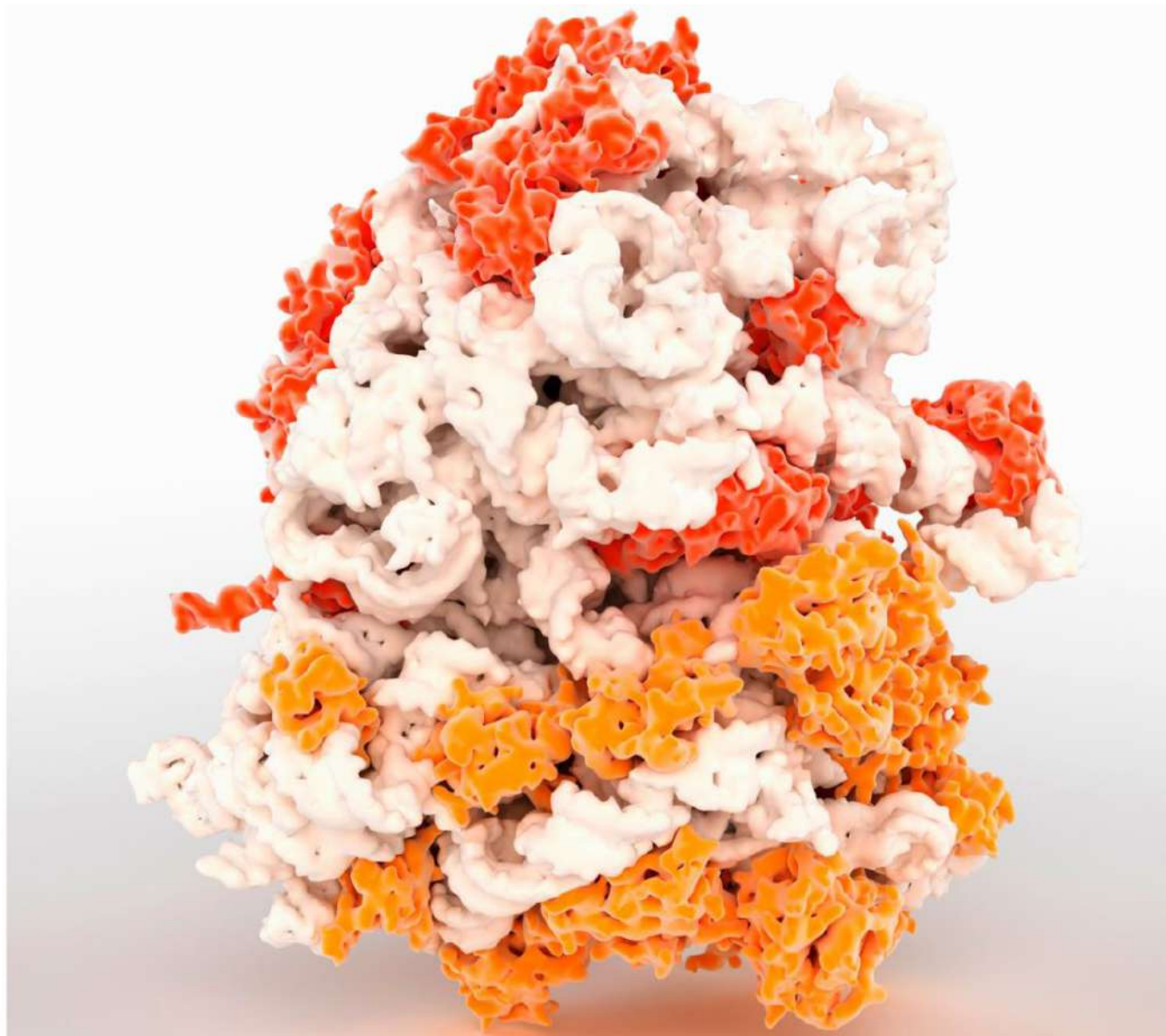


9th International Conference on

STRUCTURAL BIOLOGY

September 18-20, 2017 Zurich, Switzerland



Conference Series - America

One Commerce Center-1201, Orange St. #600, Wilmington, Zip 19899, Delaware, USA
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Hall: London A+B

conference**series**.com 08:15-08:30

Opening Ceremony

Keynote Forum

- Introduction**
- 08:30-09:10 **Title: The centers of premeltons signal the beginning and ends of genes**
Henry M Sobell, University of Rochester, USA
- 09:10-09:50 **Title: Structures and functions of seven-transmembrane helix receptors**
Shigeyuki Yokoyama, RIKEN Structural Biology Laboratory, Japan
- 09:50-10:30 **Title: Structural biology of c-di-GMP mediated signaling**
Tilman Schirmer, University of Basel, Switzerland

Networking and Refreshments Break 10:30-10:50 @ Europa Foyer

Group Photo

Special Session on Structural Biology and Single Molecules

Session Chair: Yuri L Lyubchenko, University of Nebraska Medical Center, USA

Session Introduction

- 10:50-11:10 **Title: Nanoscale structure and dynamics of centromere nucleosomes**
Yuri L Lyubchenko, University of Nebraska Medical Center, USA
- 11:10-11:30 **Title: The structure of chromatin; single-molecule experiments on model fibers and real genes**
John van Noort, Leiden University, The Netherlands
- 11:30-11:50 **Title: Deciphering and filming molecular recognition at the nano-scale with AFM**
Peter Hinterdorfer, Johannes Kepler University Linz, Austria
- 11:50-12:10 **Title: High-speed optical tweezers for the study of protein-DNA interaction**
Marco Capitanio, University of Florence, Italy
- 12:10-12:30 **Title: Sliding sleeves of XRCC4-XLF bridge DNA and connect fragments of broken DNA**
Gijs Wuite, Vrije Universiteit Amsterdam, The Netherlands
- 12:30-12:50 **Title: New applications of boxed molecular dynamics. Atomistic simulations of atomic force microscopy experiments and peptide cyclization**
Dmitrii V Shalashilin, University of Leeds, UK

Lunch Break 12:50-13:30 @ La Place AB

Hall: London A+B

Sessions: Recent Advances in Structural Biology

Session Chair: Robert Craigie, NIH, USA

Session Co-chair: Toshiya Senda, High Energy Accelerator Research Organization (KEK), Japan

Session Introduction

- 13:30-13:50 **Title: Structural insights from aptamers with base modifications**
Nebojsa Janjic, SomaLogic, Inc., USA
- 13:50-14:10 **Title: HIV-1 integrase assembles multiple discrete intasomes that are active for DNA integration *in vitro***
Robert Craigie, National Institutes of Health, USA
- 14:10-14:30 **Title: Allosteric control of transcription regulation by nuclear receptors: An integrative structural biology approach**
Dino Moras, IGBMC, France

- 14:30-14:50** Title: **Complexes of malaria parasite and human proteins drive formation of cytoadherent assemblies at the surface of infected red blood cells**
John Vakonakis, University of Oxford, United Kingdom
- 14:50-15:10** Title: **Microrobotics enables non-contact, fully automated protein crystal harvesting**
David Sargent, ETH Zurich, Switzerland
- 15:10-15:30** Title: **The native (Sulfur) SAD method in Photon Factory**
Toshiya Senda, High Energy Accelerator Research Organization (KEK), Japan
- 15:30-15:50** Title: **Structural mechanisms of nucleosome recognition as revealed by methyl-TROSY**
Yawen Bai, National Institutes of Health, USA
- 15:50-16:10** Title: **New insights into pRN1 priming: Structural changes support specific DNA recognition and catalysis**
Julien Boudet, ETH-Hönggerberg, Switzerland
- 16:10-16:30** Title: **A new protocol to investigate conformational population patterns in the enzymatic activity cycle of proteins using molecular dynamics and normal mode analysis**
Luis Paulo. B Scott, Universidade Federal do ABC, Brazil
- 16:30-16:50** Title: **Cryo-electron microscopy grid preparation from nanoliter-sized protein samples and single-cell extracts**
Thomas Braun, University of Basel, Switzerland

Networking and Refreshments Break 16:50-17:10 @ Europa Foyer

Sessions: Molecular Modelling and Drug Designing

Session Chair: Christina Scharnagl, Technical University of Munich, Germany

Session Co-chair: Shuanghong Huo, Clark University, USA

Session Introduction

- 17:10-17:30** Title: **Structure based drug discovery on membrane protein targets: New developments and advancements**
Michael Hennig, leadXpro AG, Switzerland
- 17:30-17:50** Title: **Structure-based drug design of the Eg5 inhibitor NVP-BQS481**
Dirksen E. Bussiere, Novartis Institutes for BioMedical Research, USA
- 17:50-18:10** Title: **Does the dynamics of their transmembrane domain qualify bitopic membrane proteins as substrates for intramembrane proteolysis?**
Christina Scharnagl, Technical University of Munich, Germany
- 18:10-18:30** Title: **The dynamics of a protein during its insertion into a membrane**
Andreas Kuhn, University of Hohenheim, Germany
- 18:30-18:50** Title: **Extract the thermodynamic and kinetic information from protein simulations using dimensionality reduction**
Shuanghong Huo, Clark University, USA
- 18:50-19:10** Title: **Dynamics of knotted and entangled neurotoxic polypeptides**
Marek Cieplak, Institute of Physics PAS, Poland
- 19:10-19:30** Title: **What docking studies tell us about the role of disordered protein fragments in macromolecular assembly**
Chantal Prévost, CNRS, France

Hall: Athens

Sessions: 3 Dimensional Structure Determination | Computational Approaches | Structural Molecular Biology

Session Chair: Kurt Ballmer-Hofer, Paul Scherrer Institut, Switzerland

Session Co-chair: Jianyong Li, Virginia Tech, USA

Session Introduction

- 13:30-13:50** Title: **Structural analysis of vascular endothelial growth factor receptors reveals drug-targetable allosteric sites regulating angiogenesis**
Kurt Ballmer-Hofer, Paul Scherrer Institut, Switzerland

- 13:50-14:10** **Title: A structure complex of a bacterial effort and an interacting protein: Insights into the transfer of virulence effector by pathogenic bacteria**
Jianyong Li, Virginia Tech, USA
- 14:10-14:30** **Title: Complex structure of mammalian cytochrome c–cytochrome c oxidase reveals a novel protein-protein interaction mode**
Kyoko Shinzawa-Itoh, Hyogo University, Japan
- 14:30-14:50** **Title: Oxidative stress, methionine oxidation, and calmodulin structure and function**
Jeffrey L Urbauer, The University of Georgia, USA
- 14:50-15:10** **Title: Molecular mechanism of SHP2 activation by CagA from *Helicobacter pylori***
Miki Senda, High Energy Accelerator Research Organization (KEK), Japan
- 15:10-15:30** **Title: Integrative approaches to study the structure and motions of DNA sliding clamps**
Alfredo De Biasio, Elettra-Sincrotrone Trieste, Italy
- 15:30-15:50** **Title: An atomistic view of microtubule stabilization by GTP**
Liliane Mouawad, Institut Curie, France
- 15:50-16:10** **Title: Structure and function of a chloride pump rhodopsin from marine bacteria**
Hyun-Soo Cho, Yonsei University, South Korea
- 16:10-16:30** **Title: Construction of structural mimetics of the thyrotropin receptor intracellular domain**
Stanislav Engel, Ben-Gurion University, Israel
- 16:30-16:50** **Title: Structural basis of sodium/citrate symporter as a secondary transporter**
Mi Sun Jin, Gwangju Institute of Science and Technology, South Korea

Networking and Refreshments Break 16:50-17:10 @ Europa Foyer

Sessions: Frontiers in Structural Biology

Session Chair: Petra Fromme, Arizona State University, USA

Session Co-chair: Maria Bykhovskaia, Wayne State University, USA

Session Introduction

- 17:10-17:30** **Title: Dynamics of biomolecules “In Action” studied with X-ray free electron lasers**
Petra Fromme, Arizona State University, USA
- 17:30-17:50** **Title: Protein machinery regulating the synaptic vesicle fusion**
Maria Bykhovskaia, Wayne State University, USA
- 17:50-18:10** **Title: Designer Biologics: BMP Chimeras and their clinical potential**
Senyon Teddy Choe, Mogam Institute, Korea and University of California San Diego, USA
- 18:10-18:30** **Title: Structural mechanism of partial agonists and antagonists of PPAR γ for use as antidiabetics**
John B Bruning, The University of Adelaide, Australia
- 18:30-18:50** **Title: How conformational dynamics descriptors may help in remodeling of allosteric regulation in proteins**
Luba Tchertanov, CMLA ENS, France
- 18:50-19:10** **Title: Study on the conformational transition between the alternative and collapsed form of prethrombin-2: Targeted molecular dynamics and free energy sampling**
Sangwook Wu, Pukyong National University, South Korea
- 19:10-19:30** **Title: Structural and molecular dynamics analysis of the super secondary motifs from TIM barrel proteins: Implications for folding and engineering of foldable building blocks for the assembly of TIMs**
Ramakrishna Vadrevu, Birla Institute of Technology and Science, India

Panel Discussion

Day 2 September 19, 2017

Hall: London A+B

Keynote Forum

- 08:30-09:10** **Title: Membrane protein structure, dynamics & function: Oriented sample and magic angle sample spinning solid state NMR**
Timothy A Cross, Florida State University and National High Magnetic Field Lab, USA
- 09:10-09:50** **Title: Reproducibility in biomedical sciences - Big Data Perspective**
Wladek Minor, University of Virginia, USA
- 09:50-10:30** **Title: Protein-protein interaction and amyloid cascade hypothesis for Alzheimer's disease**
Yuri L Lyubchenko, University of Nebraska Medical Center, USA

Networking and Refreshments Break 10:30-10:50 @ Europa Foyer

Special Session on Structural Biology of Biomembranes @ 10:50-12:30

Session Chair: Qiu-Xing Jiang, University of Florida, USA

Session Introduction

- 10:50-11:15** **Title: Mechanisms underlying lipid-sensing by the nicotinic acetylcholine receptor in both normal and diseased states**
John E. Baenziger, University of Ottawa, Canada
- 11:15-11:40** **Title: When structure leads to function: Protein complexes at the membrane in endocytosis**
Carsten Mim, KTH Royal Institute of Technology, Sweden
- 11:40-12:05** **Title: Role of the nucleotidyl cyclase helical domain in catalytically active dimer formation**
Volodymyr M Korkhov, Paul Scherrer Institute, Switzerland
- 12:05-12:30** **Title: Structural basis for the lipid-dependent gating of a Kv channel**
Qiu-Xing Jiang, University of Florida, USA

Lunch Break 12:30-13:30 @ La Place AB

Hall: London A+B

Sessions: Structural Biology in Complexity Arenas

Session Chair: Charles W. Carter, Jr, University of North Carolina at Chapel Hill, USA

Session Co-Chair: Ulf Skoglund, Okinawa Institute of Science and Technology, Japan

Session Introduction

- 13:30-13:50** **Title: How does domain motion contribute to transition-state stabilization? Combinatorial thermodynamic cycle analysis of conformational coupling during tryptophan activation**
Charles W. Carter, Jr, University of North Carolina at Chapel Hill, USA
- 13:50-14:10** **Title: Structure of Human IgM in complex with the Malaria protein PfEMP1**
Ulf Skoglund, Okinawa Institute of Science and Technology, Japan
- 14:10-14:30** **Title: Is nucleoid complexity hence cell diameter limited by the eclipse?**
Arieh Zaritsky, Ben-Gurion University of the Negev, Israel
- 14:30-14:50** **Title: Inter-domain communication through intrinsically disordered region (IDR) revealed through the ensemble structure analysis**
Shin-ichi Tate, Hiroshima University, Japan
- 14:50-15:10** **Title: Solution NMR relaxation and μ s molecular dynamics simulations of dynamic protein-protein and protein-membrane complexes**
Matthias Buck, Case Western Reserve University, USA
- 15:10-15:30** **Title: Functional protein conformation networks probed by NMR nanorulers**
Beat Vögeli, University of Colorado at Denver, USA

- 15:30-15:50 **Title: On two ways to predict the protein folding process over a chaotic model**
Christophe Guyeux, Université de Bourgogne Franche-Comté, France
- 15:50-16:10 **Title: Antibodies as research tools to find new chemical matter**
Marta Westwood, UCB Celltech, UK
- 16:10-16:30 **Title: Structural genomics of integral membrane proteins - Past successes and future directions**
Brian Kloss, New York Structural Biology Center, USA

Networking and Refreshments Break 16:30-16:50 @ Europa Foyer

- 16:50-17:10 **Title: Geometrical principles of homeric β -barrels and β -helices: Applications to modelling amyloid protofilaments**
Steven Hayward, University of East Anglia, UK
- 17:10-17:30 **Title: Exploring conformational equilibria of a heterodimeric ABC transporter by electron paramagnetic resonance**
Enrica Bordignon, Ruhr-Universität Bochum, Germany
- 17:30-17:50 **Title: Microscopic calculation of conformational thermodynamics in bio-macromolecular complexes**
J Chakrabarti, S. N. Bose National Centre for Basic Sciences, India

Hall: Athens

Sessions: Signalling Biology

Session Chair: Joachim Krebs, Max Planck Institute for Biophysical Chemistry, Germany

Session Co-Chair: Vesa P Hytönen, University of Tampere, Finland

Session Introduction

- 13:30-13:50 **Title: Calcium, calmodulin and the plasma membrane calcium pump**
Joachim Krebs, Max Planck Institute for Biophysical Chemistry, Germany
- 13:50-14:10 **Title: Structural insights into cholesterol regulation of inwardly-rectifying K⁺ channels**
Irena Levitan, University of Illinois, USA
- 14:10-14:30 **Title: Structural aspects of cell signaling**
Carol A Heckman, Bowling Green State University, USA
- 14:30-14:50 **Title: Mechanical stability of Talin Rod controls traction force generation and cell migration**
Vesa P. Hytönen, University of Tampere, Finland
- 14:50-15:10 **Title: Photoinduced electron transfer in cytochrome bc₁: Kinetics of ubiquinone transfer from the Q_o site to the Q_i site, and evidence for communication between the monomers in the dimer**
Francis Millett, University of Arkansas, USA
- 15:10-15:30 **Title: Mapping energy transfer channels in fucoxanthin–chlorophyll protein complex**
Leonas Valkunas, Vilnius University, Lithuania
- 15:30-15:50 **Title: PIP₂ modulation of KCNQ1 channels**
Jianmin Cui, Washington University in St. Louis, USA
- 15:50-16:10 **Title: LD motif interacting networks in cell-matrix adhesion**
Igor L. Barsukov, University of Liverpool, UK
- 16:10-16:30 **Title: Structural conformational changes report biased agonism: The case of Galanin receptors**
Arfaxad Reyes Alcaraz, Korea University, South Korea

Networking and Refreshments Break 16:30-16:50 @ Europa Foyer

- 16:50-17:10 **Title: A biophysical and structural approach to investigate calcium sensor properties of plant calmodulin-like proteins**
Alessandra Astegno, University of Verona, Italy

17:10-17:30 Title: **Structural insights into the mechanism of how polyphenols suppresses amyloid fibrillation**

He Jianwei, Liaoning University, China

17:30-17:50 Title: **Type I BIR domain inhibitors in cancer therapy: Designing drugs to modulate the NF- κ B pathway**

Federica Cossu, Institute of Biophysics at the National Research Council (IBF-CNR), Italy

Poster Presentations 17:50-18:30 @ Europa Foyer

**Workshop on Solutions for studying protein complexes in structural biology and drug development by Tobias Pfluger, NanoTemper Technologies, Germany
@ Hall: London A+B @ 18:30-19:30**

Day 3 September 20, 2017

Hall: London A+B

Sessions: Structural Biology in Cancer Research | Current Trends

Session Chair: Guo-Ping Zhou, Gordon Life Science Institute, Boston, USA

Session Co-Chair: Tzu-Ching Meng, Academia Sinica, Taiwan

Session Introduction

09:00-09:20 Title: **The NMR studies of the interaction between polysialic acid (polySA) and the PSTD peptide in ST8Sia IV polysialyltransferase**

Guo-Ping Zhou, Gordon Life Science Institute, Boston, USA

09:20-09:40 Title: **Understanding differential selectivity of arrestins toward the phosphorylation state of G-protein-coupled receptors**

Ozge Sensoy, Istanbul Medipol University, Turkey

09:40-10:00 Title: **Structural basis for the cooperative allosteric activation of the free fatty acid receptor GPR40**

Stephen M Soisson, Merck Research Laboratories, USA

10:00-10:20 Title: **Conformational dynamics revealed by ensemble cryo-EM**

Andrei Korostelev, UMass Medical School, USA

Networking and Refreshments Break 10:20-10:40 @ Europa Foyer

10:40-11:00 Title: **Structural basis for PTPN3-p38gamma complex involved in colon cancer progression**

Tzu-Ching Meng, Academia Sinica, Taiwan

11:00-11:20 Title: **Holliday junction resolvase GEN1 functions as a versatile DNA sensor and processor**

Christian Biertümpfel, Max Planck Institute of Biochemistry, Germany

11:20-11:40 Title: **Monitoring protein structural changes on a proteome-wide scale**

Paola Picotti, ETH Zurich, Switzerland

11:40-12:00 Title: **Slow domain reconfiguration causes power law kinetics in a two-state enzyme**

Hagen Hofmann, Weizmann Institute of Science, Israel

12:00-12:20 Title: **Structural and dynamic studies of DENV and ZIKV proteases and its insight into inhibitor design**

CongBao Kang, Agency for Science, Technology and Research (A*STAR), Singapore

12:20-12:40 Title: **Assembly mechanism of foreign dsDNA-sensing inflammasomes**

Jungsan Sohn, Johns Hopkins University, USA

Lunch Break 12:40-13:40 @ La Place AB

Hall: London A+B

- 13:40-14:00 **Title: Functional divergence in protein families: A co-variation analysis**
Marie Chabbert, University of Angers, France
- 14:00-14:20 **Title: RNA-binding domain disorder modulates the RNA destabilizing activity in the TTP family of proteins**
Francesca Massi, University of Massachusetts Medical School, USA
- 14:20-14:40 **Title: Role of conformational equilibrium in molecular recognition and capsid assembly: the case of flavivirus capsid proteins**
Fabio C L Almeida, Federal University of Rio de Janeiro, Brazil
- 14:40-15:00 **Title: Integrative approaches for variant interpretation in coding regions**
Sushant Kumar, Yale University, USA
- 15:00-15:20 **Title: Generation of long acting therapies using glycosylated linkers**
Abdulrahman Alshehri, University of Sheffield, UK
- 15:20-15:40 **Title: Hydrogen bond interaction with trypanosomal adenosine kinase; ornithine decarboxylase and triose phosphate isomerase could not be involved in the antitrypanosomal activity of stigmaterol: An *in silico* study**
Aminu Mohammed, Ahmadu Bello University, Nigeria

Hall: Athens

Young Researchers Forum

- 13:40-14:00 **Title: XFEL structures of the M2 proton channel of influenza A reveal pH-dependent water networks under room temperature conditions**
Jessica L Thomaston, UCSF, USA
- 14:00-14:20 **Title: Crystal structure of DNA-Binding Domain-CbnR with its promoter reveals the basis of the LysR-Type Transcriptional Regulator recognition**
Maharani Pertiwi Koentjoro, Gifu University, Japan
- 14:20-14:40 **Title: Delivery methods for Free Electron Lasers: direct protein crystallization on solid supports economizes sample consumption in serial femtosecond crystallography**
Nadia L Opara, Paul Scherrer Institute, Switzerland
- 14:40-15:00 **Title: The challenge of improve disease treatment with protein engineering. The contributions of X-ray crystallography**
Stephanie Bath de Moraes, FIOCRUZ, Brazil

Award Ceremony @ Hall: London A+B

Networking and Refreshments Break 15:00-16:00 @ Europa Foyer

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