

JOINT MEETING ON MEDICINAL CHEMISTRY Prague, June 27–30, 2019

FINAL PROGRAMME







FACULTY OF PHARMACY IN HRADEC KRÁLOVÉ Charles University





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Good to Know



WELCOME MESSAGE

Dear colleagues, JMMC-2019 participants,

Welcome to the 11th Joint Meeting on Medicinal Chemistry 2019 organized by the Faculty of Pharmacy, Charles University on occasion of its 50th anniversary, under the auspices of the European Federation for Medicinal Chemistry in June 27-30, 2019 in Prague, the heart of Europe and the capital of the Czech Republic.

In 2019, it will be 20 years of history of this traditional Joint Meetings, founded in 1999 by Prof. G. Ronsivalle (Italy) together with Prof. A. Lipkowski (Poland) and Prof. G. Toth (Hungary). On behalf of National Chemical Societies of Italy, Poland and Hungary, Prof G. Ronsivalle together with Prof. Z. Chilmonczyk (Poland) and Prof. P. Matyus (Hungary) organized the first meeting in Taormina in 1999, particularly to promote Medicinal Chemistry, attract young scientists and foster relationships between medicinal chemists of the participating countries. After Taormina, JMMC was held in Budapest 2001, Krakow 2003, Vienna 2005, Portorož 2007, Budapest 2009, Catania 2011, Lublin 2013, Athens 2015 and Dubrovnik 2017, Since the first meeting, number of participating countries has increased to nine - Austria, Croatia, Czech Republic, Greece, Hungary, Italy, Poland, Slovakia and Slovenia. The success of the last 10th JMMC 2017 (249 participants from 28 countries) illustrates an interest in this kind of meetings. We are pleased to invite medicinal chemists from all over the world, not only the participating countries, to come, stimulate discussion in drug discovery and development and to promote collaboration between medicinal chemistry scientists, both young and experienced.

The Organizing Committee wishes you a memorable stay in Prague, filled with new experience and fruitful personal contacts. Enjoy the 11th JMMC.

Jamila Timora Mali Dolial

Prof. RNDr. Jarmila Vinšová, Ph.D. Conaress President

Prof. PharmDr. Martin Doležal, Ph.D. President of the Czech Pharmaceutical Society



CONGRESS COMMITTEE

National Organizing Committee

Jarmila Vinšová Martin Doležal Radim Nencka Martin Krátký Jan Zitko Marta Kučerová-Chlupáčová

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Dariusz Matosiuk (Medical University of Lublin, Lublin, Poland)
Danijel Kikelj (University of Ljubljana, Ljubljana, Slovenia)
Emmanuel Mikros (National and Kapodistrian University of Athens, Athens, Greece)
Andrej Boháč (Comenius University in Bratislava, Bratislava, Slovakia)

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CONGRESS ORGANIZERS

Czech Pharmaceutical Society



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EFMC European Federation for Medicinal Chemistry

Faculty of Pharmacy in Hradec Kralove



FACULTY OF PHARMACY IN HRADEC KRÁLOVÉ Charles University

Charles University





PROGRAMME

THURSDAY, JUNE 27, 2019

13:00–19:00		Registration
15:00–15:30		Opening of the Meeting
15:30–16:15	PL-1	Moderator: Dr. Radim Nencka Prof. Michal Hocek: Substituted or hetero-fused 7-deazapurine nucleoside cytostatics with complex mechanism of action
16:15–16:45	KL-1	Assoc. Prof. Izidor Sosič : Development of non-peptidic and subunit-selective inhibitors of immunoproteasome
16:45–17:30	PL-2	Prof. Jakub Fichna : Challenges in design of novel treatment options in inflammatory bowel diseases employing gold and silver
17:30–18:00	KL-2	Dr. Zlatko Janeba : Development of polysubstituted pyrimidines as potent inhibitors of prostaglandin E_2 production
18:00–19:30		Welcome Cocktail



FRIDAY, JUNE 28, 2019

Moderator: Prof. Sanja Tomič

- **09:00–09:45** PL-3 Prof. **Szilvia Bősze**: Cargo-dependent mode of drug uptake with improved efficacy and bioavailability: the design and evaluation of target cell selective transporters and drug-conjugates
- 09:45–10:15 KL-3 Dr. Theodora Calogeropoulou: Constrained miltefosine derivatives. The journey towards NMT-A2, a new drug lead for visceral leishmaniasis
- 10:15–10:45 Coffee break

Moderator: Prof. Szilvia Bősze

- **10:45–11:30** PL-4 Assoc. Prof. **Janez Ilaš**: Inhibitors of topoisomerases: from antibacterial to anticancer agents
- **11:30–12:00** KL-4 Dr. **Zsuzsa Baranyai**: Synthesis and *in vitro* biological evaluation of drug-peptide conjugates against glioblastoma
- **12:00–12:30** KL-5 Assoc. Prof. **Angeliki Kourounakis**: Morpholine: A privileged scaffold for the development of multi-target bioactive molecules
- 12:30–13:45 Lunch
- 13:45–15:00 Poster Session I (odd numbers)

Moderator: Prof. Gabriele Costantino

- 15:00–15:45 PL-5 Prof. Sanja Tomić: The Role(s) of Dipeptidyl Peptidase III in Humans
- **15:45–16:15** KL-6 Prof. **Michael Schnürch**: Leoligin-inspired Synthetic Lignans with Selectivity for Cell-type and Bioactivity, Relevant for Cardiovascular Disease
- 16:15–16:45 Coffee break



Moderator: Assoc. Prof. Janez Ilaš

- **16:45–17:30** PL-6 Prof. **Gabriele Costantino**: Chasing target essentiality in the search for new antibacterials
- 17:30–18:00 KL-7 Assoc. Prof. Martina Hrast: Covalent warheads as new MurA inhibitors
- **18:00–18:20** L-1 **Miriam Girardini**: Characterizing a new series of efflux-pumps inhibitors as potential anti-tubercular adjuvants
- **18:20–18:40** L-2 Prof. **Barbara Nawrot**: Nanostructured conjugates of DNA oligonucleotides and boron clusters as potential dual-action anti-EGFR therapeutic nucleic acids

19:30–22:30 Congress dinner



SATURDAY, JUNE 29, 2019

08:30–09:30 09:30–10:00	KL-8	Moderator: Prof. Michal Hocek Invited lecture Dr. Tomas Cihlar : Discovery and Development of Antiviral Therapeutics for Emerging and Neglected Viral Infections Dr. Jose Miguel Ferreira de Oliveira : Regulation of cyclin and cyclin-dependent kinase expression by 3',4'-dihydroxyflavonol in human <i>in vitro</i> models
10:00–10:30		Coffee break
11:15–11:45	KL-9	Moderator: Prof. Danijel Kikelj Assoc. Prof. Manolis Fousteris: New artemisinin hybrid molecules with antileukemic and antimalarial activities Assoc. Prof. Zrinka Rajić : Harmicines as novel antiplasmodial leads
11:45–12:15	KL-10	Prof. Tibor Kurtan: Bioactive benzene-condensed heterocycles
12:15–13:15		Lunch
13:15–14:30		Poster session II (even numbers)
14:30–15:15	PL-8	Moderator: Assoc. Prof. Vittorio Pace Prof. Yoel Rodríguez: <i>In silico</i> Design of Chemical Modulators for Chromatin Biology
15:15–15:45	KL-11	Dr. Lars Richter: Time is running – Large scale matched molecular pair analysis to domesticate binding kinetics
15:45–16:15	L-3	Dr. David Peralta : Why Was My Paper Rejected? Tips from an Editor on How to Get Published
16:15–16:35		Coffee break
		Moderator: Prof. Yoel Rodríguez
16:35–17:20	PL-9	Assoc. Prof. Vittorio Pace : Building-up molecular complexity with carbenoids: New vistas in homologation chemistry
17:20–17:50 17:50–18:10	KL-12 L-4	Dr. Magdaléna Májeková : Targeting SERCA through drug design Assoc. Prof. Diego Muñoz-Torrero : A novel class of chroman-based multitarget anti-Alzheimer hybrids: design, synthesis, <i>in vitro</i> profiling and <i>in vivo</i> proof-of-concept



SUNDAY, JUNE 30, 2019

Moderator: Prof. Martin Doležal

09:00-09:30	KL-13	Dr. Ana Amić : Anthraquinones as potential free radical scavengers and P-glycoprotein inhibitors
09:30-10:00	KL-14	Dr. Lucia Kováčiková : Isosteric replacement brought markedly improved selectivity of aldose reductase inhibitors
10:00–10:30	KL-15	Dr. Jan Zitko : Structural modifications of pyrazinamide – rational design towards new potential anti-microbial compounds
10:30–10:50	L-5	Dr. Muhammed İhsan Han : Design, synthesis and biological activity evaluation of aryl-sulfonylthiosemicarbazides as antiproliferative agents and COX-2 inhibitors
10:50–11:20		Coffee break
		Moderator: Dr. Jan Zitko
11:20–11:50	KL-16	Prof. Agostino Marrazzo : From haloperidol to new selective sigma receptor ligands
11:50–12:20	KL-17	Dr. Anna Wieckowska: Serotonin 5HT-6 receptor antagonists and cholinesterase inhibitors with $A\beta$ antiaggregation properties in the development of multifunctional ligands against Alzheimer's disease
12:20-12:40	L-6	Belgin Sever : New pyrazoline derivatives clubbed with thiazole scaffold as anticancer agents targeting EGFR
12:40-13:00	L-7	Dr. Constantin Tanase : New carbocyclic nucleoside analogues with an optically active substituted bicyclo[2.2.1]heptane fragment as a glycoside moiety linked to the base by a methylene group
13:00–13:30		Winning Posters Flash presentations
13:30–14:00		Closing



SPEAKERS

Invited Lecture

Discovery and Development of Antiviral Therapeutics for Emerging and Neglected Viral Infections



Dr. Tomas Cihlar

Vice President of Virology at Gilead Sciences, San Francisco Bay Area, USA

Plenary Lecture Cargo-dependent mode of drug uptake with improved efficacy and bioavailability: the design and evaluation of target cell selective transporters and drug-conjugates



Prof. Szilvia Bősze MTA-ELTE Research Group of Peptide Chemistry, Eötvös Loránd University, Budapest, Hungary

Plenary Lecture Chasing target essentiality in the search for new antibacterials



Prof. Gabriele Costantino *Professor of Medicinal Chemistry and Director of Department of Food and Drugs, University of Parma, Parma, Italy*



Plenary Lecture Challenges in design of novel treatment options in inflammatory bowel diseases employing gold and silver



Prof. Jakub Fichna *Medical University Lodz, Lodz, Poland*

Plenary Lecture New artemisinin hybrid molecules with antileukemic and antimalarial activities



Assoc. Prof. Manolis Fousteris Assistant Professor in Medicinal Chemistry, Department of Pharmacy, University of Patras, Patras, Greece

Plenary Lecture Substituted or hetero-fused 7-deazapurine nucleoside cytostatics with complex mechanism of action



Prof. Michal Hocek

Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Prague, Czech Republic

Plenary Lecture Inhibitors of topoisomerases: from antibacterial to anticancer agents



Assoc. Prof. Janez Ilaš Faculty of Pharmacy, University of Ljubljana, Ljubljana, Slovenia



Plenary Lecture Building-up molecular complexity with carbenoids: new vistas in homologation chemistry



Assoc. Prof. Vittorio Pace Department of Pharmaceutical Chemistry, University of Vienna, Vienna, Austria

Plenary Lecture In silico Design of Chemical Modulators for Chromatin Biology



Prof. Yoel Rodríguez Department of Natural Sciences, Hostos Community College of CUNY, New York, USA

Plenary Lecture The Role(s) of Dipeptidyl Peptidase III in Humans



Prof. Sanja Tomić

Head of Laboratory for Protein Biochemistry and Molecular Modelling, Ruđer Bošković Institute, Zagreb, Croatia



KEYNOTE SPEAKERS

Austria

Dr. Lars Richter University of Vienna TIME IS RUNNING – LARGE SCALE MATCHED MOLECULAR PAIR ANALYSIS TO DOMESTICATE BINDING KINETICS

Prof. Michael Schnürch Institute of Applied Synthetic Chemistry, Vienna University of Technology LEOLIGIN-INSPIRED SYNTHETIC LIGNANS WITH SELECTIVITY FOR CELL-TYPE AND BIOACTIVITY, RELEVANT FOR CARDIOVASCULAR DISEASE

Croatia

Dr. Ana Amić Josip Juraj Strossmayer University of Osijek ANTHRAQUINONES AS POTENTIAL FREE RADICAL SCAVENGERS AND P-GLYCOPROTEIN INHIBITORS

Assoc. Prof. **Zrinka Rajić** Faculty of Pharmacy and Biochemistry, University of Zagreb **HARMICINES AS NOVEL ANTIPLASMODIAL LEADS**

Czech Republic

Dr. Zlatko Janeba Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences DEVELOPMENT OF POLYSUBSTITUTED PYRIMIDINES AS POTENT INHIBITORS OF PROSTAGLANDIN E2 PRODUCTION

Dr. Jan Zitko Faculty of Pharmacy in Hradec Králové, Charles University STRUCTURAL MODIFICATIONS OF PYRAZINAMIDE – RATIONAL DESIGN TOWARDS NEW POTENTIAL ANTI-MICROBIAL COMPOUNDS

Greece

Dr. Theodora Calogeropoulou Institute of Biology, Medicinal Chemistry and Biotechnology National Hellenic Research Foundation CONSTRAINED MILTEFOSINE DERIVATIVES. THE JOURNEY TOWARDS NMT-A2, A NEW DRUG LEAD FOR VISCERAL LEISHMANIASIS



Assoc. Prof. Angeliki Kourounakis University of Athens MORPHOLINE: A PRIVILEGED SCAFFOLD FOR THE DEVELOPMENT OF MULTI-TARGET BIOACTIVE MOLECULES

Hungary

Dr. Zsuzsa Baranyai MTA-ELTE Research Group of Peptide Chemistry SYNTHESIS AND IN VITRO BIOLOGICAL EVALUATION OF DRUG-PEPTIDE CONJUGATES AGAINST GLIOBLASTOMA

Prof. Tibor Kurtan University Debrecen BIOACTIVE BENZENE-CONDENSED HETEROCYCLES

Italy

Prof. Agostino Marrazzo University of Catania FROM HALOPERIDOL TO NEW SELECTIVE SIGMA RECEPTOR LIGANDS

Poland

Dr. Anna Wieckowska Faculty of Pharmacy, Jagiellonian University Medical College SEROTONIN 5-HT6 RECEPTOR ANTAGONISTS AND CHOLINESTERASE INHIBITORS WITH Aβ ANTIAGGREGATION PROPERTIES IN THE DEVELOPMENT OF MULTIFUNCTIONAL LIGANDS AGAINST ALZHEIMER'S DISEASE

Portugal

Dr. Jose Miguel Ferreira de Oliveira LAQV, REQUIMTE, Laboratory of Applied Chemistry, Faculty of Pharmacy, University of Porto REGULATION OF CYCLIN AND CYCLIN-DEPENDENT KINASE EXPRESSION BY 3',4'-DIHYDROXYFLAVONOL IN HUMAN *IN VITRO* MODELS

Slovakia

Dr. Lucia Kováčiková Institute of Experimental Pharmacology & Toxicology Slovak Academy of Sciences ISOSTERIC REPLACEMENT BROUGHT MARKEDLY IMPROVED SELECTIVITY OF ALDOSE REDUCTASE INHIBITORS



Dr. **Magdaléna Májeková** Institute of Experimental Pharmacology & Toxicology Slovak Academy of Sciences **TARGETING SERCA THROUGH DRUG DESIGN**

Slovenia

Assoc. Prof. Martina Hrast Faculty of Pharmacy, University of Ljubljana COVALENT WARHEADS AS NEW MURA INHIBITORS

Assoc. Prof. **Izidor Sosič** Faculty of Pharmacy, University of Ljubljana DEVELOPMENT OF NON-PEPTIDIC AND SUBUNIT-SELECTIVE INHIBITORS OF IMMUNOPROTEASOME



INSTRUCTIONS FOR SPEAKERS

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During your lecture, you will be using the Remote Control to facilitate the progress of your presentation. All speakers are kindly requested to keep to the allocated time for their presentation.

All presentation will be deleted from all the PC used during the congress.

ABSTRACT BOOK

Abstract book in digital format can be downloaded from: <u>https://www.jmmc2019.cz/book-of-abstracts/</u>





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P-02: DEVELOPMENT OF NOVEL H2S-DONOR SIGMA RECEPTOR HYBRIDS FOR THE MANAGEMENT OF PAIN

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Welcome Cocktail - DiJazzTiva concert

Date: June 27, 2019 Time: 18:00–19:30 Venue: Pyramida hotel Price: included in the registration fee Price for accompanying person: 25 EUR

Congress Dinner

Date: June 28, 2019 Time: 19:30–22:30 Venue & Address: The Great Monastery Restaurant (Velká klášterní restaurace), Strahovské nádvoří 302, Prague 1



Meeting point: 19:20 at reception of Pyramida hotel, distance approximately 10 minutes by walk **Price:** 45 EUR per person

The Congress Dinner will be held at the Great Monastery Restaurant, located in the premises of the Premonstratensian Strahov Monastery, just a few steps from the Prague Castle.

Premonstratensian monastery at Strahov was founded in 1140 by the Bishop of Olomouc, Jindřich Zdík, with the support of the Czech Prince, and later king Vladislav II. A huge complex standing at the outset of the Royal Way offers pleasant dining in the historical Great Monastery Restaurant.

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Date: June 27 or June 30, 2019 Departures: 11:15 am Duration: 3,5 hours Price: Adults 27,20 EUR; students 24 EUR

T9 – Český Krumlov – UNESCO



Date: June 27 or June 30, 2019 Departures: 8:45 am Duration: approx. 11 hours Price: Adults 83,60 EUR; students 83,60 EUR

T10 – Karlovy Vary and Moser Factory



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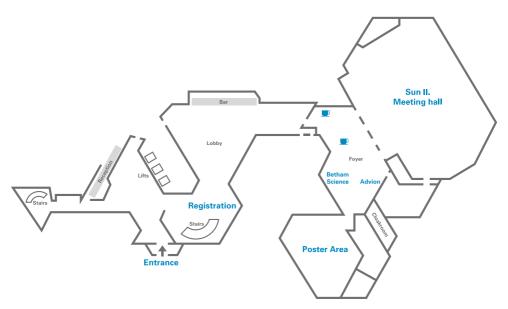
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13:00–19:30	08:30–19:00	08:00–18:30	08:30–14:00

Exhibition dismantle

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Free Wi-Fi connection is at disposal in all the Congress meeting rooms and foyer area.

Network: Pyramida No password is required.

Certificate of Attendance

Certificate of attendance will be sent via e-mail in pdf form upon request.





GOOD TO KNOW

Climate

The climate is a mixture of ocean and continental influences. The month of June is characterized by gradually rising daily temperatures, with daily highs increasing from 20 °C to 22 °C over the course of the month, exceeding 28 °C. The average probability that some form of precipitation will be observed in a given day is 60 %, with little variation over the course of the month. Throughout June, the most common forms of precipitation are moderate rain, thunderstorms, and light rain.

You can find the current weather at <u>www.weather.com</u>.

Currency and Banking

Czech Crowns are the official currency in the Czech Republic. Foreign currency exchange is available at Václav Havel Airport Prague and at most hotels, banks and exchange offices throughout the city. International credit cards are accepted for payment in hotels, restaurants and shops. Paying by cash in Euro is also possible in some restaurants and shops.

For the official exchange rates on the website of the <u>www.cnb.cz</u>.

Important Telephone Numbers

112: General Emergency for Europe150: Fire155: Ambulance156: Prague Police158: Police

Liability and Insurance

The organisers do not accept responsibility for individual medical, travel or personal insurance.

All participants are strongly advised to take out their own personal insurance before travelling to the Congress.

Programme Changes

The organisers cannot assume liability for any changes in the programme due to external or unforeseen circumstances.

Official Language

The official language of the Conference is English.



Notes		
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JOINT MEETING ON MEDICINAL CHEMISTRY Prague, June 27–30, 2019

www.jmmc2019.cz