# THE 29TH ANNUAL SYMPOSIUM OF

# **FINAL PROGRAM**



### **#PS2015**

### PROTEINSOCIETY.ORG/SYMPOSIUM









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JULY 22 - 25, 2015



### WELCOME



Welcome to the 29th Annual Symposium of the Protein Society. You probably didn't know it, but you are part of an experiment. This is the first time we have held our main meeting outside of the U.S. Moreover, it is our first meeting in Europe in four years. So I'll admit it. We were nervous. It is therefore very gratifying to see such a strong turnout: nearly 1000 delegates from more than 50 countries. The experiment is off to an auspicious start indeed.

You were no doubt attracted by the outstanding program put together by the Program Planning Committee, and the excellent workshops organized by the Mentoring and Education Committees. On behalf of the Executive Council, I would like to thank them all for their hard work.

You also know that the Protein Society Symposium is a great place to meet new people with diverse interests, centered around protein science. You can share your work at the Poster Sessions, but you should also make sure to take advantage of the mixers and networking dinners. I know I always emerge from the meeting with new ideas, new friends and often a new collaboration that I didn't expect. After all, the Protein Society Symposium is fertile ground as it brings together some of the best scientists throughout the world.

I hope you will make sure to visit the Vendor booths. It's always fun learn about new toys, especially if they can improve your science.

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

Thank you for participating in the meeting. I'm sure you'll go away inspired and I hope that you will ultimately publish the results of those inspirations in the Society's journal, Protein Science. It's your society and your journal, so only you can continue to make them thrive. Enjoy the Symposium, and enjoy Barcelona!

Best Wishes,

James U Bowie

James U. Bowie, PhD Protein Society President

THE 29<sup>th</sup> ANNUAL SYMPOSIUM of





#### **PROGRAM PLANNING COMMITTEE**

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#### **Miquel Pons**

Professor, Dept of Organic Chemistry University of Barcelona

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#### **Dimitrios Morikis**

University of California Riverside Sourav Roy University of California Riverside Louis Scott University of Western Australia K. Suresh Thallapuranam University of Arkansas Max Vasquez Adimab Sudha Veeraraghavan University of Maryland, Baltimore **Ruiying Wu** Argonne National Laboratory Serena Zanzoni University of Verona Chao Zhang University of Southern California



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# Level 1



Level 2

Level 3



FLOOR MAP

JULY 22 - 25, 2015



**GENERAL INFORMATION** 

### **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.

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### **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 22<sup>nd</sup>

11:30 AM – 1:30 PM 4:30 PM – 6:30 PM **Thursday, July 23**<sup>rd</sup> 11:30 AM – 1:30 PM 4:30 PM – 6:30 PM **Friday, July 24**<sup>th</sup> 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	PI
PROTEOMICS (PPIS, PTMS)	PJ
SYSTEMS BIOLOGY	PK
OTHER	PL
ENGINEERING & INTERPRETING THE GENOME	PM

THE 29<sup>th</sup> ANNUAL SYMPOSIUM of



Authors that have applied for the Best Poster Competition will be presenting posters on the following schedule:

POSTER SESSION 1 Wednesday, July 22, 2015

Exhibit Hall

#### **Author Presentations**

Odd Board Numbers 11:45 AM -12:30 PM Even Board Numbers 12:30 PM - 1:15 PM

THEME	BOARD #S
Cell Engineering	PA-002 – PA-003
Chemical Biology	PB-001 – PB-020
Enzyme & Pathway Engineering	PC-005 – PC-006
Folding	PD-002 – PD-010
Integrative Protein Science	PE-003 – PE-006
Intrinsically Disordered Proteins	PF-001 – PF-003
Observing Dynamics In Single Cells	PG-003
Protein Allostery & Dynamics	PH-001 – PH-005
Protein Engineering	PI-002 – PI-035
Proteomics (PPIs, PTMs)	PJ-001 – PJ-012
Systems Biology	PK-001 – PK-004
Other/No theme allocated	PL-002 – PL-021

#### **PA - CELL ENGINEERING**

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

Charlie Morgan<sup>1,2,3</sup>, Juan Diaz<sup>2,3</sup>, Jim Wells<sup>2,3</sup>

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 Sarria<sup>1</sup>, Souryadeep Bhattacharyya<sup>2</sup>, Pamela Peralta-Yahya<sup>1</sup>

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. Abboud<sup>1</sup>, Jurgen Brem<sup>1</sup>, Rasheduzzaman Chowdhury<sup>1</sup>, Ivanhoe K. H. Leung<sup>2</sup>, Timothy D. W. Claridge<sup>1</sup>, Christopher J. Schofield<sup>1</sup>

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 Acedo<sup>1</sup>, Marco van Belkum<sup>1</sup>, John Vederas<sup>1</sup>

1.-Department of Chemistry, University of Alberta

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

Yuen-Yan Chang<sup>1</sup>, Yau-Tsz Lai<sup>1</sup>, Ligang Hu<sup>1</sup>, Ya Yang<sup>1</sup>, Ailun Chao<sup>1</sup>, Hongzhe Sun<sup>1</sup> 1.-Department of Chemistry, The University of Hong Kong

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

<u>Nikolaos Eleftheriadis</u><sup>1</sup>, Stephanie Thee<sup>1</sup>, Johan te Biesebeek<sup>1</sup>, Petra van der Wouden<sup>1</sup>, Bert-Jan Baas<sup>1</sup>, Frank J. Dekker<sup>1</sup>

1.-Groningen Research Institute of Pharmacy

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

<u>Victoria Gomez</u><sup>1</sup>, Kavya Kolavasi<sup>1</sup>, Josh Beckham<sup>1</sup>, Jon Robertus<sup>1</sup> 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 Goodrich<sup>1</sup>, Dominique Frueh<sup>1</sup>

1.-Johns Hopkins University School of Medicine

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

Franca-M. Klingler<sup>1</sup>, Ewgenij Proschak<sup>1</sup>

1.-Goethe University, Institute of Pharmaceutical Chemistry

#### PB-015 Protein Carbamylation at the Chemistry-Biology interface

<u>Victoria Linthwaite</u><sup>1</sup>, Joana Janus<sup>1</sup>, David R.W. Hodgson<sup>2</sup>, Martin J. Cann<sup>1</sup> 1.-School of Biological and Biomedical Sciences, Durham University, 2.-Department of Chemistry, Durham University

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

<u>Maria-Eleni Ourailidou</u><sup>1</sup>, Paul Dockerty<sup>1</sup>, Martin Witte<sup>1</sup>, Gerrit J. Poelarends<sup>1</sup>, Frank J. Dekker<sup>1</sup>, 1.-University of Groningen

#### PC - ENZYME & PATHWAY ENGINEERING

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

<u>Tadafumi Konogami</u><sup>1</sup>, Yiwen Yang<sup>1</sup>, Mari H. Ogihara<sup>1</sup>, Juri Hikiba<sup>1</sup>, Hiroshi Kataoka<sup>1</sup>, Kazuki Saito<sup>1</sup> 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

<u>Miroslava Kopecka<sup>1, 2</sup>,</u> Zdenek Kukacka<sup>3</sup>, Petr Man<sup>3</sup>, Tomas Obsil<sup>2</sup>, Veronika Obsilova<sup>2</sup> 1.-2nd Faculty of Medicine, Charles University in Prague, 2.-Institute of Physiology of the Czech Academy of Sciences, 3.-Institute of Microbiology of the Czech Academy of Sciences

#### PD - FOLDING

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

Tania Raquel Berrocal Gama<sup>1</sup>, Jesús Renan Vergara Gutiérrez<sup>1</sup>, Andrés Escandón Flores<sup>1</sup>, Alejandro Sosa Peinado<sup>1</sup>

1.-National Autonomus University of Mexico, Faculty of Medicine



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. Garg<sup>1</sup>, Bishwajit Kundu<sup>1</sup> 1.-Indian Institute of Technology Delhi

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

. <u>Megha Goyal</u><sup>1</sup>, Tapan Kumar Chaudhuri<sup>1</sup> 1.-Indian Institute of Technology Delhi

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

<u>Tatsuya Ikenoue</u><sup>1</sup>, Lee Young-Ho<sup>1</sup>, Tetsuhei Uenoyama<sup>1</sup>, Daniel Otzen<sup>2</sup>, Yuji Goto<sup>1</sup> 1.-Institute for Protein Research, Osaka University, 2.-Interdisciplinary Nanoscience Center (iNA-NO), Aarhus University

#### **PE - INTEGRATIVE PROTEIN SCIENCE**

PE-003 **Carbohydrate Binding Modules. Structural and thermodynamic study** <u>Benjamin Garcia</u><sup>1</sup>, Patricia Cano Sánchez<sup>1</sup>, Siseth Martínez-Caballero<sup>1</sup>, Romina Rodríguez-Sanoja<sup>1</sup>, Adela Rodríguez-Romero<sup>1</sup> 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 Gustafson<sup>1</sup>, J. Chris Fromme<sup>1</sup> 1.-Cornell University

PE-006 **Studies of JMJD4-catalyzed oxidative modifications of eukaryotic release factor 1** <u>Suzana Markolovic</u><sup>1</sup>, Ivanhoe K. H. Leung<sup>2</sup>, Mathew L. Coleman<sup>3</sup>, Timothy D. W. Claridge<sup>1</sup>, Sarah E. Wilkins<sup>1</sup>, Christopher J. Schofield<sup>1</sup>

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

#### **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

Arindam Bakshi<sup>1</sup>, Srinivas Sistala<sup>2</sup>, Shruthi Sridhar<sup>1</sup>, Savithri H S<sup>1</sup>

1.-Indian institute of Science, 2.-Wipro G E Healthcare Pvt Ltd

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

<u>Giulio Chiesa</u><sup>1</sup>, Bahareh Eftekharzadeh<sup>1</sup>, Daniele Mungianu<sup>1,2</sup>, Alessandro Piai<sup>2</sup>, Jesus Garcia<sup>1</sup>, Isabella Felli<sup>2</sup>, Roberta Pieratelli<sup>2</sup>, Xavier Salvatella<sup>1,3</sup>

1.-Institute for Research in Biomedicine (IRB), 2.-Magnetic Resonance Center and Department of Chemistry, University of Florence, 3.-ICREA

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

<u>Carole Anne De Carufel</u><sup>1</sup>, Phuong Trang Nguyen<sup>1</sup>, Alexandre Arnold<sup>1</sup>, Isabelle Marcotte<sup>1</sup>, Steve Bourgault<sup>1</sup>

1.-University of Quebec in Montreal, Department of Chemistry

#### **PG - OBSERVING DYNAMICS OIN SINGLE CELLS**

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

Martin Stortz<sup>1</sup>, Luciana Bruno<sup>2</sup>, Paolo Annibale<sup>3</sup>, Enrico Gratton<sup>3</sup>, Adali Pecci<sup>1,4</sup>, Valeria Levi<sup>4,5</sup> 1.-IFIByNE-Conicet, 2.-IFIBA-Conicet & Dept. of Physics, University of Buenos Aires, 3.-LFD-University of California, 4.-Dept. of Biological Chemistry, University of Buenos Aires, 5.-IQUIBICEN-Conicet

#### **PH - PROTEIN ALLOSTERY & DYNAMICS**

PH-001 Investigation of allosteric communication pathways in human ß2-adrenergic receptor Basak Akdas<sup>1</sup>, Ozge Kurkcuoglu<sup>2</sup>, Pemra Doruker<sup>1</sup>, Demet Akten<sup>3</sup>

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

Claudia Alvarez<sup>1,2</sup>, Marijana Stagljar<sup>2</sup>, Voula Kanleis<sup>1,2,3</sup>

1.-Department of Chemistry, University of Toronto, 2.-Department of Chemical and Physical sciences, University of Toronto, 3.-Department of Chemical and Physical sciences, University of Toronto

### PH-003 Glycosylation of EGFR Extracellular Domain Induces Receptor Stability

Maryam Azimzadeh Irani<sup>1,2</sup>, Chandra Verma<sup>1,2</sup>

1.-Bioinformatics Institute (A\*-STAR), Singapore, 2.-School of Biological Sciences, Nanyang Technological University

PH-005 **Conformational Changes of the Ribose ABC Transporter Studied by EPR Spectroscopy** <u>Satchal Erramilli</u><sup>1</sup>, Michael Simon<sup>2</sup>, Matthew Clifton<sup>3</sup>, Cynthia Stauffacher<sup>1</sup> 1.-Purdue University, 2.-Washington University At St. Louis, 3.-Beryllium

#### **PI - PROTEIN ENGINEERING**

PI-002 **Mutations of a conserved tryptophan residue of the TEM-1 ß-lactamase** <u>F Ece Altinisik</u><sup>1</sup>, F Gizem Avci<sup>1</sup>, Berna Sariyar Akbulut<sup>1</sup>, Elif Özkirimli Ölmez<sup>3</sup>, Didem Vardar Ulu<sup>2</sup>, Ipek Karacan<sup>1</sup>, Duygu Sentürk<sup>1</sup>

1.-Marmara University, 2.-Wellesley College, 3.-Bogaziçi University

#### 

1.-Eindhoven University of Technology

### PI-004 Proteins as supramolecular building blocks: engineering nanoscale structures

Helen Ashmead<sup>1,2,3</sup>, Leonardo Negron<sup>1</sup>, Jack Sissons<sup>6</sup>, Kyle Webster<sup>6</sup>, Vic Arcus<sup>2,4</sup>, Juliet Gerrard<sup>1,2,5</sup> 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

Danielle Basore<sup>1,2</sup>, Rajesh Naz<sup>5</sup>, Scott Michael<sup>6</sup>, Sharon Isern<sup>6</sup>, Benjamin Wright<sup>3</sup>, Katie Saporita<sup>1</sup>, Donna Crone<sup>1</sup>, Christopher Bystroff<sup>1,2,4</sup>

1.-Biological Sciences, Rensselaer Polytechnic Institute, 2.-CBIS, Rensselaer Polytechnic Institute, 3.-Chemical and Biological Engineering, Rensselaer Polytechnic Institute, 4.-Computer Science, Rensselaer Polytechnic Institute, 5.-Obstetrics and Gynecology, West Virginia University, 6.-Biological Science, Florida Gulf Coast University



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

Esra Bozkurt<sup>1</sup>, Ruud Hovius<sup>1</sup>, Thereza A. Soares<sup>2</sup>, Ursula Rothlisberger<sup>1</sup>

1.-École Polytechnique Fédérale de Lausanne, 2.-Federal University of Pernambuco

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

Diego Caballero<sup>1,2</sup>, Corey O'Hern<sup>1,2,3,4</sup>, Lynne Regan<sup>2,5,6</sup>

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

Luis Francisco Calleja Castañeda<sup>1</sup>, José Salud Rodríguez Zavala<sup>1</sup> 1.-Instituto Nacional de Cardiología 'Ignacio Chávez'

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

H. Kay Chung<sup>1</sup>, Conor Jacobs<sup>1</sup>, Yunwen Huo<sup>2</sup>, Jin Yang<sup>3</sup>, Stefanie Krumm<sup>4</sup>, Richard Plemper<sup>4,5</sup>, Roger Tsien<sup>3,6,7</sup>, Michael Lin<sup>2,8</sup>

1.-Department of Biology, Stanford University, 2.-Department of Pediatrics, Stanford University, 3.-Department of Pharmacology, University of California San Diego, 4.-Department of Pediatrics, Emory University, 5.-Institute for Biomedical Sciences, Georgia State University, 6.-Department of Chemistry and Biochemistry, University of California San Diego, 7.-Howard Hughes Medical Institute, University of California San Diego, 8.-Department of Bioengineering, Stanford University

# $\mathsf{PI-020}$ Targeted protein degradation achieved through a combination of degrons from yeast and mammalian ornithine decarboxylase

Rushikesh Joshi<sup>1</sup>, Ratna Prabha C.<sup>1</sup>

1.-The Maharaja Sayajirao University of Baroda

#### PI-027 CXCL10 engineering: novel insights into glycan interactions

<u>Michael Nagele</u><sup>1</sup>, Martha Gschwandtner<sup>1</sup>, Patrick Sorger<sup>1</sup>, Andreas J. Kungl<sup>1</sup> 1.-Institute of Pharmaceutical Sciences, University of Graz, Universitaetsplatz 1

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

Benjamin Porebski<sup>1</sup>, Shani Keleher<sup>1</sup>, Adrian Nickson<sup>2</sup>, Emilia Marijanovic<sup>1</sup>, Mary Pearce<sup>1</sup>, Natalie Borg<sup>1</sup>, James Whisstock<sup>1</sup>, Stephen Bottomley<sup>1</sup>, Sheena McGowan<sup>1</sup>, Ashley Buckle<sup>1</sup> 1.-Department of Biochemistry and Molecular Biology, Monash University, 2.-Department of Chemistry, University of Cambridge

\_\_\_\_\_

PI-035 **Engineering APOBEC3G enzymes for altered specificity and processivity** <u>Louis Scott</u><sup>1</sup>, Muhammad Razif<sup>1</sup>, Aleksandra Filipovska<sup>1,2</sup>, Oliver Rackham<sup>1,2</sup> 1.-Harry Perkins institute of Medical Research, 2.-School of Chemistry and Biochemistry, The University of Western Australia

#### 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

<u>Devika Channaveerappa</u><sup>1</sup>, Roshanak Aslebagh<sup>1</sup>, Kathleen F. Arcaro<sup>2</sup>, Costel C. Darie<sup>1</sup> 1.-Clarkson University, 2.-University of Massachusetts

#### PJ-009 Proteomics and enology: wine yeasts study applications

Jaime Moreno García<sup>1</sup>, Juan Carlos Mauricio<sup>1</sup>, Juan Moreno<sup>2</sup>, Anna Lisa Coi<sup>3</sup>, Marilena Budroni<sup>3</sup>, Teresa García Martínez<sup>1</sup>

1.-Department of Microbiology, ceiA3, 2.-Department of Agricultural Chemistry, ceiA3, 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><sup>1</sup>, Antonio Díaz-Quintana<sup>1</sup>, Katiuska González-Arzola<sup>1</sup>, Alejandra Guerra-Castellano<sup>1</sup>, Adrián Velázquez-Campoy<sup>0</sup>, Miguel A. De la Rosa<sup>1</sup>, Irene Díaz-Moreno<sup>1</sup>

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

Gonca Ozdemir Isik<sup>1</sup>, A.Nevra Ozer<sup>1</sup>

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

#### **PK - SYSTEMS BIOLOGY**

PK-001 Effect of Three Aporphine Alkaloids on Bacillus subtilis 168 <u>Fatma Gizem Avci</u><sup>1</sup>, Berna Sariyar Akbulut<sup>1</sup> 1.-Marmara University, Department of Bioengineering

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

Sasha Weiditch<sup>1</sup>, Karen Maxwell<sup>2,4</sup>, Voula Kanelis<sup>1,3</sup>

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

#### PL - OTHER / NO THEME ALLOCATED

#### PL-002 **Prediction of binding affinity in protein complexes: contacts do matters** <u>Anna Vangone</u><sup>1</sup>, Alexandre MJJ Bonvin <sup>1</sup>

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

Anna Bychkova<sup>1</sup>, Alexandra Vladimirova<sup>1</sup>, Mariya Nezhivaya<sup>1</sup>, Tatiana Danilova<sup>1</sup>, Pavel Pronkin<sup>1</sup>, Maria Gorobets<sup>1</sup>, Alexander Tatikolov<sup>1</sup>, Vyacheslav Misin<sup>1</sup>, Mark Rosenfeld<sup>1</sup> 1.-N. M. Emanuel Institute of Biochemical Physics, Russian Academy of Science

#### PL-004 Regulation of Neuronal SNAREs by accessory proteins

<u>Shrutee Jakhanwal</u><sup>1</sup>, Reinhard Jahn<sup>1</sup> 1.-Department of Neurobiology, Max Planck Institute of Biophysical Chemistry

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

Fabian Bickel<sup>1, 2</sup>, Hans Kiefer<sup>1</sup>

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



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

Jorge Dagnino-Leone<sup>1</sup>, José Martinez-Oyanedel<sup>1</sup>, Marta Bunster-Balocchi<sup>1</sup> 1.-Universidad de Concepción

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

Zhanna Hakhverdyan<sup>1</sup>, Kelly Molloy<sup>2</sup>, Brian Chait<sup>2</sup>, Michael Rout<sup>1</sup> 1.-Laboratory of Cellular and Structural Biology, 2.-Laboratory of Mass Spectrometry and Gaseous Ion Chemistry

#### 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 Jivoon Kim<sup>1</sup>, Dylan Lawless<sup>1</sup>, Manuel Ruether<sup>2</sup>, Andrew Bowie<sup>1</sup>, Kenneth H. Mok<sup>1,3</sup>

1.-Trinity College Dublin, Trinity Biomedical Sciences Institute (TBSI), 2.-Trinity College Dublin, School of Chemistry, 3.-Trinity College Dublin, Centre for Research on Adaptive Nanostructure/ devices

### PL-019 Active site profile-based protein clustering is an efficient, accurate method to define protein functional groups

<u>Janelle Leuthaeuser</u><sup>1</sup>, Angela Harper<sup>2</sup>, Gabrielle Shea<sup>2</sup>, Patricia Babbitt<sup>3</sup>, Jacquelyn Fetrow<sup>1.2</sup> 1.-Wake Forest University, 2.-Wake Forest University, 3.-University of California San Francisco

#### PL-021 A computational investigation of tight junctions

<u>Alexis Peña</u><sup>1</sup>, Flaviyan Jerome Irudayanathan<sup>1</sup>, Shikha Nangia<sup>1</sup> 1.-Syracuse University, Dept. of Biomedical and Chemical Engineering

#### POSTER SESSION 2 Wednesday, July 22, 2015

### Exhibit Hall

#### **Author Presentations**

Odd Board Numbers 4:45 PM – 5:30 PM Even Board Numbers 5:30 PM - 6:15 PM

THEME	BOARD #S
Chemical Biology	PB-022 – PB-046
Enzyme & Pathway Engineering	PC-013 – PC-014
Folding	PD-012 – PD-020
Integrative Protein Science	PE-007 – PE-009
Protein Allostery & Dynamics	PH-008 – PH-030
Protein Engineering	PI-039 – PI-062
Proteomics (PPIs, PTMs)	PJ-013 – PJ-029
Systems Biology	PK-006 – PK-008
Other/No theme allocated	PL-023 – PL-066

#### **PB - CHEMICAL BIOLOGY**

#### PB-022 Proton solvation in protic and aprotic solvents

Emanuele Rossini<sup>1</sup>, Ernst-Walter Knapp<sup>1</sup> 1.-Institute of Chemistry and Biochemistry, Freie Universität Berlin

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

<u>Fadwa El Tahry</u><sup>1</sup>, Ingy Hashad<sup>1</sup>, Mohamed Farouk<sup>1</sup>, Mohamed Gad<sup>1</sup> 1.-German University in Cairo (GUC)

# $\mathsf{PB}\text{-}028$ Agrobacterium tumefaciens employs two distinct ClpS adaptors to modulate the N-end rule degradation pathway

Benjamin J. Stein<sup>1</sup>, Robert A. Grant<sup>1</sup>, Robert T. Sauer<sup>1</sup>, Tania A. Baker<sup>1,2</sup> 1.-Department of Biology, Massachusetts Institute of Technology, 2.-Howard Hughes Medical Institute, Massachusetts Institute of Technology

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

Jackie Thompson<sup>1</sup>, Owen Nadeau<sup>1</sup>, Gerald Carlson<sup>1</sup> 1.-Department of Biochemistry and Molecular Biology, University of Kansas Medical Center

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

<u>Christine Touma</u><sup>1</sup>, Nicolas Paquet<sup>2</sup>, Derek J. Richard<sup>2</sup>, Roland Gamsjaeger<sup>1,3</sup>, Liza Cubeddu<sup>1,3</sup> 1.-School of Science and Health, University of Western Sydney, 2.-Queensland University of Te chnology, 3.-School of Molecular Bioscience, University of Sydney

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

Luis Valencia<sup>1,2</sup>, Josh Beckham<sup>2</sup>, Oscar Villarreal, Jon Robertus<sup>2</sup> 1.-University of Texas at Austin, 2.-Freshman Research Initiative





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

Sandra Kerstin Wittmann<sup>1</sup>, Daniel Moser<sup>1</sup>, Jan Sebastian Kramer<sup>1</sup>, René Blöcher<sup>1</sup>, Janosch Achenbach<sup>3</sup>, Denys Pogoryelov<sup>2</sup>, Eugen Proschak<sup>1</sup>

1.-Institute of Pharmaceutical Chemistry, LiFF/OSF/ZAFES, Goethe-University, 2.-Institute of Biochemistry, Goethe University, 3.-BASF SE

### PB-041 Chemical-Genetic Dissection of Protein Kinase Functions

Chao Zhang<sup>1</sup>, Ying-Chu Chen<sup>1</sup>, Alvin Kung<sup>1</sup>

1.-Department of Chemistry, University of Southern California

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

<u>Francisco Tenjo Castaño</u><sup>1,2</sup>, Manuel Garavito<sup>1,2</sup>, Leonor García<sup>1,2</sup>, Silvia Restrepo<sup>2</sup>, Barbara Zimmermann<sup>1</sup>

1.-Biochemistry and Molecular Biology Research Group, Universidad de los Andes., 2.-Mycology and Plan Pathology Laboratory, Universidad de los Andes

### PC - ENZYME & PATHWAY ENGINEERING

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

Serap Pektas<sup>1, 2</sup>, Michael Knapp<sup>1</sup>

1.-University of Massachusetts Amherst, 2.-Recep Tayyip Erdogan University

### PC-014 New pharmacological therapies against congenital erythropoietic porphyria (CEP)

Pedro David Urquiza<sup>1</sup>, Ana Laín<sup>1</sup>, Arantza Sanz<sup>1</sup>, Juan Manuel Falcón<sup>1, 2</sup>, Oscar Millet<sup>1</sup> 1.-CIC bioGUNE, 2.-Ikerbasque

### PD - FOLDING

PD-012 Interaction of curcumin analogs with α-Synuclein: Modulation of Aggregation and Toxicity Narendra Jha<sup>1</sup>, A. Anoop<sup>1</sup>, Narasimham Ayyagari<sup>1</sup>, Pradeep Singh<sup>1</sup>, I.N.N. Namboothiri<sup>1</sup>, Samir Maji<sup>1</sup> 1.-Indian Institute of Technology Bombay

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

Sergio Romero Romero<sup>1</sup>, Miguel Costas<sup>2</sup>, Adela Rodríguez-Romero<sup>3</sup>, D. Alejandro Fernández-Velasco<sup>1</sup> 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-018 The structure and function of the Surrogate Light Chain

Natalia Catalina Sarmiento Alam<sup>1</sup>, Johannes Buchner<sup>1</sup>

1.-Department Chemie, Technishe Universität München

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

<u>Austin E. Smith</u><sup>1</sup>, Larry Z. Zhou<sup>1</sup>, Annelise H. Gorensek<sup>1</sup>, Michael Senske<sup>2</sup>, Gary J. Pielak<sup>1,3,4</sup> 1.-Department of Chemistry, 2.-Department of Physical Chemistry II, 3.-Department of Biochemistry and Biophysics, 4.-Lineberger Comprehensive Cancer Center

JULY 22 - 25, 2015

#### **PE - INTEGRATIVE PROTEIN SCIENCE**

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

<u>Piyanat Meekrathok</u><sup>1</sup>, Arthur T. Porfetye<sup>2</sup>, Marco Bürger<sup>2</sup>, Ingrid R. Vetter<sup>2</sup>, Wipa Suginta<sup>1</sup> 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><sup>1</sup>, Stacy Harvey<sup>1</sup>, Patrick Sammons<sup>1</sup>, Amanda Anderson<sup>2</sup>, Hema Kopalle<sup>1</sup>, Alison Banham<sup>2</sup>, Carrie Partch<sup>1</sup>

1.-University of California - Santa Cruz, 2.-University of Oxford

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

Kazem Nouri1, Mohammad Reza Ahmadian1

1.-Medical faculty of the Heinrich-Heine University

#### **PH - PROTEIN ALLOSTERY & DYNAMICS**

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

Sophie M.C. Gobeil<sup>1,2</sup>, Maximillian C.C.J.C. Ebert<sup>1,2</sup>, Jaeok Park<sup>1,4,5</sup>, Donald Gagné<sup>1,5,6</sup>, Christopher M. Clouthier<sup>1,3</sup>, Jürgen Pleiss<sup>7</sup>, Nicolas Doucet<sup>1,5,6</sup>, Albert M. Berghuis<sup>1,4,5</sup>, Joelle N. Pelletier<sup>1,2,3</sup> 1.-PROTEO, 2.-Department of Biochemistry, U. of Montreal, 3.-Department of Chemistry, U. of Montreal, 4.-Department of Biochemistry and Department of Microbiology and Immunology, McGill, 5.-GRASP, 6.-INRS–Institut Armand-Frappier, U. du Quebec, 7.-Institute of Technical Biochemistry, University Stuttgart

PH-010 Solvent models for protein simulations – the good, the bad and the applications <u>Duy Hua</u><sup>1</sup>, Amitava Roy<sup>1</sup>, He Huang<sup>1</sup>, Carol Post<sup>1</sup> 1.-Purdue University

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

<u>Alyssa Lokits</u><sup>1</sup>, Julia Koehler Leman<sup>2</sup>, Kristina Kitko<sup>1,3</sup>, Natha Alexander<sup>4</sup>, Heidi Hamm<sup>1,5</sup>, Jens Meiler<sup>1,5,6</sup> 1.-Neuroscience, Vanderbilt University Medical Center, 2.-Chemical and Biomolecular Engineering, Johns Hopkins University, 3.-Engineering, Vanderbilt University Medical Center, 4.-Pharmacology, Case Western Reserve University, 5.-Pharmacology, Vanderbilt University Medical Center, 6.-Chemistry, Vanderbilt University Medical Center

#### PH-023 How amide hydrogens exchange in native proteins

Filip Persson<sup>1</sup>, Bertil Halle<sup>1</sup>

1.-Biophysical Chemsitry, Lund University

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

Rafal Jakubowski<sup>1</sup>, Jakub Rydzewski<sup>1</sup>, Wieslaw Nowak<sup>1</sup>

1.-Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University

#### **PI - PROTEIN ENGINEERING**

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

Xin Zhou<sup>1</sup>, Linlin Fan<sup>2</sup>, Michael Lin<sup>1,3,4</sup>

1.-Department of Bioengineering, Stanford University, 2.-Department of Chemical Biology, Harvard University, 3.-Department of Pediatrics, Stanford University, 4.-Department of Chemical and System Biology, Stanford University



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

Saacnicteh Toledo Patiño<sup>1</sup>, Birte Höcker<sup>1</sup> 1.-Max Planck Institute for Developmental Biology

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

Lena Schmohl<sup>1</sup>, Felix Roman Wagner<sup>1</sup>, Michael Schümann<sup>2</sup>, Eberhard Krause<sup>2</sup>, Dirk Schwarzer<sup>1</sup> 1.-Interfaculty Institute of Biochemistry, University of Tuebingen, 2.-Laboratory of Mass Spectrometry, Leibniz-Institut Für Molekulare Pharmakologie

#### PI-042 **Directed Evolution on FucO – Structural Explanations for Changes in Substrate Scope** Käthe M. Dahlström<sup>1</sup>, Cecilia Blikstad<sup>2</sup>, Mikael Widersten<sup>2</sup>, Tiina A. Salminen<sup>1</sup>

1.-Structural Bioinformatics Laboratory, Biochemistry, Åbo Akademi University, 2.-Department of Chemistry, Uppsala University

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

<u>Masatoshi Nakatsuji</u><sup>1</sup>, Haruka Inoue<sup>1</sup>, Masaki Kohno<sup>1</sup>, Mayu Saito<sup>1</sup>, Syogo Tsuge<sup>1</sup>, Shota Shimizu<sup>1</sup>, Osamu Ishibashi<sup>1</sup>, Takashi Inui<sup>1</sup>

1.-Graduate School of Life and Environmental Sciences, Osaka Prefecture University

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

Anna Simon<sup>1</sup>, Alexis Vallée-Bélisle<sup>2</sup>, Francesco Ricci<sup>3</sup>, Kevin Plaxco<sup>1,4,5</sup>

1.-Biomolecular Science and Engineering Program, UC Santa Barbara, 2.-Département de Chimie, Université de Montréal, 3.-Dipartimento di Scienze e Tecnologie Chimiche, University of Rome, Tor Vergata, 4.-Department of Biochemistry and Chemistry, 5.-Center for Bioengineering

#### PI-048 **De novo design of protein-protein interaction using hydrophobic and electrostatic interactions** <u>Sota Yagi</u><sup>1</sup>, Satoshi Akanuma<sup>2</sup>, Akihiko Yamagishi<sup>1</sup>

1.-Tokyo University of Pharmacy and Life Sciences, Department of Applied Life Scien, 2.-Waseda University, Faculty of Human Sciences

PI-050 **Designing of a novel platinum-binding amino acid sequence on a protein surface** <u>Asumi Kaji</u><sup>1</sup>, Hiroya Niiro<sup>1</sup>, Satoshi Akanuma<sup>2</sup>, Tetsuya Uchida<sup>1</sup>, Akihiko Yamagishi<sup>1</sup> 1.-Tokyo University of Pharmacy and Life Sciences, 2.-Waseda University

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

Emma Liliana Arevalo Salina<sup>1</sup>, Joel Osuna Quintero<sup>1</sup>, Humberto Flores Soto<sup>1</sup>, Gloria Saab Rincón<sup>1</sup> 1.-Instituto de Biotecnología, Universidad Nacional Autónoma de México

# $\mathsf{PI-062}$ A novel secondary structure element assembly protocol for the design of artificial (\$\$\mathcal{\beta}\$\$). A novel secondary structure element assembly protocol for the design of artificial (\$\$\mathcal{\beta}\$\$). A novel secondary structure element assembly protocol for the design of artificial (\$\$\mathcal{\beta}\$\$). A novel secondary structure element assembly protocol for the design of artificial (\$\$\mathcal{\beta}\$\$). A novel secondary structure element assembly protocol for the design of artificial (\$\$\mathcal{\beta}\$\$). A novel secondary structure element assembly protocol for the design of artificial (\$\$\mathcal{\beta}\$\$). A novel secondary structure element assembly protocol for the design of artificial (\$\$\mathcal{\beta}\$\$). A novel secondary structure element assembly protocol for the design of artificial (\$\$\mathcal{\beta}\$\$). A novel secondary structure element assembly protocol for the design of artificial (\$\$\mathcal{\beta}\$\$). A novel secondary structure element assembly protocol for the design of artificial (\$\$\mathcal{\beta}\$\$). A novel secondary structure element assembly protocol for the design of artificial (\$\$\mathcal{\beta}\$\$). A novel secondary structure element assembly protocol for the design of artificial (\$\$\$\mathcal{\beta}\$\$). A novel secondary structure element assembly protocol for the design of artificial (\$\$\$\mathcal{\beta}\$\$). A novel secondary structure element assembly protocol for the design of artificial (\$\$\$\$). A novel secondary structure element assembly protocol for the design of artificial (\$\$\$\$\$ as a novel secondary structure element assembly protocol for the design of artificial (\$\$\$\$\$ as a novel secondary structure element assembly protocol for the design of artificial (\$\$\$\$\$ as a novel secondary structure element as a novel se

<u>Cristina Elisa Martina</u><sup>1</sup>, Steven Combs<sup>2</sup>, Rocco Moretti<sup>2</sup>, Maximiliano Figueroa<sup>1</sup>, Cecile Van De Weerdt<sup>1</sup>, Andre Matagne<sup>1</sup>, Jens Meiler<sup>2</sup>

1.-University of Liege, 2.-Vanderbilt University

#### **PJ - PROTEOMICS (PPIs, PTMS)**

#### PJ-013 **Protein plasticity improves protein-protein binding description** <u>Chiara Pallara</u><sup>1</sup>, Juan Fernández-Recio<sup>1</sup>

1.-Joint BSC-CRG-IRB Research Program In Computational Biology

JULY 22 - 25, 2015

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

Haoling Qi<sup>1</sup>, François-Xavier Cantrelle<sup>2</sup>, Amina Kamah<sup>1</sup>, Clément Despres<sup>1</sup>, Sudhakaran Prabakaran<sup>2</sup>, Jeremy Gunawardena<sup>2</sup>, Guy Lippens<sup>1</sup>, Isabelle Landrieu<sup>1</sup>

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

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

Kelly Wormwood<sup>1</sup>, Armand Ngounou Wetie<sup>1</sup>, Laci Charette<sup>2</sup>, Jeanne Ryan<sup>2</sup>, Emmalyn Dupree<sup>1</sup>, Alisa Woods<sup>1,2</sup>, Costel Darie<sup>1</sup>

1.-Clarkson University, 2.-SUNY Plattsburgh

# 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><sup>1</sup>, Michal Jamroz<sup>1</sup>, Maciej Blaszczyk<sup>1</sup>, Andrzej Kolinski<sup>1</sup>, Sebastian Kmiecik<sup>1</sup> 1.-Department of Chemistry, University of Warsaw

#### PJ-024 **Developing a Technique to Detect Deamidated Proteins and Peptides Using Rig-I** <u>Sandy On<sup>1</sup></u>, Pinghui Feng<sup>2</sup>

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

#### **PK - SYSTEMS BIOLOGY**

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

<u>Roall Espersen</u><sup>1</sup>, Milena Gonzalo<sup>3</sup>, Samuel Jacquiod<sup>3</sup>, Waleed Abu-Alsud<sup>3</sup>, Søren J. Sørensen<sup>3</sup>, Jakob R. Winther<sup>4</sup>, Per Hägglund<sup>2</sup>, Birte Svensson<sup>1</sup>

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

Sangjin Han<sup>1</sup>, Jihye Hwang<sup>2</sup>, Inhae Kim<sup>1</sup>, Sanguk Kim<sup>1,2</sup>

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

#### PL - OTHER / NO THEME ALLOCATED

#### PL-023 Mysterious world of stress-responding sigma factors in Bacillus subtilis <u>Olga Ramaniuk</u><sup>1</sup>

1.-Institute of Microbiology, Academy of Sciences of The Czech Republic

THE 29<sup>th</sup> ANNUAL SYMPOSIUM of



#### PL-026 Appearance of stabilizing interactions in the evolution of a dimeric TIM barrel

Mariana Schulte-Sasse<sup>1</sup>, Nancy O. Pulido Mayoral<sup>1</sup>, Miguel Costas-Basín<sup>2</sup>, Enrique García-Hernández<sup>3</sup>, Adela Rodríguez-Romero<sup>3</sup>, D. Alejandro Fernández-Velasco<sup>1</sup>

1.-National Autonomous University of Mexico, Faculty of Medicine, 2.-National Autonomous University of Mexico, Faculty of Chemistry, 3.-National Autonomous University of Mexico, Institute of Chemistry

#### PL-036 Thermal and structural stability of ß-Glucosidades GH1

Maira Artischeff Frutuoso1

1.-Departamento de Bioquímica do Instituto de Química da Universidade de São Paulo

#### PL-038 Structural determinants for human RNase 6 antimicrobial mechanism of action

Javier Arranz Trullén<sup>1</sup>, Guillem Prats-Ejarque<sup>1</sup>, Jose Antonio Blanco<sup>1</sup>, Marcel Albacar<sup>1</sup>, Diego Velazquez<sup>1</sup>, David Púlido<sup>2</sup>, Mohammed Moussaoui<sup>1</sup>, Ester Boix<sup>1</sup>

1.-Department of Biochemistry and Molecular Biology, Biosciences Faculty, UAB, 2.-Department of Life Sciences, Imperial College

#### PL-039 Covalent Structure of Single-Stranded Fibrinogen and Fibrin Oligomers Cross-Linked by FXIIIa. The influence of free radical oxidation

Anna Bychkova<sup>1</sup>, Vera Leonova<sup>1</sup>, Alexander Shchegolikhin<sup>1</sup>, Marina Biryukova<sup>1</sup>, Elizaveta Kostanova<sup>1</sup>, Mark Rosenfeld<sup>1</sup>

1.-N. M. Emanuel Institute Of Biochemical Physics, Russian Academy Of Sciences

#### PL-040 Structural and thermodynamic analysis of co-stimulation receptor CD28 phosphopeptide interactions with Grb2, Gads, and PI3-kinese SH2 domains

Satomi Inaba<sup>1</sup>, Nobutaka Numoto<sup>2</sup>, Hisayuki Morii<sup>3</sup>, Teikichi Ikura<sup>2</sup>, Ryo Abe<sup>4</sup>, Nobutoshi Ito<sup>2</sup>, Masayuki Oda<sup>1</sup>

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-044 Study of denaturation of proteins by surfactant using the taylor dispersion analysis and dynamic light scattering

<u>Anna Lewandrowska</u><sup>1</sup>, Aldona Jelińska<sup>1</sup>, Agnieszka Wiśniewska<sup>1</sup>, Robert Hołyst<sup>1</sup> 1.-Institute of Physical Chemistry Polish Academy of Sciences

## PL-046 Paraoxonase 1 (Pon1) regulates water homeostasis by controlling the expression of Fxr and Aqp2 proteins in mice

Marianna Wieloch<sup>1,2</sup>, Hieronim Jakubowski<sup>1,2,3</sup>

1.-Institute of Bioorganic Chemistry, 2.-Department of Biochemistry and Biotechnology, University of Life Sciences, 3.-Dep.of Microbiology Biochemistry & Molecular Genetics, Rutgers-New Jersey Medical

#### PL-050 Ab initio modelling of structurally uncharacterised antimicrobial peptides Mara Kozic<sup>1</sup>

1.-Institute of Integrative Biology, University of Liverpool

#### PL-054 Functional Clustering of the Crotonase Superfamily

Julia Hayden<sup>1</sup>, Janelle Leuthaeuser<sup>2</sup>, Patricia Babbit<sup>3</sup>, Jacquelyn Fetrow<sup>4</sup>

1.-Dickinson College, Molecular Biology and Chemistry Department, 2.-Department of Molecular Genetics, Wake Forest University, 3.-Department of Pharm. Chem., University of California, San Francisco, CA, 4.-Department of Chemistry, University of Richmond

JULY 22 - 25, 2015

#### PL-056 A search for anti-melioidosis drug candidates targeted to sedoheptulose-7-phosphate isomerase from Burkholderia pseudomallei

Jimin Park<sup>1</sup>, Daeun Lee<sup>1</sup>, Sang A Yeo<sup>1</sup>, Mi-Sun Kim<sup>1</sup>, Dong Hae Shin<sup>1</sup> 1.-College of Pharmacy, Global Top5 Research Program, Ewha Womans University

### PL-057 Mapping the Structure of Laminin Using Cross-linking and Mass Spectrometry

Gad Armony<sup>1</sup>, Toot Moran<sup>1</sup>, Yishai Levin<sup>2</sup>, Deborah Fass<sup>1</sup>

1.-Weizmann Institute of Science, Department of Structural Biology, 2.-Weizmann Institute of Science, Israel Center for Personalized Medicine

### PL-059 Effects of Cell-Like Infrastructures on Transient Protein Interactions

Ciara Kyne<sup>1</sup>, Peter Crowley<sup>1</sup>

1.-School of Chemistry, National University of Ireland Galway

#### PL-060 A search for anti-melioidosis drug candidates targeted to D-glycero-D-manno-heptose-1,7-bisphosphate phosphatase from Burkholderia pseudomallei

Jimin Park<sup>1</sup>, Sang A Yeo<sup>1</sup>, Daeun Lee<sup>1</sup>, Mi-Sun Kim<sup>1</sup>, Dong Hae Shin<sup>1</sup> 1.-College of Pharmacy, Global Top5 Research Program, Ewha Womans University

#### PL-061 Crystal structure of dimeric D-glycero-D-manno-heptose-1,7-bisphosphate phosphatase from Burkholderia thailandensis

<u>Jimin Park</u><sup>1</sup>, Mi-Sun Kim<sup>1</sup>, Daeun Lee<sup>1</sup>, Keehyung Joo<sup>2</sup>, Gil-Ja Jhon<sup>3</sup>, Jooyoung Lee<sup>2</sup>, Dong Hae Shin<sup>1</sup>

1.-Collegy of Pharmacy, Global Top5 Research Program, Ewha Womans University, 2.-School of Computational Sciences, Korea Institute for Advanced Study, 3.-Department of Chemistry and Nano Science, Ewha Womans University

# PL-064 Biochemical characterization of the substrate specificity of two unique members of the mammalian protein arginine methyltransferase family, PRMT7 and PRMT9

Andrea Hadjikyriacou<sup>1</sup>, You Feng<sup>1</sup>, Yanzhong Yang<sup>2</sup>, Mark Bedford<sup>3</sup>, Steven Clarke<sup>1,4</sup>

1.-Department of Chemistry and Biochemistry, University of California Los Angeles, 2.-Department of Radiation Biology, Beckman Research Institute, City of Hope, 3.-Department of Epigenetics and Molecular Carcinogenesis UT MD Anderson Cancer, 4.-Molecular Biology Institute, University of California Los Angeles

### PL-066 Fish ß-parvalbumin acquires allergenic properties by amyloid assembly

Javier Martínez<sup>1</sup>, Rosa Sánchez<sup>1</sup>, Milagros Castellanos<sup>2</sup>, Ana M. Fernández-Escamilla<sup>3</sup>, Sonia Vázquez-Cortés<sup>4</sup>, Montserrat Fernández-Rivas<sup>4</sup>, María Gasset<sup>1</sup>

1.-Instituto Química-Física 'Rocasolano', CSIC, 2.-Centro Nacional de Biotecnología, CSIC, 3.-Estación Experimental del Zaidín, CSIC, 4.-Allergy Department, Hospital Clínco San Carlos, IdISSC

THE 29<sup>th</sup> ANNUAL SYMPOSIUM of



#### POSTER SESSION 3

#### Thursday, July 23, 2015 Exhibit Hall

#### **Author Presentations**

Odd Board Numbers 11:45 AM -12:30 PM Even Board Numbers 12:30 PM - 1:15 PM

BOARD #S
PB-050 – PB-070
PC-015 – PC-026
PD-024 – PD-032
PE-010 – PE-015
PF-007 – PF-024
PH-032 – PH-047
PI-066 – PI-079
PJ-035 – PJ-044
PL-069 – PL-076

#### **PB – CHEMICAL BIOLOGY**

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

Maria Winiewska<sup>1</sup>, Jarosław Poznański<sup>1</sup>

1.-Institute of Biochemistry and Biophysics Polish Academy of Sciences

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

Kaitlyn M. Towle<sup>1</sup>, Christopher T. Lohans<sup>2</sup>, Marco J. van Belkum<sup>1</sup>, Mark Miskolzie<sup>1</sup>, John C. Vederas<sup>1</sup> 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

Roxana Yesenia Pastrana Alta<sup>1</sup>, Maria Teresa Machini<sup>2</sup>, Breno Pannia Espósito<sup>1</sup>

1.-Laboratory for Bioinorganic Chemistry and Metallodrugs, Instituto de Química, 2.-Laboratory of Peptide Chemistry, Instituto de Química, Universidade de São Paulo

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

Amaris Torres-Delgado<sup>1</sup>, Robert T. Sauer<sup>1</sup>, Tania A. Baker<sup>1,2</sup>

1.-Department of Biology, Massachusetts Institute of Technology, 2.-Howard Hughes Medical Institute

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

<u>Ewelina Guca</u><sup>1</sup>, François Hoh<sup>2</sup>, Jean-François Guichou<sup>2</sup>, Henri Vial<sup>1</sup>, Rachel Cerdan<sup>1</sup> 1.-DIMNP, UMR 5235, University of Montpellier, 2.-Centre de Biochimie Structurale, INSERM UMR 1054, CNRS UMR 5048

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

<u>Aishling M. Doolan</u><sup>1</sup>, Maike C. Jürgens<sup>1</sup>, Amir R. Khan<sup>2</sup>, Peter B. Crowley<sup>1</sup> 1.-School of Chemistry, National University of Ireland Galway, 2.-School of Biochemistry and Immunology, Trinity College Dublin

JULY 22 - 25, 2015

#### PB-066 Macromolecular crowding modulates enzyme catalysis

Annelise Gorensek<sup>1</sup>, Luis Acosta<sup>1</sup>, Gary Pielak<sup>1,2,3</sup>

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

#### PB-068 FBP17 controls the hepatocyte morphology through Rho signaling

Jun Zhang<sup>1</sup>, Mingming Ling<sup>1</sup>, Qianying Žhang<sup>1</sup>, Yunhong Wang<sup>7</sup>, Deqiang Wang<sup>2</sup> 1.-The Department of Cell Biology and Genetics, 2.-Key Laboratory of Molecular Biology on Infectious Disease

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

Jovan Dragelj<sup>1</sup>, Anna-Lena Woelke<sup>1</sup>, Ulrike Alexiev<sup>2</sup>, Ernst-Walter Knapp<sup>1</sup> 1.-Fachbereich Biologie, Chemie, Pharmazie/Institute of Chemistry and Biochemistry, 2.-Fachbereich Physik/Department of Physics

### PB-070 Efficient Methods in the Production of Unnatural Amino Acid Containing Proteins <u>Christopher Walters</u><sup>1</sup>, Solongo Batjargal, Anne Wagner, E. James Petersson

1.-University of Pennsylvania

#### PC – ENZYME & PATHWAY ENGINEERING

### 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><sup>1</sup>, Misaki Kinoshita<sup>1</sup>, Takahisa Ikegami<sup>1,2</sup>, Genji Kurisu<sup>1</sup>, Yuji Goto<sup>1</sup>, Toshiharu Hase<sup>1</sup>, Young-Ho Lee<sup>1</sup>

1.-Institute for Protein Research, Osaka University, 2.-Yokohama City University

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

Lisa Ngu<sup>1</sup>, Kevin Ramos<sup>1</sup>, Nicholas DeLateur<sup>1</sup>, Penny Beuning<sup>1</sup>, Mary Jo Ondrechen<sup>1</sup>

1.-Department of Chemistry & Chemical Biology, Northeastern University

### $\mathsf{PC}\text{-}020$ Structure-Function Relationships of human Aldo-Keto Reductase 1B15, AN enzyme active with 9-cis-Retinaldehyde

Joan Giménez Dejoz<sup>1</sup>, Michal H. H. Kolář<sup>2,3</sup>, Francesc Xavier Ruiz<sup>4</sup>, Isidro Crespo<sup>1</sup>, Alexandra Cousido-Siah<sup>4</sup>, Alberto Podjarny<sup>4</sup>, Jindřich Fanfrlík<sup>2</sup>, Xavier Parés<sup>1</sup>, Jaume Farrés<sup>1</sup>, Sergio Porté<sup>1</sup>

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

<u>Olumide Kayode<sup>1, 2</sup>,</u> Thomas R. Caulfield<sup>3</sup>, Ruiying Wang<sup>2</sup>, Devon Pendlebury<sup>2</sup>, Alexei Soares<sup>4</sup>, Evette S. Radisky<sup>2</sup>

1.-Mayo Graduate School, 2.-Department of Cancer Biology, Mayo Clinic Cancer Center, 3.-Department of Neuroscience, Mayo Clinic College of Medicine, 4.-Biology Department, Brookhaven National Laboratory

# PC-022 Determinants for regioselectivity in Lytic Polysaccharide MonoOxygenases (LP-MOs)

<u>Barbara Danneels</u><sup>1</sup>, Magali Tanghe<sup>1</sup>, Henk-Jan Joosten<sup>2</sup>, Tom Desmet<sup>1</sup> 1.-Centre for Industrial Biotechnology and Biocatalysis, University of Ghent, 2.-Bioprodict





# $\mathsf{PC}\text{-}026$ The development of a coupled enzyme assay to detect isochorismate pyruvate lyase activity

Linda Jäger<sup>1</sup>, Christian Jäckel<sup>1</sup>, Peter Kast<sup>1</sup>, Donald Hilvert<sup>1</sup> 1.-LOC, ETH Zürich

### PD – FOLDING

#### PD-024 Biophysical analysis of partially folded states of myoglobin in presence of 2,2,2-trifluoroethanol

Paurnima Talele<sup>1</sup>, Nand Kishore<sup>1</sup> 1.-Indian Institute of Technology Bombay

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

Estella Newcombe<sup>1</sup>, Yasmin Ramdzan<sup>1</sup>, Ashish Sethi<sup>1</sup>, Michael Lee<sup>2</sup>, Dorothy Loo<sup>3</sup>, Bim Graham<sup>2</sup>, James Swarbrick<sup>2</sup>, Anthony Purcell<sup>3</sup>, Paul Gooley<sup>1</sup>, Danny Hatters<sup>1</sup>

1.-Department of Biochemistry and Molecular Biology, University of Melbourne, 2.-Monash Institute of Pharmaceutical Science, Monash University, 3.-Department of Biochemistry and Molecular Biology, Monash University

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

Iratxe Macias<sup>1</sup>, Arantza Sanz<sup>1</sup>, Ana Laín<sup>1</sup>, Oscar Millet<sup>1</sup> 1.-CIC bioGUNE

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

Benjamin Walcott<sup>1,2</sup>, Luís Garreta<sup>3</sup>, Christopher Bystroff<sup>1,2,4</sup>

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 Rao<sup>1</sup>, Shachi Gosavi<sup>1</sup>

1.-National Centre for Biological Sciences, Tata Institute of Fundamental Research

#### PD-032 **Tuning cooperativity on the free energy landscape of protein folding** Pooja Malhotra<sup>1</sup>, Jayant Udgaonkar<sup>1</sup>

1.-National Centre for Biological Sciences, Tata Institute of Fundamental Research

### **PE – INTEGRATIVE PROTEIN SCIENCE**

# 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><sup>1</sup>, Jhon Alexander Rodríguez<sup>1</sup>, Alain Ibáñez de Opakua<sup>1</sup>, Nekane Merino<sup>1</sup>, Maider Villate<sup>1</sup>, Tammo Diercks<sup>1</sup>, Pietro Roversi<sup>2</sup>, Adriana L. Rojas<sup>1</sup>, Francisco J. Blanco<sup>1,3</sup> 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 Palakurti<sup>1</sup>, Ramakrishna Vadrevu<sup>1</sup>

1.-Department of Biological Sciences, BITS-PILANI HYDERABAD CAMPUS

JULY 22 - 25, 2015

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

<u>Rafael Palomino</u><sup>1</sup>, Glenn Millhauser<sup>2</sup>, Pietro Sanna<sup>2</sup> 1.-University of California Santa Cruz, 2.-The Scripps Research Institute

### PE-015 Theoretical Volume Profiles as a Tool for Probing Protein Folding Kinetics

Heather Wiebe<sup>1</sup>, Noham Weinberg<sup>1,2</sup>

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

#### **PF – INTRINSICALLY DISORDERED PROTEINS**

PF-007 **Solution structure and celullar functional studies of bovine cathelicidin Bt-6 (BMAP-27)** <u>Anna Hastings</u><sup>1</sup>, Manuel Ruether<sup>2</sup>, H. Paul Voorheis<sup>1</sup>, Ken H. Mok<sup>1,3</sup>

1.-Trinity College Dublin, School of Biochemistry and Immunology, 2.-Trinity College Dublin, School of Chemistry, 3.-TCD, Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN)

PF-010 **Biophysical characterization of phosducin and its complex with the 14-3-3 protein** <u>Miroslava Kacirova</u><sup>1,2</sup>, Jiri Novacek<sup>3</sup>, Petr Man<sup>1,4</sup>, Alan Kadek<sup>1,4</sup>, Veronika Obsilova<sup>2</sup>, Tomas Obsil<sup>1,2</sup> 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-016 New insights into amyloidogenesis of Tau protein induced by enantiomers of polyglutamic acid

Bartosz Nizynski<sup>1,2,3,4</sup>, Hanna Nieznanska<sup>2</sup>, Krzysztof Nieznanski<sup>2</sup>, Wojciech Dzwolak<sup>3,4</sup>

1.-College of Inter-Faculty Individual Studies in Mathematics and Natural Sciences, 2.-Department of Biochemistry, Nencki Institute of Experimental Biology, 3.-Institute of High Pressure Physics, 4.-Department of Chemistry, Biological and Chemical Research Centre

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

<u>Cesyen Cedeno</u><sup>1</sup>, Nani Van Gerven<sup>1</sup>, Wim Jonckheere<sup>1</sup>, Imke Van den Broek<sup>1</sup>, Han Remaut<sup>1</sup>, Peter Tompa<sup>1</sup>

1.-VIB, Structural Biology Research Center

### $\mathsf{PF}\text{-}021$ SDS-PAGE analysis of Aß oligomers is disserving research into Alzheimer's disease: a call for ESI-IM-MS

<u>Sílvia Vilaprinyó-Pascual</u><sup>1</sup>, Rosa Pujol-Pina<sup>1</sup>, Roberta Mazzucato<sup>1</sup>, Annalisa Arcella<sup>2</sup>, Marta Vilaseca<sup>3</sup>, Modesto Orozco<sup>2,4</sup>, Natàlia Carulla<sup>1</sup>

1.-Institute for Research in Biomedicine (IRB Barcelona), 2.-Joint IRB-BSC Research Program in Computational Biology, 3.-Mass Spectrometry Core Facility, IRB Barcelona, 4.-Department of Biochemistry and Molecular Biology, University of Barcelona

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

Pallavi Sabharwal<sup>1</sup>, Rashmi Panigrahi<sup>1</sup>, Srinivas Sistala<sup>2</sup>, Savithri H S<sup>1</sup> 1.-Indian institute of Science, 2.-Wipro G E Healthcare Pvt Ltd

#### **PH – PROTEIN ALLOSTERY & DYNAMICS**

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

<u>Veronika Navratilova</u><sup>1</sup>, Marketa Paloncyova<sup>1</sup>, Michaela Kajsova<sup>1</sup>, Karel Berka<sup>1</sup>, Michal Otyepka<sup>1</sup> 1.-RCPTM, Department of Physical Chemistry, Faculty of Science, Palacky University

### PH-034 Antibiotic binding drives catalytic activation of aminoglycoside kinase APH(2")-la Shane Caldwell<sup>1</sup>, Albert Berghuis<sup>1</sup>

1.-McGill University





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

Ryan Godwin<sup>1</sup>, William Gmeiner<sup>2</sup>, Freddie Salsbury<sup>1</sup>

1.-Wake Forest University - Department of Physics, 2.-Wake Forest University Health Sciences - Department of Cancer Biology

# $\rm PH-037~$ Structural characterization of calmodulin bound to the intracellular calmodulin binding domain of Kv7.2 channels by NMR

Ganeko Bernardo Seisdedos <sup>1,2</sup>, Álvaro Villarroel <sup>2</sup>, Oscar Millet <sup>1</sup> 1.-CIC-Biogune, 2.-Unidad de Biofísica (CSIC-UPV/EHU)

# $\mathsf{PH}\text{-}041$ $\,$ Quercetin effect on the stability and regeneration of the G-protein-coupled receptor rhodopsin

Maria Guadalupe Herrera Hernández<sup>1,3</sup>, Xiaoyun Dong<sup>1</sup>, Cecylia S. Lupala<sup>2</sup>, Juan J. Perez<sup>2</sup>, Pere Garriga<sup>1</sup>

1.-GBMI, Centre de Biotecnologia Molecular, Universitat Politecnica de Catalunya, 2.-GBMI, ET-SEIB, Universitat Politècnica de Catalunya, 3.-Unidad de Biotecnología. Campo Experimental Bajío (INIFAP)

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

Pablo Herrera Nieto<sup>1</sup>, James Dalton<sup>1</sup>, Jesús Giraldo<sup>1</sup>

1.-Universidad Autónoma de Barcelona

### PH-047 Dynamical Variability in the Clan MA of Metalloproteases

Henrique F. Carvalho<sup>1,2</sup>, Ana Cecília A. Roque<sup>1</sup>, Olga Iranzo<sup>2,3</sup>, Ricardo J. F. Branco<sup>11</sup>.-UCIBIO, RE-QUIMTE, Faculdade de Ciências e Tecnologia, Universidade Nova Lisboa, 2.-ITQB António Xavier, Universidade Nova de Lisboa, 3.-Aix Marseille Université, Centrale Marseille

### **PI – PROTEIN ENGINEERING**

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

Helen Farrants<sup>1</sup>, Oliver Hantschel<sup>1</sup>, Kai Johnsson<sup>1</sup>

1.-École Polytechnique Fédérale de Lausanne (EPFL)

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

<u>Arnab Nayek</u><sup>1</sup>, Shyamashree Banerjee<sup>1</sup>, Parth Sarthi Sen Gupta<sup>1</sup>, Biswa pratap Sur<sup>1</sup>, Pratay Seth<sup>1</sup>, Sunit Das<sup>1</sup>, Nathan A Baker<sup>2</sup>, Amal K Bandyopadhyay<sup>1</sup>

1. Department of Biotechnology, The University of Burdwan

2. Pacific Northwest National Laboratory

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

Peter Suon, Mario Navarro, John Love 1.-San Diego State University, 2.-San Diego State University, 3.-San Diego State University

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

Melissa Lokensgard<sup>1</sup>, John Love<sup>1</sup>

1.-San Diego State Uniersity

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

<u>Dorottya Németh</u><sup>1</sup>, Balázs Schäfer<sup>1</sup>, Éva Hunyadi-Gulyás<sup>2</sup>, Zsuzsanna Darula<sup>2</sup>, Csaba Tömböly<sup>1</sup> 1.-Biological Research Centre, Instute of Biochemisty, Laboratory of Chemical Biology, 2.-Biological Research Centre, Laboratory of Proteomics Research

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

<u>Martijn Van Rosmalen</u><sup>1</sup>, Remco Arts<sup>1</sup>, Brian Janssen<sup>1</sup>, Natalie Hendrikse<sup>1</sup>, Dave Wanders<sup>1</sup>, Maarten Merkx<sup>1</sup>

1.-Laboratory of Chemical Biology / Institute of Complex Molecular Systems

#### PJ - PROTEOMICS (PPIs, PTMs)

#### 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 Bielińska<sup>1</sup>, Łukasz Marczak<sup>1</sup>, Hieronim Jakubowski<sup>1,2</sup>

1.-Institute of Bioorganic Chemistry, Polish Academy of Sciences, 2.-Rutgers University, New Jersey Medical School

#### 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><sup>1</sup>, Sarah A. Graham<sup>1</sup>, Pelagia Deriziotis<sup>1</sup>, Swathi Mookonda Chinnappa<sup>1</sup>, Simon E. Fisher<sup>1,2</sup>

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)

Deqiang Wang<sup>1</sup>, Chen Ke<sup>1</sup>, Jun Zhang<sup>2</sup>

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

### $\mathsf{PJ}\text{-}039$ A new hydrophobicity scale of amino acids based on IEF-MST calculated log P and log D

<u>William J. Zamora</u><sup>1</sup>, Josep M. Campanera<sup>1</sup>, F. Javier Luque<sup>1</sup>, Jody McGinness<sup>1</sup> 1.-Departament de Fisicoquímica and Institut de Biomedicina (IBUB)

#### PJ-040 Docking-based tools for discovery of protein-protein modulators

Mireia Rosell Oliveras<sup>1</sup>, Juan Fernández Recio<sup>2</sup>

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

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

Inhae Kim<sup>1</sup>, Sangjin Han<sup>1</sup>, Jihye Hwang<sup>2</sup>, Sanguk Kim<sup>1</sup>

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-Sámano<sup>1</sup>, <u>Luis Ángel Rodríguez-Lumbreras<sup>1</sup></u>, Juan Fernández-Recio<sup>1</sup> 1.-Joint BSC-CRG-IRB Research Program in Computational Biology

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

<u>Alejandra Guerra-Castellano</u><sup>1</sup>, Katiuska González-Arzola<sup>1</sup>, Francisco Rivero-Rodríguez<sup>1</sup>, Adrián Velázquez-Campoy<sup>2</sup>, Miguel Ángel De la Rosa<sup>1</sup>, Irene Díaz-Moreno<sup>1</sup>, Antonio Díaz-Quintana<sup>1</sup> 1.-IBVF – CIC Cartuja, University of Seville - CSIC, 2.-BIFI-IQFR, University of Saragossa - CSIC

BEST POSTER COMPETITION



#### PL – OTHER/NO THEME ALLOCATED

#### PL-069 Evaluation of human salivary α-defensins by LC-ESI-MS

<u>Nadia Ashrafi</u><sup>1</sup>, Cris Lapthorn<sup>1</sup>, Fernando Naclerio<sup>2</sup>, Frank Pullen<sup>1</sup>, Birthe Nielsen<sup>1</sup>, Yue Fu<sup>2</sup>, Jack Miller<sup>2</sup>, Christian Watkinson<sup>2</sup>, Marcos Seijo<sup>2</sup>

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

#### PL-070 **Characterising interactions between alginates of different sizes and ß-lactoglobulin** <u>Emil G. P. Stender</u><sup>1</sup>, Sanaullah Khan<sup>2</sup>, Outi E. Mäkinen<sup>3</sup>, Kristoffer Almdal<sup>2</sup>, Peter Westh<sup>4</sup>, Richard Ibsen<sup>2</sup>, Maher Abou Hachem<sup>1</sup>, Birte Svensson<sup>1</sup>

1.-Technical University of Denmark – DTU – Department of Systems Biology, 2.-2Technical University of Denmark – DTU – Department of Micro- and Nanotechnology, 3.-University of Copenhagen – Department of Food Science, 4.-Roskilde University – RUC – Department of Science, Systems and Models

#### PL-071 Validation of a LC-MS method for the detection of human salivary α-defensins

Nadia Ashrafi<sup>1</sup>, Cris Lapthorn<sup>1</sup>, Birthe Nielsen<sup>1</sup>, Fernando Naclerio<sup>2</sup>, Frank Pullen<sup>1</sup>, Patricia Wright<sup>1</sup> 1.-University of Greenwich (Faculty of Engineering and Science), 2.-University of Greenwich (Centre for Sport Science and Human Performance)

#### PL-072 Moonlighting proteins: relevance for biotechnology and biomedicine

Luis Franco Serrano<sup>1</sup>, Sergio Hernández<sup>1</sup>, Alejandra Calvo<sup>2</sup>, Gabriela Ferragut<sup>2</sup>, Isaac Amela<sup>1</sup>, Juan Cedano<sup>2</sup>, Enrique Querol<sup>1</sup>

1.-Institut de Biotecnologia i Biomedicina. Universitat Autònoma de Barcelona, 2.-Laboratorio de Inmunología, Universidad de la República Regional Norte-Salto

### PL-073 Correlation between potential human neutrophil antimicrobial peptides (HNP 1-3) and stress hormones in human saliva

Nadia Ashrafi<sup>1</sup>, Frank Pullen<sup>1</sup>, Birthe Nielse<sup>1</sup>, Cris Lapthorn<sup>1</sup>, Fernando Naclario<sup>2</sup>

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

#### PL-075 Refolding and activation of recombinant trypsin i from sardine fish (Sardinops sagax caerulea)

<u>Manuel Carretas-Valdez</u><sup>1</sup>, Francisco Cinco-Moroyoqui<sup>1</sup>, Marina Ezquerra-Brauer<sup>1</sup>, Enrique Marquez-Rios<sup>1</sup>, Rogerio Sotelo-Mundo<sup>2</sup>, Idania Quintero-Reyes<sup>3</sup>, Aldo Arvizu-Flores<sup>3</sup>

1.-Úniversidad de Sonora, Departamento de Investigación en Alimentos, 2.-Centro de Investigación en Alimentación y Desarrollo, A.C., 3.-Universidad de Sonora, Departamento de Ciencias Químico Biológicas

#### **POSTER SESSION 4**

#### Thursday, July 23, 2015 Exhibit Hall

#### **Author Presentations**

Odd Board Numbers 4:45 PM – 5:30 PM Even Board Numbers 5:30 PM - 6:15 PM

THEME	BOARD #S
Chemical Biology	PB-072 – PB-085
Folding	PD-033 – PD-054
Integrative Protein Science	PE-020 – PE-029
Intrinsically Disordered Proteins	PF-026 – PF-032
Protein Engineering	PI-080 – PI-106
Other/No theme allocated	PL-077 – PL-085

#### **PB - CHEMICAL BIOLOGY**

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

<u>Caitlyn Mills</u><sup>1</sup>, Pengcheng Yin<sup>1</sup>, Penny Beuning<sup>1</sup>, Mary Jo Ondrechen<sup>1</sup> 1.-Northeastern University

PB-073 Directly observing the synergistic dynamics in F-actin and microtubule assembly Jun Zhang<sup>1</sup>, Deqiang Wang<sup>2</sup>

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

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

Wouter Engelen<sup>1</sup>, Brian Janssen<sup>1</sup>, Maarten Merkx<sup>1</sup> 1.-Eindhoven University of Technology

PB-082 Establishing a tool box for generating designer nucleosomes

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

PB-083 **Evaluating cation-pi and pi-pi interaction in proteins using various biophysical methods** <u>Jinfeng Shao</u><sup>1</sup>, Andy-Mark W.H. Thunnissen<sup>1</sup>, Jaap Broos<sup>1</sup> 1.-Laboratory of Biophysical Chemistry, University of Groningen

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

Julia Sindlinger<sup>1</sup>, Alexander Dose<sup>1</sup>, Jan Bierlmeier<sup>1</sup>, Frank Essmann<sup>1</sup>, Markus Hartl<sup>2</sup>, Iris Finkemeier<sup>3</sup>, Dirk Schwarzer<sup>1</sup>

1.-Interfaculty Institute of Biochemistry, University of Tuebingen, 2.-Max Planck Institute of Biochemistry, 3.-Max Planck Institute for Plant Breeding Research

PB-085 **Exploring the Substrate Selectivity of Oxygen Sensing Prolyl Hydroxylases** <u>Kerstin Lippl</u><sup>1</sup>, Martine Abboud<sup>1</sup>, Christoph Loenarz<sup>2</sup>, Christopher Schofield<sup>1</sup> 1.-Department of Chemistry, University of Oxford, United Kingdom, 2.-Department of Chemistry, University of Nottingham, United Kingdom



#### PD – FOLDING

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

Eriko Aoki<sup>1</sup>, Kazuo Fujiwara<sup>1</sup>, Masamichi Ikeguchi<sup>1</sup>

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 Kakimoto<sup>1</sup>, Hideya Nakano<sup>1</sup>, Yuji Nakai<sup>2</sup>, Kazuhiro Shiozaki<sup>3</sup>, Kohei Akioka<sup>4</sup>, Konosuke Otomaru<sup>5</sup>, Mitsuharu Matsumoto<sup>6</sup>, Masanobu Nagano<sup>7</sup>, Yasushi Sugimoto<sup>8</sup>, <u>Hiroaki Kanouchi<sup>1</sup></u>

1.-Department of Veterinary Pathobiology, Kagoshima University, 2.-Institute for Food Sciences, Hirosaki University, 3.-Faculty of Fisheries, Kagoshima University, 4.-Department of Veterinary Histopathology, Kagoshima University, 5.-Veterinary Clinical Training Center, Kagoshima University, 6.-Department of Veterinary Anatomy, Kagoshima University, 7.-Sakamoto Kurozu Inc., 8.-The United Graduate School of Agricultural Sciences, Kagoshima University

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

Nurriza Ab Latif<sup>1,2</sup>, Paul Engel<sup>1</sup>

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

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

Connie Tenorio<sup>1</sup>, Liam Longo<sup>1</sup>, Ozan S. Kumru<sup>2</sup>, C. Russell Middaugh<sup>2</sup>, Michael Blaber<sup>1</sup> 1.-Department of Biomedical Sciences, Florida State University, 2.-Department of Pharmaceutical Chemistry, University of Kansas

#### **PE – INTEGRATIVE PROTEIN SCIENCE**

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

<u>Ho Zee (Charles) Kong</u><sup>1</sup>, Conrad Perera<sup>1</sup>, Ivanhoe Leung<sup>1</sup>, Nazimah Hamid<sup>2</sup>, Viji Sarojini<sup>1</sup> 1.-School of Chemical Sciences, The University of Auckland., 2.-School of Applied Sciences, Auckland University of Technology

### $\mathsf{PE}\text{-}026$ A novel in vivo characterization method predicting the physicochemical parameters of an antibiotic efflux pump

Anisha M Perez<sup>1</sup>, Erin L O'Brien<sup>1</sup>, Marcella M Gomez<sup>1</sup>, Matthew R Bennett<sup>1</sup>, Yousif Shamoo<sup>1</sup> 1.-Department of BioSciences

#### PE-027 Structural Analysis of KCNE1 Transmembrane Mutant Yielding KCNE3-like Function Cheryl Law, Charles Sanders

1.-Vanderbilt University Biochemistry Department, 2.-Vanderbilt University Center for Structural Biology, 3.-Vanderbilt University School of Medicine

# PE-028 Biochemical characterization of Brassica napus diacylglycerol acyltransferase 1 and its regulatory domain

<u>Kristian Mark Caldo</u><sup>1</sup>, Rashmi Panigrahi<sup>2</sup>, Michael Greer<sup>1</sup>, Guanqun Chen<sup>1</sup>, M. Joanne Lemieux<sup>2</sup>, Randall Weselake<sup>1</sup>

1.-Alberta Innovates Phytola Centre, University of Alberta, 2.-Department of Biochemistry, University of Alberta

## PE-029 Alteration of lysine and arginine content as a strategy to modify protein solubility: a test for E. coli proteins

M. Alejandro Carballo-Amador<sup>1</sup>, Jim Warwicker<sup>1</sup>, Alan J. Dickson<sup>1</sup> 1.-Faculty of Life Sciences, University of Manchester

#### **PF – INTRINSICALLY DISORDERED PROTEINS**

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

<u>Francesco Simone Ruggeri</u><sup>1</sup>, Sophie Vieweg<sup>2</sup>, Denise Galante<sup>3</sup>, Cristina D'arrigo<sup>3</sup>, Hilal Lashuel<sup>2</sup>, Giovanni Dietler<sup>1</sup>

1.-École polytechnique fédérale de Lausanne - LPMV, 2.-École polytechnique fédérale de Lausanne - LMNN, 3.-National Research Council

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

Petr Tesina<sup>1, 2, 3</sup>, Kateřina Čermáková<sup>4</sup>, Magdalena Hořejší <sup>3</sup>, Milan Fábry<sup>3</sup>, Frauke Christ<sup>4</sup>, Jonas Demeulemeester<sup>4</sup>, Zeger Debyser<sup>4</sup>, Jan De Rijck<sup>4</sup>, Václav Veverka<sup>1</sup>, Pavlína Řezáčová<sup>3</sup>,

1.-IOCB AS CR, 2.-IMG AS CR, 3.-Faculty of Science, Charles University in Prague, 4.-KU Leuven

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

Serene W. Chen<sup>1</sup>, Srdja Drakulic<sup>2</sup>, Emma Deas<sup>3</sup>, Myriam Ouberai<sup>4</sup>, Francesco A. Aprile<sup>1</sup>, German Rivas<sup>5</sup>, Andrey Y. Abramov<sup>3</sup>, Jose Maria Valpuesta<sup>2</sup>, Christopher M. Dobson<sup>1</sup>, Nunilo Cremades<sup>1</sup> 1.-Department of Chemistry, University of Cambridge, 2.-Department of Macromolecular Structure, Centro Nacional de Biotecnologia, 3.-Department of Molecular Neuroscience, University College London, 4.-Nanoscience Centre, Department of Engineering, University of Cambridge, 5.-Department of Cellular and Molecular Biology

#### PF-031 Metal ions modulate the conformation of Starmaker-like protein from Oryzias latipes <u>Mirosława Różycka</u><sup>1</sup>, Magdalena Wojtas<sup>1</sup>, Natalie Mutter<sup>2</sup>, Benjamin Schuler<sup>2</sup>, Jacek Gapiński <sup>3,4</sup>, Andrzej Ożyhar<sup>1</sup>

1.-University of Technology, Department of Biochemistry, 2.-University of Zurich, Department of Biochemistry, 3.-Molecular Biophysics Department, Faculty of Physics, Adam Mickiewicz University, 4.-NanoBioMedical Center, Adam Mickiewicz University

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

Aleksandra Porebska<sup>1</sup>, Andrzej Ozyhar<sup>1</sup>, Piotr Dobryszycki<sup>1</sup>

1 - Wroclaw University of Technology, Department of Biochemistry

#### **PI – PROTEIN ENGINEERING**

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

<u>Silvia Scarabelli</u><sup>1</sup>, Thomas Vorherr<sup>2</sup>, Kai Johnsson<sup>1</sup>

1.-Ecole Polytechnique Fédérale de Lausanne, 2.-Novartis Institute for BioMedical Research

#### PI-083 Luminescent sensor proteins for antibody detection in solution

<u>Remco Arts</u><sup>1</sup>, Susann Ludwig<sup>1</sup>, Marina van Vliembergen<sup>1</sup>, Vito Thijssen<sup>1</sup>, Stan van der Beelen<sup>1</sup>, Ilona den Hartog<sup>1</sup>, Stefan Zijlema<sup>1</sup>, Maarten Merkx<sup>1</sup>

1.-Eindhoven University of Technology


#### PI-084 **Tertiary Structural Propensities Reveal Fundamental Sequence-Structure Relationships** <u>Fan Zheng</u><sup>1</sup>, Jian Zhang<sup>2</sup>, Gevorg Grigoryan<sup>1,2</sup>

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

#### PI-086 Synthesis of selectively functionalized adiponectin

Andreas Mattern<sup>1</sup>, Annette Beck-Sickinger<sup>1</sup>

1.-University of Leipzig, Institute of Biochemistry

PI-089 **The purification, crystallization and preliminary characterization of SdrE from S. aureus** Deqiang Wang<sup>1</sup>, Ke Chen<sup>1</sup>, Jun Zhang<sup>2</sup>

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** <u>David Leibly</u><sup>1,2</sup>, Julien Jorda<sup>2</sup>, Sunny Chun<sup>3</sup>, Alan Pang<sup>2</sup>, Michael Sawaya<sup>2</sup>, Todd Yeates<sup>1,2,3</sup> 1.-Department of Chemistry and Biochemistry, University of California, 2.-UCLA-DOE Institute for Genomics and Proteomics, 3.-Molecular Biology Institute, University of California

## $\mathsf{PI-092}$ Continuous directed evolution of receptor-selective $\partial\text{-endotoxins}$ for overcoming insecticidal resistance

<u>Ahmed Badran</u><sup>1,2</sup>, Victor Guzov<sup>3</sup>, Qing Huai<sup>3</sup>, Melissa Kemp<sup>3</sup>, Prashanth Vishwanath<sup>3</sup>, Artem Evdokimov<sup>3</sup>, Farhad Moshiri<sup>3</sup>, Meiying Zheng<sup>3</sup>, Keith Turner<sup>3</sup>, David Liu<sup>1,2</sup>

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 Maniaci<sup>1</sup>, Collin Lipper<sup>2</sup>, John J. Love<sup>1</sup> 1.-San Diego State University, 2.-University of California

# PI-094 Continuous Evolution of Site-Specific Recombinases With Highly Reprogrammed DNA Specificities

<u>Jeffrey L Bessen<sup>1,2</sup></u>, David B Thompson<sup>1,2</sup>, David R. Liu<sup>1,2</sup> 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 <u>Aleardo Morelli</u><sup>1</sup>, Burckhard Seelig<sup>1</sup>

1.-University of Minnesota

#### PI-097 Computational Design of Tighter Protein-Ligand Interfaces

Brittany Allison<sup>1</sup>, Brian Bender<sup>2</sup>, Jens Meiler<sup>1,2</sup> 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 Gonzalez<sup>1</sup>, Ste<sup>f</sup>ano Capaldi<sup>1</sup>, Maria Elena Carrizo<sup>1</sup>, Laura Destefanis<sup>1</sup>, Michele Bovi<sup>1</sup>, Massimiliano Perduca<sup>1</sup>, Hugo Luis Monaco<sup>1</sup>

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

<u>Conor Jacobs</u><sup>1</sup>, Yang Geng<sup>2</sup>, Ryan Badiee<sup>1</sup>, Tiffany Nguyen<sup>3</sup>, Andrew Evans<sup>4</sup>, Hokyung Chung<sup>1</sup>, Ying Yang<sup>2</sup>, Mehrdad Shamloo<sup>4</sup>, Roger Y. Tsien<sup>5</sup>, Michael Z. Lin<sup>2, 6</sup>

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

JULY 22 - 25, 2015

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

Edyta Kopera<sup>1</sup>, Maria Pietrzak<sup>1</sup>, Agnieszka Macioła<sup>1</sup>, Anna Maria Protas-Klukowska<sup>1</sup>, Konrad Zdanowski<sup>1</sup>, Beata Gromadzka<sup>2</sup>, Krystyna Grzelak<sup>1</sup>, Zenon Minta<sup>3</sup>, Krzysztof Śmietanka<sup>3</sup>, Bogusław Szewczyk<sup>2</sup> 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-104 Mining the structural universe for de novo design

<u>Craig Mackenzie</u><sup>1</sup>, Gevorg Grigoryan<sup>1</sup> 1.-Dartmouth College

PI-106 **Sortase-mediated synthesis of protein-DNA conjugates for sensitive biosensing** <u>Bedabrata Saha</u><sup>1</sup>, Marieke op de Beeck<sup>1</sup>, Remco Arts<sup>1</sup>, Maarten Merkx<sup>1</sup> 1.-Department of Biomedical Engineering, Eindhoven University of Technology

#### PL – OTHER/NO THEME ALLOCATED

PL-078 **Unraveling the Nature of TDP-43 Aggregates from its Putative Aggregation Domain** <u>Miguel Mompeán</u><sup>1</sup>, Rubén Hervás<sup>2</sup>, Yunyao Xu<sup>3</sup>, Timothy H. Tran<sup>4</sup>, Emanuele Buratti<sup>5</sup>, Francisco Baralle<sup>5</sup>, Liang Tong<sup>4</sup>, Mariano Carrión-Vázquez<sup>2</sup>, Ann E. McDermott<sup>3</sup>, Douglas V Laurents<sup>1</sup> 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 Alonazi<sup>1,2</sup>, Paul Engel<sup>1</sup>

1.-School of Biomolecular and Biomedical Science, Conway Institute, UCD., 2.-King Saud University, Sciences, Biochemistry department

# PL-080 Molecular characterization of specific positively selected sites in mammalian visual pigment evolution

<u>Miguel A. Fernández-Sampedro</u><sup>1</sup>, Eva Ramon<sup>1</sup>, Brandon M. Invergo<sup>2</sup>, Jaume Bertranpetit<sup>2</sup>, Pere Garriga<sup>1</sup>

1.-Grup de Biotecnologia Molecular i Industrial., 2.-IBE – Institute of Evolutionary Biology

#### PL-083 Induced oxidative modification of plasma and cellular fibrin-stabilizing factor

Anna Bychkova<sup>1</sup>, Tatiana Danilova<sup>1</sup>, Alexander Shchegolikhin<sup>1</sup>, Vera Leonova<sup>1</sup>, Marina Biryukova<sup>1</sup>, Elizaveta Kostanova<sup>1</sup>, Alexey Kononikhin<sup>1,2</sup>, Anna Bugrova<sup>1</sup>, Evgeny Nikolaev<sup>1,2</sup>, Mark Rosenfeld<sup>1</sup>, 1.-N. M. Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, 2.-Institute for Energy Problems of Chemical Physics, Russian Academy of Sciences



## TRAVEL AWARDS

The following outstanding students and early-career investigators received travel assistance to attend the 29th Annual Symposium 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, The University of Texas at Austin

#### **GRADUATE STUDENTS**

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## TRAVEL AWARDS

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

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TRAVEL AWARDS

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 assistance. These opportunities are made possible in part by support from:

#### Finn Wold Travel Award Donors

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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
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## **CALL FOR NOMINATIONS**

## 2016 AWARDS OF THE PROTEIN SOCIETY

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

The 2016 awards will be presented at the 30th Anniversary Symposium of The Protein Society on July 16-19, 2016, in Baltimore, Maryland. The deadline for submitting complete award nomination packages for the 2016 Awards cycle will be noon (EDT) on September 18, 2015.

#### Stein and Moore Award

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

#### Hans Neurath Award

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

#### **Dorothy Crowfoot Hodgkin Award**

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

#### Emil Thomas Kaiser Award

Recognizes a recent, highly significant contribution in applying chemistry to the study of proteins.

#### **Christian B. Anfinsen Award**

Recognizes significant technological achievements and/or methodological advancements in protein research.

#### Carl Brändén Award

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

#### **Protein Science Young Investigator Award**

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





## **MEETING AT A GLANCE**

WEDNESDAY 22 JULY		THUF 23 J	RSDAY JULY	FRIDAY 24 JULY		SATURDAY 25 JULY			
07:00	07:00		New Member We Members Bus	elcome Breakfast / siness Meeting					
08:30	Opening Ple Enzyme & Pathway Engineering	Proteomics (PTMs, PPIs)	Folding	Chemical Biology	Intrinsically Disordered Proteins	Observing Dynamics in Single Cells	08:30	Systems Biology	Integrative Protein Science
11:30			Lunch: Exhibits	& Poster Displays			10:50	2015 Stein & Mo	bore Award Talk
	Workshop:	Career Panel	Mentoring Comr How to Write ar	nittee Workshop:					
Noon - 01:00	on - Undergraduate Student Research Session		Educator's Lu Primary Literature Teach Foundational Sci	Incheon: Using in the Classroom to Concepts of Protein ence	Mentoring Committee Workshop: How to Give a Great Talk				
	Exhibitor Lunch Workshop: Malvern		Exhibitor Lunch	Workshop: Wyatt					
01:30	Protein Engineering	Cell Engineering	Protein Allostery & Dynamics	Engineering & Interpreting the Genome	Plenary Awards Session				
04:30	Poster Displays & Exhibits Open		Poster D Exhibi	Poster Displays & Exhibits Open					
05:30	0 Mix & Mingle Reception		Mix & Ming	le Reception					
06:30	06:30								
	Happy Hour in Honor of the 2015 Young Investigator Speakers (09:00 - 11:00 pm) <i>Level</i> 3				<b>2015 Memb</b> (08:00 - Hotel Catalonia	e <b>rs Reception</b> 10:00 pm) <i>Barcelona Plaza</i>			

Program Key		
Auditorium		
Room 6		
(room 5 - overflow)		
Main hall		
Room 3		
Room 8		
Room 4		



## WEDNESDAY, JULY 22

#### 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 am Auditorium

- 09:40 am Intro from Chair: Francesc Xavier Aviles, Universitat Autònoma de Barcelona. Barcelona, Spain.
- 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
   Yeast Proteome Dynamics from Single Cell Imaging and Automated Analysis.

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

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#### 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.
10:45 am	Young Investigator Speaker: 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 PROTEIN ENGINEERING 01:30 - 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.

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#### 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 Ebisuva, RIKEN Quantitative Biology Center, Kobe, Japan. Young Investigator Speaker: 02:05 pm Bottom-up Construction of a Synthetic Carboxysome. Shiksha Mantri, ETH Zurich. Engineering Light-Activatable Proteins for Controlling Cell Signaling Pathways. 02:20 pm Brian Kuhlman, University of North Carolina Chapel Hill, NC, United States, 25-min Coffee Break 02:50 pm 03:15 pm Phasing and Dephasing Cell Morphogenesis. Stephen Michnick. University of Montreal. Montreal. QC. Canada. Young Investigator Speaker: 03:45 pm 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. **Engineering Cell-cell Interactions.** 04:00 pm Zev Gartner, University of California San Francisco, CA, 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




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## **THURSDAY, JULY 23**

08:30 am

#### New Member Welcome Breakfast / Members Business Meeting 07:00 - 08:30 am Room 4

#### CONCURRENT MORNING SYMPOSIA FOLDING 08:30 - 11:30 am Auditorium

Intro from Chair: Irene Díaz-Moreno, Universidad de Sevilla CSIC. Sevilla. Spain.

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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 am	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
	Young Investigator Speaker:
10:45 am	Semi-Chemical Synthesis and Characterization of a Small Heat Shock Protein Bearing a Nonenzymatic Posttranslational Modification Found In Vivo.
	Maria Matveenko, University of Vienna. Vienna, Austria.
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.
	Maninouu Nasi, Halvalu Meuical School. Doston, MA, Ohiteu 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	Is it possible to understand in a quantitative manner a living system ? Luis Serrano, Centre for Genomic Regulation / ICREA. Barcelona, Spain.
	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

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### 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.
09:05 am	Young Investigator Speaker: 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	Imaging Neuronal Voltage Dynamics in Vivo with Millisecond-timescale Precision.
	Francois St. Pierre, Stanford University. Stanford, CA, United States.
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
	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 Give a Great Talk Noon - 01:00 pm Room 3

#### PLENARY AWARDS SESSION 01:30 - 06:00 pm Auditorium

- 01:30 pm Introduction from James Bowie, Protein Society President
- 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 pmVisualizing Molecular Complexity by cryo-EM to Understand Biological Function.<br/>Eva Nogales, University of California Berkeley/HHMI. Barkeley, CA, United States.02:25 pmPresentation of the Protein Science 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.
05:15 pm	Acknowledgement of the 2015 Neurath Award and Stein & Moore Award recipients
05:20 pm	Presentation of the Protein Science Best Paper Awards
05:30 pm	Presentation of the Protein Society Service Awards
05:40 pm	Presentation of the Best Poster Competition Prizes
	*Sponsored by the Hans Neurath Foundation **Sponsored by Genentech ***Sponsored by Rigaku
07:00 pm	2015 Members Reception (Catalonia Plaza Hotel)

FIRDAY, JULY 24





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### **SATURDAY, JULY 25**

#### CONCURRENT MORNING SYMPOSIA SYSTEMS BIOLOGY 08:30 - 10:20 am Auditorium

- **08:30 am** Intro from Chair: **Anne-Claude Gavin-Perrin**, *European Molecular Biology Laboratory. Heidelberg, Germany.*
- 08:35 am Disease-Associated 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 Correia, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland.
- 09:50 am Lipid-protein Networks. Anne-Claude Gavin-Perrin, European Molecular Biology Laboratory. Heidelberg, Germany.

#### 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.*

JULY 22 - 25, 2015

	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.
	<b>Debora Foguel,</b> 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

 Presenting the Stein & Moore Award to 2015 winner Bill DeGrado

 William F. DeGrado, University of California San Francisco.

 De Novo Protein Design.



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## 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).

#### 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.



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

#### Talk: Wednesday July 22 @ 03:45 PM | Protein Engineering



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.







# MARK YOUR CALENDAR

JULY 16 – 19, 2016 THE HYATT REGENCY BALTIMORE BALTIMORE, MD, USA

## **PROGRAM PLANNING COMMITTEE:**

Brenda Schulman (*Chair*), St. Jude Children's Research Hospital Nieng Yan, Tsinghua University Andreas Plückthun, University of Zurich Ralf Langen, University of Southern California

SESSIONS:

## **BIRTH, LIFE, & DEATH OF PROTEINS**

**PROTEIN EVOLUTION & DESIGN** 

**PROTEIN FOLDING & MISFOLDING** 

EMERGING METHODS FOR PROTEIN RESEARCH

MEMBRANE PROTEIN FOLDING & FUNCTION

**PROTEINS ON THE MOVE** 

**APPLIED PROTEIN RESEARCH** 

INTERFACE BETWEEN PROTEINS & NUCLEIC ACIDS

DYNAMIC MODULATION OF PROTEIN FUNCTION

FORCE IN BIOLOGY

**PROTEINS SHAPING MEMBRANES** 

INTERDISCIPLINARY APPROACHES TO PROTEIN SCIENCE

- Full-length Contributed Talk Slots In Each Session
- Celebrate 30 Years of the Society & 25 Years of Protein Science
- Free Registration for Undergraduates
- Return of the Traditional Symposium Banquet
- Short Young Investigator Talks Still Available



#### WORKSHOP - Malvern

#### Wednesday, July 22<sup>nd</sup>. 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 lsothermal 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 23<sup>rd</sup>. 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.

750 Vassar Avenue, Suite 2 Lakewood NJ, 08701 – 6929 United States Phone: +1 732 370 1300 Fax: +1 732 370 1303 Email: flo@avivbiomedical.com 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

Booth 29

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**

Unit 6, Goodwin Business Park, Willie Snaith Road, Newmarket CB8 7SQ Suffolk United Kingdom Phone: +44 (0) 778 722 9495 or +44 (0) 163 856 1051 Fax: +44 (0) 163 866 0674 Email: Jessica@moleculardimensions.com Web: www.moleculardimensions.com

At Molecular Dimensions, our love for all things crystallography drives who we are and what we do, every hour of every day. Our vision is to simply provide all our customers with the best products and intelligent solutions out there for crystallography.

Booth 3

#### NanoTemper Technologies GmbH

EXHIBITOR DIRECTOR

#### **Occhio Biotech**

Floessergasse 4 81369 Munich Germany

Phone: +49 176 110 366 00 Email: Francois.ogi@nanotemper.de

Web: www.nanotemper.de

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4 rue des Chasseurs Ardennais 4031 Angleur Belgium Phone: +32 424 300 14 Fax: +32 424 300 15 Email: info@occhio.be Web: www.occhio-biotech.com

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Booth 20

Booth 16

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#### Booth 26:



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#### PA - CELL ENGINEERING

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

<u>Bryan Berger</u><sup>1</sup>, Zhou Yang<sup>2</sup>, Leah Spangler<sup>1</sup>, Victoria Berard<sup>1</sup>, Qian He<sup>2</sup>, Li Lu<sup>2</sup>, Robert Dunleavy<sup>1</sup>, Christopher Kiely<sup>2</sup>, Steven McIntosh<sup>1</sup>

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<sup>1,2,3</sup>, Juan Diaz<sup>2,3</sup>, Jim Wells<sup>2,3</sup>

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 Sarria<sup>1</sup>, Souryadeep Bhattacharyya<sup>2</sup>, Pamela Peralta-Yahya<sup>1</sup>

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. Abboud<sup>1</sup>, Jurgen Brem<sup>1</sup>, Rasheduzzaman Chowdhury<sup>1</sup>, Ivanhoe K. H. Leung<sup>2</sup>, Timothy D. W. Claridge<sup>1</sup>, Christopher J. Schofield<sup>1</sup>

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 Acedo<sup>1</sup>, Marco van Belkum<sup>1</sup>, John Vederas<sup>1</sup>

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 Arosio<sup>1</sup>, Thomas Müller<sup>1</sup>, Luke Rajah<sup>1</sup>, Francesco Aprile<sup>1</sup>, Tom Scheidt<sup>1</sup>, Jackie Carrozza<sup>1</sup>, Maya Wright<sup>1</sup>, Michele Vendruscolo<sup>1</sup>, Christopher Dobson<sup>1</sup>, Tuomas Knowles<sup>1</sup> 1.-Department of Chemistry, University of Cambridge

### $\mathsf{PB}\text{-}004$ Using $\alpha\text{-}chymotrypsin$ and elastase enzymatic degradation to control peptide self-assembly

<u>Valeria Castelletto</u><sup>1</sup>, Ian Hamley<sup>1</sup> 1.-School of Chemistry, University of Reading

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

<u>Yuen-Yan Chang</u><sup>1</sup>, Yau-Tsz Lai<sup>1</sup>, Ligang Hu<sup>1</sup>, Ya Yang<sup>1</sup>, Ailun Chao<sup>1</sup>, Hongzhe Sun<sup>1</sup> 1.-Department of Chemistry, The University of Hong Kong

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

Irene Díaz-Moreno<sup>1</sup>, Isabel Cruz-Gallardo<sup>1</sup>, Sofía M. García-Mauriño<sup>1</sup>, Rebecca Del Conte<sup>2</sup>, B. Göran Karlsson<sup>3</sup>, Andres Ramos<sup>4</sup>, María L. Martínez-Chantar<sup>5</sup>, Francisco J. Blanco<sup>5</sup>, Myriam Gorospe<sup>6</sup>, Jacqueline A. Wilce<sup>7</sup>

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

<u>Mariapina D'Onofrio</u><sup>1</sup>, Filippo Favretto<sup>1</sup>, Serena Zanzoni<sup>1</sup>, Silvia Perez Santero<sup>1</sup>, Michael Assfalg<sup>1</sup>, Henriette Molinari<sup>1</sup>, Carlo Santambrogioc<sup>2</sup>, Rita Grandor<sup>2</sup>

1.-Department of Biotechnology, University of Verona, 2.-Department of Biotechnology and Biosciences, University of Milano-Bicocca

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

<u>Nyssa Drinkwater</u><sup>1</sup>, Shailesh Mistry<sup>2</sup>, Komagal Kannan Sivaraman<sup>1</sup>, Alessandro Paiardini<sup>3</sup>, Vicky Avery<sup>4</sup>, Peter Scammells<sup>2</sup>, Sheena McGowan<sup>1</sup> PB-033

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><sup>1</sup>, Stephanie Thee<sup>1</sup>, Johan te Biesebeek<sup>1</sup>, Petra van der Wouden<sup>1</sup>, Bert-Jan Baas<sup>1</sup>, Frank J. Dekker<sup>1</sup>

1.-Groningen Research Institute of Pharmacy

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

<u>Victoria Gomez</u><sup>1</sup>, Kavya Kolavasi<sup>1</sup>, Josh Beckham<sup>1</sup>, Jon Robertus<sup>1</sup> 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 Goodrich<sup>1</sup>, Dominique Frueh<sup>1</sup>

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<sup>1, 2</sup>

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

#### PB-013 **Peptide conjugates: From self-assembly towards applications in biomedicine** <u>lan Hamley</u><sup>1</sup>

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

<u>Franca-M. Klingler</u><sup>1</sup>, Ewgenij Proschak<sup>1</sup> 1.-Goethe University, Institute of Pharmaceutical Chemistry





#### PB-015 Protein Carbamylation at the Chemistry-Biology interface

Victoria Linthwaite<sup>1</sup>, Joana Janus<sup>1</sup>, David R.W. Hodgson<sup>2</sup>, Martin J. Cann<sup>1</sup>

1.-School of Biological and Biomedical Sciences, Durham University, 2.-Department of Chemistry, Durham University

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

Annelise de Carvalho<sup>1</sup>, Jennifer Chu<sup>2</sup>, Céline Meinguet<sup>3</sup>, Robert Kiss<sup>1</sup>, Guy Vandenbussche<sup>4</sup>, Bernard Masereel<sup>3</sup>, Yohan Wouters<sup>3</sup>, Jerry Pelletier<sup>2</sup>, <u>Véronique Mathieu<sup>1</sup></u>

1.-Laboratoire de Cancérologie et Toxicologie Expérimentale, Faculté de Pharmacie, 2.-Biochemistry Department, 3.-Namur Medicine and Drug Innovation Center (NAMEDIC-NARILIS), 4.-Laboratory for the Structure and Function of Biological Membranes

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

Maria Matveenko<sup>1</sup>, Christian Becker<sup>1</sup>

1.-Institute of Biological Chemistry, Department of Chemistry, University of Vienna

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

Manasi Mishra<sup>1</sup>, Jiri Brynda<sup>1</sup>, Michael Mares<sup>1</sup>

1.-Institute of Organic Chemistry and Biochemistry, AS CR

### PB-019 Role of the ABCC2 transporter in the mode of action of the Bacillus thuringiensis Cry1Ac toxin in the Diamond Back Moth Plutella xylostella

<u>Josué Ocelotl</u><sup>1</sup>, Jorge Sánchez<sup>2</sup>, Raquel Arroyo<sup>1</sup>, Isabel Gómez<sup>1</sup>, Gopalan Unnithan<sup>2</sup>, Bruce Tabashnik<sup>2</sup>, Alejandra Bravo<sup>1</sup>, Mario Soberón<sup>1</sup>

1.-Instituto de Biotecnología, Universidad Nacional Autónoma de México, 2.-Department of Entomology, University of Arizona

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

<u>Maria-Eleni Ourailidou</u><sup>1</sup>, Paul Dockerty<sup>1</sup>, Martin Witte<sup>1</sup>, Gerrit J. Poelarends<sup>1</sup>, Frank J. Dekker<sup>1</sup>, 1.-University of Groningen

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

<u>Arlen Peña-Cardeña</u><sup>1</sup>, Alejandra Bravo<sup>1</sup>, Mario Soberón<sup>1</sup>, Isabel Gómez<sup>1</sup> 1.-Instituto de Biotecnología, Universidad Nacional Autónoma de México

#### PB-022 Proton solvation in protic and aprotic solvents

Emanuele Rossini<sup>1</sup>, Ernst-Walter Knapp<sup>1</sup>

1.-Institute of Chemistry and Biochemistry, Freie Universität Berlin

## 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

Lana Saleh<sup>1</sup>, Esta Tamanaha, June Pais<sup>1</sup>, Romualdas Vaisvila<sup>1</sup>, Nan Dai<sup>1</sup>, Shengxi Guan<sup>1</sup>, Ivan Correa<sup>1</sup>, Christopher Noren<sup>1</sup>, Richard Roberts<sup>1</sup>, Yu Zheng<sup>1</sup> 1.-New England biolabs

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

<u>Fadwa El Tahry</u><sup>1</sup>, Ingy Hashad<sup>1</sup>, Mohamed Farouk<sup>1</sup>, Mohamed Gad<sup>1</sup> 1.-German University in Cairo (GUC)

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

<u>Christina Schroeder</u><sup>1</sup>, Sónia Henriques<sup>2</sup>, Mehdi Mobli<sup>2</sup>, Stephanie Chaousis<sup>1</sup>, Phillip Walsh<sup>1</sup>, Panumart Thongyoo<sup>1</sup>, David Craik<sup>1</sup>

1.-Institute for Molecular Bioscience, The University of Queensland, 2.-Centre for Advanced Imaging, The University of Queensland

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

<u>Montserrat Serra-Batiste</u><sup>1</sup>, Mariam Bayoumi<sup>2</sup>, Margarida Gairí<sup>3</sup>, Martí Ninot-Pedrosa<sup>1</sup>, Giovanni Maglia<sup>2</sup>, Natàlia Carulla<sup>1</sup>

1.-Institute for Research in Biomedicine (IRB Barcelona), 2.-Biochemistry, Molecular and Structural Biology Section, University of Leuven, 3.-NMR Facility, Scientific and Technological Centers, University of Barcelona

PB-027 **Molecular dynamics study on the key catalytic intermediates of threonine synthase** <u>Mitsuo Shoji</u><sup>1</sup>, Yuzuru Ujiie<sup>1</sup>, Ryuhei Harada<sup>1</sup>, Megumi Kayanuma<sup>1</sup>, Yasuteru Shigeta<sup>1</sup>, Takeshi Murakawa<sup>2</sup>, Hideyuki Hayashi<sup>2</sup>

1.-Univeristy of Tsukuba, 2.-Osaka Medical College

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

Benjamin J. Stein<sup>1</sup>, Robert A. Grant<sup>1</sup>, Robert T. Sauer<sup>1</sup>, Tania A. Baker<sup>1,2</sup>

1.-Department of Biology, Massachusetts Institute of Technology, 2.-Howard Hughes Medical Institute, Massachusetts Institute of Technology

PB-029 Interactions between U24 from HHV-6A and 7 and Nedd4 or Smurf2 WW domains Yurou Sang<sup>1</sup>, Rui Zhang<sup>1</sup>, Walter R.P. Scott<sup>1</sup>, A. Louise Creagh<sup>2</sup>, Charles A. Haynes<sup>2</sup>, S<u>uzana K. Straus<sup>1</sup></u>

1.-Department of Chemistry, University of British Columbia, 2036 Main Mall, 2.-Michael Smith Labs, University of British Columbia

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

Jinwoo Lee<sup>1</sup>, Sonia Gregory<sup>1</sup>, <u>Lukas Tamm<sup>1</sup></u> 1.-University of Virginia

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

Jackie Thompson<sup>1</sup>, Owen Nadeau<sup>1</sup>, Gerald Carlson<sup>1</sup>

1.-Department of Biochemistry and Molecular Biology, University of Kansas Medical Center

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

<u>Christine Touma</u><sup>1</sup>, Nicolas Paquet<sup>2</sup>, Derek J. Richard<sup>2</sup>, Roland Gamsjaeger<sup>1,3</sup>, Liza Cubeddu<sup>1,3</sup> 1.-School of Science and Health, University of Western Sydney, 2.-Queensland University of Te chnology, 3.-School of Molecular Bioscience, University of Sydney



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

Luis Valencia<sup>1,2</sup>, Josh Beckham<sup>2</sup>, Oscar Villarreal, Jon Robertus<sup>2</sup> 1.-University of Texas at Austin, 2.-Freshman Research Initiative

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

<u>Pedro Alberto Valiente Flores</u><sup>1</sup>, Maarten G Wolf<sup>2</sup>, Yasel Guerra<sup>3</sup>, Isel Pascual<sup>1</sup>, Isabelle Florent<sup>4</sup>, Enrique Rudiño<sup>3</sup>, Pedro Geraldo Pascutti<sup>5</sup>, Tirso Pons<sup>6</sup>, Gerrit Groenhof<sup>2</sup>

1.-Center of Protein Studies, Faculty of Biology, University of Havana., 2.-Max Planck Institute of Biophysical Chemistry, 3.-Biotechnology Institute. UNAM, 4.-CNRS-MNHN, 5.-Biophysics Institute. Federal University of Rio de Janeiro, 6.-Spanish National Cancer Research Centre

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

Antonello Melrino<sup>1</sup>, Irene Russo Krauss<sup>2</sup>, Marco Caterino<sup>1</sup>, <u>Alessandro Vergara<sup>1</sup></u> 1.-Dept. Chemical Sciences, University of Naples Federico II, 2.-Institute of Biostructures and Bioimaging, CNR

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

<u>Martin Witte<sup>1</sup></u>, Jonas Lohse<sup>1</sup>, Remko Welker<sup>1</sup> 1.-Stratingh Institute for Chemistry, University of Groningen

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

Sandra Kerstin Wittmann<sup>1</sup>, Daniel Moser<sup>1</sup>, Jan Sebastian Kramer<sup>1</sup>, René Blöcher<sup>1</sup>, Janosch Achenbach<sup>3</sup>, Denys Pogoryelov<sup>2</sup>, Eugen Proschak<sup>1</sup>

1.-Institute of Pharmaceutical Chemistry, LiFF/OSF/ZAFES, Goethe-University, 2.-Institute of Biochemistry, Goethe University, 3.-BASF SE

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

Hassan Zanna<sup>1</sup>, Andrew Nok<sup>2</sup>, Sani Ibrahim<sup>2</sup>, Hauwa Inuwa<sup>2</sup>

1.-University of Maiduguri, 2.-Ahmadu Bello University

#### PB-040 Ubiquitin-nanoparticle interactions by solution NMR spectroscopy

<u>Serena Zanzoni</u><sup>1</sup>, Michael Assfalg<sup>1</sup>, Rajesh K Singh<sup>2</sup>, Marco Pedroni<sup>3</sup>, Adolfo Speghini<sup>3</sup>, David Fushman<sup>2</sup>, Mariapina D'Onofrio<sup>1</sup>

1.-NMR Laboratory, Department of Biotechnology, University of Verona, 2.-Center For Biomolecular Structure and Organization, Department of Chemistry and Biochemistry, University of Maryland, 3.-Solid State Chemistry Laboratory, Department of Biotechnology, University of Verona

#### PB-041 Chemical-Genetic Dissection of Protein Kinase Functions

Chao Zhang<sup>1</sup>, Ying-Chu Chen<sup>1</sup>, Alvin Kung<sup>1</sup>

1.-Department of Chemistry, University of Southern California

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

Chi-Ming Ho<sup>1</sup>, Jun-Long Zhang<sup>1</sup>, <u>Cong-Ying Zhou<sup>1</sup></u>, On-Yee Chan<sup>1</sup>, Jessie Jing Yan<sup>1</sup>, Fu-Yi Zhang<sup>1</sup>, Jie-Sheng Huang<sup>1</sup>, Chi-Ming Che<sup>1</sup>

1.-The University of Hong Kong

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

Jia-Cherng Horng<sup>1</sup>, Kuei-Yen Huang<sup>1</sup>

1.-Department of Chemistry, National Tsing Hua University

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

Bashkim Kokona<sup>1</sup>, Carrie A. May<sup>2</sup>, Nicole R. Cunningham<sup>1</sup>, Franklin J. Garcia<sup>1</sup>, Kathleen M. Ulrich<sup>1</sup>, Christine M. Roberts<sup>4</sup>, Christopher D. Link<sup>4</sup>, Walter F. Stafford<sup>3</sup>, Thomas M. Laue<sup>2</sup>, Robert Fairman<sup>1</sup> 1.-Department of Biology, Haverford College, 2.-Department Of Molec., Cell., and Biomed. Sci., University of New Hampshire, 3.-Boston Biomedical Research Institute, 4.-Integrative Physiology, University of Colorado Boulder

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

<u>Robert Fairman</u><sup>1</sup>, Bashkim Kokona<sup>1</sup>, Emily S. Winesett<sup>2</sup>, Alfred N. von Krusenstiern<sup>2</sup>, Max J. Cryle<sup>3</sup>, Louise K. Charkoudian<sup>2</sup>

1.-Department of Biology, Haverford College, 2.-Department of Chemistry, Haverford College, 3.-Max Planck Institute for Medical Research

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

<u>Francisco Tenjo Castaño</u><sup>1,2</sup>, Manuel Garavito<sup>1,2</sup>, Leonor García<sup>1,2</sup>, Silvia Restrepo<sup>2</sup>, Barbara Zimmermann<sup>1</sup>

1.-Biochemistry and Molecular Biology Research Group, Universidad de los Andes., 2.-Mycology and Plan Pathology Laboratory, Universidad de los Andes

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

<u>Walter Scott</u><sup>1</sup>, Vivien Schubert<sup>2</sup>, Andi Mainz<sup>2</sup>, Suzana K. Straus<sup>1</sup>, Roderich Suessmuth<sup>2</sup> 1.-Department of Chemistry, University of British Columbia, 2.-Institut fuer Chemie, Technische Universitaet Berlin

### PB-048 Studying the Outer Membrane ß-barrel Protein LptD, the Target of a New Peptidomimetic Antibiotic

<u>Katja Zerbe</u><sup>1</sup>, Gloria Andolina<sup>1</sup>, Laszlo Bencze<sup>1</sup>, Kerstin Moehle<sup>1</sup>, John A. Robinson<sup>1</sup> 1.-Department of Chemistry, University Zurich

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

<u>Wioletta Zmudzinska</u><sup>1</sup>, Marcel Thiel<sup>1</sup>, Stanislaw Oldziej<sup>1</sup> 1.-IFB, University of Gdansk and Medical University of Gdansk

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

Maria Winiewska<sup>1</sup>, Jarosław Poznański<sup>1</sup>

1.-Institute of Biochemistry and Biophysics Polish Academy of Sciences





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

<u>Kaitlyn M. Towle</u><sup>1</sup>, Christopher T. Lohans<sup>2</sup>, Marco J. van Belkum<sup>1</sup>, Mark Miskolzie<sup>1</sup>, John C. Vederas<sup>1</sup> 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

Roxana Yesenia Pastrana Alta<sup>1</sup>, Maria Teresa Machini<sup>2</sup>, Breno Pannia Espósito<sup>1</sup>

1.-Laboratory for Bioinorganic Chemistry and Metallodrugs, Instituto de Química, 2.-Laboratory of Peptide Chemistry, Instituto de Química, Universidade de São Paulo

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

<u>Przemyslaw Glaza</u><sup>1</sup>, Tomasz Wenta<sup>1</sup>, Jerzy Osipiuk<sup>2,3</sup>, Agnieszka Kowalska<sup>1</sup>, Ewa Gebal<sup>1</sup>, Dorota Zurawa-Janicka<sup>1</sup>, Adam Lesner<sup>4</sup>, Barbara Lipinska<sup>1</sup>

1.-Department of Biochemistry, Faculty of Biology, University of Gdansk, 2.-Midwest Center for Structural Genomics, Argonne National Laboratory, 3.-Structural Biology Center, Biosciences Division, Argonne National Laboratory, 4.-Department of Biochemistry, Faculty of Chemistry, University of Gdansk

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

<u>Katarzyna Kuciñska</u><sup>1</sup>, Maria Winiewska<sup>1</sup> Jarosław Poznański<sup>1</sup> 1.-Institute of Biochemistry and Biophysics Polish Academy of Sciences

#### PB-056 Antibody Activation using DNA-Based Logic Gates

<u>Maarten Merkx</u><sup>1</sup>, Brian Janssen<sup>1</sup>, Martijn van Rosmalen<sup>1</sup>, Lotte van Beek<sup>1</sup> 1.-Laboratory of Chemical Bology, Eindhoven University of Technology

### PB-057 Insights of a novel kind of cell wall binding domain that cleaves the peptidoglycan muropeptide: the CW\_7 motif

<u>Noemí Bustamante<sup>1,3</sup>, Manuel</u> Iglesias, Noella Silva-Martín, Isabel Uson, Pedro García, Juan Hermoso, Marta Bruix, Margarita Menéndez

1.-Institute of Physical-Chemistry 'Rocasolano', CSIC, 2.-Institute of Physical-Chemistry 'Rocasolano', CSIC, 3.-Ciber of Respiratory Diseases (CIBERES), 4.-Center of Biological Research (CIB), CSIC, 5.-Institucio Catalana de Recerca i Estudis Avançats, CSIC-IBMB

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

Amaris Torres-Delgado<sup>1</sup>, Robert T. Sauer<sup>1</sup>, Tania A. Baker<sup>1,2</sup>

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

Yazan Alhadid<sup>1</sup>, Benjamin Allen<sup>2</sup>, Sangyoon Chung<sup>1</sup>, Dylan Taatjes<sup>2</sup>, Shimon Weiss<sup>1</sup> 1.-University of California, Los Angeles, 2.-University of Colorado Boulder

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

<u>Ewelina Guca</u><sup>1</sup>, François Hoh<sup>2</sup>, Jean-François Guichou<sup>2</sup>, Henri Vial<sup>1</sup>, Rachel Cerdan<sup>1</sup> 1.-DIMNP, UMR 5235, University of Montpellier, 2.-Centre de Biochimie Structurale, INSERM UMR 1054, CNRS UMR 5048

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

Anniek Den Hamer<sup>1</sup>, Lenne Lemmens<sup>1</sup>, Tom de Greef<sup>1</sup>, Christian Ottmann<sup>1</sup>, Maarten Merkx<sup>1</sup>, Luc Brunsveld<sup>1</sup>

1.-Eindhoven University of Technology

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

Luca Sorrentino<sup>1</sup>, Laura Rigamonti<sup>1</sup>, Mirvan Krasnigi<sup>1</sup>, Alessandra Calogero<sup>1</sup>, Vittorio Pandini<sup>1</sup>, Maria Antonietta Vanoni<sup>1</sup>, Alessandro Aliverti<sup>1</sup>

1.-Department of Biosciences, Università degli Studi di Milano

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

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1.-Dipartimento di Bioscienze, Università degli Studi di Milano, 2.-Dipartimento di Scienze Veterinarie e Sanità Pubblica. Università degli Studi di

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

Beata Wielgus-Kutrowska<sup>1</sup>, Joanna Krasowska<sup>1</sup>, Agnieszka Bzowska<sup>1</sup>, László Forró<sup>2</sup>, Andrzej Sienkiewicz<sup>2,3</sup>

1.-Department of Biophysics, Institute of Experimental Physics, Warsaw University, 2.-Laboratory of Physics of Complex Matter (LPMC), 3.-ADSresonances

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

Aishling M. Doolan<sup>1</sup>, Maike C. Jürgens<sup>1</sup>, Amir R. Khan<sup>2</sup>, Peter B. Crowley<sup>1</sup> 1.-School of Chemistry, National University of Ireland Galway, 2.-School of Biochemistry and Immunology, Trinity College Dublin

#### PB-066 Macromolecular crowding modulates enzyme catalysis

Annelise Gorensek<sup>1</sup>, Luis Acosta<sup>1</sup>, Garv Pielak<sup>1,2,3</sup>

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

#### PB-067 Biophysical and biochemical characterization of Arabidopsis thaliana Calmodulinlike protein CML14

Rosario Vallone<sup>1</sup>, Valentina La Verde<sup>1</sup>, Mariapina D'Onofrio<sup>1</sup>, Alessandra Astegno<sup>1</sup>, Paola Dominici<sup>1</sup> 1.-Biotechnology Department, University of Verona

#### PB-068 FBP17 controls the hepatocyte morphology through Rho signaling

Jun Zhang<sup>1</sup>, Mingming Ling<sup>1</sup>, Qianying Zhang<sup>1</sup>, Yunhong Wang<sup>1</sup>, Degiang Wang<sup>2</sup> 1.-The Department of Cell Biology and Genetics, 2.-Key Laboratory of Molecular Biology on

Infectious Disease

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

Jovan Dragelj<sup>1</sup>, Anna-Lena Woelke<sup>1</sup>, Ulrike Alexiev<sup>2</sup>, Ernst-Walter Knapp<sup>1</sup>

1.-Fachbereich Biologie, Chemie, Pharmazie/Institute of Chemistry and Biochemistry, 2.-Fachbereich Physik/Department of Physics

#### PB-070 Efficient Methods in the Production of Unnatural Amino Acid Containing Proteins Christopher Walters<sup>1</sup>, Solongo Batjargal, Anne Wagner, E. James Petersson

1.-University of Pennsylvania





### PB-071 Function and modularity of CW\_7 motives in the C-terminal region of the endolysin CpI-7 encoded by the Cp7 pneumococcal bacteriophage

Manuel Iglesias-Bexiga<sup>1,2</sup>, Noelia Bernardo-García<sup>3</sup>, Rubén Martínez-Buey<sup>4</sup>, Noemí Bustamante<sup>1,2</sup>, Guadalupe García<sup>1,2</sup>, Marta Bruix<sup>1</sup>, Juan Hermoso<sup>3</sup>, Margarita Menéndez<sup>1,2</sup>

1.-Dept. of Biological Physical-Chemistry, IQFR-CSIC, 2.-Ciber of Respiratory Diseases (CIBERES), 3.-Department of Crystallography and Structural Biology, IQFR-CSIC, 4.-University of Salamanca

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

<u>Caitlyn Mills</u><sup>1</sup>, Pengcheng Yin<sup>1</sup>, Penny Beuning<sup>1</sup>, Mary Jo Ondrechen<sup>1</sup> 1.-Northeastern University

### PB-073 **Directly observing the synergistic dynamics in F-actin and microtubule assembly** Jun Zhang<sup>1</sup>, Deqiang Wang<sup>2</sup>

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

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

<u>Jeroen Briels</u><sup>1</sup>, Maria Bartel<sup>1</sup>, Elvan Yilmaz<sup>2</sup>, Philipp Thiel<sup>3</sup>, Markus Kaiser<sup>2</sup>, Christian Ottmann<sup>1</sup> 1.-Laboratory of Chemical Biology, Eindhoven University of Technology, 2.-Centre for Medical Biotechnology, University of Duisburg-Essen, 3.-Department of Computer Science, University of Tübingen

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

Tomasz Kochanczyk<sup>1</sup>, Michal Nowakowski<sup>2</sup>, Dominika Wojewska<sup>1</sup>, <u>Artur Krezel<sup>1</sup></u> 1.-Laboratory of Chemical Biology, Faculty of Biotechnology, University of Wroclaw, 2.-Laboratory of NMR Spectroscopy, Center of New Technology, University of Warsaw

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

Wouter Engelen<sup>1</sup>, Brian Janssen<sup>1</sup>, Maarten Merkx<sup>1</sup> 1.-Eindhoven University of Technology

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

Giuseppina De Simone<sup>1</sup>, Simone Carradori<sup>2</sup>, Emma Langella<sup>1</sup>, Simona Maria Monti<sup>1</sup>, Claudiu T. Supuran<sup>3</sup>, <u>Katia D'Ambrosio<sup>1</sup></u>

1.-Istituto di Biostrutture e Bioimmagini-CNR, 2.-Department of Pharmacy, 'G. D'Annunzio' University of Chieti-Pescara, 3.-Università D egli Studi Di Firenze, NEUROFARBA Department

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

Ana Bernardo Gancedo<sup>1</sup> 1.-University of Cambridge

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

Anna Di Fiore<sup>1</sup>, Giuseppina De Simone<sup>1</sup>, Alessandro Vergara<sup>1,2</sup>, Marco Caterino<sup>2</sup>, Vincenzo Alterio<sup>1</sup>, Simona M. Monti<sup>1</sup>, Joanna Ombouma<sup>3</sup>, Pascal Dumy<sup>3</sup>, Claudiu T. Supuran<sup>4</sup>, Jean-Yves Winum<sup>3</sup> 1.-Istituto di Biostrutture e Bioimmagini-CNR, via Mezzocannone 16 - 80134 Naples., 2.-University of Naples Federico II, Via Cinthia - 80126, Naples., 3.-Institut des Biomolécules Max Mousseron-CNRS, Université de Montpellier., 4.-Università Degli Studi Di Firenze, NEUROFARBA Department

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

<u>Heather Findlay</u><sup>1</sup>, Sowmya Purushothaman<sup>2</sup>, Oscar Ces<sup>2</sup>, Paula Booth<sup>1</sup> 1.-Kings College London, 2.-Imperial College London

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

Emma Langella<sup>1</sup>, Ida Autiero<sup>1</sup>, Michele Saviano<sup>2</sup>

1.-National Research Council, Institute of Biostructures and Bioimaging, 2.-National Research Council, Institute of Crystallography

#### PB-082 Establishing a tool box for generating designer nucleosomes

Diego Aparicio Pelaz<sup>62945</sup>, Henriette Mahler, Dirk Schwarzer, Wolfgang Fischle

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

<u>Jinfeng Shao</u><sup>1</sup>, Andy-Mark W.H. Thunnissen<sup>1</sup>, Jaap Broos<sup>1</sup> 1.-Laboratory of Biophysical Chemistry, University of Groningen

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

Julia Sindlinger<sup>1</sup>, Alexander Dose<sup>1</sup>, Jan Bierlmeier<sup>1</sup>, Frank Essmann<sup>1</sup>, Markus Hartl<sup>2</sup>, Iris Finkemeier<sup>3</sup>, Dirk Schwarzer<sup>1</sup>

1.-Interfaculty Institute of Biochemistry, University of Tuebingen, 2.-Max Planck Institute of Biochemistry, 3.-Max Planck Institute for Plant Breeding Research

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

<u>Kerstin Lippl</u><sup>1</sup>, Martine Abboud<sup>1</sup>, Christoph Loenarz<sup>2</sup>, Christopher Schofield<sup>1</sup> 1.-Department of Chemistry, University of Oxford, United Kingdom, 2.-Department of Chemistry, University of Nottingham, United Kingdom

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

<u>Alina Filip</u><sup>1</sup>, Judith H Bartha-Vári<sup>1</sup>, Gergely Bánóczy<sup>2</sup>, László Poppe<sup>2</sup>, Csaba Paizs<sup>1</sup>, Florin-Dan Irimie<sup>1</sup> 1.-Biocatalysis and Biotransformation Research Group, Department of Chemistry, UBB, 2.-Department of Organic Chemistry and Technology

#### PB-087 High affinity synthetic antibodies as biological tools

<u>Mateusz Lugowski</u><sup>1</sup>, Malgorzata Nocula-Lugowska<sup>1</sup>, Somnath Mukherjee<sup>1</sup>, Anthony Kossiakoff<sup>1</sup> 1.-Department of Biochemistry and Molecular Biology, The University of Chicago

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

Tai Kubo1, Mohammed Naimuddin1, Seigo Ono1

1.-National Institute of Advanced Industrial Science and Technology (AIST)

#### PB-089 Stereoselectivity of PAL under non-optimal conditions

<u>Andrea Varga</u><sup>1</sup>, Botond Nagy<sup>1</sup>, Melinda Miklós<sup>1</sup>, Florin-Dan Irimie<sup>1</sup>, László Poppe<sup>2</sup>, Csaba Paizs<sup>1</sup> 1.-Biocatalysis and Biotransformation Research Group, Department of Chimie, UBB

#### PC - ENZYME & PATHWAY ENGINEERING

### PC-001 Biochemical Characterization and Amino Acid Sequence Analysis of Thermostable Endo-ß-1, 4-glucanase from Trichoderma viride

Nidhee Chaudhary<sup>1</sup>, Monendra Grover<sup>2</sup>

1.-Amity Institute of Biotechnology, Amity University Uttar Pradesh, Sector-125, 2.-1Centre for Agricultural Bioinformatics, IASRI





### $\mathsf{PC}\text{-}002$ $\,$ Modulation of the enzymatic activity of protein arginine methyltransferase 1 by small molecules

Wey-Jing Lin<sup>1</sup>

1.-National Yang-Ming University

PC-003 **Oligomerisation properties of light-dependent protochlorophyllide oxidoreductase** <u>Michal Gabruk</u><sup>1</sup>, Anna Piszczek<sup>1</sup>, Bozena Skupien-Rabian<sup>1</sup>, Sylwia Kedracka-Krok<sup>1,2</sup>, Jerzy Kruk<sup>1</sup>, Beata Mysliwa-Kurdziel<sup>1</sup>

1.-Faculty of Biochemistry, Biophysics and Biotechnology, Jagiellonian University, 2.-Malopolska Centre of Biotechnology, Jagiellonian University

#### PC-004 **Preparation of insect prothoracicotropic hormone with complicated disulfide-bond** structure, by the heterologous expression in Brevibacillus choshinensis

<u>Kazuki Saito</u><sup>1</sup>, Tadafumi Konogami<sup>1</sup>, Yiwen Yang<sup>1</sup>, Yusuke Yamashita<sup>1</sup>, Masatoshi Iga<sup>1</sup>, Tamari Hoshikawa<sup>1</sup>, Hiroshi Kataoka<sup>1</sup>

1.-Dept. of Integrated Biosciences, Grad. Sch. of Frontier Sciences, Univ. of Tokyo

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

Tadafumi Konogami<sup>1</sup>, Yiwen Yang<sup>1</sup>, Mari H. Ogihara<sup>1</sup>, Juri Hikiba<sup>1</sup>, Hiroshi Kataoka<sup>1</sup>, Kazuki Saito<sup>1</sup> 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

Miroslava Kopecka<sup>1, 2</sup>, Zdenek Kukacka<sup>3</sup>, Petr Man<sup>3</sup>, Tomas Obsil<sup>2</sup>, Veronika Obsilova<sup>2</sup> 1.-2nd Faculty of Medicine, Charles University in Prague, 2.-Institute of Physiology of the Czech Academy of Sciences, 3.-Institute of Microbiology of the Czech Academy of Sciences

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

Tyler Korman<sup>1</sup>, Paul Opgenorth<sup>1</sup>, James Bowie<sup>1</sup>

1.-Department of Chemistry and Biochemistry, University of California Los Angeles

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

Soon Goo Lee<sup>1</sup>, Joseph Jez<sup>1</sup>

1.-Washington University in St. Louis

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

<u>Masahiro Matsumiya</u><sup>1</sup>, Hiromi Kakizaki<sup>1</sup>, Mana Ikeda<sup>1</sup> 1.-College of Bioresource Sciences, Nihon University

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

Mohd Shukuri Mohamad Ali<sup>1,2</sup>, Ira Maya Haris<sup>1,2</sup>, Raja Noor Zaliha Raja Abd Rahman<sup>1,2</sup>, Mahiran Basri<sup>2,3</sup>, Abu Bakar Salleh<sup>1,2</sup>

1.-Enzyme and Microbial Technology Research Center, 2.-Faculty of Biotechnology and Biomolecular Sciences, 3.-Faculty of Science

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

<u>Malgorzata Nocula-Lugowska</u><sup>1</sup>, Mateusz Lugowski<sup>1</sup>, Anthony A. Kossiakoff<sup>1</sup> 1.-The University of Chicago

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

Bhumika S. Shah<sup>1</sup>, Karl A. Hassan A. Hassan<sup>1</sup>, Heather E. Clift<sup>1</sup>, Stephen J. Harrop<sup>2</sup>, Ian T. Paulsen<sup>1</sup>, Bridget C. Mabbutt<sup>1</sup>

1.-Department of Chemistry and Biomolecular Sciences, Macquarie University, 2.-School of Physics, University of New South Wales

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

Serap Pektas<sup>1, 2</sup>, Michael Knapp<sup>1</sup>

1.-University of Massachusetts Amherst, 2.-Recep Tayyip Erdogan University

PC-014 New pharmacological therapies against congenital erythropoietic porphyria (CEP) Pedro David Urquiza<sup>1</sup>, Ana Laín<sup>1</sup>, Arantza Sanz<sup>1</sup>, Juan Manuel Falcón<sup>1, 2</sup>, Oscar Millet<sup>1</sup> 1.-CIC bioGUNE, 2.-Ikerbasque

#### 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><sup>1</sup>, Misaki Kinoshita<sup>1</sup>, Takahisa Ikegami<sup>1,2</sup>, Genji Kurisu<sup>1</sup>, Yuji Goto<sup>1</sup>, Toshiharu Hase<sup>1</sup>, Young-Ho Lee<sup>1</sup>

1.-Institute for Protein Research, Osaka University, 2.-Yokohama City University

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

Lisa Ngu<sup>1</sup>, Kevin Ramos<sup>1</sup>, Nicholas DeLateur<sup>1</sup>, Penny Beuning<sup>1</sup>, Mary Jo Ondrechen<sup>1</sup> 1.-Department of Chemistry & Chemical Biology, Northeastern University

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

Benjamin Saylor<sup>1</sup>

1 -San Diego State University

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

Ju-Yi Hsieh<sup>1</sup>, Yi-Liang Liu<sup>1</sup>, Guang-Yaw Liu<sup>2</sup>, Hui-Chih Hung<sup>1</sup>

1.-Department of Life Sciences and Institute of Bioinformatics, National Chung Hsin, 2.-Institute of Microbiology & Immunology, Chung Shan Medical University, and Divis

### $\mathsf{PC}\text{-}020$ Structure-Function Relationships of human Aldo-Keto Reductase 1B15, AN enzyme active with 9-cis-Retinaldehyde

Joan Giménez Dejoz<sup>1</sup>, Michal H. H. Kolář<sup>2,3</sup>, Francesc Xavier Ruiz<sup>4</sup>, Isidro Crespo<sup>1</sup>, Alexandra Cousido-Siah<sup>4</sup>, Alberto Podjarny<sup>4</sup>, Jindřich Fanfrlík<sup>2</sup>, Xavier Parés<sup>1</sup>, Jaume Farrés<sup>1</sup>, Sergio Porté<sup>1</sup> 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

<u>Olumide Kavode<sup>1, 2</sup>,</u> Thomas R. Caulfield<sup>3</sup>, Ruiying Wang<sup>2</sup>, Devon Pendlebury<sup>2</sup>, Alexei Soares<sup>4</sup>, Evette S. Radisky<sup>2</sup>

1.-Mayo Graduate School, 2.-Department of Cancer Biology, Mayo Clinic Cancer Center, 3.-Department of Neuroscience, Mayo Clinic College of Medicine, 4.-Biology Department, Brookhaven National Laboratory



#### PC-022 Determinants for regioselectivity in Lytic Polysaccharide MonoOxygenases (LPMOs)

Barbara Danneels<sup>1</sup>, Magali Tanghe<sup>1</sup>, Henk-Jan Joosten<sup>2</sup>, Tom Desmet<sup>1</sup> 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-Morande<sup>1</sup>, Victor Castro-Fernández<sup>1</sup>, Felipe Merino<sup>1</sup>, César Ramírez-Sarmiento<sup>1</sup>, Francisco Fernández<sup>2</sup>, Cristina Vega<sup>2</sup>, <u>Victoria Guixé<sup>1</sup></u>

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

Laura Acquasaliente<sup>1</sup>, Giulia Pontarollo<sup>1</sup>, Alexiej V. Sokolov<sup>2</sup>, Simone Tescari<sup>1</sup>, Vadim B. Vasilyev<sup>2</sup>, Vincenzo De Filippis<sup>1</sup>

1.-Department of Pharmaceutical and Pharmacological Sciences, University of Padua, 2.-State University of Saint-Petersburg

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

<u>Benoit Villiers</u><sup>1</sup>, François Stricher<sup>1</sup> 1.-Global Bioenergies

 $\mathsf{PC}\text{-}026$   $\,$  The development of a coupled enzyme assay to detect isochorismate pyruvate lyase activity

Linda Jäger<sup>1</sup>, Christian Jäckel<sup>1</sup>, Peter Kast<sup>1</sup>, Donald Hilvert<sup>1</sup> 1.-LOC, ETH Zürich

#### PD - FOLDING

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

Mostafa Ahmed<sup>1,2</sup>, Martin Safo<sup>1,2</sup>, J. Neel Scarsdale<sup>1,3</sup>, Glen Kellogg<sup>1,2</sup>

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)

Tania Raquel Berrocal Gama<sup>1</sup>, Jesús Renan Vergara Gutiérrez<sup>1</sup>, Andrés Escandón Flores<sup>1</sup>, Alejandro Sosa Peinado<sup>1</sup>

1.-National Autonomus University of Mexico, Faculty of Medicine

PD-003 A hypothesis to reconcile the physical and chemical unfolding of proteins <u>Guilherme de Oliveira</u>, Jerson Silva

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

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

<u>Feng Ding</u><sup>1</sup>, Praveen Nedumpully-Govindan<sup>1</sup> 1.-Clemson Unversity

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

David Gnutt<sup>1</sup>, Michael Senske<sup>1</sup>, <u>Simon Ebbinghaus</u><sup>1</sup> 1.-Department of Physical Chemistry II, Ruhr-University Bochum, Germany

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

Angelo Figueiredo<sup>1</sup>, Sivanandam Veeramuthu<sup>2</sup>, Oscar Millet<sup>2</sup>, Eurico Cabrita<sup>1</sup>

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. Garg<sup>1</sup>, Bishwajit Kundu<sup>1</sup> 1.-Indian Institute of Technology Delhi

#### PD-008 GroEL assisted folding of multiple recombinant proteins simultaneously overexpressed in E.coli

<u>Megha Goyal</u><sup>1</sup>, Tapan Kumar Chaudhuri<sup>1</sup> 1.-Indian Institute of Technology Delhi

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

Shuanghong Huo<sup>1</sup>, Mojie Duan<sup>1,2</sup>, Hanzhong Liu<sup>1</sup>, Minghai Li<sup>1</sup> 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

<u>Tatsuya Ikenoue</u><sup>1</sup>, Lee Young-Ho<sup>1</sup>, Tetsuhei Uenoyama<sup>1</sup>, Daniel Otzen<sup>2</sup>, Yuji Goto<sup>1</sup> 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><sup>1</sup>, Ewelina Krysztofinska<sup>1</sup>, Santiago Martínez-Lumbreras<sup>1</sup>, Arjun Thapaliya<sup>1</sup> 1.-Chemistry Department, King's College London

#### $\mathsf{PD}\text{-}012$ Interaction of curcumin analogs with $\alpha\text{-}Synuclein\text{:}$ Modulation of Aggregation and Toxicity

<u>Narendra Jha</u><sup>1</sup>, A. Anoop<sup>1</sup>, Narasimham Ayyagari<sup>1</sup>, Pradeep Singh<sup>1</sup>, I.N.N. Namboothiri<sup>1</sup>, Samir Maji<sup>1</sup> 1.-Indian Institute of Technology Bombay

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

Adrian Nickson<sup>1</sup>, Jeff Hollins<sup>1</sup>, Ola Nilsson<sup>2</sup>, Gunnar von Heijne<sup>2</sup>, Jane Clarke<sup>1</sup>

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 Pandey<sup>1</sup>, Barry Farmer<sup>2</sup>

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><sup>1</sup>, Hagan Bayley<sup>2</sup>

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

<u>Sergio Romero</u><sup>1</sup>, Miguel Costas<sup>2</sup>, Adela Rodríguez-Romero<sup>3</sup>, D. Alejandro Fernández-Velasco<sup>1</sup>

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 Saad<sup>1</sup>, Jiri Vlach<sup>1</sup>, Ruba Ghanam<sup>1</sup>

1.-Department of Microbiology, University of Alabama at Birmingham

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

Natalia Catalina Sarmiento Alam<sup>1</sup>, Johannes Buchner<sup>1</sup>

1.-Department Chemie, Technishe Universität München

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

Arnaldo Serrano<sup>1</sup>, Ling-Hsien Tu<sup>2</sup>, Daniel Raleigh<sup>2</sup>, Martin Zanni<sup>1</sup>

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

<u>Austin E. Smith</u><sup>1</sup>, Larry Z. Zhou<sup>1</sup>, Annelise H. Gorensek<sup>1</sup>, Michael Senske<sup>2</sup>, Gary J. Pielak<sup>1,3,4</sup> 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

<u>Ramakrishna Vadrevu</u><sup>1</sup>, Jagadeesh Gullipalli<sup>1</sup>, Rajashekar Kadumuri<sup>1</sup>, Srividya Subramanian<sup>1</sup>, Koushik Chandra<sup>2</sup>, Hanudutta Atreya<sup>2,3</sup>

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<sup>1,2</sup>, Lien Chu<sup>1,2</sup>, Xiaolin Wang<sup>1,2</sup>, Christopher A. Waudby<sup>1,2</sup>, John Christodoulou<sup>1,2</sup>, Lisa D. Cabrita<sup>1,2</sup>

1.-Institute of Structural and Molecular Biology, University College London, 2.-Institute of Structural and Molecular Biology, Birkbeck College London

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

Sangyeol Kim<sup>1,2,4</sup>, Wookyung Yu<sup>2,3</sup>, Bora Kwon<sup>2,3</sup>, Seongjun Park<sup>2</sup>, Iksoo Chang<sup>1,2,3</sup>

1.-Research Institute, Daegu Gyeongbuk Institute of Science and Technology, 2.-Center for Proteome Biophysics, Daegu Gyeongbuk Institute of Science and Technolo, 3.-Department of Brain Science, Daegu Gyeongbuk Institute of Science and Technology, 4.-Department of Physics, Pusan National University

### PD-024 Biophysical analysis of partially folded states of myoglobin in presence of 2,2,2-trifluoroethanol

Paurnima Talele<sup>1</sup>, Nand Kishore<sup>1</sup>

1.-Indian Institute of Technology Bombay

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

Hector Zamora-Carreras<sup>1</sup>, Roberto Silva-Rojas<sup>1</sup>, Beatriz Maestro<sup>2</sup>, Erik Strandberg<sup>3</sup>, Anne Ulrich<sup>0</sup>, Jesús M Sanz<sup>2</sup>, Marta Bruix<sup>1</sup>, <u>M Angeles Jimenez<sup>1</sup></u>

1.-Instituto de Química Fisica Rocasolano (IQFR-CSIC), 2.-Instituto de Biología Molecular y Celular, Universidad Miguel Hernández, 3.-Institute of Biological Interfaces, Karlsruhe Institute of Technology (KIT), 4.-dInstitute of Organic Chemistry, Karlsruhe Institute of Technology (KIT)

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

Joanna Makowska<sup>1</sup>, Dorota Uber<sup>1</sup>, Wioletta Żmudzińska<sup>2</sup>, Caterina Tiberi<sup>3</sup>, Lech Chmurzyński<sup>1</sup>, Anna Maria Papini<sup>3</sup>

1.-Faculty of Chemistry, University of Gdansk, 2.-Laboratory of Biopolymer Structure, Intercollegiate Faculty of Biotechnology, Medical University of Gdansk, 3.-Dipartimento di Chimica Organica 'Ugo Schiff ', Universit'a di Firenze

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

Estella Newcombe<sup>1</sup>, Yasmin Ramdzan<sup>1</sup>, Ashish Sethi<sup>1</sup>, Michael Lee<sup>2</sup>, Dorothy Loo<sup>3</sup>, Bim Graham<sup>2</sup>, James Swarbrick<sup>2</sup>, Anthony Purcell<sup>3</sup>, Paul Gooley<sup>1</sup>, Danny Hatters<sup>1</sup>

1.-Department of Biochemistry and Molecular Biology, University of Melbourne, 2.-Monash Institute of Pharmaceutical Science, Monash University, 3.-Department of Biochemistry and Molecular Biology, Monash University

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

Iratxe Macias<sup>1</sup>, Arantza Sanz<sup>1</sup>, Ana Laín<sup>1</sup>, Oscar Millet<sup>1</sup> 1.-CIC bioGUNE

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

<u>Daisuke Sato</u><sup>1</sup>, Hideaki Ohtomo<sup>1</sup>, Atsushi Kurobe<sup>1</sup>, Satsuki Takebe<sup>1</sup>, Yoshiteru Yamada<sup>2</sup>, Kazuo Fujiwara<sup>1</sup>, Masamichi Ikeguchi<sup>1</sup>

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

Benjamin Walcott<sup>1,2</sup>, Luís Garreta<sup>3</sup>, Christopher Bystroff<sup>1,2,4</sup>

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 Rao<sup>1</sup>, Shachi Gosavi<sup>1</sup>

1.-National Centre for Biological Sciences, Tata Institute of Fundamental Research

#### PD-032 **Tuning cooperativity on the free energy landscape of protein folding** <u>Pooja Malhotra</u><sup>1</sup>, Jayant Udgaonkar<sup>1</sup>

1.-National Centre for Biological Sciences, Tata Institute of Fundamental Research

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

Eriko Aoki<sup>1</sup>, Kazuo Fujiwara<sup>1</sup>, Masamichi Ikeguchi<sup>1</sup>

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 Kakimoto<sup>1</sup>, Hideya Nakano<sup>1</sup>, Yuji Nakai<sup>2</sup>, Kazuhiro Shiozaki<sup>3</sup>, Kohei Akioka<sup>4</sup>, Konosuke Otomaru<sup>5</sup>. Mitsuharu Matsumoto<sup>6</sup>. Masanobu Nagano<sup>7</sup>. Yasushi Sugimoto<sup>8</sup>. Hiroaki Kanouchi<sup>1</sup>

1.-Department of Veterinary Pathobiology, Kagoshima University, 2.-Institute for Food Sciences. Hirosaki University, 3.-Faculty of Fisheries, Kagoshima University, 4.-Department of Veterinary Histopathology, Kagoshima University, 5.-Veterinary Clinical Training Center, Kagoshima University, 6.-Department of Veterinary Anatomy, Kagoshima University, 7.-Sakamoto Kurozu Inc., 8.-The United Graduate School of Agricultural Sciences, Kagoshima University

#### PD-035 Cold Denaturation of Alpha-Synuclein Amyloid Fibrils

Young-Ho Lee<sup>1</sup>, Tatsuya Ikenoue<sup>1</sup>, Yasushi Kawata<sup>2</sup>, Yuji Goto<sup>1</sup>

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

Ángel Piñeiro<sup>1</sup>, Miguel Costas<sup>2</sup>, Andrea Gutiérrez-Quezada<sup>2</sup>

1.-Dept of Applied Physics, University of Santiago de Compostela, 2.-Lab. of Biophys. Chem., Dept of Physical Chemistry, Fac, of Chemistry, UNAM

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

Salvador Ventura<sup>1</sup>, Ricardo Sant'Anna<sup>1</sup>, Maria Rosário Almeida<sup>2</sup>, Natàlia Reixach<sup>3</sup>, Raul Insa<sup>4</sup>, Adrian Velazquez-Campoy<sup>5</sup>, David Reverter<sup>1</sup>, Núria Reig<sup>4</sup>

1.-Universitat Autònoma de Barcelona, 2.-Instituto de Biologia Molecular e Celular, ICBAS, 3.-The Scripps Research Institute, 4.-SOM-Biotech, 5.-Universidad de Zaragoza

PD-038 Neurometals as modulators of protein aggregation in neurodegenerative diseases Sónia S. Leal<sup>1</sup>, Joana S. Cristóvão<sup>1</sup>, Cláudio M. Gomes<sup>1</sup> 1.-Faculdade de Ciências Universidade de Lisboa - BioISI, FCUL

#### PD-039 Single-molecule FRET reveals proline dynamics in transmembrane helices

Gustavo Fuertes<sup>1,2,3</sup>, Ismael Mingarro<sup>3</sup>, Edward A. Lemke<sup>1</sup>

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<sup>1,2</sup>, Sara Kim<sup>1</sup>, Margaret Patchin<sup>1</sup>, Britt Benner<sup>1</sup>, Susan White<sup>1</sup>

1.-Department of Chemistry, Bryn Mawr College, 2.-Department of Biology, Haverford College

PD-041 Role of a non-native  $\alpha$ -helix in the folding of equine  $\beta$ -lactoglobulin Takahiro Okabe<sup>1</sup>, Toshiaki Miyajima<sup>1</sup>, Kanako Nakagawa<sup>1</sup>, Seiichi Tsukamoto<sup>1</sup>, Kazuo Fujiwara<sup>1</sup>, Masamichi Ikeguchi1

1.-Department of Bioinformatics, Soka University

#### PD-042 Impact of the chaperonin CCT in α-Synuclein(A53T) amyloid fibrils assembly assembly

Ahudrey Leal Quintero<sup>1</sup>, Javier Martinez-Sabando<sup>1</sup>, Jose María Valpuesta<sup>1</sup>, Begoña Sot<sup>1</sup> 1.-Centro Nacional de Biotecnología (CNB/CSIC)

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

Daniela Marasco<sup>1</sup>, Concetta Di Natale<sup>1</sup>, Valentina Punzo<sup>1</sup>, Domenico Riccardi<sup>1</sup>, Pasqualina Scognamiglio<sup>1</sup>, Roberta Cascella<sup>2</sup>, Cristina Cecchi<sup>2</sup>, Fabrizio Chiti<sup>2</sup>, Marilisa Leone<sup>3</sup>, Luigi Vitagliano<sup>3</sup> 1.-Department of Pharmacy, CIRPEB: Centro Interuniversitario di Ricerca sui Pepti, 2.-Section of Biochemistry, Department of Biomedical Experimental and Clinical Scie, 3.-Institute of Biostructures and Bioimaging

### $\label{eq:pd-044} PD-044 \quad \mbox{Transition from $\alpha$-helix to $\beta$-sheet structures occurs in myoglobin in deuterium oxide solution under exposure to microwaves}$

Emanuele Calabrò, Salvatore Magazù

1.-Department of Physics and Earth Sciences, University of Messina, 2.-Department of Physics and Earth Sciences, University of Messina

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

<u>Nicola Harris</u><sup>1</sup>, Kalypso Charalambous<sup>1</sup>, Eamonn Reading<sup>1</sup>, Paula Booth<sup>1</sup> 1.-Kings College London, Department of Chemistry

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

<u>Frederic Greco</u><sup>1</sup>, Audrey Toinon<sup>1</sup>, Nadege Moreno<sup>1</sup>, Marie Claire Nicolaï<sup>1</sup>, Catherine Manin<sup>1</sup>, Francoise Guinet-Morlot<sup>1</sup>, Frederic Ronzon<sup>1</sup>

1.-Sanofi Pasteur, Analytical Research and Development, Biophysical and Biochemical

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

Exequiel Medina<sup>1</sup>, Sandro L. Valenzuela<sup>1</sup>, Cristóbal Córdova<sup>1</sup>, César A. Ramírez-Sarmiento<sup>1</sup>, Jorge Babul<sup>1</sup>

1.-Departamento de Biología, Facultad de Ciencias, Universidad de Chile

### $\mathsf{PD}\text{-}048$ $\,$ Determining the coupled interactions that stabilize the structural framework of the ß-propeller fold

Loretta Au<sup>1</sup>, David Green<sup>2,3,4</sup>

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** <u>Stanislaw Oldziej</u><sup>1</sup>, Wioletta Żmudzińska<sup>1</sup>, Anna Hałabis <sup>1</sup> 1.-Intercollegiate Faculty of Biotechnology, UG and MUG

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

<u>Michael Sanders</u><sup>1</sup>, Heather Findlay<sup>1</sup>, Paula Booth<sup>1</sup> 1.-Department of Chemistry, King's college London

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

Gowoon Kim, Taekyung Yu, Jeongyong Suh

1.-Department of Agricultural Biotechnology, Seoul National University, 2.-Department of Agricultural Biotechnology, Seoul National University, 3.-Department of Agricultural Biotechnology, Seoul National University





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

Nurriza Ab Latif<sup>1,2</sup>, Paul Engel<sup>1</sup>

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

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

<u>Connie Tenorio</u><sup>1</sup>, Liam Longo<sup>1</sup>, Ozan S. Kumru<sup>2</sup>, C. Russell Middaugh<sup>2</sup>, Michael Blaber<sup>1</sup> 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** <u>Robert Fieldhouse</u><sup>1,2</sup>, Sikander Hayat<sup>1,2</sup>, Robert Sheridan<sup>1</sup>, Debora Marks<sup>2</sup>, Chris Sander<sup>1</sup> 1.-Computational Biology Center, Memorial Sloan Kettering Cancer Center, 2.-Systems Biology, Harvard Medical School

PD-056 **Developing SHuffle as a platform for expression and engineering of antibodies** Na Ke<sup>1</sup>, Alana Ali-Reynolds<sup>1</sup>, Bryce Causey<sup>1</sup>, Mehmet Berkmen<sup>1</sup> 1.-New England Biolabs

#### **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 Abriata<sup>1</sup>, Matteo Dal Peraro<sup>1</sup> 1.-École Polytechnique Fédérale de Lausanne

#### PE-002 Protein-ligand interactions

<u>Aldona Jelińska</u><sup>1</sup>, Anna Lewandrowska<sup>1</sup>, Robert Hołyst<sup>1</sup> 1.-Institute of Physical Chemistry Polish Academy of Sciences

#### PE-003 Carbohydrate Binding Modules. Structural and thermodynamic study

Benjamin Garcia<sup>1</sup>, Patricia Cano Sánchez<sup>1</sup>, Siseth Martínez-Caballero<sup>1</sup>, Romina Rodríguez-Sanoja<sup>1</sup>, Adela Rodríguez-Romero<sup>1</sup>

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

<u>Margaret Gustafson</u><sup>1</sup>, J. Chris Fromme<sup>1</sup> 1.-Cornell University

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

<u>Sumit Handa</u><sup>1</sup>, Blair G Paul<sup>2</sup>, Kharissa L Shaw<sup>1</sup>, David L Valentine<sup>2</sup>, Partho Ghosh<sup>1</sup> 1.-Department of Chemistry and Biochemistry, University of California San Diego, 2.-Marine Science Institute, University of California Santa Barbara

JULY 22 - 25, 2015

#### PE-006 Studies of JMJD4-catalyzed oxidative modifications of eukaryotic release factor 1

<u>Suzana Markolovic</u><sup>1</sup>, Ivanhoe K. H. Leung<sup>2</sup>, Mathew L. Coleman<sup>3</sup>, Timothy D. W. Claridge<sup>1</sup>, Sarah E. Wilkins<sup>1</sup>, Christopher J. Schofield<sup>1</sup>

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 Meekrathok<sup>1</sup>, Arthur T. Porfetye<sup>2</sup>, Marco Bürger<sup>2</sup>, Ingrid R. Vetter<sup>2</sup>, Wipa Suginta<sup>1</sup>

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><sup>1</sup>, Stacy Harvey<sup>1</sup>, Patrick Sammons<sup>1</sup>, Amanda Anderson<sup>2</sup>, Hema Kopalle<sup>1</sup>, Alison Banham<sup>2</sup>, Carrie Partch<sup>1</sup>

1.-University of California - Santa Cruz, 2.-University of Oxford

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

Kazem Nouri<sup>1</sup>, Mohammad Reza Ahmadian<sup>1</sup>

1.-Medical faculty of the Heinrich-Heine University

### 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><sup>1</sup>, Jhon Alexander Rodríguez<sup>1</sup>, Alain Ibáñez de Opakua<sup>1</sup>, Nekane Merino<sup>1</sup>, Maider Villate<sup>1</sup>, Tammo Diercks<sup>1</sup>, Pietro Roversi<sup>2</sup>, Adriana L. Rojas<sup>1</sup>, Francisco J. Blanco<sup>1.3</sup> 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 Palakurti<sup>1</sup>, Ramakrishna Vadrevu<sup>1</sup> 1.-Department of Biological Sciences, BITS-PILANI HYDERABAD CAMPUS

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

Rafael Palomino<sup>1</sup>, Glenn Millhauser<sup>2</sup>, Pietro Sanna<sup>2</sup>

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

### $\mathsf{PE}\text{-}013$ Evidence of a proteolytic phenomenon in the starch binding domain of the $\alpha\text{-}amylase$ from Lactobacillus amylovorus

Zaira Esmeralda Sánchez Cuapio<sup>1</sup>, Alejandra Hernández Santoyo<sup>2</sup>, Sergio Sánchez Esquivel<sup>1</sup>, Romina Rodríguez Sanoja<sup>1</sup>

1.-Instituto de Învestigaciones Biomédicas, Universidad Nacional Autónoma de México, 2.-Instituto de Química, Universidad Nacional Autónoma de México

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

Changlin Tian<sup>1</sup>

1.-University of Science and Technology of China

#### PE-015 Theoretical Volume Profiles as a Tool for Probing Protein Folding Kinetics

Heather Wiebe<sup>1</sup>, Noham Weinberg<sup>1,2</sup>

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

Alfredo De Biasio<sup>1</sup>, Alain Ibáñez de Opakua<sup>1</sup>, Gulnahar Mortuza<sup>2</sup>, Rafael Molina<sup>3</sup>, Tiago Cordeiro<sup>4</sup>, Francisco Castillo<sup>5</sup>, David Gil-Cartón<sup>1</sup>, Pau Bernadó<sup>4</sup>, Guillermo Montoya<sup>2</sup>, <u>Francisco Blanco<sup>1,6</sup></u>

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

Lucie Zemanova<sup>1</sup>, Hana Stambergova<sup>1</sup>, Tereza Lundova<sup>1</sup>, Rudolf Andrys<sup>1</sup>, Jiri Vondrasek<sup>2</sup>, Vladimir Wsol<sup>1</sup>

1.-Faculty Of Pharmacy in Hradec Kralove, Charles University in Prague, 2.-Institute of Organic Chemistry and Biochemistry, AS CR

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

Bong-Jin Lee1, Ki-Young Lee1

1.-College of Pharmacy, Seoul National University

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

<u>Sungjo Park</u><sup>1</sup>, In-Wook Hwang<sup>1</sup>, Tatsuya Kato<sup>2</sup>, Enoch Park<sup>2</sup>, Andre Terzic<sup>1</sup> 1.-Center for Regenerative Medicine, Mayo Clinic, 2.-Laboratory of Biotechnology, Shizuoka University

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

<u>Ho Zee (Charles) Kong</u><sup>1</sup>, Conrad Perera<sup>1</sup>, Ivanhoe Leung<sup>1</sup>, Nazimah Hamid<sup>2</sup>, Viji Sarojini<sup>1</sup> 1.-School of Chemical Sciences, The University of Auckland., 2.-School of Applied Sciences, Auckland University of Technology

### $\mathsf{PE}\text{-}021$ Development of Fungal-Specific Calcineurin Inhibitors Based on Molecular Structure and Dynamics

<u>Ronald Venters</u><sup>1</sup>, Leonard Spicer<sup>1,2</sup>, Joseph Heitman<sup>3</sup>, William Steinbach<sup>3,4</sup>, Praveen Juvvadi<sup>4</sup>, Maria Schumacher<sup>2</sup>

1.-Duke University NMR Center, 2.-Duke University Biochemistry Department, 3.-Duke University Department of Molecular Genetics and Microbiology, 4.-Duke University Department of Pediatrics

# 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<sup>1,2</sup>

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 Cohen<sup>1</sup>, Gary Pielak<sup>1,2,3</sup>

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

Joanna Szewczak<sup>1</sup>, Weronika Surmacz-Chwedoruk<sup>1</sup>, Bożena Tejchman-Małecka<sup>1</sup>, Jacek Stadnik<sup>1</sup>, Grażyna Tronczyńska-Lubowicz<sup>1</sup>, Agnieszka Romanik-Chruścielewska<sup>1</sup>, Jarosław Antosik<sup>1</sup>, Piotr Borowicz<sup>1</sup>, Iwona Sokołowska<sup>1</sup>, Dorota Stadnik<sup>1</sup>,

1.-Institute of Biotechnnology and Antibiotics

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

Inho Choi<sup>1</sup>, Taesik Gwag<sup>1</sup>, Kyoungsook Park<sup>2</sup>, Kyoungbong Ha<sup>1</sup>, Joo-hee Lee<sup>3</sup>, Youn-Kyu Kim<sup>3</sup> 1.-College of Science and Technology, Yonsei University, 2.-Molecular Therapy Research Center, Sungkyunkwan University, 3.-Korea Aerospace Research Institute

### $\mathsf{PE}\text{-}026$ A novel in vivo characterization method predicting the physicochemical parameters of an antibiotic efflux pump

Anisha M Perez<sup>1</sup>, Erin L O'Brien<sup>1</sup>, Marcella M Gomez<sup>1</sup>, Matthew R Bennett<sup>1</sup>, Yousif Shamoo<sup>1</sup> 1.-Department of BioSciences

#### PE-027 Structural Analysis of KCNE1 Transmembrane Mutant Yielding KCNE3-like Function Cheryl Law<sup>Vanderbilt Universit</sup>, Charles Sanders<sup>0</sup>

1.-Vanderbilt University Biochemistry Department, 2.-Vanderbilt University Center for Structural Biology, 3.-Vanderbilt University School of Medicine

### PE-028 Biochemical characterization of Brassica napus diacylglycerol acyltransferase 1 and its regulatory domain

<u>Kristian Mark Caldo</u><sup>1</sup>, Rashmi Panigrahi<sup>2</sup>, Michael Greer<sup>1</sup>, Guanqun Chen<sup>1</sup>, M. Joanne Lemieux<sup>2</sup>, Randall Weselake<sup>1</sup>

1.-Alberta Innovates Phytola Centre, University of Alberta, 2.-Department of Biochemistry, University of Alberta

### PE-029 Alteration of lysine and arginine content as a strategy to modify protein solubility: a test for E. coli proteins

M. Alejandro Carballo-Amador<sup>1</sup>, Jim Warwicker<sup>1</sup>, Alan J. Dickson<sup>1</sup>

1.-Faculty of Life Sciences, University of Manchester

#### **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

Arindam Bakshi<sup>1</sup>, Srinivas Sistala<sup>2</sup>, Shruthi Sridhar<sup>1</sup>, Savithri H S<sup>1</sup>

1.-Indian institute of Science, 2.-Wipro G E Healthcare Pvt Ltd

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

<u>Giulio Chiesa</u><sup>1</sup>, Bahareh Eftekharzadeh<sup>1</sup>, Daniele Mungianu<sup>1,2</sup>, Alessandro Piai<sup>2</sup>, Jesus Garcia<sup>1</sup>, Isabella Felli<sup>2</sup>, Roberta Pieratelli<sup>2</sup>, Xavier Salvatella<sup>1,3</sup>

1.-Institute for Research in Biomedicine (IRB), 2.-Magnetic Resonance Center and Department of Chemistry, University of Florence, 3.-ICREA

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

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

Kendra Frederick<sup>1</sup>, Robert Griffin<sup>2</sup>, Susan Lindquist<sup>1,3</sup>

1.-Whitehead Institute for Biomedical Research, 2.-Francis Bitter Magnet Lab and Department of Chemistry, MIT, 3.-Howard Hughes Medical Institute, Department of Biology, MIT

### $\mathsf{PF}\text{-}005$ Genetic instability within regions encoding repetitive proteins as a driver of adaptation

Stephen Fuchs<sup>1</sup>

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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

Marie Dujardin<sup>1</sup>, Vanesa Madan<sup>2</sup>, Roland Montserret<sup>3</sup>, Puneet Ahuja<sup>1</sup>, Isabelle Huvent<sup>1</sup>, Helene Launay<sup>1</sup>, Ralf Bartenschlager<sup>2</sup>, François Penin<sup>3</sup>, Guy Lippens<sup>1</sup>, <u>Xavier Hanoulle<sup>1</sup></u>

1.-CNRS UMR 8576, UGSF, Lille University, 2.-Department of Infectious Diseases, Molecular Virology, University of Heidelberg, 3.-CNRS UMR 5086, IBCP, LabEx Ecofect, Lyon 1 University

#### PF-007 **Solution structure and celullar functional studies of bovine cathelicidin Bt-6 (BMAP-27)** Anna Hastings<sup>1</sup>, Manuel Ruether<sup>2</sup>, H. Paul Voorheis<sup>1</sup>, Ken H. Mok<sup>1,3</sup>

1.-Trinity College Dublin, School of Biochemistry and Immunology, 2.-Trinity College Dublin, School of Chemistry, 3.-TCD, Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN)

#### PF-008 Engineered binding proteins to amyloidogenic intrinsically disordered proteins

Hamed Shaykhalishahi<sup>1,2</sup>, Ewa Mirecka<sup>1</sup>, Aziz Gauhar<sup>1</sup>, Clara Grüning<sup>1</sup>, Michael Wördehoff<sup>1</sup>, Sophie Feuerstein<sup>2</sup>, Matthias Stoldt<sup>1,2</sup>, Torleif Härd<sup>3</sup>, Dieter Willbold<sup>1,2</sup>, <u>Wolfgang Hoyer<sup>1,2</sup></u>

1.-Physikalische Biologie, Heinrich Heine University, 2.-Structural Biochemistry (ICS-6), Research Centre Jülich, 3.-Chemistry and Biotechnology, Swedish University of Agricultural Sciences (SLU) PF-009 Interaction Profiling through Proteomic Peptide Phage Display

Cecilia Blikstad<sup>1</sup>, Moon-Hyeong Seo<sup>2</sup>, Norman Davey<sup>3</sup>, Roland Arnold<sup>2</sup>, Sachdev S Sidhu<sup>2</sup>, Philip M Kim<sup>2</sup>, <u>Ylva Ivarsson<sup>1</sup></u>

1.-Department of Chemistry - BMC, 2.-Donnelly Centre

PF-010 **Biophysical characterization of phosducin and its complex with the 14-3-3 protein** <u>Miroslava Kacirova</u><sup>1,2</sup>, Jiri Novacek<sup>3</sup>, Petr Man<sup>1,4</sup>, Alan Kadek<sup>1,4</sup>, Veronika Obsilova<sup>2</sup>, Tomas Obsil<sup>1,2</sup> 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

<u>Can Kayatekin</u><sup>1</sup>, Kent Matlack<sup>1</sup>, William Hesse<sup>2</sup>, Yinghua Guan<sup>3</sup>, Sohini Chakrabortee<sup>1</sup>, Gregory Newby<sup>2</sup>, Jenny Russ<sup>4</sup>, Erich Wanker<sup>4</sup>, Jagesh Shah<sup>3</sup>, Susan Lindquist<sup>1,2,5</sup>

1.-Whitehead Institute For Biomedical Research, 2.-Massachusetts Institute of Technology, 3.-Harvard Medical School, 4.-Max Delbrück Center For Molecular Medicine, 5.-Howard Hughes Medical Institute

#### PF-012 Structuring disorder: the case of the intrinsically disordered Unique domain of c-Src Mariano Maffei<sup>1</sup>

1.-BioNMR lab - Faculty of Organic Chemistry - University of Barcelona

#### PF-013 **The Yeast GRASP Grh1 displays features of an Intrinsically Disordered Protein** <u>Raquel Fonseca-Maldonado</u><sup>1</sup>, Felipe Mendes<sup>1</sup>, Luana Meleiro<sup>1</sup>, Assuero Garcia<sup>1</sup>, Antonio Costa-Filho<sup>1</sup> 1.-Universidade de São Paulo-FFCLRP

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

André F. Faustino<sup>1</sup>, Gabriela M. Guerra<sup>1</sup>, Roland G. Huber<sup>2</sup>, Axel Hollmann<sup>1</sup>, Peter J. Bond<sup>2</sup>, Miguel A.R.B. Castanho<sup>1</sup>, Andrea T. Da Poian<sup>3</sup>, Fábio C.L. Almeida<sup>3</sup>, Nuno C. Santos<sup>1</sup>, <u>Ivo Martins<sup>1</sup></u> 1.-Instituto de Medicina Molecular, Faculdade de Medicina, Universidade de Lisboa, 2.-Bioinformatics Institute, A\*STAR, 3.-Instituto De Bioquímica Médica, Universidade Federal Do Rio de Janeiro

#### PF-015 **Developing mechanistic insight into modulators of tau aggregation**

Eri Nakatani-Webster<sup>1</sup>, Hannah Baughman<sup>1</sup>, Shaylin Higgins<sup>1</sup>, <u>Abhinav Nath<sup>1</sup></u> 1.-Department of Medicinal Chemistry, University of Washington

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

Bartosz Nizynski<sup>1,2,3,4</sup>, Hanna Nieznanska<sup>2</sup>, Krzysztof Nieznanski<sup>2</sup>, Wojciech Dzwolak<sup>3,4</sup>

1.-College of Inter-Faculty Individual Studies in Mathematics and Natural Sciences, 2.-Department of Biochemistry, Nencki Institute of Experimental Biology, 3.-Institute of High Pressure Physics, 4.-Department of Chemistry, Biological and Chemical Research Centre

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

Ras Pandey<sup>1</sup>, Peter Mirau<sup>2</sup>, Barry Farmer<sup>2</sup>

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

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

<u>Cesyen Cedeno</u><sup>1</sup>, Nani Van Gerven<sup>1</sup>, Wim Jonckheere<sup>1</sup>, Imke Van den Broek<sup>1</sup>, Han Remaut<sup>1</sup>, Peter Tompa<sup>1</sup>

1.-VIB, Structural Biology Research Center

#### PF-019 Coupled folding and binding of transcription factors

Sarah Shammas<sup>1</sup>, Alexandra Travis<sup>1</sup>, Jane Clarke<sup>1</sup>

1.-Department of Chemistry, University of Cambridge

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

Harm Jan (Arjan) Snijder<sup>1</sup>, Maria Saline<sup>1</sup>, Tomas Jacso<sup>1</sup>, Frank Janssen<sup>1</sup>, Mattias Rohman<sup>1</sup>, Tyrrell Norris<sup>1</sup>

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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><sup>1</sup>, Rosa Pujol-Pina<sup>1</sup>, Roberta Mazzucato<sup>1</sup>, Annalisa Arcella<sup>2</sup>, Marta Vilaseca<sup>3</sup>, Modesto Orozco<sup>2,4</sup>, Natàlia Carulla<sup>1</sup>

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

Yinghao Wu1

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

Barbara Zambelli<sup>1</sup>, Francesco Musiani<sup>1</sup>, Stefano Ciurli<sup>1</sup> 1.-University of Bologna, Dept. of Pharmacy and Biotechnology





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

<u>Pallavi Sabharwal</u><sup>1</sup>, Rashmi Panigrahi<sup>1</sup>, Srinivas Sistala<sup>2</sup>, Savithri H S<sup>1</sup> 1.-Indian institute of Science, 2.-Wipro G E Healthcare Pvt Ltd

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

<u>Priscila Ferreira</u><sup>1</sup>, Carolina Andrade<sup>1</sup>, Antonio Neves<sup>4</sup>, Herbert Pereira<sup>2</sup>, Fernando Palhano<sup>1</sup>, Marcia Cruz<sup>3</sup>, Debora Foguel<sup>1</sup>

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

<u>Francesco Simone Ruggeri</u><sup>1</sup>, Sophie Vieweg<sup>2</sup>, Denise Galante<sup>3</sup>, Cristina D'arrigo<sup>3</sup>, Hilal Lashuel<sup>2</sup>, Giovanni Dietler<sup>1</sup>

1.-École polytechnique fédérale de Lausanne - LPMV, 2.-École polytechnique fédérale de Lausanne - LMNN, 3.-National Research Council

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

Petr Tesina<sup>1, 2, 3</sup>, Kateřina Čermáková<sup>4</sup>, Magdalena Hořejší <sup>3</sup>, Milan Fábry<sup>3</sup>, Frauke Christ<sup>4</sup>, Jonas Demeulemeester<sup>4</sup>, Zeger Debyser<sup>4</sup>, Jan De Rijck<sup>4</sup>, Václav Veverka<sup>1</sup>, Pavlína Řezáčová<sup>-3</sup>, 1.-IOCB AS CR, 2.-IMG AS CR, 3.-Faculty of Science, Charles University in Prague, 4.-KU Leuven

#### PF-028 Exploring Anti- amyloidogenic Attributes of Lantibiotic Nisin Deovrat Begde<sup>1</sup>

1.-Department of Biochemistry & Biotechnology, Dr. Ambedkar College, Deekshabhoom

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

<u>Yasushi Sugimoto</u><sup>1</sup>, Yoshiki Kamada<sup>1</sup>, Yusuke Nawata<sup>1</sup>, Takahiro Kusakabe<sup>2</sup> 1.-Kagoshima University, The United Graduate School of Agri. Sci., 2.-Kyushu University

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

Serene W. Chen<sup>1</sup>, Srdja Drakulic<sup>2</sup>, Emma Deas<sup>3</sup>, Myriam Ouberai<sup>4</sup>, Francesco A. Aprile<sup>1</sup>, German Rivas<sup>5</sup>, Andrey Y. Abramov<sup>3</sup>, Jose Maria Valpuesta<sup>2</sup>, Christopher M. Dobson<sup>1</sup>, Nunilo Cremades<sup>1</sup> 1.-Department of Chemistry, University of Cambridge, 2.-Department of Macromolecular Structure, Centro Nacional de Biotecnologia, 3.-Department of Molecular Neuroscience, University College London, 4.-Nanoscience Centre, Department of Engineering, University of Cambridge, 5.-Department of Cellular and Molecular Biology

PF-031 **Metal ions modulate the conformation of Starmaker-like protein from Oryzias latipes** <u>Mirosława Różycka</u><sup>1</sup>, Magdalena Wojtas<sup>1</sup>, Natalie Mutter<sup>2</sup>, Benjamin Schuler<sup>2</sup>, Jacek Gapiński <sup>3,4</sup>, Andrzej Ożyhar<sup>1</sup>

1.-University of Technology, Department of Biochemistry, 2.-University of Zurich, Department of Biochemistry, 3.-Molecular Biophysics Department, Faculty of Physics, Adam Mickiewicz University, 4.-NanoBioMedical Center, Adam Mickiewicz University

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

Aleksandra Porebska<sup>1</sup>, Andrzej Ozyhar<sup>1</sup>, Piotr Dobryszycki<sup>1</sup>

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

<u>Marta Kolonko</u><sup>1</sup>, Katarzyna Ożga<sup>1</sup>, Rafał Hołubowicz<sup>1</sup>, Andrzej Ożyhar<sup>1</sup>, Beata Greb-Markiewicz<sup>1</sup> 1.-Wroclaw University of Technology

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

Eleni Malideli<sup>1</sup>, Erika Andreetto<sup>1</sup>, Li-Mei Yan<sup>1</sup>, Michael Kracklauer<sup>1</sup>, Karine Farbiarz<sup>1</sup>, Marianna Tatarek-Nossol<sup>2</sup>, <u>Aphrodite Kapurniotu</u>

1.-Division of Peptide Biochemistry, Technische Universität München, 2.-Institute of Biochemistry and Molecular Cell Biology, RWTH Aachen University

PF-035 **Preparation of homogenous recombinant FKBP39 protein from Tribolium castaneum** <u>Aneta Tarczewska</u><sup>1</sup>, Małgorzata Kozłowska <sup>1</sup>, Andrzej Ożyhar <sup>1</sup> 1.-Department of Biochemistry, Faculty of Chemistry, Wrocław University of Technology

#### **PG - OBSERVING DYNAMICS IN SINGLE CELLS**

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

Robert Gahl<sup>1</sup>, Yi He<sup>1</sup>, Shiqin Yu<sup>1</sup>, Nico Tjandra<sup>1</sup> 1.-Biochemistry and Biophysics Center, NHLBI, NIH

#### PG-002 Bacterial cell division in super resolution

<u>Jie Xiao</u>, Carla Coltharp, Jackson Buss, Xinxing Yang 1.-Department of Biophysics and Biophysical Chemistry, Johns Hopkins School of Medicine

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

Martin Stortz<sup>1</sup>, Luciana Bruno<sup>2</sup>, Paolo Annibale<sup>3</sup>, Enrico Gratton<sup>3</sup>, Adali Pecci<sup>1,4</sup>, Valeria Levi<sup>4,5</sup> 1.-IFIByNE-Conicet, 2.-IFIBA-Conicet & Dept. of Physics, University of Buenos Aires, 3.-LFD-University of California, 4.-Dept. of Biological Chemistry, University of Buenos Aires, 5.-IQUIBICEN-Conicet 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

Basak Akdas<sup>1</sup>, Ozge Kurkcuoglu<sup>2</sup>, Pemra Doruker<sup>1</sup>, Demet Akten<sup>3</sup>

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

Claudia Alvarez<sup>1,2</sup>, Marijana Stagljar<sup>2</sup>, Voula Kanleis<sup>1,2,3</sup>

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#### PH-003 **Glycosylation of EGFR Extracellular Domain Induces Receptor Stability** <u>Maryam Azimzadeh Irani</u><sup>1,2</sup>, Chandra Verma<sup>1,2</sup>

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

Richard Baxter<sup>1</sup>

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

Satchal Erramilli<sup>1</sup>, Michael Simon<sup>2</sup>, Matthew Clifton<sup>3</sup>, Cynthia Stauffacher<sup>1</sup>

1.-Purdue University, 2.-Washington University At St. Louis, 3.-Beryllium

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

L. David Finger<sup>1</sup>, Ian A. Bennet<sup>1</sup>, Andrea Hounslow<sup>2</sup>, Jack C. Exell<sup>1</sup>, Nicola J. Baxter<sup>2</sup>, Jon P. Waltho<sup>2,3</sup>, Jane A. Grasby<sup>1</sup>

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#### PH-007 **Dynamical structure changes in binding of pharmaceutical target proteins** <u>Hideaki Fujitani</u><sup>1</sup>

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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<sup>1,2</sup>, Maximillian C.C.J.C. Ebert<sup>1,2</sup>, Jaeok Park<sup>1,4,5</sup>, Donald Gagné<sup>1,5,6</sup>, Christopher M. Clouthier<sup>1,3</sup>, Jürgen Pleiss<sup>7</sup>, Nicolas Doucet<sup>1,5,6</sup>, Albert M. Berghuis<sup>1,4,5</sup>, Joelle N. Pelletier<sup>1,2,3</sup>

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### $\mathsf{PH}\text{-}009$ Conformations of the RNA polymerase clamp throughout the transcription cycle studied by single-molecule FRET

Sarah Sarah<sup>1</sup>, Andreas Gietl<sup>1</sup>, Philip Tinnefeld<sup>1</sup>, Finn Werner<sup>2</sup>, Dina Grohmann<sup>1,3</sup>

1.-Physikalische Chemie - NanoBioSciences, Technische Universität Braunschweig, 2.-Institute of Structural and Molecular Biology, University College London, 3.-Institute of Microbiology - Single-Molecule Biochemistry, University Regensburg

#### PH-010 Solvent models for protein simulations – the good, the bad and the applications <u>Duy Hua</u><sup>1</sup>, Amitava Roy<sup>1</sup>, He Huang<sup>1</sup>, Carol Post<sup>1</sup> 1.-Purdue University

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

<u>Anwar Iqbal</u><sup>1</sup>, Fabio C. L. Almeida<sup>1</sup>, Catarina Miyomoto<sup>2</sup>, Ana P Valente<sup>3</sup>, Francisco Gomes Neto<sup>4</sup> 1.-National Center of Nuclear Magnetic Ressonance, Insti of Medical Biochemistry, 2.-Faculdades Integradas de Três Lagoas-AEMS,, 3.-Center of Structural Biology and Bioimaging (CENABIO), UFRJ, 4.-Laboratory of Toxicology, Instituto Oswaldo Cruz, Fiocruz

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### $\mathsf{PH}\text{-}012$ $\,$ In-vitro and in-silico studies of ligand binding to the nuclear receptor PPARgamma using FRET and MD $\,$

<u>Narutoshi Kamiya</u><sup>1</sup>, Gert-Jan Bekker<sup>1</sup>, Takuma Shiraki<sup>2</sup>, Haruki Nakamura<sup>1</sup> 1.-IPR, Osaka University, 2.-Kinki University

### <code>PH-013</code> Atomic Insight into kinetic mechanism for sumoylation of UBC9 with substrate motif ( $\Psi$ -K-x-D/E) by molecular dynamic simulation

Mooseok Kang<sup>1</sup>, Wookyung Yu<sup>1</sup>, Juhwan Lee<sup>1</sup>, Iksoo Chang<sup>1</sup>

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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<sup>1,2</sup></u>, Wade Van Horn<sup>0</sup>, Jarrod Smith<sup>1,2</sup>, David Nannemann<sup>2,6</sup>, Jens Meiler<sup>2,6</sup>, Carlos Vanoye<sup>7</sup>, Charles Sanders<sup>1,2</sup>

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#### PH-015 Watching conformational changes in proteins by molecular dynamics simulations <u>Kresten Lindorff-Larsen<sup>1</sup></u>

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

<u>Alyssa Lokits</u><sup>1</sup>, Julia Koehler Leman<sup>2</sup>, Kristina Kitko<sup>1,3</sup>, Natha Alexander<sup>4</sup>, Heidi Hamm<sup>1,5</sup>, Jens Meiler<sup>1,5,6</sup>

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

<u>Yuan-Chao Lou</u><sup>1</sup>, Yi-Fen Kao<sup>1</sup>, Tsi-Hsuan Weng<sup>2</sup>, Yi-Chuan Li<sup>2</sup>, Chwan-Deng Hsiao<sup>2</sup>, Chinpan Chen<sup>1</sup> 1.-Institute of Biomedical Sciences, Academia Sinica, 2.-Institute of Molecular Biology, Academia Sinica

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

<u>Yufuku Matsushita</u><sup>1</sup>, Hiroshi Sekiguchi<sup>2</sup>, Noboru Ohta<sup>2</sup>, Keigo Ikezaki<sup>1</sup>, Yuji Goto<sup>3</sup>, Yuji Sasaki<sup>1,3</sup> 1.-The University of Tokyo, Graduate School of Frontier Science, Advanced Materials Science, 2.-SPring-8, 3.-Osaka University, Institute For Protein Research

#### PH-019 **Functional implications of co-evolving residue sectors in the Ribonuclease A family** <u>Chitra Narayanan<sup>1,2</sup></u>, Kimberly Reynolds<sup>3</sup>, Rama Ranganathan<sup>3</sup>, Nicolas Doucet<sup>1,2,4</sup>

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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

<u>Dulal Panda</u><sup>1</sup>, Shalini Srivastava<sup>1</sup>, Ilina Bareja<sup>1</sup> 1.-Indian Institute of Technology Bombay

#### PH-023 How amide hydrogens exchange in native proteins

Filip Persson<sup>1</sup>, Bertil Halle<sup>1</sup>

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### PH-024 Differences in redox reactions with NADP+/H between ferredoxin-NADP+ 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

Stephan Köhler<sup>1,2</sup>, Friederike Schmid<sup>1</sup>, Giovanni Settanni<sup>1,3</sup>

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#### PH-026 Membrane curvature – the assembler of proteins

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1.-Chemistry Department, The University of Chicago, 2.-Physico-Chimie Curie, Institut Curie

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

Adnan Sljoka, Alexandr Bezginov

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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

<u>Veronika Navratilova</u><sup>1</sup>, Marketa Paloncyova<sup>1</sup>, Michaela Kajsova<sup>1</sup>, Karel Berka<sup>1</sup>, Michal Otyepka<sup>1</sup> 1.-RCPTM, Department of Physical Chemistry, Faculty of Science, Palacky University

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

Yusu<sup>i</sup> Sato<sup>1</sup>, Yusuke Tanaka<sup>1</sup>, Hiroshi Sekiguchi<sup>2</sup>, Satomi Inaba<sup>1</sup>, Takahiro Maruno<sup>3</sup>, Yuji C. Sasaki<sup>4</sup>, Yuji Kobayashi<sup>3</sup>, Takachika Azuma<sup>5</sup>, <u>Masayuki Oda<sup>1</sup></u>

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### PH-034 Antibiotic binding drives catalytic activation of aminoglycoside kinase APH(2")-la Shane Caldwell<sup>1</sup>, Albert Berghuis<sup>1</sup>

1.-McGill University

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

Ryan Godwin<sup>1</sup>, William Gmeiner<sup>2</sup>, Freddie Salsbury<sup>1</sup>

1.-Wake Forest University - Department of Physics, 2.-Wake Forest University Health Sciences - Department of Cancer Biology

### $\mathsf{PH}\text{-}036$ Structural characterization of the binding of HIV-1 integrase to its cellular co-factor Ku70

Ekaterina Knyazhanskaya<sup>1</sup>, Andrey Anisenko<sup>2</sup>, Marina Gottikh<sup>3</sup>, Timofei Zatsepin<sup>1</sup>

1.-Moscow State University, Chemistry department, 2.-Moscow State University, Department of bioengineering and bioinformatics, 3.-Moscow State University, Belozersky institute of physico-chemical biology

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

Ganeko Bernardo Seisdedos <sup>1,2</sup>, Álvaro Villarroel <sup>2</sup>, Oscar Millet <sup>1</sup> 1.-CIC-Biogune, 2.-Unidad de Biofísica (CSIC-UPV/EHU)

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

<u>Martin Srejber</u><sup>1</sup>, Veronika Navratilova<sup>1</sup>, Michal Otyepka<sup>1</sup>, Karel Berka<sup>1</sup> 1.-RCPTM, Department of Physical Chemistry, Faculty of Science, Palacky University

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

<u>Hiroshi Sekiguchi</u><sup>1</sup>, Yufuku Matsushita<sup>2</sup>, Yuri Nishino<sup>3</sup>, Keigo Ikezaki<sup>2</sup>, Atsuo Miyazawa<sup>3</sup>, Tai Kubo<sup>4</sup>, Christele Huron<sup>5</sup>, Jean-Pierre Changeux<sup>5</sup>, Pierre-Jean Corringer<sup>5</sup>, Yuji Sasaki<sup>2</sup>

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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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1.-Department of Chemistry and Biochemistry, Arizona State University, 2.-Center for Biological Physics, Department of Physics, Arizona State University

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

<u>Maria Guadalupe Herrera Hernández</u><sup>1,3</sup>, Xiaoyun Dong<sup>1</sup>, Cecylia S. Lupala<sup>2</sup>, Juan J. Perez<sup>2</sup>, Pere Garriga<sup>1</sup>

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PH-042 Identification of prospective allosteric sites of p38 by computational methods Patricia Gomez-Gutierrez<sup>1</sup>, Juan Jesus Perez<sup>1</sup>

1.-Departament d'Enginyeria Química (ETSEIB), Universitat Politècnica de Catalunya

### $\mathsf{PH}\text{-}043$ Hydrogen/deuterium exchange-mass spectrometry provides clues on the mechanism of action of Min E

Maria T. Villar<sup>1</sup>, Kyung-Tae Park<sup>2</sup>, Joe Lutkenhaus<sup>2</sup>, Antonio Artigues<sup>1</sup>

1.-Department of Biochemistry and Molecular Biology, 2.-Department of Microbiology, Molecular Genetics & Immunology

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

Pablo Herrera Nieto<sup>1</sup>, James Dalton<sup>1</sup>, Jesús Giraldo<sup>1</sup> 1.-Universidad Autónoma de Barcelona

### 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

<u>Anna Modrak-Wojcik</u><sup>1</sup>, Monika Wisniewska<sup>1</sup>, Ryszard Stolarski<sup>1</sup> 1.-Division of Biophysics, Faculty of Physics, University of Warsaw

#### PH-046 Mapping of Thrombin - Beta2Glycoprotein I Interaction Sites

Laura Acquasaliente<sup>1</sup>, Simone Tescari<sup>1</sup>, Daniele Peterle<sup>1</sup>, Giulia Pontarollo<sup>1</sup>, Vittorio Pengo<sup>2</sup>, Vincenzo De Filippis<sup>1</sup>

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#### PH-047 Dynamical Variability in the Clan MA of Metalloproteases

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

PH-048 **X-ray crystallographic analysis of cold-adapted and thermostable glucokinase** Tokuro Oda<sup>1</sup>, Naoki Fuchita<sup>1</sup>, Hiroyuki Motoshima<sup>1</sup>, <u>Keiichi Watanabe<sup>1</sup></u> 1.-Department of Applied Biochemistry and Food Science, Saga University

### **PI - PROTEIN ENGINEERING**

#### PI-001 Genetic engineering of new formate dehydrogenases for cofactor regeneration

<u>Anastasia Alekseeva<sup>1,2</sup></u>, Irina Dolina<sup>2,3</sup>, Ivan Kargov<sup>2,3</sup>, Svyatoslav Savin<sup>2,3</sup>, Vladimir Tishkov<sup>1,2,3</sup> 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

<u>F Ece Altinisik</u><sup>1</sup>, F Gizem Avci<sup>1</sup>, Berna Sariyar Akbulut<sup>1</sup>, Elif Özkirimli Ölmez<sup>3</sup>, Didem Vardar Ulu<sup>2</sup>, Ipek Karacan<sup>1</sup>, Duygu Sentürk<sup>1</sup>

1.-Marmara University, 2.-Wellesley College, 3.-Bogaziçi University

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

Stijn Aper<sup>1</sup>, Maarten Merkx<sup>1</sup> 1.-Eindhoven University of Technology

#### PI-004 Proteins as supramolecular building blocks: engineering nanoscale structures

Helen Ashmead<sup>1,2,3</sup>, Leonardo Negron<sup>1</sup>, Jack Sissons<sup>6</sup>, Kyle Webster<sup>6</sup>, Vic Arcus<sup>2,4</sup>, Juliet Gerrard<sup>1,2,5</sup> 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

Danielle Basore<sup>1,2</sup>, Rajesh Naz<sup>5</sup>, Scott Michael<sup>6</sup>, Sharon Isern<sup>6</sup>, Benjamin Wright<sup>3</sup>, Katie Saporita<sup>1</sup>, Donna Crone<sup>1</sup>, Christopher Bystroff<sup>1,2,4</sup>

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

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

<u>Jais R. Bjelke</u><sup>1</sup>, Gorm Andersen<sup>1</sup>, Henrik  $\emptyset stergaard^1$ , Laust B. Johnsen<sup>1</sup>, Anette A. Pedersen<sup>1</sup>, Tina H. Glue<sup>1</sup>

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

<u>Esra Bozkurt</u><sup>1</sup>, Ruud Hovius<sup>1</sup>, Thereza A. Soares<sup>2</sup>, Ursula Rothlisberger<sup>1</sup> 1.-École Polytechnique Fédérale de Lausanne, 2.-Federal University of Pernambuco

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

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

<u>Stéphanie Cabantous</u><sup>1</sup>, Hau B. NGuyen<sup>3</sup>, Jean-Denis Pedelacq<sup>2</sup>, Faten Koraichi<sup>1</sup>, Anu Chaudhary<sup>3</sup>, Kumkum Ganguly<sup>3</sup>, Meghan A. Lockard<sup>3</sup>, Gilles Favre<sup>1</sup>, Thomas C. Terwilliger<sup>3</sup>, Geoffrey S. Waldo<sup>3</sup> 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

Luis Francisco Calleja Castañeda<sup>1</sup>, José Salud Rodríguez Zavala<sup>1</sup> 1.-Instituto Nacional de Cardiología 'Ignacio Chávez'

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

H. Kay Chung<sup>1</sup>, Conor Jacobs<sup>1</sup>, Yunwen Huo<sup>2</sup>, Jin Yang<sup>3</sup>, Stefanie Krumm<sup>4</sup>, Richard Plemper<sup>4,5</sup>, Roger Tsien<sup>3,6,7</sup>, Michael Lin<sup>2,8</sup>

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

<u>Bruno Correia</u><sup>1</sup>, John Bates<sup>2</sup>, Rebecca Loomis<sup>3</sup>, Chris Carrico<sup>4</sup>, Joseph Jardine<sup>5</sup>, David Baker<sup>6</sup>, Roland Strong<sup>7</sup>, James Crowe<sup>3</sup>, Phillip Johnson<sup>4</sup>, William Schief<sup>1,6,7</sup>

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

Sara H. Mejias<sup>1,2</sup>, Antonio Aires<sup>1,2</sup>, Javier López-Andarias<sup>3</sup>, Pierre Couleaud<sup>1,2</sup>, Begoña Sot<sup>1,2</sup>, Carmen Atienza<sup>3</sup>, Nazario Martín<sup>1,3</sup>, <u>Aitziber L. Cortajarena<sup>1,2</sup></u>

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#### PI-015 Engineering of proteins to develop biomimetic hematite-based biohybrid materials

Greta Faccio<sup>1</sup>, Krisztina Schrantz<sup>2</sup>, Linda Thöny-Meyer<sup>1</sup>, Artur Braun<sup>2</sup>, Julian Ihssen<sup>1</sup>

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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

Fan Zheng<sup>1</sup>, Craig Mackenzie<sup>2</sup>, Jian Zhang<sup>3</sup>, Gevorg Grigoryan<sup>1.3</sup>

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

<u>Po-Ssu Huang</u><sup>1,2</sup>, Kaspar Feldmeier<sup>3</sup>, Fabio Parmeggiani<sup>1,2</sup>, D. Alejandro Fernandez Velasco<sup>4</sup>, Birte Höcker<sup>3</sup>, David Baker<sup>1,2,5</sup>

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#### PI-019 Directed Evolution of Fluorescent Protein Function

Felix Vietmeyer<sup>1</sup>, Premashis Manna<sup>1,2</sup>, Kevin Dean<sup>3</sup>, Amy Palmer<sup>2,4</sup>, Ralph Jimenez<sup>1,2</sup>

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 **The Road Not Taken: Exploring Repeat Protein Architectures By Computational Design** <u>Fabio Parmeggiani</u><sup>1</sup>, Po-Ssu Huang<sup>1</sup>, TJ Brunette<sup>1</sup>, Damian Ekiert<sup>2</sup>, Gira Bhabha<sup>2</sup>, Susan Tsutakawa<sup>3</sup>, Greg Hura<sup>3</sup>, John Tainer<sup>3</sup>, David Baker<sup>1</sup>

1.-University of Washington, 2.-University of California, San Francisco, 3.-Lawrence Berkeley National Laboratory

PI-021 **Short peptides self-assemble in the presence of metals to produce catalytic amyloids** Caroline Rufo<sup>1</sup>, Yurii Moroz<sup>1</sup>, Olesia Moroz<sup>1</sup>, Olga Makhlynets<sup>1</sup>, Pallavi Gosavi<sup>1</sup>, Jan Stöhr<sup>2</sup>, Tyler Smith<sup>1</sup>, Xioazhen Hu<sup>3</sup>, William DeGrado<sup>3</sup>, <u>Ivan Korendovych<sup>1</sup></u>

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 Oskarsson<sup>1</sup>, Sigridur Thorbjarnardottir<sup>2</sup>, Magnus Kristjansson<sup>1</sup>

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

<u>Bishwajit Kundu</u><sup>1</sup>, Dushyant Garg<sup>1</sup> 1.-Kusuma School of Biological Sciences

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

<u>Aksana Labokha</u><sup>1</sup>, Ralph Minter<sup>1</sup> 1.-Antibody Discovery & Protein Engineering dpt, MedImmune

### PI-025 Protein engineering: what's next?

<u>Maria Fatima Lucas<sup>1,2</sup></u>, Víctor Guallar<sup>1,3</sup> 1.-Joint BSC-CRG-IRB Research Program in Computational Biology, 2.-Anaxomics Biotech, 3.-ICREA

PI-026 **Bottom-up construction of a synthetic carboxysome** <u>Shiksha Mantri</u><sup>1</sup>, Raphael Frey<sup>1</sup>, Marco Rocca<sup>1</sup>, Eita Sasaki<sup>1</sup>, Donald Hilvert<sup>1</sup> 1.-ETH Zurich

PI-027 **CXCL10 engineering: novel insights into glycan interactions** <u>Michael Nagele</u><sup>1</sup>, Martha Gschwandtner<sup>1</sup>, Patrick Sorger<sup>1</sup>, Andreas J. Kungl<sup>1</sup> 1.-Institute of Pharmaceutical Sciences, University of Graz, Universitaetsplatz 1





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

<u>Mahmoud Nasr</u><sup>1</sup>, Mike Strauss<sup>1</sup>, James Hogle<sup>1</sup>, Gerhard Wagner<sup>1</sup> 1.-Dep. of Biological Chemistry and Molecular Pharmacology, Harvard Medical School

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

<u>Hiroyuki Noji<sup>1, 2</sup></u>

1.-The University of Tokyo, 2.-CREST, JST

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

<u>Gustav Oberdorfer<sup>1,2,7</sup></u>, Po-Ssu Huang<sup>1,7</sup>, Chunfu Xu<sup>1,7</sup>, Verena Kohler<sup>2</sup>, Xue Y. Pei<sup>3</sup>, Brent L. Nannenga<sup>4</sup>, Joseph M. Rogers<sup>5</sup>, Tamir Gonen<sup>4</sup>, Karl Gruber<sup>2</sup>, David Baker<sup>1,6,7</sup>

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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

<u>Teruyo Ojima-Kato<sup>1, 2</sup>, Kansuke Fukui</u><sup>2</sup>, Takaaki Kojima<sup>2</sup>, Hideo Nakano<sup>2</sup> 1.-Aichi Science and Technology Foundation, 2.-Nagoya University

# $\mathsf{PI-032}$ Targeted protein degradation achieved through a combination of degrons from yeast and mammalian ornithine decarboxylase

Rushikesh Joshi<sup>1</sup>, Ratna Prabha C.<sup>1</sup>

1.-The Maharaja Sayajirao University of Baroda

PI-033 **Design and characterisation of a synthetic serpin with novel folding properties** <u>Benjamin Porebski</u><sup>1</sup>, Shani Keleher<sup>1</sup>, Adrian Nickson<sup>2</sup>, Emilia Marijanovic<sup>1</sup>, Mary Pearce<sup>1</sup>, Natalie Borg<sup>1</sup>, James Whisstock<sup>1</sup>, Stephen Bottomley<sup>1</sup>, Sheena McGowan<sup>1</sup>, Ashley Buckle<sup>1</sup> 1.-Department of Biochemistry and Molecular Biology, Monash University, 2.-Department of Chemistry, University of Cambridge

PI-034 **Computational Design of Shape-optimized Leucine-Rich Repeat Proteins** <u>Sebastian Rämisch</u><sup>1</sup>, Ulrich Weininger<sup>2</sup>, Jonas Martinsson<sup>1</sup>, Mikael Akke<sup>2</sup>, Ingemar André<sup>1</sup> 1.-Department for Biochemistry & Structural Biology, Lund University, 2.-Department for Biophysical Chemistry, Lund University

PI-035 **Engineering APOBEC3G enzymes for altered specificity and processivity** <u>Louis Scott</u><sup>1</sup>, Muhammad Razif<sup>1</sup>, Aleksandra Filipovska<sup>1,2</sup>, Oliver Rackham<sup>1,2</sup> 1.-Harry Perkins institute of Medical Research, 2.-School of Chemistry and Biochemistry, The University of Western Australia

PI-036 **Engineering Porous Protein Crystals as Scaffolds for Programmed Assembly** Thaddaus Huber<sup>1</sup>, Luke Hartje<sup>1</sup>, <u>Christopher Snow<sup>1</sup></u> 1.-Colorado State University

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

<u>Francois St-Pierre</u><sup>1,2</sup>, Michael Pan<sup>1,2</sup>, Helen Yang<sup>3</sup>, Xiaozhe Ding<sup>1,2</sup>, Ying Yang<sup>1,2</sup>, Thomas Clandinin<sup>3</sup>, Michael Lin<sup>1,2</sup>

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### PI-038 Assembly of Armadillo Repeat Proteins from Complementary Fragments

Erich Michel<sup>1</sup>, Randall Watson<sup>1</sup>, Martin Christen<sup>1</sup>, Fabian Bumback<sup>3</sup>, Andreas Plückthun<sup>2</sup>, <u>Oliver</u> <u>Zerbe<sup>1</sup></u>

1.-Department of Chemistry, University of Zurich, 2.-Department of Biochemistry, University of Zurich, 3.-University of Melbourne

# $\mathsf{PI-039}$ Engineering light-controllable kinases and Cas9 endonuclease with photodissociable dimeric fluorescent protein domains

Xin Zhou<sup>1</sup>, Linlin Fan<sup>2</sup>, Michael Lin<sup>1,3,4</sup>

1.-Department of Bioengineering, Stanford University, 2.-Department of Chemical Biology, Harvard University, 3.-Department of Pediatrics, Stanford University, 4.-Department of Chemical and System Biology, Stanford University

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

Saacnicteh Toledo Patiño<sup>1</sup>, Birte Höcker<sup>1</sup> 1.-Max Planck Institute for Developmental Biology

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

Lena Schmohl<sup>1</sup>, Felix Roman Wagner<sup>1</sup>, Michael Schümann<sup>2</sup>, Eberhard Krause<sup>2</sup>, Dirk Schwarzer<sup>1</sup> 1.-Interfaculty Institute of Biochemistry, University of Tuebingen, 2.-Laboratory of Mass Spectrometry, Leibniz-Institut Für Molekulare Pharmakologie

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

Käthe M. Dahlström<sup>1</sup>, Cecilia Blikstad<sup>2</sup>, Mikael Widersten<sup>2</sup>, Tiina A. Salminen<sup>1</sup>

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

<u>Maximiliano Figueroa</u><sup>1</sup>, Mike Sleutel<sup>2</sup>, André Matagne<sup>3</sup>, Christian Damblon<sup>4</sup>, Els Pardon<sup>2</sup>, Marielle Valerio-Lepiniec<sup>5</sup>, Philippe Minard<sup>5</sup>, Joseph Martial<sup>1</sup>, Cécile Van de Weerdt<sup>1</sup>

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

Pawel K. Dominik<sup>1</sup>, Marta T. Borowska<sup>1</sup>, Olivier Dalmas<sup>0</sup>, Sangwoo S. Kim<sup>1</sup>, Dawid Deneka<sup>1</sup>, Eduardo Perozo<sup>1</sup>, Robert J. Keenan<sup>1</sup>, Anthony A. Kossiakoff<sup>1</sup>

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



<u>Masatoshi Nakatsuji</u><sup>1</sup>, Haruka Inoue<sup>1</sup>, Masaki Kohno<sup>1</sup>, Mayu Saito<sup>1</sup>, Syogo Tsuge<sup>1</sup>, Shota Shimizu<sup>1</sup>, Osamu Ishibashi<sup>1</sup>, Takashi Inui<sup>1</sup>

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

Anna Simon<sup>1</sup>, Alexis Vallée-Bélisle<sup>2</sup>, Francesco Ricci<sup>3</sup>, Kevin Plaxco<sup>1,4,5</sup>

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#### PI-047 Essential and non-essential amino acid species for an ancestral protein Satoshi Akanuma<sup>1</sup>

1.-Faculty of Human Sciences, Waseda University

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

Sota Yagi<sup>1</sup>, Satoshi Akanuma<sup>2</sup>, Akihiko Yamagishi<sup>1</sup>

1.-Tokyo University of Pharmacy and Life Sciences, Department of Applied Life Scien, 2.-Waseda University, Faculty of Human Sciences

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

<u>Naoto Nemoto</u><sup>1</sup>, Ryoya Okawa<sup>1</sup>, Yuki Yoshikawa<sup>1</sup>, Toshiki Miyajima<sup>1</sup>, Shota Kobayashi<sup>1</sup> 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><sup>1</sup>, Hiroya Niiro<sup>1</sup>, Satoshi Akanuma<sup>2</sup>, Tetsuya Uchida<sup>1</sup>, Akihiko Yamagishi<sup>1</sup> 1.-Tokyo University of Pharmacy and Life Sciences, 2.-Waseda University

### PI-051 Engineering of an isolated p110α subunit of PI3Kα permits crystallization and provides a platform for structure-based drug design

<u>Alexei Brooun</u><sup>1</sup>, Ping Chen<sup>1</sup>, Ya-Li Deng<sup>1</sup>, Simon Bergqvist<sup>1</sup>, Matthew Falk<sup>1</sup>, Wei Liu<sup>1</sup>, Sergei Timofeevski<sup>1</sup>

1.-Oncology Structural Biology, Worldwide Research and Development, Pfizer Inc

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

Emma Liliana Arevalo Salina<sup>1</sup>, Joel Osuna Quintero<sup>1</sup>, Humberto Flores Soto<sup>1</sup>, Gloria Saab Rincón<sup>1</sup> 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 Newell<sup>1</sup>

1.-Independent Researcher

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

Shuhei Nakane<sup>1</sup>, Zene Matsuda<sup>2,3</sup>

1.-Green Earth Research Center, Green Earth Institute Co., Ltd., 2.-Res Ctr for Asian Infect Dis, Inst of Med Sci, the Univ of Tokyo, 3.-Lab of Struct Virol and Immunol, Institute of Biophysics, CAS

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

Buyung Santoso<sup>1</sup>, Dorain Thompson<sup>1</sup>, John Nuss<sup>1</sup>, John Dwyer<sup>1</sup>

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

<u>Carrie Huynh</u><sup>1</sup>, Lee Hoang<sup>1</sup>, Chris Suh<sup>1</sup>, Jonathan Grambow<sup>1</sup> 1.- PhyNexus in San Jose

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

Kam Zhang<sup>1</sup>, Arnout Voet<sup>1</sup>, Hiroki Noguchi<sup>2</sup>, Christine Addy<sup>2</sup>, Jeremy Tame<sup>2</sup>

1.-Structural Bioinformatics Team, DSSB, CLST, RIKEN, 2.-Drug Design Laboratory, GSMLS, Yokohama City University

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

Chwan-Deng Hsiao<sup>1</sup>, Min-Guan Lin<sup>1</sup>, Long-Liu Lin<sup>2</sup>, Yuh-Ju Sun<sup>3</sup>

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

Anja Paatero<sup>1</sup>, Katja Rosti<sup>1</sup>, Alexander Shkumatov<sup>2</sup>, Cecilia Brunello<sup>3</sup>, Kai Kysenius<sup>3</sup>, Prosanta Singha<sup>1</sup>, Henri Huttunen<sup>3</sup>, <u>Tommi Kajander<sup>1</sup></u>

1.-Institute of Biotechnology, University of Helsinki2.-Dept of Pharmaceutical and Pharmacological Sciences, KU Leuven, 3.-Neuroscience Center, University of Helsinki

### PI-060 Computational design of phenylalanine binder

Olga Khersonsky<sup>1</sup>, Gil Benezer<sup>1</sup>, Sarel Fleishman<sup>1</sup>

1.-Department of Biological Chemistry, Weizmann Institute of Science

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

<u>Bjarni Ásgeirsson</u><sup>1</sup>, Manuela Magnúsdóttir<sup>1</sup>, Jens Hjörleifsson<sup>1</sup>, Gaetano Invernizzi<sup>2</sup>, Elena Papaleo<sup>2</sup> 1.-Department of Biochemistry, Science Institute, University of Iceland, 2.-University of Milano

### $\mathsf{PI-062}$ A novel secondary structure element assembly protocol for the design of artificial (\$\beta\articles\$-barrel proteins using ROSETTA

<u>Cristina Elisa Martina</u><sup>1</sup>, Steven Combs<sup>2</sup>, Rocco Moretti<sup>2</sup>, Maximiliano Figueroa<sup>1</sup>, Cecile Van De Weerdt<sup>1</sup>, Andre Matagne<sup>1</sup>, Jens Meiler<sup>2</sup>

1.-University of Liege, 2.-Vanderbilt University

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

<u>Shota Shimizu</u><sup>1</sup>, Masatoshi Nakatsuji<sup>1</sup>, Keisuke Yamaguchi<sup>1</sup>, Yuya Sano<sup>1</sup>, Yuya Miyamoto<sup>1</sup>, Takashi Inui<sup>1</sup>

1.-Graduate School of Life and Environmental Sciences, Osaka Prefecture University

### PI-064 Formation of Cytochrome cb562 Oligomers by Domain Swapping

Takaaki Miyamoto<sup>1</sup>, Mai Kuribayashi<sup>1</sup>, Satoshi Nagao<sup>1</sup>, Yasuhito Shomura<sup>2</sup>, Yoshiki Higuchi<sup>3,4</sup>, Shun Hirota<sup>1</sup> 1.-Graduate School of Materials Science, Nara Institutte of Science and Technology, 2.-Graduate School of Science and Engineering, Ibaraki University, 3.-Department of Life Science, Graduate School of Life Science, University of Hyogo, 4.-RIKEN SPring-8 Center

# 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





<u>Jens Hjörleifsson</u><sup>1</sup>, Bjarni Ásgeirsson<sup>1</sup> 1.-Department of Biochemistry, Science Institute, University of Iceland

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

<u>Helen Farrants</u><sup>1</sup>, Oliver Hantschel<sup>1</sup>, Kai Johnsson<sup>1</sup> 1.-École Polytechnique Fédérale de Lausanne (EPFL)

PI-067 **LIL traptamers: artificial transmembrane proteins with minimal chemical diversity** <u>Daniel DiMaio</u><sup>1</sup>, Erin Heim<sup>1</sup>, Ross Federman<sup>1</sup>, Lisa Petti<sup>1</sup>, Jez Marston<sup>1</sup> 1.-Yale Unversity School of Medicine

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

Yusuke Azuma<sup>1</sup>, Donald Hilvert<sup>1</sup>

1.-Laboratory of Organic Chemistry, ETH Zurich

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 Ito<sup>1</sup>, <u>Yurie Enomoto<sup>1</sup></u>, Shuhei Umemura<sup>1</sup>, Aiko Fujiyama<sup>1</sup>, Ryoko Mieno<sup>1</sup>, Yukiko Kato<sup>1</sup>, Daiichiro Kato<sup>1</sup>

1.-Graduate School of Science and Engineering, kagoshima University

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

Yang-Gyun Kim<sup>1</sup>, Xu Zheng<sup>1</sup>, So-Young Park<sup>1</sup> 1.-Department of Chemistry, Sungkyunkwan University

#### PI-071 Photo switching of protein conformation

Frank D. Sönnichsen<sup>1</sup>, Matthias Lipfert<sup>1</sup>, Hauke Kobarg<sup>1</sup>, Anne Müller<sup>1</sup>, Thisbe K. Lindhorst<sup>1</sup> 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 Nayek<sup>1</sup>, Shyamashree Banerjee<sup>1</sup>, Parth Sarthi Sen Gupta<sup>1</sup>, Biswa pratap Sur<sup>1</sup>, Pratay Seth<sup>1</sup>, Sunit Das<sup>1</sup>, Nathan A Baker<sup>2</sup>, Amal K Bandyopadhyay<sup>1</sup>

1. Department of Biotechnology, The University of Burdwan

2. Pacific Northwest National Laboratory

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

Anna Wojciechowska-Bason<sup>1</sup>, Clare Jones<sup>2</sup>, Chris Lloyd<sup>3</sup>

1.-Postdoctoral Fellow, ADPE, Medimmune, Cambridge, 2.-RIA, Medimmune, Cambridge, 3.-ADPE, Medimmune, Cambridge

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

Maria Antonietta Carillo<sup>1</sup>, Daniel Varon Silva<sup>1</sup>

1.-Max Planck Institute of Colloids and Interfaces, Biomolecular System department

### 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

<u>Melissa Lokensgard</u><sup>1</sup>, John Love<sup>1</sup> 1.-San Diego State Uniersity

PI-077 **Development of a semisynthetic method for the cell surface presentation of proteins** <u>Dorottya Németh</u><sup>1</sup>, Balázs Schäfer<sup>1</sup>, Éva Hunyadi-Gulyás<sup>2</sup>, Zsuzsanna Darula<sup>2</sup>, Csaba Tömböly<sup>1</sup> 1.-Biological Research Centre, Instute of Biochemisty, Laboratory of Chemical Biology, 2.-Biological Research Centre, Laboratory of Proteomics Research

#### PI-078 **Transmembrane domain dimerization drives p75NTR partitioning to lipid rafts** <u>Irmina García Carpio</u>, Marçal Vilar

1.-Sociedad de Biofísica de España

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

<u>Martijn Van Rosmalen</u><sup>1</sup>, Remco Arts<sup>1</sup>, Brian Janssen<sup>1</sup>, Natalie Hendrikse<sup>1</sup>, Dave Wanders<sup>1</sup>, Maarten Merkx<sup>1</sup> 1.-Laboratory of Chemical Biology / Institute of Complex Molecular Systems

### $\mathsf{PI-080}$ $\,$ Genetically encoded biosensor for cell permeability of inhibitors of the p53-HDM2 interaction

Silvia Scarabelli<sup>1</sup>, Thomas Vorherr<sup>2</sup>, Kai Johnsson<sup>1</sup>

1.-Ecole Polytechnique Fédérale de Lausanne, 2.-Novartis Institute for BioMedical Research

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

Jaume Bonet<sup>1</sup>, Javier Garcia-Garcia<sup>1</sup>, Joan Planas-Iglesias<sup>2</sup>, Narcis Fernandez-Fuentes<sup>3</sup>, Baldo Oliva<sup>1</sup>

1.-Structural Bioinformatics Lab, GRIB, UPF, 2.-Division of Metabolic and Vascular Health, University of Warwick, 3.-IBERS, Abersystwyth University

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

Taras Redchuk<sup>1</sup>, Evgeniya Omelina<sup>1</sup>, Konstantin Chernov<sup>1</sup>, Vladislav Verkhusha<sup>1,2</sup>

1.-Dept. of Biochemistry, Faculty of Medicine, University of Helsinki, 2.-Dept. of Anatomy and Structural Biology, Albert Einstein College of Medicine

### PI-083 Luminescent sensor proteins for antibody detection in solution

<u>Remco Arts</u><sup>1</sup>, Susann Ludwig<sup>1</sup>, Marina van Vliembergen<sup>1</sup>, Vito Thijssen<sup>1</sup>, Stan van der Beelen<sup>1</sup>, Ilona den Hartog<sup>1</sup>, Stefan Zijlema<sup>1</sup>, Maarten Merkx<sup>1</sup>

1.-Eindhoven University of Technology

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

Fan Zheng<sup>1</sup>, Jian Zhang<sup>2</sup>, Gevorg Grigoryan<sup>1,2</sup>

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

### PI-085 Exploiting natural sequence diversity for protein crystallization

Sergio Martínez-Rodríguez<sup>1</sup>, Valeria A. Risso<sup>1</sup>, Jose M. Sanchez-Ruiz<sup>1</sup>, Jose A. Gavira<sup>2</sup>

1.-Departamento de Química-Física, Universidad de Granada

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

### PI-086 Synthesis of selectively functionalized adiponectin

118 Andreas Mattern<sup>1</sup>, Annette Beck-Sickinge





1.-University of Leipzig, Institute of Biochemistry

#### PI-087 De novo catalysis in ancestral protein scaffolds

<u>Valeria A. Risso</u><sup>1</sup>, Sergio Martinez-Rodriguez<sup>1</sup>, Adela M. Candel<sup>1</sup>, David Pantoja-Uceda<sup>2</sup>, Mariano Ortega-Muñoz<sup>3</sup>, Francisco Santoyo-Gonzalez<sup>3</sup>, Marta Bruix<sup>2</sup>, José A Gavira<sup>4</sup>, Jose M. Sanchez-Ruiz<sup>1</sup> 1.-Departamento de Quimica Fisica, Facultad de Ciencias University of Granada, 2.-Dpto. de Quimica Fisica Biologica. Instituto de Quimica Fisica Rocasolano, 3.-Departamento de Quimica Organica, Facultad de Ciencias University of Granada, 4.-Laboratorio de Estrudios Cristalograficos, IACT-CSIC-UGR Granada

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

<u>Sierra Hansen</u><sup>1</sup>, Jiusheng Lin<sup>1</sup>, Mark Wilson<sup>1</sup> 1.-University of Nebraska, Lincoln

### $\mathsf{PI-089}$ $\,$ The purification, crystallization and preliminary characterization of SdrE from S. aureus

Deqiang Wang<sup>1</sup>, Ke Chen<sup>1</sup>, Jun Zhang<sup>2</sup>

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

<u>David Leibly</u><sup>1,2</sup>, Julien Jorda<sup>2</sup>, Sunny Chun<sup>3</sup>, Alan Pang<sup>2</sup>, Michael Sawaya<sup>2</sup>, Todd Yeates<sup>1,2,3</sup> 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><sup>1</sup>, Doga Findik<sup>1</sup>, Arzu Uyar<sup>1</sup>, Deniz Turgut<sup>2</sup>, Rahmi Ozisik<sup>2</sup>, Turkan Haliloglu<sup>1</sup>, Pemra Doruker<sup>1</sup>

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

### $\mathsf{PI-092}$ Continuous directed evolution of receptor-selective $\partial\text{-endotoxins}$ for overcoming insecticidal resistance

<u>Ahmed Badran</u><sup>1,2</sup>, Victor Guzov<sup>3</sup>, Qing Huai<sup>3</sup>, Melissa Kemp<sup>3</sup>, Prashanth Vishwanath<sup>3</sup>, Artem Evdokimov<sup>3</sup>, Farhad Moshiri<sup>3</sup>, Meiying Zheng<sup>3</sup>, Keith Turner<sup>3</sup>, David Liu<sup>1,2</sup>

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

<u>Brian Maniaci</u><sup>1</sup>, Collin Lipper<sup>2</sup>, John J. Love<sup>1</sup> 1.-San Diego State University, 2.-University of California

# PI-094 Continuous Evolution of Site-Specific Recombinases With Highly Reprogrammed DNA Specificities

Jeffrey L Bessen<sup>1,2</sup>, David B Thompson<sup>1,2</sup>, David R. Liu<sup>1,2</sup>

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

<u>Aleardo Morelli</u><sup>1</sup>, Burckhard Seelig<sup>1</sup> 1.-University of Minnesota

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

1 - Institut de Pharmacologie et de Biologie Structurale

### PI-097 Computational Design of Tighter Protein-Ligand Interfaces

Brittany Allison<sup>1</sup>, Brian Bender<sup>2</sup>, Jens Meiler<sup>1,2</sup>

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 Gonzalez<sup>1</sup>, Stefano Capaldi<sup>1</sup>, Maria Elena Carrizo<sup>1</sup>, Laura Destefanis<sup>1</sup>, Michele Bovi<sup>1</sup>, Massimiliano Perduca<sup>1</sup>, Hugo Luis Monaco<sup>1</sup>

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**

<u>Conor Jacobs</u><sup>1</sup>, Yang Geng<sup>2</sup>, Ryan Badiee<sup>1</sup>, Tiffany Nguyen<sup>3</sup>, Andrew Evans<sup>4</sup>, Hokyung Chung<sup>1</sup>, Ying Yang<sup>2</sup>, Mehrdad Shamloo<sup>4</sup>, Roger Y. Tsien<sup>5</sup>, Michael Z. Lin<sup>2, 6</sup>

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 Arts<sup>1</sup>, <u>Susann Ludwig</u><sup>1</sup>, Byron Martina<sup>2</sup>, Maarten Merkx<sup>1</sup> 1.-Eindhoven University of Technology, 2.-Erasmus Medical Center Rotterdam

### PI-101 Delivery of biologics against intracellular targets

Paulina Kolasinska-Zwierz<sup>1</sup>, Pawel Stocki<sup>1</sup>, Bina Mistry<sup>1</sup>, Sandrine Guillard<sup>1</sup>, Alison Smith<sup>1</sup>, Rose Marwood<sup>1</sup>, Ben Kemp<sup>1</sup>, Anna Czyz<sup>1</sup>, Ronald Jackson<sup>1</sup>, Ralph Minter<sup>1</sup>, Tristan Vaughan<sup>1</sup> 1.-ADPE Cambridge, MedImmune, Milstein Building

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

Edyta Kopera<sup>1</sup>, Maria Pietrzak<sup>1</sup>, Agnieszka Macioła<sup>1</sup>, Anna Maria Protas-Klukowska<sup>1</sup>, Konrad Zdanowski<sup>1</sup>, Beata Gromadzka<sup>2</sup>, Krystyna Grzelak<sup>1</sup>, Zenon Minta<sup>3</sup>, Krzysztof Śmietanka<sup>3</sup>, Bogusław Szewczyk<sup>2</sup> 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-104 Mining the structural universe for de novo design

<u>Craig Mackenzie</u><sup>1</sup>, Gevorg Grigoryan<sup>1</sup> 1.-Dartmouth College

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

Bedabrata Saha<sup>1</sup>, Marieke op de Beeck<sup>1</sup>, Remco Arts<sup>1</sup>, Maarten Merkx<sup>1</sup> 1.-Department of Biomedical Engineering, Eindhoven University of Technology

### PI-085 Exploiting natural sequence diversity for protein crystallization

Sergio Martínez-Rodríguez<sup>1</sup>, <u>Valeria A. Risso<sup>1</sup></u>, Jose M. Sanchez-Ruiz<sup>1</sup>, Jose A. Gavira<sup>2</sup> 1.-Departamento de Química-Física, Universidad de Granada, 18071, Granada, Spain, 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

<u>Devika Channaveerappa</u><sup>1</sup>, Roshanak Aslebagh<sup>1</sup>, Kathleen F. Arcaro<sup>2</sup>, Costel C. Darie<sup>1</sup> 1.-Clarkson University, 2.-University of Massachusetts

#### PJ-002 Leukolike Vectors: leukocyte-inspired nanoparticles

<u>Claudia Corbo</u><sup>1,2</sup>, Alessandro Parodi<sup>1,2</sup>, Roberto Palomba<sup>1,2</sup>, Roberto Molinaro<sup>1</sup>, Michael Evangelopoulos<sup>1</sup>, Francesco Salvatore<sup>2,3</sup>, Ennio Tasciotti<sup>1</sup>

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 Holding<sup>1</sup>

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

<u>Olivier Julien</u><sup>1</sup>, Min Zhuang<sup>1</sup>, Arun Wiita<sup>1</sup>, James Wells<sup>1</sup> 1.-University of California

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

John LaCava<sup>1,2</sup>, Kelly Molloy<sup>1</sup>, Martin Taylor<sup>3</sup>, David Fenyö<sup>2</sup>, Lixin Dai<sup>3</sup>, Brian Chait<sup>1</sup>, Jef Boeke<sup>2</sup>, Michael Rout<sup>1</sup>

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 Lee<sup>1</sup>, Trung Thanh Thach<sup>1</sup>, Namsoo Lee<sup>1</sup>, Donghyuk Shin<sup>1</sup>, Seungsu Han<sup>1</sup>, Gyuhee Kim<sup>1</sup>, Hongtae Kim<sup>1</sup>

1.-Department of Biological Sciences, Sungkyunkwan University

PJ-008 **Optimization of a protein extraction method for the proteomic study of pozol** <u>Cynthia Teresa Leyva-Arguelles</u><sup>1</sup>, Carmen Wacher<sup>2</sup>, Rosario Vera<sup>3</sup>, Romina Rodríguez-Sanoja<sup>1</sup> 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

Jaime Moreno García<sup>1</sup>, Juan Carlos Mauricio<sup>1</sup>, Juan Moreno<sup>2</sup>, Anna Lisa Coi<sup>3</sup>, Marilena Budroni<sup>3</sup>, Teresa García Martínez<sup>1</sup>

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### 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><sup>1</sup>, Antonio Díaz-Quintana<sup>1</sup>, Katiuska González-Arzola<sup>1</sup>, Alejandra Guerra-Castellano<sup>1</sup>, Adrián Velázquez-Campoy<sup>0</sup>, Miguel A. De la Rosa<sup>1</sup>, Irene Díaz-Moreno<sup>1</sup>

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?

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

Gonca Ozdemir Isik<sup>1</sup>, A.Nevra Ozer<sup>1</sup> 1.-Department of Bioengineering, Faculty of Engineering, Marmara University

#### PJ-013 Protein plasticity improves protein-protein binding description

Chiara Pallara<sup>1</sup>, Juan Fernández-Recio<sup>1</sup>

1.-Joint BSC-CRG-IRB Research Program In Computational Biology

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

<u>Vincent Puard</u><sup>1</sup>, Kit-Yee Tan<sup>1</sup>, Kurt Baldwin<sup>1</sup>, Enitan Carrol<sup>2</sup>, Rebecca Patisson<sup>3</sup>, Rob Beynon<sup>3</sup>, Christian Tiede<sup>4</sup>, Michael McPherson<sup>4</sup>, Darren Tomlinson<sup>4</sup>, Paul Ko Ferrigno<sup>1</sup>

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><sup>1</sup>, François-Xavier Cantrelle<sup>2</sup>, Amina Kamah<sup>1</sup>, Clément Despres<sup>1</sup>, Sudhakaran Prabakaran<sup>2</sup>, Jeremy Gunawardena<sup>2</sup>, Guy Lippens<sup>1</sup>, Isabelle Landrieu<sup>1</sup>

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-Mora<sup>1</sup>, Lydie Vamparys<sup>1</sup>, Alessandra Carbone<sup>2</sup>

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 Wilkins<sup>1</sup>, Kuo-Feng Hsu<sup>1</sup>, Christopher Schofield<sup>1</sup> 1.-Chemistry Research Laboratory, Oxford University

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

<u>Kelly Wormwood</u><sup>1</sup>, Armand Ngounou Wetie<sup>1</sup>, Laci Charette<sup>2</sup>, Jeanne Ryan<sup>2</sup>, Emmalyn Dupree<sup>1</sup>, Alisa Woods<sup>1,2</sup>, Costel Darie<sup>1</sup>

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### PJ-019 Understanding protein recognition using structural features

Manuel A. Marin-Lopez<sup>1</sup>, Joan Planas-Iglesias<sup>2</sup>, Jaume Bonet<sup>3</sup>, Daniel Poglayen<sup>1</sup>, Javier García-García<sup>1</sup>, Narcís Fernández-Fuentes<sup>1</sup>, Baldo Oliva<sup>1</sup>

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### PJ-020 Structural Characterization of the Cytoplasmic mRNA Export Platform

Javier Fernandez-Martinez<sup>1</sup>, Yi Shi<sup>2</sup>, Seung Joong Kim<sup>3</sup>, Paula Upla<sup>4</sup>, Riccardo Pellarin<sup>3</sup>, Daniel



Zenklusen<sup>5</sup>, David L. Stokes<sup>4</sup>, Andrej Sali<sup>3</sup>, Brian T. Chait<sup>2</sup>, Michael P. Rout<sup>1</sup>

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

Carla Oliveira<sup>1</sup>, Anael Alberto<sup>1</sup>, Mônica Freitas<sup>2</sup>, Luiz Alves<sup>1</sup>

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### 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><sup>1</sup>, Michal Jamroz<sup>1</sup>, Maciej Blaszczyk<sup>1</sup>, Andrzej Kolinski<sup>1</sup>, Sebastian Kmiecik<sup>1</sup> 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><sup>1</sup>, Michal Jamroz<sup>1</sup>, Mateusz Kurcinski<sup>1</sup>, Agata Szczasiuk<sup>1</sup>, Andrzej Kolinski<sup>1</sup>, Sebastian Kmiecik<sup>1</sup>

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PJ-024 **Developing a Technique to Detect Deamidated Proteins and Peptides Using Rig-I** <u>Sandy On</u><sup>1</sup>, Pinghui Feng<sup>2</sup>

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### PJ-025 Mass spectrometric evaluation of recombinant hemagglutinin structure conformations

Joanna Szewczak<sup>1</sup>, <u>Anna Bierczyńska-Krzysik<sup>1</sup></u>, Agnieszka Romanik-Chruścielewska<sup>1</sup>, Iwona Sokołowska<sup>1</sup>, Marcin Zieliński<sup>1</sup>, Piotr Baran<sup>1</sup>, Violetta Sączyńska<sup>1</sup>, Małgorzata Kęsik-Brodacka<sup>1</sup>, Drota Stadnik<sup>1</sup>, Grażyna Płucienniczak<sup>1</sup>

1.-Institute of Biotechnology and Antibiotics

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

Carlos Correa-Netto<sup>1,2</sup>, Ricardo Araújo<sup>1,2</sup>, Marcelo Strauch<sup>1</sup>, Leonora Brazil-Más<sup>1</sup>, Marcos Machado<sup>3</sup>, Moema Leitão-Araújo<sup>4</sup>, Paulo Melo<sup>3</sup>, Débora Foguel<sup>2</sup>, Juan Calvete<sup>5</sup>, Russolina Zingali<sup>2</sup>

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#### PJ-027 **A comprehensive analysis of scoring functions for protein-protein docking** Didier Barradas<sup>1</sup>, Juan Fernandez-Recio<sup>1,2</sup>

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)

<u>Isamu Kameshita</u><sup>1</sup>, Noriyuki Sueyoshi<sup>1</sup>, Yasunori Sugiyama<sup>1</sup> 1.-Kagawa University

PJ-029 A comprehensive analysis of scoring functions for protein-protein docking Didier Barradas<sup>1</sup>, Juan Fernandez-Recio<sup>1,2</sup>



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

Leonor Carvalho<sup>1</sup>, Vimal Parkash<sup>1</sup>, Heli Elovaara<sup>2</sup>, Sirpa Jalkanen<sup>2</sup>, Xiang-Guo Li<sup>3,4</sup>, Tiina Salminen<sup>1</sup> 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 Middleton<sup>1</sup>, Catherine Day<sup>1</sup>

1.-Department of Biochemistry, University of Otago

PJ-032 The two chromophorylated linkers of R-Phycoerythrin in Gracilaria chilensis <u>Marta Bunster</u><sup>1</sup>, Francisco Lobos-González<sup>1</sup>, José Aleikar Vásquez<sup>1</sup>, Carola Bruna<sup>1</sup>, José Martínez-Oyanedl<sup>1</sup> 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 Uchikoga<sup>1</sup>, Masahito Ohue<sup>2</sup>, Yuri Matsuzaki<sup>3</sup>, Yutaka Akiyama<sup>2.3</sup>, 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 Orlikowska<sup>1</sup>, Grzegorz Bujacz<sup>1</sup>

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# 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

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

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

Sara B. Estruch<sup>1</sup>, Sarah A. Graham<sup>1</sup>, Pelagia Deriziotis<sup>1</sup>, Swathi Mookonda Chinnappa<sup>1</sup>, Simon E. Fisher<sup>1,2</sup> 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)

Deqiang Wang<sup>1</sup>, Chen Ke<sup>1</sup>, Jun Zhang<sup>2</sup>

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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. Zamora<sup>1</sup>, Josep M. Campanera<sup>1</sup>, F. Javier Luque<sup>1</sup>, Jody McGinness<sup>1</sup>





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

#### PJ-040 Docking-based tools for discovery of protein-protein modulators

Mireia Rosell Oliveras<sup>1</sup>, Juan Fernández Recio<sup>2</sup>

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

Inhae Kim<sup>1</sup>, Sangjin Han<sup>1</sup>, Jihye Hwang<sup>2</sup>, Sanguk Kim<sup>1</sup>

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

Sergio Mares-Sámano<sup>1</sup>, <u>Luis Ángel Rodríguez-Lumbreras<sup>1</sup></u>, Juan Fernández-Recio<sup>1</sup> 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<sup>1</sup>, Blas Moreno-Beltrán<sup>1</sup>, Jonathan Martínez-Fábregas<sup>1</sup>, Carlos A. Elena-Real<sup>1</sup>, Antonio Díaz-Quintana<sup>1</sup>, Irene Díaz-Moreno<sup>1</sup>, Miguel Á. De la Rosa<sup>1</sup> 1.-Instituto de Bioquímica

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

<u>Alejandra Guerra-Castellano</u><sup>1</sup>, Katiuska González-Arzola<sup>1</sup>, Francisco Rivero-Rodríguez<sup>1</sup>, Adrián Velázquez-Campoy<sup>2</sup>, Miguel Ángel De la Rosa<sup>1</sup>, Irene Díaz-Moreno<sup>1</sup>, Antonio Díaz-Quintana<sup>1</sup> 1.-IBVF – CIC Cartuja, University of Seville - CSIC, 2.-BIFI-IQFR, University of Saragossa - CSIC

### PJ-046 MSbiodata Analysis Tool, a web tool to extract relevant information from proteomics experiments

Pau M. Muñoz Torres<sup>1</sup>, Robert Beluzic<sup>1</sup>, Ivana Grbesa<sup>1</sup>, Oliver Vugrek<sup>1</sup> 1.-Translational Medicine Group. Department of Molecular Medicine, Rudjer Bošković Institute

#### **PK - SYSTEMS BIOLOGY**

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

Fatma Gizem Avci<sup>1</sup>, Berna Sariyar Akbulut<sup>1</sup>

1.-Marmara University, Department of Bioengineering

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

Liudmila Lysenko<sup>1</sup>, Nadezda Kantserova<sup>1</sup>, Marina Krupnova<sup>1</sup>, Nina Nemova<sup>1</sup> 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<sup>1,2</sup>

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 Weiditch<sup>1</sup>, Karen Maxwell<sup>2,4</sup>, Voula Kanelis<sup>1,3</sup>

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><sup>1</sup>, Antonio Varriale<sup>2</sup>, Angelo Facchiamo<sup>2</sup>, Sabato D'Auria<sup>2</sup>, Maria Elena Raggi<sup>3</sup>, Anna Marabotti<sup>1</sup>

1.- Dept. Chemistry and Biology, University of Salerno, 2.- Institute of Food Science, CNR, 3.- RCCS "E. Medea" Ass. "La Nostra Famiolia"

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

<u>Roall Espersen</u><sup>1</sup>, Milena Gonzalo<sup>3</sup>, Samuel Jacquiod<sup>3</sup>, Waleed Abu-Alsud<sup>3</sup>, Søren J. Sørensen<sup>3</sup>, Jakob R. Winther<sup>4</sup>, Per Hägglund<sup>2</sup>, Birte Svensson<sup>1</sup>

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 Hwang<sup>1</sup>, Sangjin Han<sup>2</sup>, Inhae Kim<sup>2</sup>, Sanguk Kim<sup>2</sup>

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

Sangjin Han<sup>1</sup>, Jihye Hwang<sup>2</sup>, Inhae Kim<sup>1</sup>, Sanguk Kim<sup>1,2</sup>

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PK-009 Engineering a Stable, Symmetric Membrane Protein Scaffold

Amanda Duran<sup>1</sup>, Jens Meiler<sup>1</sup>

1.-Vanderbilt University-Department of Chemistry

### PL - OTHER

PL-001 Intrinsically Disordered Proteins Drive Heritable Transformations of Biological Traits Daniel Jarosz<sup>1</sup>, James Byers<sup>1</sup>, Sohini Chakrabortee<sup>2</sup>, Sandra Jones<sup>3</sup>, Amelia Chang<sup>2</sup>, David Garcia<sup>1</sup> 1.-Stanford University, 2.-Whitehead Institute for Biomedical Research, 3.-Rockefeller University

PL-002 **Prediction of binding affinity in protein complexes: contacts do matters** <u>Anna Vangone</u><sup>1</sup>, Alexandre MJJ Bonvin <sup>1</sup> 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><sup>1</sup>, Alexandra Vladimirova<sup>1</sup>, Mariya Nezhivaya<sup>1</sup>, Tatiana Danilova<sup>1</sup>, Pavel Pronkin<sup>1</sup>, Maria Gorobets<sup>1</sup>, Alexander Tatikolov<sup>1</sup>, Vyacheslav Misin<sup>1</sup>, Mark Rosenfeld<sup>1</sup>

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PL-004 Regulation of Neuronal SNAREs by accessory proteins Shrutee Jakhanwal<sup>1</sup>, Reinhard Jahn<sup>1</sup>

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

<u>Aldo A. Arvizu-Flores</u><sup>1</sup>, Eduardo Guevara-Hernandez<sup>2</sup>, Enrique F. Velazquez-Contreras<sup>1</sup>, Francisco J. Castillo-Yañez<sup>1</sup>, Luis G. Brieba<sup>3</sup>, Rogerio R. Sotelo-Mundo<sup>2</sup>

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

<u>Aldo A. Arvizu-Flores</u><sup>1</sup>, Manuel I. Carretas-Valdez<sup>2</sup>, Francisco J. Castillo-Yañez<sup>1</sup>, Karina D. Garcia-Orozco<sup>3</sup>, Carmen A. Contreras-Vergara<sup>3</sup>, Rogerio R. Sotelo-Mundo<sup>3</sup>, Maria A. Islas-Osuna<sup>1,3</sup>

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

Heejeong Lee<sup>1</sup>, <u>Dong Gun Lee<sup>1</sup></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

Krishna Chaitanya Bhattiprolu, Evelyne Schrank, Klaus Zangger

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

Fabian Bickel<sup>1, 2</sup>, Hans Kiefer<sup>1</sup>

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

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

Eva S. Cunha<sup>1</sup>, Pedro Sfriso<sup>2</sup>, Adriana Rojas<sup>1</sup>, Adam Hospital<sup>2</sup>, Modesto Orozco<sup>2</sup>, Nicola Abrescia<sup>1</sup> 1.-Structural Biology Unit, CIC bioGUNE, 2.-Institute for Research in Biomedicine (IRB Barcelona)

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

Jorge Dagnino-Leone<sup>1</sup>, José Martinez-Oyanedel<sup>1</sup>, Marta Bunster-Balocchi<sup>1</sup> 1.-Universidad de Concepción

#### PL-013 Novel practical strategies to access artificial metalloenzymes

Marco Filice<sup>1</sup>, Jose Miguel Palomo<sup>1</sup>

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

Zhanna Hakhverdyan<sup>1</sup>, Kelly Molloy<sup>2</sup>, Brian Chait<sup>2</sup>, Michael Rout<sup>1</sup>

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#### PL-015 Active Site Clustering Identifies Functional Families of the Peroxiredoxin Superfamily Angela Harper<sup>1</sup>, Janelle Leuthaeuser<sup>2</sup>, Patricia Babbitt<sup>2</sup>, Jacquelyn Fetrow<sup>3</sup>

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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 Karska<sup>1</sup>, Andrea D. Lipińska<sup>2</sup>, Małgorzata Graul<sup>2</sup>, Franciszek Kasprzykowski<sup>1</sup>, Emilia Sikorska<sup>1</sup>, Igor Zhukov<sup>3</sup>, Magdalena J. Ślusarz<sup>1</sup>, <u>Sylwia Rodziewicz-Motowidło<sup>1</sup></u> 1.-Faculty of Chemistry, University of Gdansk, 2.-Intercollegiate Faculty of Biotechnology, University of Gdansk, 3.-Nano Bio Medical Centre University of Poznan

### PL-017 Functional and mechanistic studies of dysferlin, an essential protein in cell membrane repair

<u>Colin Johnson</u><sup>1</sup>, Sara Codding<sup>1</sup> 1.-Oregon State University

# 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

Jiyoon Kim<sup>1</sup>, Dylan Lawless<sup>1</sup>, Manuel Ruether<sup>2</sup>, Andrew Bowie<sup>1</sup>, Kenneth H. Mok<sup>1,3</sup>

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### PL-019 Active site profile-based protein clustering is an efficient, accurate method to define protein functional groups

Janelle Leuthaeuser<sup>1</sup>, Angela Harper<sup>2</sup>, Gabrielle Shea<sup>2</sup>, Patricia Babbitt<sup>3</sup>, Jacquelyn Fetrow<sup>1,2</sup> 1.-Wake Forest University, 2.-Wake Forest University, 3.-University of California San Francisco

### PL-020 Insertion of the hydrophobic C-terminal domain of apoptotic BH3-only proteins into biological membranes

Ismael Mingarro<sup>1</sup>, Vicente Andreu-Fernández<sup>2</sup>, Manuel Bañó-Polo<sup>1</sup>, Maria J. García-Murria<sup>1</sup>, Mar Orzáez<sup>2</sup>

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### PL-021 A computational investigation of tight junctions

<u>Alexis Peña</u><sup>1</sup>, Flaviyan Jerome Irudayanathan<sup>1</sup>, Shikha Nangia<sup>1</sup> 1.-Syracuse University, Dept. of Biomedical and Chemical Engineering

# 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)

Idania Emedith Quintero Reyes<sup>1</sup>, Francisco Javier Castillo Yáñez<sup>1</sup>, Enrique fernando Velázquez Contreras<sup>1</sup>, Rocío Sugich Miranda<sup>1</sup>, David Octavio Corona Martínez<sup>1</sup>, Aldo Alejandro Arvizu Flores<sup>1</sup>, Ivet Cervantes Domínguez<sup>1</sup>

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#### PL-023 Mysterious world of stress-responding sigma factors in Bacillus subtilis <u>Olga Ramaniuk</u><sup>1</sup>





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#### PL-024 Assessing the costs and benefits of protein aggregation

<u>Natalia Sanchez de Groot</u><sup>1</sup>, Marc Torrent Burgas<sup>2</sup>, Charles N. J. Ravarani<sup>1</sup>, Salvador Ventura<sup>3</sup>, M. Madan Babu<sup>1</sup>

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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

Marta A. Silva<sup>1</sup>, <u>Telma C. Santos<sup>1</sup></u>, Teresa Catarino<sup>2</sup>, Carlos A. Salgueiro<sup>1</sup>

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#### PL-026 Appearance of stabilizing interactions in the evolution of a dimeric TIM barrel

<u>Mariana Schulte-Sasse</u><sup>1</sup>, Nancy O. Pulido Mayoral<sup>1</sup>, Miguel Costas-Basín<sup>2</sup>, Enrique García-Hernández<sup>3</sup>, Adela Rodríguez-Romero<sup>3</sup>, D. Alejandro Fernández-Velasco<sup>1</sup>

1.-National Autonomous University of Mexico, Faculty of Medicine, 2.-National Autonomous University of Mexico, Faculty of Chemistry, 3.-National Autonomous University of Mexico, Institute of Chemistry

### PL-027 Receptor Protein-Tyrosine Phosphatases: Dimerization, receptor kinase interaction and allosteric modulation

Elizabeth Dembicer<sup>1</sup>, <u>Damien Thevenin<sup>1</sup></u>

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### PL-028 Inhibiting EGFR dimerization and signaling through targeted delivery of juxtamembrane domain peptide mimics using pHLIP

Anastasia Thevenin<sup>1</sup>, Kelly Burns<sup>1</sup>, Janessa Guerre-Chaley<sup>1</sup>, Damien Thevenin<sup>1</sup> 1.-Department of Chemistry, Lehigh University

# PL-029 The thumb subdomain of yeast mitochondrial RNA polymerase is involved in processivity, transcript fidelity and mitochondrial transcription factor binding.

Gilberto Velazquez<sup>1</sup>, Luis Brieba<sup>2</sup>, Rui Sousa<sup>3</sup>

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

<u>Vladimir Yarov-Yarovoy</u><sup>1</sup>, Diane Nguyen<sup>1</sup> 1.-University of California Davis

#### PL-031 **Coordinated gripping of substrate by subunits of a AAA+ proteolytic machine** <u>Ohad Yosefson</u><sup>1</sup>, Andrew Nager<sup>1</sup>, Tania Baker<sup>1</sup>, Robert Sauer<sup>1</sup>

1.-Department of Biology, Massachusetts Institute of Technology

PL-032 Structure and function of the Toc159 M-domain, and its role in targeting the preprotein receptor to the chloroplast outer envelope membrane

Matthew Smith<sup>1</sup>, Shiu-Cheung Lung<sup>2</sup>, Prem Nichani<sup>1</sup>, Nicholas Grimberg<sup>1</sup>, J. Kyle Weston<sup>1</sup>, Shane

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### PL-033 Structural investigation of NIpC/P60 protein acquired by Trichomonas vaginalis through a lateral gene transfer event

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# PL-034 Novel DNA polymerases from Red Sea brine-pools: New potential polymerases for PCR application

<u>Masateru Takahashi</u><sup>1</sup>, Etsuko Kimura<sup>1</sup>, Mohamed Salem<sup>1</sup>, Ulrich Stingl<sup>1</sup>, Samir Hamdan<sup>1</sup> 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

<u>Ming-Hon Hou</u><sup>1</sup>, Shing-Yen Lin<sup>1</sup>, Chia-Ling Liu<sup>1</sup>, Yu-Ming Chang<sup>2</sup>, Jincun Zhao<sup>3</sup>, Stanley Perlman<sup>3</sup> 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

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### 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

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#### 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><sup>1</sup>, Vera Leonova<sup>1</sup>, Alexander Shchegolikhin<sup>1</sup>, Marina Biryukova<sup>1</sup>, Elizaveta Kostanova<sup>1</sup>, Mark Rosenfeld<sup>1</sup>

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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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#### PL-041 Novel kinetochore protein complex from silkworm holocentric chromosomes

Takahiro Kusakabe<sup>1</sup>, Hiroaki Mon<sup>1</sup>, JaeMan Lee<sup>1</sup> 1.-Kyushu University Graduate School

### PL-042 Inactivation of betaine aldehyde dehydrogenase from spinach by its physiological substrate betaine aldehyde

Rosario A. Muñoz-Clares<sup>1</sup>, Andrés Zárate-Romero<sup>1</sup>, Dario S. Murillo-Melo<sup>1</sup>, Carlos Mújica-Jiménez<sup>1</sup>, Carmina Montiel<sup>1</sup>

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PL-044 Study of denaturation of proteins by surfactant using the taylor dispersion analysis and dynamic light scattering

<u>Anna Lewandrowska</u><sup>1</sup>, Aldona Jelińska<sup>1</sup>, Agnieszka Wiśniewska<sup>1</sup>, Robert Hołyst<sup>1</sup> 1.-Institute of Physical Chemistry Polish Academy of Sciences

### PL-046 Paraoxonase 1 (Pon1) regulates water homeostasis by controlling the expression of Fxr and Aqp2 proteins in mice

Marianna Wieloch<sup>1,2</sup>, Hieronim Jakubowski<sup>1,2,3</sup>

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### PL-047 Development and application of novel non-Ewald methods for calculating electrostatic interactions in molecular simulations

Ikuo Fukuda<sup>1</sup>, Narutoshi Kamiya<sup>1</sup>, Han Wang<sup>2</sup>, Kota Kasahara<sup>1</sup>, Haruki Nakamura<sup>1</sup> 1.-Institute for Protein Research, Osaka University, 2.-Freie Universitaet Berlin

#### PL-048 Isolation and characterisation of the zearalenone degrading hydrolase ZenA

<u>Sebastian Fruhauf</u><sup>1</sup>, Michaela Thamhesl<sup>1</sup>, Patricia Fajtl<sup>1</sup>, Verena Klingenbrunner<sup>1</sup>, Elisavet Kunz-Vekiru<sup>2</sup>, Gerhard Adam<sup>3</sup>, Gerd Schatzmayr<sup>1</sup>, Wulf-Dieter Moll<sup>1</sup>

1.-Biomin Research Center, 2.-Christian Doppler Laboratory for Mycotoxin Metabolism (IFA-Tulln), 3.-IAGZ, University of Natural Resources and Life Sciences

#### PL-049 A new biding site for snake venom C-type lectins?

<u>Maria Cristina Nonato Costa</u><sup>1</sup>, Ricardo Augusto Pereira de Pádua<sup>1</sup>, Marco Aurelio Sartim<sup>1</sup>, Suely Vilela Sampaio<sup>1</sup>

1.-University of São Paulo, FCFRP, Av. Café S/N Monte Alegre

#### PL-050 **Ab initio modelling of structurally uncharacterised antimicrobial peptides** Mara Kozic<sup>1</sup>

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#### PL-051 Surface Aggregation-Propensity as a Constraint on Globular Proteins Evolution

<u>Susanna Navarro</u><sup>1</sup>, Marta Diaz<sup>2</sup>, Pablo Gallego<sup>2</sup>, David Reverter<sup>2</sup>, Salvador Ventura<sup>1</sup> 1.-Institut de Biotecnologia i Biomedicina and Departament de Bioquimica i Biologia, 2.-Institut de

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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><sup>1</sup>, Noreen Gonzales<sup>1</sup>, Gabriele Marchler<sup>1</sup>, Myra Derbyshire<sup>1</sup>, James Song<sup>1</sup>, Roxanne Yamashita<sup>1</sup>, Christina Zheng<sup>1</sup>, Stephen Bryant<sup>1</sup>, Aron Marchler-Bauer<sup>1</sup>, Farideh Chitsaz<sup>1</sup>

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# PL-053 Biophysical characterization of the Sema3A C-terminal basic domain interaction with glycosaminoglycans

Roman Bonet<sup>1</sup>, Miriam Corredor<sup>1</sup>, Cecilia Domingo<sup>1</sup>, Jordi Bujons<sup>1</sup>, Yolanda Perez<sup>1</sup>, Ignacio Alfonso<sup>1</sup>, Angel Messeguer<sup>1</sup>

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### PL-054 Functional Clustering of the Crotonase Superfamily

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1.-Dickinson College, Molecular Biology and Chemistry Department, 2.-Department of Molecular Genetics, Wake Forest University, 3.-Department of Pharm. Chem., University of California, San Francisco, CA, 4.-Department of Chemistry, University of Richmond

### PL-055 Peptidic Probes for Intravascular Molecular Imaging of Inflammation Using Clinically Translatable Polymeric Microbubbles

<u>Olga Iranzo</u><sup>1,2</sup>, Ana C. Fernandes<sup>1</sup>, Teresa Sorbo<sup>2</sup>, Ivan Duka<sup>2</sup>, Lia Christina Appold<sup>3</sup>, Marianne Ilbert<sup>4</sup>, Fabian Kiessling<sup>3</sup>, Ricardo J. F. Branco<sup>5</sup>

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# PL-056 A search for anti-melioidosis drug candidates targeted to sedoheptulose-7-phosphate isomerase from Burkholderia pseudomallei

Jimin Park<sup>1</sup>, Daeun Lee<sup>1</sup>, Sang A Yeo<sup>1</sup>, Mi-Sun Kim<sup>1</sup>, Dong Hae Shin<sup>1</sup> 1.-College of Pharmacy, Global Top5 Research Program, Ewha Womans University

#### PL-057 **Mapping the Structure of Laminin Using Cross-linking and Mass Spectrometry** Gad Armonv<sup>1</sup>, Toot Moran<sup>1</sup>, Yishai Levin<sup>2</sup>, Deborah Fass<sup>1</sup>

1.-Weizmann Institute of Science, Department of Structural Biology, 2.-Weizmann Institute of Science, Israel Center for Personalized Medicine

### PL-058 Non-sequential protein structure alignment program MICAN and its applications

Shintaro Minami<sup>1</sup>, George Chikenji<sup>2</sup>, Motonori Ota<sup>1</sup>

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### PL-059 Effects of Cell-Like Infrastructures on Transient Protein Interactions

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PL-060 A search for anti-melioidosis drug candidates targeted to D-glycero-D-mannoheptose-1,7-bisphosphate phosphatase from Burkholderia pseudomallei Jimin Park<sup>1</sup>, Sang A Yeo<sup>1</sup>, Daeun Lee<sup>1</sup>, Mi-Sun Kim<sup>1</sup>, Dong Hae Shin<sup>1</sup>





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### PL-061 Crystal structure of dimeric D-glycero-D-manno-heptose-1,7-bisphosphate phosphatase from Burkholderia thailandensis

Jimin Park<sup>1</sup>, Mi-Sun Kim<sup>1</sup>, Daeun Lee<sup>1</sup>, Keehyung Joo<sup>2</sup>, Gil-Ja Jhon<sup>3</sup>, Jooyoung Lee<sup>2</sup>, Dong Hae Shin<sup>1</sup>

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PL-062 **Refined crystal structure of predicted fructose-specific enzyme IIB(fruc) from E. coli** <u>Jimin Park</u><sup>1</sup>, Daeun Lee<sup>1</sup>, Mi-Sun Kim<sup>1</sup>, Keehyung Joo<sup>2</sup>, Gil-Ja Jhon<sup>3</sup>, Jooyoung Lee<sup>2</sup>, Dong Hae Shin<sup>1</sup>

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#### PL-063 NMR studies of the insertase BamA in three different membrane mimetics

<u>Leonor Morgado</u><sup>1</sup>, Kornelius Zeth<sup>0</sup>, Björn M. Burmann<sup>1</sup>, Timm Maier<sup>1</sup>, Sebastian Hiller<sup>1</sup> 1.-Biozentrum, University of Basel, 2.-Department of Biochemistry, University of the Basque Country, 3.-Ikerbasque - Basque Foundation for Research

### PL-064 Biochemical characterization of the substrate specificity of two unique members of the mammalian protein arginine methyltransferase family, PRMT7 and PRMT9

Andrea Hadjikyriacou<sup>1</sup>, You Feng<sup>1</sup>, Yanzhong Yang<sup>2</sup>, Mark Bedford<sup>3</sup>, Steven Clarke<sup>1,4</sup>

1.-Department of Chemistry and Biochemistry, University of California Los Angeles, 2.-Department of Radiation Biology, Beckman Research Institute, City of Hope, 3.-Department of Epigenetics and Molecular Carcinogenesis UT MD Anderson Cancer, 4.-Molecular Biology Institute, University of California Los Angeles

### PL-065 Ornithine decarboxylase participates in autophagy by ultraviolet B-induced cell injury

Guang-Yaw Liu<sup>1</sup>, Yen-Hung Lin<sup>2</sup>, Hui-Chih Hung<sup>2</sup>

1.-Institute of Microbiology & Immunology, Chung Shan Medical University, and Divi, 2.-Department of Life Sciences, National Chung Hsing University (NCHU)

#### PL-066 Fish ß-parvalbumin acquires allergenic properties by amyloid assembly

Javier Martínez<sup>1</sup>, Rosa Sánchez<sup>1</sup>, Milagros Castellanos<sup>2</sup>, Ana M. Fernández-Escamilla<sup>3</sup>, Sonia Vázquez-Cortés<sup>4</sup>, Montserrat Fernández-Rivas<sup>4</sup>, María Gasset<sup>1</sup>

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### PL-067 Peptidylarginine Deiminase 2 Assigns Activated T Cell Autonomous Death

<u>Guang-Yaw Liu<sup>1</sup></u>, Wen-Hao Lin<sup>2</sup>, Hui-Chih Hung<sup>2</sup>

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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 Yuliana Raynova<sup>1</sup>, Krassimira Idakieva<sup>1</sup>, Vaclav Motyka<sup>2</sup>, Petre Dobrev<sup>2</sup>, Yuliana Markovska<sup>3</sup>, Milka

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#### PL-069 Evaluation of human salivary α-defensins by LC-ESI-MS

<u>Nadia Ashrafi</u><sup>1</sup>, Cris Lapthorn<sup>1</sup>, Fernando Naclerio<sup>2</sup>, Frank Pullen<sup>1</sup>, Birthe Nielsen<sup>1</sup>, Yue Fu<sup>2</sup>, Jack Miller<sup>2</sup>, Christian Watkinson<sup>2</sup>, Marcos Seijo<sup>2</sup>

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

#### PL-070 **Characterising interactions between alginates of different sizes and ß-lactoglobulin** <u>Emil G. P. Stender</u><sup>1</sup>, Sanaullah Khan<sup>2</sup>, Outi E. Mäkinen<sup>3</sup>, Kristoffer Almdal<sup>2</sup>, Peter Westh<sup>4</sup>, Richard Ibsen<sup>2</sup>, Maher Abou Hachem<sup>1</sup>, Birte Svensson<sup>1</sup>

1.-Technical University of Denmark – DTU – Department of Systems Biology, 2.-2Technical University of Denmark – DTU – Department of Micro- and Nanotechnology, 3.-University of Copenhagen – Department of Food Science, 4.-Roskilde University – RUC – Department of Science, Systems and Models

#### PL-071 Validation of a LC-MS method for the detection of human salivary α-defensins

Nadia Ashrafi<sup>1</sup>, Cris Lapthorn<sup>1</sup>, Birthe Nielsen<sup>1</sup>, Fernando Naclerio<sup>2</sup>, Frank Pullen<sup>1</sup>, Patricia Wright<sup>1</sup> 1.-University of Greenwich (Faculty of Engineering and Science), 2.-University of Greenwich (Centre for Sport Science and Human Performance)

#### PL-072 Moonlighting proteins: relevance for biotechnology and biomedicine

Luis Franco Serrano<sup>1</sup>, Sergio Hernández<sup>1</sup>, Alejandra Calvo<sup>2</sup>, Gabriela Ferragut<sup>2</sup>, Isaac Amela<sup>1</sup>, Juan Cedano<sup>2</sup>, Enrique Querol<sup>1</sup>

1.-Institut de Biotecnologia i Biomedicina. Universitat Autònoma de Barcelona, 2.-Laboratorio de Inmunología, Universidad de la República Regional Norte-Salto

### PL-073 Correlation between potential human neutrophil antimicrobial peptides (HNP 1-3) and stress hormones in human saliva

Nadia Ashrafi<sup>1</sup>, Frank Pullen<sup>1</sup>, Birthe Nielse<sup>1</sup>, Cris Lapthorn<sup>1</sup>, Fernando Naclario<sup>2</sup>

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### PL-074 Gwidd: genome-wide docking database

<u>Madhurima Das</u><sup>1</sup>, Varsha D. Badal<sup>1</sup>, Petras J. Kundrotas<sup>1</sup>, Ilya A. Vakser<sup>1</sup> 1.-Center for Computational Biology, The University of Kansas

### PL-075 Refolding and activation of recombinant trypsin i from sardine fish (Sardinops sagax caerulea)

<u>Manuel Carretas-Valdez</u><sup>1</sup>, Francisco Cinco-Moroyoqui<sup>1</sup>, Marina Ezquerra-Brauer<sup>1</sup>, Enrique Marquez-Rios<sup>1</sup>, Rogerio Sotelo-Mundo<sup>2</sup>, Idania Quintero-Reyes<sup>3</sup>, Aldo Arvizu-Flores<sup>3</sup> 1.-Universidad de Sonora, Departamento de Investigación en Alimentos, 2.-Centro de Investigación en Alimentación y Desarrollo, A.C., 3.-Universidad de Sonora. Departamento de Ciencias Químico Biológicas

#### PL-076 **WapA and SMU\_63c are Amyloidogenic Proteins of Streptococcus mutans** Richard Besingi<sup>1</sup>, <u>L. Jeannine Brady<sup>1</sup></u>

1.-Department of Oral Biology, University of Florida

# $\mathsf{PL}\text{-}077$ Characterization of the membrane-localized interaction network between the GTP-ase Rheb and the FKBP12-like protein FKBP38 by NMR

Maristella De Cicco<sup>1</sup>, Sonja A. Dames<sup>1</sup>





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PL-078 **Unraveling the Nature of TDP-43 Aggregates from its Putative Aggregation Domain** <u>Miguel Mompeán</u><sup>1</sup>, Rubén Hervás<sup>2</sup>, Yunyao Xu<sup>3</sup>, Timothy H. Tran<sup>4</sup>, Emanuele Buratti<sup>5</sup>, Francisco Baralle<sup>5</sup>, Liang Tong<sup>4</sup>, Mariano Carrión-Vázquez<sup>2</sup>, Ann E. McDermott<sup>3</sup>, Douglas V Laurents<sup>1</sup> 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

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### PL-080 Molecular characterization of specific positively selected sites in mammalian visual pigment evolution

<u>Miguel A. Fernández-Sampedro</u><sup>1</sup>, Eva Ramon<sup>1</sup>, Brandon M. Invergo<sup>2</sup>, Jaume Bertranpetit<sup>2</sup>, Pere Garriga<sup>1</sup>

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PL-081 **Natural Evolution Sheds Light on Modern Drug Resistance in Protein Kinases** <u>Marc Hoemberger</u><sup>1</sup>, Christopher Wilson<sup>1</sup>, Roman Agafonov<sup>1</sup>, Dorothee Kern<sup>1</sup> 1.-HHMI & Department of Biochemistry, Brandeis University

#### PL-082 An Evolutionary View of The Cold Adapted Catalysis of Enzymes

Vy Nguyen<sup>1</sup>, Christopher Wilson<sup>1</sup>, Dorothee Kern<sup>1</sup>

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PL-083 Induced oxidative modification of plasma and cellular fibrin-stabilizing factor

Anna Bychkova<sup>1</sup>, Tatiana Danilova<sup>1</sup>, Alexander Shchegolikhin<sup>1</sup>, Vera Leonova<sup>1</sup>, Marina Biryukova<sup>1</sup>, Elizaveta Kostanova<sup>1</sup>, Alexey Kononikhin<sup>1,2</sup>, Anna Bugrova<sup>1</sup>, Evgeny Nikolaev<sup>1,2</sup>, Mark Rosenfeld<sup>1</sup>, 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-084 Performance and quality. Making microcalorimetry simple with microcal peaq-itc

<u>Natalia Markova</u><sup>1</sup>, Ronan O'Brien<sup>1</sup>, Mark Arsenault<sup>1</sup> 1.-MicroCal, Malvern Instruments Ltd.

### PL-085 Glutamine-rich activation domain of transcription factor Sp1- biochemical activity and structure

Jun Kuwahara<sup>1</sup>, Chisana Uwatoko<sup>1</sup>, Emi Hibino<sup>2</sup>, Katsumi Matsuzaki<sup>2</sup>, Masaru Hoshino<sup>2</sup>

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# PL-086 CHIPping Away at the Yeast Proteome: Redesigning an E3 Ubiquitin Ligase for Targeted Protein Degradation

Michael Hinrichsen<sup>1</sup>, Lynne Regan<sup>1</sup>

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### **PM - ENGINEERING & INTERPRETING THE GENOME**

### PM-001 Functional characterization of proteins by domain architecture

Roxanne Yamashita<sup>1</sup>, Lewis Geer<sup>1</sup>, Lianyi Han<sup>1</sup>, Lanczycki Christopher<sup>1</sup>, Shennan Lu<sup>1</sup>, Jane He<sup>1</sup>, Josie Wang<sup>1</sup>, CDD Curation Team<sup>1</sup>, Aron Marchler-Bauer<sup>1</sup>

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