THE 29TH ANNUAL SYMPOSIUM OF



FINAL PROGRAM



TABLE OF CONTENTS



Welcome	3
Committees	4
2015 Protein Society Awards	7
Palau de Congressos de Barcelona Floor Map	8
General information	9
Travel awards	10
Meeting at a glance	12
Program	15
Exhibition	24





Dear Colleagues,

As the President of the Protein Society, I would like to encourage your company to participate in the 29th Annual Symposium of The Protein Society. A unique, 3.5 day forum focusing on all aspects of protein science, the meeting will take place in Barcelona, Spain, July 22-25, 2015.

With an outstanding program developed by the 2015 Program Planning Committee, the meeting will be the can't-miss event for scientists seeking to stay on top of the latest advances and developments.

The longstanding significance of the meeting derives from its unique, trans-disciplinary focus on proteins per se, rather than a narrower focus on a particular protein type, biological field, or experimental method. This shared interest in proteins draws thought leaders from from around the world who are conducting molecular biological, genetic, biochemical, biophysical and computational experiments at leading institutions in more than 50 nations. Put simply, the Protein Society Symposium is the meeting for learning and presenting the latest results in protein science from all scientific disciplines. And, consequently, it serves as a singular opportunity for vendors and sponsors who offer services and technologies aimed at proteins in the lab. There are numerous sponsorship offerings that are designed to cost-effectively boost your company's visibility, and we work with our exhibitors to drive traffic and ensure your return on investment.

Please take a look at the information below and get in touch if you have any questions or suggestions.

I hope you will be able to make it, and look forward to meeting many of you in Barcelona!

Best Wishes,

James U. Bowie, PhD

James U Bowie

Protein Society President



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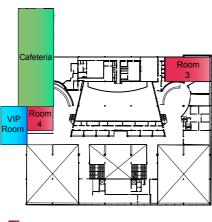




Level 1



Level 2

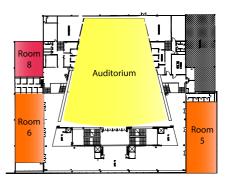


Lunch Time Workshops

Speaker Room

Cafeteria

Level 3



Lunch Time Workshops

Plenary Room

Parallel Rooms



SCIENTIFIC REGISTRATION - HALL

The Registration Area will open at 3:00 PM on Tuesday, July 21st (refer to hours below). Registration includes admission to all scientific and poster sessions, exhibits, one copy of the Final Program and one tote bag. Registration does not include any meals.

HOURS

 Tuesday, 21st:
 3:00 pm - 6:00 pm

 Wednesday, 22nd:
 7:30 am - 6:30 pm

 Thursday, 23rd:
 6:30 am - 6:30 pm

 Friday, 24th:
 8:00 am - 6:30 pm

 Saturday, 25th:
 8:00 am - 12:00 pm

REGISTRATION FEES

Full Member Registration:	535€
Emeritus Member Registration:	405€
Staff Member Registration:	420€
Graduate Student Member Registration:	195€
Undergrad Member Registration:	FREE
Early-Career Member Registration:	390€
Regular Non-Member Registration:	775€
Non-Member Student:	270€
Non-Member Lab Staff / Emeritus:	665€
Non-Member Corporate:	1350€
One-day Registration:	270€
Guest Registration (Networking Events):	100€
Guest Registration (Exhibition Hall Only):	390€

BADGE/ DELEGATE BAG PICKUP - MAIN HALL

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

CAMERAS/VIDEO RECORDING

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

MOBILE DEVICES

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

MEAL FUNCTIONS / CAFETERIA OPENING HOURS

Meals are not included with the Symposium registration fee.

There is a Cafeteria inside the venue for attendees to purchase sandwiches and drinks. It will be open from 8.30 am - 04.30 pm and is located in level 2. Nearby restaurants also offer some affordable menus (further information available in the Symposium app).

COMPLIMENTARY INTERNET ACCESS

There is free wi-fi internet access at the meeting venue. The network name is PS2015 and is open to all attendees.

TAXIS

Taxis in Barcelona may be ordered by phone, picked up at authorized taxi stands or flagged down in the street. Taxis must usually be paid in cash though some accept credit cards.

Radio Taxi: 0034 933 033 033

Taxi for disabled people: 0034 935 519 368

USEFUL TELEPHONES

For emergencies: 112 Municipal Police 092 Airport: 0034 902 404 704

Railway company (Renfe): 0034 902 320 320

Bus station: 0034 934 913 183

CURRENCY

The currency in Spain is the Euro. All fees and rates are charged in Euros. No other currency will be accepted.

TOURS FOR ACCOMPANYING PERSONS

Icono Serveis offers a wide variety of tours during the week. Please refer to the Symposium app for further information



POSTER SET UP & REMOVAL

Posters can be mounted from 8:30 AM to 11:00 AM on Wednesday, July 22nd. Note that all posters must be no larger than 150 cm height x 90 cm width. No 'landscape' posters will be accepted. Main Hall. Posters can remain mounted until 01:00 PM on Saturday, July 24th. Any posters remaining after that point will be discarded.

POSTER VIEWING TIMES

Posters are on display from Wednesday morning until Saturday morning. During the following shifts, exhibitors will be on hand and--during the 2 afternoon shifts—a Mix & Mingle networking reception taking place:

Wednesday, July 22nd 11:30 AM – 1:30 PM 4:30 PM – 6:30 PM Thursday, July 23rd 11:30 AM – 1:30 PM 4:30 PM – 6:30 PM

Friday, July 24th 11:30 AM – 1:30 PM

POSTER SESSION KEY

CELL ENGINEERING	PA
CHEMICAL BIOLOGY	PB
ENZYME & PATHWAY ENGINEERING	PC
FOLDING	PD
INTEGRATIVE PROTEIN SCIENCE	PE
INTRINSICALLY DISORDERED PROTEINS	PF
OBSERVING DYNAMICS IN SINGLE CELLS	PG
PROTEIN ALLOSTERY & DYNAMICS	PH
PROTEIN ENGINEERING	PΙ
PROTEOMICS (PPIS, PTMS)	PJ
SYSTEMS BIOLOGY	PK
OTHER	PL

Authors will be presenting posters on the following schedule:

Wednesday, july 22nd

4:30 PM - 5:30 PM

Even/Odd numbered posters P-P - TBD

Thursday, july 23rd 4:30 PM – 5:30 PM

Even/Odd numbered posters P-P - TBD



The following outstanding students and early-career investigators received travel assistance to attend the 29th Annual Symopsium of The Protein Society from The Finn Wold Travel Awards fund and The Protein Science Young Investigator Travel Grants:

UNDERGRADUATE STUDENTS

Devika Channaveerappa, Clarkson University Joana M Dantas, Universidade Nova de Lisboa Tania Raquel Berrocal Gama, Universidad Nacional Autónoma de México Angela Faye Harper, Wake Forest University Shrutee Jakhanwal, Max Planck Institute for Biophysical Chemistry, Goettingen Sandy On, University of Southern California Alexis Noelli Peña, Syracuse University Luis Valencia, The University of Texas at Austin Oscar Villarreal, University of Texas at Austin

GRADUATE STUDENTS

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Arnab Nayek, The University of Burdwan

Estella Newcombe, University of Melbourne

Bartosz Nizynski, Nencki Institute of Experimental Biology

Anisha Maria Perez, Rice University

V. V. Hemanth Giri Rao, National Centre for Biological Sciences, Bengaluru, India





Mariana Schulte-Sasse, Universidad Nacional Autónoma de México

Austin E. Smith, University of North Carolina-Chapel Hill

Teresa Vitali, Università degli Studi di Milano

Marina Warepam, University of Delhi

Heather Wiebe, Simon Fraser University

EARLY-CAREER RESEARCHERS

- Dr. Deovrat Begde, Dr. Ambedkar College
- Dr. Sinisa Bjelic, Linnaeus University
- Dr. Savita Bhutoria, Yeshiva University
- Dr. Minttu Virkki de Marothy, Stockholm University
- Dr. Nyssa Drinkwater, Monash University
- Dr. Priscila Ferreira, Universidade Federal do Rio de Janeiro
- Dr. Pedro Alberto Valiente Flores, University of Havana
- Dr. Robert Gahl, National Institutes of Health
- Dr. Olivier Julien, University of California San Francisco
- Dr. Tyler Korman, University of California Los Angeles
- Dr. Brett Kroncke, Vanderbilt University School of Medicine
- Dr. Manasi Mishra, Academy of Sciences of Czech Republic, Prague
- Dr. Peter B. Oparin, Russian Academy of Sciences
- Dr. Sebastian Rämisch, Lund University
- Dr. Christina Schroeder, Institute for Molecular Bioscience
- Dr. Arnaldo Serrano, University of Wisconsin-Madison
- Dr. Gyanesh Sharma, Lady Davis Institute, McGill University
- Dr. Christopher Snow, Colorado State University
- Dr. Anna Vangone, Utrecht University
- Dr. Conny Wing-Heng Yu, University College London
- Dr. Lucie Zemanova, Charles University in Prague, Czech Republic



Thank you, on behalf of the leadership and Executive Council of the Protein Society, to the recent donors to the Finn Wold Travel Awards Fund. In 2015, greater than 50 students and young investigators will be able to attend and take part in the 29th Annual Symposium because they received some form of travel assisstance. These opportunities are made possible in part by support from:

Finn Wold Travel Award Donors

Roger Acher Spencer Anthony-Cahill Len Banaszak Dorothy Beckett George R. Bousfield Donna E. Crone Timothy A Cross Anne Gershenson Jenny P. Glusker Jacob M. Goldberg Flizabeth Goldsmith Norma J Greenfield Tijana Z. Grove John R Helliwell Mark A. Hermodson Yao-Te Huang Joel Janin Edyth Malin Andreas Matouschek

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

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

Tatsuya Ikenoue, Institute for Protein Research, Osaka University
 Olivier Julien, PhD, University of California, San Francisco
 Ivo C. Martins, PhD, Universidade de Lisboa
 Shruti Mittal, University of Delhi
 Arnaldo L. Serrano, PhD, University of Wisconsin, Madison
 Austin E. Smith, University of North Carolina, Chapel Hill
 Heather Wiebe. Simon Fraser University







MEETING AT A GLANCE







WEDNESDAY, JULY 22

Germany.

OPENING PLENARY SESSION & THE 2015 HANS NEURATH AWARD TALK 08:30 - 09:10 am Auditorium

08:30 am	Introduction & welcome from Protein Society President James Bowie, University of California Los Angeles. Los Angeles, CA, United States.
08:35 am	Presentation of the 2015 Hans Neurath Award* to Marina Rodnina
08:40 am	The Ribosome in Action: Following Protein Synthesis in Real Time. Marina Rodnina, Max Planck Institute for Biophysical Chemistry. Göttingen, Germany. *Sponsored by the Hans Neurath Foundation
09:10 am	Morning Meet-Up Coffee Break

CONCURRENT MORNING SYMPOSIA PROTEOMICS (PTMs, PPIs) 09:40 am - 11:30 pm

Auditorium

09:40 am	Intro from Chair: Francesc Xavier Aviles , <i>Universitat Autònoma de Barcelona. Barcelona, Spain.</i>
09:45 am	Chemical Cross-linking/Mass Spectrometry and the Structural Biology Toolbox. Ruedi Aebersold, Eidgenössische Technische Hochschule Zürich. Zürich, Switzerland.
10:15 am	Integrative Structural Biology. Andrej Sali, University of California San Francisco, CA, United States.
	Young Investigator Speaker:
10:45 am	Global Kinetic Analysis of Caspase-2 and Caspase-6 Proteolysis in Cellular Extract Reveals Target Specificity Beyond the Substrate Primary Sequence. Olivier Julien, University of California San Francisco, CA, United States.
11:00 am	Lipid-protein Networks. Anne-Claude Gavin-Perrin, Furopean Molecular Biology Laboratory, Heidelberg

CONCURRENT MORNING SYMPOSIA ENZYME & PATHWAY ENGINEERING

09:40 - 11:30 am

Room 6 (room 5 - overflow)

09:40 am Intro from Chair: F. Xavier Gomis-Rüth, IBMB-CSIC. Barcelona, Spain.

09:45 am New Recipes for Biocatalysis: Expanding the Cytochrome P450 Reaction Landscape

for Non-natural Chemistry.

Eric Brustad, University of North Carolina Chapel Hill. Chapel Hill, NC, United States.

10:15 am Assembly Line Biosynthesis of Polyketide Antibiotics.

Chaitan Khosla, Stanford University. Stanford, CA, United States.

Young Investigator Speaker:

10:45 am Conformation-Specific Antibodies as Enhancers and Inhibitors of Phosphatase

Activity of DEP 1.

Malgorzata Nocula-Lugowska, University of Chicago, Chicago, IL, United States.

11:00 am Novel Strategies for Pathway Engineering In Vivo.

Lynne Regan, Yale University. New Haven, CT, United States.

LUNCH

Poster Displays and Exhibits Open - Exhibit Hall

11:30 - 01:30 pm

Workshop: Career Panel Noon - 01:00 pm Room 3

Undergraduate Student Research Session

Noon - 01:00 pm Room 8

Enabling high resolution protein interaction analysis with PEAQ-ITC.

Presented by: **Dr. Natalia Markova**Noon - 01:00 pm
Room 4

CONCURRENT AFTERNOON SYMPOSIA

CELL ENGINEERING

01:30 - 04:30 pm Room 6 (room 5 - overflow)





01:30 pm	Intro from Chair: Bryan Berger, Lehigh University. Bethlehem, PA, United States.
01:35 pm	Reconstitution of an Intercellular Symmetry Breaking Mechanism Driven by Delta-Notch Signaling. Miki Ebisuya, RIKEN Quantitative Biology Center. Kobe, Japan.
02:05 pm	Young Investigator Speaker:
02:20 pm	Engineering Light-Activatable Proteins for Controlling Cell Signaling Pathways. Brian Kuhlman, University of North Carolina Chapel Hill, NC, United States.
02:50 pm	25-min Coffee Break
03:15 pm	Phasing and Dephasing Cell Morphogenesis. Stephen Michnick, University of Montreal. Montreal, QC, Canada.
03:45 pm	Young Investigator Speaker: Development and Use of a Molecular Purge Valve to Maintain Reduction/ Oxidation Balance in Synthetic Biochemistry Systems. Tayler Korman, University of California Los Angeles, CA, United States.
04:00 pm	Engineering Cell-cell Interactions. Zev Gartner, University of California San Francisco, CA, United States.

CONCURRENT AFTERNOON SYMPOSIA PROTEIN ENGINEERING

01:30 - 04:30 pm

1:30 - 04:30 pm Auditorium

01:30 pm	Intro from Chair: Beatriz Ibarra-Molero, Universidad de Granada. Granada, Spain
01:35 pm	Engineering the Specificity and Delivery of Genome-Editing Proteins. David Liu, Harvard University/HHMI. Cambridge, MA, United States.
02:05 pm	Young Investigator Speaker: Parametric Design of Alpha-helical Barrels and Pore-like Assemblies with Very High Thermodynamic Stabilities. Gustav Oberdorfer, University of Washington. Seattle, WA, United States.
02:20 pm	Ribonuclease A: From kcat/KM to the Clinic Ronald Raines, University of Wisconsin. Madison, WI, United States.
02:50 pm	25-min Coffee Break
03:15 pm	Engineering Protein-Protein Interaction for Tunable Assembly and Release of Molecular Cargos from Protein Cages. Sierin Lim, Nanyang Technological University. Singapore, Republic of Singapore.
03:45 pm	Protein Science Best Paper Speaker: Folding of Aquaporin 1: How Marginally Hydrophobic Transmembrane Helices Can Shape Membrane Protein Folding Minttu Virkki, Stockholm University. Stockholm, Sweden.
04:00 pm	Modifying Biological Function Using Conformational Trapping by Customized Synthetic Antibodies. Anthony Kossiakoff, University of Chicago. Chicago, IL, United States.

Poster Displays, Exhibits Open 04:30 - 06:30 pm

Mix & Mingle Reception 05:30 pm

Happy Hour in Honor of the 2015 Young Investigator Speakers 09:00 - 11:00 pm





THURSDAY, JULY 23

New Member Welcome Breakfast / Members Business Meeting 07:00 - 08:30 am

CONCURRENT MORNING SYMPOSIA FOLDING

08:30 - 11:30 am Auditorium

08:30 pm	Intro from Chair: Irene Díaz-Moreno, Universidad de Sevilla CSIC. Sevilla, Spain.
08:35 am	Structural Observations of Protein Folding on the Ribosome. John Christodoulou, University College London & Wellcome Trust. London, United Kingdom.
	Young Investigator Speaker:
09:05 am	In Vitro Folding Mechanisms Determine the Forces Applied During Co-translational Folding.
	Adrian Nickson, University of Cambridge. Cambridge, United Kingdom.
09:20 am	Folding to the Rhythm of Translation Rate.
	Patricia Clark, University of Notre Dame. Notre Dame, IN, United States.
09:50 am	25-min Coffee Break
10:15 am	The Unfolded N- and C-termini of TAp63a regulate p63's Transcriptional Activity by Locking the Protein in an Inhibited, Dimeric Conformation Volker Dötsch, Johann Wolfgang Goethe Universität. Frankfurt am Main, Germany.
	Young Investigator Speaker:
10:45 am	Single-molecule Vectorial Folding and Unfolding Through Membrane Pores. David Rodriguez-Larrea, University of the Basque Country. Leioa, Spain.
11:00 am	Structural Insight into the Biogenesis of Beta-Barrel Membrane Proteins. Susan Buchanan, NIDDK, National Institutes of Health. Bethesda, MD, United States.

CONCURRENT MORNING SYMPOSIA

CHEMICAL BIOLOGY

08:30 - 11:30 am

Room 6 (room 5 - overflow)

08:30 pm	Intro from Chair: Francisco Blanco, CIC bioGUNE. Elexalde Derio, Spain.
08:35 am	Probing Dynamic Protein Lipidation: From Chemical Proteomics to Drug Discovery.
	Edward Tate, Imperial College. London, United Kingdom.
09:05 am	Young Investigator Speaker: Ubiquitin-Nanoparticle Interactions by Solution NMR Spectroscopy. Serena Zanzoni, University of Verona. Verona, Italy.
09:20 am	Protein Methyltransferase Inhibitors as Personalized Cancer Therapeutics. Robert Copeland, Epizyme, Inc. Cambridge, MA, United States.
09:50 am	25-min Coffee Break
10:15 am	Dynamic Regulation of Metabolic Enzymes and Pathways by O-Glycosylation. Linda Hsieh-Wilson, California Institute of Technology/HHMI. Pasadena, CA, United States.
10:45 am	Young Investigator Speaker: Semi-Chemical Synthesis and Characterization of a Small Heat Shock Protein Bearing a Nonenzymatic Posttranslational Modification Found In Vivo. Maria Matveenko, <i>University of Vienna. Vienna, Austria.</i>
11:00 am	Peptides and Molecular Recognition at Protein Surfaces. Ernest Giralt, Institut de Recerca Biomèdica. Barcelona, Spain.

LUNCH
Poster Displays & Exhibits open – Exhibit Hall
11:30 - 01:30 pm

Mentoring Committee Workshop: How to Write an Effective Paper.

Noon - 01:00 pm

Room 3



Educator's Luncheon - Using Primary Literature in the Classroom to Teach Foundational Concepts of Protein Science Noon - 01:00 pm Room 8

Molar Mass, Size, Charge and Interactions: the Light Scattering Toolkit for Essential Biophysical Characterization and Quality Control.

Presented by: Dr. Dan Some.

Noon - 01:00 pm

Room 4



CONCURRENT AFTERNOON SYMPOSIA PROTEIN ALLOSTERY & DYNAMICS

01:30 - 04:30 pm Auditorium

01:30 pm	Intro from Chair: Modesto Orozco, IRB Barcelona. Barcelona, Spain.
01:35 pm	Deciphering the 'Ubiquitin Code': Conformations and Molecular Recognition of Polyubiquitin Signals. David Fushman, University of Maryland. College Park, MD, United States.
02:05 pm	Young Investigator Speaker: The Role of the Mg(II) Ion on Integrin-collagen Interactions: Regulating Affinity Through Conformational Fluctuations. Anna Monica Nunes, Rutgers University. Newark, NJ, United States.
02:20 pm	Multifaceted BAR-domain Proteins to Shape Cell Membranes. Patricia Bassereau, Institut Curie Centre de Recherche. Paris, France.
02:50 pm	25-min Coffee Break
03:15 pm	Mapping Allosteric Sites Across the Apoptotic Caspases. Jeanne Hardy, University of Massachusetts. Amherst, MA, United States.
03:45 pm	Protein Science Best Paper Speaker: Crystal Structure of the Campylobacter Jejuni CmeC Outer Membrane Channel. Chih-Chia (Jack) Su, Iowa State University. Ames, IA, United States.
04:00 pm	Allosteric Inhibition of FGF-FGFR-Complex by Small Molecules. Harald Schwalbe, Johann Wolfgang Goethe Universität. Frankfurt am Main, Germany.

CONCURRENT AFTERNOON SYMPOSIA ENGINEERING & INTERPRETING THE GENOME 01:30 - 04:30 pm

Room 6 (room 5 - overflow)

01:30 pm	Intro from Chair: Maria Solà Vilarrubias, IBMB. Barcelona, Spain.
01:35 pm	Structural Basis for RNA-dependent DNA Cleavage and PAM Recognition by CRISPR-Cas9.
	Osamu Nureki, University of Tokyo. Fukuoka, Japan.
	Young Investigator Speaker:
02:05 pm	Creating Large Covalently Circularized Nanodiscs and Their Application in Studying Viral Entry and Genome Translocation. Mahmoud Nasr, Harvard Medical School. Boston, MA, United States.
02:20 pm	CRISPR Tools for Genome Engineering and Cell Reprogramming. Stanley Qi, University of California. San Francisco, CA, United States.
02:50 pm	25-min Coffee Break
03:15 pm	Defining, Improving, and Altering the Specificities of CRISPR-Cas9 Nucleases. Keith Joung, Massachusetts General Hospital. Charlestown, MA, United States.
	Young Investigator Speaker:
03:45 pm	Prion-like Proteins Sequester and Suppress the Toxicity of Huntingtin Exon 1. Can Kayatekin, Whitehead Institute. Cambridge, MA, United States.
04:00 pm	How Nature Evolves New Enzyme Functions. Patricia Babbitt, University of California San Francisco, CA, United States.

Poster Displays, Exhibits Open 04:30 - 06:30 pm

Mix & Mingle Reception 05:30 pm



FRIDAY, JULY 24

CONCURRENT MORNING SYMPOSIA INTRINSICALLY DISORDERED PROTEINS 08:30 - 11.30 am

Auditorium

08:30 am	Intro from Chair: Xavier Salvatella, IRB Barcelona. Barcelona, Spain.
08:35 am	Fuzzy Interactions and Context Dependence of Proteins. Monika Fuxreiter, Debreceni Egyetem. Debrecen, Hungary.
	Young Investigator Speaker:
09:05 am	Structuring Disorder: the Case of the Intrinsically Disordered Unique Domain of c-Src. Mariano Maffei, University of Barcelona. Barcelona, Spain.
09:20 am	Single-Molecule Spectroscopy of Intrinsically Disordered Proteins. Ben Schuler, Universität Zürich. Zürich, Switzerland.
09:50 am	25-min Coffee Break
10:15 am	Identifying Order in Intrinsically Disordered Proteins. Robert Konrat, University of Vienna. Vienna, Austria.
	Young Investigator Speaker:
10:45 am	Intrinsically Disordered Proteins Drive Heritable Transformations of Biological Traits.
	Daniel Jarosz, Stanford University. Stanford, CA, United States.
11:00 am	The Role of Protein Disorder and Self-Association in the Formation of Cellular Bodies. Tanja Mittag, St. Jude Children's Research Hospital. Memphis, TN, United States.
	,,

CONCURRENT MORNING SYMPOSIA OBSERVING DYNAMICS IN SINGLE CELLS

08:30 - 11.30 am Room 6 (room 5 - overflow)

08:30 am	Intro from Chair: Eva Nogales, University of California, Berkeley/HHMI. Berkeley,
	CA, United States.

08:35 am A Single Cell Systems Based View of Immunity and Cancer.
Garry Nolan, Stanford School of Medicine. Palo Alto, CA, United States.

Young Investigator Speaker:

09:05 am In Situ Membrane Protein Structure and Function Analysis using Site-Specific Unnatural Amino Acid Incorporation and Spectroscopy Methods.

Changlin Tian, University of Science and Technology of China. Hefei, China.

09:20 am ORACLs: Optimized Reporter cell lines for Annotating Compound Libraries

Across Diverse Drug Classes Via Imaged Based Phenotypic Screens. Lani Wu, University of Texas, Southwestern Medical Center. Dallas, TX, United

States.

09:50 am 25-min Coffee Break

10:15 am Does Engineering Functional Enzymes Require Preserving Protein

Dynamics?

Joelle Pelletier, University of Montreal. Montreal, QC, Canada.

Young Investigator Speaker:

10:45 am Live-cell Measurements of the Conformational Rearrangements in Bax at the

Initiation of Apoptosis.

Robert Gahi. The National Institutes of Health. Bethesda. MD. United States.

11:00 am Imaging the Genome in Living Cells.

Bo Huang, University of California San Francisco, CA, United States.

Lunch - Poster Displays and Exhibits Open – Exhibit Hall 11:30 - 01:30 pm

Mentoring Committee Workshop: How to Bive a Great Talk
Noon - 01:00 pm
Room 3

PLENARY AWARDS SESSION

01:30 - 06:00 pm Auditorium

01:30 pm Intro from Chair: James Bowie, Protein Society President, University of California

Los Angeles. Los Angeles. CA, United States

01:35 pm Presenting The Hans Neurath Outstanding Promise Awards*

01:50 pm Claudio Ciferri, Genentech - Presenting the Dorothy Crowfoot Hodgkin

Award** to Eva Nogales

01:55 pm Visualizing Molecular Complexity by cryo-EM to Understand Biological Function.

Eva Nogales, University of California Berkeley/HHMI. Barkeley, CA, United States.



02:25 pm	Presentation of the <i>Protein Science</i> Young Investigator Award to Nieng Yan
02:30 pm	Structural and Mechanistic Investigation of Glucose Transporters. Nieng Yan, Tsinghua University/HHMI. Beijing, China.
03:00 pm	Presenting The Emil T. Kaiser Award to Anna Mapp
03:05 pm	Dissecting Transcriptional Protein Networks. Anna Mapp, University of Michigan. Ann Arbor, MI, United States.
03:35 pm	30-min Coffee Break
04:05 pm	Presenting the Christian B. Anfinsen Award to Sachdev Sidhu
04:10 pm	Synthetic Proteins in the Real World. Sachdev Sidhu, University of Toronto. Toronto, ON, Canada.
04:40 pm	Presenting The Carl Brändén Award*** to C. Robert Matthews
04:45 pm	Superoxide Dismutase: From Folding and Stability to Potential Therapeutics for ALS C. Robert Matthews, University of Massachusetts Medical School. Worcester, MA, USA.
04:45 pm 05:15 pm	Therapeutics for ALS C. Robert Matthews, University of Massachusetts Medical School.
·	Therapeutics for ALS C. Robert Matthews, University of Massachusetts Medical School. Worcester, MA, USA.
05:15 pm	Therapeutics for ALS C. Robert Matthews, University of Massachusetts Medical School. Worcester, MA, USA. Acknowledgement of the 2015 Neurath Award and Stein & Moore Award recipients
05:15 pm 05:20 pm	Therapeutics for ALS C. Robert Matthews, University of Massachusetts Medical School. Worcester, MA, USA. Acknowledgement of the 2015 Neurath Award and Stein & Moore Award recipients Presentation of the Protein Science Best Paper Awards
05:15 pm 05:20 pm 05:30 pm	Therapeutics for ALS C. Robert Matthews, University of Massachusetts Medical School. Worcester, MA, USA. Acknowledgement of the 2015 Neurath Award and Stein & Moore Award recipients Presentation of the Protein Science Best Paper Awards Presentation of the Protein Society Service Awards

SATURDAY, JULY 25

CONCURRENT MORNING SYMPOSIA SYSTEMS BIOLOGY

08:30 - 10:20 am Auditorium

08:30 am Intro from Chair: **Luis Serrano**, *Centre for Genomic Regulation / ICREA*.

Barcelona, Spain.

08:35 am Disease-ssociated Mutations and Coding Variation in Human Transcription

Factors.

Martha Bulyk, Brigham & Women's Hospital and Harvard Medical School.

Boston, MA, United States.

09:05 am Dynamic Heterogeneity in the ERK and AMPK Networks and its Role in

Human Disease.

John Albeck, University of California. Davis, CA, United States.

Young Investigator Speaker:

09:35 am Proof of Principle for Epitope-focused Vaccine Design.

Bruno Correa, École Polytechnique Fédérale de Lausanne. Lausanne, Switzerland.

09:50 am Yeast Proteome Dynamics from Single Cell Imaging and Automated Analysis.

Brenda Andrews, University of Toronto. Toronto, ON, Canada.

CONCURRENT MORNING SYMPOSIA INTEGRATIVE PROTEIN SCIENCE

08:30 - 10:20 am Room 6 (room 5 - overflow)

08:30 am Intro from Chair: Miguel Ángel de la Rosa, University of Sevilla. Sevilla. Spain.

Lorne Conference on Protein Structure and Function Guest Speaker

08:35 am Targeting the Plasmodium Falciparum Neutral Aminopeptidases for Development

of Novel Antimalarial Agents.

Sheena McGowan, Monash University. Clayton, VIC, Australia.

Sponsored by the Lorne Conference on Protein Structure and Function.

09:05 am NMR Analysis of Protein Structure and Dynamics with Computational and

Information Sciences.

Takanori Kigawa, RIKEN Quantitative Biology Center. Yokohama, Japan.



Young Investigator Speaker:

09:35 am Experimental and Computational Studies of the Effects of Highly Concentrated

Solutes on Proteins: Insights Into the Causes and Consequences of Quinary

Protein Structure and Cytoplasmic Organization.

Luciano Abriata, École Polytechnique Fédérale de Lausanne. Lausanne, Switzerland.

Latin American Protein Society Guest Speaker

09:50 am Studies with the Amyloidogenic Protein Transthyretin: from the Patients to

the Protein.

Debora Foguel, Universidade de Federal do Rio de Janeiro. Rio de Janeiro, Brazil.

Sponsored by the Latin American Protein Society.

10:20 am Coffee Break

CLOSING PLENARY SESSION & THE 2015 STEIN & MOORE AWARD TALK 10:50 am Auditorium

10:50 am Introduction from James Bowie, Protein Society President

De Novo Protein Design.

William F. DeGrado, Presenting the Stein & Moore Award to 2015 winner Bill

DeGrado, University of California - San Francisco.



PROGRAM PLANNING COMMITTEE



James Wells (Chair)
Professor & Chair, Dept of Pharmaceutical Chemistry University of California San
Francisco

James A. Wells, PhD, focuses on development of enabling technologies for engineering proteins and for identifying small molecules to aid in drug discovery for challenging targets such as allosteric regulation and protein-protein interactions.

He is interested in the discovery and design of small molecules and enzymes that trigger or modulate cellular processes in inflammation and cancer. Using small molecules and engineered proteins, the Wells lab is studying how activation of particular signaling nodes involving protease, kinases, or ubiquitin ligases drives cell biology. The lab has focused much on a set of proteases, known as caspases, responsible for fate determining cellular decisions involved in apoptosis and innate inflammation among others. These enzymes act as cellular remodelers and help us understand the essential protein struts that support life. These targets also provide leads for developing new cancer therapeutics and biomarkers for cancer treatment.

Wells is a professor and chair of the Department of Pharmaceutical Chemistry in the UCSF School of Pharmacy. He holds a combined appointment as professor in the Department of Cellular & Molecular Pharmacology in the School of Medicine. He joined UCSF in 2005 as holder of the Harry Wm. and Diana V. Hind Distinguished Professorship in Pharmaceutical Sciences. Wells also founded and directs the Small Molecule Discovery Center (SMDC) located at UCSF's Mission Bay campus. He earned a PhD degree in biochemistry from Washington State University with Professor Ralph Yount in 1979 and completed postdoctoral work at Stanford University School of Medicine with Professor George Stark in 1982. Before joining UCSF, Wells was a founding scientist in Genentech's Protein Engineering Department and in 1998 co-founded Sunesis Pharmaceuticals.

Wells is a recipient of the Hans Neurath Award by the Protein Society, the Pfizer Award and Smissman Award given by the American Chemical Society, the Perlman Lecture Award given by the ACS Biotechnology Division, the du Vigneaud Award given by the American Peptide Society, the Merck Award from the ASBMB and in 1999 a member of the National Academy of Sciences and in 2015 a member of the American Academy of Arts and Sciences.



Sarah Teichmann

Research Group Leader EMBL-European Bioinformatics Institute & Wellcome Trust Sanger Institute.

Dr Sarah Teichmann is a research group leader at EMBL-EBI and senior group leader at the Wellcome Trust Sanger Institute. She is also a Principle Research Associate in the Dept Physics/Cavendish Laboratory, and a fellow of Trinity College, Cambridge.

She is a leader in systems biology, which aims to explain how individual molecules within a cell co-operate to produce the cell's overall behaviour. Previously, she was a Programme Leader at the MRC Laboratory of Molecular Biology, from 2001 to 2012. Dr Teichmann gained her PhD in 2000 at the University of Cambridge and MRC Laboratory of Molecular Biology, and was a Beit Memorial Fellow for Biomedical Research, University College London, in 2000/01. Dr Teichmann is an EMBO member and a Fellow of the Academy of Medical Sciences, and has just been awarded the EMBO Gold Medal (2015).

SYMPOSIUM OF





Mark Lemmon
Professor & Chair, Dept of Biochemistry & Biophysics University of Pennsylvania
Perelman School of Medicine

Mark Lemmon is the George W. Raiziss Professor and Chair of Biochemistry and Biophysics at the University of Pennsylvania Perelman School of Medicine, and an Investigator in the Abramson Family Cancer Research Institute.

He received his BA (Hons) in Biochemistry from the University of Oxford (Hertford College), England in 1988, and then completed his Ph.D. with Don Engelman in Yale University's Department of Molecular Biophysics and Biochemistry in 1993. During a postdoc with Joseph Schlessinger at New York University Medical Center (Pharmacology) in Manhattan, as a Damon Runyon Fellow, he worked on mechanisms of receptor tyrosine kinase signaling and Pleckstrin Homology domains, among other things. In 1996, Mark took a position as Assistant Professor in the Department of Biochemistry and Biophysics (and Johnson Foundation) at the University of Pennsylvania Perelman School of Medicine in Philadelphia. At Penn, Mark's laboratory has focused on mechanistic and structural aspects of signaling by growth factor receptors (especially the EGF receptor) and through phosphoinositides. He was promoted to Associate Professor in 2001, to full Professor in 2004, and was appointed Chair of Biochemistry and Biophysics at Penn in 2010. He serves on the Editorial Boards of Cell and Molecular Cell, as well as being a Deputy Chair (and Vice Chair for the Americas) for the Biochemical Journal. Mark received the Protein Society's 2012 Dorothy Crowfoot Hodgkin Award. In 2015, he will move to Yale University as Sackler Professor of Cancer Biology and co-director of the new Cancer Biology Institute.



Miquel Pons
Professor, Dept of Organic Chemistry University of Barcelona

Miquel Pons studied simultaneously biology and chemistry at the University of Barcelona. Obtained his PhD at the University of London under the supervision of Prof. Dennis Chapman. He is full professor and the scientific director of the Large Scale NMR facility at the University of Barcelona. He is interested in dynamics proteins, including intrinsically disordered proteins, supramolecular systems, lipid-protein interactions and NMR methodology.



Oscar Millet Structural Biology Unit CIC BioGUNE

Degree in Chemistry (Univ. Ramon Llull,1994) and Chemical Engineering (IQS, 1995). Ph D in Organic Chemistry (University of Barcelona, 1999) and post-doctoral fellow the group of Lewis Kay (University of Toronto, 2000-2004). Ramon y Cajal fellow at the Parc Cientific de Barcelona (2004-2006), currently group leader at the Structural Biology Unit of the CIC bioGUNE.

My research line focuses of the use of nuclear magnetic resonance (NMR) to the study of biologically relevant proteins and enzymes, paying special attention to the delicate balance existing between protein stability and dynamics. Prize of the Real Sociedad Española de Química (2004) and the Spanish NMR group prize (2005).



Gary Pielak
Distinguished Term Professor of Chemistry, University of North Carolina, Chapel Hill

Gary J. Pielak earned a B.A. in Chemistry from Bradley University in Peoria, Illinois and a Ph.D. in Biochemistry from Washington State University in Pullman, Washington. He was a postdoctoral fellow in the laboratory of Michael Smith at the University of British Columbia in Vancouver, Canada and in the laboratory of Robert J.P. Williams at the University of Oxford in England.

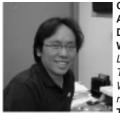
Gary is Kenan Distinguished Term Professor of Chemistry, Biochemistry and Biophysics at the University of North Carolina-Chapel Hill. His research focuses on understanding protein chemistry in cells and undecrowded conditions in vitro.





BEST PAPER AWARD WINNERS

At the beginning of each year, 2 "best papers" are selected from articles published in Protein Science during the preceding 12 months. A junior author (typically the first author) is designated as the award winner and invited to give a talk at the annual Protein Society Symposium.



Chih-Chia (Jack) Su Assistant Scientist, Biological Systems Department of Chemistry at Iowa State University

Winning Paper: Chih-Chia Su, Abhijith Radhakrishnan, Nitin Kumar, Feng Long, Jani Reddy Bolla, Hsiang-Ting Lei, Jared A. Delmar, Sylvia V. Do, Tsung-Han Chou, Kanagalaghatta R. Rajashankar, Qijing Zhang, Edward W. Yu (2014) Crystal structure of the Campylobacter jejuni CmeC outer membrane channel. Protein Sci. 23:954-961



Talk: Thursday July 23 @ 03:45 PM | Protein Allostery and Dynamics

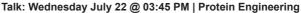
Jack Su received his Bachelor's degree in Life Science from National Dong-Hwa University, Taiwan. He received his Ph.D. in the Department of Biochemistry, Biophysics and Molecular Biology from Iowa State University (ISU). Currently, he is an assistant research scientist at ISU, working on the structure/function relationships of bacterial antimicrobial efflux proteins, which include the C. jejuni CmeABC, N.

gonorrhoeae MtrCDE and E. coli CusCBA tripartite efflux systems. He uses X-ray crystallography, single-molecule FRET, isothermal titration calorimetry, and drug accumulation and efflux assays to elucidate the action mechanisms of these protein machines. Ultimately, he would like to pursue a career in academic research and study disease-related proteins using biophysical techniques.



Minttu Virkki Graduate Student

Department of Biochemistry and Biophysics at Stockholm University Winning Paper: Minttu Virkki, Nitin Agrawal, Elin Edsbacker, Susana Cristobal, Arne Elofsson, Anni Kauko (2014) Folding of aquaporin 1: Multiple evidence that helix 3 can shift out of the membrane core. Protein Sci. 23:981-992





Minttu Virkki's path to her award-winning manuscript was not entirely straightforward. She was born and attended school in Finland and planned to go to medical school. While studying for the entrance exams, however, she "fell in love" with cells, which led her to take a course in molecular biology in Sweden at Stockholm University. This led to further courses on a variety of subjects with her interest focusing more and more on proteins. After obtaining her Master's degree she began Ph.D. studies on

membrane proteins with Arne Elofsson.

WORKSHOP - MALVERN

Wednesday, July 22nd. Noon - 01:00pm. Room 4

ENABLING HIGH RESOLUTION PROTEIN INTERACTION ANALYSIS WITH MICROCAL PEAQ-ITC.

Dr. Natalia Markova, Principal Scientist - MicroCal, Malvern Instruments

Dynamic interactions involving biomolecules drive and regulate all biological processes. Studies of biomolecular interactions are fundamentally important in all areas of life sciences. Data provided by Isothermal Titration Calorimetry (ITC) enables scientists in academia and industry to directly and quantitatively characterize these interactions in solution.

This workshop is aimed at addressing the current bottlenecks in interaction analysis. We will start with a Q&A panel session with calorimetry users and continue with the presentation of the new MicroCal PEAQ-ITC system.

MicroCal PEAQ-ITC, the latest generation of MicroCal ITC instrumentation, offers a whole range of solutions for addressing current pains associated with interaction analysis. Among the most recognized challenges are the needs to adequately address a broad range of binding affinities and to reliably interpret binding data complicated by the presence of inactive protein fraction or inherent uncertainty in the concentration of a ligand.

MicroCal PEAQ-ITC is designed to improve signal stability, mixing, and signal-to-noise characteristics. The improved performance along with an advanced experimental design feature of the easy-to-use all new data analysis software facilitate optimization of experiments for the studies of interactions.

Consistently high performance of MicroCal PEAQ-ITC enables increased confidence and data resolution when measuring low heats at low or uncertain sample concentrations and complex binding modes.

The new MicroCal PEAQ-ITC analysis software allows for automated data analysis, minimizing analysis time and user subjectivity in assessing data quality. Data quality is determined and advanced fitting performed in a few seconds per experiment allowing for analysis of large data sets of 50 or more experiments in a matter of seconds.

Come, join us for lunch and find out more!

WORKSHOP - WYATT

Thusday, July 23rd. Noon - 01:00pm. Room 4

MOLAR MASS, SIZE, CHARGE AND INTERACTIONS: THE LIGHT SCATTERING TOOLKIT FOR ESSENTIAL BIOPHYSICAL CHARACTERIZATION AND QUALITY CONTROL

Dr. Dan Some, Principal Scientist & Director of Marketing, Wyatt

Biophysical characterization and protein quality assessments are central capabilities in any laboratory that seeks qualified, reproducible results in biomolecular or biochemical research. This seminar describes a comprehensive suite of tools based on static and dynamic light scattering that provides biophysical characterization and quality screening from first-principles.

Common uses of the light scattering toolkit include determination of molecular weight and size, native oligomeric or aggregation state, protein-protein binding parameters, and the composition of glycoproteins or other conjugated macromolecules. All measurements are performed entirely in solution and without any form of labeling, offering valuable alternatives to less general methods.





Aviv Biomedical, INc.

Booth 29

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Web: http://www.avivbiomedical.com/

Aviv Biomedical Inc. manufactures scientific and clinical instruments. Products include a fluorescence accessory (AU-FDS) for the Beckman Analytical Ultracentrifuge, model XLA/XLI. Sales, service and support of Aviv Spectrometers, Aviv Spectrophotometers and Aviv Fluorometers.

Malvern Instruments

Booth 27

30 Rue Jean Rostand 91893 Orsay cedex

France

Phone: +33 (0) 169 351 808 Fax: +33 (0) 160 191 326 Email: contact@malvern.com Web: http://www.malvern.com

After buying MicroCal in July 2014, Malvern Instruments launches new PEAQ-ITC in April 2015 and the workshop organized on Wednesday 22th of July will be the first official presentation in Europe. Malvern offers also 4 new devices for characterizing proteins: Viscosizer using the Taylor dispersion to study viscosity and size of proteins and peptides solutions at high concentration, Archimedes to characterize protein aggregates, Helix, combining Raman DLS to identify chemical bonds and study secondary and tertiary structure and finally Nanosight for counting nanoparticles in complex media like serums.

Molecular Dimensions

Booth 3

Unit 6, Goodwin Business Park, Willie Snaith Road, Newmarket CB8 7SQ Suffolk United Kingdom

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Booth 26

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Sigma-Aldrich, a leading Life Science and High Technology company focused on enhancing human health and safety, manufactures and distributes more than 230,000 chemicals, biochemicals and other essential products to more than 1.4 million customers globally in research and applied labs as well as in industrial and commercial markets. With three distinct business units – Research, Applied and SAFC Commercial – Sigma-Aldrich is committed to enabling science to improve the quality of life. The Company operates in 37 countries, has more than 9,000 employees worldwide and had sales of \$2.7 billion in 2013.

St. Jude Children's Research Hospital

Booth 28

262 Danny Thomas Place Memphis, TN 38105, United States

Phone: +1 901 595 2750 Fax: +1 901 595 5376 Email: postdoc@stjude.org Web: www.stjude.org/postdoc

St. Jude is a non-profit biomedical research institution in Memphis, Tennessee where researchers study the molecular basis of both normal and diseased cellular processes. Over 100 faculty investigators perform basic research in close association with 90 clinical faculty, creating an excellent environment for translational research. Visit our booth to discuss postdoctoral fellowship opportunities.

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The Protein Society

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Email: staff@proteinsociety.org Web: www.proteinsociety.org

Wiley Booth 2

The Atrium PO19 8SQ Chichester United Kingdom

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Booth 19

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United States

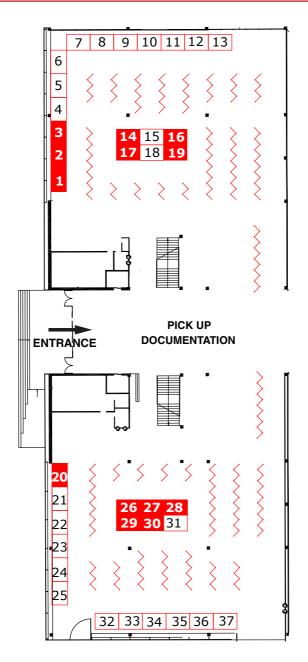
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Booth 2:

WILEY

Booth 3:



Booth 14:

SIGMA-ALDRICH®

Booth 16:



Booth 17:



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Booth 19:



Booth 20:



Booth 26:



Booth 27:



Booth 28:



Booth 29:



Booth 30:







PA - CELL ENGINEERING

PA-001 Scalable biosynthesis of quantum dots: evolution of size selectivity, solubility and extracellular production

<u>Bryan Berger</u>¹, Zhou Yang², Leah Spangler¹, Victoria Berard¹, Qian He², Li Lu², Robert Dunleavy¹, Christopher Kiely², Steven McIntosh¹

1.-Department of Chemical and Biomolecular Engineering, Lehigh University, 2.-Department of Materials Science and Engineering, Lehigh University

PA-002 Protein and Cellular Engineering Platform for Selective and Inducible Apoptotic Proteolysis

Charlie Morgan^{1,2,3}, Juan Diaz^{2,3}, Jim Wells^{2,3}

1.-Chemistry and Chemical Biology Graduate Program, UCSF, 2.-Pharmaceutical Chemistry Department, UCSF, 3.-Molecular and Cellular Pharmacology, UCSF

PA-003 Improving microbial medium-chain fatty acid production using GPCR-based chemical sensors

Stephen Sarria¹, Souryadeep Bhattacharyya², Pamela Peralta-Yahya¹

- 1.- School of Chemistry and Biochemistry, Georgia Institute of Technology
- 2.- School of Chemical and Biomolecular Engineering, Georgia Institute of Technology

PB - CHEMICAL BIOLOGY

PB-001 Applications of 19F-NMR to study protein-ligand interactions and protein conformational changes in solution

Martine I. Abboud¹, Jurgen Brem¹, Rasheduzzaman Chowdhury¹, Ivanhoe K. H. Leung², Timothy D. W. Claridge¹, Christopher J. Schofield¹

1.-University of Oxford, Department of Chemistry, 2.-University of Auckland, School of Chemical Sciences

PB-002 NMR solution structure of lacticin Q, a broad spectrum leaderless antimicrobial protein from Lactococcus lactis QU 5

Jeella Acedo¹, Marco van Belkum¹, John Vederas¹

1.-Department of Chemistry, University of Alberta

PB-003 Sizing and interactions of proteins under native conditions from microfluidic diffusion measurements: application to molecular chaperones and single-step immunoassay Paolo Arosio¹, Thomas Müller¹, Luke Rajah¹, Francesco Aprile¹, Tom Scheidt¹, Jackie Carrozza¹, Maya Wright¹, Michele Vendruscolo¹, Christopher Dobson¹, Tuomas Knowles¹

1.-Department of Chemistry, University of Cambridge

PB-004 Using  alpha-chymotrypsin and elastase enzymatic degradation to control peptide self-assembly

Valeria Castelletto1, Ian Hamley1

1.-School of Chemistry. University of Reading

PB-005 Fluorescence-based techniques for the investigation of localization and functions of proteins

Yuen-Yan Chang¹, Yau-Tsz Lai¹, Ligang Hu¹, Ya Yang¹, Ailun Chao¹, Hongzhe Sun¹

1.-Department of Chemistry, The University of Hong Kong

PB-006 MRNA Fate is Controlled by Highly-Regulated RNA Binding Proteins

<u>Irene Díaz-Moreno</u>¹, Isabel Cruz-Gallardo¹, Sofía M. García-Mauriño¹, Rebecca Del Conte², B. Göran Karlsson³, Andres Ramos⁴, María L. Martínez-Chantar⁵, Francisco J. Blanco⁵, Myriam Gorospe⁶, Jacqueline A. Wilce⁷

1.-IBVF - CICCartuja, University of Seville - CSIC, 2.-CERM, Department of Chemistry, University of Florence, 3.-Swedish NMR Centre, University of Gothenburg, 4.-Molecular Structure Division, MRC National Institute for Medical Research, 5.-CIC bioGUNE, 6.-Laboratory of Genetics, National Institute on Aging-Intramural Research Program, 7.-Department of Biochemistry and Molecular Biology, Monash University

PB-007 Understanding promiscuous and selective ligand binding by liver FABP

Mariapina D'Onofrio¹, Filippo Favretto¹, Serena Zanzoni¹, Silvia Perez Santero¹, Michael Assfalg¹, Henriette Molinari¹

1.-Department of Biotechnology, University of Verona

PB-008 Antimalarial Agents With a Novel Mode of Action: Dual Inhibition of P. falciparum M1 and M17 Metalloaminopeptidases

Nyssa Drinkwater¹, Shailesh Mistry², Komagal Kannan Sivaraman¹, Alessandro Paiardini³, Vicky Avery⁴, Peter Scammells², Sheena McGowan¹

1.-Department of Biochemistry & Molecular Biology, Monash University, 2.-Monash Institute of Pharmaceutical Sciences, Monash University, 3.-Dipartmento di Scienze Biochimiche, Sapienza Universita di Roma, 4.-Eskitis Institute for Drug Discovery, Griffith University

PB-009 Different classes of inhibitors for human 15-lipoxygenase-1

<u>Nikolaos Eleftheriadis</u>¹, Stephanie Thee¹, Johan te Biesebeek¹, Petra van der Wouden¹, Bert-Jan Baas¹, Frank J. Dekker¹

1.-Groningen Research Institute of Pharmacy

PB-010 Identification of Novel Inhibitors of 6-Phosphogluconate Dehydrogenase (6PGDH) in Trypanosoma brucei Through Virtual Drug Screening

Victoria Gomez¹, Kayva Kolavasi¹, Josh Beckham¹, Jon Robertus¹

1.-The University of Texas at Austin College of Natural Science

PB-011 NMR studies of the structural influence of phosphopantetheinylation in nonribosomal peptide synthetase carrier proteins and impact on binding affinities

Andrew Goodrich¹. Dominique Frueh¹

1.-Johns Hopkins University School of Medicine

PB-012 Functional analysis of of conditional analog-sensitive alleles of essential protein kinases in the fission yeast Schizosaccharomyces pombe

Juraj Gregan^{1, 2}

1.-Mfpl/imp, 2.-Comenius University

PB-013 Peptide conjugates: From self-assembly towards applications in biomedicine lan Hamley¹

1.-University Of Reading, Dept Of Chemistry

PB-014 Approved Drugs containing Thiols as Inhibitors of Metallo-ß-Lactamases: a Strategy to Combat Multidrug-Resistant Bacteria

Franca-M. Klingler¹, Ewgenij Proschak¹

1.-Goethe University, Institute of Pharmaceutical Chemistry





PB-015 Protein Carbamylation at the Chemistry-Biology interface

Victoria Linthwaite¹, Joana Janus¹, David R.W. Hodgson², Martin J. Cann¹

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PB-016 A beta-carboline substituted derivative displays selective anti-cancer activity through inhibition of translation

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PB-017 Semi-chemical synthesis and characterization of a small heat shock protein bearing a nonenzymatic posttranslational modification found in vivo

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PB-018 A new scaffold for inhibition of cysteine proteases: structural and functional characterization of Kunitz inhibitors from potato

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PB-019 Role of the ABCC2 transporter in the mode of action of the Bacillus thuringiensis Crv1Ac toxin in the Diamond Back Moth Plutella xylostella

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PB-020 Metabolic alkene labeling and in vitro detection of histone acylation via the aqueous oxidative Heck reaction

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PB-021 "Study of Bacillus thuringiensis Cry1Ab and Cry1Ac protoxins interaction with cadherin-like receptor from Manduca sexta"

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PB-022 Proton solvation in protic and aprotic solvents

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PB-023 Biochemical characterization of two evolutionary distant ten-eleven translocation enzymes and their utility in 5-methylcytosine sequencing in the genomes at single-base resolution

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PB-024 Contribution of Connexin37 Gene Polymorphism (C1019T) in the Incidence of Acute Myocardial Infarction in the Egyptians

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PB-025 Delineating toxin: lipid:ion channel interactions for rationally sodium channel inhibitors design

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PB-026 Micelles promote Aß42 assembly into pore-forming oligomers

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PB-027 **Molecular dynamics study on the key catalytic intermediates of threonine synthase** <u>Mitsuo Shoji</u>¹, Yuzuru Ujiie¹, Ryuhei Harada¹, Megumi Kayanuma¹, Yasuteru Shigeta¹, Takeshi Murakawa², Hideyuki Hayashi²

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PB-028 Agrobacterium tumefaciens employs two distinct ClpS adaptors to modulate the N-end rule degradation pathway

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PB-029 Interactions between U24 from HHV-6A and 7 and Nedd4 or Smurf2 WW domains Yurou Sang¹, Rui Zhang¹, Walter R.P. Scott¹, A. Louise Creagh², Charles A. Haynes², Suzana K. Straus¹.

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PB-030 Ebola Virus Surface Glycoprotein GP2 Forms a Hydrophobic Fist to Enter Cells by Membrane Fusion

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PB-031 Zero-Length Crosslinking of the ß Subunits of the Phosphorylase Kinase Complex by Periodate

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PB-032 HSSB1 is involved in the cellular response to oxidative DNA damage

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PB-033 Virtual Screening for Novel Inhibitors of Acetoacetyl-CoA Reductase of Burkholderia pseudomallei

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PB-034 Use of Principal Component Analysis and Molecular Docking to Identify Novel Selective Plasmepsin II Non-Competitive Inhibitors with Antimalarial Activity

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PB-035 Ain't gold all that glitters: missing gold atoms in the structure of lysozyme crystals used to co-crystallize gold nanoparticles

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PB-036 Finding a novel treatment for the biological weapon threat of epidemic typhus by targeting ß-ketoacyl-ACP-reductase in Rickettsia prowazekii

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PB-037 Diazotransfer reagents to selectively functionalize a protein of interest with azido groups

Martin Witte¹, Jonas Lohse¹, Remko Welker¹

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PB-038 Peng: a neural gas-based approach for pharmacophore elucidation, method design, validation, and virtual screening for novel ligands of Ita4h

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PB-039 Stabilization of aspergillus parasiticus cytosine deaminase by immobilization on calcium alginate beads improved enzyme operational stability

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PB-040 Ubiquitin-nanoparticle interactions by solution NMR spectroscopy

<u>Serena Zanzoni</u>¹, Michael Assfalg¹, Rajesh K Singh², Marco Pedroni³, Adolfo Speghini³, David Fushman², Mariapina D'Onofrio¹

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3.-Solid State Chemistry Laboratory, Department of Biotechnology, University of Verona

PB-041 Chemical-Genetic Dissection of Protein Kinase Functions

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PB-042 Selective modification of proteins and peptides by ruthenium porphyrin-catalyzed carbene transfer reaction

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PB-043 Modulating the affinities of phophopeptides to human Pin1 WW domain using 4-substituted proline derivatives

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PB-044 Applying an analytical ultracentrifuge equipped with fluorescence detection to the study of polyglutamine aggregation in Caenorhabditis elegans

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PB-045 Probing the selectivity of peptide carrier protein-tailoring enzyme interactions using analytical ultracentrifugation

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PB-046 Uridine Monophosphate Synthase: Architecture Versatility in the Service of Late Blight Control

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PB-047 Three Antimicrobial Peptides: MD Simulation Studies Supporting Experiment

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$\mathsf{PB}\text{-}048$ Studying the Outer Membrane ß-barrel Protein LptD, the Target of a New Peptidomimetic Antibiotic

<u>Katja Zerbe</u>¹, Gloria Andolina¹, Laszlo Bencze¹, Kerstin Moehle¹, John A. Robinson¹ 1.-Department of Chemistry. University Zurich

PB-049 Structure and catalytic properties of peptides based on sequences of P-loop from ATP binding domains

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PB-050 The atp-binding site of ck2 carries two regions with antagonistic electrostatic potential that atracts charged ligands

Maria Winiewska¹, Jarosław Poznański¹

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PB-052 NMR Solution Structure Elucidation of Phenol Soluble Modulins; Virulence Factors in Staphylococcus aureus

<u>Kaitlyn M. Towle</u>¹, Christopher T. Lohans², Marco J. van Belkum¹, Mark Miskolzie¹, John C. Vederas¹ 1.-University of Alberta, 2.-University of Oxford

PB-053 Mitochondrial iron as a potential therapeutic target in friedreich's ataxia neurodegeneration: desferioxamine-peptide conjugate

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PB-054 The proteolytic activity and oligomerization status of the human HtrA3 protease functioning as a tumor suppressor

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PB-055 Cyclodextrins moderately affects binding of halogenated benzotriazoles by protein kinase ck2

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PB-056 Antibody Activation using DNA-Based Logic Gates

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PB-057 Insights of a novel kind of cell wall binding domain that cleaves the peptidoglycan muropeptide: the CW_7 motif

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PB-058 Engagement of the CIpS NTE by the CIpAP machinery inhibits substrate recognition and processing

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PB-059 Single-molecule assay development for studying Human RNA Polymerase II Promoter-Proximal Pausing

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PB-060 Structural characterization of Plasmodium falciparum CCT and fragment-based drug design approach for targeting phospholipid biosynthesis pathway

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PB-061 14-3-3 proteins as a scaffold for small-molecule controlled signaling platforms

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PB-062 The G308E variant of the apoptosis inducing factor, responsible of a rare encephalopathy, is hampered in NAD+/H binding

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PB-063 Understanding the mechanism of action of human MICAL1, a multidomain flavoenzyme controlling cytoskeleton dynamics

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PB-064 Protective function of enhanced green fluorescent protein against reactive oxygen species photo-sensitized by N-doped nanoTiO2

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PB-065 Selective Recognition and Assembly in Protein-Small molecule Interactions

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PB-066 Macromolecular crowding modulates enzyme catalysis

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PB-067 Biophysical and biochemical characterization of Arabidopsis thaliana Calmodulin-like protein CML14

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PB-068 FBP17 controls the hepatocyte morphology through Rho signaling

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PB-069 Energetics of proton transport in Cytochrome c oxidase: Investigation of proton entry in the K-channel of Paracoccus denitrificans

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PB-070 Efficient Methods in the Production of Unnatural Amino Acid Containing Proteins Christopher Walters¹, Solongo Batjargal, Anne Wagner, E. James Petersson

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PB-071 Function and modularity of CW_7 motives in the C-terminal region of the endolysin Cpl-7 encoded by the Cp7 pneumococcal bacteriophage

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PB-072 Utilizing computational and experimental chemistry to characterize the functions of Structural Genomics proteins in the Crotonase Superfamily

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PB-073 Directly observing the synergistic dynamics in F-actin and microtubule assembly Jun Zhang¹, Deqiang Wang²

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PB-074 Bivalent phosphonate inhibitors for extracellular 14-3-3 protein targets

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PB-075 Probing the extremely high metal-to-protein affinity of interprotein zinc hook domain of Rad50 protein from P. furiosus

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PB-076 DNA-directed control of enzyme-inhibitor complex formation: A modular approach to reversibly switch enzyme activity

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PB-077 Carboxylic acids: a versatile classe of carbonic anhydrase inhibitors

Giuseppina De Simone¹, Simone Carradori², Emma Langella¹, Simona Maria Monti¹, Claudiu T. Supuran³, <u>Katia D'Ambrosio</u>¹

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PB-078 Exploring the mechanism of fibril formation using fluorescently labelled human lysozyme variants

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PB-079 A new lead compound for the development of carbonic anhydrase inhibitors

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PB-080 Secondary transporter structure and function in synthetic lipid bilayer systems

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PB-081 Targeting Abeta oligomers by Trehalose-conjugated peptides: a molecular dynamics study

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PB-082 Establishing a tool box for generating designer nucleosomes

Diego Aparicio Pelaz 62945, Henriette Mahler, Dirk Schwarzer, Wolfgang Fischle

PB-083 Evaluating cation-pi and pi-pi interaction in proteins using various biophysical methods

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PB-084 Synthesis and application of chemical probes for histone deacetylases

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PB-085 Exploring the Substrate Selectivity of Oxygen Sensing Prolyl Hydroxylases

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PB-086 Non-natural aminoacids via the MIO-enzyme toolkit

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PB-087 High affinity synthetic antibodies as biological tools

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PB-088 In vitro evolution from pluripotent peptide libraries with natural neurotoxin scaffolds to target receptors, proteases and trophic factors

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PB-089 Stereoselectivity of PAL under non-optimal conditions

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PC - ENZYME & PATHWAY ENGINEERING

PC-001 Preparation of insect prothoracicotropic hormone with complicated disulfide-bond structure, by the heterologous expression in Brevibacillus choshinensis

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PC-002 Modulation of the enzymatic activity of protein arginine methyltransferase 1 by small molecules

Wey-Jing Lin1

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PC-003 Oligomerisation properties of light-dependent protochlorophyllide oxidoreductase Michal Gabruk¹, Anna Piszczek¹, Bozena Skupien-Rabian¹, Sylwia Kedracka-Krok^{1,2}, Jerzy Kruk¹, Beata Mysliwa-Kurdziel¹

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PC-004 Biochemical Characterization and Amino Acid Sequence Analysis of Thermostable Endo-ß-1, 4-glucanase from Trichoderma viride

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PC-005 Role of the disulfide bridges in the transmembrane region of the insect prothoracicotropic-hormone receptor, Torso

<u>Tadafumi Konogami</u>¹, Yiwen Yang¹, Mari H. Ogihara¹, Juri Hikiba¹, Hiroshi Kataoka¹, Kazuki Saito¹ 1.-Dept. of Integrated Biosciences, Grad. Sch. of Frontier Sciences, Univ. of Tokyo

PC-006 Structural study of the yeast enzyme neutral trehalase Nth1 and pNth1:Bmh1 protein complex

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PC-007 Development and use of a molecular purge valve to maintain reduction/oxidation balance in synthetic biochemistry systems

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PC-008 Evolution of Structure and Mechanistic Divergence in Di-Domain Methyltransferases from Nematode Phosphocholine Biosynthesis

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PC-009 Glycoside hydrolase family18 chitinase from the stomach of fish: characteristics of isozymes

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PC-010 A bifunctional cold active lipase with protease activity isolated from an Antarctic yeast, Glaciozyma antarctica PI12

Mohd Shukuri Mohamad Ali^{1,2}, Ira Maya Haris^{1,2}, Raja Noor Zaliha Raja Abd Rahman^{1,2}, Mahiran Basri^{2,3}, Abu Bakar Salleh^{1,2}

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PC-011 Conformation-specific antibodies as enhancers and inhibitors of phosphatase activity of DEP 1

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PC-012 Investigating Acinetobacter baumannii pathogenesis: crystal structure of WbjB epimerase from a polysaccharide biosynthesis cluster

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PC-013 Role of the Hydrogen Bonding Interactions in the O2 Sensitivity of HIF-Prolyl Hydroxylase (PHD2)

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PC-014 New pharmacological therapies against congenital erythropoietic porphyria (CEP) Pedro David Urquiza¹, Ana Laín¹, Arantza Sanz¹, Juan Manuel Falcón^{1, 2}, Oscar Millet¹

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PC-015 Delicate Balance of Noncovalent Forces Control the Electron Transfer Complex between Ferredoxin and Sulfite Reductase to Optimize Enzymatic Activity

<u>Juyaen Kim</u>¹, Misaki Kinoshita¹, Takahisa Ikegami¹.², Genji Kurisu¹, Yuji Goto¹, Toshiharu Hase¹, Young-Ho Lee¹

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PC-016 Ornithine transcarbamylase has a spatially extended active site as computationally predicted

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PC-018 Identification, Characterization, and Modification of Fatty Acid Alkyl Esterases Found in Staphylococcus aureus

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PC-019 Functional elements of a human antizyme essential for binding and inhibiting human ornithine decarboxylase

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PC-020 Structure-Function Relationships of human Aldo-Keto Reductase 1B15, AN enzyme active with 9-cis-Retinaldehyde

<u>Joan Giménez Dejoz</u>¹, Michal H. H. Kolář^{2,3}, Francesc Xavier Ruiz⁴, Isidro Crespo¹, Alexandra Cousido-Siah⁴, Alberto Podjarny⁴, Jindřich Fanfrlík², Xavier Parés¹, Jaume Farrés¹, Sergio Porté¹ 1.-Universitat Autònoma de Barcelona, 2.-Institute of Organic Chemistry and Biochemistry, 3.-Institute of Neuroscience and Medicine and Institute for Advanced Simulation, 4.-Institut de Génétique et de Biologie Moléculaire et Cellulaire

PC-021 Significance of protein substrate structure and dynamics in proteolysis: insights from Kunitz-BPTI family canonical serine protease inhibitors

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- Mayo Graduate School, 2.-Department of Cancer Biology, Mayo Clinic Cancer Center,
 Department of Neuroscience, Mayo Clinic College of Medicine,
 Biology Department,
 Brookhaven National Laboratory
- PC-022 **Determinants for regioselectivity in Lytic Polysaccharide MonoOxygenases (LPMOs)** Barbara Danneels¹, Magali Tanghe¹, Henk-Jan Joosten², Tom Desmet¹
- 1.-Centre for Industrial Biotechnology and Biocatalysis, University of Ghent, 2.-Bioprodict
- PC-023 Folding topology determines substrate binding order in the ribokinase superfamily Alejandra Herrera-Morandé¹, Victor Castro-Fernández¹, Felipe Merino¹, César Ramírez-Sarmiento¹, Francisco Fernández², Cristina Vega², Victoria Guixé¹
- 1.-Departamento de Biología, Facultad de Ciencias, Universidad de Chile., 2.-Centro de Investigaciones Biológicas (CIB-CSIC)

PC-024 Thrombin Proteolytically Hinders the Antioxidant Activity of Human Ceruloplasmin: Implications in the Pathogenesis of Rheumatoid Arthritis

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PC-025 An artificial pathway for isobutene production by direct fermentation : combining metabolic engineering and protein engineering

Benoit Villiers1. François Stricher1

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PC-026 The development of a coupled enzyme assay to detect isochorismate pyruvate lyase activity

<u>Linda Jäger</u>¹, Christian Jäckel¹, Peter Kast¹, Donald Hilvert¹ 1.-LOC, ETH Zürich

PD - FOLDING

PD-001 3-D interaction homology. Do hydropathic microenvironments dictate amino acid sidechain conformations?

Mostafa Ahmed^{1,2}, Martin Safo^{1,2}, J. Neel Scarsdale^{1,3}, Glen Kellogg^{1,2}

- 1.-Institute For Structural Biology and Drug Discovery, Virginia Commonwealth University, 2.-Department of Medicinal Chemistry, Virginia Commonwealth University, 3.-Center For The Study
- of Biological Complexity, Virginia Commonwealth University

PD-002 Folding studies of independent domains of Lysine, Arginine, Ornithine binding protein (LAO)

<u>Tania Raquel Berrocal Gama</u>¹, Jesús Renan Vergara Gutiérrez¹, Andrés Escandón Flores¹, Alejandro Sosa Peinado¹

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PD-003 A hypothesis to reconcile the physical and chemical unfolding of proteins

Guilherme de Oliveira, Jerson Silva

1.-Instituto de Bioquímica Médica, Universidade Federal do Rio de Janeiro

PD-004 Zinc: A Promoter or Inhibitor for IAPP aggregation?

Feng Ding¹, Praveen Nedumpully-Govindan¹

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PD-005 Macromolecular Crowding: From the test tube to the cell

David Gnutt¹, Michael Senske¹, Simon Ebbinghaus¹

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PD-006 Breaking the deleterious effect of urea-unfolded state: consequences for the reversibility of intermediate species

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1.-Faculdade De Ciências E Tecnologia, Universidade Nova De Lisboa, 2.-CIC BioGUNE, Structural Biology Unit and Metabolomics Unit

PD-007 Highly concerted domain folding and subunit association of a multidomain multimeric L asparaginase from hyperthermophile: A mechanistic underpinning of complex protein folding in extreme environement

Dushyant K. Garq1, Bishwajit Kundu1

1.-Indian Institute of Technology Delhi

PD-008 GroEL assisted folding of multiple recombinant proteins simultaneously over-expressed in E.coli

Megha Goyal¹, Tapan Kumar Chaudhuri¹

1.-Indian Institute of Technology Delhi

PD-009 Complexity of the Post-transition State Folding of Rd-apocytochrome b562

Shuanghong Huo¹, Mojie Duan^{1,2}, Hanzhong Liu¹, Minghai Li¹

1.-Clark University, 2.-Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences

PD-010 Establishment of thermodynamics of protein aggregation using isothermal titration calorimetry

Tatsuva Ikenoue¹, Lee Young-Ho¹, Tetsuhei Uenoyama¹, Daniel Otzen², Yuji Goto¹

1.-Institute for Protein Research, Osaka University, 2.-Interdisciplinary Nanoscience Center (iNANO), Aarhus University

PD-011 Molecular Mechanisms of Cytoplasmic Protein Quality Control

<u>Rivka Isaacson</u>¹, Ewelina Krysztofinska¹, Santiago Martínez-Lumbreras¹, Arjun Thapaliya¹ 1.-Chemistry Department, King's College London

PD-012 Interaction of curcumin analogs with α -Synuclein: Modulation of Aggregation and Toxicity

Narendra Jha¹, A. Anoop¹, Narasimham Ayyagari¹, Pradeep Singh¹, I.N.N. Namboothiri¹, Samir Maji¹ 1.-Indian Institute of Technology Bombay



PD-013 In vitro folding mechanisms determine the forces applied during co-translational folding

Adrian Nickson¹, Jeff Hollins¹, Ola Nilsson², Gunnar von Heijne², Jane Clarke¹

1.-Department of Chemistry, University of Cambridge, 2.-Department of Biochemistry and Biophysics, Stockholm University

PD-014 Can the structure of a protein (H3.1) depend on the treatment of a solvent medium (explicit vs effective) in a coarse-grained computer simulation?

Ras Pandey¹, Barry Farmer²

1.-University of Southern Mississippi, 2.-Air Force Research Laboratory

PD-015 Single-molecule vectorial folding and unfolding through membrane pores

<u>David Rodriguez-Larrea</u>¹, Hagan Bayley²

1.-University of the Basque Country, Dept. Biochemistry and Molecular Biology, 2.-University of Oxford, Dept. of Chemistry

PD-016 Reversibility and two state behavior in the thermal unfolding of oligomeric TIM barrel proteins from three bacterial phyla

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1.-Facultad de Medicina, Universidad Nacional Autónoma de México., 2.-Facultad de Química, Universidad Nacional Autónoma de México., 3.-Instituto de Química, Universidad Nacional Autónoma de México

PD-017 Structural insights into HIV-1 Gag binding to the plasma membrane during virus assembly

Jamil Saad¹, Jiri Vlach¹, Ruba Ghanam¹

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PD-018 The structure and function of the Surrogate Light Chain

Natalia Catalina Sarmiento Alam¹, Johannes Buchner¹

1.-Department Chemie, Technishe Universität München

PD-019 2D IR spectroscopy reveals a ß-sheet intermediate that dictates the fiber formation of hIAPP

Arnaldo Serrano¹, Ling-Hsien Tu², Daniel Raleigh², Martin Zanni¹

1.-Department of Chemistry, University of Wisconsin-Madison, 2.-Department of Chemistry, Stony Brook University

PD-020 The temperature dependence of protein stability in living cells

Austin E. Smith¹, Larry Z. Zhou¹, Annelise H. Gorensek¹, Michael Senske², Gary J. Pielak^{1,3,4}

1.-Department of Chemistry, 2.-Department of Physical Chemistry II, 3.-Department of Biochemistry and Biophysics, 4.-Lineberger Comprehensive Cancer Center

PD-021 Molecular crowding effects on the native and equilibrium intermediate state of a 29 kDa TIM Barrel protein

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1.-Dept. of Biological Sciences, Birla Institute of Technology & Science, 2.-NMR Research Centre, Indian Institute of Science, 3.-Solid State and Structural Chemistry Unit, Indian Institute of Science

PD-022 Co-translational protein folding studies of alpha-1 antitrypsin

Conny Wing-Heng Yu^{1,2}, Lien Chu^{1,2}, Xiaolin Wang^{1,2}, Christopher A. Waudby^{1,2}, John Christodoulou^{1,2}, Lisa D. Cabrita^{1,2}

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PD-023 pH and Temperature dependent Folding-Unfolding transition of BBL protein under various Urea concentration

Sangyeol Kim^{1,2,4}, Wookyung Yu^{2,3}, Bora Kwon^{2,3}, Seongjun Park², Iksoo Chang^{1,2,3}

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PD-024 Biophysical analysis of partially folded states of myoglobin in presence of 2.2.2-trifluoroethanol

Paurnima Talele¹, Nand Kishore¹

1.-Indian Institute of Technology Bombay

PD-025 Structural duality in peptides derived from choline binding repeats

Hector Zamora-Carreras¹, Roberto Silva-Rojas¹, Beatriz Maestro², Erik Strandberg³, Anne Ulrich⁰, Jesús M Sanz², Marta Bruix¹, <u>M Angeles Jimenez¹</u>

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PD-026 Conformational analysis of fragments of the human Pin1 protein: the influence of charged amino-acid residues on the ß-hairpin structure

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PD-027 Understanding the biology of Huntington's disease via the pathogenic huntingtin monomer

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PD-028 Molecular basis of tyrosinemia and identification of possible pharmacological chaperones targets

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1 -CIC bioGUNE

PD-029 Repulsion between net charges of subunits during ferritin assembly

<u>Daisuke Sato</u>¹, Hideaki Ohtomo¹, Atsushi Kurobe¹, Satsuki Takebe¹, Yoshiteru Yamada², Kazuo Fujiwara¹, Masamichi Ikeguchi¹

1.-Department of Bioinformatics, Graduate School of Engineering, Soka University, 2.-JASRI/ SPring-8



PD-030 Improved modeling of protein unfolding rates and pathways through solvation and modeling of beta-barrels

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1.-Department of Biology, Rensselaer Polytechnic Institute, 2.-Center for Biotechnology and Interdisciplinary Studies, 3,-Department of Computer Science, Universidad del Valle, 4,-Department of Computer Science, Rensselaer Polytechnic Intitute

PD-031 In the Multi-domain Protein Adenylate Kinase, Domain Insertion Facilitates Cooperative Folding while Accommodating Function at Domain Interfaces

V. V. Hemanth Giri Rao1, Shachi Gosavi1

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PD-032 Tuning cooperativity on the free energy landscape of protein folding Pooja Malhotra¹, Jayant Udgaonkar¹

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PD-033 Role of electrostatic repulsion between unique arginine residues on the assembly of a trimeric autotransporter translocator domain

Eriko Aoki¹, Kazuo Fujiwara¹, Masamichi Ikeguchi¹

1.-Department of Bioinformatics, Graduate School of Engineering, Soka University

PD-034 Kurozu Increases HSPA1A Expression and Ameliorates Cognitive Dysfunction in Aged SAM P8 Mice

Toshiaki Kakimoto¹, Hideya Nakano¹, Yuji Nakai², Kazuhiro Shiozaki³, Kohei Akioka⁴, Konosuke Otomaru⁵, Mitsuharu Matsumoto⁶, Masanobu Nagano⁷, Yasushi Sugimoto⁸, Hiroaki Kanouchi¹

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PD-035 Cold Denaturation of Alpha-Synuclein Amyloid Fibrils

Young-Ho Lee¹, Tatsuya Ikenoue¹, Yasushi Kawata², Yuji Goto¹

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PD-036 Key structural differences between TbTIM and TcTIM revealed by thermal unfolding molecular dynamics simulations

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PD-037 Repositioning SOM0226 as a potent inhibitor of transthyretin amyloidogenesis and its associated cellular toxicity

Salvador Ventura¹, Ricardo Sant'Anna¹, Maria Rosário Almeida², Natàlia Reixach³, Raul Insa⁴, Adrian Velazquez-Campoy⁵, David Reverter¹, Núria Reig⁴

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PD-038 Neurometals as modulators of protein aggregation in neurodegenerative diseases Sónia S. Leal¹, Joana S. Cristóvão¹, Cláudio M. Gomes¹

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PD-039 Single-molecule FRET reveals proline dynamics in transmembrane helices <u>Gustavo Fuertes</u>^{1,2,3}, Ismael Mingarro³, Edward A. Lemke¹

1.-Structural and Computational Biology Unit, European Molecular Biology Laboratory, 2.-European Molecular Biology Laboratory, 3.-Department of Biochemistry and Molecular Biology, University of Valencia

PD-040 Thermodynamic contributions of specific mutations of L30e protein in the RNA: protein interface region measured by analytical ultracentrifugation and gel shift assay.

Bashkim Kokona^{1,2}, Sara Kim¹, Margaret Patchin¹, Britt Benner¹, Susan White¹

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PD-041 Role of a non-native α -helix in the folding of equine β -lactoglobulin

<u>Takahiro Okabe</u>¹, Toshiaki Miyajima¹, Kanako Nakagawa¹, Seiichi Tsukamoto¹, Kazuo Fujiwara¹, Masamichi Ikeguchi¹

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PD-042 Impact of the chaperonin CCT in α-Synuclein (A53T) amyloid fibrils assembly assembly Ahudrey Leal Quintero¹, Javier Martinez-Sabando¹, Jose María Valpuesta¹, Begoña Sot¹

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PD-043 Amyloid-like aggregation of Nucleophosmin regions associated with acute myeloid leukemia mutations

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PD-044 Transition from α -helix to β -sheet structures occurs in myoglobin in deuterium oxide solution under exposure to microwaves

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PD-045 Investigating the insertion and folding of membrane proteins into lipid bilayers using a cell free expression system

Nicola Harris¹, Kalypso Charalambous¹, Eamonn Reading¹, Paula Booth¹

1.-Kings College London, Department of Chemistry

PD-047 Domain swapping of the DNA-binding domain of human FoxP1 is facilitated by its low folding stability

Exequiel Medina¹, Sandro L. Valenzuela¹, Cristóbal Córdova¹, César A. Ramírez-Sarmiento¹, <u>Jorge</u> Babul¹

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PD-048 $\,$ Determining the coupled interactions that stabilize the structural framework of the $\,$ B-propeller fold

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1.-Department of Statistics, The University of Chicago, 2.-Department of Applied Mathematics and Statistics, Stony Brook University, 3.-Graduate Program in Biochemistry and Structural Biology, Stony Brook University, 4.-Laufer Center of Physical and Quantitative Biology, Stony Brook University



PD-049 Temperature induced conformational changes of the villin headpiece miniprotein Stanislaw Oldziej¹, Wioletta Żmudzińska¹, Anna Hałabis ¹

1.-Intercollegiate Faculty of Biotechnology, UG and MUG

PD-050 Comparative equilibrium folding of a membrane transporter within detergent and lipid environments

Michael Sanders¹, Heather Findlay¹, Paula Booth¹

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PD-051 NMR Investigation of pH-induced unfolding of B domain of an Escherichia Coli mannitol transporter IlMannitol in the bacterial phosphotransferase system

Gowoon Kim, Taekyung Yu, Jeongyong Suh

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PD-052 Can site-directed mutagenesis shed light on the refolding pattern of human glucose 6-phosphate dehydrogenase (G6PD)?

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1.-Conway Institute, Univerversity College Dublin, 2.-Faculty of Biosciences and Medical Engineering, Universiti Teknologi Malaysia

PD-053 Monitoring nascent membrane protein insertion using unnatural amino acids Eamonn Reading¹

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PD-054 A single aromatic core mutation converts a designed 'primitive' protein from halophile to mesophile folding

Connie Tenorio¹, Liam Longo¹, Ozan S. Kumru², C. Russell Middaugh², Michael Blaber¹

1.-Department of Biomedical Sciences, Florida State University,, 2.-Department of Pharmaceutical Chemistry, University of Kansas

PD-055 From Sequence Data to Protein 3D Structure Using Evolutionary Couplings

Robert Fieldhouse^{1,2}, Sikander Hayat^{1,2}, Robert Sheridan¹, Debora Marks², Chris Sander¹

1.-Computational Biology Center, Memorial Sloan Kettering Cancer Center, 2.-Systems Biology, Harvard Medical School

PD-046 Study of rabies virus by Differential Scanning Calorimetry: Identification of Proteins Involved in Thermal Transitions

<u>Frederic Greco</u>¹, Audrey Toinon¹, Nadege Moreno¹, Marie Claire Nicolaï¹, Catherine Manin¹, Francoise Guinet-Morlot¹, Frederic Ronzon¹

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PE - INTEGRATIVE PROTEIN SCIENCE

PE-001 Experimental and computational studies of the effects of highly concentrated solutes on proteins: Insights into the causes and consequences of quinary protein structure and cytoplasmic organization

Luciano Abriata¹, Matteo Dal Peraro¹

1.-École Polytechnique Fédérale de Lausanne

PE-003 Carbohydrate Binding Modules, Structural and thermodynamic study

<u>Benjamin Garcia</u>¹, Patricia Cano Sánchez¹, Siseth Martínez-Caballero¹, Romina Rodríguez-Sanoja¹, Adela Rodríguez-Romero¹

1.-Instituto de Química, UNAM

PE-004 Initiating vesicle formation at the Golgi complex: auto-regulation and protein interactions govern the Arf-GEFs Gea1 and Gea2

Margaret Gustafson¹, J. Chris Fromme¹

1.-Cornell University

PE-005 Sequence variation in Archaea through diversity-generating retroelements

Sumit Handa¹, Blair G Paul², Kharissa L Shaw¹, David L Valentine², Partho Ghosh¹

1.-Department of Chemistry and Biochemistry, University of California San Diego, 2.-Marine Science Institute, University of California Santa Barbara

PE-006 **Studies of JMJD4-catalyzed oxidative modifications of eukaryotic release factor 1** <u>Suzana Markolovic</u>¹, Ivanhoe K. H. Leung², Mathew L. Coleman³, Timothy D. W. Claridge¹, Sarah E. Wilkins¹, Christopher J. Schofield¹

1.-Chemistry Research Laboratory, Department of Chemistry, University of Oxford, 2.-School of Chemical Sciences, University of Auckland, 3.-School of Cancer Sciences, University of Birmingham

PE-007 Functional and structural analysis of a GH20 ß-N-acetylglucosaminidase from the marine bacterium Vibrio harveyi

Piyanat Meekrathok¹, Arthur T. Porfetye², Marco Bürger², Ingrid R. Vetter², Wipa Suginta¹

1.-Biochemistry-Electrochemistry Research Unit, Suranaree University of Technology, 2.-Max Planck Institute of Molecular Physiology

PE-008 Silencing the molecular timekeeper in human cancer

<u>Alicia Michael</u>¹, Stacy Harvey¹, Patrick Sammons¹, Amanda Anderson², Hema Kopalle¹, Alison Banham², Carrie Partch¹

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PE-009 New insights into the interaction between IQGAP1 and Rho family proteins

Kazem Nouri¹, Mohammad Reza Ahmadian¹

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PE-010 Structural Characterization of the Tumor Suppressor ING5 as a Bivalent Reader of Histone H3 Trimethylated at Lysine 4

<u>Georgina Ormaza Hernandez</u>¹, Jhon Alexander Rodríguez¹, Alain Ibáñez de Opakua¹, Nekane Merino¹, Maider Villate¹, Tammo Diercks¹, Pietro Roversi², Adriana L. Rojas¹, Francisco J. Blanco^{1,3} 1.-CIC bioGUNE, Structural Biology Unit, 2.-Oxford University, Department of Biochemistry, 3.-IKERBASQUE, Basque Foundation for Science

PE-011 Abelson tyrosine kinase, a new enzyme target for alzheimer's disease: exploring multiple e-pharmoacophore modeling, virtual screening, selectivity assessment for potential inhibitors

Ravichand Palakurti¹, Ramakrishna Vadrevu¹

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PE-012 The Role of Syndecans in Melanocortin Signaling and Energy Balance

Rafael Palomino¹. Glenn Millhauser². Pietro Sanna²

1.-University of California Santa Cruz, 2.-The Scripps Research Institute



PE-013 Evidence of a proteolytic phenomenon in the starch binding domain of the α -amylase from Lactobacillus amylovorus

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PE-014 In Situ Membrane Protein Structure and Function Analysis using Site-Specific Unnatural Amino Acid Incorporation and Spectroscopy Methods Changlin Tian¹

1.-University of Science and Technology of China

PE-015 Theoretical Volume Profiles as a Tool for Probing Protein Folding Kinetics Heather Wiebe¹, Noham Weinberg^{1,2}

1.-Department of Chemistry, Simon Fraser University, 2.-Department of Chemistry, University of the Fraser Valley

PE-016 Structure of the p15paf/pcna complex and implications for clamp sliding on the dna during replication and repair

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PE-017 DHRS7 enzyme – important player in human health and diseases?

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PE-018 Structure-based functional identification of Helicobacter pylori HP0268 as a nuclease with both DNA nicking and Rnase activities

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PE-019 High-fidelity recombinant protein production in a silkworm bioreactor

Sungjo Park¹, In-Wook Hwang¹, Tatsuya Kato², Enoch Park², Andre Terzic¹

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PE-020 Studies exploring potential applications of synthetic antifreeze proteins in the frozen food industry

Ho Zee (Charles) Kong¹, Conrad Perera¹, Ivanhoe Leung¹, Nazimah Hamid², Viji Sarojini¹

1.-School of Chemical Sciences, The University of Auckland., 2.-School of Applied Sciences, Auckland University of Technology

PE-021 Development of Fungal-Specific Calcineurin Inhibitors Based on Molecular Structure and Dynamics

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PE-022 Lupin (Lupinus angustifolius L.) b-conglutin proteins: Structure functional features, catalytic mechanism modeling and cross-allergenicity identification using protein threading and molecular docking methods

Jose C. Jimenez-Lopez^{1,2}

1.-Department of Biochemistry, Cell and Molecular Biology of Plants; EEZ-CSIC, 2.-The UWA Institute of Agriculture; The University of Western Australia

PE-023 Intracellular pH and quinary structure

Rachel Cohen¹, Gary Pielak^{1,2,3}

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

PE-024 Advanced analytical tools for monitoring and control in production processes of recombinant hemagglutinin influenza vaccine

<u>Joanna Szewczak</u>¹, Weronika Surmacz-Chwedoruk¹, Bożena Tejchman-Małecka ¹, Jacek Stadnik¹, Grażyna Tronczyńska-Lubowicz ¹, Agnieszka Romanik-Chruścielewska ¹, Jarosław Antosik¹, Piotr Borowicz¹, Iwona Sokołowska ¹, Dorota Stadnik¹,

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PE-025 Muscle cell atrophy via HSP gene silencing was counteracted by celastrol-mediated HSP overexpression

Inho Choi¹, Taesik Gwag¹, Kyoungsook Park², Kyoungbong Ha¹, Joo-hee Lee³, Youn-Kyu Kim³ 1.-College of Science and Technology, Yonsei University, 2.-Molecular Therapy Research Center, Sungkyunkwan University, 3.-Korea Aerospace Research Institute

PE-026 A novel in vivo characterization method predicting the physicochemical parameters of an antibiotic efflux pump

<u>Anisha M Perez</u>¹, Erin L O'Brien¹, Marcella M Gomez¹, Matthew R Bennett¹, Yousif Shamoo¹ 1.-Department of BioSciences

PE-027 Structural Analysis of KCNE1 Transmembrane Mutant Yielding KCNE3-like Function Cheryl Law Vanderbilt Universit, Charles Sanders⁰

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$\mbox{PE-}028$ Biochemical characterization of Brassica napus diacylglycerol acyltransferase 1 and its regulatory domain

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PF - INTRINSICALLY DISORDERED PROTEINS

PF-001 Role of C terminal disordered domain of Sesbania mosaic virus RNA dependent RNA polymerase in the modulation of its activity and oligomeric status

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PF-002 Aggregation of androgen receptor in spinal bulbar muscular atrophy is a multistep process

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PF-003 Destabilizing the Transient Helical Conformation of Islet Amyloid Polypeptide Hastens Peptide Self-Assembly and Potentiates Cytotoxicity

<u>Carole Anne De Carufel</u>¹, Phuong Trang Nguyen¹, Alexandre Arnold¹, Isabelle Marcotte¹, Steve Bourgault¹

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PF-004 Towards in vivo NMR: Putting prions in context

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PF-005 Genetic instability within regions encoding repetitive proteins as a driver of adaptation

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PF-006 A Proline-Tryptophan turn in the intrinsically disordered domain 2 of NS5A protein is essential for Hepatitis C virus RNA replication

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PF-007 Solution structure and celullar functional studies of bovine cathelicidin Bt-6 (BMAP-27)

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PF-008 Engineered binding proteins to amyloidogenic intrinsically disordered proteins

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PF-009 Interaction Profiling through Proteomic Peptide Phage Display

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PF-010 **Biophysical characterization of phosducin and its complex with the 14-3-3 protein** Miroslava Kacirova^{1,2}, Jiri Novacek³, Petr Man^{1,4}, Alan Kadek^{1,4}, Veronika Obsilova², Tomas Obsil^{1,2} 1.-Faculty of Science, Charles University in Prague, 2.-Institute of Physiology, Czech Academy of Sciences, 3.-Masaryk University, CEITEC – Central European Institute of Technology, 4.-Institute of Microbiology. Czech Academy of Sciences

PF-011 Prion-like proteins sequester and suppress the toxicity of huntingtin exon 1

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PF-012 Structuring disorder: the case of the intrinsically disordered Unique domain of c-Src Mariano Maffei¹

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PF-013 The Yeast GRASP Grh1 displays features of an Intrinsically Disordered Protein

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PF-014 Conformational changes governing dengue virus capsid protein function and its inhibition by pep14 23

André F. Faustino¹, Gabriela M. Guerra¹, Roland G. Huber², Axel Hollmann¹, Peter J. Bond², Miguel A.R.B. Castanho¹, Andrea T. Da Poian³, Fábio C.L. Almeida³, Nuno C. Santos¹, Ivo Martins¹

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PF-015 Developing mechanistic insight into modulators of tau aggregation

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PF-016 New insights into amyloidogenesis of Tau protein induced by enantiomers of polyglutamic acid

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PF-017 Self-organizing structures of alpha-synulceins and its aggregates by a coarse-grained Monte Carlo simulation

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PF-018 Tear down the wall: dismantling the biofilm scaffold of E.coli

<u>Cesyen Cedeno</u>¹, Nani Van Gerven¹, Wim Jonckheere¹, Imke Van den Broek¹, Han Remaut¹, Peter Tompa¹

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PF-019 Coupled folding and binding of transcription factors

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PF-020 Alternative hit finding strategies for intrinsically disordered proteins, exemplified by forkhead-box transcription factors

<u>Harm Jan (Arjan) Snijder</u>¹, Maria Saline¹, Tomas Jacso¹, Frank Janssen¹, Mattias Rohman¹, Tyrrell Norris¹

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PF-021 SDS-PAGE analysis of Aß oligomers is disserving research into Alzheimer's disease: a call for ESI-IM-MS

<u>Sílvia Vilaprinyó-Pascual</u>¹, Rosa Pujol-Pina¹, Roberta Mazzucato¹, Annalisa Arcella², Marta Vilaseca³, Modesto Orozco^{2,4}, Natàlia Carulla¹

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PF-022 Coarse-grained simulation of protein association: application to rate prediction and implication for association mechanisms

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$\mbox{PF-}023 \quad \mbox{(Un)structure-function relationships on the UreG enzyme in the nickel-dependent urease system}$

Barbara Zambelli¹, Francesco Musiani¹, Stefano Ciurli¹

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PF-024 Molecular insights into the VPg-Pro interaction from Pepper Vein Banding Virus: Implication in protease activity

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PF-025 A novel mutant that prevents tetramerization of amyloidogenic transthyretin protein involved in family cardiac amyloidosis (FAC)

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PF-026 Misfolding and Aggregation of Intrinsically Disordered Proteins: Nanoscale Structural Characterization by AFM-IR

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PF-027 Multiple cellular proteins interact with LEDGF/p75 through a conserved unstructured consensus motif

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PF-028 Exploring Anti- amyloidogenic Attributes of Lantibiotic Nisin Deovrat Beade¹

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PF-029 Amyloidogenic lysozyme accumulates in the endoplasmic reticulum tangling with GRP78/BiP and evokes ER stress

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PF-030 Structural characterization of toxic oligomers that are kinetically trapped during alpha-synuclein fibril formation

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PF-031 **Metal ions modulate the conformation of Starmaker-like protein from Oryzias latipes** <u>Mirosława Różycka</u>¹, Magdalena Wojtas¹, Natalie Mutter², Benjamin Schuler², Jacek Gapiński ^{3,4}, Andrzej Ożyhar¹

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PF-032 Intrinsically disordered recombinant 57K fragment of human DMP1 influences the in vitro crystallization of CaCO3

<u>Aleksandra Porebska</u>¹, Andrzej Ozyhar¹, Piotr Dobryszycki¹ 1.-Wroclaw University of Technology, Department of Biochemistry

PF-033 Structural analysis of the C-terminal domain of Drosophila melanogaster Methoprene tolerant protein (Met)

<u>Marta Kolonko</u>¹, Katarzyna Ożga¹, Rafał Hołubowicz¹, Andrzej Ożyhar¹, Beata Greb-Markiewicz¹ 1.-Wroclaw University of Technology

PF-034 Designed cross-amyloid inhibitors of amyloid self-assembly

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PF-035 Preparation of homogenous recombinant FKBP39 protein from Tribolium castaneum Aneta Tarczewska¹, Małgorzata Kozłowska¹, Andrzej Ożyhar¹

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PG - OBSERVING DYNAMICS IN SINGLE CELLS

PG-001 Live-cell Measurements of the Conformational Rearrangements in Bax at the Initiation of Apoptosis

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PG-002 Bacterial cell division in super resolution

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PG-003 Mapping transcription factors dynamics and interactions by advanced fluorescence microscopy techniques

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PG-004 Assembly of membrane pores as a mechanism for amyloid cytotoxicity by the bacterial prionoid RepA-WH1

<u>Cristina Fernández</u>, Rafael Núñez-Ramirez, Mercedes Jimenez, Germán Rivas, Rafael Giraldo 1.-Centro de Investigaciones Biológicas, CSIC

PH - PROTEIN ALLOSTERY & DYNAMICS

PH-001 Investigation of allosteric communication pathways in human ß2-adrenergic receptor

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1.-Department of Chemical Eng. and Polymer Research Center, Bogazici University, 2.-Department of Chemical Engineering, Istanbul Technical University, 3.-Department of Bioinformatics and Genetics, Kadir Has University

PH-002 Neonatal diabetes and congenital hyperinsulinism mutations change molecular interactions in SUR1 NBD1

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PH-003 Glycosylation of EGFR Extracellular Domain Induces Receptor Stability Maryam Azimzadeh Irani^{1,2}, Chandra Verma^{1,2}

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PH-004 Dynamic protein complexes mediate reactivity and specificity of complement-like immunity in Anopheles gambiae

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PH-005 Conformational Changes of the Ribose ABC Transporter Studied by EPR Spectroscopy

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PH-006 The Catalytic Cycle of hFEN1 Requires Protein and DNA Conformational Changes, but Are They Rate-Limiting?

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PH-007 Dynamical structure changes in binding of pharmaceutical target proteins Hideaki Fuiitani¹

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PH-008 Structure-based recombination of drug resistance enzymes: structural and functional tolerance to new dynamics in artificially-evolved enzymes

Sophie M.C. Gobeil^{1,2}, Maximillian C.C.J.C. Ebert^{1,2}, Jaeok Park⁰, Donald Gagné⁰, Christopher M. Clouthier^{1,3}, Jürgen Pleiss⁷, Nicolas Doucet⁰, Albert M. Berghuis⁰, Joelle N. Pelletier⁰

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PH-009 Conformations of the RNA polymerase clamp throughout the transcription cycle studied by single-molecule FRET

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PH-010 Solvent models for protein simulations – the good, the bad and the applications <u>Duy Hua</u>¹, Amitava Roy¹, He Huang¹, Carol Post¹

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PH-011 Dissection of the water cavity of yeast Thioredoxin 1: the effect of a hydrophobic residue in the cavity

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PH-012 In-vitro and in-silico studies of ligand binding to the nuclear receptor PPARgamma using FRET and MD

Narutoshi Kamiya¹, Gert-Jan Bekker¹, Takuma Shiraki², Haruki Nakamura¹ 1.-IPR, Osaka University, 2.-Kinki University

PH-013 Atomic Insight into kinetic mechanism for sumoylation of UBC9 with substrate motif (Ψ-K-x-D/E) by molecular dynamic simulation

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PH-014 Bending over Backwards for Water: How KCNE3 Helix Curvature and Flexibility Influence a Human Potassium Channel's Conduction Profile

<u>Brett Kroncke</u>^{1,2}, Wade Van Horn⁰, Jarrod Smith^{1,2}, David Nannemann^{2,6}, Jens Meiler^{2,6}, Carlos Vanoye⁷, Charles Sanders^{1,2}

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PH-015 Watching conformational changes in proteins by molecular dynamics simulations Kresten Lindorff-Larsen¹

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PH-016 Coupling Conformational and Energetic Changes in G Protein Signaling

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PH-017 Structure and dynamics of the polymyxin-resistance-associated response regulator PmrA in complex with the promoter DNA

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PH-018 Time-resolved X-ray Observations of Nano-scale Protein Assembly Networks

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PH-019 Functional implications of co-evolving residue sectors in the Ribonuclease A family Chitra Narayanan^{1,2}, Kimberly Reynolds³, Rama Ranganathan³, Nicolas Doucet⁰

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PH-020 Effects of KCI on the Dynamics and Catalytic Mechanism of a Halophilic Enzyme -Dihydrofolate Reductase (hvDHFR) from Haloferax volcanii

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PH-021 Structure and dynamics of the octameric iron-, heme- and cobalamin-binding protein HbpS from the soil bacterium Streptomyces reticuli

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PH-022 A centrosomal protein FOR20 regulates microtubule assembly through a direct interaction with tubulin

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PH-023 How amide hydrogens exchange in native proteins

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Differences in redox reactions with NADP+/H between ferredoxin-NADP+ PH-024 oxidoreductases from Bacillus subtilis and Rhodopseudomonas palustris

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PH-025 The internal dynamics of fibrinogen and its implications for coagulation and adsorption

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PH-026 Membrane curvature - the assembler of proteins

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PH-027 Transmission of rigidity at a distance - new insights into allosteric signalling in G-Protein Coupled Receptors

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PH-028 Comparing the intrinsic dynamics of multiple proteins using elastic network models reveals global similarities based on their overall shape

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PH-029 Oxygen-Affinity and Cooperativity of Hemoglobin (Hb) are Regulated by 4D Structural Changes (Protein Dynamics), rather than 3D Structural Changes

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PH-030 On the Role of Metal lons in Synaptic Proteins Assembly

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PH-031 The role of the Mg(II) ion on integrin-collagen interactions: regulating affinity through conformational fluctuations

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PH-032 Effect of Membrane Composition on the Structure of Membrane-Attached Cytochrome P450 3A4

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PH-033 Generation of single-chain Fv antibody against (4-hydroxy-3-nitrophenyl)acetyl and analysis of its structural dynamics

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PH-034 Antibiotic binding drives catalytic activation of aminoglycoside kinase APH(2")-la Shane Caldwell¹, Albert Berghuis¹

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PH-035 Disease Related Mutation Effects on Conformations and Dynamics of the Zinc-Finger NEMO

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PH-036 Structural characterization of the binding of HIV-1 integrase to its cellular co-factor Ku70

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PH-037 Structural characterization of calmodulin bound to the intracellular calmodulin binding domain of Kv7.2 channels by NMR

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PH-038 Cytochrome P450 Oxidoreductase Simulations: Cofactors Movement and Structural Changes

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PH-039 Single Molecule Motion Map of Pentameric Ligand Gated Ion Channel by Diffracted X-ray Tracking

<u>Hiroshi Sekiguchi</u>¹, Yufuku Matsushita², Yuri Nishino³, Keigo Ikezaki², Atsuo Miyazawa³, Tai Kubo⁴, Christele Huron⁵, Jean-Pierre Changeux⁵, Pierre-Jean Corringer⁵, Yuji Sasaki²

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$\,$ PH-040 $\,$ Evolutionary hinge migration sheds light on the mechanism of green-to-red photoconversion in GFP-like proteins

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PH-041 Quercetin effect on the stability and regeneration of the G-protein-coupled receptor rhodopsin

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PH-042 Identification of prospective allosteric sites of p38 by computational methods Patricia Gomez-Gutierrez¹, Juan Jesus Perez¹

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PH-043 Hydrogen/deuterium exchange-mass spectrometry provides clues on the mechanism of action of Min E

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PH-044 Biased signalling and heteromization of the Dopamine D2 receptor in Schizophrenia and Parkinson's disease

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PH-045 Bis-ANS as a tool to monitor conformational changes upon assembly of binary and ternary complexes of eIF4E, 4E-BP1 inhibitory protein, and the mRNA 5'cap

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PH-046 Mapping of Thrombin - Beta2Glycoprotein I Interaction Sites

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PH-047 Dynamical Variability in the Clan MA of Metalloproteases

<u>Henrique F. Carvalho</u>^{1,2}, Ana Cecília A. Roque¹, Olga Iranzo^{2,3}, Ricardo J. F. Branco¹1.-UCIBIO, REQUIMTE, Faculdade de Ciências e Tecnologia, Universidade Nova Lisboa, 2.-ITQB António Xavier, Universidade Nova de Lisboa, 3.-Aix Marseille Université, Centrale Marseille

$\hbox{PH-}048\quad \hbox{X-ray crystallographic analysis of cold-adapted and thermostable glucokinase}$

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PI - PROTEIN ENGINEERING

PI-001 **Genetic engineering of new formate dehydrogenases for cofactor regeneration**<u>Anastasia Alekseeva</u>^{1,2}, Irina Dolina^{2,3}, Ivan Kargov^{2,3}, Svyatoslav Savin^{2,3}, Vladimir Tishkov⁰ 1.-A.N. Bach Institute of Biochemistry, Russian Academy of Sciences, 2.-Innovations and High Technologies MSU Ltd, 3.-Chemistry Faculty, M.V. Lomonosov Moscow State University

PI-002 Mutations of a conserved tryptophan residue of the TEM-1 ß-lactamase

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PI-003 Light-switchable Zn2+ binding proteins to study the role of intracellular Zn2+ signaling

Stijn Aper¹, Maarten Merkx¹

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PI-004 **Proteins as supramolecular building blocks: engineering nanoscale structures**<u>Helen Ashmead</u>^{1,2,3}, Leonardo Negron¹, Jack Sissons⁶, Kyle Webster⁶, Vic Arcus^{2,4}, Juliet Gerrard⁰ 1.-Callaghan Innovation, 2.-Biomolecular Interaction Centre, University of Canterbury, 3.-School of Biological Sciences, University of Canterbury, 4.-Faculty of Science & Engineering, University of Waikato, 5.-School of Biological Sciences, University of Auckland, 6.-School of Biological Sciences, Victoria University



PI-005 A Structure Based Approach to Engineering Contraceptive Vaccine Antigens

<u>Danielle Basore</u>^{1,2}, Rajesh Naz⁵, Scott Michaele, Sharon Iserne, Benjamin Wright, Katie Saporita, Donna Crone, Christopher Bystroff

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PI-006 Protein carriers for passage of the blood-brain barrier Sinisa Bielic¹

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PI-007 Medium-throughput multistep purification of coagulation factor VIIa

 $\underline{\mathsf{Jais}\ R.\ Bjelke}^{\scriptscriptstyle 1},\ \mathsf{Gorm\ Andersen}^{\scriptscriptstyle 1},\ \mathsf{Henrik}\ \emptyset \mathtt{stergaard}^{\scriptscriptstyle 1},\ \mathsf{Laust\ B.\ Johnsen}^{\scriptscriptstyle 1},\ \mathsf{Anette\ A.\ Pedersen}^{\scriptscriptstyle 1},\ \mathsf{Tina}\ \mathsf{H.\ Glue}^{\scriptscriptstyle 1}$

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PI-008 Biomimetic sequestration of co2: reprogramming the b1 domain of protein g through a combined computational and experimental approach

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PI-009 The roles of entropy and packing efficiency in determining protein-peptide interaction affinities

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1.-Physics, Yale University, 2.-Integrated Graduate Program in Physical and Engineering Biology, Yale University, 3.-Mechanical Engineering and Materials Science, Yale University, 4.-Applied Physics, Yale University, 5.-Molecular Biophysics and Biochemistry, Yale University, 6.-Chemistry, Yale University

PI-010 Monitoring protein-protein interactions using tripartite split-GFP complementation assays

<u>Stéphanie Cabantous</u>¹, Hau B. NGuyen³, Jean-Denis Pedelacq², Faten Koraichi¹, Anu Chaudhary³, Kumkum Ganguly³, Meghan A. Lockard³, Gilles Favre¹, Thomas C. Terwilliger³, Geoffrey S. Waldo³ 1.-Cancer Research Center of Toulouse, 2.-CNRS- IPBS, UMR 5089, 205 Route De Narbonne, 3.-Los Alamos National Laboratory, Los Alamos NM

PI-011 Role of residues Cys301 and Cys303 in the active site of human ALDH2

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PI-012 Small molecule-assisted shutoff: A widely applicable method for tunable and reversible control of protein production

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PI-013 Proof of principle for epitope-focused vaccine design

<u>Bruno Correia</u>¹, John Bates², Rebecca Loomis³, Chris Carrico⁴, Joseph Jardine⁵, David Baker⁶, Roland Strong⁷, James Crowe³, Phillip Johnson⁴, William Schief^{1,6,7}

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PI-014 Designed repeat proteins as templates for photoactive molecules and fluorescent nanoclusters

Sara H. Mejias¹², Antonio Aires¹², Javier López-Andarias³, Pierre Couleaud¹², Begoña Sot¹², Carmen Atienza³, Nazario Martín¹³, <u>Aitziber L. Cortajarena¹²</u>

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PI-015 **Engineering of proteins to develop biomimetic hematite-based biohybrid materials** Greta Faccio¹, Krisztina Schrantz², Linda Thöny-Meyer¹, Artur Braun², Julian Ihssen¹

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PI-016 Correcting Free Energy Expressions for Thermal Motion

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PI-017 Tertiary Structural Propensities Reveal Fundamental Sequence/Structure Relationships

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PI-018 De novo design of an ideal TIM-barrel scaffold

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PI-019 Directed Evolution of Fluorescent Protein Function

Felix Vietmeyer¹, Premashis Manna^{1,2}, Kevin Dean³, Amy Palmer^{2,4}, Ralph Jimenez^{1,2}

1.-JILA, University of Colorado and NIST, 2.-Dept. of Chemistry & Biochemistry, University of Colorado, 3.-University of Texas Southwestern Medical Center, 4.-BioFrontiers Institute, University of Colorado

PI-020 Targeted protein degradation achieved through a combination of degrons from yeast and mammalian ornithine decarboxylase

Rushikesh Joshi¹. Ratna Prabha C.¹

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PI-021 Short peptides self-assemble in the presence of metals to produce catalytic amyloids Caroline Rufo¹, Yurii Moroz¹, Olesia Moroz¹, Olga Makhlynets¹, Pallavi Gosavi¹, Jan Stöhr², Tyler Smith¹, Xioazhen Hu³, William DeGrado³, Ivan Korendovych¹

1.-Syracuse University, 2.-Institute for Neurodegenerative Diseases and Department of Neurology, UCSF, 3.-Department of Pharmaceutical Chemistry, UCSF

PI-022 Rational design of the cold active subtilisin-like serine protease VPR with improved catalytic properties and thermal stability

Kristinn Oskarsson¹, Sigridur Thorbjarnardottir², Magnus Kristjansson¹

1.-Science Institute, University of Iceland, Department of Biochemistry, 2.-Institute of Biology, University of Iceland

PI-023 Critical peptide stretches may not serve as faithful experimental mimics for protein amyloidogenesis

Bishwajit Kundu¹, Dushyant Garg¹

1.-Kusuma School of Biological Sciences

PI-024 A Systematic Exploration Of Protein Uptake And Trafficking Into Intracellular Compartments

Aksana Labokha¹, Ralph Minter¹

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PI-025 Protein engineering: what's next?

Maria Fatima Lucas^{1,2}, Víctor Guallar^{1,3}

1.-Joint BSC-CRG-IRB Research Program in Computational Biology, 2.-Anaxomics Biotech, 3.-ICREA

PI-026 Bottom-up construction of a synthetic carboxysome

Shiksha Mantri¹, Raphael Frey¹, Marco Rocca¹, Eita Sasaki¹, Donald Hilvert¹ 1-FTH Zurich

PI-027 CXCL10 engineering: novel insights into glycan interactions

Michael Nagele¹, Martha Gschwandtner¹, Patrick Sorger¹, Andreas J. Kungl¹

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PI-028 Creating large covalently circularized nanodiscs and their application in studying viral entry and genome translocation

Mahmoud Nasr¹, Mike Strauss¹, James Hogle¹, Gerhard Wagner¹

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PI-029 Single molecule DNA-based in vitro translation in femtoliter chamber array for directed evolution

Hiroyuki Noji1, 2

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PI-030 Parametric design of alpha-helical barrels and pore-like assemblies with very high thermodynamic stabilities

<u>Gustav Oberdorfer</u>^{1,2,7}, Po-Ssu Huang^{1,7}, Chunfu Xu^{1,7}, Verena Kohler², Xue Y. Pei³, Brent L. Nannenga⁴, Joseph M. Rogers⁵, Tamir Gonen⁴, Karl Gruber², David Baker¹,^{6,7}

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PI-031 Leucine Zipper fused Fab; Enhancement of active Fab formation in E. coli in vitro and in vivo expression systems

Teruyo Ojima-Kato^{1, 2}, Kansuke Fukui², Takaaki Kojima², Hideo Nakano²

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PI-032 The Road Not Taken: Exploring Repeat Protein Architectures By Computational Design

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PI-033 Design and characterisation of a synthetic serpin with novel folding properties

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PI-034 Computational Design of Shape-optimized Leucine-Rich Repeat Proteins

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PI-035 Engineering APOBEC3G enzymes for altered specificity and processivity

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PI-036 Engineering Porous Protein Crystals as Scaffolds for Programmed Assembly

Thaddaus Huber¹, Luke Hartje¹, Christopher Snow¹

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PI-037 Engineering ultrasensitive protein probes of voltage dynamics for imaging neural activity in vivo

<u>Francois St-Pierre</u>^{1,2}, Michael Pan^{1,2}, Helen Yang³, Xiaozhe Ding^{1,2}, Ying Yang^{1,2}, Thomas Clandinin³, Michael Lin^{1,2}

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PI-038 Assembly of Armadillo Repeat Proteins from Complementary Fragments

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PI-039 Engineering light-controllable kinases and Cas9 endonuclease with photodissociable dimeric fluorescent protein domains

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PI-040 Exploring the evolution of folds and its application for the design of functional hybrid proteins

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PI-041 Semisynthesis and initial characterization of sortase A mutants containing selenocysteine and homocysteine

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PI-042 Directed Evolution on FucO – Structural Explanations for Changes in Substrate Scope

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PI-043 Aided-Crystallization of the artificial protein Octarellin V.1 by alpha-Reps and nanobodies

<u>Maximiliano Figueroa</u>¹, Mike Sleutel², André Matagne³, Christian Damblon⁴, Els Pardon², Marielle Valerio-Lepiniec⁵, Philippe Minard⁵, Joseph Martial¹, Cécile Van de Weerdt¹

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PI-044 Generation of synthetic antibodies against membrane proteins in nanodiscs for use in structural biology

<u>Pawel K. Dominik</u>¹, Marta T. Borowska¹, Olivier Dalmas⁰, Sangwoo S. Kim¹, Dawid Deneka¹, Eduardo Perozo¹, Robert J. Keenan¹, Anthony A. Kossiakoff¹

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PI-045 A novel drug delivery system for poorly water-soluble anti-tumor drug SN-38 utilizing intravital transporter protein

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PI-046 Intrinsic Disorder as Biomimetic Strategies for the Introduction of Hill-Type Cooperativity into Biomolecular Receptors

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PI-047 Essential and non-essential amino acid species for an ancestral protein Satoshi Akanuma¹

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PI-048 De novo design of protein-protein interaction using hydrophobic and electrostatic interactions

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PI-049 In Vitro Selection of Liposome Anchoring Peptide by cDNA display

Naoto Nemoto¹, Ryoya Okawa¹, Yuki Yoshikawa¹, Toshiki Miyajima¹, Shota Kobayashi¹ 1.-Graduate School of Science and Engineering, Saitama University

PI-050 Designing of a novel platinum-binding amino acid sequence on a protein surface

<u>Asumi Kaji</u>¹, Hiroya Niiro¹, Satoshi Akanuma², Tetsuya Uchida¹, Akihiko Yamagishi¹ 1.-Tokyo University of Pharmacy and Life Sciences, 2.-Waseda University

PI-051 Engineering of an isolated p110 α subunit of PI3K α permits crystallization and provides a platform for structure-based drug design

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PI-052 Identification of structural determinants involved in the differential conformational changes of EF-hand modules

Emma Liliana Arevalo Salina¹, Joel Osuna Quintero¹, Humberto Flores Soto¹, Gloria Saab Rincón¹ 1.-Instituto de Biotecnología, Universidad Nacional Autónoma de México

PI-053 Mapping side chain interactions at the N- and C-termini of protein helices Nicholas Newell¹

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PI-054 Generation of fluorescent protein-tagged gp120 mutants to analyze the intracellular distribution of HIV-1 envelope protein

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PI-055 NGS-Guided Phage Panning: Comparison to Conventional Panning Strategy

Buyung Santoso¹, Dorain Thompson¹, John Nuss¹, John Dwyer¹

1.-Ferring Research Institute

PI-056 Fully Automated Mini, Midi, and Maxi Plasmid Prep on the AutoPlasmid MEA Instrument

Carrie Huynh¹, Lee Hoang¹, Chris Suh¹, Jonathan Grambow¹

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PI-057 RE3Volutionary Computational Design of Symmetric Proteins That Biomineralize Nano-Crystals

Kam Zhang¹, Arnout Voet¹, Hiroki Noguchi², Christine Addy², Jeremy Tame²

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PI-058 Bacillus licheniformis Trehalose-6-phosphate Hydrolase structures suggest keys to substrate specificity

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1.-Institute of Molecular Biology, Academia Sinica, 2.-Department of Applied Chemistry, National Chiayi University, 3.-Department of Life Science, National Tsing Hua University



PI-059 Crystal structure of engineered LRRTM2 synaptic adhesion molecule and a model for neurexin binding

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PI-060 Computational design of phenylalanine binder

Olga Khersonsky¹, Gil Benezer¹, Sarel Fleishman¹

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PI-061 Dimer dynamics in a cold-active enzyme: the case of alkaline phosphatase

<u>Bjarni Ásgeirsson</u>¹, Manuela Magnúsdóttir¹, Jens Hjörleifsson¹, Gaetano Invernizzi², Elena Papaleo² 1.-Department of Biochemistry, Science Institute, University of Iceland, 2.-University of Milano

PI-062 A novel secondary structure element assembly protocol for the design of artificial $(\beta\alpha)$ 8-barrel proteins using ROSETTA

<u>Cristina Elisa Martina</u>¹, Steven Combs², Rocco Moretti², Maximiliano Figueroa¹, Cecile Van De Weerdt¹, Andre Matagne¹, Jens Meiler²

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PI-063 Construction of protein capsule possessing drugs controlled release ability

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PI-064 Formation of Cytochrome cb562 Oligomers by Domain Swapping

<u>Takaaki Miyamoto</u>¹, Mai Kuribayashi¹, Satoshi Nagao¹, Yasuhito Shomura², Yoshiki Higuchi⁰, Shun Hirota¹

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PI-065 A highly buried and conserved tryptophan residue close to the dimer interface in a cold-adapted phosphatase is phosphorescent and important for activity

Jens Hjörleifsson¹, Bjarni Ásgeirsson¹

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PI-066 Modulating protein-protein interaction with a molecular tether

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PI-067 LIL traptamers: artificial transmembrane proteins with minimal chemical diversity

Daniel DiMaio¹, Erin Heim¹, Ross Federman¹, Lisa Petti¹, Jez Marston¹

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PI-068 Efficient Encapsulation of Enzymes in an Engineered Protein Cage

Yusuke Azuma1, Donald Hilvert1

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PI-069 Identification of disease-related antigen-specific human antibodies by a method that combines biopanning and high throughput sequencing from patient-derived scFv antibody library

Yuji Ito¹, <u>Yurie Enomoto</u>¹, Shuhei Umemura¹, Aiko Fujiyama¹, Ryoko Mieno¹, Yukiko Kato¹, Dai-ichiro Kato¹

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PI-070 Biochemical analysis of the recognition helix of Z-DNA binding proteins: Roles in conformational specificity

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PI-071 Photo switching of protein conformation

<u>Frank D. Sönnichsen</u>¹, Matthias Lipfert¹, Hauke Kobarg¹, Anne Müller¹, Thisbe K. Lindhorst¹ 1.-Otto Diels Institute for Organic Chemistry, Christian-Albrechts-University

PI-072 ADSETMEAS: Automated Determination of Salt-bridge Energy Terms and Micro Environment from Atomic Structures using APBS method, version 1.0

Arnab Nayek¹, Shyamashree Banerjee, Parth Sarthi Sen Gupta, Biswa pratap Sur, Pratay Seth, Sunit Das, Nathan A Baker, Amal K Bandyopadhyay

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PI-073 Next generation analgesics – targeting ion channels with antibody-drug conjugates (ADCs)

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PI-074 Semi-synthesis and Evaluation of Parasitic GPI-Anchored Proteins

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PI-075 Assessment of UCH-L3 Substrate Selectivity using Engineered Ubiquitin Fusions with Varying Linker Lengths

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PI-076 Beta-hairpins: Molecular Accessories for Helical Peptide Expression

Melissa Lokensgard¹, John Love¹

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PI-077 Development of a semisynthetic method for the cell surface presentation of proteins

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PI-078 Transmembrane domain dimerization drives p75NTR partitioning to lipid rafts Irmina García Carpio, Marcal Vilar

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PI-079 Bioluminescent sensor proteins for therapeutic drug monitoring of the monoclonal antibody Cetuximab

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PI-080 Genetically encoded biosensor for cell permeability of inhibitors of the p53-HDM2 interaction

Silvia Scarabelli¹, Thomas Vorherr², Kai Johnsson¹

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PI-081 Archer: Predicting protein function using local structural features. A helpful tool for protein redesign

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PI-082 Light-induced interaction of protomers in bacterial phytochrome from Rhodopseudomonas palustris

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PI-083 Luminescent sensor proteins for antibody detection in solution

Remco Arts¹, Susann Ludwig¹, Marina van Vliembergen¹, Vito Thijssen¹, Stan van der Beelen¹, Ilona den Hartog¹, Stefan Zijlema¹, Maarten Merkx¹

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PI-084 Tertiary Structural Propensities Reveal Fundamental Sequence-Structure Relationships

Fan Zheng¹, Jian Zhang², Gevorg Grigoryan⁰

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PI-085 Exploiting natural sequence diversity for protein crystallization

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2.-Laboratorio de Estudios Cristalográficos, IACT-CSIC-UGR Granada

PI-086 Synthesis of selectively functionalized adiponectin

Andreas Mattern, Annette Beck-Sickinger

1.-University of Leipzig, Institute of Biochemistry, 2.-University of Leipzig, Institute of Biochemistry

PI-087 De novo catalysis in ancestral protein scaffolds

<u>Valeria A. Risso</u>¹, Sergio Martinez-Rodriguez¹, Adela M. Candel¹, David Pantoja-Uceda², Mariano Ortega-Muñoz³, Francisco Santoyo-Gonzalez³, Marta Bruix², José A Gavira⁴, Jose M. Sanchez-Ruiz¹

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PI-088 Exploring the Importance of Dimerization for DJ-1 Function through Engineered Domain Fusions

Sierra Hansen¹, Jiusheng Lin¹, Mark Wilson¹

1.-University of Nebraska, Lincoln

PI-089 The purification, crystallization and preliminary characterization of SdrE from S. aureus

Degiang Wang¹, Ke Chen¹, Jun Zhang²

1.-Key Laboratory of Molecular Biology on Infectious Disease, 2.-The Department of Cell Biology and Genetics

PI-090 Structure based modifications of the bacterial microcompartment shell protein PduA

David Leibly^{1,2}, Julien Jorda², Sunny Chun³, Alan Pang², Michael Sawaya², Todd Yeates⁰

1.-Department of Chemistry and Biochemistry, University of California, 2.-UCLA-DOE Institute for Genomics and Proteomics, 3.-Molecular Biology Institute, University of California

PI-091 Targeted conformational transitions of large and multimeric proteins by an efficient elastic network based technique

<u>Yasemin Yesiltepe</u>¹, Doga Findik¹, Arzu Uyar¹, Deniz Turgut², Rahmi Ozisik², Turkan Haliloglu¹, Pemra Doruker¹

1.-Bogazici University and Polymer Research Center, 2.-Rensselaer Polytechnic Institute

PI-092 Continuous directed evolution of receptor-selective ∂-endotoxins for overcoming insecticidal resistance

<u>Ahmed Badran</u>^{1,2}, Victor Guzov³, Qing Huai³, Melissa Kemp³, Prashanth Vishwanath³, Artem Evdokimov³, Farhad Moshiri³, Meiying Zheng³, Keith Turner³, David Liu¹.²

1.-Department of Chemistry and Chemical Biology, Harvard University, 2.-Howard Hughes Medical Institute, Harvard University, 3.-Monsanto Company

PI-093 Optimization of a Designed Protein-Protein Interface

Brian Maniaci¹, Collin Lipper², John J. Love¹

1.-San Diego State University, 2.-University of California

PI-094 Directed Evolution of Site-Specific Recombinases for Targeted Integration into Unmodified Human Cells

Jeffrey L Bessen^{1,2}, David B Thompson^{1,2}, David R, Liu^{1,2}

1.-Department of Chemistry & Chemical Biology, Harvard University, 2.-Howard Hughes Medical Institute, Harvard University

PI-095 Generation of comprehensive deletion libraries mediated by in vitro transposition Aleardo Morelli¹, Burckhard Seelig¹

1.-University of Minnesota

PI-096 Structural characterization of PpsC, a multi-domain polyketide synthase from Mycobacterium tuberculosis using a fragment-based approach

Alexandre Faille¹, Nawel Slama1¹, Anna Grabowska¹, David Ricard¹, Annaik Quémard¹, Lionel Mourey¹, <u>Jean-Denis Pedelacq¹</u>

1.-Institut de Pharmacologie et de Biologie Structurale

PI-097 Computational Design of Tighter Protein-Ligand Interfaces

Brittany Allison¹, Brian Bender², Jens Meiler⁰

1.-Vanderbilt University, Department of Chemistry, 2.-Vanderbilt University, Department of Pharmacology



PI-098 Structural studies of human acidic fibroblast-growth factor (FGF1) mutants with a probable anticancer activity

Maria Cecilia Gonzalez¹, Stefano Capaldi¹, Maria Elena Carrizo¹, Laura Destefanis¹, Michele Bovi¹, Massimiliano Perduca¹, Hugo Luis Monaco¹

1.-Biocristallography Laboratory, Department of Biotechnology, University of Verona

PI-099 Drug-controllable protein tags for the selective visualization or selective shutoff of newly synthesized proteins of interest in mammalian cells and in vivo

Conor Jacobs¹, Yang Geng², Ryan Badiee¹, Tiffany Nguyen³, Andrew Evans⁴, Hokyung Chung¹, Ying Yang², Mehrdad Shamloo⁴, Roger Y. Tsien⁵, Michael Z. Lin².6

- 1.-Department of Biology, Stanford University, 2.-Department of Pediatrics, Stanford University,
- 3.-Department of Neurology and Neurological Sciences, Stanford University, 4.-Department of Neurosurgery, Stanford University, 5.-Department of Pharmacology, UC San Diego, 6.-Department of Bioengineering, Stanford University

PI-100 BRET-based antibody switches for detection of Dengue serotype 1 antibodies

Remco Arts¹, Susann Ludwig¹, Byron Martina², Maarten Merkx¹

1.-Eindhoven University of Technology, 2.-Erasmus Medical Center Rotterdam

PI-101 Delivery of biologics against intracellular targets

<u>Paulina Kolasinska-Zwierz</u>¹, Pawel Stocki¹, Bina Mistry¹, Sandrine Guillard¹, Alison Smith¹, Rose Marwood¹, Ben Kemp¹, Anna Czyz¹, Ronald Jackson¹, Ralph Minter¹, Tristan Vaughan¹ 1.-ADPE Cambridge, MedImmune, Milstein Building

PI-102 Recombinant H5 antigen based on hydrolytic domain with deletion of polybasic cleavage site forms functional oligomers

<u>Edyta Kopera</u>¹, Maria Pietrzak¹, Agnieszka Macioła ¹, Anna Maria Protas-Klukowska¹, Konrad Zdanowski¹, Beata Gromadzka², Krystyna Grzelak¹, Zenon Minta³, Krzysztof Śmietanka³, Bogusław Szewczyk²

1.-Institute of Biochemistry and Biophysics, Polish Academy of Sciences, 2.-University of Gdansk and Medical University of Gdansk, 3.-National Veterinary Research Institute, Department of Poultry Diseases

PI-103 Alteration of lysine and arginine content as a strategy to modify protein solubility: a test for E. coli proteins

M. Alejandro Carballo-Amador¹, Jim Warwicker¹, Alan J. Dickson¹

1 - Faculty of Life Sciences, University of Manchester

PI-104 Mining the structural universe for de novo design

Craig Mackenzie¹, Gevorg Grigoryan¹

1.-Dartmouth College

PI-105 Engineering a Stable, Symmetric Membrane Protein Scaffold

Amanda Duran¹, Jens Meiler¹

1.-Vanderbilt University-Department of Chemistry

PI-106 Sortase-mediated synthesis of protein-DNA conjugates for sensitive biosensing

Bedabrata Saha¹, Marieke op de Beeck¹, Remco Arts¹, Maarten Merkx¹

1.-Department of Biomedical Engineering, Eindhoven University of Technology

PI-085 Exploiting natural sequence diversity for protein crystallization

Sergio Martínez-Rodríguez¹, Valeria A. Risso¹, Jose M. Sanchez-Ruiz¹, Jose A. Gavira²

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2.-Laboratorio de Estudios Cristalográficos, IACT-CSIC-UGR Granada

PJ - PROTEOMICS (PPIS, PTMS)

PJ-001 Mass Spectrometry based Proteomics to Identify the Protein Differences in Human Breast Milk from Breast Cancer Patients and Controls

Devika Channaveerappa¹, Roshanak Aslebagh¹, Kathleen F. Arcaro², Costel C. Darie¹

1.-Clarkson University, 2.-University of Massachusetts

PJ-002 Leukolike Vectors: leukocyte-inspired nanoparticles

<u>Claudia Corbo</u>^{1,2}, Alessandro Parodi^{1,2}, Roberto Palomba^{1,2}, Roberto Molinaro¹, Michael Evangelopoulos¹, Francesco Salvatore⁰, Ennio Tasciotti¹

1.-The Houston Methodist Research Institute, 2.-Fondazione IRCCS SDN, 3.-CEINGE-, Biotecnologie Avanzate

PJ-003 Visualising gene regulation: a combined proteomic and genomic approach for the structural analysis of steroid hormone receptor complexes

Andrew Holding¹

1.-Cancer Research UK Cambridge Institute, University of Cambridge

PJ-004 Global kinetic analysis of caspase protein substrates in cell lysate reveals selective roles and target specificity

Olivier Julien¹, Min Zhuang¹, Arun Wiita¹, James Wells¹

1.-University of California

PJ-005 A chemical proteomics approach reveals direct 'readers' of histone variant gammaH2AX involved in the DNA damage response

Ralph Kleiner, Priyanka Verma, Kelly Molly, Brian Chait, Tarun Kapoor

1.-The Rockefeller University, 2.-The Rockefeller University, 3.-The Rockefeller University, 4.-The Rockefeller University, 5.-The Rockefeller University

PJ-006 Interactomic and Enzymatic Analyses of Distinct Affinity Isolated Human Retrotransposon Intermediates

<u>John LaCava</u>^{1,2}, Kelly Molloy¹, Martin Taylor³, David Fenyö², Lixin Dai³, Brian Chait¹, Jef Boeke², Michael Rout¹

1.-The Rockefeller University, 2.-New York University School of Medicine, 3.-Johns Hopkins University School of Medicine

PJ-007 Polyubiquitin recognition by continuous ubiquitin binding domains of Rad18 probed by modeling, small-angle X-ray scattering and mutagenesis

Sangho Lee¹, Trung Thanh Thach¹, Namsoo Lee¹, Donghyuk Shin¹, Seungsu Han¹, Gyuhee Kim¹, Hongtae Kim¹

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PJ-008 Optimization of a protein extraction method for the proteomic study of pozol

<u>Cynthia Teresa Leyva-Arguelles</u>¹, Carmen Wacher², Rosario Vera³, Romina Rodríguez-Sanoja¹ 1.-Instituto de Investigaciones Biomédicas, UNAM., 2.-Facultad de Química, UNAM., 3.-Instituto de Biotecnología, UNAM

PJ-009 Proteomics and enology: wine yeasts study applications

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- 3.-Dipartimento di Agraria





PJ-010 Additional binding sites for cytochrome c on its redox membrane partners facilitate its turnover and sliding mechanisms within respiratory supercomplexes

<u>Blas Moreno-Beltrán</u>¹, Antonio Díaz-Quintana¹, Katiuska González-Arzola¹, Alejandra Guerra-Castellano¹, Adrián Velázquez-Campoy⁰, Miguel A. De la Rosa¹, Irene Díaz-Moreno¹

1.-IBVF, CICCartuja, Universidad de Sevilla - CSIC, 2.-BIFI - IQFR (CSIC), Universidad de Zaragoza, 3.-Departamento de Bioquímica y Biología Molecular Celular, Universidad de Zaragoza, 4.-ARAID Foundation, Government of Aragon

PJ-011 Can Bio-functionalities be deciphered from Protein Sequence Information using Computational Approaches?

Norbert Nwankwo1

1.-University of Port Harcourt

PJ-012 Prediction of Cleavage Specificity in HCV NS3/4A Serine Protease and AdV2 Cysteine Protease Systems by Biased Sequence Search Threading

Gonca Ozdemir Isik1, A.Nevra Ozer1

1.-Department of Bioengineering, Faculty of Engineering, Marmara University

PJ-013 Protein plasticity improves protein-protein binding description

Chiara Pallara¹, Juan Fernández-Recio¹

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PJ-014 Affimers, new Affinity Reagents for Life Science Research

<u>Vincent Puard</u>¹, Kit-Yee Tan¹, Kurt Baldwin¹, Enitan Carrol², Rebecca Patisson³, Rob Beynon³, Christian Tiede⁴, Michael McPherson⁴, Darren Tomlinson⁴, Paul Ko Ferrigno¹

1.-Avacta Life Sciences, 2.-Institute of Infection and Global Health, University of Liverpool, 3.-Centre for Proteome Research, University of Liverpool, 4.-Biomedical Health Research Centre, University of Leeds

PJ-015 NMR study of ERK-mediated hyperphosphorylation of the neuronal Tau protein

<u>Haoling Qi</u>¹, François-Xavier Cantrelle², Amina Kamah¹, Clément Despres¹, Sudhakaran Prabakaran², Jeremy Gunawardena², Guy Lippens¹, Isabelle Landrieu¹

1.-UMR 8576 CNRS-USTL, Lille University, 2.-Department of Systems Biology, Harvard Medical School

PJ-016 How binding incorrect partners can lead to the prediction of correct interfaces: Results from a massive cross-docking study on proteins

Sophie Sacquin-Mora¹, Lydie Vamparys¹, Alessandra Carbone²

1.-Laboratoire de Biochimie Théorique, 2.-Génomique Analytique, Université Pierre et Marie Curie

PJ-017 Whole-protein mass spectrometry reveals global changes to histone modification patterns in hypoxia

Sarah Wilkins¹, Kuo-Feng Hsu¹, Christopher Schofield¹

1.-Chemistry Research Laboratory, Oxford University

PJ-018 Mass Spectrometry-Based Protein Biomarker Discovery in Neurodevelopmental Disorders

<u>Kelly Wormwood</u>¹, Armand Ngounou Wetie¹, Laci Charette², Jeanne Ryan², Emmalyn Dupree¹, Alisa Woods⁰, Costel Darie¹

1.-Clarkson University, 2.-SUNY Plattsburgh

PJ-019 Understanding protein recognition using structural features

<u>Manuel A. Marin-Lopez</u>¹, Joan Planas-Iglesias², Jaume Bonet³, Daniel Poglayen¹, Javier García-García¹, Narcís Fernández-Fuentes¹, Baldo Oliva¹

1.-Structural Bioinformatics Lab (GRIB-IMIM), Department of Experimental and Health, Universitat Pompeu Fabra, 2.-Division of Metabolic and Vascular Health, University of Warwick, 3.-Laboratory of Protein Design & Immunoengineering, School of Engineering, Ecole Polytechnique Federale De Lausanne

PJ-020 Structural Characterization of the Cytoplasmic mRNA Export Platform

<u>Javier Fernandez-Martinez</u>¹, Yi Shi², Seung Joong Kim³, Paula Upla⁴, Riccardo Pellarin³, Daniel Zenklusen⁵, David L. Stokes⁴, Andrej Sali³, Brian T. Chait², Michael P. Rout¹

1.-Laboratory of Cellular and Structural Biology, The Rockefeller University., 2.-Laboratory of Mass Spectrometry and Gaseous Ion Chemistry, The Rockefeller Univ., 3.-University of California, 4.-The New York Structural Biology Center, 5.-Department of Biochemistry, Faculty of Medicine, University of Montreal

PJ-021 Study of candidate proteins to pore associated with P2X7 receptor in different cell types

Carla Oliveira¹, Anael Alberto¹, Mônica Freitas², Luiz Alves¹

1.-Laboratório de Comunicação Celular – FIOCRUZ, 2.-Centro Nacional de Ressonância Magnética Nuclear – UFRJ

PJ-022 CABS-dock web server for protein-peptide docking with significant conformational changes and without prior knowledge of the binding site

<u>Mateusz Kurcinski</u>¹, Michal Jamroz¹, Maciej Blaszczyk¹, Andrzej Kolinski¹, Sebastian Kmiecik¹ 1.-Department of Chemistry, University of Warsaw

PJ-023 Web server tools for modeling of protein structure, flexibility, aggregation properties and protein-peptide interactions

<u>Maciej Blaszczyk</u>¹, Michal Jamroz¹, Mateusz Kurcinski¹, Agata Szczasiuk¹, Andrzej Kolinski¹, Sebastian Kmiecik¹

1.-University of Warsaw, Faculty of Chemistry

PJ-024 **Developing a Technique to Detect Deamidated Proteins and Peptides Using Rig-I** Sandy On¹, Pinghui Feng²

1.-University of Southern California, Keck School of Medicine, 2.-USC Norris Comprehensive Cancer Center

PJ-025 Mass spectrometric evaluation of recombinant hemagglutinin structure conformations

Joanna Szewczak¹, <u>Anna Bierczyńska-Krzysik¹</u>, Agnieszka Romanik-Chruścielewska¹, Iwona Sokołowska¹, Marcin Zieliński¹, Piotr Baran¹, Violetta Sączyńska¹, Małgorzata Kęsik-Brodacka¹, Drota Stadnik¹, Grażyna Płucienniczak¹

1 -Institute of Biotechnology and Antibiotics

PJ-026 Monoclonal-based antivenomics and biological activities revealing conserved neutralizing epitopes across elapidae family

<u>Carlos Correa-Netto</u>^{1,2}, Ricardo Araújo^{1,2}, Marcelo Strauch¹, Leonora Brazil-Más¹, Marcos Machado³, Moema Leitão-Araújo⁴, Paulo Melo³, Débora Foguel², Juan Calvete⁵, Russolina Zingali²

1.-Instituto Vital Brazil, 2.-Instituto de Bioquimica Medica-UFRJ, 3.-Programa de Farmacologia e Química Medicinal-UFRJ, 4.-Fundação Zoobotânica do Rio Grande do Sul, 5.-Instituto de Biomedicina de Valencia-CSIC



PJ-027 A comprehensive analysis of scoring functions for protein-protein docking Didier Barradas¹, Juan Fernandez-Recio^{1,2}

1.-Barcelona Supercomputing Center, 2.-Joint BSC-CRG-IRB Research Program in Computational Biology

PJ-028 Multi-PTK Antibody: A Powerful Tool to Detect a Wide Variety of Protein Tyrosine Kinases (PTKs)

Isamu Kameshita¹, Noriyuki Sueyoshi¹, Yasunori Sugiyama¹

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PJ-029 A comprehensive analysis of scoring functions for protein-protein docking

Didier Barradas¹, Juan Fernandez-Recio^{1,2}

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PJ-030 Analysis of the Siglec-9 and hVAP-1 interactions

<u>Leonor Carvalho</u>¹, Vimal Parkash¹, Heli Elovaara², Sirpa Jalkanen², Xiang-Guo Li^{3,4}, Tiina Salminen¹ 1.-Structural Bionformatics Laboratory, Department of Biosciences, 2.-MediCity Research Laboratory, 3.-Department of Pharmacology, Drug Development and Therapeutics, 4.-Turku PET Center

PJ-031 Molecular basis of polyubiquitin chain formation by Ube2K

Adam Middleton¹, Catherine Day¹

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PJ-032 The two chromophorylated linkers of R-Phycoerythrin in Gracilaria chilensis

Marta Bunster¹, Francisco Lobos-González¹, José Aleikar Vásquez¹, Carola Bruna¹, José Martínez-Oyanedl¹

1.-Fac de Cs Biol., Universidad de Concepción

PJ-033 Post-docking analysis by physicochemical properties of protein-protein interactions generated from rigid-body docking processes.

Nobuyuki Uchikoga¹, Masahito Ohue², Yuri Matsuzaki³, Yutaka Akiyama^{2,3},

1.-Dept. of Phys., Chuo Univ., 2.-Grad. Sch. of Inform. Sci. and Eng., Tokyo Tech, 3.-ACLS, Tokyo Tech

PJ-034 The structural studies of the two thermostable laccases from the white-rot fungi Pycnoporus sanguineus

Marta Orlikowska¹, Grzegorz Bujacz¹

1.-Institute of Technical Biochemistry, Lodz University of Technology

PJ-035 Analysis of liver proteome in cystathionine ß-synthase deficient mice using 2D IEF/SDS-PAGE gel electrophoresis, MALDI-TOF mass spectrometry, and label-free based relative quantitative proteomics

Izabela Bielińska¹, Łukasz Marczak¹, Hieronim Jakubowski^{1,2}

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PJ-036 Identification of N-homocysteinylation sites in mouse plasma albumin and hemoglobin from cystathionine ß-synthase deficient mice

Marta Sikora¹, ŁukaszMarczak¹, Hieronim Jakubowski¹

1.-Institute of Bioorganic Chemistry, Polish Academy of Sciences, 2.-Department of Biochemistry and Biotechnology, University of Life Sciences, 3.-Rutgers-New Jersey Medical School, International Center for Public Health

PJ-037 Investigating protein-protein interactions of the language-related transcription factor FOXP2 in live cells with bioluminescence resonance energy transfer

<u>Sara B. Estruch</u>¹, Sarah A. Graham¹, Pelagia Deriziotis¹, Swathi Mookonda Chinnappa¹, Simon E. Fisher^{1,2}

1.-Max Planck Institute for Psycholinguistics, Language and Genetics Department, 2.-Donders Institute for Brain, Cognition and Behaviour, Radboud University

PJ-038 The directly interaction between PreS1 of Human virus B and Human Heat Shock protein 70 (HSP70)

Degiang Wang¹, Chen Ke¹, Jun Zhang²

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PJ-039 A new hydrophobicity scale of amino acids based on IEF-MST calculated log P and log D

William J. Zamora¹, Josep M. Campanera¹, F. Javier Luque¹, Jody McGinness¹

1.-Departament de Fisicoquímica and Institut de Biomedicina (IBUB)

PJ-040 **Docking-based tools for discovery of protein-protein modulators** Mireia Rosell Oliveras¹, Juan Fernández Recio²

1.-Barcelona Supercomputing Center, 2.-Barcelona Supercomputing Center

PJ-041 Identification of transient protein complexes by using intrinsic disorder and network topology

Inhae Kim¹, Sangjin Han¹, Jihye Hwang², Sanguk Kim¹

1.-Department of Life Sciences, Pohang University of Science and Technology, 2.-Division of IT Convergence Engineering, Pohang University of Science and Technol

PJ-042 Expanding template-based protein-protein complex prediction using ab-initio docking

Sergio Mares-Sámano¹, <u>Luis Ángel Rodríguez-Lumbreras¹</u>, Juan Fernández-Recio¹ 1.-Joint BSC-CRG-IRB Research Program in Computational Biology

PJ-043 A Common Role for Cytochrome c in Programmed Cell Death in Humans and Plants Katiuska González-Arzola Instituto de Bioquím, Blas Moreno-Beltránº, Jonathan Martínez-Fábregasº, Carlos A. Elena-Realº, Antonio Díaz-Quintanaº, Irene Díaz-Morenoº, Miguel Á. De la Rosaº Falta Afiliation

PJ-044 Phosphorylation of Cytochrome c at Positions 28 and 47 could affect its Double Role in the Cell

<u>Alejandra Guerra-Castellano</u>¹, Katiuska González-Arzola¹, Francisco Rivero-Rodríguez¹, Adrián Velázquez-Campoy², Miguel Ángel De la Rosa¹, Irene Díaz-Moreno¹, Antonio Díaz-Quintana¹ 1.-IBVF – CIC Cartuja, University of Seville - CSIC, 2.-BIFI-IQFR, University of Saragossa - CSIC

PJ-045 Glucose-stimulated 4-hydroxynonenal (4-HNE) modification of the circadian rhythm protein, Cry1, in a murine model of insulin exocytosis

<u>Dean Wiseman</u>¹, Xianyin Lai², Frank Witzmann²

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PK - SYSTEMS BIOLOGY

PK-001 Effect of Three Aporphine Alkaloids on Bacillus subtilis 168

Fatma Gizem Avci¹, Berna Sariyar Akbulut¹

1.-Marmara University, Department of Bioengineering

PK-002 Protein degradation systems in the control of salmonid fish growth

Liudmila Lysenko¹, Nadezda Kantserova¹, Marina Krupnova¹, Nina Nemova¹

1.-The Institute of Biology, Karelian Research Centre of Russian Academy of Science

PK-003 Solving the proteomic organization of fitness-related genes in Uropathogenic Escherichia coli

Marc Torrent Burgas^{1,2}

1.-Microbiology Department, Vall d'Hebron Institut de Recerca, 2.-Biochemistry Department, Universitat Autònoma de Barcelona

PK-004 Elucidating the molecular mechanisms by which the HNH endonuclease gp74 activates the terminases in bacteriophage HK97

Sasha Weiditch¹, Karen Maxwell^{2,4}, Voula Kanelis^{1,3}

1.-Cell & Systems Biology, University of Toronto, 2.-Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, 3.-Chemical & Physical Sciences, University of Toronto, 4.-Department of Molecular Genetics, University of Toronto

PK-005 Analysis of the binding of mycotoxins to proteins involved in ASD with a combined computational/experimental approach

<u>Bernardina Scafuri</u>, Antonio Varriale, Angelo Facchiamo, Sabato D'Auria, Maria Elena Raggi, Anna Marabotti

1.-Dept. Chemistry and Biology, University of Salerno Bernardina Scafuri, 2.-Institute of Food Science, CNR Antonio Varriale, 3.-IRCCS "E. Medea" Ass. "La Nostra Famiglia" Maria Elena Raggi, 4.-2 Sabato D'auria, 5.-2 Angelo Facchiano, 6.-2 Anna Marabotti, 7.-1 Anna Marabotti

PK-006 Developing of microbial consortia for enzymatic valuable conversion of keratin-rich slaughter-house waste

Roall Espersen¹, Milena Gonzalo³, Samuel Jacquiod³, Waleed Abu-Alsud³, Søren J. Sørensen³, Jakob R. Winther⁴, Per Hägglund², Birte Svensson¹

1.-Enzyme and Protein Chemistry, Department of Systems Biology, Technical Universit, 2.-Protein and Immune Systems Biology, Department of Systems Biology, Technical Uni, 3.-Section of Microbiology, Department of Biology, University of Copenhagen, 4.-Section for Biomolecular Sciences, Department of Biology, University of Copenhag

PK-007 A comprehensive protein domain analysis to map cancer-type-specific somatic mutations

Jihye Hwang¹, Sangjin Han², Inhae Kim², Sanguk Kim²

1.-Department of IT Convergence and Engineering, POSTECH, 2.-Department of Life Science, POSTECH

PK-008 Identification of cancer-type-specific modules comprised of cancer-type-specific variants through phenotype similarity between cancer types

Sangjin Han¹, Jihye Hwang², Inhae Kim¹, Sanguk Kim⁰

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PL - OTHER

PL-001 Intrinsically Disordered Proteins Drive Heritable Transformations of Biological Traits Daniel Jarosz¹, James Byers¹, Sohini Chakrabortee², Sandra Jones³, Amelia Chang², David Garcia¹ 1.-Stanford University, 2.-Whitehead Institute for Biomedical Research, 3.-Rockefeller University

PL-002 Prediction of binding affinity in protein complexes: contacts do matters Anna Vangone¹, Alexandre MJJ Bonvin ¹

1.-Computational Structural Biology group, Bijvoet Center for Biomolecular Research

PL-003 Free radical oxidation – a new method for obtaining stable protein coatings on magnetic nanoparticles

<u>Anna Bychkova</u>¹, Alexandra Vladimirova¹, Mariya Nezhivaya¹, Tatiana Danilova¹, Pavel Pronkin¹, Maria Gorobets¹, Alexander Tatikolov¹, Vyacheslav Misin¹, Mark Rosenfeld¹

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PL-004 Evaluation of human salivary α-defensins by LC-ESI-MS

Nadia Ashrafi¹, Cris Lapthorn¹, Fernando Naclerio², Frank Pullen¹, Birthe Nielsen¹, Yue Fu², Jack Miller², Christian Watkinson², Marcos Seijo²

1.-University of Greenwich (Faculty of Engineering and Science), 2.-University of Greenwich (Centre for Sport Science and Human Performance)

PL-005 Binding of thymidine nucleotides to a viral thymidine monophosphate kinase

<u>Aldo A. Arvizu-Flores</u>¹, Eduardo Guevara-Hernandez², Enrique F. Velazquez-Contreras¹, Francisco J. Castillo-Yañez¹, Luis G. Brieba³, Rogerio R. Sotelo-Mundo²

1.-Universidad de Sonora, Departamento de Ciencias Químico Biológicas, 2.-Centro de Investigación en Alimentación y Desarrollo, A.C., 3.-Laboratorio Nacional de Genómica para la Riodiversidad

PL-006 A cold-adapted trypsin in sardine fish (Sardinops sagax caerulea): molecular modeling and recombinant expression

<u>Aldo A. Arvizu-Flores</u>¹, Manuel I. Carretas-Valdez², Francisco J. Castillo-Yañez¹, Karina D. Garcia-Orozco³, Carmen A. Contreras-Vergara³, Rogerio R. Sotelo-Mundo³, Maria A. Islas-Osuna¹.³

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PL-007 Fungicidal mechanism of scolopendin 2, a cationic antimicrobial peptide from centipede

Heejeong Lee¹, <u>Dong Gun Lee¹</u>

1.-Kyungpook National University

PL-008 Structural and functional investigation of the far C-terminal domain (CTD) of the bifunctional enzyme Tral using NMR Spectroscopy

<u>Krishna Chaitanya Bhattiprolu</u>, Evelyne Schrank, Klaus Zangger No hay afiliation

PL-009 Sodium Chloride induced Aggregation of Monoclonal Antibodies at low pH: Prevention by Additives

Fabian Bickel^{1, 2}, Hans Kiefer¹

1.-Institute of Applied Biotechnology, Biberach University of Applied Sciences, 2.-International Graduate School in Molecular Medicine Ulm. Ulm University



PL-010 Antigenic characterization of the HCMV gH/gL/gO and Pentamer cell entry complexes reveals binding sites for potently neutralizing human antibodies

Ciferri Claudio¹

1.- Genentech Inc

PL-011 Conformational Flexibility of CD81 Cellular Receptor Head-subdomain – Implications on Hepatitis C Binding Modes

<u>Eva S. Cunha</u>¹, Pedro Sfriso², Adriana Rojas¹, Adam Hospital², Modesto Orozco², Nicola Abrescia¹ 1.-Structural Biology Unit, CIC bioGUNE, 2.-Institute for Research in Biomedicine (IRB Barcelona)

PL-012 Allophycocyanin of Gracilaria chilensis: From Gene to function

<u>Jorge Dagnino-Leone</u>¹, José Martinez-Oyanedel¹, Marta Bunster-Balocchi¹ 1.-Universidad de Concepción

PL-013 Novel practical strategies to access artificial metalloenzymes

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PL-014 Proteomic examination of the yeast nuclear pore complex dynamics

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PL-015 Active Site Clustering Identifies Functional Families of the Peroxiredoxin Superfamily Angela Harper¹, Janelle Leuthaeuser², Patricia Babbitt², Jacquelyn Fetrow³

1.-Department of Physics, Wake Forest University, 2.-Department of Molecular Genetics and Genomics, Wake Forest University, 3.-Departments of Physics and Computer Science, Wake Forest University

PL-016 Synthesis and conformational studies of glycoprotein N homolog of bovine herpesvirus 1 (BHV-1) by using CD. NMR and molecular modelling

Natalia Karska¹, Andrea D. Lipińska², Małgorzata Graul², Franciszek Kasprzykowski¹, Emilia Sikorska¹, Igor Zhukov³, Magdalena J. Ślusarz¹, <u>Sylwia Rodziewicz-Motowidło¹</u>

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PL-017 Functional and mechanistic studies of dysferlin, an essential protein in cell membrane repair

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PL-018 Exploring the therapeutic potential of a peptide derived from a poxviral immune evasion protein: NMR determination of the solution structure of VIPER and its inactive mutant

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PL-019 Active site profile-based protein clustering is an efficient, accurate method to define protein functional groups

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PL-020 Insertion of the hydrophobic C-terminal domain of apoptotic BH3-only proteins into biological membranes

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PL-021 A computational investigation of tight junctions

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PL-022 Determination of Optimal Conditions for an Isothermal Titration Calorimetry Essay to Obtain Kinetic Parameters of Trypsin I from Pyloric Caeca of Monterey Sardine (Sardinops sagax caerulea)

<u>Idania Emedith Quintero Reyes</u>¹, Francisco Javier Castillo Yáñez¹, Enrique fernando Velázquez Contreras¹, Rocío Sugich Miranda¹, David Octavio Corona Martínez¹, Aldo Alejandro Arvizu Flores¹, Ivet Cervantes Domínguez¹

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PL-023 Mysterious world of stress-responding sigma factors in Bacillus subtilis Olga Ramaniuk¹

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PL-024 Assessing the costs and benefits of protein aggregation

Natalia Sanchez de Groot¹, Marc Torrent Burgas², Charles N. J. Ravarani¹, Salvador Ventura³, M. Madan Babu¹

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PL-025 Revealing the key role of negatively charged residues of heme sensor proteins involved in Geobacter sulfurreducens' signal transduction pathways

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PL-026 Appearance of stabilizing interactions in the evolution of a dimeric TIM barrel

<u>Mariana Schulte-Sasse</u>¹, Nancy O. Pulido Mayoral¹, Miguel Costas-Basín², Enrique García-Hernández³, Adela Rodríguez-Romero³, D. Alejandro Fernández-Velasco¹

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PL-027 Receptor Protein-Tyrosine Phosphatases: Dimerization, receptor kinase interaction and allosteric modulation

Elizabeth Dembicer¹, Damien Thevenin¹

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PL-028 Inhibiting EGFR dimerization and signaling through targeted delivery of juxtamembrane domain peptide mimics using pHLIP

Anastasia Thevenin¹, Kelly Burns¹, Janessa Guerre-Chaley¹, Damien Thevenin¹

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PL-029 The thumb subdomain of yeast mitochondrial RNA polymerase is involved in processivity, transcript fidelity and mitochondrial transcription factor binding.

Gilberto Velazguez, Luis Brieba, Rui Sousa

1.-Universidad de Guadalajara, 2.-Langebio cinvestav, 3.-University of Texas Health Science Center at San Antonio

PL-030 Design principles of membrane protein structures

Vladimir Yarov-Yarovoy1, Diane Nguyen1

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PL-031 Coordinated gripping of substrate by subunits of a AAA+ proteolytic machine

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Structure and function of the Toc159 M-domain, and its role in targeting the preprotein receptor to the chloroplast outer envelope membrane

Matthew Smith1, Shiu-Cheung Lung2, Prem Nichani1, Nicholas Grimberg1, J. Kyle Weston1, Shane Szalai¹, Simon Chuong²

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PL-033 Structural investigation of NIpC/P60 protein acquired by Trichomonas vaginalis through a lateral gene transfer event

Jully Pinheiro^{1,2}, Augusto Simoes-Barbosa¹, David Goldstone²

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PL-034 Novel DNA polymerases from Red Sea brine-pools: New potential polymerases for PCR application

Masateru Takahashi¹, Etsuko Kimura¹, Mohamed Salem¹, Ulrich Stingl¹, Samir Hamdan¹ 1.-King Abdullah University of Science and Technology

PL-035 Structural Basis for the Identification of the N-Terminal Domain of Coronavirus **Nucleocapsid Protein as an Antiviral Target**

Ming-Hon Hou¹, Shing-Yen Lin¹, Chia-Ling Liu¹, Yu-Ming Chang², Jincun Zhao³, Stanley Perlman³ 1.-Institute of Genomics and Bioinformatics, National Chung Hsing University., 2.-Institute of Biological Chemistry, Academia Sinica., 3.-Department of Microbiology, The University of Iowa

PL-036 Thermal and structural stability of ß-Glucosidades GH1

Maira Artischeff Frutuoso¹

Life Sciences, Imperial College

1.-Departamento de Bioquímica do Instituto de Química da Universidade de São Paulo

PL-037 Computational modeling of INI1/SMARCB1 and novel insights into its interaction with HIV-1 Integrase

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PL-038 Structural determinants for human RNase 6 antimicrobial mechanism of action Javier Arranz Trullén¹, Guillem Prats-Ejarque¹, Jose Antonio Blanco¹, Marcel Albacar¹, Diego

Velazquez¹, David Púlido², Mohammed Moussaoui¹, Ester Boix¹ 1.-Department of Biochemistry and Molecular Biology, Biosciences Faculty, UAB, 2.-Department of

PL-039 Covalent Structure of Single-Stranded Fibrinogen and Fibrin Oligomers Cross-Linked by FXIIIa. The influence of free radical oxidation

<u>Anna Bychkova</u>¹, Vera Leonova¹, Alexander Shchegolikhin¹, Marina Biryukova¹, Elizaveta Kostanova¹, Mark Rosenfeld¹

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PL-040 Structural and thermodynamic analysis of co-stimulation receptor CD28 phosphopeptide interactions with Grb2, Gads, and Pl3-kinese SH2 domains

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1.-Graduate School of Life and Environmental Sciences, Kyoto Prefectural University, 2.-Medical Research Institute, Tokyo Medical and Dental University (TMDU), 3.-National Institute of Advanced Industrial Science and Technology, 4.-Research Institute for Biomedical Sciences, Tokyo University of Science

PL-041 Novel kinetochore protein complex from silkworm holocentric chromosomes

Takahiro Kusakabe¹, Hiroaki Mon¹, JaeMan Lee¹

1.-Kyushu University Graduate School

PL-042 Inactivation of betaine aldehyde dehydrogenase from spinach by its physiological substrate betaine aldehyde

Rosario A. Muñoz-Clares¹, Andrés Zárate-Romero¹, Dario S. Murillo-Melo¹, Carlos Mújica-Jiménez¹, Carmina Montiel¹

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PL-043 AFFINImeter: a new software for a more complete characterization of protein-ligand binding processes by Isothermal Titration Calorimetry experiments

Ángel Piñeiro^{1,2}, Eva Muñoz², Juan Sabín², Javier Rial², Philippe Dumas³, Eric Ennifar³

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PL-044 Study of denaturation of proteins by surfactant using the taylor dispersion analysis and dynamic light scattering

Anna Lewandrowska¹, Aldona Jelińska¹, Agnieszka Wiśniewska¹, Robert Hołyst¹ 1.-Institute of Physical Chemistry Polish Academy of Sciences

PL-045 Protein-ligand interactions

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PL-046 Paraoxonase 1 (Pon1) regulates water homeostasis by controlling the expression of Fxr and Aqp2 proteins in mice

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PL-047 Development and application of novel non-Ewald methods for calculating electrostatic interactions in molecular simulations

Ikuo Fukuda¹, Narutoshi Kamiya¹, Han Wang², Kota Kasahara¹, Haruki Nakamura¹

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PL-048 Isolation and characterisation of the zearalenone degrading hydrolase ZenA

<u>Sebastian Fruhauf</u>¹, Michaela Thamhesl¹, Patricia Fajtl¹, Verena Klingenbrunner¹, Elisavet Kunz-Vekiru², Gerhard Adam³, Gerd Schatzmayr¹, Wulf-Dieter Moll¹

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3.-IAGZ, University of Natural Resources and Life Sciences

PL-049 A new biding site for snake venom C-type lectins?

Maria Cristina Nonato Costa¹, Ricardo Augusto Pereira de Pádua¹, Marco Aurelio Sartim¹, Suely Vilela Sampaio¹

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PL-050 Ab initio modelling of structurally uncharacterised antimicrobial peptides Mara Kozic¹

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PL-051 Surface Aggregation-Propensity as a Constraint on Globular Proteins Evolution

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PL-052 Utilizing 3D structure for the annotation of structural motifs in the Conserved Domain Database

<u>Narmada Thanki-Cunningham</u>¹, Noreen Gonzales¹, Gabriele Marchler¹, Myra Derbyshire¹, James Song¹, Roxanne Yamashita¹, Christina Zheng¹, Stephen Bryant¹, Aron Marchler-Bauer¹ 1.-Conserved Domain Database. Structure Group CBB/NCBI/NLM/NIH

PL-053 Biophysical characterization of the Sema3A C-terminal basic domain interaction with glycosaminoglycans

Roman Bonet¹, Miriam Corredor¹, Cecilia Domingo¹, Jordi Bujons¹, Yolanda Perez¹, Ignacio Alfonso¹, Angel Messeguer¹

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PL-054 Functional Clustering of the Crotonase Superfamily

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$PL-055 \ \ \textbf{Peptidic Probes for Intravascular Molecular Imaging of Inflammation Using Clinically Translatable Polymeric Microbubbles$

<u>Olga Iranzo</u>^{1,2}, Ana C. Fernandes¹, Teresa Sorbo², Ivan Duka², Lia Christina Appold³, Marianne Ilbert⁴, Fabian Kiessling³, Ricardo J. F. Branco⁵

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PL-056 A search for anti-melioidosis drug candidates targeted to sedoheptulose-7-phosphate isomerase from Burkholderia pseudomallei

Jimin Park¹, Daeun Lee¹, Sang A Yeo¹, Mi-Sun Kim¹, Dong Hae Shin¹

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PL-057 Mapping the Structure of Laminin Using Cross-linking and Mass Spectrometry Gad Armony¹, Toot Moran¹, Yishai Levin², Deborah Fass¹

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PL-058 Non-sequential protein structure alignment program MICAN and its applications Shintaro Minami¹, George Chikenji², Motonori Ota¹

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PL-059 Effects of Cell-Like Infrastructures on Transient Protein Interactions

Ciara Kyne¹, Peter Crowley¹

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PL-060 A search for anti-melioidosis drug candidates targeted to D-glycero-D-manno-heptose-1,7-bisphosphate phosphatase from Burkholderia pseudomallei

Jimin Park¹, Sang A Yeo¹, Daeun Lee¹, Mi-Sun Kim¹, Dong Hae Shin¹

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PL-061 Crystal structure of dimeric D-glycero-D-manno-heptose-1,7-bisphosphate phosphatase from Burkholderia thailandensis

<u>Jimin Park</u>¹, Mi-Sun Kim¹, Daeun Lee¹, Keehyung Joo², Gil-Ja Jhon³, Jooyoung Lee², Dong Hae Shin¹

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PL-063 NMR studies of the insertase BamA in three different membrane mimetics

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PL-064 Biochemical characterization of the substrate specificity of two unique members of the mammalian protein arginine methyltransferase family, PRMT7 and PRMT9

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PL-065 Ornithine decarboxylase participates in autophagy by ultraviolet B-induced cell injury

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PL-066 Fish ß-parvalbumin acquires allergenic properties by amyloid assembly

<u>Javier Martínez</u>¹, Rosa Sánchez¹, Milagros Castellanos², Ana M. Fernández-Escamilla³, Sonia Vázquez-Cortés⁴, Montserrat Fernández-Rivas⁴, María Gasset¹

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PL-067 **Peptidylarginine Deiminase 2 Assigns Activated T Cell Autonomous Death** Guang-Yaw Liu¹, Wen-Hao Lin², Hui-Chih Hung²

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PL-068 Studies on secondary metabolites production and proteins and enzymes of in vitro cultivated Artemisia alba Turra and relations with some endogenous phytohormones

<u>Yuliana Raynova</u>¹, Krassimira Idakieva¹, Vaclav Motyka², Petre Dobrev², Yuliana Markovska³, Milka Todorova¹, Antoaneta Trendafilova¹, Ljuba Evstatieva⁴, Evelyn Wolfram⁵, Kaliva Danova¹

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PL-069 Regulation of Neuronal SNAREs by accessory proteins

Shrutee Jakhanwal¹. Reinhard Jahn¹

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PL-070 Characterising interactions between alginates of different sizes and ß-lactoglobulin Emil G. P. Stender¹, Sanaullah Khan², Outi E. Mäkinen³, Kristoffer Almdal², Peter Westh⁴, Richard Ibsen², Maher Abou Hachem¹, Birte Svensson¹

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PL-071 Validation of a LC-MS method for the detection of human salivary α -defensins

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PL-072 Moonlighting proteins: relevance for biotechnology and biomedicine

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PL-073 **WapA and SMU_63c are Amyloidogenic Proteins of Streptococcus mutans** Richard Besingi¹, <u>L. Jeannine Brady</u>¹

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PL-074 Gwidd: genome-wide docking database

Madhurima Das¹, Varsha D. Badal¹, Petras J. Kundrotas¹, Ilya A. Vakser¹

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PL-075 Refolding and activation of recombinant trypsin i from sardine fish (Sardinops sagax caerulea)

<u>Manuel Carretas-Valdez</u>¹, Francisco Cinco-Moroyoqui¹, Marina Ezquerra-Brauer¹, Enrique Marquez-Rios¹, Rogerio Sotelo-Mundo², Idania Quintero-Reyes³, Aldo Arvizu-Flores³

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PL-076 Correlation between potential human neutrophil antimicrobial peptides (HNP 1-3) and stress hormones in human saliva

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PL-077 Characterization of the membrane-localized interaction network between the GTP-ase Rheb and the FKBP12-like protein FKBP38 by NMR

Maristella De Cicco¹, Sonja A. Dames¹

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PL-078 Unraveling the Nature of TDP-43 Aggregates from its Putative Aggregation Domain Miguel Mompeán¹, Rubén Hervás², Yunyao Xu³, Timothy H. Tran⁴, Emanuele Buratti⁵, Francisco Baralle⁵, Liang Tong⁴, Mariano Carrión-Vázquez², Ann E. McDermott³, Douglas V Laurents¹ 1.-Instituto Química Física Rocasolano, 2.-Instituto Cajal, IC-CSIC, 3.-Department of Chemistry, Columbia University, 4.-Department of Biological Sciences, Columbia University, 5.-International Centre for Genetic Engineering and Biotechnology

PL-079 The role of the structural NADP+ binding site in human glucose 6-phosphate dehydrogenase

Mona Alonazi1,2, Paul Engel1

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PL-080 Molecular characterization of specific positively selected sites in mammalian visual pigment evolution

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PL-081 Natural Evolution Sheds Light on Modern Drug Resistance in Protein Kinases

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PL-082 An Evolutionary View of The Cold Adapted Catalysis of Enzymes

Vy Nguyen¹, Christopher Wilson¹, Dorothee Kern¹

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PL-083 Induced oxidative modification of plasma and cellular fibrin-stabilizing factor

Anna Bychkova¹, Tatiana Danilova¹, Alexander Shchegolikhin¹, Vera Leonova¹, Marina Biryukova¹, Elizaveta Kostanova¹, Alexey Kononikhin⁰, Anna Bugrova¹, Evgeny Nikolaev⁰, Mark Rosenfeld¹, 1.-N. M. Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, 2.-Institute for Energy Problems of Chemical Physics, Russian Academy of Sciences

PL-062 **Refined crystal structure of predicted fructose-specific enzyme IIB(fruc) from E. coli** Jimin Park¹, Daeun Lee¹, Mi-Sun Kim¹, Keehyung Joo², Gil-Ja Jhon³, Jooyoung Lee², Dong Hae

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PM - ENGINEERING & INTERPRETING THE GENOME

PM-001 Functional characterization of proteins by domain architecture

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