



11th International Meeting on Cholinesterases



4-9 June 2012
Kazan, Russia

11th International Meeting on Cholinesterases

PROGRAM

June 4-9, 2012
Kazan, Russia

ORGANIZERS



Russian Academy of Sciences



Kazan (Volga Region) Federal University



Lomonosov Moscow State University



Emanuel Institute of Biochemical Physics



Kazan Scientific Center of Russian Academy of Sciences



Arbuzov Institute of Organic and Physical Chemistry



Kazan State Medical University



Kazan Institute of Biochemistry and Biophysics



Institute of Physiologically Active Compounds

Monday, 4 June 2012	
9:00	Registration Poster mounting Testing MS Power Point Presentation
16:00	Opening Welcome addresses
16:30-17:00	Alexander Konovalov (Kazan, Russia) Kazan school of chemistry: from foundation to present
17:00-17:45	Sergei Varfolomeev (Moscow, Russia) History of cholinesterase research in USSR and Russia
17:45-18:00	Zrinka Kovarik (Zagreb, Croatia) Tribute to Elsa Reiner
Plenary lectures	
Chairpersons: Patrick Masson (France), Sergei Varfolomeev (Russia)	
18:00-18:45 PL-1	The EMBO Plenary lecture Joel Sussman (Rehovot, Israel) Acetylcholinesterase: from 3D structure to drug design
18:45-19:30 PL-2	Oksana Lockridge (Omaha, USA) Human butyrylcholinesterase: from basic structure to medical applications
20:00	Welcome party

Tuesday, 5 June 2012		
Session 1: Structure and dynamics of cholinesterases and related α/β hydrolase-fold proteins		
Chairpersons: Fredrik Ekström (Sweden), Joel Sussman (Israel)		
8:00-8:20	L1-1	Palmer Taylor (La Jolla, USA) Approaching forty: the cholinesterases leading the α,β -hydrolase-fold structure-function quest
8:25-8:45	L1-2	Pascale Marchot (Marseille, France) Recent structural and mutagenesis insights into allosteric inhibition of AChE by peptidic ligands
8:50-9:00	L1-3	Schroeder Noble (Silver Spring, USA) Crystal structures of acetylcholinesterase in complex with novel bis-imidazoloxime reactivators
9:05-9:25	L1-4	Fredrik Ekström (Umeå, Sweden) Targeting acetylcholinesterase; from high throughput screening of a chemical library to quantitative structure-activity relationships
9:30-9:45	Coffee Break	
9:45-9:55	L1-5	Anna Linusson (Umeå, Sweden) Enantiomers define non-covalent interactions in the catalytic site of acetylcholinesterase
10:00-10:20	L1-6	Judith Peters (Grenoble, France) Acetylcholinesterase dynamics investigated by incoherent neutron scattering
10:25-10:45	L1-7	Martin Weik (Grenoble, France) Structural dynamics of acetylcholinesterase as studied by kinetic crystallography
10:50-11:00	L1-8	Arlan Gonçalves (Guarapari, Brazil) Molecular dynamics simulations and QM/MM studies of the reactivation by 2-PAM of tabun inhibited human acethylcholinesterase
11:05-11:15	L1-9	Sofya Lushchekina (Moscow, Russia) Computational modeling of hysteresis in Ala328Cys mutant of human butyrylcholinesterase
11:20-11:30	L1-10	Swapna David (Coimbatore, India) Why human butyrylcholinesterase L307P variant is not structurally stable: a molecular dynamics simulation study
11:35-11:50	Coffee Break	

Session 2: Interaction of cholinesterases with substrates, inhibitors and reactivators.		
Chairpersons: Terrone Rosenberry (USA), Yaacov Ashani (Israel)		
11:50-12:00		Patrick Masson (Grenoble, France) Tribute to Sergei Moralev
12:00-12:20	L2-1	Israel Silman (Rehovot, Israel) Reversible and irreversible inhibition of acetylcholinesterase by the photosensitizer methylene blue
12:25-12:45	L2-2	Terrone Rosenberry (Jacksonville, USA) The rate-limiting step for the second-order hydrolysis of acetylcholine analogs by acetylcholinesterase (k_{cat}/K_M) is gated entry to the catalytic triad
12:50-13:10	L2-3	Jure Stojan (Ljubljana, Slovenia) The significance of low substrate concentration measurements for mechanistic interpretation in cholinesterases
13:15-14:15	Lunch	
14:15-14:25	L2-4	Alexander Nemukhin (Moscow, Russia) QM/MM approaches to resolve the catalytic mechanism of cholinesterases
14:30-14:50	L2-5	Chang-Guo Zhan (Lexington, USA) Reaction pathways of cholinesterases with various types of compounds: computational insights and implication for rational drug design
14:55-15:15	L2-6	Paul Carlier (Blacksburg, USA) Designing inhibitors for potency against the G119S resistant mutant of <i>Anopheles gambiae</i> acetylcholinesterase
15:20-15:30	L2-7	Kamil Kuča (Hradec Kralove, Czech Republic) Quaternary compounds designed for cholinesterase inhibition and modulation of cholinergic receptors
15:35-15:45	L2-8	Donald Maxwell (Aberdeen Proving Ground, USA) A common mechanism for resistance of agent-inhibited acetylcholinesterase to oxime reactivation based on QSAR of nerve agent analogues of sarin, cyclosarin and tabun
15:50-16:10	Coffee Break	

16:10-16:30	L2-9	Zrinka Kovarik (Zagreb, Croatia) Reactivation of tabun-phosphorylated cholinesterases probed by mutagenesis and new oximes
16:35-16:55	L2-10	Apurba Bhattacharjee (Silver Spring, USA) Discovery of non-oxime reactivators of OP-inhibited acetylcholinesterase (AChE) using <i>in silico</i> generated pharmacophore models
17:00-17:10	L2-11	Julien Renou (Rouen, France) Synthesis of new uncharged reactivators for acetylcholinesterase
17:15-17:25	L2-12	Pierre-Yves Renard (Rouen, France) <i>In vitro</i> evaluation of 3-hydroxy 2-pyridinaldoxime conjugates as efficient uncharged reactivators for the dephosphylation of poisoned human acetylcholinesterase
17:30-17:50	Coffee Break	
Session 7A: Novel approaches to the treatment of Alzheimer disease. Chairpersons: Ezio Giacobini (Switzerland), Giancarlo Pepeu (Italy)		
17:50-18:10	L7A-1	Ezio Giacobini (Geneva, Switzerland) Cholinesterase inhibitors: from neurotoxic agents to drugs of choice to treat Alzheimer disease
18:15-18:35	L7A-2	Giancarlo Pepeu (Florence, Italy) Cholinesterase inhibitors affect attention and memory
18:40-19:00	L7A-3	Gabriel Gold (Geneva, Switzerland) Cholinesterase inhibitors in the treatment of non-Alzheimer types of dementia
19:05-19:25	L7A-4	Taher Darreh-Shori (Stockholm, Sweden) The role of cholinesterases in AD pathology: implications for improving efficacy of cholinesterase inhibitors
19:30-19:50	L7A-5	Sultan Darvesh (Halifax, Canada) Butyrylcholinesterase radioligands to image Alzheimer disease brain
19:55-20:05	L7A-6	Ricardo Souza (Curitiba, Brazil) Association analysis between K and -116 variants of butyrylcholinesterase and Alzheimer's disease in a Brazilian population

Wednesday, 6 June 2012

Session 3: Anticholinesterases: Mechanisms of toxicity, detection and analytical methods, diagnosis of exposure, detoxification and therapy; counter-terrorism strategies.

Chairpersons: Oksana Lockridge (USA), Franz Worek (Germany)

8:00-8:20	L3-1	Oksana Lockridge (Omaha, USA) Mass spectrometry for detection of exposure to organophosphorus compounds
8:25-8:35	L3-2	Judit Marsillach (Seattle, USA) Human butyrylcholinesterase, a mass spectrometric biomarker for organophosphorus exposure
8:40-8:50	L3-3	Mariya Liyasova (Omaha, USA) Butyrylcholinesterase is a biomarker of exposure to tri-ortho-cresyl phosphate, an agent implicated in “aerotoxic syndrome”
8:55-9:05	L3-4	Marcel van der Schans (Rijswijk, The Netherlands) Methods for unequivocal assessment of exposure to chemical warfare agents based on covalent protein adducts
9:10-9:20	L3-5	Robert VanDine (Sarasota, USA) A point of care 10 minute assay for detection of blood protein adducts resulting from low level exposure to organophosphate nerve agents
9:25-9:45	L3-7	Hermona Soreq (Jerusalem, Israel) Prophylactic antagomiRs-mediated enhancement of host acetylcholinesterase protects from organophosphate poisoning
9:50-10:10	L3-8	Bhupendra Doctor (Silver Spring, USA) A unique combination of (-)-Huperzine A and (+)-Huperzine A effectively and reversibly inhibits acetylcholinesterase as well as reduces NMDA-induced seizures and glutamate-induced toxicity
10:15-10:35	L3-9	Franz Worek (Munich, Germany) Structural requirements for effective oximes — a kinetic <i>in vitro</i> study with phosphorylated human AChE and structurally different oximes
10:40-11:10	Coffee Break	

11:10-11:20	L3-10	Tsung-Ming Shih (Aberdeen Proving Ground, USA) Searching for an effective <i>in vivo</i> reactivator for OP nerve agent-inhibited AChE in the central nervous system
11:25-11:35	L3-11	Christophor Dishovsky (Sofia, Bulgaria) <i>In vitro</i> investigation of efficacy of new reactivators of cholinesterase on OPC-inhibited rat brain AChE
11:40-11:50	L3-12	Janice Chambers (Starkville, USA) Development of novel brain-penetrating oxime reactivators of acetylcholinesterase inhibited by organophosphates
11:55-12:05	L3-13	John Graham (Aberdeen Proving Ground, USA) Facilitated transport of reactivators across the blood brain barrier
12:10-12:30	L3-14	Marloes Joosen (Rijswijk, The Netherlands) Timing of decontamination and treatment in case of percutaneous poisoning with VX
12:35-12:55	L3-15	Guy Testylier (La Tronche, France) Ketamine combinations for the field treatment of soman-induced self-sustaining status epilepticus. Review of the current data and perspectives

13:00-14:00 Lunch

Session 4: Stoichiometric and catalytic bioscavengers against anticholinesterase agents; nanobiotechnology for cholinesterases and related therapeutic aspects.

Chairpersons: Douglas Cerasoli (USA), Patrick Masson (France).

14:00-14:20	L4-1	Douglas Cerasoli (Aberdeen Proving Ground, USA) The protective efficacy of human butyrylcholinesterase against exposure to organophosphorus nerve agents
14:25-14:45	L4-2	Helen Mumford (Salisbury, UK) Human plasma-derived BuChE as a stoichiometric bioscavenger for treatment of nerve agent poisoning
14:50-15:00	L4-3	Yvonne Rosenberg (Rockville, USA) Protection by aerosolized recombinant macaque butyrylcholinesterase against aerosolized paraoxon exposure in homologous macaques

15:05-15:25	L4-4	Tsafrir Mor (Tempe, USA) Plant-produced butyrylcholinesterase variants as versatile bioscavengers
15:30-15:50	L4-5	Nageswaraao Chilukuri (Aberdeen Proving Ground, USA) The use of adenovirus to deliver therapeutic levels of bioscavengers against anticholinesterase agents
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15:55-16:25	Coffee Break	
16:25-16:45	L4-6	Yakov Ashani (Rehovot, Israel) Analysis of the inputs required for estimating catalytic scavenger doses needed to protect against OP intoxication
17:50-17:10	L4-7	Moshe Goldsmith (Rehovot, Israel) Directed evolution of serum paraoxonase 1 for broad spectrum G-agent hydrolysis
17:15-17:25	L4-8	Tamara Otto (Aberdeen Proving Ground, USA) Identification and characterization of novel catalytic bioscavengers
17:30-17:40	L4-9	Manojkumar Valiyaveettil (Silver Spring, USA) Crossroads in therapeutic evaluation of paraoxonase 1 in nerve agent toxicity
18.45-18.05		Elena Efremenko (Moscow, Russia) Bacterial phosphotriesterases, effective enzymes for degradation of OPs: genetic engineering, applications to destruction of CWA and decontamination
19:00	Conference dinner	

Thursday, 7 June 2012		
Session 4: Stoichiometric and catalytic bioscavengers against anticholinesterase agents; nanobiotechnology for cholinesterases and related therapeutic aspects (continued)		
Chairpersons: Douglas Cerasoli (USA), Patrick Masson (France).		
8:00-8:10	L4-10	Sean Hodgins (Aberdeen Proving Ground, USA) Biochemical characterization and <i>in vivo</i> anti-OP protective efficacy of recombinant huPON1 expressed in <i>Trichoplusia ni</i> larvae
8:15-8:25	L4-11	Shane Kasten (Aberdeen Proving Ground, USA) <i>The in vitro</i> specificity and <i>in vivo</i> protective efficacy of PON1 variants against exposure to organophosphorus nerve agents
8:30-8:50	L4-12	Alexander Kabanov (Moscow, Russia) Nanozymes as potential bioscavengers for prevention and reparation of damage caused by OP compounds
8:55-9:05	L4-13	Stephen Kirby (Aberdeen Proving Ground, USA) An engineered mutant of human platelet activating factor acetylhydrolase hydrolyzes organophosphorus nerve agents
9:10-9:20	L4-14	Robert diTargiani (Aberdeen Proving Ground, USA) Catalytic activity of human prolidase and its variants against nerve agents
9:25-9:55	Coffee Break	
9:55-10:05	L4-15	Pierre-Yves Renard (Rouen, France) Strategies for the selection of catalytic antibodies against OP nerve agents
10:10-10:30	L4-16	Alexander Gabibov (Moscow, Russia) Catalytic antibodies reacting with OP compounds
10:35-10:45	L4-17	François Estour (Rouen, France) Functionalized cyclodextrins – a promising way to degrade nerve agents
10:50-11:10	L4-18	Steve Brimijoin (Rochester, USA) Progress toward gene transfer of modified human BuChE as a therapy for cocaine addiction

11:15-11:25	L4-19	Yang Gao (Rochester, USA) Cocaine hydrolase and anti-cocaine antibody combine to reduce cocaine stimulation and toxicity
11:30-12:00		Coffee Break
Session 5: Enzymes other than cholinesterases reacting with anticholinesterase agents.		
Chairpersons: Clement Furlong (USA), Galina Makhaeva (Russia)		
12:00-12:20	L5-1	John Casida (Berkeley, USA) Anticholinesterase insecticide retrospective
12:25-12:45	L5-2	Philip Potter (Memphis, USA) Carboxylesterases as targets for anticholinesterase agents
12:50-13:10	L5-3	Rudy Richardson (Ann Arbor, USA) Neuropathy target esterase: overview and future
13:15-13:35	L5-4	Clement Furlong (Seattle, USA) Tert-butylated triaryl phosphates are not readily metabolized to serine esterase inhibitors
13:40-14:40	Lunch	
14:40-15:00	L5-5	Eugenio Vilanova (Elche, Spain) Differential interactions of neuropathy inducers, non-inducers and promoters with soluble and membrane esterases: Kinetic approaches
15:05-15:25	L5-6	Galina Makhaeva (Chernogolovka, Russia) Organophosphorus compound esterase profiles as predictors of therapeutic and toxic effects
15:30-15:50	L5-7	Dragomir Draganov (Ashland, USA) How does Paraoxonase 1 work <i>in vivo</i> – the indirect model
15:55-16:15	L5-8	Giuseppe Manco (Napoli, Italy) Hyperthermophilic phosphotriesterases/lactonases: structure, function and possible applications
16:20-16:50		Coffee Break

3D Session

Chairpersons: Zoran Radić (USA), Martin Weik (France)

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- 16:50-17:20 3D-1 **Florian Nachon** (La Tronche, France)
Structural aspects of the inhibition of cholinesterases by cresyl saligenin phosphate (CBDP)
- 17:25-17:55 3D-2 **Zoran Radić** (La Jolla, USA)
Mechanism of interaction of novel uncharged, centrally active reactivators with OP-hAChE conjugates
- 18:00-18:15 3D-3 **Rathanam Boopathy** (Coimbatore, India)
Structure based repurposing of FDA approved drugs as acetylcholinesterase inhibitors
- 18:20-18:50 3D-4 **Eric Chabrière** (Marseille, France)
Structural Biology contributions in the understanding and increase of phosphotriesterase activities
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Friday, 8 June 2012

Session 6: Molecular biology and cell biology of cholinesterases and alternative functions of cholinesterases.

Chairpersons: Karl Tsim (China), Arnaud Chatonnet (France)

9:00-9:10		Claire Legay (Paris, France) Tribute to Jean Massoulié
9:10-9:30	L6-1	Claire Legay (Paris, France) Developmental consequences of the ColQ/MuSK interaction
9:35-9:55	L6-2	Karl Tsim (Hong Kong, China) Molecular assembly of PRiMA-linked acetylcholinesterase: the roles of t-peptide, FHB domain and N-linked glycosylation
10:00-10:10	L6-3	Paul Layer (Darmstadt, Germany) Alternative functions of cholinesterases during embryonic development of chick and mouse
10:15-10:25	L6-4	Janez Sketelj (Ljubljana, Slovenia) Several mechanisms regulate acetylcholinesterase-associated collagen Q expression in slow and fast muscle fibers of rat muscles
<hr/> 10:30-11:00 Coffee Break		
11:00-11:20	L6-5	Leo Pezzementi (Birmingham, USA) Do the MRL proteins - MIG-10, RIAM, and lamellipodin - interact with acetylcholinesterase and butyrylcholinesterase?
11:25-11:45	L6-6	Susan Greenfield (Oxford, UK) Non-hydrolytic effects of AChE: the actions of peptides derived from the C-terminal
11:50-12:10	L6-7	Zoran Grubič (Ljubljana, Slovenia) Classical and alternative roles of acetylcholinesterase in the <i>in vitro</i> innervated human skeletal muscle
12:15-12:25	L6-8	Astrid Vogel-Höpker (Darmstadt, Germany) Alternative cholinolytic function of Acetylcholinesterase in skeletogenesis

12:30-12:40	L6-9	Nicolas Lenfant (Montpellier, France) Proteins with an α/β hydrolase fold: how to decipher new functions in an ever growing superfamily?
12:45-13:45		Lunch
13:45-13:55	L6-10	Xue Jun Zhang (Shanghai, China) Regulation of acetylcholinesterase expression in cell apoptosis
14:00-14:10	L6-11	Anthony Turner (Leeds, UK) Acetylcholinesterase and Alzheimer's disease: novel interactions and regulatory mechanisms
14:15-14:25	L6-12	Yifan Han (Hong Kong, China) Novel dimeric anticholinesterases derived from Chinese herb: molecular basis for unexpected neuroprotection via multiple targets
14:30-14:40	L6-14	Ebru Bodur (Ankara, Turkey) Effects of exercise and conjugated linoleic acid (CLA) usage on BChE and obesity in men
16:00		Excursion

Saturday, 9 June 2012

Session 7B: Diseases related to cholinesterases, and cholinesterase inhibitors therapy.

Chairpersons: Eric Krejci (France), Enver Bogdanov (Russia)

9:00-9:20	L7B-1	Kinji Ohno (Nagoya, Japan) Specific binding of collagen Q to the neuromuscular junction is exploited to cure congenital myasthenia and to explore bases of myasthenia gravis
9:25-9:35	L7B-2	Lupe Furtado-Alle (Curitiba, Brazil) -116A and K BCHE gene variants associated with obesity and hypertryglyceridemia in adolescents from Southern Brazil
9:40-9:50	L7B-3	Ricardo Souza (Curitiba, Brazil) Copy number variation at 7q22 and 3q26 in sporadic breast cancer
9:55-10:15	L7B-4	Eric Krejci (Paris, France) A novel insight into acetylcholinesterase functions in the nervous system provided by the mutant mice
10:20-10:40	L7B-5	Cecilio Vidal (Murcia, Spain) The AChE membrane binding tail PRiMA is down-regulated in muscle and nerve of mice with muscular dystrophy by merosin deficiency

10:45-11:15 Coffee Break

11:15-11:25	L7B-6	Anna Hrabovska (Bratislava, Slovakia) Studying cholinesterases in biological samples
11:30-11:40	L7B-7	Ian Macdonald (Halifax, Canada) Radioligands for imaging cholinesterases in brain
11:45-12:05	L7B-8	Konstantin Petrov (Kazan, Russia) Tissue-specific inhibitors of acetylcholinesterase for treatment of myasthenia gravis
12:25-12:35	L7B-9	Irina Kovyazina (Kazan, Russia) Nitric oxide is an endogenous regulator of acetylcholinesterase activity in mammalian neuromuscular junction

12:40-12:50	L7B-10	Madhusoodana P. Nambiar (Silver Spring, USA) Modulation of cholinergic pathways in blast-induced traumatic brain injury
12:55-13:10	L7B-11	Natalya Zalutskaya (St.Petersburg, Russia) Results of monotherapy in patients with Alzheimer's disease and vascular dementia by anticholinesterase drug Axamon
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13:15-14:15 Lunch		
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3D Session (continued)		
Chairpersons: Zoran Radić (USA), Martin Weik (France)		
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14:15-14:45	3D-5	Yves Bourne (Marseille, France) Structural bases for a novel mechanism of AChE inhibition
14:50-15:20	3D-6	Yechun Xu (Shanghai, China) The dynamic behavior of residues along the long active-site gorge of AChE and their relationship to the ligand traffic
15:25-15:40	3D-7	Gianluca Santoni (Grenoble, France) Conformational variabilities in human and <i>Torpedo californica</i> acetylcholinesterases studied by MD simulations and kinetic crystallography
15:45-16:15	3D-8	Jacques-Philippe Colletier (Grenoble, France) Structural evidence for the interaction of acetylcholinesterase and the amyloid-beta peptide
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16:20-16:50	Coffee Break	
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17:00	Closing	
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Patrick Masson (Grenoble, France), Zoran Radić (La Jolla, USA) Summing up of the 11 th Meeting on Cholinesterases Farewell addresses		

LIST OF POSTERS

Session 1: Structure and dynamics of cholinesterases and related α/β hydrolase-fold proteins.

- P1-1. PROLINE RICH PEPTIDES FROM SOLUBLE TETRAMERIC FETAL BOVINE SERUM ACETYLCHOLINESTERASE AND HORSE BUTYRYLCHOLINESTERASE
K. Biberoglu, L.M. Schopfer, A. Saxena, O. Tacal, O. Lockridge
- P1-2. COMPUTATIONAL STUDY OF THE CHOLINESTERASE DYNAMICS
D.A. Novichkova, S.V. Luschkina, P. Masson, A.V. Nemukhin, S.D. Varfolomeev
- P1-3. ANALYSIS AND COMPARISON OF 3D-STRUCTURES OF ACETYLCHOLINESTERASE
V.S. Polomskih, **S.V. Luschkina**, A.V. Nemukhin, S.D. Varfolomeev
- P1-4. DYNAMICS, ACTIVITY AND STABILITY RELATIONSHIP WITHIN THE CHOLINESTERASE FAMILY
M.Trovaslet, M. Trapp, F.Nachon, M.Tehei, M.Weik, P.Masson, J.Peters

Session 2: Interaction of cholinesterases with substrates, inhibitors and reactivators.

- P2-1. THE ACETYLCHOLINESTERASE SITES EFFECTS ON THE INTERACTION OF SER203 WITH PYRIDOXINE DERIVATIVES
R. Ch. Ayupov, N.I. Akberova, D.S. Tarasov
- P2-2. EXPLORING THE LIGAND-BINDING PROPERTIES OF ACETYLCHOLINESTERASE - THE IMPORTANCE OF WEAK HYDROGEN BONDS
L. Berg, Fr. Ekström, A. Linusson
- P2-3. SCREENING FOR NATURALLY OCCURRING P-SITE INHIBITORS OF ACETYLCHOLINESTERASE THAT BLOCK ORGANOPHOSPHATE INACTIVATION
V. Beri, T. Rosenberry
- P2-4. A COMPUTATIONAL PERSPECTIVE OF MOLECULAR INTERACTIONS THROUGH PHARMACOPHORE BASED VIRTUAL SCREENING FOR IDENTIFYING POTENTIAL BIVALENT INHIBITORS OF NATURAL ORIGIN AGAINST HUMAN ACETYLCHOLINESTERASE AND BUTYRYLCHOLINESTERASE
L. Venkatachalam, S. K. Venkatesan, E. Selvaraj, R. Boopathy

- P2-5. STRUCTURE-ACTIVITY RELATIONSHIP IN INTERACTIONS OF CHOLINESTERASES WITH BISDIMETHYLCARBAMATES
A. Bosak, I. Gazić, V. Vinković, G. Šinko, A. Štimac, Z. Kovarik
- P2-6. OXIME REACTIVATION OF NERVE AGENT-INHIBITED ACETYLCHOLINESTERASE (ACHE) PROBED USING RECOMBINANT HUMAN AChE MUTANT ENZYMES
C. Chambers, C. Luo, A. Saxena
- P2-7. STRUCTURES OF RECOMBINANT HUMAN ACETYLCHOLINESTERASE COMPLEXED WITH FAS-2 WITH BOUND ACTIVE SITE INHIBITORS
J. Cheung, M. Franklin, M. Rudolph, F. Burshteyn, M. Cassidy, E. Gary, J. Height, W. Hendrickson, W. Appel
- P2-8. EFFECT OF DIFFERENT BUFFERS ON ELLMAN'S REAGENT ACTION
D. Dingová, A. Hrabovská
- P2-9. HI-6 AND OBIDOXIME IMPLICATION IN OXIDATIVE STRESS: GUINEA PIG MODEL
L. Drtinova, M. Pohanka, V. Sepsova, F. Zemek, J. Zdarova Karasova, Z. Krenkova, J. Misik, J. Korabecny
- P2-10. MOLECULAR ASPECTS OF THE REACTIVATION OF ACETYLCHOLIN-ESTERASE INHIBITED BY THE CARBAMATE CARBOFURAN
K.S. Matos, T.C.C. França, E.F.F. Cunha, T.C. Ramalho, K. Kuca
- P2-11. DOCKING STUDIES OF SARIN-INHIBITED ACETYLCHOLINESTERASE: MOLECULAR DOCKING VERSUS *IN VITRO* DATA
T.C.C. França, J.S.F.D. Almeida, A.P. Guimarães, M. N. Rennó, T.C. Ramalho, A.S. Gonçalves, M.C. de Koning
- P2-12. INTERACTIONS OF PYRIDINIUM OXIMES WITH THE PERIPHERAL ALOSTERIC SITE LIMIT THEIR EFFICIENCY IN REACTIVATION OF PHOSPHORYLATED AChE
M. Katalinić, N. Maček, G. Šinko, Z. Kovarik
- P2-13. IDENTIFICATION OF COMPOUNDS THAT PROTECT AND REACTIVATE ACETYLCHOLINESTERASE
F.S. Katz, L. Schneider, M. Luzac, A. Hastings-Robinson, D.W. Landry, M.N. Stojanovic
- P2-14. SYNTHESIS, BIOLOGICAL ASSESSMENT AND MOLECULAR MODELING OF NOVEL TACRINE-7 METHOXYTACRINE HETERODIMERS FOR ALZHEIMER DISEASE TREATMENT
J. Korabecny, S. Hamuľakova, K. Babkova, A. Horova, K. Musilek, K. Spilovska, J. Imrich, V. Opletalova, Z. Gazova, J. Zdarova Karasova, J. Hroudova, Z. Fisar, L. Gaľa, M. Valko, J. Kassa, K. Kuca

- P2-15. STUDY OF NEW DERIVATES OF CARBAMATES AND THEIR INHIBITION OF ACETYLCHOLINESTERASE
M. Kovářová, K. Komers, Š. Štěpánková
- P2-16. KINETICS AND COMPUTATIONAL PREDICTIONS OF FLUORINATED CARBETHOXY 1-AMINOPHOSPHONATE REACTIVITY WITH SERINE ESTERASES
S.V. Lushchekina, G.F. Makhaeva, O.G. Serebryakova, A.Y. Aksinenko, R.J. Richardson
- P2-17. COMPUTATIONAL MODELING OF INTERACTION BETWEEN CHOLINESTERASES AND CRESYL SALIGENIN PHOSPHATE
S.V. Luschevskaya, V.S. Polomskih, P. Masson, A.V. Nemukhin, S.D. Varfolomeev
- P2-18. EXPLORING THE PERIPHERAL SITE OF BUTYRYLCHOLINESTERASE
I.R. Macdonald, E. Martin, S. Darvesh
- P2-19. NOVEL AND RE-EVALUATED ACTIVITIES IN THE SERIES OF N-ALKYLATED-TACRINE DERIVATIVES: SYNTHESIS, BIOLOGICAL EVALUATION AND MOLECULAR MODELING
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- P3-3. A PHARMACOKINETIC PROFILE OF HI-6 DMS IN THE CONSCIOUS GUINEA PIG
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- P6-12. PC12 CELLS AS A RELIABLE MODEL FOR CHARACTERIZING BIOACTIVITY OF ACHE PEPTIDES.
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L.O. Guimarães, T.E. Setoguchi, G.F. Bono, M.B. Brandão, E.A.C.F. Maia, I.C.R. dos Santos, G. Picheth, R.R. Réa, A.C.R. de A. Faria, **R.L.R. Souza**, L.F. Alle
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- P7-7. THE INTERACTION OF TACRINE AND 7-MEOTA WITH NEURONAL NICOTINIC RECEPTOR
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- P7-10. THE INTERACTION OF REVERSIBLE ACETYLCHOLINESTERASE INHIBITORS WITH THE NICOTINIC RECEPTORS - *IN VITRO* TESTING
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- P3D-1. TEMPLATE DESIGNING FOR ALZHEIMER'S DISEASE DRUG: TOWARDS PREDICTION OF BEST KNOWN INHIBITORS FOR CHOLINESTERASES
L. Venkatachalam, R. Boopathy

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