

Day 1 - Thursday, 14 May 2026		
15:00-17:30	Check-In & Onsite Registration	
Day 2 - Friday, 15 May 2026		
8:00	Check-In & Onsite Registration	
9:00	Opening Ceremony	
9:20	Plenary	Learn, Unlearn, Relearn - A Formula to Transformative Peptide Therapeutics Prof. Dr. Richard DiMarchi (<i>Indiana University, USA</i>)
10:00	Plenary	TBA Prof. Dr. Ma Dawei (<i>Shanghai Institute of Organic Chemistry, CAS, China</i>)
10:40	Tea Break	
11:10	Plenary	TBA Prof. Dr. Chen Fener (<i>Fudan University, China</i>)
S1. Chemical Biology for Drug Discovery		
11:50	Session Introduction	
11:55	Keynote	Molecular Design of mRNA Based on Chemistry and its Utilization in Drug Discovery Technology Prof. Dr. Hiroshi Abe (<i>Nagoya University, Japan</i>)
12:25	Lunch	
13:30	Oral	A family of compounds highly potent against Plasmodium and Leishmania with a novel mechanism of action targeting protein condensates Prof. Dr. Xavier Fernández-Busquets (<i>The Barcelona Institute of Science and Technology, Spain</i>)
13:45	Oral	G3BP1/2-Targeting PROTAC Disrupts Stress Granules Dependent ATF4 Migracytosis as Cancer Therapy Dr. Xiaohui Liu (<i>Chinese Academy of Medical Sciences & Peking Union Medical College, China</i>)
14:00	Oral	Pharmacological Activation of NAD⁺ Biosynthesis for Neuroprotection Assoc. Prof. Gelin Wang (<i>Shanghai Jiao Tong University School of Medicine, China</i>)
14:15	Oral	Small molecules reveal molecular mechanisms of SARM1 activation and inhibition Dr. Yun Shi (<i>Monash University, Australia</i>)
14:30	Oral	Fragment-Induced Enhancement of Extracellular Growth via Metabolic Reprogramming Huiyuan Meng (<i>University of Manchester, UK</i>)
14:45	Keynote	Chimeric Oligonucleotide drugs for targeting RNA and protein degradation Prof. Dr. Xinjing Tang (<i>Peking University, China</i>)
15:15	Tea Break	
S2. Medicinal Chemistry Tales		
15:45	Session Introduction	
15:50	Keynote	TBA Prof. Dr. Hong Liu (<i>Shanghai Institute of Materia Medica, CAS, China</i>)

16:20	Oral	Discovery of Covalent and Non-covalent Isoform-Selective NADPH Oxidase Inhibitors through Ultra-Large Virtual Screening and Medicinal Chemistry Optimization: New Tools for Cancer and Neuroprotection <i>Prof. Dr. Antonello Mai (Sapienza University of Rome, Italy)</i>
16:35	Oral	Discovery and Mechanism Study of Novel HBV CpAMs with High Potency and Broad Anti-drug Resistance Activity <i>Dr. Shujing Xu (Shandong University, China)</i>
16:50	Oral	Functionalizing Thiosemicarbazones for Biomedical Targets <i>Prof. Dr. Axel Klein (University of Cologne, Germany)</i>
17:05	Oral	Discovery of a Novel Class of Potent Inhibitors of the m6A Demethylase FTO for the Treatment of Severe CNS Disorders <i>Dr. Ana Mallo-Abreu (University of Barcelona, Spain)</i>
17:20	Keynote	Chemical Adaptation in Kinase Drug Design <i>Prof. Dr. Ke Ding (Shanghai Institute of Organic Chemistry, CAS, China)</i>
17:50	Poster Session	
19:00	Banquet Dinner	
Day 3 - Saturday, 16 May 2026		
S3. Natural Products in Drug Discovery		
9:00	Session Introduction	
9:05	Keynote	Small Molecules That Potentiate Antitumor Immunity <i>Prof. Dr. Motonari Uesugi (Kyoto University, Japan)</i>
9:35	Oral	Discovery and Total Synthesis of Anhydrotuberosin as a STING Antagonist for Treating Autoimmune Diseases <i>Dr. Fusheng Guo (Peking University, China)</i>
9:50	Oral	Natural product AW126 inhibits pancreatic cancer growth via TGF-β/MAPK pathway <i>Prof. Jun-Li Yang (Lanzhou Institute of Chemical Physics, CAS, China)</i>
10:05	Oral	Identification of Chalcone 17 and Chalcone 30 Protein Targets in the nematode <i>Caenorhabditis elegans</i>: new nematocides mode of action (MOA) <i>Dr. Alejandro Calderon-Urrea (California State University, USA)</i>
10:20	Oral	Anti-osteoporosis lead compounds from marine fungi <i>Prof. Dr. Xiaowei Luo (Guangxi University of Chinese Medicine, China)</i>
10:35	Tea Break	
11:05	Keynote	Natural Product-Driven Innovative Drug Discovery <i>Prof. Dr. Yefeng Tang (Tsinghua University, China)</i>
11:35	Keynote	Identification of Cellular Targets for Natural Bioactive Molecules <i>Prof. Dr. Kewu Zeng (Peking University, China)</i>
12:05	Oral	Triptolide Enhances Valve Interstitial Cell Autophagy-Lysosomal Function to Alleviate Calcific Aortic Valve Disease <i>Dr. Zhengfeng Fan (Huazhong University of Science and Technology, China)</i>
12:20	Oral	Genome Mining for the Discovery of Novel Marine Natural Products <i>Dr. Nedeljka Rosic (Southern Cross University, Australia)</i>
12:35	Lunch	
13:00	Poster Session	
S4. AI for Drug Discovery		
14:00	Session Introduction	

14:05	Keynote	Drug Discovery towards Undruggable Targets <i>Prof. Dr. Luhua Lai (Peking University, China)</i>
14:35	Oral	Machine Learning Approaches for Predicting ADMET Parameters in Drug Development: Integrating Molecular Descriptors and Deep Learning <i>Prof. Dr. Rino Ragno (Sapienza University of Rome, Italy)</i>
14:50	Oral	Integrating HPC and AI to Advance Protein-ligand Binding Interaction Prediction <i>Prof. Dr. Niu Huang (National Institute of Biological Sciences, China)</i>
15:05	Oral	Assessment of affinity prediction approaches in small molecular drug discovery <i>Dr. Yao Wu (China Innovation Center of Roche, China)</i>
15:20	Keynote	A Small Molecule Targeting Every Human Protein: Harnessing AI to Realize the Dream <i>Dr. Albert Antolin Hernandez (Vall d'Hebron Institute of Oncology, Spain)</i>
15:50	Tea Break	
S5. Drug Discovery Targeting GPCRs and Ion Channels		
16:20	Session Introduction	
16:25	Keynote	Psychedelics-inspired drug discovery: structure-based design of subtype-selective 5-HT_{2A} agonists <i>Prof. Dr. Jianjun Cheng (ShanghaiTech University, China)</i>
16:55	Oral	Photocrosslinking-assisted platform for GPCR deorphanization and related drug discovery <i>Prof. Dr. Miao Jing (Chinese Institute for Brain Research, China)</i>
17:10	Oral	Selective activation of the kappa-opioid receptor by diphenethylamines, HS665 and HS666, for an effective and safer pain treatment <i>Prof. Dr. Mariana Spetea (University of Innsbruck, Austria)</i>
17:25	Oral	Discovery of Novel Adenosine A_{2A}R/A_{2B}R Dual Antagonists for Cancer Immunotherapy <i>Assoc. Prof. Qiong Xie (Fudan University, China)</i>
17:40	Keynote	Beyond Single Targets: Serotonin System Polypharmacology and Prodrug Development in Alzheimer's Disease <i>Prof. Dr. Christophe Rochais (University of Caen Normandy, France)</i>
Day 4 - Sunday, 17 May 2026		
S6. New Proximity-Based Drug Modalities		
9:00	Session Introduction	
9:05	Keynote	DNA Encoded Library Technology Development and its Application for Proximity -Based Drug Discovery <i>Prof. Dr. Xiaojie Lu (Shanghai Institute of Materia Medica, CAS, China)</i>
9:35	Oral	Extracellular HSP90-Facilitated Degradation of Extracellular and Membrane Proteins by Bifunctional Small Molecules <i>Assoc. Prof. He Chen (Tianjin Medical University, China)</i>
9:50	Oral	Targeting E3 Pseudoligases via Proximity-Based Protein Abundance Control: TRIM15 as a Case Study <i>Dr. Chengliang Zhu (Zhejiang University, China)</i>

10:05	Oral	RIMTAC: A Novel Degradation Design Platform by Indirect VHL-Recruitment via RIPK1 <i>Assoc. Prof. Yudao Shen (Shanghai Jiao Tong University, China)</i>
10:20	Oral	Hijacking Phosphatases for Target Protein Dephosphorylation with Phosphorylation Targeting Chimeras (PhosTACs) <i>Prof. Zhenyi Hu (Shanghai Institute of Organic Chemistry, China)</i>
10:35	Tea Break	
11:05	Oral	PSMA-Mediated Target Protein Degradation Enables Selective and Effective Therapy for Prostate Cancer <i>Assoc. Prof. Xufen Yu (Fudan University, China)</i>
11:20	Oral	Proximity-Based Small Molecules for Induced Dephosphorylation <i>Prof. Dr. Lei Wang (China Pharmaceutical University, China)</i>
11:35	Oral	Targeted Degradation of TDP-43: A PROTAC-Based Therapeutic Approach for ALS and Alzheimer's Disease <i>Javier Sánchez (University of Barcelona, Spain)</i>
11:50	Oral	Synthesis of PTP1B-Targeting PROTACs and Their Anti-Type 2 Diabetes Activity <i>Assoc. Prof. Zunhua Yang (Jiangxi University of Chinese Medicine, China)</i>
12:05	Lunch	
13:00	Poster Session	
14:00	Keynote	Molecular Glue Degraders: Discovery and Therapeutic Potential <i>Prof. Dr. Ting Han (National Institute of Biological Sciences, China)</i>
14:30	Oral	The converging mechanism of a molecular glue degrader and cancer gain-of-function mutations <i>Asst. Prof. Xiaowen Xie (Peking University, China)</i>
S7. Biocatalysis for Natural Product and Drug Synthesis		
14:45	Session Introduction	
14:50	Keynote	Biosynthesis of Enethioether Crosslinked, Peptide Natural Products <i>Prof. Dr. Wen Liu (Shanghai Institute of Organic Chemistry, CAS, China)</i>
15:20	Oral	Novel Oxidative Amidases for the Efficient Synthesis of Amides <i>Kangdelong Hu (Peking University, China)</i>
15:35	Tea Break	
16:05	Keynote	TBA <i>Prof. Dr. Jason Micklefield (Imperial College London, UK)</i>
16:35	Oral	Merging Natural and Unnatural Reactivity of Reductive Aminases for Stereoselective Thioamination Cascade Reactions <i>Dr. Dongshan Wu (Peking University, China)</i>
16:50	Oral	Convergent Total Synthesis and Structural Revision of (-)-Papililone A via Pd-Catalyzed Alkenylation/Cyclization Cascade <i>Assoc. Prof. Sihua Hou (Shanghai Jiao Tong University, China)</i>
17:05	Oral	Biosynthesis and chemoenzymatic synthesis of ADP-heptoses <i>Prof. Dr. Yihua Chen (Institute of Microbiology, CAS, China)</i>
17:20	Oral	Biocatalytic Synthesis of Chiral Amines toward Novel Drug Discovery <i>Asst. Prof. Licheng Yang (Chinese Academy of Medical Sciences & Peking Union Medical College, China)</i>
17:35	Award Ceremony & Closing Speech	