

# 32<sup>nd</sup> Protein Structure Determination in Industry conference

## PSDI 2024

November 10-12, 2024 · Paris

### PSDI 2024 Program

Sunday, 10th of November

SESSION	TIME	TALK
	11 am – 1 pm	Conference registration
	<b>1 pm – 2 pm</b>	<b>Bus 1/2/3 to SOLEIL, Meeting point in front of NOVOTEL</b>
	2 pm – 2:20 pm	Welcome session - <i>Sonja Kuhn (Servier), Jean Susini (Director of Synchrotron SOLEIL)</i>
<b>Session 1: Emerging Technologies</b> <i>Chairs: Pierre Legrand, Sonja Kuhn</i>	2:20 pm - 2:40 pm	Drugging the Undruggable – Rationalizing Targeted Protein Degradation - <i>Georg Petzold (Monte Rosa Therapeutics Inc)</i>
	2:40 pm – 3 pm	Identifying small molecules binding sites in RNA conformational ensembles with SHAMAN - <i>Paraskevi Gkeka (Sanofi)</i>
	3 pm – 3:20 pm	3D Structure of Monoclonal Antibodies In Solution By Electron Density Topography - <i>Joseph D. Ferrara (Rigaku Americas Corp)</i>
<b>COFFEE BREAK – 30 min</b>		
<b>Session 2: Cryo-EM advancements in sample preparation &amp; data processing</b> <i>Chair: Pierre Legrand</i>	3:50 pm – 4:05 pm	EasyGrid: Automated Sample Preparation and Control for Cryo-Imaging Experiments - <i>Gergely Papp (EMBL Grenoble)</i>
	4:05 pm – 4:25 pm	CCPEM Pipeliner and Doppio: Software For End-To-End CryoEM Data Processing - <i>Matthew G. Iadanza (CCP-EM, STFC Rutherford Appleton Laboratory)</i>
	4:25 pm – 4:40 pm	Biomolecular Conformational Landscapes By MDSPACE: Cryo-EM Image Analysis Based On MD Simulations For Biomedical Applications - <i>Slavica Jonic (Sorbonne University &amp; CNRS)</i>
	4:40 pm – 5 pm	Image processing warnings for the use of CryoEM to drug discovery – <i>Carlos Oscar Sorzano (CSIC)</i>
	<b>5:15 pm – 6 pm</b>	<b>Bus 1 Return to NOVOTEL</b>
	5 pm – 6 pm	SOLEIL Tour (optional)
	<b>6:15 pm – 7 pm</b>	<b>Bus 2&amp;3 Return to NOVOTEL</b>
	7:15 pm – 9:30 pm	Exhibition, poster session, dinner

Monday, 11<sup>th</sup> of November

SESSION	TIME	TALK
	9 am – 9:15 am	Welcome session – <i>Sonja Kuhn (Servier), Pierre Legrand (SOLEIL)</i>
<b>Session 3: Challenging targets: Cryo-EM of membrane proteins</b> <i>Chair: Dave Brown</i>	9:15 am – 9:45 am	Enabling Structure-based Drug Discovery for Membrane Proteins: Insights Into Lipid-mediated Activation of GPR55 - <i>Dietmar Weichert (Boehringer Ingelheim)</i>
	9:45 am – 10:15 am	Cryo-EM on Solute Carriers – Basic Research and Drug interaction - <i>Christian Löw (EMBL Hamburg)</i>
	10:15 am – 10:45 am	Structural Dynamics of Insulin receptor signalling - implications for drug design - <i>Gerd Schluckebier (NovoNordisk)</i>
<b>COFFEE BREAK – 30 min</b>		
<b>Session 4: Structural Biophysics</b> <i>Chair: Alexey Rak</i>	11:15 am – 11:30 am	Integral Membrane Proteins for Biophysics and Cryo-EM applications. Case Study: Ion Channel TrpML3 - <i>Nathan R. Zaccai (Domainex Ltd.)</i>
	11:30 am – 11:45 am	NMR-Driven Discovery of Cryptic Pockets in IL13 for Fragment Drug Discovery - <i>Roberto Maya-Martinez (Signature Discovery)</i>
	11:45 am – 12:15 pm	Advanced Structural Mass Spectrometry in Vaccinology Research - <i>Natalie Norais (GSK)</i>
<b>Gold Sponsor talks</b>	12:15 pm – 12:25 pm	BIOSAXS GmbH: Beyond the Algorithm: Why Solution SAXS Still Matters in the Age of AI-Driven Design
	12:25 pm – 12:35 pm	Refeyn: Biomolecular characterization with mass photometry
	12:35 pm – 12:45 pm	Thermo Fisher: Advancing Drug Discovery With Cryo-Electron Microscopy
	12:45 pm – 12:55 pm	CryoCLOUD: Speeding Up Cryo-EM Data Analysis With Scalable Cloud Infrastructure And Novel Algorithms
<b>LUNCH TIME</b>		
<b>Session 5: Structural Biophysics: NMR in SBDD</b> <i>Chair: Alexey Rak</i>	2:30 pm – 3:10 pm	NMR versatility: fast, cheap, exact - <i>Roland Riek (ETH Zuerich)</i>
	3:10 pm – 3:35 pm	Harnessing Advanced NMR Methodologies to Enhance Biophysics and Structural Biology in Drug Discovery - <i>Nicola Salvi (Sanofi)</i>
	3:35 pm – 3:55 pm	Insights From Three Decades Of Hands-on Use Of Protein Structures In The Pharma Industry - <i>Steven LaPlante (NMX Research and Solutions, inc.)</i>
<b>COFFEE BREAK – 30 min</b>		
<b>Session 6: Synergies AI &amp; experimental approaches</b> <i>Chair: Christian Wiesmann</i>	4:30 pm – 5 pm	Functional design of soluble analogs of integral membrane proteins - <i>Casper Goverde (EPFL, Switzerland)</i>
	5 pm – 5:30 pm	Let AI Be Your Guide: Protein Engineering, Hypothesis Building And Beyond - <i>Matthias Haffke (Novartis)</i>
	5:30 pm – 6 pm	The future of macromolecular crystallography in the age of machine learning - <i>Arwen Pearson (University of Hamburg)</i>
<b>FREE EVENING</b>		
	7 pm – 10 pm	Seine Cruise & dinner (bring your dinner ticket)

Tuesday, 12<sup>th</sup> of November

SESSION	TIME	TALK
<b>Session 7: Emerging Technologies</b> Chair: Chun-Wa Chung	9 am – 9:30 am	Growing bigger to see small, running with cryoEM scissors, and other Adventures in Structureland - <i>James Kiefer (Genentech)</i>
	9:30 am – 10 am	Fuelling an Open Science Approach to Early-Stage Drug Discovery - <i>Martin A. Walsh (Diamond Light Source)</i>
	10 am – 10:30 am	In Situ Structures and Architectures of $\beta$ -amyloid and Tau Pathology within Alzheimer's Disease Patient Brain - <i>Madeleine A.G. Gilbert (University of Leeds)</i>
COFFEE BREAK – 30 min		
<b>Session 8: Case studies</b> Chair: Djordje Musil	11 am – 11:30 am	The unprecedented mechanism of lipid transport inhibition by the antibiotic Zosurabalpin - <i>Thomas Clairfeuille (Roche)</i>
	11:30 am – 12 pm	The novel structure of Salt inducible kinase 3 reveals determinants for isoform selective design - <i>Helena Käck (AstraZeneca)</i>
<b>Gold Sponsor talks</b>	12 pm – 12:10 pm	Nuvisan: Your trusted partner in gene-to-high resolution structure and challenging membrane targets.
	12:10 pm – 12:20 pm	ALPX: Accelerating Drug Discovery: ALPX Advanced Automated Crystallography And Cutting-Edge Screening Pipelines
	12:20 pm – 12:30 pm	Selvita: Integrated Fragment-Based Drug Discovery at Selvita
	12:30 pm – 12:40 pm	Cube Biotech: Characterizing membrane protein in near-native conditions using the NativeMP polymer suite
LUNCH TIME		
<b>Session 9: Case studies</b> Chair: Andreas Kuglstatler	2 pm – 2:35 pm	Discovery of ASTX295: A bone-marrow sparing MDM2 antagonist. From concept to clinic - <i>Martin Noble (Newcastle University, CRUK Newcastle Drug Discovery Unit)</i>
	2:35 pm – 2:50 pm	Fragment-Based Discovery of Allosteric Modulators of $\beta$ -Glucocerebrosidase - <i>Pravin Mahajan (Astex Pharmaceuticals)</i>
	2:50 pm – 3:20 pm	The Discovery of AZD5305: A PARP1–DNA Trapper with High Selectivity for PARP1 over PARP2 and Other PARPs - <i>Marianne Schimpl (AstraZeneca)</i>
	3:20 pm – 3:45 pm	Closing remarks
END		