

33rd Annual Symposium
Program



June 30 - July 3, 2019
www.proteinsociety.org



Mission

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.



#PS33
1986 - 2019

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Welcome



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.

Kind Regards,

Charles L. Brooks III, Ph.D.
President

#PS33



Program Planning Committee

Seattle | June 30 - July 3, 2019



C. Robert Matthews,
CHAIR, University of
Massachusetts
Medical School



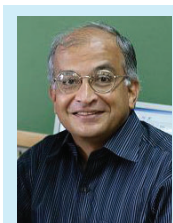
Michael Feig,
Michigan State
University



Karen Fleming,
John Hopkins University



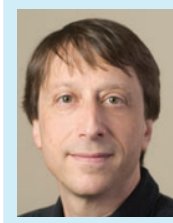
Sheena Radford,
University of Leeds



Jayant Udgaonkar,
Indian Institute of Science
Research & Education



Gerhard Wagner,
Harvard University



William Weis,
Stanford University

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Andrew Vendel, Ph.D.

Eli Lilly

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William Holmes

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Kathryn McMenimen, Ph.D.

Mount Holyoke College

Denise Okafor, Ph.D.

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Priyanka Narayan,

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Donald Spratt

Clark University

Vishwa Trivedi

Bethune-Cookman University



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Prem Kumarathasan, Ph.D.
Health Canada

Jinsong Liu, Ph.D.
MD Anderson

Sanela Marfic, Ph.D.
Oakland University

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Argonne National Laboratory

Cesar Ramirez-Sarmiento, Ph.D.
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Philipp Schmidpeter, Ph.D.
Weill Cornell Medical College

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Brian Shilton, Ph.D.
University of Western Ontario

Jeffrey L Urbauer, Ph.D.
University of Georgia

Jill Zeilstra-Ryalls, Ph.D.
Bowling Green State University



Corporate Support

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

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Thank you for helping us celebrate 33 years of impact.

#PS33 Registration

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

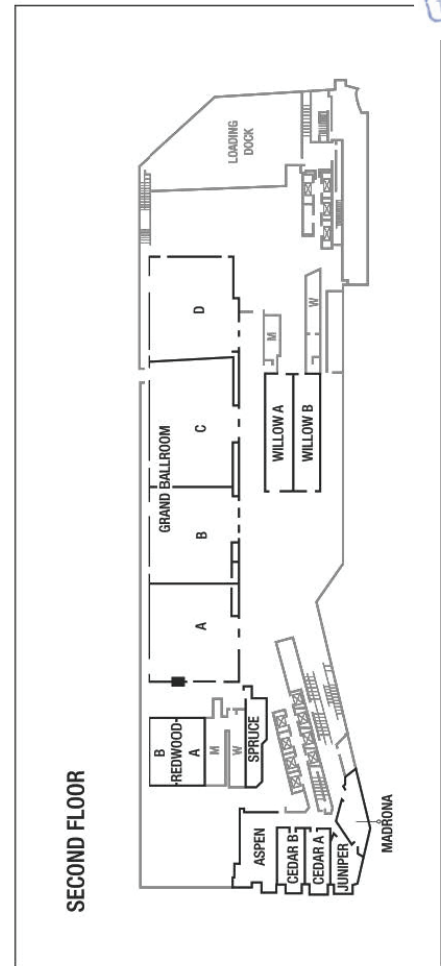
Saturday, June 29:	5:00 p.m. - 8:00 p.m.
Sunday, June 30:	7:00 a.m. - 6:30 p.m.
Monday, July 1:	7:30 a.m. - 7:00 p.m.
Tuesday, July 2:	8:30 a.m. - 7:00 p.m.
Wednesday, July 3:	8:30 a.m. - 12:00 p.m.

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



Him

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
The Protein Society Councilor

Elizabeth Meiering
The Protein Society Councilor

Charney Robinson-Williams
Director of Events and Communications for The Protein Society

Posters



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.

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!





General Info

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.com/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 station 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

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 download, for both iPhone and Android.



Cameras/Video Recording

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

Mobile Devices

As a courtesy to your fellow attendees, please silence all cell phones 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: PS33 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.



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TPS Membership



	1 Year Price/ Discount Code	2 Year Price/ Discount Code	5 Year Price/ Discount Code
Undergraduate	Regular Rate: \$25 Early-Bird Rate: \$20 Code: kxuesyfv	Regular Rate: \$50 Early-Bird Rate: \$40 Code: hzapbec9	
Graduate	Regular Rate: \$50 Early-Bird Rate: \$40 Code: vt8bupqd	Regular Rate: \$90 Early-Bird Rate: \$75 Code: xdhsxh4	
Early-Career	Regular Rate: \$100 Early-Bird Rate: \$80 Code: ppb3r6vt	Regular Rate: \$180 Early-Bird Rate: \$150 Code: vhnemwn	Regular Rate: \$475 Early-Bird Rate: \$375 Code: ujnuurf
Lab Staff	Regular Rate: \$50 Early-Bird Rate: \$40 Code: axkbqrhu	Regular Rate: \$90 Early-Bird Rate: \$75 Code: azsjdkhf	Regular Rate: \$230 Early-Bird Rate: \$180 Code: gjkfzsfb
Full	Regular Rate: \$200 Early-Bird Rate: \$150 Code: zkmbg6wx	Regular Rate: \$380 Early-Bird Rate: \$285 Code: 7sj9cxrk	Regular Rate: \$950 Early-Bird Rate: \$700 Code: kzxgwn99
Emeritus	Regular Rate: \$25 Early-Bird Rate: \$20 Code: 7d4dmat9	Regular Rate: \$50 Early-Bird Rate: \$40 Code: wurmkky	Regular Rate: \$115 Early-Bird Rate: \$90 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.



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 Editor-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



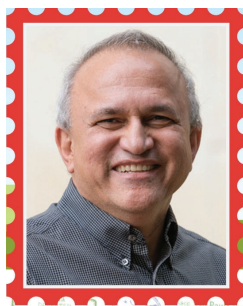
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2019 Protein Society

Award Winners

Dave Thirumalai, Ph.D., University of Texas at Austin

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



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.

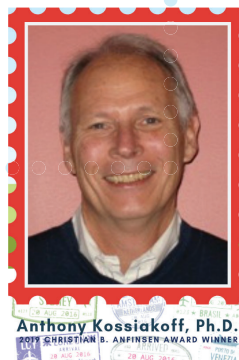
Dame Carol Robinson, Ph.D., University of Oxford

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



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

Hao Wu, Ph.D., Harvard University

2019 Dorothy Crowfoot Hodgkin Award Winner - Sponsored by Genentech



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.



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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 BRÄNDÉN AWARD WINNER

The 2019 recipient of this award is Professor Minoru Kanehisa (Kyoto University). Professor Kanehisa is one of the world leaders in the bioinformatics field. The KEGG (Kyoto Encyclopedia of Genes and Genomes) database, which he established in 1995 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 systems from the organismal-level, to the cell-level, to the molecular level and includes genomic, chemical, and human health data both for understanding biological systems and practical applications in society. Professor 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 Asia Pacific Protein Association (APPA).

Shahriar Mobashery, Ph.D., University of Notre Dame
2019 Emil Thomas Kaiser Award Winner



Shahriar Mobashery, Ph.D.
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.



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



Gabriel Lander, Ph.D.
2019 PROTEIN SCIENCE YOUNG INVESTIGATOR AWARD WINNER

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

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 protein 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 understanding of the determinants of protein structure and stability that leads to consistent predictive capabilities, including the ability to design protein shapes and functions as desired.



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Protein Science Best Paper Award Winners

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



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.

As noted by Dr. McCammon, "Mindy is a remarkably versatile young theoretician of protein 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 represents a novel opportunity for drug discovery. In addition to her outstanding research, Mindy has been active in mentorship of students in the groups 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.
PALL CORPORATION

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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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 Travel 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



2019 Protein Science Young Investigator Travel Award Recipients

Jun Liu, University of California, San Francisco
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
Ari 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 Outstanding 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
Purna Sharma, Arizona State University
Jonathan Williams, Rutgers University

#PS33

At A Glance

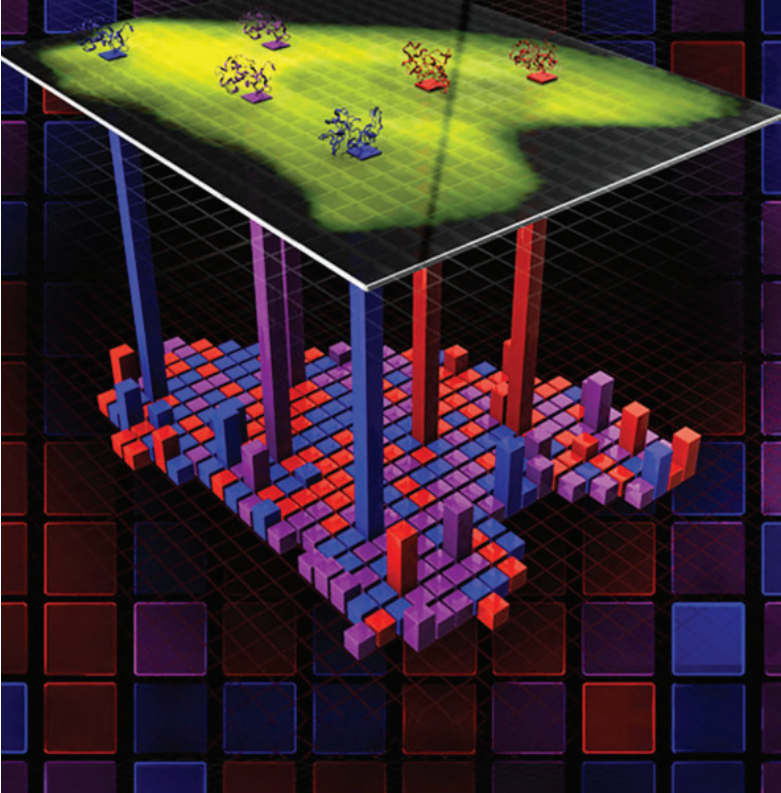


	Sat., 6/29	Sun., 6/30	Mon., 7/1		Tues., 7/2	Wed., 7/3		
7:15 a.m.			New Member Welcome Breakfast/ Member Business Meeting (7:30 – 8:15 a.m.) Cedar A & B					
7:30 a.m.								
8:30 a.m.		Opening Plenary Session Grand Ballroom A & B	Chaperoning Aggregation and Proteostasis: Life and Death in a Cell Grand Ballroom A	Folding, Function & Quality Control of Membrane Proteins Grand Ballroom B	Selectivity in Protein-Protein Interactions: From Design to Control Grand Ballroom A	What Do Proteins Do When They Are Crowded? Does it Matter? Grand Ballroom B	Structural Elucidation of Protein Complexes by Mass Spectrometry Grand Ballroom A	Signaling Across the Membrane, G-Protein Coupled Receptors Grand Ballroom B
9:10 a.m.		CryoEM Workshop Cedar A & B						
9:40 a.m.		Mechanobiology – Force- Dependent Protein Interactions with Cytoskeleton Grand Ballroom A	Timing is of the Essence: Dynamics and Kinetics of Biological Function via Experiment and Simulation Grand Ballroom B					
11:30 a.m.		Exhibits Open Grand Ballroom C & D (11:30 a.m. – 1 p.m.) ForteBio Exhibitors' Workshop Cedar A & B (11:30 a.m. – 1 p.m.)	Exhibits Open Grand Ballroom C & D (11:45 a.m. – 1 p.m.) Educators' Workshop – Willow A & B (Noon – 1:10 p.m.) Wiley Publisher's Workshop – Cedar A & B (Noon – 1:10 p.m.)	Exhibits Open Grand Ballroom C & D (11:45 a.m. – 1:30 p.m.) Undergrad Research Session Willow A & B (12:15 – 1:30 p.m.)	Closing Plenary Session (10:20 – 11:45 a.m.) Grand Ballroom A			
1:10 p.m.		Mechanisms of Protein Aggregation Grand Ballroom A	Protein Folding and Dynamics: Experiments and Simulations Grand Ballroom B	Proteins in the Membrane: Dynamics and Recognition Grand Ballroom A	Unrestricted Bullies in the Cell - Large Protein Systems in Solution Grand Ballroom B	Plenary Awards Session Grand Ballroom A & B		
4:30 p.m.		Posters Open/Exhibits/Mix & Mingle (4:30 – 6:30 p.m.) – Grand Ballroom CD						
		Networking Event – RSVP ONLY (6:45 – 7:45 p.m.) Grand Ballroom B	Mentoring Panel Willow A & B (6:45 – 7:45 p.m.)		Posters Open/Exhibits/Mix & Mingle (5:30 – 7:30 p.m.) Grand Ballroom C & D			
	Sounders' Game Century Link Field (7 p.m.)				Members' Reception – ALL WELCOME Grand Ballroom B (8:30 – 10 p.m.)			

PROTEIN SCIENCE

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Special Issue: Proteins in the Cell



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 Program

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*
Eva-Maria Strauch, University of Georgia;
Athens, Georgia; United States

9:45 - 10:15 a.m. *Dissecting Structural Mechanisms of Force-sensitive
Actin Binding*
Greg Alushin, 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*
Pearl Magala, 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*
Timothy Springer, Harvard University; Cambridge,
Massachusetts; United States

28 * travel support provided by Fred Hutchinson Cancer Research Center

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

9:40 - 9:45 a.m. *Introduction From Chair*
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

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

#PS33 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
- 1:15 - 1:45 p.m. *Amyloid Fibrils: Structure, Energetics, and Function*
David Eisenberg, University of California, Los Angeles; 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 Ozelik, 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
- 3:45 - 4:00 p.m. *Dynamics of Amyloid Fibrils Play a Role in Seeding and Propagating the Aggregation of α -Synuclein*
Jonathan Williams, Rutgers University; New Brunswick, 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



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*
Karin Crowhurst, 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
Abhay Thakur, 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*
Shachi Gosavi, 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*
Martin Gruebele, University of Illinois; Urbana-Champaign, Illinois; United States

Poster Presentation and Mix & Mingle Reception, 4:30 - 6:30 p.m. | Grand Ballroom C & D

Networking Event | 6:45 - 7:45 p.m. | Grand Ballroom B



#PS33

Program

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*
Mark Herzik, University of California, San Diego;
San Diego, California; United States
- 8:35 - 9:05 a.m. *Chaperone Functions in Protein Folding and Proteome Maintenance*
Ulrich Hartl, 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, Georgia; United States
- 11:15 - 11:45 a.m. *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 Schleich, Indiana University; Bloomington, Indiana; United States
- 9:05 - 9:35 a.m. *Unfolding and Refolding of Individual Bacteriorhodopsin Molecules Probed with 1- μ s 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 p13II 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



Program

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*
Stephan Grzesiek, 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**
- 3:15 - 3:45 p.m. *Receptor Clustering and Activation Driven by its Transmembrane Anchor*
James Chou, Harvard Medical School; Cambridge, Massachusetts; United States
- 3:45 - 4:00 p.m. *Native-state Prolyl Isomerization is Involved in the Activation of a CNG Channel*
Phillip Schmidpeter, Weill Cornell Medical College; New York, New York; United States
- 4:00 - 4:30 p.m. *The Chaperonin TRiC/CCT Associates with Prefoldin Through a Conserved Electrostatic Interface Essential for Cellular Proteostasis*
Daniel Gestaut, Stanford University; Palo Alto, California; United States

Day 2 - Monday, July 1, 2019 (cont.)

CONCURRENT AFTERNOON SESSION 2

Unrestricted 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*
Mikaela Stewart, Texas Christian University; Fort Worth, Texas; United States
- 1:15 - 1:45 p.m. *Structural Basis for the Binding of Non-native Proteins by Molecular Chaperones*
Charalampos Kalodimos, St. Jude Children's Research Hospital; Memphis, Tennessee; United States
- 1:45 - 2:15 p.m. *Targeting KRAS Oncoprotein at Biological Membranes*
Mitsu Ikura, 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-jump X-ray Crystallography and Solution Scattering*
Michael Thompson, 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*
Stefan Bibow, University of Basel; Basel, Switzerland
- 4:00 - 4:30 p.m. *Activation of the Exocyst Tethering Complex for Snare Complex Regulation and Membrane Fusion*
Mary Munson, University of Massachusetts Medical School; Worcester, Massachusetts; United States

Poster Presentation and Mix & Mingle Reception 4:30 - 6:30 p.m. | Grand Ballroom C & D

Mentoring Panel | 6:45 - 7:45 p.m. | Willow A & B

#PS33 Program

Day 3 - Tuesday, July 2, 2019



CONCURRENT MORNING SESSION 1

Selectivity 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*
Jeanine Amacher, Western Washington University; Bellingham, Washington; United States
- 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. *Engineering Linkage-Specific Polyubiquitin Antibodies: Tools for Elucidation of Novel Signaling Pathways*
Marissa Matsumoto, Genentech; San Francisco, 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

Coffee Break | 9:50 - 10:15 a.m. | Grand Ballroom C & D

- 10:15 - 10:45 a.m. *From Systems Biology to Systems Biologics*
Dev Sidhu, University of Toronto; Toronto, Canada
- 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. *A Molecular View of the Liquid to Gel Phase Transition of Heterochromatin Protein HP1 α*
Galia Debelouchina; University of California, San Diego; San Diego, California; United States

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

CONCURRENT MORNING SESSION 2

What do Proteins do When They Are Crowded? Does it Matter?
8:30 - 11:45 a.m. | Grand Ballroom B

- 8:30 - 8:35 a.m. *Introduction From Chair*
David Ban, Merck; Kenilworth, New Jersey; United States
- 8:35 - 9:05 a.m. *Exploring the Determinants of Protein Crowding Effects by Molecular Simulation*
Rebecca Wade, Heidelberg Institute for Theoretical Studies gGmbH; Heidelberg; Germany
- 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
- 9:35 - 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
Yu-ming "Mindy" Huang; University of California San Diego; San Diego, California; United States

Coffee Break | 9:50 - 10:15 a.m. | Grand Ballroom C & D

- 10:15 - 10:45 a.m. *Protein Folding, Aggregation and Phase Separation in the Cell*
Simon Ebbinghaus, Ruhr-Universität Bochum; Bochum; Germany
- 10:45 - 11:15 a.m. *Protein Crowding at Membrane Surfaces*
Jeanne C. Stachowiak, University of Texas at Austin; Austin, Texas; United States
- 11:15 - 11:45 a.m. *Critical Phenomena in the Temperature-pressure-crowding Phase Diagram of a Protein*
Margaret Cheung; University of Houston; Houston, Texas; United States

Box Lunch Pickup | 11:45 a.m. - 1:30 p.m. | Grand Ballroom C & D

Undergrad Research Session | 12:15 - 1:30 p.m. | Willow A & B

#PS33 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
1:40 - 2:10 p.m. GroEL and RNA Chaperones as Stochastic Machines
2019 Hans Neurath Award Winner **Dave Thirumalai**, University of Texas at Austin; Austin, Texas, United States
- 2:10 - 2:15 p.m. Presentation - Dorothy Crowfoot Hodgkin Award
2:15 - 2:45 p.m. 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. Presentation - Christian B. Anfinsen Award
2:50 - 3:20 p.m. 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. |
Grand Ballroom B

Day 4 - Wednesday, July 3, 2019

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
Benjamin Garcia, 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
Stephanie Zimmerman, 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 β 2AR-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
David Baker, University of Washington; Seattle, Washington; United States

11:30 - 11:45 a.m. *Closing*
Charles L. Brooks III, University of Michigan

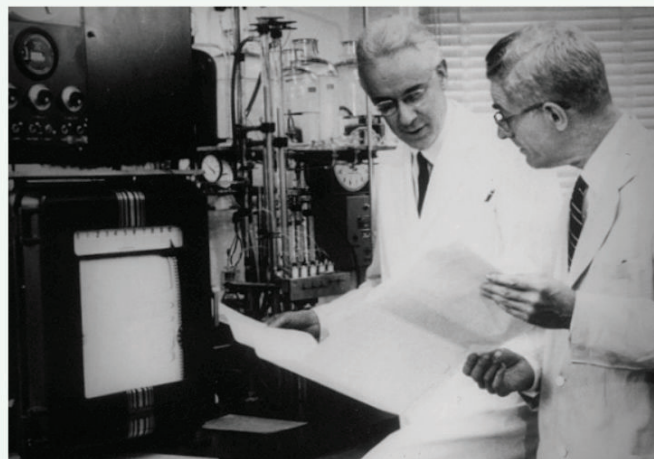


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educator's workshop



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



WILLOW ROOM

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 #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



mentoring
panel

Monday, July 1
6:45 - 7:45 p.m.
Willow Room



THE
PROTEIN
SOCIETY

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Exhibitor Directory

BECKMAN COULTER

5350 Lakeview Parkway S. Drive
Indianapolis, Indiana 46268, United States
Phone: 800-742-2345
Email: oadiguida@beckman.com
Web: www.beckman.com

BOOTH 8

Beckman Coulter Life Sciences develops, manufactures and markets products that simplify, automate and innovate complex biomedical testing. For more than 75 years, our products have been making a difference in people's lives by improving the productivity of medical professionals and scientists, supplying critical information for improving patient health and delivering trusted solutions for research and discovery. Scientists use our life science research instruments to study complex biological problems including causes of disease and potential new therapies or drugs.

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BOOTH 5

Bon Opus Biosciences is a NJ-based Contract Research Organization. Our areas of expertise include gene synthesis, custom protein expression, and custom antibody production. All proteins have activity and purity data testing performed and reported. In addition to our vast recombinant protein catalog featuring up to 2,000 protein products, we also carry a comprehensive catalog of over 3,000 primary antibodies, both monoclonal and polyclonal. Each antibody has distinct data recorded on their datasheet. Bon Opus has built several service programs that are specifically designed to support the development of targeted therapeutics -in particular, antigen production and monoclonal antibodies.

CELL FREE SCIENCES

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Email: tech-sales@cfsciences.com
Web: http://www.cfsciences.com/eg/
Web: http://www.cfsciences.com/jp/index.html

BOOTH 10

CellFree Sciences (CFS) is an ISO9001:2015 certified provider of comprehensive solutions for wheat germ cell-free protein production and analysis using the ENDEXT® Technology Platform originally developed in the laboratory of Prof. Yaeta Endo at Ehime University in Japan. With our different WEPRO® wheat germ protein expression extracts, CFS is serving the research community and customers in industry with protein synthesis services, reagents, and the fully automated Protomist® robotic protein production systems.

FLUIDIC ANALYTICS

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Web: https://www.fluidic.com/

BOOTH 4

Fluidic Analytics' vision is that protein science will transform our understanding of how the biological world operates in real time, a transformation every bit as revolutionary as the one we've seen in DNA sequencing. And Fluidic Analytics aim to make this vision a reality by developing products that enable easier, faster, more convenient and more accurate protein characterisation. Our first product – the Fluidity One – measures changes in protein size caused by folding, aggregation or interactions in solution in biologically relevant timescales, without the need for matrices or surfaces and without a bias towards large species. And because measurement is fast and requires as little as 50 nanograms of protein this makes the Fluidity One perfect for rapid quantification and characterisation - from small peptides to large complexes and over a wide range of concentrations.

#PS33 Exhibitor Directory

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Molecular Devices, LLC.
3860 N First Street
San Jose, CA 95134 USA
Phone: 800/635-5577
Gemma.Milan@moldev.com
Web: <https://www.moleculardevices.com/products/biologics>

ForteBio, a business unit of Molecular Devices LLC, offering products that span multiple technology vectors including analytical instrumentation and software, clone picking and imaging, and customized engineering solutions. We partner with our customers in biologics and other life sciences segments to unlock workflow bottlenecks, provide best-in-class products and first-class service.

MALVERN ANALYTICAL **BOOTH 9**
117 Flanders Road
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Web: www.malvern.com

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Web: www.nicoyalife.com

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Biochemistry
117 Schweitzer Hall
University of Missouri
Columbia, MO 65211
Phone: 573/882-4845
<https://pncc.labworks.org/>
chapmanms@missouri.edu

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68 Elm Street
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Phone: 800-762-4000
Email: customercareUS@perkinelmer.com
Web: www.perkinelmer.com

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<https://www.refeyn.com/>

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262 Danny Thomas Place, MS 276
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Canyon Country, California 91386, United States
Phone: 844-377-6834
Email: staff@proteinsociety.org | Web: www.proteinsociety.org

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call for nominations

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.

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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

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Poster/Abstract

June 30, 2019

AbS	Board (BOD)	Track	Date
ABS008	1	1. Amyloid and aggregation	6/30/2019
ABS145	2	1. Amyloid and aggregation	6/30/2019
ABS019	3	1. Amyloid and aggregation	6/30/2019
ABS147	4	1. Amyloid and aggregation	6/30/2019
ABS041	5	1. Amyloid and aggregation	6/30/2019
ABS062	6	1. Amyloid and aggregation	6/30/2019
ABS053	7	1. Amyloid and aggregation	6/30/2019
ABS057	8	1. Amyloid and aggregation	6/30/2019
ABS134	9	1. Amyloid and aggregation	6/30/2019
ABS040	10	1. Amyloid and aggregation	6/30/2019
ABS044	11	1. Amyloid and aggregation	6/30/2019
ABS434	12	10. Folding	6/30/2019
ABS226	13	10. Folding	6/30/2019
ABS276	14	10. Folding	6/30/2019
ABS443	15	10. Folding	6/30/2019
ABS274	16	10. Folding	6/30/2019
ABS034	17	11. Intrinsically disordered proteins	6/30/2019
ABS138	18	11. Intrinsically disordered proteins	6/30/2019
ABS150	19	11. Intrinsically disordered proteins	6/30/2019
ABS087	20	12. Membrane proteins	6/30/2019
ABS020	21	12. Membrane proteins	6/30/2019
ABS092	22	12. Membrane proteins	6/30/2019
ABS029	23	12. Membrane proteins	6/30/2019
ABS143	24	12. Membrane proteins	6/30/2019
ABS037	25	12. Membrane proteins	6/30/2019
ABS211	26	12. Membrane proteins	6/30/2019
ABS214	27	14. Motors & machines	6/30/2019
ABS424	28	14. Motors & machines	6/30/2019
ABS102	29	15. Peptides	6/30/2019
ABS295	30	15. Peptides	6/30/2019
ABS202	31	15. Peptides	6/30/2019
ABS017	32	16. Protein interactions and assemblies	6/30/2019
ABS009	33	16. Protein interactions and assemblies	6/30/2019
ABS011	34	16. Protein interactions and assemblies	6/30/2019
ABS099	35	16. Protein interactions and assemblies	6/30/2019
ABS038	36	16. Protein interactions and assemblies	6/30/2019
ABS016	37	16. Protein interactions and assemblies	6/30/2019
ABS035	38	16. Protein interactions and assemblies	6/30/2019
ABS108	39	16. Protein interactions and assemblies	6/30/2019
ABS071	40	16. Protein interactions and assemblies	6/30/2019
ABS049	41	16. Protein interactions and assemblies	6/30/2019
ABS068	42	16. Protein interactions and assemblies	6/30/2019
ABS055	43	17. Proteins in cells	6/30/2019
ABS144	44	16. Protein interactions and assemblies	6/30/2019
ABS082	45	16. Protein interactions and assemblies	6/30/2019

AbS	Board (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	72	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	76	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	84	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS249	85	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS331	86	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

Poster/Abstract

June 30, 2019

Abs	Board (BOD)	Track	Date
ABS351	93	21. Structure (x-ray/NMR/EM)	6/30/2019
ABS028	94	24. Therapeutics and antibodies	6/30/2019
ABS070	95	24. Therapeutics and antibodies	6/30/2019
ABS077	96	24. Therapeutics and antibodies	6/30/2019
ABS113	97	24. Therapeutics and antibodies	6/30/2019
ABS194	98	24. Therapeutics and antibodies	6/30/2019
ABS253	99	24. Therapeutics and antibodies	6/30/2019
ABS271	100	24. Therapeutics and antibodies	6/30/2019
ABS272	101	24. Therapeutics and antibodies	6/30/2019
ABS186	102	25. Transcription/translation/post-translational modifications	6/30/2019
ABS275	104	25. Transcription/translation/post-translational modifications	6/30/2019
ABS204	105	3. Chaperones	6/30/2019
ABS207	106	3. Chaperones	6/30/2019
ABS030	107	4. Chemical biology	6/30/2019
ABS021	108	4. Chemical biology	6/30/2019
ABS110	109	4. Chemical biology	6/30/2019
ABS184	110	4. Chemical biology	6/30/2019
ABS454	111	12. Membrane proteins	6/30/2019
ABS310	112	4. Chemical biology	6/30/2019
ABS369	113	4. Chemical biology	6/30/2019
ABS374	114	4. Chemical biology	6/30/2019
ABS025	115	5. Computational modeling/simulation	6/30/2019
ABS048	116	5. Computational modeling/simulation	6/30/2019
ABS237	117	5. Computational modeling/simulation	6/30/2019
ABS122	118	5. Computational modeling/simulation	6/30/2019
ABS321	119	5. Computational modeling/simulation	6/30/2019
ABS322	120	5. Computational modeling/simulation	6/30/2019
ABS032	121	6. Design/engineering	6/30/2019
ABS056	122	6. Design/engineering	6/30/2019
ABS043	124	6. Design/engineering	6/30/2019
ABS256	125	6. Design/engineering	6/30/2019
ABS084	126	6. Design/engineering	6/30/2019
ABS094	127	6. Design/engineering	6/30/2019
ABS166	128	6. Design/engineering	6/30/2019
ABS278	129	6. Design/engineering	6/30/2019
ABS107	130	6. Design/engineering	6/30/2019
ABS180	131	6. Design/engineering	6/30/2019
ABS212	132	6. Design/engineering	6/30/2019
ABS223	133	6. Design/engineering	6/30/2019
ABS072	134	6. Design/engineering	6/30/2019
ABS262	135	6. Design/engineering	6/30/2019
ABS171	136	6. Design/engineering	6/30/2019
ABS146	137	6. Design/engineering	6/30/2019
ABS063	138	7. Dynamics and allostery	6/30/2019
ABS174	139	7. Dynamics and allostery	6/30/2019

Abs	Board (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

Abs	Board (BOD)	Track	Date
ABS073	1	1. Amyloid and aggregation	7/1/2019
ABS078	2	1. Amyloid and aggregation	7/1/2019
ABS196	3	1. Amyloid and aggregation	7/1/2019
ABS213	4	1. Amyloid and aggregation	7/1/2019
ABS290	5	1. Amyloid and aggregation	7/1/2019
ABS230	6	1. Amyloid and aggregation	7/1/2019
ABS389	7	1. Amyloid and aggregation	7/1/2019
ABS254	8	1. Amyloid and aggregation	7/1/2019
ABS294	9	1. Amyloid and aggregation	7/1/2019
ABS363	10	1. Amyloid and aggregation	7/1/2019
ABS292	11	1. Amyloid and aggregation	7/1/2019
ABS450	12	1. Amyloid and aggregation	7/1/2019
ABS198	13	1. Amyloid and aggregation	7/1/2019
ABS337	14	10. Folding	7/1/2019
ABS340	15	10. Folding	7/1/2019
ABS329	16	8. Enzymology	7/1/2019
ABS152	17	11. Intrinsically disordered proteins	7/1/2019
ABS156	18	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	21	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	27	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

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Abs	Board (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	56	17. Proteins in cells	7/1/2019
ABS341	57	17. Proteins in cells	7/1/2019
ABS367	58	18. Proteomics	7/1/2019
ABS375	59	18. Proteomics	7/1/2019
ABS165	60	19. Proteostasis and quality control	7/1/2019
ABS403	61	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	66	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	73	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS359	74	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS136	75	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS364	76	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS151	77	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS370	78	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS378	79	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS162	80	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS420	81	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS433	82	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS182	83	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS435	84	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS479	85	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS218	86	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS481	87	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS076	88	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS221	89	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS288	90	21. Structure (x-ray/NMR/EM)	7/1/2019
ABS289	91	21. Structure (x-ray/NMR/EM)	7/1/2019

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Poster/Abstract

July 1, 2019

Abs	Board (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	133	6. Design/engineering	7/1/2019
ABS142	134	6. Design/engineering	7/1/2019
ABS282	135	7. Dynamics and allostery	7/1/2019
ABS406	136	7. Dynamics and allostery	7/1/2019

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Abs	Board (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

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Abs	Board (BOD)	Track	Date
ABS299	1	1. Amyloid and aggregation	7/2/2019
ABS315	2	1. Amyloid and aggregation	7/2/2019
ABS429	3	1. Amyloid and aggregation	7/2/2019
ABS432	4	1. Amyloid and aggregation	7/2/2019
ABS457	5	1. Amyloid and aggregation	7/2/2019
ABS004	6	10. Folding	7/2/2019
ABS311	7	10. Folding	7/2/2019
ABS357	8	10. Folding	7/2/2019
ABS277	9	11. Intrinsically disordered proteins	7/2/2019
ABS320	10	11. Intrinsically disordered proteins	7/2/2019
ABS334	11	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	14	12. Membrane proteins	7/2/2019
ABS168	15	12. Membrane proteins	7/2/2019
ABS199	16	12. Membrane proteins	7/2/2019
ABS216	17	12. Membrane proteins	7/2/2019
ABS217	18	12. Membrane proteins	7/2/2019
ABS234	19	12. Membrane proteins	7/2/2019
ABS269	20	12. Membrane proteins	7/2/2019
ABS286	21	12. Membrane proteins	7/2/2019
ABS313	22	12. Membrane proteins	7/2/2019
ABS438	23	12. Membrane proteins	7/2/2019
ABS459	24	12. Membrane proteins	7/2/2019
ABS465	25	12. Membrane proteins	7/2/2019
ABS015	26	13. Metabolic engineering/energy applications	7/2/2019
ABS338	27	15. Peptides	7/2/2019
ABS393	28	15. Peptides	7/2/2019
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	7/2/2019
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

Abs	Board (BOD)	Track	Date
ABS437	46	17. Proteins in cells	7/2/2019
ABS059	47	18. Proteomics	7/2/2019
ABS093	48	18. Proteomics	7/2/2019
ABS455	50	18. Proteomics	7/2/2019
ABS026	51	19. Proteostasis and quality control	7/2/2019
ABS079	52	19. Proteostasis and quality control	7/2/2019
ABS153	53	19. Proteostasis and quality control	7/2/2019
ABS330	54	19. Proteostasis and quality control	7/2/2019
ABS163	55	2. Bioinformatics	7/2/2019
ABS179	56	2. Bioinformatics	7/2/2019
ABS307	57	2. Bioinformatics	7/2/2019
ABS318	58	2. Bioinformatics	7/2/2019
ABS449	59	2. Bioinformatics	7/2/2019
ABS473	60	2. Bioinformatics	7/2/2019
ABS219	61	20. Single molecule studies	7/2/2019
ABS298	62	20. Single molecule studies	7/2/2019
ABS446	63	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	67	21. Structure (x-ray/NMR/EM)	7/2/2019
ABS383	68	21. Structure (x-ray/NMR/EM)	7/2/2019
ABS390	69	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	85	24. Therapeutics and antibodies	7/2/2019
ABS468	86	24. Therapeutics and antibodies	7/2/2019
ABS485	87	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

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Abs	Board (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	5. Computational modeling/simulation	7/2/2019
ABS193	107	5. Computational modeling/simulation	7/2/2019
ABS319	108	5. Computational modeling/simulation	7/2/2019
ABS362	109	5. Computational modeling/simulation	7/2/2019
ABS366	110	5. Computational modeling/simulation	7/2/2019
ABS405	111	5. Computational modeling/simulation	7/2/2019
ABS418	112	5. Computational modeling/simulation	7/2/2019
ABS426	113	5. Computational modeling/simulation	7/2/2019
ABS440	114	5. Computational modeling/simulation	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	120	6. Design/engineering	7/2/2019
ABS257	121	6. Design/engineering	7/2/2019
ABS260	122	6. Design/engineering	7/2/2019
ABS327	124	6. Design/engineering	7/2/2019
ABS343	125	6. Design/engineering	7/2/2019
ABS355	126	6. Design/engineering	7/2/2019
ABS360	127	6. Design/engineering	7/2/2019
ABS373	128	6. Design/engineering	7/2/2019
ABS447	129	6. Design/engineering	7/2/2019
ABS470	130	6. Design/engineering	7/2/2019
ABS483	131	6. Design/engineering	7/2/2019
ABS123	132	7. Dynamics and allostery	7/2/2019
ABS173	133	7. Dynamics and allostery	7/2/2019
ABS205	134	7. Dynamics and allostery	7/2/2019
ABS209	135	7. Dynamics and allostery	7/2/2019
ABS235	136	7. Dynamics and allostery	7/2/2019
ABS279	137	7. Dynamics and allostery	7/2/2019
ABS280	138	7. Dynamics and allostery	7/2/2019

Abs	Board (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



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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

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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 sAB-based 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.

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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 β -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

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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 CYCLE: 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 McCammon^{1,2,3}

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- 3 Department of Chemistry and Biochemistry, University of California, San Diego
- 4 Department of Chemistry, The University of Utah, Salt Lake City

Abstract Malate dehydrogenase (MDH) and citrate synthase (CS) are two pace-making enzymes involved in the tricarboxylic acid (TCA) 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 wild-type 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.

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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 β -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 β -barrel protein, cellular retinoic acid-binding protein 1 (CRABP1), 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-local 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-terminal regions, which are involved in closure of the native β -barrel. In addition, CSPs support the presence of two features in the denatured state: a major hydrophobic cluster involving residues from various parts of the sequence and a native-like interaction similar to one identified in previous studies as forming early in folding (Budyak et al., *Structure* 21,476 [2013]). 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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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 Rockefeller 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. Blanchard (1)

(1) *Weill Cornell Medical College*

G. Glenn Gregorio^{1*}, Matthieu Masureel^{2*}, Daniel Hilger^{2*}, Daniel S. Terry¹, Manuel Juethe¹, Hong Zhao¹, Zhou Zhou¹, Jose Manuel Perez-Aguilar^{1,9}, Maria Hauge^{3,5,7,8}, Signe Mathiasen^{3,5}, Jonathan A. Javitch^{3,4,5}, Harel Weinstein^{1,6}, Brian K. Kobilka^{2†},

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

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 β_2 adrenergic receptor (β_2 AR) 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 β_2 AR-Gs complexes are formed and the efficiency of nucleotide exchange leading to Gs activation. These data also reveal transient nucleotide-bound β_2 AR-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, NNF Center for Basic Metabolic Research, University of Copenhagen
- 8 Present address: IBM Thomas J. Watson Research Center, Yorktown Heights, New York, USA
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ULTRAVIOLET PHOTODISSOCIATION MASS SPECTROMETRY FOR CHARACTERIZATION 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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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 top-down 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.

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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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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

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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)

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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

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)

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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)

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Protein-protein and protein-RNA interactions range widely in strength, from strong 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

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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 β_1 -adrenergic GPCR (β_1 AR) 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 - ^{15}N chemical shifts in a detergent-solubilized thermostabilized mutant of the turkey β_1 AR [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 β_1 AR in various complexed forms from precise measurements of four types of ^{15}N 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 binding pocket. The pivoting explains (i) the increased affinity of agonist ligands upon G protein/Nb80 binding, which results from a compression of the binding pocket by the TM6 motion, (ii) the higher 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)

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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 ELONGATION ELUCIDATED BY KINETIC NETWORK MODELS

Xuhui Huang (1)

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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 elongation 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)

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RAS proteins are frequently mutated in cancer (~30% of all human tumours) and an estimated world-wide death toll 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 downstream 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

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Tepei 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 THA1718, 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

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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 S100 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)

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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

Raquel L. Lieberman (1)

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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)

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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.

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ENGINEERING LINKAGE-SPECIFIC POLYUBIQUITIN ANTIBODIES: TOOLS FOR ELUCIDATION OF NOVEL SIGNALING PATHWAYS

Marissa L. Matsumoto (1)

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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 poly-ubiquitin 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 MOLECULES PROBED WITH 1-MS RESOLUTION

Thomas T. Perkins (1)

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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 $<10 \mu\text{s}$. 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 $\Delta\Delta G_0$ 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)

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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 alters 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 MECHANOSENSORS IN THE $\alpha\beta$ T CELL LINEAGE

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$\alpha\beta$ 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 $\alpha\beta$ 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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PROBING SEQUENCE CONSTRAINTS ASSOCIATED WITH THE COTRANSLATIONAL FOLDING AND MISFOLDING OF INTEGRAL MEMBRANE PROTEINS

Jonathan P. Schleich (1)

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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 ApoE4. 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 Biasseti, Kevin Staras.

HOW DO MEMBRANE PROTEIN EXTRACELLULAR DOMAINS REGULATE INTRACELLULAR 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 MOLECULAR SIMULATION

Rebecca C. Wade (1), (2)

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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 macromolecular 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

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.

References

R. Marchante, D.M. Beal, N. Koloteva-Levine, T.J. Purton, M.F. Tuite, W.-F. Xue, The physical dimensions of amyloid aggregates control their infective potential as prion particles, *eLife*, 6 (2017).

D.M. Beal, M. Tournus, R. Marchante, T. Purton, D.P. Smith, M.F. Tuite, M. Doumic, W.-F. Xue, The Division of Amyloid Fibrils, *BioRxiv*, (2018) 506386.

THE STABILITY OF MECHANOSENSING FORCE-TRANSMISSION SUPRAMOLECULAR LINKAGES

Jie Yan (1), (2)

(1) *Mechanobiology Institute, National University of Singapore*

(2) *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-molecule detector assay for the mechanical stability of force-bearing inter-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,
National Institute of Immunology

(1)

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
University of Illinois at Urbana-Champaign

(1)

ABS008/BOD1

Transthyretin Disassembly Mechanism and Metal-Induced Oxidation Degradation Pathway Studied via Native Mass Spectrometry and Surface-Induced Dissociation

Mehdi Shirzadeh, 1
Texas A&M University

(1)

ABS009/BOD9

Unlocking the mechanism of HIV-1 viral assembly nucleation with native mass spectrometry

Samantha Sami, 1, Erik Olson, Shuohui Liu, Karin Musier-Forsyth, Vicki Wysocki

(1) Ohio State Biochemistry Program, The Ohio State University

ABS010/BOD145

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

Shoyab Ansari, 1
Jamia Millia Islamia University, New Delhi, INDIA

(1)

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

(1)

ABS013/BOD72

Snapshots of irreversible FGFR1 inhibition

Maria Kalyukina, 1, Yuliana Yosaatmadja, Adam Patterson, Jeff Smail, 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. Loffis, 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
Agricultural Biotechnology Research Center, Academia Sinica

(1)

ABS016/BOD37

Kinetic Trapping and Robustness in Proteasome Assembly

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

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ABS017/BOD32

Oscillatory Mechanism of a Circadian Clock System

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

(1)

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

(1)

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

Posters

ABS020/BOD21

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

Philipp Schmidpeter,1, Crina Nimigean
Weill Cornell Medicine

(1)

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

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ABS022/BOD69

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

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ABS023/BOD107

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

Tokyo University of Agriculture & Technology

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ABS024/BOD69

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

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

(1)

ABS025/BOD115

Advanced clustering, machine learning and conformational change: new methods and some applications

Freddie Salisbury,1, Ryan Melvin, Jiajie Xiao
Wake Forest University

(1)

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
UC Riverside

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ABS027/BOD50

An Analytical Revolution: Introducing the Next Generation Optima AUC

Chad Schwartz,1

Ex Beckman Coulter Employee

(1)

ABS028/BOD94

High throughput glycan profiling for improved quality control of therapeutic glycoproteins

Baolin Zhang,1, Lei Zhang, Shen Luo
Food and Drug Administration

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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

(1)

ABS030/BOD107

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

University of California, San Francisco

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ABS031/BOD70

Protein Synthesis Studies on Single Molecule Level

Joerg Fitter,1, Henning Hoefig, Alexandros Katranidis
Research Centre Juelich

(1)

ABS032/BOD121

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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Posters

ABS033/BOD66

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

Amy Chau, I, Yuxin Hao, Clare Canavan, Susan Taylor, Rodrigo Maillard

(1) Department of Chemistry, Georgetown University

ABS034/BOD17

Recruitment of Amyloid- β Oligomers by the Prion Protein

Priyanka Madhu, I, Samrat Mukhopadhyay

(1) 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, I, Dulal Panda

(1) 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, I, 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, I, Matthias Roos, Venkata Mandala,

Alexander Shcherbakov

(1) MIT

ABS038/BOD36

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

Neel Shah, I, 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, I, Ritu Gurung, Sharifah Albariki, Aaron Dhandu, Carol Otey, Wayne Vogl, Julian Guttman

(1) Wichita State University

ABS040/BOD10

Real-Time Monitoring of α -Synuclein-Induced Cell Membrane Disruption in Parkinson's Disease

Jacob Parres-Gold, I, Stephanie Wong Su, Andy Chieng, Yixian Wang

(1) California State University, Los Angeles

ABS041/BOD5

Rutin Interacts Weakly with α -Synuclein and Suppresses its Aggregation by Modulating its Fibrillation Pathway

Geetika Verma, I, 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, I, Gabriela Uceda-Cortez,

Svetlana Shestopal, Timothy K Lee, Andrey Sarafanov

(1) 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, I, Satoshi Nagao, Chunguang Ren,

Mohan Zhang, Akiya Oda, Yoshiki Higuchi

(1) Graduate School of Science and Technology Division of Materials Science, Nara Institute of Science and Technology

ABS044/BOD11

Molecular Mechanisms of Peptide Self-Assembly in Hydrogel Formation

Gabriel Braun, I, Sara Linse, Karin Åkerfeldt,

(1) Department of Chemistry, Haverford College

Posters

ABS045/BOD63

UniProt: A universal hub of protein knowledge

Alex Bateman, 1,
EMBL-EBI

(1)

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

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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
Medicine, University of Florida, USA

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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 Brüscheweiler,
Department of Chemistry and Biochemistry, The Ohio State
University

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ABS049/BOD41

Effect of Ethanol and Protein Content on the Gelation of Almond, Lentil, and Pea Proteins

Nahla kreidly, 1, Graciela Padua, Hakime Yavuz,
University of Illinois at Urbana Champaign

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ABS051/BOD67

Bioinformatics for Sperm Capacitation

Nailis Syifa', 1, Jiahn-Haur Liao, Tzu-Hua Wu*,
Taipei Medical University

(1)

ABS052/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

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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

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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,
College of Pharmacy, University of Houston

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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,
University of Iceland

(1)

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
Mathematics, Department of Chemistry and Integrative
Biosciences (IB) Program

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ABS059/BOD47

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

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

(1)

Posters

ABS060/BOD65

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

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ABS062/BOD6

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, Butler University

(1)

ABS064/BOD110

Distinct chaperone activities in nascent protein folding

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

(1)

ABS065/BOD73

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, University of Washington

(1)

ABS066/BOD56

Vasoinhibin Inhibits Thrombin-Induced Angiogenesis, Vasopermeability, Platelet Aggregation, and Cancer Invasion

Juan Pablo Robles, 1, Magdalena Zamora, Gonzalo Martínez de la Escalera, Carmen Clapp, Instituto de Neurobiología, UNAM (Universidad Nacional Autónoma de México)

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

(1)

ABS069/BOD60

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,

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University of Washington

ABS070/BOD95

Translesion Synthesis Pathway as Target for Anti-Cancer Drug Design

Dmitry Korzhnev, 1, Department of Molecular Biology & Biophysics, University of Connecticut Health Center

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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

Posters

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 Walzothelini, Ruedi Aebersold, Wah Chiu, Judith Frydman,

(1) Stanford University

ABS075/BOD123

Engineering halogen bonds to affect protein stability, activity, and recognition

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

(1) 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,

(1) 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,

(1) McGill University

ABS080/BOD55

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,

(1) Michel Roberge, Lawrence McIntosh, University of British Columbia

ABS083/BOD30

Modulation of ligand and receptor state in DDR-collagen interactions

Gunjan Agarwal,1,

(1) Ohio State University

ABS084/BOD126

Elucidating a code for RNA sequence recognition

Wei Zhou,1, Daniel Melamed,

(1) University of Washington

Posters

ABS085/BOD142

Activation dynamics of USP7 deubiquitinase

Irina Bezonova,1, Gabrielle Valles, Dmitry Korzhnev,
UCONN Health

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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,
California State University Long Beach

(1)

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

(1)

ABS088/BOD126

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,
University of Washington

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ABS089/BOD22

Expression of Band 3, a Membrane Protein

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

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ABS091/BOD67

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

Sayeeda Chowdhury,1, Ram Bhusal,
Monash University

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ABS092/BOD22

Discovering Novel Antibodies Against Peptidisc Stabilized Membrane Proteins

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

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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,
Univ. of Mass. Boston

(1)

ABS094/BOD127

De novo design of self-assembling helical protein filaments

Hao Shen,1,
Institute for Protein Design, University of Washington

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ABS095/BOD92

Distinct pathways of activation of human small heat shock protein HSPB5 by different stress factors

Maria Janowska,1, Rachel Klevit,
University of Washington

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ABS097/BOD48

Determining the Mechanism of Action of the Antibiotic Argirin B

Chris Swanson,1, Riley Roberts, Jessica Mantchev, Catie Shelton,
Justin Walter, Bassam Haddad, P. Clint Spiegel,
Western Washington University

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ABS098/BOD33

A Molecular View of the Liquid to Gel Phase Transition of Heterochromatin Protein HP1a

Bryce Ackermann,1,
University of California, San Diego

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ABS099/BOD35

Impact of Oxidative Stress on the Structural Conformation and Chemical Integrity of Soluble CLIC1

Olga Faerch,1, Stoyan Stoychev, Heini Dirr,
PSFRU, School of Molecular and Cell Biology, Faculty of Science,
University of the Witwatersrand, Johannesburg

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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,
Institute of Biomedical Sciences, Academia Sinica

(1)

Posters

ABS102/BOD29

Novel hevein-like defense peptides from wild cereals

- (1) Eugene Rogozhin,1, Dmitry Ryazantsev, Sergey Zavriev, Shemyakin And Ovchinnikov Institute Of Bioorganic Chemistry Russian Academy Of Sciences

ABS104/BOD49

The Structure of the interleukin 11 signalling complex

- (1) Riley D. Metcalfe,1, 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 Molecular Science and Biotechnology Institute, University of Melbourne, Parkville, Victoria 3010, Australia

ABS105/BOD130

Directed Evolution of sensor proteins for GPCR signaling mechanisms

- (1) Andre Berndt,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

- (1) 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, University of Melbourne

ABS107/BOD130

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

- (1) Oana-Nicoleta Antonescu,1, Kristoffer Enøe Johansson, Jakob Rahr Winther, Linderstrøm-Lang Centre for Protein Science, University of Copenhagen

ABS108/BOD39

The Interaction of IAA-94 with the Soluble Conformation of the CLIC1 Protein and its Structural Homolog hGSTP1-1

- (1) Roland Worth,1, Heinrich Dirr, University of the Witwatersrand

ABS109/BOD93

Microfluidic methods reveal the thermodynamics of chaperone binding

- (1) Therese Herling,1, Anais Cassaignau, John Christodoulou, Tuomas Knowles, 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

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

ABS111/BOD43

Calcium Binding Proteins and the Regulation of the Visual Sensory System: from Molecules to Networks

- (1) Daniele Dell'Orco,1, University of Verona

ABS112/BOD25

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

- (1) 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

- (1) Joseph Curtis,1, Amy Xu, Monica Castellanos, Kevin Mattison, NIST

ABS114/BOD90

Taking a Magic Leap into Augmented Reality Protein Structure Visualization

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

Posters

ABS115/BOD64

Evaluating the Molecular Function Families of Phosducins Using Multi-iterative Sequence Searching Technique

Sarah Hosler, I., Jacquelyn Fetrow,
Albright College

(1)

ABS116/BOD146

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

Duygu Aydemir, I., Firdevs Gecili, Nalan Ozdemir, Nuriye Nuray Ulusu,
Koc University School of Medicine Department of Medical Biochemistry

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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, I., Kristinn Ragnar Óskarsson,
Magnús Már Kristjánsson,
University of Iceland

(1)

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, I., Yijuan Sun,
Fox Chase Cancer Center

(1)

ABS119/BOD47

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

Chynna Denham, I., Shilpi Agrawal, T.K.S. Kumar,
University of Arkansas

(1)

ABS120/BOD66

Properties for predicting protein function

Caitlyn L. Mills, I., Lydia A. Ruffner, Penny J. Beuning,
Northeastern University

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ABS122/BOD118

Network-Level Analysis of Molecular Dynamics Simulations Reveals Allosteric Properties of Calcium Sensor proteins

Valerio Marino, I., Daniele Dell'Orco,
University of Verona

(1)

ABS124/BOD148

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

Arnor Saevarsson, I., Brynjar Ellertsson,
University of Iceland

(1)

ABS125/BOD40

Generation of 13 full length proteins of the cGAS-STING Pathway for drug tractability assessment

Yong Jiang, I.,
GSK

(1)

ABS126/BOD46

Bid as a novel interacting partner of IRE1: A differential modulator determining diverse outputs of its RNase activity

Samirul Bashir, I., Maryam Banday, Ozaira Qadri, Arif Bashir, Nazia Hilal,
Department of Blotechnology, University of Kashmir

(1)

ABS127/BOD132

A Generative Algorithm For Proteins From The Ntf2-Like Superfamily

Benjamin Basanta, I., Mathew Bick, Ted Baughman, Philip Leung, Eric Nalefski, David Baker,
Institute for Protein Design

(1)

ABS128/BOD118

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

Maksim Kouza, I., Andrzej Kolinski, Irina Buhimschi, Andrzej Kloczkowski,
Nationwide Childrens Hospital

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ABS129/BOD72

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

Mi Li, I.,
Leidos Biomedical Research, Inc

(1)

Posters

ABS130/BOD27

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

Gerhard Wagner, I, William Shih, Meng Zhang, Krishna Das, Harvard Medical School

(1)

ABS131/BOD14

The Structure of Discoidal High-density Lipoprotein Particles

Stefan Bibow, I, Yevhen Polyhach, Cédric Eichmann, Celestine Chi, Henning Stahlberg, Gunnar Jeschke, Roland Riek, University of Basel

(1)

ABS132/BOD61

5112 isolated from *Aquilegia nivalis*, provokes dual inhibition of Ire1 α and perk arms of Unfolded Protein Response signaling

Nazia Hilal, I, Aarif Bashir, Samirul Bashir, University of Kashmir

(1)

ABS133/BOD49

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

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

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University of Washington Department of Genome Sciences

ABS134/BOD9

Dynamics of Amyloid Fibrils Play a Role in Seeding and Propagating the Aggregation of α -Synuclein

Jonathan Williams, I, Xue Yang, Jean Baum, Rutgers University

(1)

ABS135/BOD49

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

Margaret Stratton, I, University of Massachusetts, Amherst

(1)

ABS136/BOD75

Visualizing Conformational Changes of the Magnesium Channel CorA using Synthetic Antibodies

Satchal Erramilli, I, Piotr Tokarz, Kamil Nosol, Przemyslaw Dutka, Blazej Skrobek, Pawel Dominik, Somnath Mukherjee, Anthony Kossiakoff,

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ABS137/BOD52

High-throughput identification of dominant negative polypeptides in yeast

Michael Dorrity, I, Michael Dorrity, Christine Queitsch, Stanley Fields,

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University of Washington

ABS138/BOD18

EPR reveals different conformations of LcrG

Pallavi Guha Biswas, I, Pavanjeet Kaur, Andrew McShan, Kawaljit Kaur, Likai Song, Roberto De Guzman, University of Kansas

(1)

ABS139/BOD121

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

Julia Koehler Leman, I, Brian Weitzner, Douglas Renfrew, Richard Bonneau,

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Simons Foundation / NYU

ABS140/BOD105

Mechanical properties of designed protein fibers

Neville Bethel, I, Matt Bick, David Baker, Institute for Protein Design, University of Washington

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ABS141/BOD80

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

Amritangshu Chakravarty, I, Helen Peng, Dr Roberto N De Guzman,

(1)

University of Kansas

ABS142/BOD134

Computational Protein Design with Multisite lambda Dynamics

Ryan Hayes, I, Jonah Vilseck, Charles Brooks III, University of Michigan

(1)

Posters

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

(1)

ABS144/BOD44

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

(1)

ABS145/BOD2

Novel α -sheet secondary structure in amyloid β -peptide drives aggregation and toxicity in Alzheimer's Disease

Valerie Daggett,1, University of Washington

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ABS146/BOD137

Generation of Polymeric Recombinant Hemoglobin Using PEG-azide Dendrimers and DBCO-modified Hemoglobin

Dedeepya Gudipati,1, Johann Sigurjonsson, Leah Huey, Spencer Anthony-Cahill,

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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

(1)

ABS148/BOD57

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

Jared Mohr,1, Juan Chavez, James Bruce, University of Washington

(1)

ABS149/BOD153

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

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

(1)

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, Oregon State University

(1)

ABS151/BOD77

Examination of Substrate Binding and Specificity in a PEPX from L. helveticus

Nicholas Bratt,1, Tera Almaw, Kent Jones, Douglas Juers, Whitworth University

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ABS152/BOD17

Mutual communication between the Kibra WW domains modulates interactions with LATS1

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

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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 Hemmerlich, Douglas Rusch, Jens Meiler, Jonathan Schleich,

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ABS154/BOD62

Rapid Pharmacological Profiling of Genetic Variants by Deep Mutational Scanning

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

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ABS155/BOD128

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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ABS156/BOD18

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

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

(1)

ABS158/BOD20

Combining smFRET and DEER Distance Measurements to Characterize Disordered Proteins

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

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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, I, Yue Yuan, Zhong Liang, Shaun Lee, Victoria Ploplis,
Francis Castellino,

(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, I, Dagmara Kisiela, Angelo Ramos,
Wendy Thomas, Evgeni Sokurenko, Rachel Klevit,
University of Washington

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ABS163/BOD55

Engaging the Protein Science Community to Expand Protein Literature Representation and Annotations in UniProt

Cecilia Arighi, I, Hongzhan Huang, Yongxing Chen,
Qinghua Wang, Peter McGarvey, Cathy Wu, UniProt Consortium,
UniProt Consortium, UniProt Consortium,

(1) Protein Information Resource, University of Delaware

ABS164/BOD100

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

Sunhee Hwang, I,
Stanford University

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ABS165/BOD60

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

Laura Chamness, I, Charles Kuntz, Wesley Penn, Jens Meiler,
Jonathan Schleich,

(1) Indiana University

ABS166/BOD128

Programmable Design of Orthogonal Protein Heterodimer

Zibo Chen, I, Scott Boyken, Mengxuan Jia, Florian Busch, David Flores-Solis, Matthew Bick, Peilong Lu, Zachary VanAernum, Aniruddha Sahasrabudhe, Robert Langan, Sherry Bermeo, T.J. Brunette, Vikram Mulligan, Vicki Wysocki, Frank DiMaio, David Baker

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ABS167/BOD149

Design of catalytic de novo proteins

Shane Caldwell, I, Susana Vazquez Torres, Cathleen Zeymer,
Ian Haydon, Don Hilvert, David Baker,

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ABS168/BOD15

Nanopore-confined lipid bilayers for oriented sample EPR and NMR studies of membrane proteins

Sergey Milikisiyants, I, Melanie Chestnut, Morteza Jafarabadi,
Antonin Marek, Maxim Voinov, Alexander Nevzorov,

(1) NCSU

ABS169/BOD144

High Pressure Optical Spectroscopy (HiPOS) and Real-Time Analysis of Enzymes Kinetics at Elevated Hydrostatic Pressure

Gary Smejkal, I, Alana Murphy, Vera Smejkal, Nicole Cutri,
Ed Ting, Alexander Lazarev,

(1) Pressure Biosciences

ABS171/BOD136

Design of Novel Lectins by Computer-Aided Directed Evolution

Perna Sharma, I, Ismail C Kazan, Sefika B Ozkan, Giovanna Ghirlanda,

(1) Arizona State University

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ABS172/BOD56

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

Shannon Speer, I, Alex Guseman, Gary Pielak,
Department of Chemistry, University of North Carolina at
Chapel Hill

(1)

ABS173/BOD133

***Staphylococcus aureus* IsdH: the chemical and dynamic basis of heme extraction from human hemoglobin**

Ken Ellis-Guardiola, I, Joseph Clayton, Brendan Mahoney,
Clarissa Pham, Sinan Sabuncu, Jeff Wereszczynski,
Pierre Moenne-Loccoz, Robert Clubb,
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ABS174/BOD139

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

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

(1)

ABS175/BOD141

Force-dependent allosteric enhancement of α E-catenin binding to F-actin by vinculin

Nicolas Bax, I, Derek Huang, Sabine Pokutta, Alexander Dunn,
William Weis,

Structural Biology, Stanford University

(1)

ABS177/BOD82

The cyclic nucleotide-binding homology domain of the integral membrane protein CNNM mediates dimerization and is required for Mg^{2+} efflux activity

Yu Seby Chen, I, Guennadi Kozlov, Rayan Fakhri, Yosuke Funato,
Hiroaki Miki, Kalle Gehring,
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, I, Tobias Schmidt, Siegfried Gessulat, Bernhard
Kuster, Mathias Wilhelm,

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ABS180/BOD131

Computational design of multipass transmembrane proteins

Peilong Lu, I, Chunfu Xu, Duyoung Min, Frank Dimairo,
Tamer El-Din, Lance Stewart, Justin Kollman, Tomoaki Matsuura,
William A. Catterall, James U. Bowie, David Baker,
University of Washington

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ABS181/BOD21

Coming Together in the DNA Damage Response: Interactions with the Intrinsically Disordered Region of BRCA1

Christine Hurd, I, Brian Morote-Costas,
Texas Christian University

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ABS182/BOD83

Five reasons to pay attention to CASP-SAXS

Susan Tsutakawa, I, Greg Hura, Andry Kryshchuk,
Krzysztof Fidelis, John Tainer,
Lawrence Berkeley National Laboratory

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ABS183/BOD115

The Limits of Tethering in Kinase Signaling Reactions

Elizabeth Speltz, I, TJ Brunette, Fabio Parmeggiani, David Baker,
Jesse Zalatan,

University of Washington

(1)

ABS184/BOD110

Molecular Basis of GPCR Biased Agonist Recognition

John McCorvy, I,
Medical College of Wisconsin

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ABS185/BOD99

Systematic Identification of Recognition Motifs for the Hub Protein LC8

Aidan Estelle, I, Nathan Jespersen, David Hendrix, Ylva Ivarsson,
Norman Davey,

Department of Biochemistry and Biophysics, Oregon State
University

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ABS186/BOD102

The Structural and Functional Organization of Ribosomal Compartment in the Cell: The new model with highly ordered network of ribosomes

- Elizaveta Karpova, I,
(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, I, Tracey Rouault,
(1) nih

ABS188/BOD116

Protein shape sculpting using rigid helical junctions

- TJ Brunette, I, 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, I, Matthew C Johnson, Joseph Watson,
Logesh Somasundaram, Hannele Ruohola-Bake,
Emmanuel Derivery, David Baker,
(1) 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, I, 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, I, Andy LiWang, Joel Heisler,
Yonggang Chang,
(1) University of California, Merced

ABS192/BOD94

Structural Analysis of DnaJ Protein ERdj6 and Non-Native Proinsulin

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

ABS193/BOD107

Predicting protein function from experimental and predicted structures using Graph Convolutional Neural Networks

- Vladimir Gligorijevic, I, Douglas Renfrew, Richard Bonneau,
(1) Flatiron Institute, Simons Foundation

ABS194/BOD98

Exploring Composition of Peptide Linker to Enhance Stability of Antibody Fragments for Cancer Therapeutics

- Jeong Min Han, I, 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, I, Allison Newel, Ashwag Binmahfooz,
(1) California State University San Marcos

ABS197/BOD31

Comparison of Strategies for the Enrichment of Cross-Linked Peptides

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

ABS198/BOD13

Computational Study on Aggregation and Disruption of Amyloid Fibrils

- Seokmin Shin, I, Kyunghee Lee, MinJun Lee, Jeseong Yoon,
(1) Seoul National University

ABS199/BOD16

Mapping accessibility in the bacterial mechanosensitive channel MscS to a small photoreactive probe

- Gabriela Elena Gómez, I, Yan Wang, Andriy Anishkin,
Sergei Sukharev,
(1) University of Buenos Aires

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ABS200/BOD149

Ionic Strength Modulates Dimerization and Enzyme Activity of a β -Glycosidase

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

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ABS201/BOD117

Design of Light Harvesting Proteins for Photosynthesis

Nathan Ennist,1, Adam Moyer, Derrick Hicks, Chunfu Xu, TJ Brunette, David Baker,

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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)

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ABS203/BOD151

Structural and biochemical studies of Mtb L-asparaginase reveal survival mechanism of Mycobacterium tuberculosis inside macrophages

Arfi Kataria,1, Bishwajit Kundu,

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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

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ABS207/BOD106

Alternative Forms of Energy Modulate Group II Chaperonin Activity

Kevin Goncalves,1, Tom Lopez, Judith Frydman, Stanford University

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ABS208/BOD147

Molecular mechanism of Ubiquitin E2 enzyme activation in ERAD

Tobias Ritterhoff,1, Christian Lips, Thomas Sommer, Rachel Klevit, University of Washington

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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,

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ABS210/BOD33

Applications Of Ultracentrifugation In Purification And Characterization Of Biomolecules

Akash Bhattacharya,1, Ross Verheul, Eric Von Seggern, Stephen Otts,

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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,

Department of Genome Sciences, University of Washington

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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, Colorado State University

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ABS213/BOD4

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

- (1) Sashank Agrawal,1, Woei-Chyn Chu, Hanna S. Yuan,
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ABS214/BOD27

Molecular mechanisms of the interhead coordination by interhead tension in cytoplasmic dyneins

- (1) 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 inner-membrane fusion

- (1) Luke Chao,1, Yifan Ge, Sivakumar Boopathy, Julie McDonald,
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ABS217/BOD18

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

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

ABS218/BOD86

Protein, Ligand and Water Characterization by Multiple Solvent Crystal Structures

- (1) Sorabh Agarwal,1, Mychal Smith, Miriam Segura-Totten,
Carla Mattos,
Northeastern University

ABS219/BOD61

Direct observation of target site bypassing during rotation-coupled protein diffusion on DNA

- (1) 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

ABS220/BOD83

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

- (1) Priyanka Goyal,1, Steve Seibold, Mark Richter, George Wilson,
Scott Lovell,
University of Kansas

ABS221/BOD89

A Structural and Functional Analysis of BshA: Insights into the Catalytic Mechanism and Feedback Inhibition by Bacillithiol

- (1) Paul Cook,1, Christopher Royer, Kelsey Winchell,
Grand Valley State University

ABS222/BOD104

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

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

ABS223/BOD133

Engineering Sortase A: Activity and Selectivity of New Hybrid and Ancestral Variants of Sortase A

- (1) Sarah Struyvenberg,1, Jordan Valgardson, Nick Horvath,
John Antos, Jeanine Amacher,
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ABS224/BOD23

Use of Spin-Labeled Nanodiscs to Improve Structural Determination of Membrane Proteins by ESR

- (1) Chieh-Chin Li,1, Yun-Wei Chiang,
Department of Chemistry, National Tsing Hua University

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ABS225/BOD143

Protein Local Dynamics and Its Coupling to Solvent

Yun-Hsuan Kuo, I, Yun-Wei Chiang,

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ABS226/BOD13

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

Chien-Lun Hung, I, Yun-Wei Chiang,

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ABS227/BOD92

Structural Insights into Chloramphenicol-metabolizing Enzyme from Metagenome

Sang-Hoon Kim, I,

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ABS228/BOD34

Biochemical Analysis of PriA Helicases from Gram-positive Bacteria Reveals Distinct DNA Unwinding Activity in DNA Replication Restart

Chwan-Deng Hsiao, I, Min-Guan Lin, Yi-Ching Li,

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ABS229/BOD150

Effects of Reactive Glutamines and a Binding Site Region on the Factor XIII Substrate Specificity for Fibrinogen α C (233-425)

Muriel Maurer, I, Mohammed Hindi, Francis D.O. Ablan,

Chad Stephens, Kelly Mouapi

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ABS230/BOD6

Identify the amyloidogenic peptides and create photocontrollable probes for neurodegenerative disease

Jen-Tse Huang, I,

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ABS231/BOD119

Thermal Reconstruction of Protein Nano-Building Block Complexes Using an Ultra-Stable de Novo Protein Domain

Ryoichi Arai, I, Naoya Kimura, Naoya Kobayashi,

(1) Shinshu University

ABS232/BOD35

Reversible and Orthogonal Four Helix Bundle Heterodimers

Ajasja Ljubetic, I, Ryan Kibler, Zibo Chen, Sherry Bermeo, Roman Jerala, David Baker,

(1) 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, I, Morgan Gibbs, Rajesh Gumpena,

David Waugh,

(1) Basic Science Program, Frederick National Laboratory for Cancer Research

ABS234/BOD19

Structural and Functional Characterization of p13II Protein from Human T-cell Leukemia Virus Type 1

Elka R Georgieva, I, 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, I, Elihu Ihms, Weicheng Li, Cameron Jamshidi,

Vicki Wysocki, Paul Gollnick,

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ABS237/BOD117

The Structural and Functional Roles of Disulphide Bridges in the Solanum tuberosum Plant Specific Insert, a Saposin-Like Protein

John H. Dupuis, I, Rickey Y. Yada,

(1) 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, I, Matthias Langhorst, Gavin Young, Daniel Cole,

Phillipp Kukura,

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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,1, 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,

(1) Western Washington University

ABS242/BOD59

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

ABS243/BOD120

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

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

(1) University of Washington

ABS245/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

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ABS248/BOD112

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

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

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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) University of Washington

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

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ABS252/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, Indiana University School of Medicine

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ABS253/BOD99

Influence of the Endoplasmic Reticulum Localization Sequence on the Cytotoxicity of Pseudomonas Exotoxin A-based Recombinant Immunotoxins

Jillian Baker,1, John Weldon, Towson University

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ABS254/BOD8

Natural and Pathogenic Protein Sequence Variation Affecting Prion-Like Domains Within and Across Human Proteomes

Sean Cascarina,1, Eric Ross, Colorado State University

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ABS255/BOD102

High Throughput sialylation measurement on Octet label free instrument for cell line development

Sunny Song,1, Molecular Devices

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ABS256/BOD125

Development of LOCKR-Activating Logic Circuits

Ryan Kibler,1, Zibo Chen, Marc Lajoie, Bobby Langan, David Baker, University of Washington

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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,1, Thomas E. Edwards, Donald Lorimer, Bart L. Staker, Robin Stacy, David Veessler, Gabriele Varani, Lance J. Stewart, Wesley C. Myler, Peter J. Myler, Pacific Northwest National Laboratory

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ABS259/BOD38

Amelogenin - A Multi-Pronged Approach to Identify Structural Features Guiding Enamel Formation

Garry W. Buchko,1, Jinhui Tao, Rajith J. Arachchige, Sarah D. Burton, Yongsoo Shin, Bojana Ginovska, Barbara J. Tarasevich, Wendy J. Shaw, Pacific Northwest National Laboratory

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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

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ABS261/BOD101

Non-ideality of Protein-based Therapeutics in Biological Environments

Hayli Larsen,1, University of Washington Department of Medicinal Chemistry

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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

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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, Suranaree University of Technology

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ABS264/BOD140

Genetic selections for the discovery of new reductases and oxidases of methionine

Bruno Manta,1, Mehmet Berkmen,
New England Biolabs

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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,
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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

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ABS268/BOD154

Report from the Ribosome: The Origins of Protein Folding

Loren Williams,1,
Georgia Tech

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ABS269/BOD20

Modulation of rod opsin stability, function and membrane supramolecular organization by flavonoids

Joseph T Ortega,1, Tanu Parmar, Beata Jastrzebska,
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ABS270/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,
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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,

(1) University of Washington

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,
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ABS274/BOD16

Knock-out mutations in a knotted protein improve the success of folding

John Finke,1,
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ABS275/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,
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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,
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ABS277/BOD9

Exploiting Autoinhibition Mechanism for Screening of Small Molecules that Modulate DNA Binding to ETS Transcription Factors

Jennifer Bui, I, 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 Jiang, I,

(1) University of Washington

ABS279/BOD137

Understanding the Interface: Exploring Malate Dehydrogenase using Computational and Experimental Approaches

Ellis Bell, I, 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, I, 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

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ABS281/BOD141

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

Jessica Bell, I, Joseph Provost, Ellis Bell,

(1) University of San Diego

ABS282/BOD135

The Role of dynamics in transcription factor DNA-binding specificity

Karlton Scheu, I, Soymya De, Lawrence McIntosh,

(1) University of British Columbia

ABS283/BOD32

Electrostatics Govern Membrane Interactions of the HSV-1 Nuclear Egress Complex

Mike Thorsen, I, 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, I, Natalia Maltseva,

(1) Argonne National Laboratory

ABS285/BOD34

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,

(1) University of Arkansas

ABS286/BOD21

The Unique amino acid composition of the chromophore-binding pocket contributes to the retinal binding specificity in human cone opsins

Beata Jastrzebska, I, Joseph Ortega, Kota Katayama, Sahil Gulati, Krzysztof Pakczewski,

(1) 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, I, 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 Cefazidime and its Transition State Analog

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

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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,

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ABS290/BOD5

Discovery and Characterization of a PAP248-286/Lipid Co-Assembly: The Messicle Story

Eleanor W Vane, 1, Abhinav Nath,

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ABS291/BOD39

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

Adalberto Diaz-Casas, 1, Walter Chazin,

(1) 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,

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ABS293/BOD50

Functional and Structural Study on HERC4

Young Sun Lee, 1, Donald Spratt,

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ABS294/BOD9

SUMO-derived Peptides as Inhibitors of α -Synuclein Aggregation

Zhaohui Liang, 1, Junqing Yang, Ho Yin Edwin Chan, Ming Ming Marianne Lee, Michael Kenneth Chan

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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,

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ABS296/BOD35

Expression and Characterization of the *Drosophila melanogaster* (Dm)IKK β : γ 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,

(1) Lawrence Livermore National Laboratory

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 Sierceki,

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ABS299/BOD1

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

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

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ABS300/BOD84

Crystal Structures Of Snx11 Reveal The Membrane Binding Mechanism

Xu Tingting, 1, Liu Jinsong,

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ABS301/BOD142

Catalytic Mechanism of TiaS5 in Tiacumicin B Biosynthesis Pathway

- (1) Yongzhi Lu,1, Yan Dong, Mingze Sun, Jinsong Liu, 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

- (1) 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

ABS303/BOD148

Structural and Biochemical Analysis of the HECT E3 Ubiquitin Ligase HECW2

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

ABS304/BOD77

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

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

ABS305/BOD143

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

- (1) 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

ABS306/BOD150

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

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

ABS307/BOD57

Prediction of deleterious protein mutants

- (1) Andrzej Kloczkowski,1, Robert Jernigan, Eshel Faraggi, Maksim Kouza, Nationwide Children's Hospital

ABS308/BOD79

Trimeric Immune Traps for Blockade of PD-1 and LPS Signaling in Combination Cancer Immunotherapy

- (1) 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

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

ABS310/BOD112

Biophysical and Structural Analysis of Drosophila Transcription Factors

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

ABS311/BOD7

The Measurement of Volume Change by Capillary Dilatometry

- (1) Peter Kahn,1, Rutgers University

ABS312/BOD24

Oligomerization of lipid membrane bound Cytochrome P450

- (1) Nirupama Sumangala,1, Thirupathi Ravula, Ayyalusamy Ramamoorthy, 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,

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ABS314/BOD103

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

Cecilia Arighi, 1, Hongzhan Huang, Karen Ross, Jia 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,

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ABS317/BOD123

Generative Modeling for Protein Structures

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

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ABS318/BOD58

Using Deep Learning Neural Networks for Inverse Protein Folding Predictions

Alyssa La Fleur, 1, Tera Almar, Deanna Ojennus, Kent Jones, Whitworth University

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ABS319/BOD108

Novel perspectives on olfactory receptor-odorant dynamics simulations

Chiquito Crasto, 1, Peter Lai, 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,

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ABS321/BOD119

The Rational Discovery and Design of Disordered Protein Ligands

David Baggett, 1, Abhinav Nath, University of Washington

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ABS322/BOD120

Analysis of Loop Motions in 1 μ s Simulations of OXA-66 Reveals Striking Differences in Flexibility between Mutants

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ABS323/BOD95

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

Isabel Zecua, 1, Blake Gillespie, CSU Channel Islands

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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

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ABS325/BOD37

Biophysical Examination of Ubiquitin E3 Ligase, HECTD1: An Important Regulator in Neurological Development

Misa Mai, 1, Donald Spratt, Clark University

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ABS326/BOD51

Structural Examination of the HECT E3 Ligase Are1 and its Implications in Apoptosis

Emily Ladda, 1, Donald Spratt, Clark University

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ABS327/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 Riddell, David Baker,
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ABS328/BOD91

Structure and Intrinsic Hydrolysis of NRas Q61 Mutants

Derion Reid,1, Spiro Pavlopoulos, Carla Mattos,
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ABS329/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,
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ABS330/BOD54

Molecular Basis of ClpP Protease Activation by Small Molecules

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ABS331/BOD86

Structure-Activity Relationships In The Metamorphic, Antimicrobial Protein Xcl1

Acacia Dishman,1, Michelle Lee, Gerard Wong, Brian Volkman,
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ABS333/BOD65

Functionally Relevant Clustering of the Arsenate Reductase (ArsC) Superfamily

Mikaela Rosen,1, Jacquelyn Fetrow, Carol Parish, Janelle Leuthaeuser,
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ABS334/BOD11

Defining GP41-1 Extein Splice Junction

Carla Madrid,1, Thuy Nguyen, Kimberly Reynolds, Kendra Frederick,
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ABS335/BOD64

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

Mark Herzik,1, Mengyu Wu, Gabriel Lander,
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ABS336/BOD53

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

Jordan Valgardson,1, Sarah Struyvenberg, Zach Sailer, Jeanine Amacher,
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ABS337/BOD14

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

Rama Reddy Goluguri,1, Mourad Sadqi, Victor Munoz,
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ABS338/BOD27

De Novo Peptide Design For Enhanced Cell Permeability, Oral Bioavailability And Blood-Brain Barrier Traversal

Gaurav Bhardwaj,1, Stephen Rettie, Jacob O'Connor, Yen-Hua Huang, David Craik, David Baker,
University of Washington, Seattle

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ABS339/BOD41

Novel Fc-Poly His Tag Leads To High Order Oligomerization

Zebulun Lapoint,1, Zebulun Lapoin, John Hall, Matteo Binda, DeeAnn Martinez-Guzman, Susan Hilt, Pranti Das, Charles Holz, Jody Berry, Peter Schwind, Elizabeth Booth, Vincenzo Favalaro, Grifols Diagnostic Solutions

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ABS340/BOD15

Optimization of Protein Structure and Function: The Importance of Loop Length

Neha Nandwani,1, Praneeth Reddy, Manjula Ramu, Jayant Udgaonkar, Shachi Gosavi,
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ABS341/BOD57

Biophysical and Biochemical Characterization of HACE1, a HECT E3 Ubiquitin Ligase Implicated in Cancer and Huntington's Disease

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ABS342/BOD65

Room Temperature Crystallography of Retinal Proteins: Investigating the Retinal Isomerization Mechanism

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ABS343/BOD125

Designer Proteins - From Fold To Applications

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ABS344/BOD44

Identifying "Hot Spot" Residues At The Etv6 Pnt Domain Polymerization Interface

Sophia Cho,1, Chloe Gerak, Michel Roberge,
Lawrence McIntosh,

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ABS345/BOD119

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,

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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,
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ABS347/BOD155

Resurrection of Ancestral Effector Caspases Identifies Novel Networks for Evolution of Substrate Specificity

Clay Clark,1, Robert Grinshpon, Suman Shrestha,
James Tifus-McQuillan, Paul Hamilton, Paul Swartz,
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ABS348/BOD38

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,
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ABS349/BOD96

ParABS, Chromosome Partitioning System

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ABS350/BOD92

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

Bidisha Acharya,1, Snigdha Maiti, Aditya Jyoti Basak,
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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,
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ABS352/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,

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ABS353/BOD73

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

Aditya Jyoti Basak, I, Snigdha Maiti, Anita Hansda, Dhruvajyoti Mahata, Woonghee Lee, Gayatri Mukherjee, Soumya De, Dibyendu Samanta,
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ABS354/BOD58

Contribution of Cleavage and MHCII Binding Events to the Generation of Hemagglutinin Immunodominant Peptides

Tynan Becker, I, Thomas Kuhn,
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ABS355/BOD126

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

Nihal Korkmaz, I, TJ Brunette, David Baker,
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ABS356/BOD66

The Supramolecular Structure Of The Bacterial Stressosome Revealed By Cryo-Em Unveils Its Mechanism Of Activation

Allison Williams, I,
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ABS357/BOD8

Crystal Structure Of A Protein Folding Intermediate

Jinquan Luo, I,
Janssen R&D

(1)

ABS358/BOD145

Identification and Characterization of an Oxalyl CoA-Synthetase from Grass Pea (Lathyrus sativus L.)

Moshe Goldsmith, I, Shirir Barad, Orly Dym, Shira Albeck, Yoav Peleg, Ziv Reich,
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ABS359/BOD74

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

Balint Nagy, I, Zsofia Zambo, Agnes Hubert, Martin Polak, Eszter Szabo, Jiri Novacek, Frank Jordan, Vera Adam-Vizi,
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ABS360/BOD127

Automated Design Of Interface Structure For Targeted Binders

Yu Zhao, I, Gevorg Grigoryan,
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ABS361/BOD146

New CRISPR/Cas9 Characterization Broadens The Protospacer-Adjacent Motif Recognition

Trung Thach, I, Nam Hyeong Kim, Junho Hur, Sang-Seob Lee, Yong Ho Kim,
Sungkyunkwan University

(1)

ABS362/BOD109

Computational Modeling of S-phase kinase-associated protein 2 (Skp2) E3 Ligase and Novel Inhibitors Interactions

Shuxing Zhang, I,
MD Anderson Cancer Center

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ABS363/BOD10

The Yeast Sup35 Protein Forms A Large Number Of Infectious Structures

Yu-Wen Huang, I, Chih-Yen King,
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ABS364/BOD76

eIF2B-Catalyzed Nucleotide Exchange And Phosphoregulation By The Integrated Stress Response

Lillian Kenner, I,
UCSF

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ABS365/BOD142

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

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

(1)

Posters

ABS366/BOD110

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

Narutoshi Kamiya, I., Gert-Jan Bekker,
University of Hyogo

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ABS367/BOD58

Cytotoxic Activity Of Non-Specific Lipid Transfer Protein (NsLTP) From Fennel (Foeniculum Vulgare) Seeds

Mekdes Megeessa, I., Yamna Khurshid, Aftab Ahmed,
Chapman University

(1)

ABS368/BOD98

Photosensitive handles for selective manipulations of biosynthetic proteins

Rasa Rakauskaite, I., Giedre Urbanaviciute, Viktoras Masevicius,
Aušra Vaiteikaite, Aurelija Žvirbliene,
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ABS369/BOD113

Differential Localization Of An Engineered RAS Rheostat Reveals Unique RAS-ERK Signaling Dynamics

Emily M Dieter, I., John Rose, Dustin Maly,
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ABS370/BOD78

Exploring the Novel Structure of Human Myeloid-Derived Growth Factor

Valeriu Bortnov, I., Marco Tonelli, Woonghee Lee, John Markley,
Deane Mosher,
University of Wisconsin-Madison

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ABS371/BOD120

Engineering Orthogonality into the Chemokine-GPCR Interface Using Rosetta

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

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Medical College of Wisconsin

ABS372/BOD67

Hydrophobic Ligands Influence the Structure, Stability, and Processing of the Major Cockroach Allergen Bla g 1

Alexander Foo, I., Peter Thompson, Lalith Perera, Simrat Arora,
Eugene DeRose, Jason Williams, Geoffrey Mueller,
National Institute of Environmental Health Sciences

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ABS373/BOD128

Capturing The Structural Flexibility Of Single-Layer Beta-Sheet Within Isomorphous Crystals Revealed By Comprehensive Structure Determinations

Koki Makabe, I., Hideki Fujiwara, Kenta Hongo, Yuki Hori,
Norio Yoshida,
Yamagata university

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ABS374/BOD114

Cysteine Scanning Mass Spectrometry Towards Elucidation of Intramolecular Structure-Function Relationships in Multi-Domain Kinases

Zachary E. Potter, I., Dr. Dustin Maly,
Department of Chemistry, University of Washington

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ABS375/BOD59

Proteomic and Cytotoxic Characterization of Proteins from Cuscuta (Dodder) Tendrils

Umaima Akhtar, I., Mekdes Megeessa, Basir Syed,
Ishtiaq Ahmed Khan, Keykavous Parang, Aftab Ahmed,
Chapman University

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ABS376/BOD113

A Chemoproteomic Method For Characterizing Kinase Complexes

Linglan Fang, I.,
University of Washington

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ABS377/BOD139

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

Abha Jain, I., Nikolay Dokholyan, Andrew Lee,
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ABS378/BOD79

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

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

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ABS379/BOD80

Characterization of Proteins by Microfluidic CE-SDS

April Blodgett,1,

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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

ABS381/BOD114

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

Thualfeqar Almohanna,1, George Popescu, Sorina Popescu,

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ABS382/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,

(1) Argonne National Laboratory

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,

(1) IBT, UNAM

ABS385/BOD137

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,

(1) Novartis Institutes for BioMedical Research

ABS387/BOD81

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,

(1) 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

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ABS390/BOD69

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

(1) Cheng-Yu Chen, I. Woonghee Lee, William Montfort, University of Arizona, Department of Chemistry and Biochemistry

ABS391/BOD147

Functional Evolution of TRPM2 Channels

(1) Jordan Iordanov, I. 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

(1) Djamali Muhoza, I. Paul Adams, University of Arkansas

ABS393/BOD28

Sequence Specificity for Peptide Substrates in Thioether Crosslinking Reaction Catalyzed by Radical SAM Enzyme QhpD

(1) Toshinori Oozeki, I. 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

(1) Toshihide Okajima, I. Takeshi Murakawa, Seiki Baba, Satoshi Kanagawa, Hideyuki Hayashi, Takato Yano, Takashi Kumasaka, Katsuyuki Tanizawa, Osaka University

ABS395/BOD154

Regulatory Role of 5'-AMP in cAMP Signaling Dynamics

(1) Nikhil Tulsian, I. Abhijeet Ghode, 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

(1) Akinobu Senoo, I. Satoru Nagatoishi, Kouhei Yoshida, Sho Ito, Go Ueno, Takumi Tashima, Shota Kudou, Kouhei Tsumoto, Department of Chemistry and Biotechnology, School of Engineering, The University of Tokyo

ABS397/BOD12

How Nature Harnesses Entropy To Tune Protein Function

(1) Zachary Wood, I. Nick Keul, Krishnadev Oruganty, Elizabeth Schaper Bergman, Nathan Beattie, Weston McDonald, Renuka Kadirvelraj, Michael Gross, Robert Phillips, Stephen Harvey, University of Georgia

ABS398/BOD29

Structural Modeling of Antimicrobial Peptides in the Database of Antimicrobial Activity and Structure of Peptides

(1) Anthony Armstrong, I. Phil Cruz, Andrei Gabrielian, Mindia Chubinidze, Malak Pirtskhalava, Darrell Hurt, Alex Rosenthal, Mike Tartakovsky, 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

(1) Rodrigo Arreola-Barroso, I. Wendy Xolalpa-Villanueva, Leticia Olvera-Rodriguez, Gloria Saab-Rincón, Institute of Biotechnology, UNAM

ABS400/BOD152

Functional Elements Of A Human Antizyme Essential For Binding And Inhibiting Human Ornithine Decarboxylase

(1) Ju-Yi Hsieh, I. Hui-Chih Hung, Institute of Biochemistry, Microbiology & Immunology, Chung Shan Medical University

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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, Zhifeng Chen, Eberhard Durr, James Cook, Kerim Babaoglu, Stephen Soisson, Lan Zhang, Kalpit Vora, Alexei Brooun, Merck and Co., Inc., Computational and Structural Chemistry

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ABS402/BOD144

Evaluation Of The Effect Of Heat Capacity On The Catalysis Of A Dimeric Enzyme

Ekaferina Jalomo Khayrova,1, Christopher Bahl, Gloria Saab Rincón,

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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,

(1) The Scripps Research Institute

ABS404/BOD103

Modulating Receptor Signaling using Variobody; 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,

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ABS405/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-Pyrazoliny-1-Carbothioamide

Beom Soo Kim,1, Sangho Ji, Sang Won Jung,

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ABS406/BOD136

Functional networks study of Ga using coevolution analysis

Minjae Seo,1,

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ABS407/BOD26

Bifurcated H-Bonding in Membrane Proteins

Esther S Brielle,1, Isaiah T Arkin,

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ABS408/BOD82

Engineering Therapeutics for the Treatment of Anemia in Oncology Patients

Ning Yang,1, Marina Chemerovski-Glikman, Lia Cardarelli, Jarrett Adams, Sachdev Sidhu,

(1) Donnelly Center for Cellular and Biomolecular Research, 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

ABS410/BOD117

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

Sujata Chakraborty,1, Ethan Ahler, Linglan Fang, Emily Dieter,

(1) University of Washington

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,

(1) The University of Akron

ABS412/BOD153

Atomistic View of an Unfolding Pathway in a Seven-Helical Membrane Protein

Peng Xiao,1, David Bolton, Vladimir Ladizhansky,

(1) University of Guelph

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ABS413/BOD39

Mechanism of microtubule nucleation in the PCM

Shiou-Lan Lin,1,

- (1) Institute of Bioinformatics and Structural Biology,
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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

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,

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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

Rajji Kawade,1, Daisuke Kuroda, Jose Caaveiro, Hiroki Akiba, Shigeru Okumura, Toshiaki Maruyama, Kevin Entzminger, Kouhei Tsumoto,

- (1) The University of Tokyo

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,

- (1) Lei Brüscheweiler-Li, Rafael Bru'schweiler,
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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

- (1)

ABS423/BOD68

Developing Orthogonal Single-Molecule Constructs Using HUH Endonucleases and DNA Handle Self-Assembly

Andrew Nelson,1, Cassidy Tompkins, Blake Everett, Klaus Lovendahl, Wendy Gordon,

- (1) University of Minnesota- Twin Cities

ABS424/BOD28

Protein Disorder in Reconstituted Dynein Cargo Attachment Subcomplex

Kayla Jara,1, Cat Hoang, Sanjana Saravanan, Elisar Barbar,

- (1)

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ABS425/BOD96

Biasing Binding Orientation of the C-terminal Strand Exchange Limits Chaperone Function in Human Alpha-B Crystallin

(1) James Hebda, I, Derrick Draeger, Khan Nguyen, Anna Nevels, Austin College

ABS426/BOD113

pH Dependence on Binding and Release of Folate by Folic Acid Receptor a

(1) Thomas Paul, I, Hedieh Torabifard, Jonah Vilsack, Ryan Hayes, Charles Brooks
Department of Chemistry, University of Michigan

ABS427/BOD138

AMP Regulation of Bifunctional ADP-dependent Sugar Kinases from Archaea: Evolutionary History and Kinetic Characterization

(1) Gabriel Vallejos, I, Sixto M Herrera, Victor Castro-Fernandez, Departamento de Biología, Facultad de Ciencias, Universidad de Chile

ABS428/BOD127

Characterizing Catch Bond Clusters Using DNA Origami and Atomic Force Microscopy

(1) Molly Mollica, I, Olga Yakovenko, Nathan Sniadecki, Wendy Thomas,
University of Washington

ABS429/BOD3

Design and Validation of De Novo Designed Protein Mini Binders of Ribosomal RNA Small Subunit Methyltransferase A From *Burkholderia pseudomallei*

(1) Bradley Hammerson, I, 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 Disease Research

ABS430/BOD74

Novel Structure of Flavohemoglobin from *Malassezia yamatoensis* Determined by SAD Phasing

(1) Madison Bolejack, I, Jan Abendroth, David Fox III, Thomas Edwards, Peter Myler, Stephen Mayclin,
SSGCID/UCB

ABS431/BOD151

Discerning the biochemical function for the catalytic domain of the Plasmodium BEM46-like protein (PBLP)

(1) Anna Groat Carmona, I, Koryn Aguon, Misaki Seto,
University of Washington Tacoma

ABS432/BOD4

Characterization of mechanisms involved in Sbp1 reversible protein aggregation on *Saccharomyces cerevisiae*

(1) Jesus Ruiz Flores, I, Francisco Torres Quiroz,
National Autonomous University of Mexico

ABS433/BOD82

Structural Insights into the Evolution of the CAZy GT8 Glycosyltransferase Glycogenin

(1) Hyun Woo Kim, I, Msano Mandalasi, Zachary Wood, Christopher West,
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

(1) Exequiel Medina, I, Ricardo Coñuecar, Cesar A. Ramirez-Sarmiento,
Departamento de Biología, Facultad de Ciencias, Universidad de Chile

ABS435/BOD84

Structure-based Design of Selective Inhibitors Against the BACE Protein Family

(1) Emma Lendy, I, Emilio Cardenas, Yu-Chen Yen, Arun Ghosh, Andrew Mesecar,
Department of Biochemistry, Purdue University

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ABS436/BOD41

Towards Synthetic Allosteric Transcriptional Modulators: Defining the Role of Conformational Entropy in Coactivator Complexes

Amanda Peiffer, I, Charles Brooks III, Anna Mapp
University of Michigan

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ABS437/BOD46

Analysis of Calmodulin-Interacting Proteins Captured in Live Cells by Photoactivated Cross-linking: Evidence for an Active Ca²⁺ Signaling Microdomain

Anthony Persechini, I, DJ Black, Quang-Kim Tran,
Andrew Keightley, Ameya Chinawalker, Cole McMullin,
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ABS438/BOD23

The development of E. coli expression system for G protein-coupled receptors

Nanao Suzuki, I, Yuuki Takamuku, Chika Yoshida, Takeshi Murata,
Graduate School of Science, Chiba University

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ABS439/BOD150

Intra-Melanosomal Domains of Human Recombinant Tyrosinases Prone to Protein Aggregation at Physiological Temperatures

Monika Dolinska, I, Claudia Kassouf, Paul Wingfield, Yuri Sergeev,
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ABS440/BOD114

Engineering scFv Antibody Against Conserved Regions of Dengue Virus Envelope Protein

Abhishek S Rathore, I, Rinkoo D Gupta,
Colorado State University

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ABS441/BOD83

A Rationally Designed Plant-Produced IgA Has Improved Yield And Exhibits Cross Serotype Protection Against Enterohemorrhagic Escherichia Coli

Adam Chin-Fatt, I, Rima Menassa,
Western University

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ABS442/BOD93

Structure of the PR Domain from PRDM3 and its Function in Acute Myeloid Leukemia

Sharon Loa, I, Tung-Chung Mou, Kelly McGlynn,
Archibald Perkins, Stephen Sprang, Klara Briknarova,
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ABS443/BOD15

Influences of unstructured hinge polypeptides on the folding, and purification of a conventional kinesin heavy chain motor protein

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Taipei Medical University

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ABS444/BOD139

Mutation-Based Tuning of the Rice Cyclophilin LRT2

Nathan Korson, I, Lucila Andrea Acevedo, Linda Nicholson,
Cornell University

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ABS445/BOD140

Conformational Dynamics of Deubiquitinase A in Regulation and Substrate Specificity

Ying Li, I, Ashish Kabra, Efsita Rumpa,
University of Louisville

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ABS446/BOD63

Single-molecule force spectroscopy reveals cooperative interfacial metal sites in human antibacterial protein S100A12 homodimer

Peng Zheng, I,
Nanjing University

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ABS447/BOD129

Altering the conformational specificity of DNA binding proteins

Seul Ki Lee, I, Chan Yang Park, Chaehee Park, Hee-Jung Choi,
Yang-Gyun Kim,
Sungkyunkwan University

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ABS448/BOD75

Protein-induced structural deviations of Z-DNA

Hyuk Won, I, Chaehee Park, Ji-Ye Yun, Young Eun Won,
Hee-Jung Choi, Yang-Gyun Kim,
Sungkyunkwan University

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ABS449/BOD59

Coarse-Grained Protein Modelling with SURPASS

- (1) Dominik Gront, I, Justyna Kryś,
University of Warsaw Faculty of Chemistry

ABS450/BOD12

An Evolutionarily Conserved Mechanism of Amylin Misfolding in Type 2 Diabetes

- (1) Caitlyn Fields, I, Justin Lomont, Kacie Rich, Sidney Dicke,
Megan Petti, Martin Zanni,
University of Wisconsin, Madison

ABS451/BOD89

Investigating the fitness effect of mutations in the diphthamide histidine of human elongation factor 2

- (1) John Weldon, I, Brian Masters, Nadim Alkharouf, Benjamin Atha,
Jack Sanford, Lauren Russell, John Cyprien,
Towson University

ABS452/BOD151

An inactivated dimeric Vibrio alkaline phosphatase converts to a state with a different promiscuous activity

- (1) Jens Gudmundur Hjörleifsson, I, Kristófer Arnar Eiríksson,
Bjarni Ásgeirsson,
University of Iceland

ABS453/BOD84

Nonlinear Partial Correlation To Identify Contribution Of Residues In Global Conformational Dynamics

- (1) Amitava Roy, I, Michael Bender, Rong Yang, Paula Lei,
KC Cheng, Frank Arnold,
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ABS454/BOD29

Hx to measure membrane protein electrostatics

- (1) Esther Brielle, I, Isaiah T Arkin,
The Alexander Grass Center for Bioengineering,
The Hebrew University of Jerusalem, Edmond J. Safra Campus

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

- (1) Won-Kyu Lee, I, 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
Innovation Foundation

ABS456/BOD85

Comparison of kinetics of purified antibody and animal cell expression sup using BLI system

- (1) Myung ho Sohn, I, Myung ho Sohn, HOJIN Yoo, Won-Kyu Lee,
Sora Park, Saehae Choi, So-Young Choi,
New Drug Development Center, Osong Medical Innovation
Foundation

ABS457/BOD5

Amyloid- β 42 Aggregate Structure from Large-scale Mutational Data

- (1) Floriane Ngako Kameni, I, Vanessa E. Gray, Katherine A. Sitko,
Douglas M. Fowler,
Seattle Children's Research Institute

ABS458/BOD42

Chromatin as Viewed by Ubiquitin Writers: Determinants of H2A Site Specificity by RING Ubiquitin E3 ligases, BRCA1/BARD1 and Ring1b/Bmi1

- (1) Sam Witus, I, Alex Zelter, Evie Henry, Mikaela Stewart,
Trisha Davis, Rachel Klevit,
University of Washington School of Medicine

ABS459/BOD24

Engineered Virus-Like-Particles for GPCR Specific Therapeutic Antibody Discovery

- (1) Mart Ustav, I, Jarrett Adams, Sachdev Sidhu,
University of Toronto

ABS460/BOD154

Predicting Protein-Protein Interface Domains Using Multiple Scale Analysis

- (1) Ben Tribelhorn, I, Mike Bailey,
University of Portland

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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

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ABS462/BOD44

MAF1b from Toxoplasma gondii Interacts with Human RaiGAPa1, Potentially Altering Host Immune Signalling

Cameron Powell,1, Matthew Blank, Reece Hoffman, John Burke, John Boyle, Martin Boulanger, University of Victoria

(1)

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,

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(1)

ABS464/BOD77

Cis-acting Glycan Drives Protein-Protein Interactions of Skp1 in Dictyostelium and Toxoplasma

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ABS465/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, Merck & Co.

(1)

ABS466/BOD129

Engineering the Next Generation of SH2 Superbinders to Probe the Phosphoproteome and Antagonize cancer cell signalling

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ABS467/BOD97

Increasing Surface Charge Converts Spy Into A More Efficient Chaperone

Wei He,1, Jiayin Zhang, East China University of Science and Technology

(1)

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

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ABS469/BOD131

Construction of Chimeric Calbindin D9k Proteins Showing a Ca2+ Induced -Conformational Change

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ABS470/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

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ABS471/BOD155

Substrate-based Allosteric Regulation of a Homodimeric Enzyme

Christopher Di Pietrantonio,1, Pedram Mehrabi, Tae Hun Kim, Adnan Sijoka, Christopher Ing, Regis Pomes, Emil F. Pai, R. Scott Prosser, Department of Chemistry, University of Toronto

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ABS472/BOD155

Assessing The Resilience of Proteins to the Effects of Drugs

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ABS473/BOD60

A Scalable Compute Framework for Generating and Assessing Protein Mutants

Dylan Carpenter,1, Michael Albert, Sam Herr, Filip Jagodzinski, Western Washington University

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Posters

ABS474/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,

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ABS475/BOD122

Integrating the influence of pH in NMR chemical shift prediction Methods

Efrosini Artikis,1, Charles Brooks III, Graduate Student

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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

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ABS478/BOD62

Regulatory mechanisms of the deubiquitinase BAP1

Maxime Uriarte,1, Salima Daou, Haitthem 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

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ABS479/BOD85

Structural Characterization of the LC8-RavP Complex Reveals a New Role for LC8 in Lyssavirus Phosphoproteins

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ABS480/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, University of Minnesota

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ABS481/BOD87

Determination of Protein Complex Architecture Guided by Low-Resolution Cryo-Electron Microscopy Density

Daniel Farrell,1, Frank DiMaio, University of Washington

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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 Environmental Health Sciences

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ABS483/BOD131

Computational Design of a De Novo, Modular Mini-protein Targeting PD-1

Cassie Bryan,1, Gabriel Rocklin, David Baker, University of Washington

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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

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ABS485/BOD87

Subunit Mass Analysis for Monitoring Multiple Attributes of Monoclonal Antibodies

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ABS486/BOD55

Interaction Studies of Calmodulin-Like Protein 19 (CML19), the Centrin 2 of Arabidopsis thaliana, with RAD4 and SAC3B target peptides

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