

**XV ITALIAN-HUNGARIAN SYMPOSIUM ON SPECTROCHEMISTRY
PHARMACOLOGICAL RESEARCH AND ANALYTICAL APPROACHES**

PISA, 12 – 16 JUNE, 2016

PROGRAMME

Sunday, 12 June, 2016

19.00 Welcome reception

Monday, 13 June, 2016

8.00 Registration of participants

9.00 *Opening ceremony of the Symposium and welcome address*

Massimo Mario Augello (Chancellor, UNIPi, Pisa), Sergio Caroli (SSFA, Milan), Roger Fuoco (UNIPi, Pisa), Loredana Musmeci (ISS, Roma), Marco Romano (SSFA, Milan), Beáta Sperlágh (MFT, Budapest), Gyula Záray (ELTE, Budapest)

Oral session 1

New trends in pharmacological research

Chairpersons: Marco Romano (SSFA, Milan), Beáta Sperlágh (MFT, Budapest)

09.30 Key-note lecture 1

Pierluigi Navarra (Catholic University, Rome), The process of drug discovery and the Yin/Yang of small-molecule/biotech option

10.00 Key-note lecture 2

György Keserű (MTA, Budapest), Finding the sweet spot: the role of nature and nurture in medicinal chemistry

10.30 General discussion

11.00 Coffee break

11.30 Beáta Sperlágh (MFT, Budapest), Translation of genetic findings to animal models: a gateway to find new therapies for psychiatric disorders

11.50 Giacomo Pozzoli (Catholic University, Rome), New advances in cancer therapy

12.10 Péter Ferdinandy (Semmelweis University, Budapest), Why do we still not have cardioprotective drugs? Need for unbiased “omics” approach and co-morbidity models to find valid targets

12.30 Laura Calzà, Vito Antonio Baldassarro, Alessandra Marchesini, Luisa Stella Dolci, Luciana Giardino (University of Bologna), To increase soundness of *in vitro* pharmacological preclinical research: focus on the appropriate cellular system, high-content analysis and regulatory considerations

12.50 Diego La Mendola (University of Pisa), Maria Letizia Trincavelli, Chiara Giacomelli, Orjan Hansson, Cristina Satriano, Enrico Rizzarelli, Claudia Martini, The interplay of copper ions and the protein angiogenin as new target in cancer therapy

13.10 Lunch break

Oral session 2

The legal framework

Chairpersons: Antonella Di Gioia (Chiesi Farmaceutici, Parma), Viktor G. Mihucz (ELTE, Budapest)

14.30 Key-note lecture 3

Marco Romano (Società di Scienze Farmacologiche Applicate, Milan), The Italian Society for Applied Pharmacological Science (SSFA): its main goals, activities, working groups and cooperation

14.50 Key-note lecture 4

Umberto Filibeck (Tor Vergata University, Rome), Eleonora Sanzi, GCP and quality in Regulation (EU) No. 536/2014 on clinical trials on medicinal products for human use

15.20 Andrew Gray (MHRA, London), Challenges and opportunities associated with the application of a single international standard to non-clinical safety studies

15.50 Vittorio Tarditi (JRC, Ispra), Meeting multiple needs with a quality management system: a challenge for an evolving scientific organisation

16.10 Péter Arányi (Medical Research Council of Hungary, Budapest), Ethical aspects of drug development

16.30 Isabella Andreini (RTC, Pomezia, Rome), Modern challenges of preclinical regulatory safety assessment

16.50 Mario Carere (ISS, Rome), Robert Kase, Estrogen and EDC monitoring towards regulatory options for water quality management

17.10 Sergio Caroli (SSFA, Milan), Paola Bottoni, Residues and metabolites of pharmaceutical products in food commodities

17.30 General discussion

17.40 Closure of day 1

Tuesday, 14 June, 2016

Oral session 3

Advances in analytical techniques

Chairpersons: Roger Fuoco (UNIPi, Pisa), Gyula Záray (ELTE, Budapest)

09.00 Key-note lecture 5

Fabio Di Francesco (UNIPi, Pisa), Francesca Bellagambi, Silvia Ghimenti, Tommaso Lomonaco, Pietro Salvo, Roger Fuoco, Advances in breath and saliva analysis

09.30 Mikołaj Mizera (Poznań University of Medical Sciences, Poznań, Poland), Irena Oszczapowicz, Judyta Cielecka-Piontek, FT-IR/Raman spectroscopy coupled with quantum mechanics modelling for assessment of complexation ability of β -lactam analogs and cyclodextrins

09.50 Barbara Roda (University of Bologna), Pierluigi Reschiglian, Andrea Zattoni, Valentina Marassi, Sonia Casolari, Hollow-fiber field flow fractionation, an analytical tool for the characterization and quality control of new biotechnological protein based drugs

- 10.10 Viktor G. Mihucz (ELTE, Budapest), Christina Dunster, Tamás Szigeti, Zsófia Kertész, Martina Giannoni, Franco Lucarelli, Frank J. Kelly, Gyula Záray, Integrated method development for chemical characterization and oxidative potential determination of indoor particulate matter
- 10.30 Tommaso Lomonaco (UNIFI, Pisa), Silvia Ghimenti, Isabella Piga, Denise Biagini, Massimo Onor, Roger Fuoco, Aldo Paolicchi, Lucia Ruocco, Giovanni Pellegrini, Maria Giovanna Trivella, Fabio Di Francesco, Monitoring of warfarin therapy by saliva analysis: an open issue on the way to clinical practice
- 10.50 Coffee break
- 11.10 Anikó Vasanits-Zsigrai (ELTE, Budapest), Main challenges of analytical method development for multiresidue analysis of pharmaceuticals in environmental water samples
- 11.30 Raviraj M. Kalunke, Gerardo Grasso (CNR, Rome), Renato D'Ovidio, Roberto Dragone, Chiara Frazzoli, Ciprofloxacin residues detection in cow milk: development of a novel and rapid optical β -galactosidase-based screening assay

Oral session 4

Medical devices: current challenges and future prospects

Chairpersons: Salvatore Bianco (Akros Biosciences, Pomezia, Rome), Sándor Kerpel-Fronius (Semmelweis University, Budapest)

- 11.50 Key-note lecture 6
Salvatore Bianco (Akros Biosciences, Pomezia), Alfredo Nunziata, Development of medical devices containing active pharmaceutical ingredients
- 12.20 Lucia Bonadonna (ISS, Rome), Rossella Briancesco, Maurizio Semproni, Microbiological quality control of different types of medical devices
- 12.50 Fabio Geremia, Domenico Capestrani (CTP System, Milan), Quality aspects for medical devices, quality system and certification process
- 13.10 Stefania Marcheggiani (ISS, Rome), Cristina Romanelli, Loredana Musmeci, Carmine Guarino, Cinzia Grasso, Anna Maria D'Angelo, Elio Pierdominici, Silvana Cacioli, Camilla Puccinelli, Roberto Giuseppetti, Emilio D'Ugo, Filippo Chiudioni, Massimiliano Bugarini, Elisabetta Volpi, Fabrizio Volpi, Mario Figliomeni, Maria Rosaria Lombardi, Giuseppina Terzulli, Graziella Quinci, Laura Mancini, Italian Guidelines on microbiological quality of the water used in the medical devices industry
- 13.30 Laura Laffranchi (University of Brescia), Lorenzo Sala, Corrado Paganelli, Evaluation of subacute and subchronic systemic toxicity of metal dental alloys, guidelines and reference standards.

13.50 General discussion

14.00 Lunch break

Oral Session 5/a (parallel session)

Personalized medicine from genetics to analytics

Chairpersons: Isabella Andreini (RTC, Pomezia), Katalin Monostory (Hungarian Academy of Science, Budapest)

15.00 Key-note lecture 7

- Erika Pintér, János Szolcsányi (University of Pécs), New perspectives in personalized pharmacotherapy of pain and inflammation
- 15.30 Davide Seripa (IRCCS Casa Sollievo della Sofferenza, San Giovanni Rotondo, Foggia), F. Panza, M. Lozupone, G. Miscio, M. Urbano, C. Gravina, A. Bellomo, A. Greco, Stefano Angelo Santini, Genetics of tailored medicine: the CYP system
- 15.50 István Peták (Semmelweis University, Budapest), Csilla Hegedus, Zsófia Binder, Janos Hodsagi, György Keri, Molecular evidence-based targeting of rare driver gene alterations in cancer
- 16.10 Loredana Serpe (University of Turin), Pier Luigi Calvo, Andrea Brunati, Antonio Amoroso, Renato Romagnoli, Roberto Canaparo, Pharmacogenetics as a tool to tailor the immunosuppressive therapy: focus on azathioprine and tacrolimus
- 16.30 Csaba Szántay (Richter Gedeon Co., Budapest), The structure behind the drug, the man behind the structure: scrutinizing molecules by NMR and MS with a human eye
- 16.50 General discussion

Oral Session 5/b (parallel session)

Pharmaceuticals and the environment

Chairpersons: Anna Barra Caracciolo (CNR, Rome), Paola Bottoni (ISS, Rome)

- 15.00 Key-note lecture 8
Ettore Zuccato (Istituto di Ricerche Farmacologiche Mario Negri, Milan), Sara Castiglioni, Francesco Riva, Pharmaceuticals as environmental contaminants: analysis, levels and significance
- 15.30 Key-note lecture 9
György Heltai (Szent István University, Gödöllő), Zoltán Győri, Ilona Fekete, Gábor Halász, Katalin Kovács, Anita Takács, Norbert Boros, Márk Horváth, Potentially toxic elements in the soil-water-sediment system by sequential extraction
- 16.00 Anna Barra Caracciolo (CNR, Rome), Paola Grenni, Jasmin Rauseo, Nicoletta Ademollo, M. Cardoni, Luisa Patrolecco, Effects on the natural microbial community of a fluoroquinolone antibiotic in an urbanized stretch of the river Tiber
- 16.20 Paola Grenni, Luisa Patrolecco, Nicoletta Ademollo, M. Di Lenola, Anna Barra Caracciolo (CNR, Rome), Persistence of the fibrate drug Gemfibrozil in a river water ecosystem
- 16.40 Marina Di Carro (University of Genoa), Cristiana Mirasole, Barbara Benedetti, Emanuele Magi, Pharmaceuticals as emerging pollutants, passive sampling and tandem mass spectrometry for their determination in water
- 17.00 István Sebestyén (Toxi-Coop Toxicological Research Center Plc, Budapest), Katalin Monostory, Gabor Hirka, Hungary Environmental risk assessment of human and veterinary medicinal products: Analytical challenges during the ecotoxicological studies
- 17.20 Péter Hegedűs (University of Pannonia, Veszprém), Erzsébet Szabó-Bárdos, Ottó Horváth, Photocatalytic decomposition of water contaminants over immobilized TiO₂
- 17.40 General discussion
- 18.00 Closure of day 2

Wednesday, 15 June, 2016

Oral session 6

Metabolomics

Chairpersons: Stefano Angelo Santini (Catholic University, Rome), György Heltai, (University of Gödöllő)

09.00 Key-note lecture 10

Sándor Kerpel-Fronius (Semmelweis University, Budapest), Pharmacokinetics of biological medicinal agents

09.30 Zsolt Valicsek, Ottó Horváth (University of Pannonia, Veszprém), Possible application of out-of-plane metalloporphyrins in medical sciences

09.50 Norbert Szoboszlai (ELTE, Budapest), Anikó Gaál, Gábor Orgován, Christina Streli, Comparative study of anticancer copper chelators

10.10 Tamás Tábi, Éva Szökő (Semmelweis University, Budapest), Chiral capillary electrophoresis in metabolic research

10.30 Coffee break

10.50 Annamaria Colacci (University of Bologna), The use of omics-based approaches in regulatory toxicology

11.10 Imre Klebovich (Semmelweis University, Budapest), Novel tools of radiochromatography in pharmacokinetic and drug metabolism research

11.30 Emanuela Testai (ISS, Rome), Profiling the toxicity of new drugs in an animal-free testing strategy: the relevance of integrating dynamics and biokinetics

11.50 General discussion

12.00 Round Table 1

Pharmacology and analytical chemistry: the quest for quality

Participants: Sergio Caroli (SSFA, Milan), Roger Fuoco (UNIFI, Pisa) József Posta (University of Debrecen), Valentine Sforza (Quality Associates, Anzio), Beáta Sperlág (MFT, Budapest).

13.00 Lunch Break

14.30 Round Table 2

Pharmaceuticals and the environment: challenges and remedial actions

Participants: Anna Barra Caracciolo (CNR, Rome), Paola Bottoni (ISS, Rome), Sergio Caroli (SSFA, Milan), Viktor G. Mihucz (ELTE, Budapest), István Sebestyén (Toxi-Coop Co., Budapest), Gyula Záray (ELTE, Budapest)

16.30 Social programme: visit of the San Rossore Park

20.00 Conference dinner

22.00 Closure of day 3

Thursday, 16 June, 2016

Oral session 7

Nutraceuticals

Chairpersons: Ornella Abollino (University of Turin) and Victor G. Mihucz (ELTE, Budapest)

09.00 Key-note lecture 11

- Patricia Nora Smichowski (CNEA, Buenos Aires, Argentina), A. Londonio, Evaluation of different approaches for the elemental characterization of dietary supplements
- 09.30 Ornella Abollino (University of Turin), Mery Malandrino, Carmela La Gioia, Gaia Paparella, Emanuele Magi, Agnese Giacomino, *In vitro* estimation of element bioaccessibility in Ayurvedic products
- 09.50 Anna Blázovics (Semmelweis University, Budapest), *Beta vulgaris L. ssp. esculenta var. rubra* as a functional food
- 10.10 Stefano Fogli, Germano Tarantino, Angela Fabiano, Elisa Brillì, Sara Carpi, Ylenia Zambito (UNIFI, Pisa), Sucrosomial iron and traditional iron dosage forms are compared for absorption by Caco2 cells
- 10.30 Michaela Zeiner (BOKU – University of Natural Resources and Life Sciences, Vienna, Austria), Iva Juranović Cindrić, Wolfgang Kandler, Gerhard Stingeder, Trace determination of skin-irritating metals in tea tree oil by GFAAS
- 10.50 Alessandra Bertoli (UNIFI, Pisa), Cüneyt Çirak, Fatih Seyis, *Hypericum* spp. volatile profilings and their potential significance in the quality control of new valuable raw material
- 11.10 Giovanni Rizzato (University of Venice), Elisa Scalabrin, Marta Radaelli, Daniela Cirasola, Oreste Piccolo, Gabriele Capodaglio, Exhausted roots of licorice: an unexplored potential source of bioactive compounds

11:20 General discussion

11.40 Coffee break

12.00 Poster discussion

13.30 Closure of day 4 and closure of the Symposium

Poster presentations

Monday, 13 June, through Thursday, 16 June

Poster session 1

Pharmacological research and innovation

Coordinator: Giacomo Pozzoli (Catholic University, Rome)

- Marilena Carbone (Tor Vergata University), Lucia Bonadonna, Rossella Briancesco, Maurizio Semproni, Stefania Paduano, Alessandro Talone, Emanuele Scibetta, Daniele Cecchetti, Mixed metal oxide nanoparticles as pharmacologically active biocides
- Anikó Gaál (ELTE, Budapest), Investigation of *in vitro* copper toxicity induced by chelators in human cancer cells
- Edit Háfra (MTA, Budapest), Tibor Kovács, Ádám Ferenc Kiss, Dávid Sirok, Katalin Tóth, Attila Szijártó, Katalin Monostory, The effect of portal vein occlusion on drug-metabolizing function of rat liver
- Gergely Horváth (Hungarian Academy of Sciences, Budapest), Lilla Otrókoci, Ágnes Kittel, Mária Baranyi, Beáta Sperlágh, The role of purinergic mechanisms in maternal Poly(I:C) Evoked Rodent Model of Autism spectrum disorder (ASD)
- Ádám Ferenc Kiss (Hungarian Academy of Science, Budapest), Katalin Tóth, Cintia Juhász, Edit Háfra, Manna Temesvári, József Paulik, Gábor Hirka, Katalin Monostory, Is CYP2D6 phenotype predictable from CYP2D6 genotype?

- Katalin Tóth, Dávid Sirok, Ágnes Kiss, Anita Csárdy, Márta Pátfalusi, Gábor Hirka, Katalin Monostory (Hungarian Academy of Sciences, Budapest), Utility of *in vitro* pharmacokinetic data in prediction of *in vivo* hepatic clearance of antipsychotics
- Alberto Terracina (Al. Terr. Consulting S.r.l., Rome), How to choice a clinical study management system
- Katalin Tóth (Hungarian Academy of Sciences), Dávid Sirok, Ales Belic, Gábor Csukly, István Bitter, Katalin Monostory, Contribution of CYP3A enzymes and NAT2 alleles to clonazepam metabolism
- Zsolt Valicsek (University of Pannonia, Veszprém, Hungary), Gergely Harrach, Arnold Károly Sebestyén, Bálint Németh, Ottó Horváth, Formation and photoinduced properties of silver porphyrins as promising PDT reagents

Poster session 2

The role of analytical chemistry in pharmacology

Coordinator: Viktor G. Mihucz (ELTE, Budapest)

- Palak Agarwal (St. Stephen's College, Dehli), Pragati Mishra, Nikita Gupta, Priyaranjan Sahoo, Kunal Prakash, Satish Kumar, Simple hydrazone based tweezer type receptors for the recognition of cyanide ion
- Roberta Ascrizzi (University of Pisa), Viviana Deriu, Silvio Chericoni, Mario Giusiani, Guido Flamini, Volatile fingerprints of different hashish blocks by means of HS-SPME-GC/MS
- Dilek Bakircioglu (Trakya University, Edirne, Turkey), Yasemin Bakircioglu Kurtulus, Nukte Topraksever, Meltem Kizildere, Investigation of macro, micro and toxic element concentrations of fermented traditional beverage kefir by using an inductively coupled plasma optical emission spectrometer, to improve food safety in Turkey
- Yasemin Bakircioglu Kurtulus (Trakya University, Edirne, Turkey), Dilek Bakircioglu, Alper Can Babac, Nukte Topraksever, Oil-in-water emulsion broken by heating into three-separated-phase procedure: a new approach for simultaneous separation/preconcentration of iron in solid oil samples
- Katia Buonasera (CNR, Rome), Gianni Pezzotti Escobar, Antonio Gabrielli, Alessandro Nicolosi, Rossella Briancesco, Stefania Paduano, Maurizio Semproni, Lucia Bonadonna, A completely automatic optical biosensor system for stressed bacteria in marine water
- Orsolya Fónagy (University of Pannonia, Veszprém), Erzsébet Szabó-Báros, Ottó Horváth, Krisztián Horváth, Effective mineralization of benzenesulfonic acid by heterogenous photocatalysis
- Silvia Ghimenti (University of Pisa, Italy), Tommaso Lomonaco, Francesca G. Bellagambi, Denise Biagini, Fabio Di Francesco, Roger Fuoco, Determination of warfarin and its active metabolites in dried blood spots
- Sema Gündüz (Technical University, Istanbul), Suleyman Akman, Sulfur determination in some nuts and dried fruits sold in Turkey by High Resolution Graphite Furnace Molecular Absorption Spectrometry
- Melitta Patrícia Kiss, Muhammad Imran, Zsolt Valicsek, Ottó Horváth, (University of Pannonia, Veszprém) Spectrophotometric investigation of early lanthanide (III) porphyrins for potential biomedical applications
- Katarzyna Michalska, EwaGruba, Mikołaj Mizera (Poznań University of Medical Sciences, Poznań), Kornelia Lewandowska, Elżbieta Bednarek, Wojtek Bocian, Judyta Cielecka-Piontek, Application of spectroscopic methods (FT-IR, Raman and NMR) for identification of radezolid. Experimental and DFT based approach
- Dávid Sirok (Hungarian Academy of Science, Budapest), Márta Pátfalusi, Gábor Szelezcky, Gyula Somorjai, Dávid Greskovits, Katalin Monostory, Simple and sensitive

LC/MS-MS method for simultaneous detection of acetylsalicylic acid and salicylic acid in human plasma

- István Vincze (Semmelweis University, Budapest), Tamás Tábi, Éva Szökő, Analysis of NMDA modulator D-serine and D-aspartate in biological samples using Capillary Electrophoresis-Laser-Induced Fluorescent (CE-LIF) detection method

Poster session 3

Environmental contamination by pharmaceuticals

Coordinator: Norbert Szoboszlai (ELTE, Budapest)

- Anna Barra Caracciolo, Paola Grenni, Valeria Ancona (CNR, Bari), Vito Felice Uricchio, An ecological approach to investigate the occurrence of pharmaceuticals in the aquatic environment
- Nicoletta Ademollo (CNR, Rome), Luisa Patrolecco, Jasmin Rauseo, J. S. Christiansen, S. Corsolini, Bioaccumulation of endocrine disrupting compounds in the Greenland shark *Somniosus microcephalus*
- Éva Cseperke Vizsolyi (ELTE, Budapest), Péter Dobosy, Imre Varga, József Varga, Gyula Záray, Study of chlorobenzene removal by ferrate treatment from groundwater applying GC-MS
- Péter Dobosy (ELTE, Budapest), Laura Jurecska, Katalin Barkács, Éva Fenyvesi, Gyula Záray, Characterization of cyclodextrin containing nanofilters for removal of pharmaceutical residues
- Andrea Cafuta, Erzsébet Szabó-Bárdos, Ottó Horváth, Krisztián Horváth, Péter Hegedűs (ELTE, Budapest), Sandra Babić, Irena Škorić, Photoinduced degradation of the nitrofurantoin
- Laura Jurecska (ELTE, Budapest), Katalin Barkács, Éva Fenyvesi, Ibolya Molnár-Perl, Gyula Záray, A pilot plant scale experiment aiming removal of pharmaceutical residues from biologically treated wastewater
- Katalin Kovács, Anita Takács (Szent István University, Gödöllő), Márk Horváth, Gábor Halász, György Heltai, Zoltán Győri, Kinetics study of ultrasound-assisted extraction of BCR sequential extraction procedures for potentially toxic element content of soil and sediment
- Laura Jurecska (ELTE, Budapest), Katalin Barkács, Éva Fenyvesi, Ibolya Molnár-Perl, Gyula Záray, A pilot plant scale experiment aiming removal of pharmaceutical residues from biologically treated wastewater

Poster session 4

Medical Devices

Coordinator: Fabio Geremia (CTP System, Milan)

- Anna Maria D'Angelo, Emilio D'Ugo (ISS, Rome), Stefania Marcheggiani, Roberto Giuseppetti, Elio Pierdominici, Filippo Chiudioni, Silvana Caciolli, Massimiliano Bugarini, Elisabetta Volpi, Fabrizio Volpi, Carmine Guarino, Cristina Romanelli, Laura Mancini, Microbiological quality of water used to manufacture medical devices
- Rosa Anna Grifa (Catholic University, Rome), Giacomo Pozzoli, Salvatore Bianco, Clinical investigations of medical devices, regulatory framework and methodological specificities
- Laura Mancini (ISS, Rome), Anna Maria D'Angelo, Silvana Caciolli, Stefania Marcheggiani, Camilla Puccinelli, Fabrizio Volpi, Cristina Romanelli, Carmine Guarino, Stefano Fabiani, Riccardo Grifoni, A pilot study for the wastewater reuse by medical device manufacturers

- Cristina Romanelli (ISS, Rome), Carmine Guarino, Medical devices borderline: regulatory aspects
- Laura Mancini, Cristina Romanelli (ISS, Rome), Anna Maria D'Angelo, Carmine Guarino, Cinzia Grasso, Silvana Caciolli, Camilla Puccinelli, Emilio D'Ugo, Massimiliano Bugarini, Elisabetta Volpi, Fabrizio Volpi, Mario Figliomeni, Stefania Marcheggiani, Microbiological risk linked to use of medical devices in beauty salons