

## Monday, September 25

8:30		Welcome Reception and Registration
9:00	Welcome Speech	Official Opening by UniVie Vice Rector Manuela Baccharini and MolTag Speaker Gerhard Ecker
9:15	<b>Plenary Session 1:</b> <b>Lynette Daws</b> , University of Texas Health Science Center	More than one way to transport monoamines: Uncovering novel molecular targets for therapeutics to treat psychiatric and substance use disorders; <i>Host: Marco Niello</i>
10:00	<b>Stefanie Kicking</b> , University of Copenhagen	Development of novel selective tool compounds for the nutrient amino acid transporters (SLC6A15-20); <i>Host: Marco Niello</i>
10:25	<b>Thomas Steinkellner</b> , Medical University of Vienna	Selective vulnerability of dopamine neurons in Parkinson's disease; <i>Host: Nina Kastner</i>
10:50		Coffee Break, 20 min
11:10	<b>Kusumika Saha</b> , Brigham Women's Hospital	Pharmacological chaperone-rescued cystic fibrosis CFTR-F508del mutant overcomes PRAF2-gated access to endoplasmic reticulum exit sites; <i>Host: Nina Kastner</i>
11:35	<b>Felix Mayer</b> , University of Copenhagen	Exploiting GPCR Regulation of Transporter Trafficking to Rescue Defective Neurotransmitter Homeostasis; <i>Host: Ralph Gradisch</i>
12:00	<b>Eva Hellsberg</b> , National Institutes of Health	Computational studies of molecular interactions in the human serotonin and dopamine transporters; <i>Host: Ralph Gradisch</i>
12:25		Lunch Break, 50 min
13:15	<b>Plenary Session 2:</b> <b>Robin Bon</b> , University of Leeds	Understanding TRPC1/4/5 channels through chemical biology and structural pharmacology; <i>Host: Viktor Savic</i>
14:00	<b>Konstantina Bampali</b> , University of Copenhagen	Antipsychotics and antidepressants can inhibit $\alpha 5$ -containing GABAA receptors by two distinct mechanisms; <i>Host: Florian Vogel</i>
14:25	<b>Lukáš Rýček</b> , Charles University Prague	Selaginella Natural Products as a Platform for Evaluation of New Synthetic Methods, Structural Aspects Elucidation and Drug; <i>Host: Viktor Savic</i>
14:50	<b>Kumaresan Jayaraman</b> , Laurus Bio Bangalore	Enzyme engineering to resist feedback inhibition in 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase; <i>Host: Florian Vogel</i>
15:15		Coffee Break, 20 min
15:35	Poster Flash Talks	26 Presentations, <i>Host: Gerhard Ecker</i>
17:05	Poster Session	27 Posters
18:30	End of Day 1	
19:00		Conference Dinner at <a href="#">Summerstage Pavillon</a> , directly at Donaukanal (U4 Rossauer Lände, use exit to Promenade)

## Tuesday, September 26

8:45		Welcome Reception (Tea, Coffee)
9:15	<b>Plenary Session 3:</b> <b>Marina Kasimova</b> , Novo Nordisk, Denmark	From understanding principles of ion channel functioning to design of protein modulators; <i>Host: Theres Friesacher</i>
10:00	<b>Vaibhavkumar Gawali</b> , Charles River Laboratories	Ionic and immune mechanisms of response to cancer immunotherapy and severe COVID-19; <i>Host: Michael Netzer</i>
10:25	<b>Péter Lukács</b> , Agricultural Institute of the Hungarian Academy of Sciences	Optimizing for Information Content on IonFlux Mercury Automated Patch Clamp; <i>Host Michael Netzer</i>
10:50		Coffee Break, 25 min <i>Intro by Margot Ernst;</i>
11:15	<b>Panel Discussion:</b> <b>PhD finished! What's next?</b>	Hosted by Catherine McKenzie (Discovery Scientist in Gene Therapy, Roche Basel). With: Chris Ahern, Claire Colas, Christian Knittl-Frank, Jasmin Morandell, Gaia Novarino, David Siebert
12:30		Lunch Break, 45 min
13:15	<b>Plenary Session 4:</b> <b>Stéphanie Baulac</b> , Paris Brain Institute	Somatic mosaicism in epilepsy and cortical malformations; <i>Host: Lena Schwarz</i>
14:00	<b>Jasmin Morandell</b> , University of Trento	circHTT, a novel circular RNA molecule from the Huntington's disease gene locus: functional characterization and pathophysiological implications; <i>Host: Nathalie Agudelo-Duenas</i>
14:25	<b>Julia Michalska</b> , E11 Bio	A versatile tool for the comprehensive analysis of nervous tissue organization with light microscopy; <i>Host: Nathalie Agudelo-Duenas</i>
14:50		Closing Words by MolTag Speaker Gerhard Ecker Fare Well Coffee

## Poster Session – Flash talks (No 1-24: 3 min each; 25+26: ca. 5 min)

15:35	Short introduction	Gerhard Ecker	
15:37	Visualizing the transcriptional landscape with tissue context	Nathalie Agudelo-Duenas	1
15:40	Development of Novel Fluorescent Dyes in the Making of New Biologically Active Conjugates	Sergijo Matheu Armentia	2
15:43	Assay for evaluation of proarrhythmic effects of herbal products	Bozhidar Baltov	3
15:46	Novel fluorescent probes for imaging the serotonin transporter	Oliver Belleza	4
15:49	New enrichable cross-linkers for protein-protein interaction analysis by mass spectrometry	Bogdan-Razvan Brutiu	5
15:52	Ethosuximide inhibition of GIRK channels	Theres Friesacher	6
15:55	$\beta$ subunits of GABAA receptors form proton gated ion channels	Aleksandra Garifulina	7
15:58	Ligand coupling mechanism of the human serotonin transporter differentiates substrates from inhibitors	Ralph Gradisch	8
16:01	Macrocycles as potential inhibitors of GLUT1 and GLUT4	Nejra Granulo	9
16:04	Systemic fingerprints for predicting liver related adverse even	Palle Helmke	10
16:07	ProteoMutaMetrics: Machine Learning Approaches for SLC6 Mutation Pathogenicity Prediction	Jiahui Huang	11
16:10	Characterization of MDMA derivative 1,3-Benzodioxolylbutanamine (BDB) and its structural analogs	Nina Kastner	12
16:13	Electrophysiological characterization of cardiac organoids	Michael Netzer	13
	<i>Analysing the Co-existence of Immune Reaction and LiverToxicity for Therapeutical Monoclonal Antibodies (no flash talk)</i>	Abir Omran	14
<b>6 min short break</b>			
16:22	Substituting Gaseous Reagents for Solid Alternatives	Eleni Papaplioura	15
16:25	Modified Phosphatidylinositols for the Investigation of Peptide Assemblies	Viktor Savic	16
16:28	Development of Novel Pyrazoloquinolinone Ligandsfor Selective and Site-Specific Modulation of GABA <sub>A</sub> Receptors	Dominik Schnalzer	17

<b>16:31</b>	Hidden targets of autism spectrum disorders: dissecting divergent and convergentcausal paths	Lena Schwarz	18
<b>16:33</b>	Investigating Photoswitchable Drugs: The Effect of para-Substitution on the Thermal Z/E-Isomerization Mechanism of Arylazo-pyrazoles	Nadja Singer	19
<b>16:37</b>	Identifying Differences in the Performance of Machine Learning Models for off-Targets trained on publicly available and proprietary datasets	Aljoša Smajić	20
<b>16:40</b>	Estimating thermal isomerization half- lives of arylazopyrazole photoswitches using neural network potentials	Maximilian Tiefenbacher	21
<b>16:43</b>	GABRA4 variants contribute to neurodevelopmental abnormalities with or without seizures	Florian Vogel	22
<b>16:46</b>	Development of Novel Fluorescent Dyes and Their Application as Probes to Study Biological Processes	Yi Xiao	23
<b>16:49</b>	Synthesis of FR Analogues and its Application inHuman PBMCs	Haoqi Zhang	24
<b>16:52</b>	Photoswitchable Tool Compounds for the Reversible Stabilization of G Quadruplex DNA	Katharina Schlögl	25
<b>16:57</b>	Persistent binding at dopamine transporters determines sustained psychostimulant effects	Marco Niello	26
<b>17:02</b>	End of Flash talks – Please go to the posters!		