

PROGRAM

MONDAY, May 15—7:00 PM

Opening Remarks

Martin Caffrey, Trinity College Dublin

KEYNOTE SPEAKER

Introduction by: **Martin Caffrey**, Trinity College Dublin, Ireland

Probing G protein-coupled receptors as allosteric sensors linking hormone binding to G protein activation

Roger K. Sunahara [40'+10']

Presenter affiliation: University of California at San Diego, La Jolla, California.

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MONDAY, May 15—8:00 PM

POSTER SNAPSHOTS

See Poster Session I for list of posters

Introduction by: **Martin Caffrey**, Trinity College Dublin, Ireland

TUESDAY, May 16—9:00 AM

SESSION 1 TRANSPORTERS AND CHANNELS

Chairperson: **Kaspar Locher**, ETH Zürich, Zürich, Switzerland

TRPV1 structure in lipid nanodisc by single particle cryo-EM

Yuan Gao, David Julius, Yifan Cheng [20'+5']

Presenter affiliation: University of California San Francisco, San Francisco, California.

2

Structure of respirasome

Maojun Yang [20'+5']

Presenter affiliation: Tsinghua University, Beijing, China.

3

Mechanistic relationships in the TMEM16 family of calcium activated chloride channels and lipid scramblases

Raimund Dutzler [20'+5']

Presenter affiliation: University of Zurich, Zurich, Switzerland.

4

Structural diversity in group I energy coupling factor transporters

Inokentijis Josts, Yasser Almeida Hernandez, Antonina Andreeva, Henning Tidow [10'+5']

Presenter affiliation: Institute for Biochemistry and Molecular Biology, University of Hamburg, Hamburg, Germany.

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Coffee / Tea Break

TUESDAY, May 16—11:00 AM

SESSION 2 GPCRs

Chairperson: **Karen Fleming**, Johns Hopkins University, Baltimore, Maryland, USA

Structure and mechanism of human CNS GPCRs

Daniel M. Rosenbaum [20'+5']

Presenter affiliation: UT Southwestern Medical Center, Dallas, Texas.

6

Structural biology methodology development and crystal structure of the human cannabinoid receptor CB1

Zhi-Jie Liu [20'+5']

Presenter affiliation: ShanghaiTech University, Shanghai, China.

7

Structural insight into allosteric modulation of protease-activated receptor-2

Robert K.Y. Cheng, Cedric Fiez-Vandal, Oliver Schlenker, Karl Edman, Birte Aggeler, Dean G. Brown, Giles Brown, Robert Cooke, Christopher E. Dumelin, Andrew S. Doré, Stefan Geschwindner, Christoph Grebner, Nils-Olov Hermansson, Ali Jazayeri, Patrik Johansson, Louis Leong, Rudi Prihandoko, Mathieu Rappas, Holly Souter, Arjan Snijder, Linda Sundström, Benjamin Tehan, Peter Thornton, Dawn Troast, Giselle Wiggin, Andrei Zhukov, Fiona H. Marshall, Niek Dekker [10'+5']

Presenter affiliation: Heptares Therapeutics Ltd, Welwyn Garden City, United Kingdom.

8

The cubicon method for concentrating membrane proteins in the cubic mesophase

Pikyee Ma, Dietmar Weichert, Luba A. Aleksandrov, Timothy J. Jensen, John R. Riordan, Xiangyu Liu, Brian K. Kobilka, Martin Caffrey [10'+5']

Presenter affiliation: Trinity College Dublin, Dublin, Ireland; Current: Paul Scherrer Institut, Villigen, Switzerland.

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TUESDAY, May 16—2:00 PM

POSTER SESSION I

Even # posters 2:00 pm / Odd # posters 3:15 pm

The crystal structure of the YknZ extracellular domain of ABC transporter YknWXYZ from *Bacillus amyloliquefaciens*

Jinsook Ahn, Yongbin Xu, Nam-Chul Ha

Presenter affiliation: Seoul National University, Seoul, South Korea.

10

Functional characterization of a eukaryotic copper transporter CTR

Kehan Chen, Yaping Pan, Ming Zhou

Presenter affiliation: Baylor College of Medicine, Houston, Texas.

11

Modulations of BMP binding to receptors through protein engineering and natural small molecules

Guo-Chung Dong

Presenter affiliation: National Health Research Institutes, Miaoli, Taiwan.

12

A versatile in vitro system to study translocation and functional integration of bacterial outer membrane proteins

Derrick Norell, Alexander Heuck, Thuy-Anh Tran-Thi, Hansjörg Götzke, Françoise Jacob-Dubuisson, Tim Clausen, Daniel O. Daley, Volkmar Braun, Matthias Müller, Enguo Fan

Presenter affiliation: University of Freiburg, Freiburg, Germany.

13

Structure of the tripartite macrolide-specific efflux pump MacAB-ToIC by negative-stain EM

Seok-Ho Hong, Inseong Jo, Nam-Chul Ha

Presenter affiliation: Seoul National University, Seoul, South Korea.

14

Crystal structures of <i>C. elegans</i> TRIC channels—Pore architecture and gating mechanism	
<u>Miaohui Hu</u>	
Presenter affiliation: Institute of Biophysics, Chinese Academy of Sciences, Beijing, China; University of Chinese Academy of Sciences, Beijing, China.	15
Functional reconstitution of the adenosine A_{2A} receptor in native lipid membranes via maleic acid co-polymers	
<u>Shuya K. Huang</u> , Brent Lyda, Roger K. Sunahara, Robert S. Prosser	
Presenter affiliation: University of Toronto, Toronto, Canada.	16
Structure of the tripartite multidrug efflux pump AcrAB-ToIC suggests an alternative assembly mode	
<u>Yongdae Jang</u> , Jin-Sik Kim, Jaekyung Hyun, Nam-Chul Ha	
Presenter affiliation: Seoul National University, Seoul, South Korea.	17
Interaction mediated by the putative tip regions of MdsA and MdsC in the formation of a <i>Salmonella</i>-specific tripartite efflux pump	
<u>Soyeon Jeong</u> , Saemee Song, Nam-Chul Ha	
Presenter affiliation: Seoul National University, Seoul, South Korea.	18
Cryo-EM structure of the tripartite multidrug efflux pump AcrAB-ToIC	
<u>Inseong Jo</u> , Jinsook Ahn, Nohra Park, Seok-Ho Hong, Yongdae Jang, Soyeon Jeong, Nam-Chul Ha	
Presenter affiliation: Seoul National University, Seoul, South Korea.	19
Membrane topology of Dengue NS2B and NS4B in detergent micelles	
Yan Li, Ying Ru Loh, <u>Congbao Kang</u>	
Presenter affiliation: ASTAR, Singapore.	20
Production and characterization of aquaporins of euryhaline fish	
<u>Zhengjun Li</u> , Chin Xia Liew, Jie Shin Liew, Hu Zhou, Eei Yin Lui, Qingsong Lin, Siew Hong Lam	
Presenter affiliation: National University of Singapore, Singapore.	21
Advances in MicroED development and investigating membrane protein crystals using MicroED	
<u>Shian Liu</u> , Johan Hattne, M. Jason de la Cruz, Dan Shi, Tamir Gonen	
Presenter affiliation: Howard Hughes Medical Institute, Ashburn, Virginia.	22

- Mechanism of intracellular allosteric β 2AR antagonist revealed by X-Ray crystal structure**
Xiangyu Liu, Seungkil Ahn, Alem W. Kahsai, Kai-Cheng Meng, Naomi R. Latorraca, Biswaranjan Pani, A. J. Venkatakrishnan, Ali Masoudi, William I. Weis, Ron O. Dror, Xin Chen, Robert J. Lefkowitz, Brian K. Kobilka
 Presenter affiliation: Tsinghua University, Beijing, China. 23
- Identification and characterization of interactions between MurJ (MviN) and proteins of bacterial division and elongation machineries in *E. coli***
Samir Olatunji, Mohammed Terrak
 Presenter affiliation: Trinity College Dublin, Dublin, Ireland; Université de Liège, Liège, Belgium. 24
- Characterizing ligand receptor interaction dynamics via 19F NMR studies in a class a G-protein coupled receptor**
Alexander P. Oraziotti, Libin Ye, Aditya Pandey, Advait Hasabnis, Patrick Barth, Robert S. Prosser
 Presenter affiliation: University of Toronto, Toronto, Canada. 25
- Crystal structure of a soluble fragment of the membrane fusion protein HlyD in a type I secretion system of gram-negative bacteria**
Nohra Park, Nam-Chul Ha
 Presenter affiliation: Seoul National University, Seoul, South Korea. 26
- Probing allosteric communication with long-range rigidity propagation across protein networks**
Adnan Slijoka
 Presenter affiliation: Kwansai Gakuin University, Osaka, Japan. 27
- Analysis of 138 pathogenic mutations in presenilin-1 on the in vitro production of A β 42 and A β 40 peptides by γ -secretase**
Linfeng Sun, Rui Zhou, Guanghui Yang, Yigong Shi
 Presenter affiliation: School of Life Sciences, Beijing, China. 28
- Crystal structures of the human orexin 2 receptor (OX2R) bound to the selective antagonist EMPA**
Ryoji Suno, Kanako Kimura-Terakado, Takanori Nakane, Kunio Hirata, Keitaro Yamashita, Junmei Wang, Takaaki Fujiwara, Yasuaki Yamanaka, Dohyun Im, Shoichiro Horita, Hirokazu Tsujimoto, Maki Tawaramoto S, Keiko Shimamoto, Masaki Yamamoto, Daniel M. Rosenbaum, Tatsuro Shimamura, So Iwata, Takuya Kobayashi
 Presenter affiliation: Kyoto University, Kyoto, Japan. 29

Cleavage of β -amyloid peptide by an archaeal presenilin homologue

Shangyu Dang, Shenjie Wu, Jiawei Wang, Hongbo Li, Min Huang, Wei He, Yue-Ming Li, Catherine C. L. Wong, Yigong Shi
Presenter affiliation: Tsinghua University, Beijing, China.

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The dynamic process of M_2 muscarinic acetylcholine receptor activation and allostery

Jun Xu, Yunfei Hu, Xiaogang Niu, Changwen Jin, Brian Kobilka
Presenter affiliation: Tsinghua University, Beijing, China.

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Mechanistic insight into allosteric regulation of the $A2A$ adenosine G-protein-coupled receptor by physiological cations

Libin Ye, Chris Neale, Adnan Sljoka, Brent Lyda, Dmitry Pichugin, Nobuyuki Tsuchimura, Sacha Larda, Régis Pomès, Angel García, Oliver Ernst, Roger Sunahara, Scott Prosser
Presenter affiliation: University of Toronto, Toronto, Canada.

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TUESDAY, May 16—4:30 PM

Chinese Tea and Beer Tasting

TUESDAY, May 16—7:00 PM

SESSION 3 TRANSPORTERS

Chairperson: **Edward Kunji**, Medical Research Council, Cambridge, United Kingdom

Structural and mechanistic studies of ABC transporters facilitating translocation or flipping reactions

Kaspar Locher [20'+5']
Presenter affiliation: ETH Zurich, Zurich, Switzerland.

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Pore architecture and ion selectivity filter of the mitochondrial calcium uniporter

James J. Chou, Chan Cao, Ying Dong [20'+5']
Presenter affiliation: Harvard University Medical School, Boston, Massachusetts; Institute of Biochemistry and Cell Biology, Shanghai, China.

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Mechanistic insights into the chloroplast triose-phosphate/phosphate translocator

Yongchan Lee, Tomohiro Nishizawa, Mizuki Takemoto, Kaoru Kumazaki, Keitaro Yamashita, Kunio Hirata, Ayumi Minoda, Satoru Nagatoishi, Kouhei Tsumoto, Ryuichiro Ishitani, Osamu Nureki [10'+5']

Presenter affiliation: The University of Tokyo, Tokyo, Japan.

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Coffee / Tea Break

TUESDAY, May 16—8:30 PM

DISTINGUISHED ALUMNI LECTURE

Introduction by: **Christopher Tate**, MRC Laboratory of Molecular Biology, Cambridge, United Kingdom

Is Alzheimer's disease caused by β -amyloid plaques?

Yigong Shi, Rui Zhou, Guanghui Yang, Linfeng Sun [30'+10']

Presenter affiliation: Tsinghua University, School of Life Sciences, Beijing, China.

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TUESDAY, May 16—9:00 PM

POSTER SESSION II

See Poster Session I for list of posters

Odd # posters 9:00 pm / Even # posters 9:45 pm

WEDNESDAY, May 17—9:00 AM

SESSION 4 TRANSMEMBRANE SIGNALING

Chairperson: **Raimund Dutzler**, University of Zürich, Zürich, Switzerland

Structure of the human adenosine A_{2A} receptor bound to an engineered G protein

Christopher G. Tate, Byron Carpenter, Rony Nehmé, Tony Warne, Andrew G. Leslie [20'+5']

Presenter affiliation: MRC Laboratory of Molecular Biology, Cambridge, United Kingdom.

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Structural and biochemical insights into sigma receptor function
Andrew C. Kruse [20'+5']
Presenter affiliation: Harvard Medical School, Boston, Massachusetts. 38

Activation mechanism of endothelin ET_B receptor by endothelin-1
Tomohiro Nishizawa, Wataru Shihoya, Akiko Okuta, Yoshinori Fujiyoshi, Tomoko Doi, Osamu Nureki [10'+5']
Presenter affiliation: The University of Tokyo, Tokyo, Japan. 39

Structure of CC chemokine receptor 5 (CCR5) with a potent chemokine inhibitor of HIV
Yi Zheng, Gye Won Han, Ruben Abagyan, Beili Wu, Raymond C. Stevens, Vadim Cherezov, Irina Kufareva, Tracy M. Handel [10'+5']
Presenter affiliation: University of California San Diego, La Jolla, California. 40

Coffee / Tea Break

WEDNESDAY, May 17—11:00 AM

SESSION 5 EMERGING TECHNOLOGY: FUNCTIONAL CHARACTERIZATION

Chairperson: **Nancy Carrasco**, Yale University, New Haven, Connecticut, USA

From chaperones to the membrane with a BAM!
Karen G. Fleming [20'+5']
Presenter affiliation: Johns Hopkins University, Baltimore, Maryland. 41

Understanding GPCR activation through biophysical characterization of the ensemble—Studies of the adenosine A2A receptor by NMR, EPR, optical spectroscopy, and radioligand binding
Robert S. Prosser, Libin Ye, Ned van Eps, Oliver P. Ernst, Brent Lyda, Roger Sunahara, Dennis Fernandes, Claudiu Gradinaru, Chris Neale, Adnan Sijoka [20'+5']
Presenter affiliation: University of Toronto, Toronto, Canada. 42

Probing the regulatory and transport mechanism of mitochondrial carriers with thermostability shift assays
Edmund R. Kunji [20'+5']
Presenter affiliation: University of Cambridge, Cambridge, United Kingdom. 43

Membrane protein structure determination by serial crystallography

Meitian Wang [10'+5']

Presenter affiliation: Paul Scherrer Institute, Villigen, Switzerland.

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WEDNESDAY, May 17—2:00 PM

Visit to Old Suzhou

WEDNESDAY, May 17—7:00 PM

SESSION 6 DYNAMICS OF MEMBRANE PROTEINS

Chairperson: **Aashish Manglik**, Stanford University School of Medicine, Stanford, California, USA

On symmetry and the conformational transitions of ion channels— A cryo-EM study

Eduardo Perozo [20'+5']

Presenter affiliation: University of Chicago, Chicago, Illinois.

45

Roles of membrane interactions in electrochemical coupling in voltage-sensing phosphatase

Yasushi Okamura, Akira Kawanabe, Kazuhisa Nishizawa, Souhei Sakata [20'+5']

Presenter affiliation: Graduate School of Medicine, Osaka University, Suita, Japan.

46

Structural insight into the ligand recognition mechanism of lysolipid receptor

Reiya Taniguchi, Asuka Inoue, Misa Sayama, Akiharu Uwamizu, Keitaro Yamashita, Kunio Hirata, Masahito Yoshida, Yoshiki Tanaka, Hideaki E. Kato, Yoshiko Nakada-Nakura, Yuko Otani, Tomohiro Nishizawa, Takayuki Doi, Tomohiko Ohwada, Ryuichiro Ishitani, Junken Aoki, Osamu Nureki [10'+5']

Presenter affiliation: The University of Tokyo, Tokyo, Japan.

47

The molecular basis of agonist recognition and activation of the prototypical olfactory receptor Olfr73

Shuguang Yuan, Thamani Dahoun, Horst Vogel [10'+5']

Presenter affiliation: Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland; Actelion Pharmaceutical Ltd, Basel, Switzerland.

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WEDNESDAY, May 17—8:30 PM

POSTER SESSION III

See Poster Session I for list of posters

Even # posters 8:30 pm / Odd # posters 9:15 pm

THURSDAY, May 18—9:00 AM

SESSION 7 ION CHANNELS I

Chairperson: **Nieng Yan**, Tsinghua University, Beijing, China

Structure-based mechanistic insights into the function of trimeric intracellular cation channels

Hanting Yang, Miaohui Hu, Jianli Guo, Xiaomin Ou, Tanxi Cai,
Zhenfeng Liu [20'+5']

Presenter affiliation: Institute of Biophysics, Chinese Academy of Sciences, Beijing, China; University of Chinese Academy of Sciences, Beijing, China.

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Molecular physiology of voltage-gated calcium channel auxiliary β subunits

Henry M. Colecraft [20'+5']

Presenter affiliation: Columbia University, New York, New York.

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Molecular mechanism of the ATP-dependent modulation of the Mg^{2+} channel MgtE for Mg^{2+} homeostasis

Motoyuki Hattori [10'+5']

Presenter affiliation: Fudan University, Shanghai, China.

51

Structure and function of the divalent anion/ Na^+ symporter from *Vibrio cholerae* and a humanized variant

Rongxin Nie, Steven Stark, Jindrich Symerksy, Ronald Kaplan, Min Lu [10'+5']

Presenter affiliation: Rosalind Franklin University, North Chicago, Illinois.

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Coffee / Tea Break

SESSION 8 PUTTING STRUCTURE TO WORK

Chairperson: **Scott Prosser**, University of Toronto, Toronto, Canada

Recent findings on the mechanism of the sodium/iodide symporter (NIS)

Nancy Carrasco [20'+5']

Presenter affiliation: Yale School of Medicine, New Haven, Connecticut.

53

Structure enabled drug discovery for safer opioids

Aashish Manglik [20'+5']

Presenter affiliation: Stanford University, Stanford, California.

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***In meso in situ* serial crystallography (IMISX) of soluble and membrane proteins**

Chia-Ying Huang [10'+5']

Presenter affiliation: Paul Scherrer Institute, Villigen, Switzerland; Trinity College Dublin, Dublin, Ireland.

55

Nucleotide sugar transporters—Elucidating the structure-function relationship

Joe Tiralongo [10'+5']

Presenter affiliation: Griffith University, Gold Coast, Australia.

56

Structural basis for ligand and antibody recognition of the human prostaglandin E receptor

Yosuke Toyoda, Kazushi Morimoto, Ryoji Suno, Shoichiro Horita, Keitaro Yamashita, Kunio Hirata, Yusuke Sekiguchi, Satoshi Yasuda, Mitsunori Shiroishi, Yukihiro Sugimoto, Norimichi Nomura, Masahiro Kinoshita, Takeshi Murata, Kiyoshi Takayama, Masaki Yamamoto, Shuh Narumiya, So Iwata, Takuya Kobayashi [10'+5']

Presenter affiliation: Kyoto University, Kyoto, Japan.

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THURSDAY, May 18—2:00 PM

SESSION 9 MEMBRANE COMPLEXES AND ENZYMES

Chairperson: **Irina Serysheva**, UT Health Medical School, Houston, Texas, USA

Molecular mechanism of the IP₃R calcium channel—Insights from cryo-EM studies

Guizhen Fan, Mariah R. Baker, Zhao Wang, Alexander B. Seryshev, Wah Chiu, Steven J. Ludtke, Matthew L. Baker, Irina I. Serysheva [20'+5']

Presenter affiliation: McGovern Medical School at UTHealth, Houston, Texas.

58

Realising the full potential of electron cryomicroscopy

Kutti Vinothkumar [20'+5']

Presenter affiliation: MRC Laboratory of Molecular Biology, Cambridge, United Kingdom.

59

Structures of DPAGT1 reveal substrate and inhibitor binding mechanism

Yin Y. Dong, Ashley C. Pike, Amy Chu, Simon R. Bushell, Annamaria Tessitore, Leela Shrestha, Shubhashish Mukhopadhyay, Katsiaryna Belaya, Nicola A. Burgess-Brown, David Beeson, Elisabeth P. Carpenter [10'+5']

Presenter affiliation: University of Oxford, Oxford, United Kingdom.

60

Atomic structure of anthrax PA pore elucidates toxin translocation

Hong Zhou, Jiansen Jiang, Bradley L. Pentelute, R J. Collier [10'+5']

Presenter affiliation: UCLA, Los Angeles, California.

61

An update on detergent usage in membrane protein structural biology

Edward Pryor, Ritesh Mittal, Ben Travis [10'+5']

Presenter affiliation: Anatrice, Maumee, Ohio.

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Coffee / Tea Break

THURSDAY, May 18—4:00 PM

KEYNOTE SPEAKER

Introduction by: **Ming Zhou**, Baylor College of Medicine, Houston, Texas, USA

How is electrical signal generated? Structural and mechanistic investigations of Nav and Cav channels

Nieng Yan [40'+10']

Presenter affiliation: Tsinghua University, Beijing, China.

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THURSDAY, May 18—5:00 PM

POSTER SESSION IV

See Poster Session I for list of posters

Odd # posters 5:00 pm / Even # posters 5:30 pm

THURSDAY, May 18—6:00 PM

COCKTAILS and BANQUET

FRIDAY, May 19—9:00 AM

SESSION 10 ION CHANNELS II

Chairperson: **Andy Kruse**, Harvard Medical School, Boston, Massachusetts, USA

Structure, ion permeation and mechanogating of the mechanosensitive piezo channel

Bailong Xiao [20'+5']

Presenter affiliation: Tsinghua University, Beijing, China.

64

High resolution cryo-EM structure of a eukaryotic cyclic nucleotide-gated channel

Minghui Li, Xiaoyuan Zhou, Shu Wang, Ioannis Michailidis, Ye Gong, Deyuan Su, Huan Li, Xueming Li, Jian Yang [20'+5']

Presenter affiliation: Columbia University, New York, New York;

Kunming Institute of Zoology, Kunming, China.

65

Crystal structures of human glycine receptor $\alpha 3$ bound to a novel class of analgesic potentiators

Xin Huang, Paul L. Shaffer, Shawn Ayube, Howard Bregman, Hao Chen, Soyna G. Lehto, Jason A. Luther, David J. Matson, Stefan I. McDonough, Klaus Michelsen, Matthew H. Plant, Stephen Schneider, Jeffrey R. Simard, Yohannes Teffera, Shuyan Yi, Maosheng Zhang, Erin F. DiMauro, Jacinthe Gingras [20'+5']

Presenter affiliation: Amgen Inc., Cambridge, Massachusetts.

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Coffee / Tea Break

FRIDAY, May 19—10:45 AM

SESSION 11 ION CHANNELS III

Chairperson: **Dianfan Li**, Shanghai Institute of Biochemistry and Cell Biology, Shanghai, China

Structural basis of lipoprotein signal peptidase II action and inhibition by the antibiotic globomycin

Lutz Vogeley, Toufic El Arnaout, Jonathan Bailey, Phillip J. Stansfeld, Coilin Boland, Martin Caffrey [20'+5']

Presenter affiliation: Trinity College Dublin, Dublin, Ireland.

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Novel mechanism of gating in an ATP-gated ion channel TrkH

Ming Zhou [20'+5']

Presenter affiliation: Baylor College of Medicine, Houston, Texas.

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New insight into ASIC1a channel signaling in the brain

Tian-Le Xu [20'+5']

Presenter affiliation: Shanghai Jiao Tong University School of Medicine, Shanghai, China.

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Closing Remarks

Nancy Carrasco, Yale University, USA
Tian-Le Xu, Shanghai Jiao Tong University, China