Sixth World Conference on Physico-Chemical Methods in Drug Discovery and Development & Third World Conference on ADME and DMPK
September 4-7, 2017
Zagreb, Croatia

PROGRAM
Organization of IAPC-6 Meeting is supported by

Ministry of Science and Education of the Republic of Croatia

PLIVA

Fidelta A Galápagos Company
Conference Program
Social events:
1. Welcome reception, Sunday, September 3, 20:00 Museum of Arts and Crafts
2. Zagreb sightseeing, Wednesday afternoon
3. Social dinner, Wednesday 20:00, Pivnica Medvedgrad, Ilica 49, Zagreb
4. Optional excursion to Plitvice lakes (lunch included), Thursday 7, 9:00 – 18:00*

Welcome reception, Zagreb sightseeing and Social dinner are free of charge for conference participants.
*The charge of 50 EUR is required for the excursion to the Plitvice lakes.

Important notice: It is required that participants confirm the participation at above events. They can do that at the conference desk no later than Monday 14:00. The organizer cannot guarantee the place at the particular event for late registrations.

Publications:
- the selected conference contributions will be published in Pharmaceutical Research (Springer)
- all participants are invited to contribute to the special issue of ADMET and DMPK which will be published in September and December.

Posters
Participants are strongly encouraged to mount their posters either on Sunday afternoon or on Monday between 8-9 am. Available dimensions of the poster boards are 200 (H) × 80 (W) cm. Poster dismounting should be no later than Wednesday 12:00. Posters left on the boards after the deadline will be removed by the Organizer.

Guidebook mobile application for IAPC-6
The hardcopy of the Book of abstracts will not be published and distributed among participants. Rather participants are encouraged to install and open a Guidebook IAPC-6 Meeting application on their smartphones. They can do that by clicking the link https://guidebook.com/g/iapc6/ on the smartphone. If the link is used from the desktop or laptop computer the application will ask for your mobile phone number for sending the corresponding link.

The application is responsive and it will recognize whether the smartphone is Apple or Android and it will direct the user directly to the corresponding application store from where user should install and open the Guidebook application (registration is required). Once the Guidebook installation has finished the IAPC-6 meeting can be accessed by entering the passphrase: iapc6. The application is also available on Windows phones, desktops, laptops and tablets: https://guidebook.com/g/iapc6/, option Web

The application is easy to use. The menu can be accessed from the top left icon. From the menu, various options are available such as program, list of posters, book of abstracts etc.
Sunday, September 03rd
15:00 – 19.30  Participant registration, Hotel Westin, 17th floor
20:00 – Welcome party, Museum of Arts and Crafts, Trg maršala Tita 10

All sessions will be held in Opera hall, Hotel Westin, 17th floor

Monday, September 04th
08:00  Poster mounting,
09:00 – 09:15  Opening Ceremony

Drug development Session - Moderator: Biserka Cetina Čižmek
09:15 – 10:00  Christos Reppas, University of Athens, Greece
O 01  The environment in the lower intestine and its impact on drug absorption
10:00 – 10:45  Abu Serajuddin, St. John’s University, USA
O 02  Strategies for the development of liquid, semisolid and solid lipid-based drug delivery systems
10:45 – 11:00  Coffee break
11:00 – 11:40  Mario Jug, Anita Hafner, Jasmina Lovrić, Maja Lusina Kregar, Ivan Pepić, Željka Vanić, Biserka Cetina-Čižmek, Jelena Filipović-Grčić, University of Zagreb, Croatia
O 03  In vitro dissolution/release methods for novel mucosal drug delivery systems
11:40 – 12:10  Seval Korkmaz, Biruni University, Turkey
O 04  How to increase the success of bioequivalence studies in the generic drug industry?
12:10 – 12:35  Imre Dékány, Edit Csapóa, Hajnalka Szokolai, Ádám Juhásza, Ágota Deák, László Janovák, University of Szeged, Hungary
O 05  Design of colloidal drug delivery systems for controlled release of non-steroidal anti-inflammatory drugs
12:35 – 13:00  Marieta Duvnjak Romić, Drago Špoljarić, Biserka Cetina-Čižmek, Jelena Filipović-Grčić and Anita Hafner, PLIVA, Croatia
O 06  Spray-dried melatonin-NLC loaded chitosan microspheres: development, optimisation and physicochemical characterization
13:00 – 15:00  Lunch Time

Solid State Session - Moderator: Rolf Hilfiker
15:00 – 15:45  Wei Gao, Tonglei Li, Purdue University, USA
O 07  Exploring in vivo fate of drug nanocrystals
15:45 – 16:30  Elena Boldyreva, Novosibirsk State University, Russia
O 08  Drugs as materials: processing, structure, properties
16:30 – 16:45  Coffee break

Cocrystal Session - Moderator: Alex Avdeef
16:45 – 17:45  Nair Rodriguez-Hornedo, University of Michigan, USA
O 09  Cocrystal thermodynamic and kinetic properties: Mathematical relationships and insights
17:45 – 18:30  Rafel Prohens, University of Barcelona, Spain
O 10  Application of Surface Site Interaction Points calculation to cocrystal screening
18:30 – 19:15  Rolf Hilfiker, Solvias AG, Switzerland
O 12  Co-Crystals: The role of phase diagrams in optimizing experimental strategies

Short Break
20:15 – 21:00  Nikoletta Fotaki, University of Bath, UK
O 13  Dissolution of pharmaceutical cocrystals for oral administration
21:00 – 21:45  Abu Serajuddin, St. John’s University, USA
O 14  How feasible is it to form cocrystals by acid-base interaction?
21:45 – 22:30  Alex Avdeef, In-ADME Research, USA
O 15  Cocrystal dissolution-pH mechanistic models: aqueous boundary layer convection-diffusion-reaction in rotating disk/powder methods
22:30 –  Cocrystal session closing remarks

Tuesday, September 05th

PhysChem, Permeability and Instrumental Session I - Moderator: Martí Rosés
09:00 – 09:40  Klara Valko, Biomimeic chromatography, UK
O 16  How to optimize the physicochemical and biomimetic properties of putative drug molecules?
09:40 – 10:15  Shenaz Bunally, GSK, UK
O 17  Industrialisation of physicochemical measurements in early drug discovery
10:15 – 10:50  Marina Shalaeva, Pfizer, USA
O 18  Phys Chem tool box for drug design in Beyond rule of Five chemical space
10:50 – 11:05  Coffee break

PhysChem, Permeability and Instrumental Session II - Moderator: Kin Tam
11:05 – 11:50  Annette Bauer-Brandl, University of Southern Denmark, Denmark
O 19  A new approach for HT permeability screening based on a biomimetic barrier
11:50 – 12:35  Kiyohiko Sugano, Ritsumeikan University, Japan
O 20  A mechanistic intestinal cell permeation model
12:35 – 13:00  Mare Oja, Uko Maran, University of Tartu, Estonia
O 21  Measuring, modelling and predicting pH-profiles of membrane permeability
13:00 – 15:00  Lunch

PhysChem, Permeability and Instrumental Session III - Moderator: Kiyohiko Sugano
15:00 – 15:40  Martí Rosés, Elisabet Fuguet, Xavier Subirats, Susana Amézqueta, University of Barcelona, Spain
O 22  Surrogation of ADMET processes by chromatography and capillary electrophoresis
15:40 – 16:20  John Comer, Sirius Analytical Ltd, UK
O 23  Behaviour of ionisable drugs after precipitation from aqueous solution in response to pH change
16:20 – 16:40  Theodoros Avgerinos, Nikolaos Kantiranis, Kyriakos Kachrimanis, Ioannis Nikolakakis, Aristotle University of Thessaloniki, Greece
O 24  Mechanical properties of Venlafaxine HCl solid mini matrices prepared by hot-melt extrusion and hot or ambient compression and effect of plasticizer
16:40 – 17:00  Coffee break

PhysChem, Permeability and Instrumental Session IV Moderator: Klara Valko
17:00 – 17:40  M. Abrami, G. Chiarappa, R. Farra, G. Grassi, P. Marizza, M. Grassi, University of Trieste, Italy
O 25  Use of Low field NMR for the characterisation of gels and biological tissues
17:40 – 18:20  Gesa Schad, Shimadzu Europa GmbH, Germany
O 26  Automated LC and SFC method development for new APIs: The power of selectivity and the strength to choose
18:20 – 18:50  Olivera S. Marković, Jelena M. Konstantinović, 27 N. Cvijetić, Susana Amézqueta, Klara Valko, Clara Ráfoš, Natalija D. Polović, Bogdan A. Šolaja, Tatjana Ć. Verbić, University of Belgrade, Serbia
O 27  Measurements of plasma protein binding – variety of experimental techniques
19:00 – 23:00  Poster Session
**Wednesday, September 06th**

08:00  Poster dismounting

**ADMET and DMPK Session - Moderator: Tatjana Ž. Verbić**

09:00 – 09:45  **Godefridus J Peters**, Anne-Sophie Govaerts, Hans R Hendriks, *VU University Medical Center, The Netherlands*

The role of pharmacology in European cancer drug development

09:45 – 10:30  **Susanne Winiwarter**, *AstraZeneca R&D, Sweden*

In silico ADME in drug design – aiming at the decision-to-make

10:30 – 10:50  **Ana Bokulić**, Astrid Milić, Jasna Padovan, *Fidelta d.o.o. Croatia*

Automation of ADME in vitro binding assays using HTDialysis device on Tecan Freedom EVO

10:50 – 11:20  Coffee break

**Drug Discovery Session I - Moderator: Godefridus J Peters**

11:20 – 11:45  **Bin Li**, Peng Lyu, Rui Ma, Ravikiran Mahadevappa, Xinpeng Xi, **Hang Fai Kwok**, *University of Macau, Macau*

Venom-based peptide drug discovery: enhancing specificity in cancer treatment

11:45 – 12:10  **Shao-Lin Zhang**, Zheng Yang, **Kin Yip Tam**, *University of Macau, Macau*

4-Isopropyl-3-nitro-dichloroacetophenone (INDAP) targets pyruvate dehydrogenase kinase 1 and inhibits cancer cells proliferation

12:10  Conference closing

12:30  Lunch

16:30  Organized sightseeing of Zagreb

20:00  Conference dinner, Pivnica Medvedgrad, Ilica 49, Zagreb

**Thursday, September 07th**

09:00 – 18:00  Optional excursion to the Plitvice lakes national park
LIST OF POSTERS

ID | Title | Authors
--- | --- | ---
P1 | Simultaneous Lipolysis/Permeation in vitro Model for the Estimation of Bioavailability of Lipid Based Formulations | Hanady A. Bibi, René Holm, Annette Bauer-Brandl
P2 | Small Scale Biphasic Dissolution testing of Dipyriramole Suspension | Patrick J. O’Dwyer, John Comer, Robert Taylor, Karl J. Box
P3 | Estimation of the octanol-water distribution coefficient of acidic compounds by microemulsion electrokinetic chromatography measurements | Alejandro Fernández-Pumarega, Susana Amézqueta, Elisabet Fuguet, Martí Rosés
P4 | Physicochemical classification analysis of hERG inhibitor specificity | Remigijus Didziapetris, Kiril Lanevskij
P5 | Prediction of physico-chemical properties of illegal drugs using the conformational analysis | Vera Lukić, Ružica Mićić, Biljana Arsić, Anja Jokić, Dragana Sejmanović
P6 | pH-dependent solubility profile of desipramine hydrochloride | Olívia S. Marković, Miloš P. Pešić, Tatjana Ž. Verbić, Alex Avdeef
P7 | Protolytic equilibria of rupatadine in micellar solutions of differently charged surfactants | Marija Popović Nikolić, Gordana Popović, Danica Agaba
P8 | Protolytic equilibria and stability of a pair of novel pentaaza macrocyclic chelators | Dragana D. Stoijkov, Rabindra Nath Pradhan, Goran Angelovski, Carlos Platas-Iglesias, Akhilesh Kumar Singh, Tatjana Ž. Verbić
P9 | Solid Forms Screening of Fentanyl Citrate | Rafael Barbosa, Mercé Font-Bardia, Susana Portillo, Antoni Caparrós, Rafel Prohens
P10 | Solid dispersions as expanded multicomponent systems | Lucie Gruberová, Bohumil Kratochvíl, Ežen Šárka
P11 | Quantification of residual amorphous content, by Dynamic Vapor Sorption, in predominantly crystalline drugs | Luís A. Sousa, Ana F. Santos
P12 | New cocrystals of beaxotene with pyridinecarboxamide isomers sustained by the acid–aromatic nitrogen supramolecular heterosynth | Ricardo A. E. Castro, Ana M. Cortesão, Teresa M. R. Maria, M. Ramos Silva, F. Emmerling, João Canotilho, M. Ermelinda S. Eusébio
P13 | Obtaining of cocrystals of meloxicam with carboxylic acids. Study of their structure and properties | Kseniya A. Cherkashina, Sergei G. Arkhipov, Christian Tantardini and Elena V. Boldyreva
P14 | Behaviour of the new API-API Co-Crystal of Tramadol Hydrochloride-Celecoxib (ctc) in preclinical formulation solvents | Adriana Port, Carme Almansa, José Miguel Vela, Carlos R. Plata-Salamán
P15 | Dissolution rate of cocrystals: effect of pH | Clara Ráfols, Hanan Fael, Elisabet Fuguet, Brigitte Outhwaite, Rebeca Ruiz
P16 | 3D QSAR and target fishing docking studies of novel aryldiketo acids with promising antibacterial activity toward MDR strains | Iljia N. Cvijetić, Tatjana Ž. Verbić, Pedro Ernesto de Resende, Paul Stapleton, Simon Gibbons, Mire Zloh
P17 | Lysosomal Accumulation of tyrosine kinase inhibitors in relation to molecular physico-chemical parameters | Richard J Honeywell, Letje Kathman, Gerrit Jansen, Klara Valko, Gedefridus J Peters
P18 | ADME-Tox profiling of some water soluble chitosan derivatives used to obtain nanomaterials | Adriana Isovran, Alexu Ciorsac, Vasile Ostafe
P19 | Computational assessment of pharmacokinetics and biological effects of some anabolic and androgen steroids | Marín Roman, Diana Lorisa Roman, Alexu Ciorsac, Vasile Ostafe, Adriana Isovran
P20 | Enterovirus Inhibitory Activity of substituted Urea and Thiourea derivatives of p-Benzene sulfonamide | Prashant S. Chakrasi, Min Jeong Kim, Jin Soo Shin, Soo Bong Han, and Young-Sik Jung
P21 | The relationship between the antioxidant and hepatoprotective activity of oil of Thymus mugodzharicus | A. Kazbekova, G. Atazhanova, Sh. Madieva, S. Adekenov, G. Tuleshova
P22 | Biogenic synthesis of silver nanoparticles from labisia pumila and its antioxidant efficacy | Nageswari Ramesh, Lakshmi Sammugam, Ravikiran Mahadevappo, Pasupuleti Visweswara Rao, Hang Fai Kwok
P23 | Liver protective effects of KGSP in ethanol-induced liver damage model | Ji-Hyun Lee, Sarmila-Nepali, Hyeon-Hui Ki, Young-Mi Lee, Dae-Ki Kim
P24 | Inhibitory effect of Euphorbia supina extract and its fractions on tyrosinase activity and melanin formation in B16F10 melanoma cells | Hoon-Yeon Lee, Sa-Haeng Kang, Bo-Ram Kim, Sung-Woo Hwang, Min Park, Bo-Ri Lee, Sang-Min Shin, Su-Jeong Kim, Hee-Yeon Kim, Dae-Ki Kim, Young-Mi Lee
P25 | Evaluation of the interactions between some drugs and human serum albumin (HSA) using fluorescence | Susana Amézqueta, Anna M Bolioli, José Luis Beltrán, Clara Ráfols
P27 | Estimation of skin permeation by chromatography | Sara Soriano-Meseguer, Elisabet Fuguet, Adriana Port, Martí Rosés
P28 | Estimation of biological properties of pharmaceutical interest using lecithin preparations as pseudostationary phases for capillary electrophoresis or liquid chromatography | Elisabet Fuguet, Susana Amézqueta, Sandra Farré, Daniel Luno, Alejandro Fernández-Pumarega, Martí Rosés
P29 | Vibrational spectroscopy coupled with chemometrics used in monitoring reaction for pharmaceutical and chemical industries | Dardan Hetemi
<table>
<thead>
<tr>
<th>ID</th>
<th>Title</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>P 30</td>
<td>ACD/Portal technology – bringing ACD/Percepta capabilities to a new level</td>
<td>Remigijus Didziapetris, Kiril Lanevskij</td>
</tr>
<tr>
<td>P 31</td>
<td>Confocal Micro Raman Spectroscopy approach to characterize content uniformity in pharmaceutical development</td>
<td>Elisa Melian, Beatriz Munguia, Santiago Palma, Ricardo Faccio, Laura Domínguez</td>
</tr>
<tr>
<td>P 32</td>
<td>Revisiting blood-brain barrier: a chromatographic approach</td>
<td>Xavier Subirats, Laura Muñoz-Pascual, Michael H. Abraham, Marti Rosés</td>
</tr>
<tr>
<td>P 33</td>
<td>New derivatization approach for TLC/MALDI-TOF mass spectrometry analysis of mixtures of sterols and steroids</td>
<td>Cesar Esparza, Roman Borisov, Nikolai Polovkov, Vladimir Zaikin</td>
</tr>
<tr>
<td>P 34</td>
<td>Fixed-charge derivatization of carbonyl compounds for their analysis by MALDI mass spectrometry</td>
<td>Dmitri. I. Zhiyaev, Roman. S. Borisov</td>
</tr>
<tr>
<td>P 35</td>
<td>LC-MS/MS assessment of metabolic switch in cancer cell after treatment with PDK1 inhibitors</td>
<td>Wen Zhang, Xiaohui Hu, Wei Zhou, Kin Yip Tam</td>
</tr>
<tr>
<td>P 36</td>
<td>2D inkjet printing of nanoparticles for microarray testing</td>
<td>Jonathan C. Burley, Vincenzo Taresco, Martin Garnett, et al.</td>
</tr>
<tr>
<td>P 37</td>
<td>Prolonged release system with paliperidone: micro-NIR real-time preparation process monitoring</td>
<td>Sonia Iurian, Bianca Sylvester, Ioan Tomuta</td>
</tr>
<tr>
<td>P 38</td>
<td>Exploitation of griseofulvin chloroform solvate incorporated inside polymeric matrix to improve aqueous solubility</td>
<td>Hamid Al-Obaidi, Zheng Li, Radoslaw M. Kowalczyk, Miridul Majumder, Elaine Loon</td>
</tr>
<tr>
<td>P 40</td>
<td>Mucoadhesive microspheres for vaginal administration of Cefixime: development and evaluation</td>
<td>Maestrelli F., Jug M., Kovalce I., Cirri M., Mura P.</td>
</tr>
<tr>
<td>P 41</td>
<td>Nanostructured lipid carriers (NLC) as a new drug delivery system for potential hydrochlorothiazide oral administration in the paediatric therapy</td>
<td>Maria Cirri, Francesca Maestrelli, Paola Mura, Carla Ghelardini, Lorenzo Di Cesare Mannelli</td>
</tr>
<tr>
<td>P 42</td>
<td>pH and temperature dependent release of diclofenac from wound dressing material</td>
<td>Tina Mauer, Uroš Mauer, Karin Stana Kleinschek, Dragica Maja Smrke</td>
</tr>
<tr>
<td>P 43</td>
<td>Benzocaine and pH sensitive dye in electrosprunen nanofibers for painless wound care and fast detection of wound infection</td>
<td>Manja Kurečić, Tina Mauer, Alenka Ojstršek, Uroš Mauer, Lidija Gadišnik, Silvo Hribnernik, Karin Stana Kleinschek</td>
</tr>
<tr>
<td>P 44</td>
<td>Liposomal co-encapsulation of DOX and CURC: a nanotechnological approach to increase antitumor activity against colon cancer</td>
<td>Tefas Lucia, Sersarman Alina, Sylvester Bianco, Porav Sebastian, Licarette Emilia, Rauca Valentin, Luput Lavinia, Patras Laura, Banciu Manuela, Porfire Alina</td>
</tr>
<tr>
<td>P 45</td>
<td>CANCELLED</td>
<td>Redong Song, Yanguo Lu, Xiangqin Li, Yingchao Liu, Yweli Wang, Tianqing Liu</td>
</tr>
<tr>
<td>P 46</td>
<td>CANCELLED</td>
<td>Susana S. Pinto, Luis A. Sousa</td>
</tr>
<tr>
<td>P 47</td>
<td>Anti-carcinogenic capacity of microcapsules loaded with NaF through coaxial ultrasonic atomizer</td>
<td>Suk-Young Kim, Hae-Won Choi, Sang-Hoon Rhee</td>
</tr>
<tr>
<td>P 48</td>
<td>Evaluation by PXRD and vibrational spectroscopy of spironolactone solid dispersions prepared by co-spray drying with polymers</td>
<td>Nizar Al-Zoubi, Fatem Odah, Wafsy Obeidat, Ahmad Al-Jaberi, Ioannis Partheniadis, Ioannis Nikolakakis</td>
</tr>
<tr>
<td>P 50</td>
<td>Anti-inflammatory activity of TAs associated with activation of suppressor of cytokine signaling 1 in human HaCaT keratinocyte cells</td>
<td>Hyeon-Hui Ki, Sarmila Nepali, Ji-Hyun Lee, Dae-Ki Kim, Young-Mi Lee</td>
</tr>
<tr>
<td>P 51</td>
<td>The role of protein tyrosine phosphatases in hepatocellular carcinoma</td>
<td>Qingshui Wang, Yide Huang, Yafei Zhang, Yao Lin and Hang Fai Kwok</td>
</tr>
<tr>
<td>P 52</td>
<td>Anti-neuroinflammatory effects of SLOH in Aβ-induced BV-2 microglial cells and 3xTg-2td mice involve the inhibition of GSK-3β</td>
<td>Xiaoli Wu, Jayasankar Kosaraju, Kin Yip Tam</td>
</tr>
<tr>
<td>P 53</td>
<td>Neuroprotective effect of linaglaptin in 1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine induced mouse model of Parkinson’s disease</td>
<td>Jayasankar Kosaraju, Kin Yip Tam</td>
</tr>
<tr>
<td>P 54</td>
<td>Identification of Novel M1 — Selective Muscarinic Receptor Modulator Using Virtual Screening</td>
<td>Harapriya Chakravarty, Kin Yip Tam</td>
</tr>
<tr>
<td>P 55</td>
<td>Value of intermediates in drug design — example of novel L-ascorbic acid derivatives</td>
<td>Všnja Stepanić, Andrijana Mešić, Anja Harej, Sandra Kraljević-Pavelić, Silvana Raic-Malić</td>
</tr>
<tr>
<td>P 56</td>
<td>Synthesis, structure, antibacterial and anticancer activity of new macrolide antibiotics analogs</td>
<td>Anna Janas, Krystian Pyta, Katarzyna Pyta-Klich, Joanna Domagalska, Piotr Przybylski</td>
</tr>
<tr>
<td>P 57</td>
<td>The influence of the plant food fibers and MILKYBOOM-PLUS on the children’s reactivity of nursery schools from 3 till 6 years old</td>
<td>A. A. Abdulayeva, G. T. Tuleshova</td>
</tr>
<tr>
<td>P 58</td>
<td>Rapid biomimetic screening of drug-membrane affinity using IAM HPLC</td>
<td>Klara Vaiko, Scott Anderson</td>
</tr>
</tbody>
</table>
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All participants are invited to contribute to the special issue of ADMET and DMPK which will be published in September and December.
http://pub.iapchem.org/admet