

# PROGRAMME

# ORAL SESSIONS



**PROGRAMME – ORAL SESSIONS**

**Sunday, 9**

**18.00 - 19.30 S01 Plenary Lectures**

Chair: Patrick Masson (Russia), Kamil Kuca (Czech Republic)

18.00 - 18.45 **S01-1 Chronic illness from organophosphorus toxicant exposure**

**Oksana Lockridge** (USA), Lawrence M. Schopfer

18.45 - 19.30 **S01-2 The catalytic power of phosphotriesterases for the hydrolysis and destruction of organophosphorus nerve agents**

**Frank M. Raushel** (USA)

**19.30 - 21.00 Welcome party**

Conference venue: Campus, Building A, Hradecká 1227, Hradec Králové

*Included in the registration fee*



**PROGRAMME – ORAL SESSIONS**

**Monday, 10**

**08.15 - 08.30**

**Opening ceremony**

Chair: Kamil Kuca

**08.30 - 11.30**

**S02**

**Structure and dynamics of cholinesterases and OP hydrolases**

Chair: Yuan-Ping Pang (USA), Joel Sussman (Israel)

08.30 - 08.50

**S02-1**

**Recent breakthroughs in the structure/function studies of acetylcholinesterase**

**Joel L. Sussman** (Israel), I. Silman

08.50 - 09.10

**S02-2**

**Coupling of acetylcholinesterase to the interfacial phase state**

Bernhard Fichtl, Stefan Nuschele, Konrad Kaufmann, **Israel Silman** (Israel), Matthias F Schneider

09.10 - 09.30

**S02-3**

**The other side of AChE: Allosteric sites and modulators**

Carlos Roca, Carlos Requena, Víctor Sebastián-Pérez, Sony Malhotra, Chris Radoux, Concepción Pérez, Ana Martínez, Juan Antonio Páez, Tom L. Blundell, **Nuria E. Campillo** (Spain)

09.30 - 09.50

**S02-4**

**Partial unfolding of insect acetylcholinesterase:  
Steps toward cysteine-targeting insecticides**

**Yuan-Ping Pang** (USA)

09.50 - 10.10

*COFFEE BREAK*

10.10 - 10.30

**S02-5**

**The protonation state of Glu197 and its important role in stabilizing catalytic triad of butyrylcholinesterase**

**Junjun Liu** (China), Xiao Wan

10.30 - 10.50

**S02-6**

**Recipes to design specific ligands of human butyrylcholinesterase**

**Florian Nachon** (France), Jacques-Philippe Colletier, Nicolas Coquelle, Xavier Brazzolotto

10.50 - 11.10

**S02-7**

**Exploring the evolutionary potential of the  $\alpha$ E7 carboxylesterase**

**Galen J. Correy** (Australia), Colin J. Jackson

11.10 - 11.30

**S02-8**

**Protein dynamics of phosphotriesterase: Two cations required for enzyme catalysis**

**Yuan-Ping Pang** (USA)

11.30 - 12.30

*LUNCH and POSTERS*

PROGRAMME – ORAL SESSIONS

Monday, 10

**12.30 - 15.15 S03 Interaction of cholinesterases with substrates, inhibitors and reactivators**

Chair: Terrone Rosenberry (USA), Franz Worek (Germany)

- 12.30 - 12.50 **S03-1 New Progress in Drug Design, Discovery and Development Involving Cholinesterases**  
Fang Zheng, **Chang-Guo Zhan** (USA)
- 12.50 - 13.10 **S03-2 In searching for the mechanism of butyrylcholinesterase activators**  
**Jure Stojan** (Slovenia)
- 13.10 - 13.30 **S03-3 Computational analysis of reaction mechanisms for optimization of butyrylcholinesterase-based catalytic bioscavengers against organophosphorus agents**  
**Sofya Lushchekina** (Russia), Bella Grigorenko, Alexander Nemukhin, Sergei Varfolomeev, Patrick Masson
- 13.30 - 13.50 **S03-4 Enhancement in pyridinium oxime-assisted reactivation of tabun-inhibited acetylcholinesterase achieved by active site mutations**  
**Zrinka Kovarik** (Croatia), Maja Katalinić, Nikolina Maček Hrvat, Goran Šinko, Tamara Zorbaz, Anita Bosak
- 13.50 - 14.10 **S03-5 The search for resistance-breaking and species-selective mosquitocidal inhibitors of *Anopheles gambiae* AChE**  
**Paul R. Carlier** (USA), Jeffrey R. Bloomquist, Jonah Cheung, Jianyong Li, Max Totrov
- 14.10 - 14.30 **S03-6 Steric Effects in the Decarbamylation of Carbamoylated Acetylcholinesterase**  
Kunisi S. Venkatasubban, Joseph L. Johnson, Jamie L. Thomas, Abdul Fauq, Bernadette Cusack, **Terrone L. Rosenberry** (USA)
- 14.30 - 14.45 **S03-7 Assessment of scoring functions for AChE-ligand interactions**  
**Goran Šinko** (Croatia)
- 14.45 - 15.00 **S03-8 Phenyl valerate esterase activity of human cholinesterases**  
**Jorge Estévez** (Spain), María Romo, Marina Terol, Iris Mangas, Miguel Ángel Sogorb, Eugenio Vilanova
- 15.00 - 15.15 **S03-9 Effects of memantine and its metabolite Mrz 2/373 on soman-induced inhibition of bovine erythrocyte acetylcholinesterase *in vitro***  
**Miloš P. Stojiljković** (Bosnia & Herzegovina), Ranko Škrbić, Milan Jokanović
- 15.15 - 15.40 **COFFEE BREAK**

## PROGRAMME – ORAL SESSIONS

Monday, 10

**15.40 - 18.10 S04 Reactivators of AChE, OP inhibitors – mechanism of toxicity, detection and analytical methods, diagnosis of exposure, detoxification and therapy; counter-terrorism strategies**

Chair: Franz Worek (Germany), Terrone Rosenberry (USA)

- 15.40 - 16.00 **S04-1 Oximes with ortho-positioned chlorine moiety exhibit improved physical-chemical properties, efficient reactivation of inhibited human acetylcholinesterase and reduced in vivo toxicity**  
David Malinak, Tamara Zorbaz, Adam Skarka, Martina Hrabinova, Nikola Marakovic, Jana Janockova, Ondrej Soukup, Jan Misik, Daniel Jun, Kamil Kuca, Zrinka Kovarik, **Kamil Musilek** (Czech Republic)
- 16.00 - 16.20 **S04-2 Design and synthesis of bifunctional fluoropyridinaldoxime reactivators for nerve agent-inhibited human acetylcholinesterase**  
**Jagadeesh Yerri** (France), José Dias, Florian Nachon, Rachid Baati
- 16.20 - 16.40 **S04-3 Combination of oximes with overlapping reactivation spectra: obidoxime and HI-6**  
**Timo Wille** (Germany), Horst Thiermann, Franz Worek
- 16.40 - 17.00 **S04-4 Design of broad spectrum antidotes**  
Cecilia Lindgren, Nina Forsgren, Christine Akfur, Lotta Berg, David Andersson, Franz Worek, Anna Linusson, **Fredrik Ekström** (Sweden)
- 17.00 - 17.15 **S04-5 Demonstration of the First Small Molecule Therapeutics for Resurrection of the Aged form of Acetylcholinesterase after Exposure to Organophosphorus Chemical Nerve Agents and Pesticides**  
**Andrew J. Franjesevic** (USA), Qinggeng Zhuang, Ola, Nosseir, William H. Coldren, Christopher S. Callam, Christopher M. Hadad
- 17.15 - 17.30 **S04-6 Nanotechnology strategies using oximes-loaded lipid nanoparticles for brain protection against organophosphorus poisoning**  
**Tatiana N. Pashirova** (Russia), Irina V. Zueva, Anissa Braïki, Konstantin A. Petrov, Vasily M. Babaev, Evgenia A. Burilova, Darya A. Samarkina, Ildar Kh. Rizvanov, Eliana B. Souto, Ludovic Jean, Pierre-Yves Renard, Patrick Masson, Lucia Ya. Zakharova, Oleg G. Sinyashin
- 17.30 - 17.50 **S04-7 Utilizing Structure-Activity Relationships and Mechanistic Insights to Design Non-Oxime Reactivators**  
**C. Linn Cadieux** (USA), Zachary Canter, Kevin Martin, Keith Morgan, Michael Hepperle
- 17.50 - 18.10 **S04-8 New Non-Oxime Reactivators of Organophosphate Inhibited Acetylcholinesterase with Promising Reactivation Potency**  
**Martijn de Koning** (Netherlands), Franz Worek, Gabriele Horn, Marco van Grol

PROGRAMME – ORAL SESSIONS

Tuesday, 11

**08.00 - 09.40 S05 Enzymes and proteins other than ChEs interacting with OP**

Chair: Oksana Lockridge (USA), Patrick Masson (Russia)

08.00 - 08.20 **S05-1 Identifying axonal transport-related targets for reversing the adverse effects of organophosphate exposure**

Sean X. Naughton, **Alvin V. Terry, Jr (USA)**

08.20 - 08.40 **S05-2 Diagnosis of Poisoning with O-Isobutyl-S-[2-(diethylamino)ethyl] methylphosphonothioate (VR) under Antidotal Therapy with Carboxim**

**Nadezhda L. Koryagina (Russia)**, Elena I. Savelieva, Anton I. Ukolov, Darya S. Prokofieva, Nataliia S. Khlebnikova, Tatiana I. Aliushina, Elena S. Ukolova, Andrey S. Radilov, Nikolay V. Goncharov

08.40 - 09.00 **S05-3 Copper-dependent hydrolysis of trichloronate by turkey serum and albumin**

**Damianys Almenares-López (México)**, Antonio Monroy-Noyola

09.00 - 09.20 **S05-4 Mass Spectral Detection of Diethoxyphospho-Tyrosine Adducts on Proteins from HEK293 Cells Using Monoclonal Antibody depY for Enrichment**

**Seda Onder (Turkey, USA)**, Lawrence M. Schopfer, Ozden Tacal, Thomas A. Blake, Rudolph C. Johnson, Oksana Lockridge

09.20 - 09.40 **S05-5 Innovative Biocatalysts as Tools to Detect and Inactivate Nerve Agents**

Elena Porzio, Francesca Bettazzi, Luigi Mandrich, Immacolata Del Giudice, Odile F. Restaino, Serena Laschi, Ferdinando Febbraio, Valentina De Luca, Maria G. Borzacchiello, Teresa M. Carusone, Franz Worek, Antonio Pisanti, Piero Porcaro, Chiara Schiraldi, Mario De Rosa, Ilaria Palchetti, **Giuseppe Manco (Italy)**

09.40 - 10.00 **COFFEE BREAK**

**PROGRAMME – ORAL SESSIONS**

**Tuesday, 11**

**10.00 - 12.10 S06 Stoichiometric bioscavenger, biotechnology and therapeutical aspects**

Chair: Palmer Taylor (USA)

10.00 - 10.10

**Commemoration of John Casida**

**Palmer Taylor** (USA)

10.10 - 10.30

**S06-1 Ionizable, Zwitterionic Oximes as Countermeasures to Volatile Organophosphate (OP) Exposure**

**Palmer Taylor** (USA), William C. Hou, Jeremiah Momper, Yan-Jye Shyong, Zoran Radic, John McDonough, Zrinka Kovarik, Yvonne Rosenberg, K. Barry Sharpless

10.30 - 10.50

**S06-2 Development of pre- and post-countermeasures against OP toxins in macaques**

**Yvonne Rosenberg** (USA), James Fink, Lingjun Mao, Xiaoming Jiang, Jonathan Lees, Jerry Wang, Tara Ooms, Narayanan Rajendra, Zoran Radic, Palmer Taylor

10.50 - 11.10

**S06-3 Human Plasma-Derived Butyrylcholinesterase Is Behaviorally Safe and Effective in Cynomolgus Macaques (*Macaca fascicularis*) Challenged with Soman**

**Todd M. Myers** (USA)

11.10 - 11.30

**S06-4 Design of a combined aptamer for paraoxon and acetylcholinesterase by in silico approach**

**Daria A. Belinskaia** (Russia), Pavel A. Avdonin, Nikolay V. Goncharov

11.30 - 11.50

**S06-5 Prokaryotic expression of human butyrylcholinesterase as a tool for catalytic bioscavenger development**

**Xavier Brazzolotto** (France), Alexandre Igert, Virginia Guillon, Gianluca Santoni, Florian Nachon

11.50 - 12.10

**S06-6 Bioscavengers and the medical management chain**

**Thomas M. Mann** (England), H. Rice

12.10 - 13.40

*LUNCH and POSTERS*

**PROGRAMME – ORAL SESSIONS**

**Tuesday, 11**

**13.40 - 16.00 S07 Catalytical Bioscavengers – PON and PTE**

Chair: Eugenio Vilanova (Spain), Florian Nachon (France)

- 13.40 - 13.50 **Commemoration of Doug Cerasoli**  
**Tamara C. Otto** (USA)
- 13.50 - 14.00 **S07-1 Borderline between catalytic and non-catalytic bio scavengers: the example of albumin and reversible B-esterases**  
**Eugenio Vilanova** (Spain), Jorge Estévez, Miguel Ángel Sogorb, Iris Mangas, Antonio Monroy
- 14.00 - 14.20 **S07-2 Catalytic Scavengers Provide Broad-Spectrum Protection against Organophosphorus Nerve Agents**  
Shane A. Kasten, Sandra J. DeBus, Thuy L. Dao, Michael V. Boeri, Zachary A. Canter, Sean M. Hodgins, Robyn. B. Lee, Douglas M. Cerasoli, **Tamara C. Otto** (USA)
- 14.20 - 14.40 **S07-3 Paraoxonase 1 variant I-F11 gene therapy using adeno-associated virus8 (AAV8) offers long-term protection against G-type chemical warfare nerve agents**  
Venkaiah Betapudi, Deborah M. Doctor, **Nageswararao Chilukuri** (USA)
- 14.40 - 15.00 **S07-4 Organophosphate Hydrolase (OPH) Designed as a Tethered Monomer**  
Jaffet Santiago Garcia, Cetara Baker, Richard Sweeney, **Stephen Kirby** (USA)
- 15.00 - 15.20 **S07-5 A new animal model to investigate organophosphorus poisoning and enzymatic decontamination**  
**Laetitia Poirier** (France), Pauline Jacquet, Laure Plener, Cédric Torre, Eric Ghigo, David Daudé, Eric Chabrière
- 15.20 - 15.40 **S07-6 Paraoxonase-2 dependent redox control of platelet physiology**  
**Victoria Petermann** (Germany), H.Kleinert, K.Jurk
- 15.40 - 16.00 **S07-7 Copper with chicken serum albumin show stereoselective hydrolysis of chiral phosphoramidates**  
**Antonio Monroy-Noyola** (México), Miguel Angel Sogorb, Eugenio Vilanova

**18.00**

***Walking tour around the city***

The tour will begin and finish in front of the Cathedral of the Holy Spirit.  
Free tickets at the registration desk (limited amount!)

**20.00**

***Concert in the Cathedral of the Holy Spirit***



**PROGRAMME – ORAL SESSIONS**

**Wednesday, 12**

**08.30 - 11.30 S08 3D section – structure and dynamics of  $\alpha/\beta$  hydrolases and OP hydrolases, in silico methods for designing of modulator**

Chair: Zoran Radić (USA), Jonah Cheung (USA)

08.30 - 08.55 **S08-1 Insights into the Yin and the Yang of Acetylcholinesterase Inhibition by Mechanistic X-Ray Crystallography**

M. Bartolini, M.L. Bolognesi, J. Korábečný, K. Kuca, **Doriano Lamba** (Italy), A. Pesaresi, X. Zha

08.55 - 09.20 **S08-2 Photo-induced release of an acetylcholinesterase inhibitor**

**Eugenio de la Mora** (France), Johannes Broichhagen, Peter Mayer, Elisabet Artursson, Fredrik Ekström, Joel Sussman, Israel Silman, Dirk Trauner, Giorgio Schirò, Martin Weik

09.20 - 09.45 **S08-3 Structural studies of *Anopheles gambiae* acetylcholinesterase provide insight towards improved insecticides for malaria vector control**

**Jonah Cheung** (USA), Arshad Mahmood, Ravi Kalathur, Lixuan Liu, Max Totrov, Paul Carlier

09.45 - 10.05 **COFFEE BREAK**

10.05 - 10.30 **S08-4 Room-temperature crystallography and neutron scattering studies of human acetylcholinesterase to inform the design of oxime reactivators**

Oksana Gerlits, Mikolai Fajer, Xiaolin Cheng, Donald Blumenthal, Palmer Taylor, Zoran Radić, **Andrey Kovalevsky** (USA)

10.30 - 10.55 **S08-5 Crystal structures of human cholinesterases in complex with supramolecular ligands**

**José Dias** (France), Xavier Brazzolotto, Xiao-Yu Cao, Artur Stefankiewicz, Jean-Marie Lehn, Florian Nachon

10.55 - 11.20 **S08-6 Modifications of Cholinesterase Structure and Function in Covalent Organophosphate Conjugates Visualized in 2D, 3D and VR**

Zihan Zheng, Wanlu Yu, Jacqueline Rohrer, Alexandria Tran, **Zoran Radić** (USA)

11.20 - 11.30 **Concluding sentence**

**Zoran Radić** (USA)

11.30 - 13.00 **LUNCH and POSTERS**

**13.00**

**Trips**

13.00 National Stud Farm at Kladruby nad Labem

13.15 Kuks hospital

13.30 Hrádek u Nechanic chateau

**PROGRAMME – ORAL SESSIONS**

**Thursday, 13**

**08.00 - 11.30 S09 Biological functions, development and non-cholinergic function of cholinesterases**

Chair: Shani Shenhar-Tsarfaty (Israel), Israel Silman (Israel)

08.00 - 08.15

**Commemoration of Eric Barnard**

**Israel Silman** (Israel), **Karl W. K. Tsim** (China)

08.15 - 08.35

**S09-1 Cholinergic mechanisms at the core of skeletal and retinal histogenesis**

Gesine Bachmann, Afrim Bytyqi, Florian Frohns, Matthias Rieke, Gopenath Thangaraj, **Paul G. Layer** (Germany)

08.35 - 08.55

**S09-2 Butyrylcholinesterase as a ghrelin modulator impacting anxiety, stress, obesity, and drug cravings**

**Stephen Brimijoin** (USA), Y. Gao, L.Y. Geng, V.P. Chen

08.55 - 09.15

**S09-3 Assembly of PRiMA-linked form of acetylcholinesterase in neurons: the role of enzyme inhibitor acting as chemical chaperon**

**Karl W. K. Tsim** (China), Etta Y. L. Liu, Miranda L. Xu, Xiang P. Kong, Qiyun Wu, Ran Duan, Tina T. X. Dong

09.15 - 09.35

**S09-4 Evolution of the first disulfide bond in the cholinesterase-carboxylesterase (COesterase) family: Possible consequences for cholinesterase expression in prokaryotes**

**Arnaud Chatonnet** (France), Xavier Brazzolotto, Thierry Hotelier, Nicolas Lenfant, Pascale Marchot

09.35 - 09.55

*COFFEE BREAK*

09.55 - 10.15

**S09-5 Acetylcholinesterase in neuromuscular synaptic clefts of vertebrates**

Edna Blotnick-Rubin, **Lili Anglister** (Israel)

10.15 - 10.35

**S09-6 Respiration during organophosphate and carbamate intoxication when acetylcholinesterase is not anchored at cholinergic synapses**

**Eric Krejci** (France), Aurélie Nervo, Imene Kellout, Anne Sophie Hanak, Guilhem Calas, Florian Nachon

10.35 - 10.55

**S09-7 Single nucleotide polymorphisms in the genes encoding AChE and its miR-608 regulator co-modulate anxiety and blood pressure**

**Alon Simchovitz** (Israel), Nimrod Madrer, Rotem Haviv, Geula Hanin, Shani Shenhar-Tsarfaty, Einor Ben Assayag, Shlomo Berliner, Zehava Solomon, Hermona Soreq

10.55 - 11.15

**S09-8 Dioxin suppresses AChE expression in neuron and muscle**

**Heidi Qunhui Xie** (China), Yingjie Xia, Tuan Xu, Yangsheng Chen, Yali Luo, Rui Sha, Yiyun Liu, Li Xu, Bin Zhao

11.15 - 11.30

**S09-9 Wnt3a induces the transcription of acetylcholinesterase: an enzyme playing a role in osteoblastic differentiation**

**Miranda L. Xu** (China), Etta Y. L. Liu, Qiyun Wu, Duan Ran, Tina T. X. Dong, Karl W. K. Tsim

11.30 - 12.30

*LUNCH and POSTERS*

**PROGRAMME - ORAL SESSIONS**

**Thursday, 13**

**12.30 - 14.45 S10 Alzheimer's disease and diseases related to cholinesterases**

Chair: Ana Martinez (Spain), Maria-Laura Bolognesi (Italy)

12.30 - 12.50 **S10-1 Restoring mitochondria (dys)function and acetylcholine levels as a prospective therapeutic strategy for Alzheimer's disease**

**Fernanda Borges** (Portugal)

12.50 - 13.10 **S10-2 From dual binding site AChE inhibitors to chameleon molecules: discovery of potent BuChE inhibitors**

Carlos Roca, Talita P.C. Chierrito, Concepción Perez, Loreto Martinez, Nuria Campillo, **Ana Martinez** (Spain)

13.10 - 13.30 **S10-3 Discovery and development of neuroprotective and disease-modifying anti-AD drug leads from the Chinese medicine**

Marvin Mak, Wei Cui, **Yifan Han** (China)

13.30 - 13.50 **S10-4 Fifty shades of cholinesterase immobilization and their application to drug discovery**

**Manuela Bartolini** (Italy), Anna Tramarin, Edoardo Fabini, Piotr Drączkowski, Marina Naldi, Daniele Tedesco, Krzysztof Józwiak, Vincenza Andrisano

13.50 - 14.10 **S10-5 Serum cholinesterase activity and Alzheimer disease comorbidities - can bariatric surgery change your sympathetic prone state?**

**Shani Shenhar-Tsarfaty** (Israel), Shiri Sherf-Dagan, Galia Berman, Shira Zelber-Sagi, Oren Shibolet, Itzhak Shapira, David Zeltser, Shlomo Berliner, Ori Rogowski

14.10 - 14.30 **S10-6 Indazolylketones: hit to lead optimization of a multitarget drugs**

Pedro González-Naranjo, Natalia Pérez, Concepción Pérez, Carlos Roca, Rocio Girón, Eva Sánchez-Robles, Ángeles Martín Requero, Maria L. de Ceballos, **Nuria E. Campillo** (Spain), Juan Antonio Páez

14.30 - 14.45 **S10-7 Butyrylcholinesterase genetic polymorphism and neuroimaging biomarkers in Alzheimer's disease**

**DeBay Drew R.** (Canada), Maxwell Selena, Luke David, Fisk John D., Burrell Steve, Bowen Chris V., Song Xiaowei, Black Sandra E., Darvesh Sultan

14.45 - 15.10

*COFFEE BREAK*

## PROGRAMME - ORAL SESSIONS

Thursday, 13

**15.10 - 17.40 S11 Multi-target-directed ligands in Alzheimer's disease primarily targeting cholinesterases**

Chair: Maria-Laura Bolognesi (Italy), Ana Martinez (Spain)

- 15.10 - 15.30 **S11-1 Case studies for successful combination of ChE inhibitors and GPCR ligands (cannabinoid 2 and histamine 3 receptors)**  
Dominik Dolles, Fouad H. Darras, Antonios Drakopoulos, Andrea Strasser, Hans-Joachim Wittmann, Christoph A. Sotriffer, Steffen Pockes, Bassem Sadek, Tangui Maurice, **Michael Decker** (Germany)
- 15.30 - 15.50 **S11-2 From acetylcholinesterase inhibitors to multi-target-directed ligands (MTDLs): a step forward in Alzheimer's disease drug discovery**  
**Maria-Laura Bolognesi** (Italy)
- 15.50 - 16.10 **S11-3 From selective butyrylcholinesterase inhibitors to multi-target-directed ligands as lead compounds for Alzheimer's disease**  
Urban Košak, Damijan Knez, Boris Brus, **Stanislav Gobec** (Slovenija)
- 16.10 - 16.30 **S11-4 Discovery and characterization of tacrine/huprine-tryptophan heterodimers as novel multipotent compounds against Alzheimer's disease**  
**Jan Korabecny** (Czech Republic), Katarina Spilovska, Manuela Bartolini, Barbara Monti, Dorian Lamba, Rosanna Caliendo, Alessandro Pesaresi, Vendula Hepnarova, Daniel Jun, Martina Hrabnova, Rafael Dolezal, Jana Zdarova Karasova, Ondrej Soukup, Eva Mezeiova, Eugenie Nepovimova, Maria Laura Bolognesi, Kamil Kuca
- 16.30 - 16.50 **S11-5 Novel conjugates based on  $\gamma$ -carbolines, carbazoles, phenothiazines, and aminoadamantanes as multifunctional agents for Alzheimer's disease treatment**  
**Galina F. Makhaeva** (Russia), N.P. Boltneva, N.V. Kovaleva, S.V. Lushchekina, E.V. Rudakova, R.J. Richardson, S.O. Bachurin
- 16.50 - 17.10 **S11-6 Pleiotropic prodrugs: a novel polypharmacology approach to treat neurodegenerative diseases**  
**Christophe Rochais** (France), Patrick Dallemagne
- 17.10 - 17.25 **S11-7 Toward an innovative treatment of Alzheimer's disease: Design of multi-target directed ligands (MTDLs) targeting acetylcholinesterase (AChE) and alpha-7 nicotinic receptors (alpha-7 nAChRs)**  
**Mégane Pons** (France), Buron Frédéric, Ludovic Jean, Sylvie Chalon, Sylvain Routier, Pierre-Yves Renard
- 17.25 - 17.40 **S11-8 Molecular modeling in search of new, multi-target ligands against Alzheimer's disease. Exploring the biochemical multiverse.**  
**Jakub Jończyk** (Poland), Dawid Panek, Anna Więckowska, Justyna Godyń, Marek Bajda, Tomasz Wichur, Anna Pasięka, Damijan Knez, Anja Pišlar, Jan Korabecny, Ondrej Soukup, Vendula Sepsova, Raimon Sabaté, Janko Kos, Stanislav Gobec, Barbara Malawska

**20.00****Gala dinner**

Hotel Nové Adalbertinum, Velké náměstí 32, Hradec Králové

Included in the registration fee

**PROGRAMME – ORAL SESSIONS**

**Friday, 14**

**08.00 - 09.20 S12 Varia**

Chair: Kamil Kuca (Czech Republic), Ondrej Soukup (Czech Republic)

08.00 - 08.20 **S12-1 Design of a butyrylcholinesterase mutant for detoxifying cocaine and its toxic metabolites in concurrent use of cocaine and alcohol**

**Fang Zheng** (USA), Xirong Zheng, Ting Zhang, Xiabin Chen, and Chang-Guo Zhan

08.20 - 08.40 **S12-2 7-Methoxyderivative of tacrine is a 'foot-in-the-door' blocker of GluN1/GluN2 and GluN1/GluN3 NMDA receptors**

Martina Kaniakova, Lenka Kleteckova, Katarina Lichnerova, Kristina Holubova, Kristyna Skrenkova, Miloslav Korinek, Jan Krusek, Tereza Smejkalova, Jan Korabecny, Karel Vales, Ondrej Soukup, **Martin Horak** (Czech Republic)

08.40 - 09.00 **S12-3 The *Caenorhabditis elegans* pharynx as a model system to investigate and mitigate against the effects of anti-cholinesterase drugs**

**Patricia Gonzalez** (United Kingdom), Christopher Green, John Tattersall, Lindy Holden-Dye, Vincent O'Connor

09.00 - 09.20 **S12-4 Pharmacokinetics of bis-pyridinium mono-aldoximes**

**Huba Kalász** (Hungary), Kamil Kuca, Kamil Musilek, Gellért Karvaly, Syed Nurulain, Kornélia Tekes

**09.20 - 09.30 Concluding remarks**

**10.00 Shuttle bus to Prague Airport**

# PROGRAMME

# POSTERS



## PROGRAMME – POSTERS

### S02P Structure and dynamics of cholinesterases and OP hydrolases

#### S02P-1 3D structure of natural tetrameric form of human butyrylcholinesterase obtained by Cryo-electron microscopy

**Konstantin M. Boyko** (Russia), Timur N. Baimukhametov, Yury M. Chesnokov, Michael Hons, Sofya V. Lushchekina, Peter Konarev, Alexey Lipkin, Alexandre L. Vasiliev, Patrick Masson, Vladimir Popov

#### S02P-2 Butyrylcholinesterase-proteins interactions in human blood serum

**Jacek Jasiecki** (Poland), Krzysztof Waleron, Bartosz Wasąg

#### S02P-3 Dimerization interface of cholinesterases: analysis of crystal structures, free energy molecular dynamics calculations, and *in silico* alanine screening

**Dana A. Novichkova** (Russia), Lushchekina S. V., Sussman Joel L.

### S03P Interaction of cholinesterases with substrates, inhibitors and reactivators

#### S03P-1 4-aminoquinolines as reversible inhibitors of human cholinesterase activity

**Anita Bosak** (Croatia), Dejan M. Opsenica, Goran Šinko, Matija Zlatar, Zrinka Kovarik

#### S03P-2 Synthesis of Nerve Agents' surrogates from Dialkyl Alkylphosphonates for Antidote Screening and Toxicological Studies

**Samir F. de A. Cavalcante** (Brazil, Czech Republic), Leandro B. Bernardo, Kamil Kuča, Alessandro B. C. Simas

#### S03P-3 Biological evaluation of cysteine targeted insecticides

**Martina Hrabínova, Monika Schmidt** (Czech Republic), Gorecki L., Kucera T., Psotka M., Svobodova B., Hrabcova V., Hepnarova V., Jun D., Kuca K., Musilek K., Korabecny J.

#### S03P-4 An alternative substrate for human erythrocyte Acetylcholinesterase activity detection

**Sheemona Chowdhary** (India), Rajasri Bhattacharyya, Dibyajyoti Banerjee

#### S03P-5 Acetylcholinesterase reactivators based on oxime-functionalized biodegradable ionic liquids

**Yevgen Karpichev** (Estonia), Illia Kapitanov, Nicholas Gathergood, Ondřej Soukup, Vendula Hepnarova, Daniel Jun, Kamil Kuča

#### S03P-6 *In silico* screening of novel BChE-reactivators

**Tomas Kucera** (Czech Republic), Rafael Dolezal, Kamil Musilek

#### S03P-7 Phenyltetrahydroisoquinoline-based triazole compounds are high-affinity potential reactivators of nerve agent-inhibited human acetylcholinesterase

**Nikolina Maček Hrvat** (Croatia), Jarosław Kalisiak, Antonio Zandona, Goran Šinko, Zoran Radić, K. Barry Sharpless, Palmer Taylor, Zrinka Kovarik

#### S03P-8 *In silico* and *In vitro* evaluation of two novel oximes K456 and K733 against paraoxon inhibited human acetylcholinesterase and butyrylcholinesterase

**Syed M Nurulain** (Pakistan), M. Qaiser Fatmi, Amna Iqbal, Shahrukh Malik, Huba Kalasz, Kamil Musilek, Kamil Kuca, Georg Petroianu

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- S03P-9** **Facile synthesis of cysteine-acetylcholinesterase targeted insecticides**  
**Miroslav Psoška** (*Czech Republic*), Lukas Gorecki, Barbora Svobodova, Kamil Musilek, Daniel Jun, Jan Korabecny, Kamil Kuca
- S03P-10** **Inhibition of human acetylcholinesterase and butyrylcholinesterase by methylene violet 3RAX**  
**Seda Onder** (*Turkey*), Kevser Biberoglu, Ozden Tacal
- S03P-11** **Molecular modeling studies on the interactions of aflatoxin B1 and its metabolites with peripheral and catalytic anionic sites of human acetylcholinesterase**  
**Joyce S. F. D. de Almeida** (*Brazil*), Rafael Dolezal, Samir F. de A. Cavalcante, Kamil Kuca, Kamil Musilek, Daniel Jun, Tanos C. C. França
- S03P-12** **Chlorinated pyridinium oximes are potent reactivators of acetylcholinesterase inhibited by nerve agents**  
**Tamara Zorbaz** (*Croatia*), Nikola Maraković, Kamil Musilek, Zrinka Kovarik
- S03P-13** **Bistable dynamic behavior of endogenous butyrylcholinesterase expressed in Expi293 cells**  
**Irina Zueva** (*Russia*), Sofya Lushchekina, Oksana Lockridge, Lawrence M. Schopfer, Patrick Masson
- S03P-14** **Expi 293 cells expressing an endogenous wild-type butyrylcholinesterase, and a variety of esterases that self-reactivates after phosphorylation by all types of organophosphorus agents**  
**Irina Zueva** (*Russia*), Oksana Lockridge, Lawrence M. Schopfer, Patrick Masson

## **S04P** **Reactivators of AChE, OP inhibitors – mechanism of toxicity, detection and analytical methods, diagnosis of exposure, detoxification and therapy; counter-terrorism strategies**

- S04P-1** **Reactivating efficacy of oximes K203 and K027 against a direct acetylcholinesterase inhibitor in rat diaphragm: dose-response modeling**  
**Evica Antonijevic** (*Serbia*), Kamil Musilek, Kamil Kuca, Danijela Djukic-Cosic, Marijana Curcic, Zorica Bulat, Biljana Antonijevic
- S04P-2** **Inhibition of cholinesterases following percutaneous intoxication with V agents in rats**  
**Jiri Bajgar** (*Czech Republic*), Kamil Kuca, Jiri Kassa
- S04P-3** **Near attack conformation approach for molecular modeling studies upon the prophylactic agent 7-methoxytacrine-4-pyridinealdoxime hybrid compared with other reactivators of VX-inhibited HssAChE**  
Jorge Alberto Valle da Silva, Eugenie Nepovimova, Kamil Kuča, Teodorico Castro Ramalho,  
**Tanos Celmar Costa França** (*Brazil, Czech Republic*)
- S04P-4** **Design, synthesis and *in vitro* evaluation of a promising new class of bifunctional uncharged hybrid reactivators for nerve agent-inhibited human acetylcholinesterase**  
**José Dias** (*France*), Julien De Sousa, Yeri Jagadeesh, Charlotte Courageux, Anne-Julie Gastellier, Christopher Timperley, Richard Brown, Gianluca Santoni, Martin Weik, Rachid Baati, Florian Nachon
- S04P-5** **The early tissue alteration induced by different oximes in rats**  
**Vesna Jačević** (*Republic of Serbia, Czech Republic*), Eugenie Nepovimova, Kamil Kuča



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- S04P-6**      **Cytotoxicity study of oxime@CB7 complexes for central nervous system penetration of quaternary acetylcholinesterase reactivators**  
**Petr Jost** (Czech Republic), Lubica Muckova, Jana Zdarova Karasova
- S04P-7**      **Brain Exposure of bis-Pyridinium Oxime KR-26256**  
Hyun Myung Lee, Sunjoo Ahn, Sung Hee Cho, Soo Bong Han, Hyejin Kim, Sang Ho Lee, Gyeunghaeng Hur, **Young-Sik Jung** (South Korea)
- S04P-8**      **Analysis of bis-pyridinium mono-aldoximes in serum and organs using a high-throughput high performance liquid chromatography approach**  
**Gellert Karvaly** (Hungary), Kornélia Tekes, Huba Kalász
- S04P-9**      **A comparison of the reactivating and therapeutic efficacy of a novel bispyridinium oxime K870 with commonly used pralidoxime and the oxime HI-6 in sarin-poisoned rats and mice**  
**Jiri Kassa** (Czech Republic), Vendula Hepnarova, Kamil Musilek, Daniel Jun
- S04P-10**     **The monoquaternary reactivators for the treatment of organophosphorous intoxication**  
Gorecki L., **Jan Korabecny** (Czech Republic), Svobodova B., Kucera T., Malinak D., Junova L., Hepnarova V., Hrabinoval M., Soukup O., Jun D., Musilek K., Kobrlova T., Konecny J., Psocka M., Dolezal R., Honegr J., Kuca K.
- S04P-11**     **Decontamination of warfare agent**  
**Jan Marek** (Czech Republic), Marketa Benkova, Jan Misik, Ondrej Soukup, Marek Matula, Daniel Jun
- S04P-12**     **In vitro characterization of the standard acetylcholinesterase reactivators**  
**Lubica Muckova, Vendula Hepnarova** (Czech Republic), Misik J., Jun D., Soukup O.
- S04P-13**     **Uncharged Reactivators of Cholinesterases Inhibited by Organophosphorus Nerve Agents**  
**Nicolas Probst** (France), A. Braïki, P. Warnault, J. Renou, C. Gomez, G. Mercey, T. Verdelet, R. Baati, J. Dias, G. Calas, F. Nachon, M. Weik, L. Jean, P. Y. Renard
- S04P-14**     **In vitro determination of oxidative stress induced by oxime reactivators using chromatographic methods**  
**Nela Váňová** (Czech Republic), Mišík J., Múčková L., Herman D., Pejchal J.
- S04P-15**     **In vitro evaluation of quinuclidinium oximes as reactivators of human cholinesterases inhibited by organophosphorus compounds**  
**Antonio Zandona** (Croatia), Ines Primožič, Maja Katalinić, Zrinka Kovarik

## S05P      Enzymes and proteins other than ChEs interacting with OP

- S05P-1**      **Determination of BChE Activity by Mass Spectrometric Analysis of Its Adduct with Russian Vx**  
**Ekaterina A. Murashko** (Russia), Dubrovskii Ya. A., Belyukov P.P., Radilov A.S., Babakov V.N.
- S05P-2**      **An in-vitro induction of Paraoxonase 3 activity in Hepatocytes by Resveratrol**  
**Kumari Priyanka** (India), Kiran Dip Gill, Surjit Singh, Indu Verma

## PROGRAMME – POSTERS

### S06P Stoichiometric biocavangers, biotechnology and therapeutical aspects

#### S06P-1 Smart & Innovative Tools for Cholinesterases Related Applications

**Emilie David** (France), Benoît Roubinet

#### S06P-2 *In Vitro* Evaluation of Standard Acetylcholinesterase Reactivators as Reactivators of Human Plasma Butyrylcholinesterase

**Lucie Junova** (Czech Republic), Vendula Sepsova, Kamil Musilek, Daniel Jun

#### S06P-3 Novel bisquaternary heteroaromatic compounds as potential reactivators of human butyrylcholinesterase

**David Malinak, Eugenie Nepovimova** (Czech Republic), Marketa Neugebauerova, Miroslava Hozova, Vendula Hepnarova, Daniel Jun, Rafael Dolezal, Kamil Musilek, Kamil Kuca

### S09P Biological functions, development and non-cholinergic function of cholinesterases

#### S09P-1 Butyrylcholinesterase and its variants (rs3495 & rs1803274) association with Major Depressive Disorder

**Sliha Awan** (Pakistan), Syed M Nurulain, Sadaf Munir, Sania Ghafoor, Rabia Habib, Maleeha Azam

#### S09P-2 Alkaloids derived from traditional Chinese medicine are inhibitors for inflammation and acetylcholinesterase

**Xiang P. Kong** (China), Miranda L. Xu, Etta Y. L. Liu, Qiyun Wu, Tina T. X. Dong, David C. C. Wan, Karl W. K. Tsim

#### S09P-3 Acetylcholinesterase regulates inflammatory responses in cultured macrophages: a player in cholinergic anti-inflammatory pathway

**Etta Y. L. Liu** (China), Miranda L. Xu, Xiang P. Kong, Qiyun Wu, Tina T. X. Dong, Karl W. K. Tsim

#### S09P-4 Genistein, a phytoestrogen in soybean, induces the expression of acetylcholinesterase via G protein-coupled receptor 30 in PC12 cells

**Etta Y. L. Liu** (China), Miranda L. Xu, Qiyun Wu, Tina T.X. Dong, Sibao Chen, Karl W. K. Tsim

#### S09P-5 Status of Cholinesterases in Heroin, Hashish (Cannabis) and Polydrug Addicts

**Syed M Nurulain** (Pakistan), Sliha Awan, Sadaf Munir, Tahira Javed, Sania Ghafoor, Rabia Habib

#### S09P-6 Indirect effects of dioxin on neuronal AChE expression via astrocytes

**Rui Sha** (China), Yangsheng Chen, Yiyun Liu, Li Xu, Heidi Qunhui Xie, Bin Zhao

#### S09P-7 Non-neuronal cholinergic system in rat aorta

**Kristína Szmicseková** (Slovak Republic, France), Kiliánová Z., Krajčovičová K., Krejci E., Paul Hrabovská A.

#### S09P-8 Microphthalmia-associated transcription factor regulates acetylcholinesterase expression during melanogenesis of B16F10 cells: a cholinergic regulator in pigmentation

**Qiyun Wu** (China), Aster H. Y. Fung, Miranda L. Xu, Etta Y. L. Liu, Ran Duan, Ping Yao, Tina T. X. Dong, Karl W. K. Tsim

## PROGRAMME – POSTERS

### S10P Alzheimer's disease and diseases related to cholinesterases

**S10P-1** Dual binding site inhibitors of acetylcholinesterase as therapeutic treatments for Alzheimer's disease: any need for an update?

**Konstantin Petrov** (*Russia*), I. Zueva, J. Dias, S. Lushchekina, V. Semenov, F. Nachon, E. Nikolsky, P. Masson

**S10P-2** Detection of Alzheimer's drug candidate by Surface-Enhanced Raman Spectroscopy

**Jan Proska** (*Czech Republic*), Lucie Maresova, Marek Prochazka, Eugenie Nepovimova, Kamil Kuca

### S11P Multi-target-directed ligands in Alzheimer's disease primarily targeting cholinesterases

**S11P-1** Butyrylcholinesterase inhibitors grafted with antioxidant and neuroprotective activities: novel multifunctional ligands for Alzheimer's disease

**Damijan Knez** (*Slovenia*), Nicolas Coquelle, Anja Pišlar, Simon Žakelj, Marko Jukič, Matej Sova, Janez Mravljak, Florian Nachon, Xavier Brazzolotto, Janko Kos, Jacques-Philippe Colletier, Stanislav Gobec

**S11P-2** 7-MEOTA-donepezil hybrids: Potential cholinesterase inhibitors for the treatment of Alzheimer's disease

**Katarina Spilovska** (*Czech Republic*), Eva Mezeiova, Jan Korabecny, Jana Hroudova, Vendula Hepnarova, Martina Hrabnova, Ondrej Soukup, Kamil Musilek, Daniel Jun, Kamil Kuca