, Thuy Nguyen, Kimberly Reynolds, Kendra Frederick
- UT Southwestern Medical Center (1)

### ABS335/BOD64

Achieving better-than-2-Å resolution by single-particle cryo-EM at 200 keV

- Mark Herzik, 1, Mengyu Wu, Gabriel Lander,
- University of California, San Diego (1)

### ABS336/BOD53

#### Investigating Bacterial Sortase Substrate Selectivity Using Ancestral Protein Reconstruction And Sequence Network Analysis

Jordan Valgardson, 1, Sarah Struyvenberg, Zach Sailer, Jeanine Amacher,

(1) Western Washington University

#### AB\$337/BOD14

#### Effect of experimental parameters of optical traps on folding/ unfolding dynamics of fast folding proteins

- Rama Reddy Goluguri, 1, Mourad Sadqi, Victor Munoz,
- (1) UC Merced

#### AB\$338/BOD27

#### De Novo Peptide Design For Enhanced Cell Permeability, Oral Bioavailability And Blood-Brain Barrier Traversal Gaurav Bhardwai, 1, Stephen Rettie, Jacob O'Connor,

- Yen-Hua Huang, David Craik, David Baker,
- University of Washington, Seattle

#### AB\$339/BOD41

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Novel Fc-Poly His Tag Leads To High Order Oligomerization Zebulon Lapoint, 1, Zebulon Lapoin, John Hall, Matteo Binda, DeeAnn Martinez-Guzman, Susan Hilt, Pranti Das, Charles Holz, Jody Berry, Peter Schwind, Elizabeth Booth, Vincenzo Favaloro, Grifols Diagnostic Solutions

#### ABS340/BOD15

### Optimization of Protein Structure and Function: The Importance of Loop Lenath

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Jayant Udgaonkar, Shachi Gosavi,
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- (1) Stanford University
- Neha Nandwani, 1, Praneeth Reddy, Manjula Ramu,

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#### ABS341/BOD57

Biophysical and Biochemical Characterization of HACE1, a HECT E3 Ubiquitin Ligase Implicated in Cancer and Huntington's Disease Diana Argiles Castillo, 1, Donald Spratt,

(1) Clark University

#### ABS342/BOD65

Room Temperature Crystallography of Retinal Proteins: Investigating the Retinal Isomerization Mechanism Gebhard F.X. Schertler, 1,

(1) Paul Scherrer Institut / ETH Zurich D-BIOL

#### ABS343/BOD125

- Designer Proteins From Fold To Applications
- Eva-Maria Strauch, 1, David Baker,
- (1) University of Georgia

#### ABS344/BOD44

#### Identifying "Hot Spot" Residues At The Etv6 Pnt Domain Polymerization Interface Sophia Cho, 1, Chloe Gerak, Michel Roberge,

Lawrence McIntosh, University of British Columbia

#### ABS345/BOD119

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#### Dynamics of Opening and Closing Motions of the Clamp of Bacterial RNA Polymerase Ilona Christy Unarta, 1, Kubo Shintaroh, Wei Wang, Xuhui Huang,

Shoji Takada, Xuhui Huang, Hong Kong University of Science and Technology

#### ABS346/BOD42

Cardiomyopathy Mutations in Metavinculin Disrupt Regulation of Vinculin-Induced F-Actin Assemblies Sharon Campbell,1, Muzaddid Sarker, Hyunna Lee, Lin Mei, Andrey Krokhotin, Santiago E de los Reyes, Laura Yen,

Lindsay Costantini, Jack Griffith, Nikolay Dokholyan, Greg Alushin, University of North Carolina

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#### AB\$347/BOD155

Resurrection of Ancestral Effector Caspases Identifies Novel Networks for Evolution of Substrate Specificity Clay Clark, 1, Robert Grinshpon, Suman Shrestha, James Titus-McQuillan, Paul Hamilton, Paul Swartz,

University of Texas at Arlington

### ABS348/BOD38

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Structural Biology Of The Miz-1/C-Myc Interaction To Accelerate The Development Of C-Myc Inhibitors Jean-Michel Moreau, 1, Martin Montagne, Danny Létourneau, Mikaël Bédard, Pierre Lavigne,

(1) Université de Sherbrooke

#### ABS349/BOD96

#### **ParABS, Chromosome Partitioning System** Yuh Ju Sun, 1,

 Institute of Bioinformatics and Structural Biology, National Tsing Hua University

#### ABS350/BOD92

### Elucidating the Role of Protein Partnerships in Modulating DNA Binding Specificity of Transcription Factors

Bidisha Acharya, 1, Snigdha Maiti, Aditya Jyoti Basak, Soumya De,

Indian Institute of Technology, Kharagpur

#### ABS351/BOD93

#### Homodimer Interface Mutations Of Human Galectin-7 Alter Its Biological Activity

Ngoc Thu Hang Pham, 1, Myriam Létourneau, Marlène Fortier, Carolina Perusquía Hernández, Marie-Aude Pinoteau, Jacinthe Gagnon, Philippe Egesborg, David Chatenet, Yves St-Pierre, Charles Calmettes, Nicolas Doucet,

 Centre Armand-Frappier Santé Biotechnologie, Institut National de da Recherche Scientifique (INRS), Université du Québec

### AB\$352/BOD71

#### The Structural Basis of Adhesion Regulation by the Cadherin-Catenin Complex

Allison Maker, 1, Brad Hammerson, David Dranow, Richard Mangio, Leslayann Schecterson, Bart Staker, Barry Gumbiner, University of Washington

(1) University of Washington

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#### AB\$353/BOD73

Solution state structural and dynamic studies of mouse BTNL2, an orphan T cell coinhibitory molecule

Aditya Jyoti Basak, 1, Snigdha Maiti, Anita Hansda,

Dhrubajyoti Mahata, Woonghee Lee, Gayatri Mukherjee, Soumya De, Dibyendu Samanta,

Indian Institute Of Technology Kharagpur

#### ABS354/BOD58

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Contribution of Cleavage and MHCII Binding Events to the Generation of Hemagglutinin Immunodominant Peptides Tynan Becker, 1, Thomas Kuhn,

(1) Dept. of Biology and Wildlife University of Alaska Fairbanks

#### ABS355/BOD126

#### High-throughput de novo design of stable and high-affinity binders

Nihal Korkmaz, 1, TJ Brunette, David Baker,

Institute for Protein Design, University of Washington

#### ABS356/BOD66

- The Supramolecular Structure Of The Bacterial Stressosome Revealed By Cryo-Em Unveils Its Mechanism Of Activation Allison Williams, 1,
- (1) Institut Pasteur, Department of Microbiology

#### AB\$357/BOD8

#### Crystal Structure Of A Protein Folding Intermediate

- Jinquan Luo, 1,
- (1) Janssen R&D

#### AB\$358/BOD145

- Identification and Characterization of an Oxalyl CoA-Synthetase from Grass Pea (Lathyrus sativus L.) Moshe Goldsmith, 1, Shiri Barad, Orly Dym, Shira Albeck, Yoav Peleg, Ziv Reich,
- (1) Dept. of Biomolecular Sciences

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#### ABS359/BOD74

Cryo-EM Structure of the Dihydrolipoamide Succinyltransferase (E2) Component of the Human Alpha-Ketoglutarate Dehydrogenase Complex

Balint Nagy, 1, Zsofia Zambo, Agnes Hubert, Martin Polak,

- Eszter Szabo, Jirí Novacek, Frank Jordan, Vera Adam-Vizi,
- (1) Department of Medical Biochemistry, Semmelweis University

#### ABS360/BOD127

Automated Design Of Interface Structure For Targeted Binders Yu Zhao, 1, Gevorg Grigoryan,

(1) Dartmouth college

#### ABS361/BOD146

New CRISPR/Cas9 Characterization Broadens The Protospacer-Adjacent Motif Recognition Trung Thach, 1, Nam Hyeong Kim, Junho Hur, Sang-Seob Lee, Yong Ho Kim,

(1) Sungkyunkwan University

#### AB\$362/BOD109

#### Computational Modeling of S-phase kinase-associated protein 2 (Skp2) E3 Ligase and Novel Inhibitors Interactions Shuxing Zhang, 1,

(1) MD Anderson Cancer Center

#### ABS363/BOD10

#### The Yeast Sup35 Protein Forms A Large Number Of Infectious Structures

- Yu-Wen Huang, 1, Chih-Yen King,
- ) Institute of Molecular Biology, Academia Sinica

#### ABS364/BOD76

elF2B-Catalyzed Nucleotide Exchange And Phosphoregulation By The Integrated Stress Response Lillian Kenner, 1,

(1) UCSF

#### ABS365/BOD142

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The Molecular Mechanism of Disease Mutations in Human Glutamine Synthetase and Compensatory Rescue by Secondary Mutations

Erin Thompson, 1, Avi Samelson, Martin Kampmann, James Fraser, UCSF

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#### ABS366/BOD110

#### Dynamic Docking Between an Enzyme and Its Inhibitor Using **Multicanonical MD Simulations**

- Narutoshi Kamiya, 1, Gert-Jan Bekker,
- (1)University of Hyogo

#### ABS367/BOD58

- Cytotoxic Activity Of Non-Specific Lipid Transfer Protein (NsLTP) From Fennel (Foeniculum Vulgare) Seeds Mekdes Megeressa, 1, Yamna Khurshid, Aftab Ahmed,
- Chapman University
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#### ABS368/BOD98

- Photosensitive handles for selective manipulations of biosynthetic proteins Rasa Rakauskaite, 1, Giedre Urbanaviciute, Viktoras Masevicius, Aušra Vaiteikaite, Aurelija Žvirbliene, (1)
  - Institute of Biotechnology, Vilnius University

#### AB\$369/BOD113

- Differential Localization Of An Engineered RAS Rheostat Reveals Unique RAS-ERK Signaling Dynamics Emily M Dieter, 1, John Rose, Dustin Maly,
- University of Washington

#### ABS370/BOD78

#### Exploring the Novel Structure of Human Myeloid-Derived Growth Factor

Valeriu Bortnov, 1, Marco Tonelli, Woonghee Lee, John Markley, Deane Mosher,

University of Wisconsin-Madison (1)

#### AB\$371/BOD120

Engineering Orthogonality into the Chemokine-GPCR Interface Using Rosetta

Michael Wedemeyer, 1, Benjamin K. Mueller, Jens Meiler, Brian Volkman,

Medical College of Wisconsin (1)

#### ABS372/BOD67

- Hydrophobic Ligands Influence the Structure, Stability, and Processing of the Major Cockroach Allergen Blag 1 Alexander Foo, 1, Peter Thompson, Lalith Perera, Simrat Arora, Eugene DeRose, Jason Williams, Geoffrey Mueller,
- National Institute of Environmental Health Sciences (1)

#### AB\$373/BOD128

Capturing The Structural Flexibility Of Single-Layer Beta-Sheet Within Isomorphous Crystals Revealed By Comprehensive Structure Determinations Koki Makabe, 1, Hideki Fujiwara, Kenta Hongo, Yuki Hori, Norio Yoshida,

(1) Yamagata university

#### AB\$374/BOD114

Cysteine Scanning Mass Spectrometry Towards Elucidation of Intramolecular Structure-Function Relationships in Multi-Domain Kinases Zachary E. Potter, 1, Dr. Dustin Maly,

- Department of Chemistry, University of Washington (1)

#### AB\$375/BOD59

Proteomic and Cytotoxic Characterization of Proteins from Cuscuta (Dodder) Tendrils Umaima Akhtar, 1, Mekdes Megeressa, Basir Syed, Ishtiaq Ahmed Khan, Keykavous Parang, Aftab Ahmed, Chapman University

#### AB\$376/BOD113

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A Chemoproteomic Method For Characterizing Kinase Complexes

- Linglan Fang, 1, University of Washington

#### ABS377/BOD139

Optoallostery: An Experimental Study of the Mechanism of Light-Induced Allosteric Control of Engineered Rho Family GTPases

Abha Jain, 1, Nikolay Dokholyan, Andrew Lee, (1) University of North Carolina at Chapel Hill



#### ABS378/BOD79

Molecular Mechanisms Giving Rise to Human Dihydrolipoamide Dehydrogenase Deficiency - Structural Analysis of Seven Disease-Relevant Enzyme Variants

Eszter Szabó, 1, Piotr Wilk, Bálint Nagy, Réka Mizsei, Zsófia Zámbó, Dávid Bui, Andrzej Weichsel, Palaniappa Arjunan, Beáta Törocsik, Ágnes Hubert, William Furey, William Monfort, Frank Jordan, Manfred Weiss, Vera Ádám-Vizi, Attila Ambrus

(1) Department of Medical Biochemistry, MTA-SE Laboratory for Neurobiochemistry, Semmelweis University

#### ABS379/BOD80

#### Characterization of Proteins by Microfluidic CE-SDS

- April Blodgett,1,
- I) PerkinElmer

#### ABS380/BOD99

Biochemical, Biophysical And Structural Characterization Of Isoniazid Resistance Katg Variants From Mycobacterium Tuberculosis

Brenda Uribe, 1, Xavier Soberon, Humberto Flores,

(1) Biotechnology Institute, UNAM

#### AB\$381/BOD114

#### Redox Regulation Of The Dimerization And Enzymatic Activities Of TOP1 and TOP2

Thualfeqar Almohanna, 1, George Popescu, Sorina Popescu,Mississippi state University

#### AB\$382/BOD100

Increasing User Capabilities at the GM/CA@APS X-ray Crystallography User Facility at the Advanced Photon Source Michael Becker, 1, Stephen Corcoran, Dale Ferguson, Mark Hilgart, David Kissick, Oleg Makarov, Craig Ogata, Ruslan Sanishvili, Sergey Stepanov, Nagarajan Venugopalan,

Qingping Xu, Shenglan Xu, Robert Fischetti, Janet Smith, Argonne National Laboratory

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#### ABS383/BOD68

A PsR Domain in Atg32 is Required for Mitophagy

- Xue Xia, 1, Sarah Katzenell, Erin Reinhart, Katherine Bauer,
- Maria Pellegrini, Michael Ragusa,
- (1) Dartmouth College

#### ABS384/BOD124

#### Structural Analysis Of Cytochrome BM3 For Synthesis Of Caffeic Acid

- Jorge Jimenez Niebla,1, Gloria Saab Rincón , IBT, UNAM
- AB\$385/BOD137

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#### Influence of Mechanical Force On The Lifetime Of Activated FimH-mannose Bonds

- Laura Carlucci,1, Wendy Thomas,
- (1) University of Washington, Department of Bioengineering

#### ABS386/BOD101

#### Characterization of E. coli LpxA Inhibitors Targeting Various Enzymatic States by NMR Spectroscopy

Feng Wang, 1, Andreas Frank, Andreas Lingel, Alexandra Frommlet, Wooseok Han, Xiaolei Ma, Alun Bermingham, Barbara Chie Leon, Chi-Min Ho, Patrick Lee, Min Li, Jacob Shaul, Charles Wartchow, Tsuyoshi Uehara, Novartis Institutes for BioMedical Research

#### ABS387/BOD81

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Increased Antigen Binding Affinity And Decreased Thermal Stability Of An Anti-(4-Hydroxy-3-Nitrophenyl)Acetyl Antibody Possessing A Glycine Residue At Position 95 Of The Heavy Chain Masayuki Oda, 1, Takachika Azuma,

(1) Kyoto Prefectural University

#### ABS388/BOD19

Characterizing the Intrinsically Disordered Domain of LIAT1 Akshaya Arva, 1, Christopher Brower, Yasar Kasu,

Texas Woman's University

#### ABS389/BOD7

Novel Alpha-Sheet Secondary Structure Drives Aggregation and Toxicity in Alzheimer's Disease Dylan Shea,1, Valerie Daggett,

(1) University of Washington



#### ABS390/BOD69

Solution Structure of the IWP-051-bound H-NOX from Shewanella woodyi Reveals a Conserved Binding Pocket for Soluble Guanylyl Cyclase Stimulators

Cheng-Yu Chen, 1, Woonghee Lee, William Montfort,

(1) University of Arizona, Department of Chemistry and Biochemistry

#### AB\$391/BOD147

#### Functional Evolution of TRPM2 Channels

- lordan lordanov, 1, Balázs Tóth, Andras Szollosi, László Csanády,
- ) Department of Medical Biochemistry and MTA-SE Lendület Ion Channel Research Group, Semmelweis University
- ABS392/BOD116
  - The effects of a Small Molecule Inhibitor on Cdc42, its Mutant and its Interaction with Effector Proteins
  - Djamali Muhoza, 1, Paul Adams, University of Arkansas

#### ABS393/BOD28

- Sequence Specificity for Peptide Substrates in Thioether Crosslinking Reaction Catalyzed by Radical SAM Enzyme QhpD Toshinori Oozeki, 1, Kazuki Kozakai, Tadashi Nakai, Katsuyuki Tanizawa, Toshihide Okajima,
- Osaka University

#### ABS394/BOD148

Structural Basis For Conformational Change Of The Topaquinone Cofactor During The Catalytic Reaction Of Bacterial Copper Mine Oxidase

Toshihide Okajima, 1, Takeshi Murakawa, Seiki Baba,

Satoshi Kanagawa, Hideyuki Hayashi, Takato Yano,

Takashi Kumasaka, Katsuyuki Tanizawa, Osaka University

## AB\$395/BOD154

(1)

#### Regulatory Role of 5'-AMP in cAMP Signalosome Dynamics

- Nikhil Tulsian, 1, Abhijeet Ghode,
- (1) National University of Singapore

#### ABS396/BOD102

- Disruption of Homophilic Protein-protein Interaction of P-cadherin by A Fragment Compound as A Trigger To Inhibit Cell Adhesion Akinobu Senoo, 1, Satoru Nagatoishi, Kouhei Yoshida, Sho Ito, Go Ueno, Takumi Tashima, Shota Kudou, Kouhei Tsumoto,
- (1) Department of Chemistry and Biotechnology, School of Engineering, The University of Tokyo

#### ABS397/BOD12

#### How Nature Harnesses Entropy To Tune Protein Function Zachary Wood, 1, Nick Keul, Krishnadev Oruganty, E lizabeth Schaper Bergman, Nathan Beattie, Weston McDonald, Renuka Kadirvelraj, Michael Gross, Robert Phillips, Stephen Harvey,

(1) University of Georgia

#### ABS398/BOD29

#### Structural Modeling of Antimicrobial Peptides in the Database of Antimicrobial Activity and Structure of Peptides Anthony Armstrong, 1, Phil Cruz, Andrei Gabrielian, Mindia Chubinidze, Malak Pirtskhalava, Darrell Hurt, Alex Rosenthal, Mike Tartakovsky, Office of Cyber Infrastructure & Computational Biology,

 Office of Cyber Infrastructure & Computational Biology, National Institute of Allergy and Infectious Diseases, National Institutes of Health

#### ABS399/BOD125

Modulating Enzyme Activity Between Sugar Hydrolysis
And Sugar Transfer Using An Evolutionary Approach
Rodrigo Arreola-Barroso, 1, Wendy Xolalpa-Villanueva,
Leticia Olvera-Rodriguez, Gloria Saab-Rincón,
Institute of Biotechnology, UNAM

AB\$400/BOD152

Functional Elements Of A Human Antizyme Essential For Binding And Inhibiting Human Ornithine Decarboxylase Ju-Yi Hsieh, 1, Hui-Chih Hung,

- (1) Institute of Biochemistry, Microbiology & Immunology,
- Chung Shan Medical University



#### ABS401/BOD70

#### Impacting Respiratory Therapeutic Programs Through Protein Biophysics and Structural Biology

Michael Eddins, 1, Hua-poo Su, Xiao Xiao, Jennifer Shipman, Srivanya Tummala, John Reid, Yacob Gomez Llorente, Zhifena Chen, Eberhard Durr, James Cook, Kerim Babaoalu, Stephen Soisson, Lan Zhang, Kalpit Vora, Alexei Brooun,

Merck and Co., Inc., Computational and Structural Chemistry (1)

#### AB\$402/BOD144

#### Evaluation Of The Effect Of Heat Capacity On The Catalysis Of A **Dimeric Enzyme** Ekaterina Jalomo Khayrova, 1, Christopher Bahl,

Gloria Saab Rincón,

(1) Instituto de Biotecnología, Universidad Nacional Autónoma de México

#### ABS403/BOD61

- Distinct Structural Features of the Lon Protease Drive Conserved Hand-over-Hand Substrate Translocation
- Mia Shin, 1, Ananya Asmita, Cristina Puchades, Eric Adjei,
- R. Luke Wiseman, A. Wali Karzai, Gabriel C. Lander, The Scripps Research Institute

#### AB\$404/BOD103

(1)

#### Modulating Receptor Signaling using Variabody; A Novel **Bispecific Antibody Format Enables One-pot Synthesis of** Fab-dimer Library

Yasuhisa Shiraishi, 1, Akifumi Kato, Munetake Shimabe, Jun Taneo, Minako Oogi, Kaname Kimura, Shigeyuki Yokoyama, Kensaku Sakamoto,

(1) Antibody & Biologics Research Labs, Research Functions Unit, R&D Division, Kyowa Hakko Kirin Co., Ltd.

#### AB\$405/BOD111

Calculating Potential Of Mean Force (PMF) With Umbrella Sampling Predicts Relationships Between Ligand-Based And Structure-Based Drug Design For Potential Abl Tyrosine Kinase Inhibitors Derived From 2-Pyrazolinyl-1-Carbothioamide Beom Soo Kim, 1, Sangho Ji, Sang Won Jung, Department of Brain and Cognitive Sciences, Daegu

150 Gyeongbuk Institute of Science and Technology (DGIST)

#### ABS406/BOD136

#### Functional networks study of Ga using coevolution analysis Miniae Seo.1

DGIST (Daegu Gyeongbuk Institute of Science and Technology)

#### ABS407/BOD26

(1)

- **Bifurcated H-Bonding in Membrane Proteins**
- Esther S Brielle, 1, Isaiah T Arkin,
- The Alexander Grass Center for Bioengineering.

The Hebrew University of Jerusalem, Edmond J. Safra Campus

#### AB\$408/BOD82

#### Engineering Therapeutics for the Treatment of Anemia in **Oncology Patients** Ning Yang, 1, Marina Chemerovski-Glikman, Lia Cardarelli,

Jarrett Adams, Sachdev Sidhu,

Donnelly Center for Cellular and Biomolecular Research, (1) University of Toronto

#### ABS409/BOD71

#### The Retaining Glycoside Hydrolase T26H Mutant of T4 Lysozyme Utilizes a Reverse Protonation Catalytic Mechanism Jacob Brockerman, 1, Mark Okon, Stephen Withers, Lawrence McIntosh.

(1) University of British Columbia

#### AB\$410/BOD117

#### Interrogation of the Regulatory Role of the SH4 Domain of Src Family Kinases

- Sujata Chakraborty, 1, Ethan Ahler, Linglan Fang, Emily Dieter,
- University of Washington (1)

#### ABS411/BOD28

#### Homotypic and Heterotypic Interactions of Plexin and Neuropilin TM Domains

Shaun Christie, 1, Soon-Jeung Kim, Paul Toth,

- Jeannine Muller-Greven, Matthias Buck, Adam Smith,
- The University of Akron

#### ABS412/BOD153

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#### Atomistic View of an Unfolding Pathway in a Seven-Helical Membrane Protein

Peng Xiao, 1, David Bolton, Vladimir Ladizhansky, University of Guelph



#### ABS413/BOD39

## Mechanism of microtubule nucleation in the PCM

 Institute of Bioinformatics and Structural Biology, National Tsing Hua University

#### ABS414/BOD149

Purification Of Recombinant Adipose Triglyceride Lipase (ATGL) For Biochemical, Biophysical And Mechanistic Studies Suman Shanker, 1, Kim Fennell, Nicole Caspers, Yang Cong, Erik Ralph, Jessica Calloway, Jemy Gutierrez, Benjamin Reidich, Cecile Vernochet, Francis Rajamohan,

(1) Pfizer

#### ABS415/BOD43

### Structural basis of OLA1 activation by BARD1 BRCT

Ting Chen, 1,(1) National Tsing Hua University

The University of Tokyo

#### ABS416/BOD146

Catalytic Bioscavenger with Improved Stability and Reduced Susceptibility to Oxidation to Treat Acute Poisoning with Neurotoxic Organophosphorous Compounds (OPs) Laura Job, 1, Anja Köhler, Benjamin Escher, Franz Worek, Arne Skerra.

(1) Chair of Biological Chemistry, Technical University Munich

#### ABS417/BOD88

#### Multi-subunit E.coli expression system applied to the X-ray crystallographic analysis of S. pombe Mediator complex Kayo Nozawa, 1, Thomas Schneider, Patrick Cramer,

(1) The University of Tokyo, Institute for Quantitative Biosciences

#### ABS418/BOD112

#### The Effects Of Protonation Of A Phosphorylated Amino Acid On The Molecular Recognition: Comparative Studies Of Generic Proteins And An Antibody

Raiji Kawade, 1, Daisuke Kuroda, Jose Caaveiro, Hiroki Akiba, Shigeru Okumura, Toshiaki Maruyama, Kevin Entzminger, Kouhei Tsumoto,



#### ABS419/BOD153

#### Illuminating the Evolution of Beetle Bioluminescence with Fatty Acyl-CoA Synthetases

- Spencer Adams Jr., 1, Stephen Miller,
- (1) University of Massachusetts Medical School

#### ABS420/BOD81

- NMR NOE assignments and buildup measurements of Im7 in solution: towards internal dynamics characterization from NOEs Xinyao Xiang, 1, Chunhua Yuan, Alexandar Hansen, Lei Brüschweiler-Li, Rafael Bru<sup>\*</sup>schweiler, Dongtmart of Chamittar, and Bru<sup>\*</sup>schweiler,
- (1) Department of Chemistry and Biochemistry, The Ohio State University

#### ABS421/BOD71

#### Structural and enzymatic characterization of a Penicillin Binding Protein from Leptospira interrogans Jademilson Celestino dos Santos, 1, Sumit Handa, Luis Guilherme

Virgilio Fernandes, Partho Ghosh, Ana Lucia Tabet Oller Nascimento,

(1) UCSD/Insituto Butantan

#### ABS422/BOD73

#### Structure Determination of Nontuberculosis Mycobacteria Dihydrofolate Reductase to Inform Structure-Guided Drug Discovery

Rachael Zigweid, 1, Brad Hammerson, Abe Shim, Stephen Mayclin, Jan Abendroth, Bart Staker, Peter Myler,

Seattle Children's Research Institute

#### ABS423/BOD68

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 Developing Orthogonal Single-Molecule Constructs Using HUH

 Endonucleases and DNA Handle Self-Assembly

 Andrew Nelson, 1, Kassidy Tompkins, Blake Everett,

 Klaus Lovendahl, Wendy Gordon,

 University of Minnesota- Twin Cities

#### ABS424/BOD28

#### Protein Disorder in Reconstituted Dynein Cargo Attachment Subcomplex

Kayla Jara, 1, Cat Hoang, Sanjana Saravanan, Elisar Barbar, Oregon State University



#### ABS425/BOD96

Biasing Binding Orientation of the C-terminal Strand Exchange Limits Chaperone Function in Human Alpha-B Crystallin James Hebda, 1, Derrick Draeger, Khan Nguyen, Anna Nevels,

(1) Austin College

#### ABS426/BOD113

#### pH Dependence on Binding and Release of Folate by Folic Acid Receptor a

Thomas Paul, 1, Hedieh Torabifard, Jonah Vilseck, Ryan Hayes, Charles Brooks

Department of Chemistry, University of Michigan (1)

#### AB\$427/BOD138

AMP Regulation of Bifunctional ADP-dependent Sugar Kinases from Archaea: Evolutionary History and Kinetic Characterization Gabriel Vallejos, 1, Sixto M Herrera, Victor Castro-Fernandez,

Departamento de Biología, Facultad de Ciencias, (1)

Universidad de Chile

#### AB\$428/BOD127

Characterizing Catch Bond Clusters Using DNA Origami and Atomic Force Microscopy Molly Mollica, 1, Olga Yakovenko, Nathan Sniadecki,

Wendy Thomas,

University of Washington (1)

#### ABS429/BOD3

#### Design and Validation of De Novo Designed Protein Mini Binders of Ribosomal RNA Small Subunit Methyltransferase A From Burkholderia pseudomallei

Bradley Hammerson, 1, Longxing Cao, Brian Coventry, Matt Clifton, Jan Abendroth, Banumathi Sankaran, Lance Stewart, Bart Staker, David Baker, Peter Myler,

- Seattle Childrens Research Institute Center for Global Infectious
- (1) Disease Research

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#### ABS430/BOD74

Novel Structure of Flavohemoglobin from Malassezia yamatoensis Determined by SAD Phasing

- Madison Bolejack, 1, Jan Abendroth, David Fox III,
- Thomas Edwards, Peter Myler, Stephen Mayclin,
- SSGCID/UCB

#### AB\$431/BOD151

Discerning the biochemical function for the catalytic domain of the Plasmodium BEM46-like protein (PBLP) Anna Groat Carmona, 1, Koryn Aguon, Misaki Seto,

- University of Washington Tacoma

#### ABS432/BOD4

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Characterization of mechanisms involved in Sbp1 reversible protein aggregation on Saccharomyces cerevisiae Jesus Ruiz Flores, 1, Francisco Torres Quiroz,

National Autonomous University of Mexico

#### ABS433/BOD82

Structural Insights into the Evolution of the CAZy GT8 Glycosyltransferase Glycogenin Hyun Woo Kim, 1, Msano Mandalasi, Zachary Wood, Christopher West.

(1) Department of Biochemistry and Molecular biology, University of Georgia

#### ABS434/BOD12

The Protonation State of an Evolutionarily Conserved Histidine Modulates Domain Swapping Stability of the DNA-binding Domain of Human FoxP1 Exequiel Medina, 1, Ricardo Coñuecar, Cesar A. Ramírez-Sarmiento,

Departamento de Biología, Facultad de Ciencias, (1) Universidad de Chile

#### ABS435/BOD84

Structure-based Design of Selective Inhibitors Against the BACE **Protein Family** Emma Lendy, 1, Emilio Cardenas, Yu-Chen Yen, Arun Ghosh, Andrew Mesecar,

(1) Department of Biochemistry, Purdue University

Pastens

#### AB\$436/BOD41

Towards Synthetic Allosteric Transcriptional Modulators: Defining the Role of Conformational Entropy in Coactivator Complexes Amanda Peiffer, 1, Charles Brooks III, Anna Mapp

(1) University of Michigan

#### ABS437/BOD46

Analysis of Calmodulin-Interacting Proteins Captured in Live Cells by Photoactivated Cross-linking: Evidence for an Active Ca2+ Signaling Microdomain

Anthony Persechini, 1, DJ Black, Quang-Kim Tran,

Andrew Keightley, Ameya Chinawalker, Cole McMullin, University of Missouri at Kansas City

#### AB\$438/BOD23

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#### The development of E. coli expression system for G proteincoupled receptors

Nanao Suzuki, 1, Yuuki Takamuku, Chika Yoshida, Takeshi Murata, Graduate School of Science, Chiba University

#### AB\$439/BOD150

Intra-Melanosomal Domains of Human Recombinant Tyrosinases Prone to Protein Aggregation at Physiological Temperatures Monika Dolinska, 1, Claudia Kassouf, Paul Wingfield, Yuri Sergeev, National Eye Institute/NIH

#### ABS440/BOD114

#### Engineering scFv Antibody Against Conserved Regions of **Dengue Virus Envelope Protein**

- Abhishek S Rathore, 1, Rinkoo D Gupta,
- Colorado State University

#### ABS441/BOD83

A Rationally Designed Plant-Produced IgA Has Improved Yield And Exhibits Cross Serotype Protection Against Enterohemorrhagic Escherichia Coli Adam Chin-Fatt, 1, Rima Menassa,

(1) Western University

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#### ABS442/BOD93

#### Structure of the PR Domain from PRDM3 and its Function in Acute Myeloid Leukemia

- Sharon Loa, 1, Tung-Chung Mou, Kelly McGlynn,
- Archibald Perkins, Stephen Sprang, Klara Briknarova,
- Department of Chemistry and Biochemistry,
- University of Montana

#### ABS443/BOD15

Influences of unstructured hinge polypeptides on the folding, and purification of a conventional kinesin heavy chain motor protein Tai-Chih Kuo,1, Yih-An Jian,

(1) Dept. Biochemistry & Molecular Cell Biology, Taipei Medical University

#### ABS444/BOD139

#### Mutation-Based Tuning of the Rice Cyclophilin LRT2

- Nathan Korson, 1, Lucila Andrea Acevedo, Linda Nicholson,
- (1)Cornell University

#### AB\$445/BOD140

#### Conformational Dynamics of Deubiquitinase A in Regulation and Substrate Specificity

- Ying Li, 1, Ashish Kabra, Efsita Rumpa,
- University of Louisville (1)

#### ABS446/BOD63

Single-molecule force spectroscopy reveals cooperative interfaical metal sites in human antibacterial protein \$100A12 homodimer Peng Zheng, 1,

Nanjing University

#### AB\$447/BOD129

Altering the conformational specificity of DNA binding proteins Seul Ki Lee, 1, Chan Yang Park, Chaehee Park, Hee-Jung Choi, Yang-Gyun Kim,

Sungkyunkwan University

#### ABS448/BOD75

(1)

Protein-induced structural deviations of Z-DNA Hyuk Won, 1, Chaehee Park, Ji-Ye Yun, Young Eun Won, Hee-Jung Choi, Yang-Gyun Kim, Sungkyunkwan University

(1)



#### ABS449/BOD59

#### Coarse-Grained Protein Modelling with SURPASS

- Dominik Gront, 1, Justyna Krys,
- (1) University of Warsaw Faculty of Chemistry

#### ABS450/BOD12

#### An Evolutionarily Conserved Mechanism of Amylin Misfolding in

- Type 2 Diabetes Caitlyn Fields, 1, Justin Lomont, Kacie Rich, Sidney Dicke,
- Megan Petti, Martin Zanni,
- (1) University of Wisconsin, Madison

#### ABS451/BOD89

#### Investigating the fitness effect of mutations in the diphthamide histidine of human elongation factor 2

- John Weldon, 1, Brian Masters, Nadim Alkharouf, Benjamin Atha, Jack Sanford, Lauren Russell, John Cyprien,
- (1) Towson University

#### (.)

- AB\$452/BOD151 An inactivated dimeric Vibrio alkaline phosphatase converts to a state with a different promiscuous activity Jens Gudmundur Hjörleifsson, 1, Kristófer Arnar Eiríksson, Bjarni Ásgeirsson,
- (1) University of Iceland

#### ABS453/BOD84

#### Nonlinear Partial Correlation To Identify Contribution Of Residues In Global Conformational Dynamics Amitava Roy, 1, Michael Bender, Rong Yang, Paula Lei,

KC Cheng, Frank Arnold, NIH

## (1) NH

#### ABS454/BOD29

#### **Hx to measure membrane protein electrostatics** Esther Brielle, 1, Isaiah T Arkin,

 The Alexander Grass Center for Bioengineering. The Hebrew University of Jerusalem, Edmond J. Safra Campus

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#### ABS455/BOD50

#### Studies on human epidermal growth factor receptor 2/4 (Her2/4) inhibitors that cause changes in protein expression level of protozoan parasite, Toxoplasma gondii Won-Kyu Lee, 1, Hye-Jin Ahn, Jaehui Park, Seul gi Oh,

Hyeweon Kang, Myung-Ho Sohn, Hojin Yoo, Hye-Jung Kim, Saehae Choi, Dae Young Kim, Jurang Woo, Ho-Woo Nam, New Drug Development Center, OSONG Biomedical

(1) New Drug Developmer Innovation Foundation

#### ABS456/BOD85

#### Comparison of kinetics of purified antibody and animal cell expression sup using BLI system Myung ho Sohn, 1, Myung ho Sohn, HOJIN Yoo, Won-Kyu Lee, Sora Park, Saehae Choi, So-Young Choi,

(1) New Drug Developmnet Center, Osong Medical Innovation Foundation

#### AB\$457/BOD5

#### Amyloid-642 Aggregate Structure from Large-scale Mutational Data

Floriane Ngako Kameni, 1, Vanessa E. Gray, Katherine A. Sitko, Douglas M. Fowler,

Seattle Children's Research Institute

#### ABS458/BOD42

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#### Chromatin as Viewed by Ubiquitin Writers: Determinants of H2A Site Specificity by RING Ubiquitin E3 ligases, BRCA1/BARD1 and Ring1b/Bmi1

- Sam Witus, 1, Alex Zelter, Evie Henry, Mikaela Stewart,
- Trisha Davis, Rachel Klevit,
- University of Washington School of Medicine

#### AB\$459/BOD24

#### Engineered Virus-Like-Particles for GPCR Specific Therapeutic Antibody Discovery

- Mart Ustav, 1, Jarrett Adams, Sachdev Sidhu,
- University of Toronto

#### ABS460/BOD154

Predicting Protein-Protein Interface Domains Using Multiple Scale Analysis

Ben Tribelhorn, 1, Mike Bailey, University of Portland



#### ABS461/BOD76

#### Cryo-EM Structure of the Gene Therapy Vector, Adeno-Associated Virus, with its Cell Receptor, AAVR

Nancy Meyer, 1, Guiqing Hu, Omar Davulcu, Qing Xie, Alex Noble, Craig Yoshioka, Drew Gingerich, Andrew Trzynka,

Larry David, Scott Stagg, Michael Chapman, Oregon Health and Science University

#### ABS462/BOD44

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#### MAF1b from Toxoplasma gondii Interacts with Human RalGAPa1, Potentially Altering Host Immune Signalling

Cameron Powell, 1, Matthew Blank, Reece Hoffman, John Burke, John Boyle, Martin Boulanger,

University of Victoria

#### ABS463/BOD45

Targeted Mutational Perturbations Of The Small Gtpase Ran Reveal How Pleiotropy Is Encoded In A Model Molecular Switch Christopher Mathy, 1, Tina Perica, Yang Zhang, Jiewei Xu, Gwendolyn Jang, Danielle Swaney, Nevan Krogan, Tanja Kortemme,

University of California, San Francisco

#### ABS464/BOD77

#### Cis-acting Glycan Drives Protein-Protein Interactions of Skp1 in Dictyostelium and Toxoplasma

- Hyunwoo Kim, 1, Alexander Eletsky, James Prestegard,
- (1) University of Georgia

#### AB\$465/BOD25

#### Efforts to Enhance the Expression of Functionally Active Membrane Proteins using BacMam expression system Srivanya Tummala, 1, Noel Byrne, Jennifer Shipman,

James Kostas, Richard Edwards, Kaspar Hollenstein, Harini Krishnamurthy, Alexei Brooun, Stephen Soisson,

(1)Merck & Co.

#### ABS466/BOD129

#### Engineering the Next Generation of SH2 Superbinders to Probe the Phosphoproteome and Antagonize cancer cell signalling

Greg Martyn, 1, Gianluca Veggiani, Sachdev Sidhu, 1)60 Department of Molecular Genetics, University of Toronto



ABS467/BOD97

#### Increasing Surface Charge Converts Spy Into A More Efficient Chaperone

- Wei He, 1, Jiayin Zhang,
- East China University of Science and Technology

#### ABS468/BOD86

The Multiple Conformer Story: Characterization of 10E8 Antibody Constructs by SEC, HIC and Molecular Dynamics Simulations Michael Bender, 1, Amitava Roy, Sylvie Yang, Yile Li, Xiangchun Wang, Frank Arnold, Paula Lei,

Vaccine Production Program, VRC, NIAID, NIH

#### AB\$469/BOD131

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Construction of Chimeric Calbindin D9k Proteins Showing a Ca2+ Induced -Conformational Change Emma Liliana Arévalo-Salina, 1, Humberto Flores-Soto, Joel Osuna-Quintero, Gloria Saab-Rincón,

(1) Instituto de Biotecnología, UNAM

#### AB\$470/BOD130

Machine-Learning-Guided Mutagenesis for Directed Evolution of Fluorescent Proteins

- Tomoshi Kameda, 1, Yutaka Saito, Misaki Oikawa,
- Hikaru Nakazawa, Teppei Niide, Koji Tsuda, Mitsuo Umetsu, Artificial Intelligence Research Center, AIST

#### AB\$471/BOD155

Substrate-based Allosteric Regulation of a Homodimeric Enzyme Christopher Di Pietrantonio, 1, Pedram Mehrabi, Tae Hun Kim, Adnan Sljoka, Christopher Ing, Regis Pomes, Emil F. Pai, R Scott Prosser

Department of Chemistry, University of Toronto (1)

#### AB\$472/BOD155

Assessing The Resilience of Proteins to the Effects of Drugs Tess Thackray, 1, Bodi Van Roy, Filip Jagodzinski,

Western Washington University

#### ABS473/BOD60

(1)

#### A Scalable Compute Framework for Generating and Assessing **Protein Mutants**

Dylan Carpenter, 1, Michael Albert, Sam Herr, Filip Jagodzinski, Western Washington University



#### AB\$474/BOD133

Designed Protein Logic for Ultra-Specific Cell Targeting Marc Lajoie, 1, Scott Boyken, Alexander Salter, Anusha Rajan, Robert Langan, Audrey Olshefsky, Vishaka Muhunthan, Mesfin Gewe, Alfredo Quijano Rubio, Colin Correnti, Stanley Riddell, David Baker.

Institute for Protein Design, University of Washington, Seattle, (1) WA, USA; Department of Biochemistry, University of Washington, Seattle, WA, USA

#### AB\$475/BOD122

Integrating the influence of pH in NMR chemical shift prediction Methods

- Efrosini Artikis, 1, Charles Brooks III,
- (1)Graduate Student

#### ABS476/BOD98

- Large-scale characterization of PTEN missense variants that differentially affect intracellular protein abundance and phosphatase activity
- Kenneth Matreyek, 1, Douglas Fowler, Jason Stephany, University of Washington (1)

#### AB\$478/BOD62

- Regulatory mechanisms of the deubiquitinase BAP1 Maxime Uriarte, 1, Salima Daou, Haithem Barbour, Oumamai Ahmed, Louis Masclef, Caroline Baril, Nadine Sen Nkwe, Eric Bonneil, Derek Ceccarelli, Jean-Yves Masson, Pierre Thibault, Frank Sicheri, Haining Yang, Michele Carbone, Marc Therrien, El Bachir Affar Maisonneuve-Rosemont Hospital Research Center and
- (1) Department of Medicine, University of Montréal

#### AB\$479/BOD85

Structural Characterization of the LC8-RavP Complex Reveals a
New Role for LC8 in Lyssavirus Phosphoproteins
Nathan Jespersen, 1, Cedric Leyrat, Francine Gérard,
Jean-Marie Bourhis, Danielle Blondel, Marc Jamin, Elisar Barbar,
Oregon State University

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#### AB\$480/BOD104

#### Harnessing the Natural Properties of HUH-endonucleases for Covalent Protein-DNA Linkage Technologies Kassidy Tompkins, 1, Andrew Nelson, Blake Everet,

- Andrew Lemmex, Lidia Swanson, Wendy Gordon,
- (1)University of Minnesota

#### ABS481/BOD87

#### Determination of Protein Complex Architecture Guided by Low-Resolution Cryo-Electron Microscopy Density Daniel Farrell, 1, Frank DiMaio,

(1)University of Washington

#### ABS482/BOD78

- Structural and Functional Characterization of a Tristetraprolin Family Tandem Zinc Finger Protein Stephanie Hicks, 1, Ronald Venters, Wi Lai, Monica Pillon, Perry Blackshear,
- Signal Transduction Laboratory, National Institute of (1)Environmental Health Sciences

#### ABS483/BOD131

#### Computational Design of a De Novo, Modular Miniprotein T argeting PD-1

- Cassie Bryan, 1, Gabriel Rocklin, David Baker, University of Washington

#### ABS484/BOD13

Another Reason Why Solving Lots of Protein Structures is Useful: Structural Diversity in the Mycobacteria DUF3349 Family Garry W. Buchko, 1, Jan Abendroth, John I. Robinson, Isabelle Phan, Wesley C. Van Voorhis, Peter J. Myler, Thomas E. Edwards, Pacific Northwest National Laboratory

#### ABS485/BOD87

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Subunit Mass Analysis for Monitoring Multiple Attributes of **Monoclonal Antibodies** 

Peiran Liu, 1, Bristol-Myers Squibb

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Interaction Studies of Calmodulin-Like Protein 19 (CML19), the Centrin 2 of Arabidopsis thaliana, with RAD4 and SAC3B target peptides

Matteo Trande, 1, Marco Pedretti, Paola Dominici, Alessandra Astegno,

(1) University of Verona

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