

**New Frontiers in Structure-based Drug Discovery**

**Program**

<b>Monday, Sep 23, 2019</b>		<i>Key note lectures: 35+5 min, Talks: 15+5 min, Flashtalks: 2 min</i>
12:45	<b>Welcome</b> Michael Sattler, Christian Ottmann	
	<b>SESSION 1 – Structure- and Fragment-based Drug Discovery</b>	
	Chair: <i>Christian Ottmann</i>	
13:00	<b>Keynote lecture:</b> <a href="#">Stephen Fesik</a> <i>Cancer Drug Discovery Using Fragment-Based Methods and Structure-Based Design</i>	
13:40	<b>Francesco Bosica</b> <i>Mg<sup>2</sup>-assisted small-molecule stabilisation of 14-3-3 Protein-Protein Interactions.</i>	
14:00	<b>Barak Akabayov</b> <i>Development of antibacterial agents that target the ribosomal PTC of M. tuberculosis</i>	
14:20	<b>Christian Griesinger</b> <i>Modulation of aggregating proteins studied by NMR and beyond in neuro- and cellular degeneration</i>	
14:40	<b>Madita Wolter</b> <i>Drug Discovery at the Boundary of Cancer and Infection</i>	
15:00	<b>Keynote lecture:</b> <a href="#">Mike Hann</a> <i>'PhABits – shining new light on fragment approaches for assessing target tractability'</i>	
15:40	<i>Coffee Break</i>	
	<b>SESSION 1 – cont'd</b>	
	Chair: <i>Tomáš Obšil</i>	
16:10	<b>João Neves</b> <i>Nuclear Magnetic Resonance guided screening applied to the discovery of modulators of 14-3-3 Protein-Protein Interactions</i>	
16:30	<b>Stefan Hoerer</b> <i>Allosteric Activation of Striatal-Enriched Protein Tyrosine Phosphatase (STEP, PTPN5) by a Fragment-like Molecule</i>	
16:50	<b>Keynote lecture:</b> <a href="#">Edward Tate</a> <i>Fragment-guided discovery of an irresistible antiviral protein-protein interaction inhibitor</i>	
17:30	<b>Flash Talks</b>	
18:45	-	
20:30	<b>Poster Session 1</b> with drinks	
<b>Tuesday, Sep 24, 2019</b>		
	<b>SESSION 2 – Intrinsically Disordered and Amyloidogenic Proteins</b>	
	Chair: <i>Isabelle Landrieu</i>	
09:00	<b>Keynote lecture:</b> <a href="#">Birthe Kragelund</a> <i>Disordered Protein Complexes</i>	
09:40	<b>Orgeta Zejneli</b> <i>A VHH directed against tau as a novel therapeutic approach in tauopathies</i>	
10:00	<b>Carlos Camacho</b> <i>Neuroprotection by small molecule inhibition of disordered peptide and syntaxin interaction</i>	
10:20	<i>Coffee Break</i>	
	<b>SESSION 3 – Chemical biology, targeting &amp; new concepts</b>	
	Chair: <i>Alex Dömling</i>	
10:50	<b>Keynote lecture:</b> <a href="#">Alessio Ciulli</a> <i>Targeted Protein Degradation with Small Molecules: How PROTACs work</i>	
11:30	<b>Felix Hausch</b> <i>Selective FKBP51 inhibitors enabled by transient pocket binding</i>	
11:50	<b>Markella Konstantinidou</b> <i>Discovery of proteolysis targeting chimeras for leucine-rich repeat kinase 2 (LRRK2)</i>	
12:10	<b>Nikolaos Sgourakis</b> <i>New tools for the analysis of polyclonal T cell repertoires using chaperone-mediated peptide exchange</i>	
12:30	<b>Valeria Napolitano</b> <i>Inhibition of glycosomal protein import: the sweet death of Trypanosoma</i>	
12:50	<i>Lunch</i>	
	<b>SESSION 3 – cont'd</b>	
	Chair: <i>Alex Dömling</i>	
14:20	<b>Keynote lecture:</b> <a href="#">Michelle Arkin</a> <i>Chemical Biology Approaches to Understanding the VCP/p97 Protein Interaction Network</i>	
15:00	<b>João Encarnaçã</b> <i>Bioengineering subunit B from Shiga Toxin 1 for intracellular drug delivery</i>	

**SESSION 4 – Peptides, natural products and non-small molecules**Chair: *Andrew Wilson*

15:20	<a href="#">Keynote lecture: Ora Schueler-Furman</a> <i>Peptide as leads for targeted inhibition of interactions – How free, how determined?</i>
16:00	<b>Helen Boyd</b> <i>Identification of a novel cyclic peptide that disrupts the homodimerization of the E3 ubiquitin ligase IDOL</i>
16:20	<i>Coffee Break</i>
<b>SESSION 4 – cont'd</b>	
Chair: <i>Andrew Wilson</i>	
16:50	<b>Françoise Ochsenbein</b> <i>Rational Design of Peptides and Foldamers inhibiting a New Epigenetic Target in Cancer</i>
17:10	<b>Grzegorz Dubin</b> <i>Macrocyclic mediated inhibition of PD-1/PD-L1 immune checkpoint</i>
17:30	<b>Katiuscia Pagano</b> <i>Design of antiangiogenic agents targeting Fibroblast Growth Factors-2/Tyrosine-Kinase Receptor</i>
17:50	<b>Federica De Leo</b> <i>Diflunisal targets the HMGB1/CXCL12 heterocomplex and blocks immune cell recruitment</i>
18:10	<b>Xiao-Ling Cockcroft</b> <i>New Paradigm for Finding Natural-product-like KRAS Inhibitors</i>
18:30	<a href="#">Keynote lecture: Patricia Aducci</a> <i>Fusicoccin and 14-3-3 proteins, a long story from plant pathology to drug design.</i>
19:10	<b>Poster Session 2</b>
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20:30	<b>Gala Dinner</b>
20:30	
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23:00	

**Wednesday, Sep 25, 2019****SESSION 5 – Computational Drug Discovery**Chair: *Helena Danielson*

09:00	<a href="#">Keynote lecture: Rebecca Wade</a> <i>Computational Approaches to Protein Dynamics and Binding Kinetics for Drug Discovery</i>
09:40	<b>Marcus Gastreich</b> <i>Debunking a myth - Can <math>\sigma</math>-Holes Really Drive Affinity?</i>
10:00	<b>Alessandro Paiardini</b> <i>Identification of small-molecule inhibitors of the Aurora-A/TPX2 complex</i>

**SESSION 6 – Structural biology, biophysics & methods**Chair: *Michael Nilges*

10:20	<b>Sebastian Guenther</b> <i>Serial Crystallography for Ligand-Binding Studies</i>
10:40	<b>Charlotte Softley</b> <i>Placing fragments with lanthanide tags using paramagnetic NMR</i>
11:00	<i>Coffee Break</i>
<b>SESSION 6 – cont'd</b>	
Chair: <i>Michael Nilges</i>	
11:30	<b>Claire Munier</b> <i>Small molecule stabilization of the GR 14-3-3 protein-protein interaction (PPI)</i>
11:50	<b>Daisy Paiva</b> <i>Because structure means function - Conformational changes in proteins measured with switchSENSE®</i>
12:10	<b>Charlotte Hodson</b> <i>Expanding Crystallographic methods for Fragment-based Drug Design</i>
12:30	<a href="#">Keynote lecture: Jan Steyaert</a> <i>From Nanobodies to Megabodies for applications in cryo-EM</i>
13:10	<i>Lunch</i>
14:40	<b>Announcement of Posterprizes</b> <b>END/FAREWELL</b> Michael Sattler, Christian Ottmann
14:50	<b>Workshop BioSolveIT</b>
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16:50	