Scientific Program

9th International Conference on

STRUCTURAL BIOLOGY

September 18-20, 2017  Zurich, Switzerland
Day 1  September 18, 2017

08:00-08:15 Registrations

Conference Series

08:15-08:30 Opening Ceremony

Keynote Forum

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

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

Sessions: Recent Advances in Structural Biology
Session Chair: Robert Craigie, NIH, USA
Session Co-chair: Toshiya Senda, High Energy Accelerator Research Organization (KEK), Japan

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
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

Title: Microrobotics enables non-contact, fully automated protein crystal harvesting
David Sargent, ETH Zurich, Switzerland

Title: The native (Sulfur) SAD method in Photon Factory
Toshiya Senda, High Energy Accelerator Research Organization (KEK), Japan

Title: Structural mechanisms of nucleosome recognition as revealed by methyl-TROSY
Yawen Bai, National Institutes of Health, USA

Title: New insights into pRN1 priming: Structural changes support specific DNA recognition and catalysis
Julien Boudet, ETH-Hönggerberg, Switzerland

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

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

Title: Structure based drug discovery on membrane protein targets: New developments and advancements
Michael Hennig, leadXpro AG, Switzerland

Title: Structure-based drug design of the Eg5 inhibitor NVP-BQS481
Dirksen E. Bussiere, Novartis Institutes for BioMedical Research, USA

Title: Does the dynamics of their transmembrane domain qualify bitopic membrane proteins as substrates for intramembrane proteolysis?
Christina Scharnagl, Technical University of Munich, Germany

Title: The dynamics of a protein during its insertion into a membrane
Andreas Kuhn, University of Hohenheim, Germany

Title: Extract the thermodynamic and kinetic information from protein simulations using dimensionality reduction
Shuanghong Huo, Clark University, USA

Title: Dynamics of knotted and entangled neurotoxic polypeptides
Marek Cieplak, Institute of Physics PAS, Poland

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

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

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 PPARgamma 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
### Keynote Forum

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

### 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

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

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

### 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

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<tr>
<td>13:30-13:50</td>
<td>How does domain motion contribute to transition-state stabilization? Combinatorial thermodynamic cycle analysis of conformational coupling during tryptophan activation</td>
<td>Charles W. Carter, Jr, University of North Carolina at Chapel Hill, USA</td>
</tr>
<tr>
<td>13:50-14:10</td>
<td>Structure of Human IgM in complex with the Malaria protein PfEMP1</td>
<td>Ulf Skoglund, Okinawa Institute of Science and Technology, Japan</td>
</tr>
<tr>
<td>14:10-14:30</td>
<td>Is nucleoid complexity hence cell diameter limited by the eclipse?</td>
<td>Arieh Zaritsky, Ben-Gurion University of the Negev, Israel</td>
</tr>
<tr>
<td>14:30-14:50</td>
<td>Inter-domain communication through intrinsically disordered region (IDR) revealed through the ensemble structure analysis</td>
<td>Shin-ichi Tate, Hiroshima University, Japan</td>
</tr>
<tr>
<td>14:50-15:10</td>
<td>Solution NMR relaxation and μs molecular dynamics simulations of dynamic protein-protein and protein-membrane complexes</td>
<td>Matthias Buck, Case Western Reserve University, USA</td>
</tr>
<tr>
<td>15:10-15:30</td>
<td>Functional protein conformation networks probed by NMR nanorulers</td>
<td>Beat Vögeli, University of Colorado at Denver, USA</td>
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<td>Time</td>
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<tr>
<td>15:30-15:50</td>
<td>Title: On two ways to predict the protein folding process over a chaotic model</td>
<td>Christophe Guyeux, Université de Bourgogne Franche-Comté, France</td>
</tr>
<tr>
<td>15:50-16:10</td>
<td>Title: Antibodies as research tools to find new chemical matter</td>
<td>Marta Westwood, UCB Celltech, UK</td>
</tr>
<tr>
<td>16:10-16:30</td>
<td>Title: Structural genomics of integral membrane proteins - Past successes and future directions</td>
<td>Brian Kloss, New York Structural Biology Center, USA</td>
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**Networking and Refreshments Break 16:30-16:50 @ Europa Foyer**

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

**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**

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<tr>
<td>13:30-13:50</td>
<td>Title: Calcium, calmodulin and the plasma membrane calcium pump</td>
<td>Joachim Krebs, Max Planck Institute for Biophysical Chemistry, Germany</td>
</tr>
<tr>
<td>13:50-14:10</td>
<td>Title: Structural insights into cholesterol regulation of inwardly-rectifying (K^+) channels</td>
<td>Irena Levitan, University of Illinois, USA</td>
</tr>
<tr>
<td>14:10-14:30</td>
<td>Title: Structural aspects of cell signaling</td>
<td>Carol A Heckman, Bowling Green State University, USA</td>
</tr>
<tr>
<td>14:30-14:50</td>
<td>Title: Mechanical stability of Talin Rod controls traction force generation and cell migration</td>
<td>Vesa P. Hytönen, University of Tampere, Finland</td>
</tr>
<tr>
<td>14:50-15:10</td>
<td>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</td>
<td>Francis Millett, University of Arkansas, USA</td>
</tr>
<tr>
<td>15:10-15:30</td>
<td>Title: Mapping energy transfer channels in fucoxanthin–chlorophyll protein complex</td>
<td>Leonas Valkunas, Vilnius University, Lithuania</td>
</tr>
<tr>
<td>15:30-15:50</td>
<td>Title: PIP2 modulation of KCNQ1 channels</td>
<td>Jianmin Cui, Washington University in St. Louis, USA</td>
</tr>
<tr>
<td>15:50-16:10</td>
<td>Title: LD motif interacting networks in cell-matrix adhesion</td>
<td>Igor L. Barsukov, University of Liverpool, UK</td>
</tr>
<tr>
<td>16:10-16:30</td>
<td>Title: Structural conformational changes report biased agonism: The case of Galanin receptors</td>
<td>Aftaxad Reyes Alcaraz, Korea University, South Korea</td>
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**Networking and Refreshments Break 16:30-16:50 @ Europa Foyer**

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<td>16:50-17:10</td>
<td>Title: A biophysical and structural approach to investigate calcium sensor properties of plant calmodulin-like proteins</td>
<td>Alessandra Astegno, University of Verona, Italy</td>
</tr>
</tbody>
</table>
### Structural insights into the mechanism of how polyphenols suppresses amyloid fibrillation

He Jianwei, Liaoning University, China

**Title:** Type I BIR domain inhibitors in cancer therapy: Designing drugs to modulate the NF-κB 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

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<tr>
<td>09:00-09:20</td>
<td>The NMR studies of the interaction between polysialic acid (polySA) and the PSTD peptide in ST8Sia IV polysialytranseferase</td>
<td>Guo-Ping Zhou, Gordon Life Science Institute, Boston, USA</td>
<td>Gordon Life Science Institute, Boston, USA</td>
</tr>
<tr>
<td>09:20-09:40</td>
<td>Understanding differential selectivity of arrestins toward the phosphorylation state of G-protein-coupled receptors</td>
<td>Ozge Sensoy, Istanbul Medipol University, Turkey</td>
<td>Istanbul Medipol University, Turkey</td>
</tr>
<tr>
<td>09:40-10:00</td>
<td>Structural basis for the cooperative allosteric activation of the free fatty acid receptor GPR40</td>
<td>Stephen M Soisson, Merck Research Laboratories, USA</td>
<td>Merck Research Laboratories, USA</td>
</tr>
<tr>
<td>10:00-10:20</td>
<td>Conformational dynamics revealed by ensemble cryo-EM</td>
<td>Andrei Korostelev, UMass Medical School, USA</td>
<td>UMass Medical School, USA</td>
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### Session Introduction

**Title:** The NMR studies of the interaction between polysialic acid (polySA) and the PSTD peptide in ST8Sia IV polysialytranseferase

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

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

Ozge Sensoy, Istanbul Medipol University, Turkey

**Title:** Structural basis for the cooperative allosteric activation of the free fatty acid receptor GPR40

Stephen M Soisson, Merck Research Laboratories, USA

**Title:** Conformational dynamics revealed by ensemble cryo-EM

Andrei Korostelev, UMass Medical School, USA

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

**Title:** Structural basis for PTPN3-p38gamma complex involved in colon cancer progression

Tzu-Ching Meng, Academia Sinica, Taiwan

**Title:** Holliday junction resolvase GEN1 functions as a versatile DNA sensor and processor

Christian Bierstümpfel, Max Planck Institute of Biochemistry, Germany

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

Paola Picotti, ETH Zurich, Switzerland

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

Hagen Hofmann, Weizmann Institute of Science, Israel

**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

**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

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

#### Young Researchers Forum

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

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