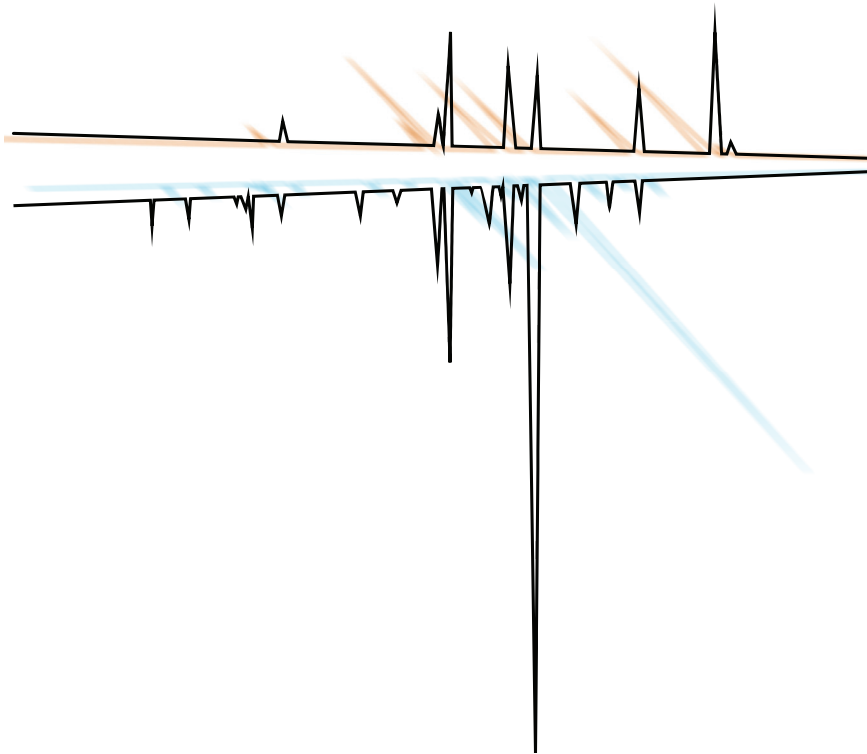


# Conference Programme



## Sunday, September 18<sup>th</sup>

- 10:00 – 12:00 & Course 1, Lecture Room “Mala dvorana”, Hotel Donat  
16:00 – 18:00 ***Polymorphs and other solid forms: identification, properties and analytical principles***  
**Rolf Hilfiker**, Solvias AG, Switzerland
- 10:00 – 12:00 & Course 2, Lecture Room “Bura”, Hotel Funimation  
16:00 – 18:00 ***Chiral recognition and separation mechanisms***  
**Nelu Grinberg**, Boehringer-Ingelheim, USA
- 10:00 – 12:00 & Course 3, Lecture Room “Novi Park”, Hotel Funimation  
16:00 – 18:00 ***QSAR analysis - principles, methods and applications***  
**Stefan Dove**, University of Regensburg, Germany
- 09:00 – 10.30 **Conference Desk open**  
15:00 – 18.30 **Participant registration**, Hotel Donat
- 20:00 **Welcome party, Hotel Adriana**

All Conference Lectures, as well as Oral Presentations will be given in the **Conference Hall, Hotel Donat**

## Monday, September 19<sup>th</sup>

- 08:00 **Poster mounting**, in front of the Conference Hall, Hotel Donat
- 09:00 **Opening Ceremony**  
Chair: Klara Valko
- 09:20 ***The importance and different approaches for the determination of permeability across an artificial membrane***  
OP 01 **Kin Y. Tam**, AstraZeneca, UK
- 10:05 ***Mechanistic prediction of oral drug absorption from physicochemical property***  
OP 02 **Kiyohiko Sugano**, Pfizer, UK
- 10:50 **Coffee break**  
Chair: Kiyohiko Sugano
- 11:10 ***Applications of bio-mimetic HPLC methods for the estimation of in vivo distribution of early drug discovery compounds***  
OP 03 **Klara Valko**, GlaxoSmithKline, UK

- 11:55 **Implementation of In Vivo Permeability Studies for Evaluation and**  
OP 04 **Improvement of Generic Drug Formulations Before Bioequivalence Studies**  
Seval Korkmaz, Abdi Ibrahim, Turkey
- 12:30 **Dynamic dissolution testing in R&D**  
OP 05 **Martin Čulen**, Jiří Dohnal, Josef Jampílek, Anna Řezáčová  
University of Veterinary and Pharmaceutical Sciences, Czech Republic
- 13:00 **Lunch**
- Chair: Kin Tam
- 15:00 **GLP determination of equilibrium solubility with special interest of ionization**  
OP 06 **and polymorphism**  
Krisztina Takács-Novák, Semmelweis University, Hungary
- 15:40 **Techniques for investigating supersaturation and the enhancement of**  
OP 07 **solubility**  
John Comer, Sirius-analytical Ltd. UK
- 16:20 **Dissolution of nanocrystalline particles for IV route: in vitro studies and in silico**  
OP 08 **modelling**  
Guillaume Louit, Xavier Pepin, Morgane Vacher, Sanofi-Aventis, France
- 16:45 **Coffee break**
- Chair: John Comer
- 17:00 **Structure-based QSAR studies on 5-HT<sub>2A</sub> partial agonists**  
OP 09 **Stefan Dove**, Maria E. Silva, Ralf Heim, Andrea Strasser, Sigurd Elz  
University of Regensburg, Germany
- 17:40 **Modeling Biorelevant Solubility and Dissolution: Effects of Molecular**  
OP 10 **Ionization**  
Michael B. Bolger, Robert Fraczek, Marvin Waldman, Dechuan Zhuang,  
Walter S. Woltoz, Simulations plus Inc. USA
- 18:20 **The relationship study of Clog P & aphicidal activity of cyantraniliprole analogs**  
OP 11 HuiBin Yang, Hua Chen, JunFeng Wang, Bin Li  
Shenyang Research Institute, China
- 18:45 **IS-CE: A fast high-throughput method for pKa determination by capillary**  
OP 12 **electrophoresis**  
Martí Rosés, Joan Marc Cabot, Elisabet Fuguet, Clara Ràfols  
University of Barcelona, Spain

## Tuesday, September 20<sup>th</sup>

Chair: Predrag Novak

09:00 ***NMR studies of peptides and proteins and their interactions: implications for drug development***  
OP 13

**Horst Kessler**, *Technical University of Munich, Germany*

09:40 ***Functional mechanisms of drugs studied by NMR: methodology and applications***  
OP 14

**Teresa Carlomagno**, *EMBL, Germany*

10:20 ***Determining the orientation of drugs in receptors by solvent paramagnetic relaxation NMR spectroscopy***  
OP 15

Simone Kosol, Christoph Göbl, Katarina Culjak, Walter Hohlweg, Predrag Novak, **Klaus Zangger**, *University of Graz, Austria*

### 10:50 Coffee break

Chair: Danièle Giron

11:10 ***The importance in drug design of resolving structural and dynamic details for membrane drug targets at the nanoscale***  
OP 16

**Anthony Watts**, *Oxford University, UK*

11:50 ***Statistically optimized Raman microscopy for detecting low levels of undesired polymorphic forms in low dose active tablets***  
OP 17

**Slobodan Šašić**, Mark Whitlock and Shawn Mehrens, *Pfizer, USA*

12:30 ***<sup>14</sup>N NQR study of polymorphism of piroxicam and nifedipine; characterization of their polymorphs and solid-solid transformations***  
OP 18

**Zoran Lavrič**, Janez Pirnat, Janko Lužnik, Zvonko Trontelj, Stane Srčič  
*University of Ljubljana, Slovenia*

### 13:00 Lunch

Chair: Biserka Cetina Čižmek

15:00 ***Challenging characterization of polyphasic drugs. Use of combined physico-chemical techniques in pharmaceutical development***  
OP 19

**Danielle Giron**, *Consultant, France*

15:40 ***Hydrates: Thermodynamics and Determination of Relevant Parameters***  
OP 20

**Rolf Hilfiker**, *Solvias AG, Switzerland*

16:20 ***The determination of dehydration mechanism of lactose monohydrate by using thermogravimetric methods***  
OP 21

**Petar Tudja**, Ernest Meštrović, *PLIVA d.o.o, Croatia*

### 16:40 Coffee break

Chair: Rolf Hilfiker

17:00 ***Solid-state chemistry and new drug forms***

OP 22 **Elena V. Boldyreva**, *Novosibirsk State University, Russia*

- 17:40 **Study of the role of molecular mobility in physical stability of amorphous of anti-inflammatory drug: Celecoxib**  
OP 23  
**Marian Paluch**, Katarzyna Grzybowska, Żaneta Wojnarowska, Kia L. Ngai  
*Institute of Physics, Poland*
- 18:10 **Tailor-made batch crystallisation of Entacapone through the use of self-assembled layers on gold single crystal surface**  
OP 24  
**Ana Kwokal**, Kevin J. Roberts, *PLIVA d.o.o. Croatia*
- 18:35 **Physical insight into tautomerization reaction in some pharmaceutically important molecules**  
OP 25  
**Zaneta Wojnarowska**, Marian Paluch, *Institute of Physics, Poland*
- 19:00 **Poster session (until 23:00)**

### Wednesday, September 21<sup>st</sup>

Chair: Pierre Parot

- 09:00 **The influence of glycosylation to biological activity of proteins**  
OP 26  
**Jasna Peter Katalinić**, *University of Münster, Germany*
- 09:45 **Mass spectrometric approaches for structural elucidation of “misfolding” - aggregating neurodegenerative proteins: Ion mobility- MS and affinity- MS**  
OP 27  
Camelia Vlad, Claudia Cozma, Marilena Manea, Marius Iurascu, Kathrin Lindner, Jieun Jung, Martin Scheffner, Marcel Leist, **Michael Przybylski**  
*University of Konstanz, Germany*
- 10:30 **Coffee break**
- Chair: Jasna Peter Katalinić
- 10:50 **Biophysical methods for identifying and characterizing protein-ligand interactions**  
OP 28  
**Geoff Holdgate**, *AstraZeneca, UK*
- 11:35 **Dynamic Force Spectroscopy for studying high affinity ligand receptor complexes**  
OP 29  
**Pierre Parot**, Jean-Luc Pellequer, *CEA Marcoule, France*
- 12:00 **TRANSIL High Sensitivity Binding Assay: A novel tool for assessing plasma binding of hardly soluble and sticky drugs**  
OP 30  
**Hinnerk Boriss**, *Sovicell GmbH, Germany*
- 12:25 **Lunch**
- 13:30 **Excursion**
- 20:30 **Conference Dinner**

## Thursday, September 22<sup>nd</sup>

Chair: Vesna Gabelica

09:00 **Chromatographic and spectroscopic studies on the chiral recognition of**  
OP 31 **sulfated  $\beta$ -cyclodextrin as chiral mobile phase additive: Enantiomeric**  
**separation of a chiral amine**

Shengli Ma, Sherry Shen, Nizar Haddad, Wenjun Tang, JingWang, Heewon Lee,  
Nathan Yee, Chris Senanayake, **Nelu Grinberg**, *Boehringer-Ingelheim, USA*

09:45 **Automated Patch Clamp in Drug Discovery – from the bench to the midfield**  
OP 32 **Morten Sunesen**, *Sophion Bioscience, Denmark*

10:30 **Coffee break**

Chair: Nelu Grinberg

10:50 **Synergistic and antagonistic effects between selected phenolic and**  
OP 33 **polyphenolic antioxidants**

**Ewelina Kowalewska**, Grzegorz Litwinienko, *University of Warsaw, Poland*

11:15 **Compressibility investigation of chewing gum bases used for API containing**  
OP 34 **direct compressed chewing gum tablet preparation**

**Peter Kása jr.**, Imre Jojart, Klára Pintye-Hódi, *University of Szeged, Hungary*

11:40 **Seminar/Workshop: Bioaffinity - Mass Spectrometry**,  
S 1 **Michael Przybylski**, *University of Konstanz, Germany*

13:00 **Conference closing**