



4<sup>th</sup> year of the Prague Summer School

## ADVANCES IN DRUG DISCOVERY

**DRUG discovery and DEVELOPMENT**  
from basic research through preclinical  
to clinical phases



Prague, Czech Republic ■ September 4<sup>th</sup> – 8<sup>th</sup>, 2017

# PROGRAMME

The course is organized by  
the University of Chemistry and Technology Prague  
and  
Institute of Organic Chemistry and Biochemistry of the CAS



UNIVERSITY OF  
CHEMISTRY AND TECHNOLOGY  
PRAGUE



ÚOCHB <sup>AV</sup>  
CR  
IOCB PRAGUE

## MEETING VENUE

### University of Chemistry and Technology Prague

*BUILDING A, ROOM AI (Technická 5, Prague 6)*

#### MONDAY, SEPTEMBER 4<sup>th</sup>

<b>11:00</b>	<i>Registration at University of Chemistry and Technology Prague (UCT)</i>
<b>14:00</b>	<i>Welcome from the IOCB director &amp; UCT rector</i> Zdeněk Hostomský (Director IOCB) Karel Melzoch (UCT rector) Opening Talks
<b>14:20</b>	Helena Mertlíková (IOCB) Overview of the Process
<b>15:00</b>	<i>Coffee break</i>
<b>15:20</b>	Dorte X. Gram (CEO) If I'm right, This could be a really Big Thing! – Daring to Challenge Status-quo in Diabetes Treatment
<b>16:00</b>	Jiří Paleček (FGU) Pain, Research and Challenging Path for New Treatments
<b>18:00</b>	<i>Welcome Party at Masaryk Dormitory (address: Thákurova 1, Prague 6)</i>

#### TUESDAY, SEPTEMBER 5<sup>th</sup>

<b>9:00</b>	James Engel (University of Michigan) Developing Therapeutics for the Worlds Most Common Inherited Genetic Disease
<b>9:45</b>	Petr Váchal (MSD) Medicinal Chemistry Enabled by Novel, Transformational Capabilities
<b>10:30</b>	<i>Coffee break</i>
<b>10:45</b>	Stanislav Rádl (Zentiva) Deuterated Drugs – A Hot Topic of Current Medicinal Chemistry
<b>11:30</b>	Stephane Daffis (Gilead) Drug Discovery and Development Strategies for HBV Cure
<b>12:15</b>	<i>Lunch at Masaryk Dormitory</i>

<b>14:00</b>	Thomas Ullrich (Novartis) Local Drug Delivery to Joints and Tendon
<b>14:45</b>	Evžen Bouřa (IOCB) Rational structure-based drug design – practical experiences
<b>15:30</b>	<i>IOCB Tour (meeting point registration desk)</i>

## WEDNESDAY, SEPTEMBER 6<sup>th</sup>

<b>9:00</b>	Ivana Šurová (MediTox s.r.o.) Preclinical Toxicology – an Important Part of Drug Development
<b>9:45</b>	Ivana Šurová (MediTox s.r.o.) Preclinical Toxicology and its Relevance to Clinical Trials
<b>10:30</b>	<i>Coffee break</i>
<b>10:45</b>	Vít Perlík (Independent consultant) Clinical Trials in Drug Development
<b>11:30</b>	Piotr Golkiewicz (Elsevier) Quick access to collated data on bioactivity of chemical compounds with help of Reaxys Medicinal Chemistry
<b>12:15</b>	<i>Lunch at Masaryk Dormitory</i>
<b>14:30</b>	<i>Prague City Tour and dinner (restaurant Staré časy – address Rytířská 4, Prague 1)</i>

## THURSDAY, SEPTEMBER 7<sup>th</sup>

<b>9:00</b>	Sergey Zozulya (ENAMINE) Discovering Drugs with a CRO
<b>9:45</b>	Ernst Plefka (Biocrates) Pharmacometabolomics in Drug Development and Precision Medicine
<b>10:30</b>	<i>Coffee break</i>
<b>10:45</b>	Stephan Bachmann (Roche) Catalysis as Key Technology in the Synthesis & Scale-up of APIs and Their Intermediates
<b>11:30</b>	Dan Svozil (UCT Prague) Introduction to Chemoinformatics and Computational Drug Design
<b>12:15</b>	<i>Lunch at Masaryk Dormitory</i>
<b>13:30</b>	Marián Hajdůch (IMTM) Personalized Medicine in Oncology
<b>14:15</b>	Tomáš Etrych (IMC) Nanosized Polymer-based Medicines for Targeted Therapy
<b>15:00</b>	<i>UCT Tour and Visit of the University Brewery (meeting point registration desk)</i>

## FRIDAY, SEPTEMBER 8<sup>th</sup>

<b>9:00</b>	Igor Linhart (UCT Prague) Clandestine Drug Design: From Mere Copying to New Psychoactive Substances
<b>9:45</b>	Pavína Řezáčová (UMG) X-ray Crystallography in Drug Design
<b>10:30</b>	<i>Coffee break</i>
<b>10:45</b>	David M.Andrews (Astra Zeneca) The discovery of AZD4547
<b>11:30</b>	Eva Kudová (IOCB) Architecture in the Syntesis of Steroidal Inhibitors of NMDA Receptors: Do Built New or Rebuilt Old?
<b>12:15</b>	Václav Veverka (IOCB) NMR and Drug Development
<b>13:00</b>	CLOSING, BEST POSTER AWARD WINNER
<b>13.30</b>	<i>Lunch at Masaryk Dormitory</i>



UCT Prague, room A1

# LIST OF POSTERS

	Last Name	First Name	Name of Abstract
<b>P1</b>	Andranovits	Stanislav	Key role of segment IS4 in Cav1.2 inactivation: link between activation and inactivation
<b>P2</b>	Andrs	Martin	The development of novel compounds with radio- and chemosensitizing properties based on the phosphatidylinositol 3-kinase inhibitor LY294002
<b>P3</b>	Bekić	Sofija	Evaluation of the steroid receptor binding affinity of some selected steroid derivatives by fluorescent cellular biosensor
<b>P4</b>	Bor	Gizem	TBA
<b>P5</b>	Górecki	Lukáš	Mono-quaternary reactivators, new lead structures for organophosphorus intoxication.
<b>P6</b>	Chechina	Nataliia	Arylglyoxals as convenient precursors for the synthesis of heterocyclic compounds
<b>P7</b>	Ibba	Roberta	Design and synthesis of new planar heteroaromatic derivatives with antiviral activity
<b>P8</b>	Janočková	Jana	Inhibition of A $\beta$ 1-42 self-aggregation process
<b>P9</b>	Janovská	Pavĺina	Casein kinase 1 $\delta/\epsilon$ is a therapeutic target in chronic lymphocytic leukemia (CLL)
<b>P10</b>	Kobřlová	Tereza	In vitro PAMPA and MDCK models for the prediction of blood brain barrier penetration
<b>P11</b>	Kodedová	Marie	The mechanism of action of halictines is dependent on the lipid composition of Candida cells
<b>P12</b>	Korábečný	Jan	Design, synthesis and in vitro evaluation of novel 7-methoxytacrine-adamantylamine hybrids: Novel cholinesterase inhibitors with potential implication for Alzheimer's disease treatment

<b>P13</b>	Kučera	Tomáš	Anti-Alzheimer or antimalarial drugs? Usage of the cross-docking in drug design
<b>P14</b>	Levin	Maxim	Engineering novel protein agents to study and manipulate the extracellular matrix
<b>P15</b>	Marchetti	Giuseppe	In vitro and computational studies of Syk inhibitors as new antimalarial drugs
<b>P16</b>	Marinovič	Maja	Use of crystallographic data, molecular dynamics and A Fluorescent cell assay to identify ligands with selectivity for estrogen or androgen receptor isoforms
<b>P17</b>	Mezeiová	Eva	Development of novel huprine derivative for Alzheimer's disease therapy
<b>P18</b>	Mohl	Gregory	In silico design and structure-activity relationship of novel influenza inhibitors
<b>P19</b>	Morozová	Alisa	Domino reactions of 3(5)-aminoisoxazoles and pyruvic acid's derivatives
<b>P20</b>	Němec	Václav	Discovery of new protein kinase inhibitors with the furo [3,2-b]pyridine core
<b>P21</b>	Pavlovská	Tetyana	Spiropyrrolidinoxindoles as potential drug candidates in target-oriented synthesis
<b>P22</b>	Plavša	Jovana	Identification of potential inhibitors of AKR1C3 and preparation for structural analyses.
<b>P23</b>	Repich	Hlib	Pi-coordination compounds of Pd(II) and Pt(II) as potential substitutes of cisplatin and its analogues
<b>P24</b>	Sanin	Eduard	Bright fluorescent squaraine rotaxanes for biomedical applications
<b>P25</b>	Shraga	Amit	Novel covalent inhibitors of the MKK7 kinase
<b>P26</b>	Stadler	Marco	Pharmacological characterization of a GLIC-GABAA beta3 chimera

<b>P27</b>	Szánti-Pintér	Eszter	Claisen-Schmidt condensation of 17-ketosteroids in the presence of switchable polarity solvents
<b>P28</b>	Tomas	Jan	Importance of tablet disintegration for pharmaceutical product performance: New approaches using texture analysis.
<b>P29</b>	Tubon Usca	Irvin Ricardo	Effects of ethanolic extracts of four ecuadorian plants on porcine aortic endothelial cells (pAECs) stability.
<b>P30</b>	Tulli	Ludovico	Dendrimers as polyfunctional scaffolds for mass cytometry applications
<b>P31</b>	Vaca Altamirano	Gabriela Liseth	Identification of a new, functional cross-talk between EphB1 receptor and mu opioid receptor
<b>P32</b>	Vodolazhenko	Mariia	One-pot synthesis of highly substituted 2-pyridones and related heterocycles via reaction of $\alpha$ -carbonyl CH-acids with DMFDMA and active methylene nitriles



UOCHB Building



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### BIOCRATES

LIFE SCIENCES

The Deep Phenotyping Company

*ESSENCE LINE*



### IOCB TTO

[www.iocb-tto.cz](http://www.iocb-tto.cz)



### ELSEVIER

### lach:ner

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of the Czech Republic (TA ČR).

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#### Organizing Secretariat: Congress Business Travel

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