Scientific Program

XXIX Symposium on Bioinformatics and Computer-Aided Drug Discovery (BCADD 2023)

Monday September 18, 2023

Chairpersons: Vladimir Poroikov and Roman Efremov

8:30*		**Opening of the Symposium**	
		Speaker	**Title**
Plenary lecture	9:00	**Roman Zubarev**	**CHEMICAL PROTEOMICS IN DRUG DESIGN**
	9:30	**Mikhail Panteleev**	**COMPUTATIONAL PHYSIOLOGY AND DRUG DEVELOPMENT**
Oral presentations	10:00	**Arli Aditya Parikesit**	**DRUG PROPERTIES AND DRUG LIGAND-BINDING COMPARISON ANALYSIS ON TENOFOVIR AND ZIDOVUDINE AS A REVERSE TRANSCRIPTASE INHIBITOR OF HIV-1**
	10:20	**Allan Kalueff**	**AI-POWERED IN VIVO SCREENS FOR NEUROACTIVE DRUG DISCOVERY USING ZEBRAFISH (DANIO RERIO)**
	10:40	**Bhaskar Ganguly**	**FUNCTIONAL PROFILING OF MATURE VERSUS IMMATURE DENDRITIC CELL EXOSOME-SHUTTLE miRNAs**
Keynote lectures	11:00	**G. Narahari Sastry**	**THE IMPACT OF PANDEMICS, EPIDEMICS, AND THE PROLIFERATION OF ARTIFICIAL INTELLIGENCE ON (COMPUTATIONAL) DRUG DISCOVERY**
	11:30	**Maria Khrenova**	**MECHANISM OF THE APTAMER RECOGNITION BY SARS-COV-2 SPIKE PROTEIN REVEALED BY NANOPORE SEQUENCING AND MOLECULAR MODELING**
Oral presentations	12:00	**Natia Samsonidze**	**DBAASP AS A VAST BASE OF MULTIFANCIONAL, NATURAL, CYCLIC ANTIMICROBIAL PEPTIDES**
	12:20	**Marat Kazanov**	**ANALYSIS OF THE THREE-DIMENSIONAL LOCALIZATION OF THE APOBEC-INDUCED MUTATIONS IN THE CELL NUCLEUS USING Hi-C DATA**
	12:40	**Prashantha Karunakar**	**VINALIGGEN: A METHOD TO GENERATE LIGPLOTS AND RETRIEVAL OF HYDROGEN AND HYDROPHOBIC INTERACTIONS FROM PROTEIN-LIGAND COMPLEXES**

lunch break 13:00-15:00

Chairpersons: Alexander Tuzikov and Dmitry Osolodkin

		Speaker	**Title**
Plenary lectures	15:00	**Alexander Tuzikov**	**COMPUTER-AIDED DISCOVERY OF NOVEL DRUG CANDIDATES AGAINST SARS-COV-2 TARGETING THE HEPTAD REPEAT DOMAIN 1 IN S2 PROTEIN**
	15:30	**Vladimir Sulimov**	**DOCKING PARADIGM IN COMPUTER-AIDED DRUG DISCOVERY**

Oral presentations	16:00	**Dmitry Osolodkin**	**THE GLAMOUR AND GLOOM OF ENSEMBLE DOCKING**
	16:20	**Yaroslav Faletrov**	**NEW FLUORESCENT ANTIFUNGAL AZOLE DERIVATIVE WITH NBD-PIPERAZINE MOIETY AND ITS DOCKING-REVEALED INTERACTION WITH SOME CYTOCHROMES P450**
	16:40	**Dmitry Shulga**	**IMPROVING ELECTROSTATICS DESCRIPTION IN SCORING FUNCTIONS - INSIGHTS FOR THEIR ROLE FOR DRUGS**
Keynote lectures	17:00	**Masha Y. Niv**	**PROGRESS AND CHALLENGES IN LIGANDS DISCOVERY FOR BITTER TASTE RECEPTORS**
	17:30	**Alexander I. Sobolevsky**	**GATING AND MOLECULAR PHARMACOLOGY OF TRP CHANNELS**
Oral presentations	18:00	**Rodrigo Costa Zeferino**	**IMMUNOMODULATORY ACTIVITY OF BENZNIDAZOLE IN EHRLICH ASCITES CARCINOMA IN SILICO AND IN VIVO**
	18:20	**Ricardo Affeldt**	**IN SILICO PREDICTIONS OF 2-PHENYL-3-(4-DIMETHYLAMINOPHENYL)QUINOXALINE ACTIVITY AND AKT1 INHIBITION**
	18:40	**Maricarmen Hernandez Rodriguez**	**DRUG REPURPOSING OF HNMT INHIBITORS AND THEIR EVALUATION IN SCOPOLAMINE-INDUCED AMNESIA MODEL**

Chairpersons: Alexander Kel **and Hanoch Senderowitz**

		Speaker	Title
Plenary lectures	9:00	**Hanoch Senderowitz**	**OPTIMIZATION OF QSAR MODELS FOR VIRTUAL SCREENING**
	9:30	**Derek van Tilborg**	**EXPOSING THE LIMITATIONS OF MOLECULAR MACHINE LEARNING WITH ACTIVITY CLIFFS**

Oral presentations	10:00	**Vincent Villanueva**	**A COMPARATIVE STUDY OF SAFETY AND PHARMACOKINETIC PARAMETERS BETWEEN STATINS, BILE ACID SEQUESTRANTS, AND EZETIMIBE AS DIFFERENT CLASSES OF LOW-DENSITY LIPOPROTEIN (LDL) CHOLESTEROL-LOWERING DRUGS IN SILICO**
	10:20	**Maxim Gureev**	**MODELING OF MIF-AIF INTERACTIONS IN FIELD OF ALLOSTERIC INHIBITORS DESIGN**
	10:40	**Humayun Wali**	**SELECTION PROCESS OF PHYTOCHEMICALS FOR UTILIZATION IN DISINFECTION OF DRINKING WATER**
	11:00	**Alexander Serbin**	**FROM BASIC PRINCIPLES TO COMPUTATIONALLY REFINED MODELS FOR A PRACTIC SYNTHESIS OF THE NANO-TARGETABLE POLYMERIC ANTIVIRALS**
	11:20	**Nehal Rami**	**PLANT EXTRACTS IN CANCER THERAPY A COMPREHENSIVE ANALYSIS OF ANTICANCER ACTIVITY AND MOLECULAR DOCKING PROFILES**
	11:40	**Stanislav Ignatov**	**CONFORMATIONAL DYNAMICS AND STABILITY OF MYCOLIC ACIDS BILAYERS FROM THE MYCOBACTERIUM TUBERCULOSIS OUTER MEMBRANE**

Keynote lectures	12:00	**Alexander Kel**	**LISTEN TO A SYMPHONY OF EPIGENOMICS WHEN SEEKING FOR DRUG TARGETS**
	12:30	**Yangyang Chen**	**DEEP GENERATIVE MODEL FOR DRUG DESIGN FROM PROTEIN TARGET SEQUENCE**

lunch break 13:00-15:00

Chairpersons: Athina Geronikaki and Alexey Lagunin

		Speaker	Title
Young Scientists flash presentations	15:00	**Christian Renz Algenio**	**IN SILICO ANALYSIS OF VARIOUS FUNGAL SECONDARY METABOLITES AND ANTIRETROVIRAL DRUGS ON ITS MOLECULAR BINDING TO NIPAH VIRUS PROTEINS INVOLVED IN CELLULAR ATTACHMENT, FUSION, AND REPLICATION**
	15:10	**Ankur Kumar**	**FIRST QSTR REPORT ON RATS CHRONIC AND SUB-CHRONIC TOXICITY OF DIVERSE CLASS OF CHEMICALS**

	15:20	**Arkaprava Banerjee**	**DEVELOPMENT OF A GLOBAL Q-RASAR MODEL FOR THE EFFICIENT QUANTITATIVE PREDICTIONS OF SKIN SENSITIZATION POTENTIAL OF DIVERSE ORGANIC CHEMICALS**
	15:30	**Upasana Hazarika**	**INVESTIGATION OF LEISHMANIA DONOVANIS KEY PATHWAYS BY COMPARATIVE NETWORK ANALYSIS TO UNCOVER NEW THERAPEUTIC TARGETS**
	15:40	**Assel Diyar**	**SPATIAL CHARACTERISTICS AND PREDICTION OF PROBABLE ACTIVITY AND TOXICITY OF STREPTOMYCIN AND ITS DERIVATIVES USING PASS-PROGRAM**
	15:50	**Maksim Perfilev**	**SEARCH FOR NEW ANXIOLYTIC SUBSTANCES BY NEURAL NETWORK MODELING USING MULTIPLE DOCKING**
	16:00	**Aleksandra Sagaidak**	**A NEW TARGET TO OVERCOME ABC TRANSPORTER ACCOSITED CHEMORESISTANCE OF TUMOR CELLS**
	16:10	**Ruslan Mallaev**	**ARTEMIS - STUDYING THE COMMUNICATION OF BIOMOLECULES USING INFORMATION THEORY**
	16:20	**Dmitrii Shkil**	**PREDICTION OF TOXICITY ENDPOINTS AS A PATHWAY TOWARDS MINIMISING RISKS IN DRUG DEVELOPMENT**
	16:30	**Daria Frolova**	**STRUCTPLM - ENHANCING PROTEIN REPRESENTATIONS WITH STRUCTURAL INFORMATION**
	16:40	**Hanna Karpenko**	**GENERATIVE HETERO-ENCODER MODEL FOR DE NOVO DESIGN OF SMALL-MOLECULE COMPOUNDS AS POTENTIAL INHIBITORS OF BCR-ABL TYROSINE KINASE**
	16:50	**Ivan Kuznetsov**	**EDGAR - A DEEP LEARNING-BASED PROGRAM FOR PREDICTION OF FOLDING ENERGY OF NUCLEIC ACIDS**
	17:00	**Anton Kolodnitsky**	**A COMPREHENSIVE DATABASE FOR PREDICTING METABOLISM OF XENOBIOTICS BY HUMAN MICROBIOME**
	17:10	**Luis Melo**	**DEVELOPMENT OF A STANDARDIZED APPROACH FOR TRANSFER LEARNING WITH QSAR MODELS**
	17:20	**Juan Felipe Avellaneda-Tamayo**	**CHEMICAL MULTIVERSE AND DIVERSITY OF FOOD CHEMICALS**
	17:30	**Massyel Martinez**	**EXPANDING THE EPIGENETIC RELEVANT CHEMICAL SPACE IDENTIFICATION OF DNA METHYLTRANSFERASE I ACTIVATORS**
	17:40	**Carlos Daniel Ramirez Marquez**	**CHEMOINFORMATIC ANALYSIS OF NATURAL PRODUCTS FROM MEXICO**
	17:50	**Mly Huiza**	**IN SILICO SCREENING OF COMMERCIAL DRUG-LIKE COMPOUNDS FOR COVALENT INHIBITION OF TC80 INSIGHTS INTO MECHANISM AND PROMISING CANDIDATES FOR THE TREATMENT AGAINST CHAGAS DISEASE**

Plenary lectures	18:00	**Andrey Rzhetsky**	**DISSECTING ETIOLOGY OF MALADIES OF THE MIND WITH VERY LARGE MEDICAL DATASETS**
	18:30	**Mikhail Pyatnitskiy**	**IT WAS TWENTY YEARS AGO TODAY: HOW OMICS HAVE SUCCEEDED IN PERSONALIZED MEDICINE**

Wednesday September 20, 2022

Chairpersons: Sophia Borisevich and Vladimir Palyulin

		Speaker	Title
Plenary lectures	9:00	**Sophia Borisevich**	**SEARCH FOR INHIBITORS OF SURFACE VIRAL PROTEINS I TYPE BY MOLECULAR MODELLING**
	9:30	**Alexey Lagunin**	**IN SILICO PREDICTION OF CELL-LINES CYTOTOXICITY OF DRUG-LIKE COMPOUNDS BASED ON THEIR STRUCTURAL FORMULA**
Oral presentations	10:00	**Urvashi Tiwari**	**EVALUATION OF SELECTED INDIGENOUS SPICES-AND HERBS-DERIVED SMALL MOLECULES AS POTENTIAL INHIBITORS OF SREBP1 AND ITS IMPLICATIONS FOR BREAST CANCER USING MD SIMULATIONS AND MMPBSA CALCULATIONS**
	10:20	**Andrey Markov**	**SEMISYNTHETIC TRITERPENOIDS AS PROMISING BLOCKERS OF AGGRESSIVENESS-RELATED TRAITS IN GLIOBLASTOMA MULTIFORME IN SILICO, IN VITRO, AND IN VIVO APPROACHES**
	10:40	**Vladimir Ostrovskii**	**COMPUTER PREDICTION AND IN VITRO STUDY OF ANTIVIRAL ACTIVITY OF HETEROCYCLIC SYSTEMS CONTAINING THIOPYRANO2,3-bQUINOLINE AND TETRAZOLE MOIETIES**
Keynote lectures	11:00	**Kunal Roy**	**Q-RASAR VS. QSAR: EFFICIENT PREDICTIONS OF ACTIVITY/PROPERTY/ TOXICITY ENDPOINTS**
	11:30	**Vladimir Palyulin**	**MOLECULAR MODELLING AND RECENT EXPERIMENTAL STUDIES OF AMPA RECEPTOR MODULATORS: BINDING MODES AND PHYSIOLOGICAL EFFECT**
Oral presentations	12:00	**Grigory Mokrov**	**COMPUTER-AIDED DESIGN OF NOVEL TSPO-LIGANDS - POTENTIAL NEUROPSYCHOTROPIC AGENTS**
	12:20	**Pavel Vassiliev**	**CONSENSUS MODELING OF ANXIOLYTIC ACTIVITY OF CHEMICAL COMPOUNDS BY CONVOLUTIONAL NEURAL NETWORKS**
	12:40	**Daria Novikova**	**A FRESH ANGLE ON P-GLYCOPROTEIN TO OVERCOME TUMOR CHEMORESISTANCE**

lunch break 13:00-16:00

Chairpersons: Narahari G. Sastry and Maria Khrenova

		Speaker	Title
Oral presentations	16:00	**Eugene Radchenko**	**MACHINE LEARNING PREDICTION OF MYCOBACTERIAL CELL WALL PERMEABILITY OF DRUGS AND DRUG-LIKE COMPOUNDS**

	16:20	**Alexey Mishin**	**A CASE STUDY OF STRUCTURE-BASED DRUG DESIGN WITH CYSTEINYL LEUKOTRIENE G-PROTEIN COUPLED RECEPTORS**
	16:40	**Anna Kulakova**	**MOLECULAR MODELING OF GLUTAMATE ACYLATION MECHANISM IN THE ACTIVE SITE OF N-ACETYLGLUTAMATE SYNTHASE**
Plenary lectures	17:00	**José Medina-Franco**	**EXPANDING THE CHEMICAL SPACE AND MULTIVERSE OF NATURAL PRODUCTS AND FOOD CHEMICALS**
	17:30	**Robert J. Woods**	**AUTOMATING THE RATIONAL DESIGN OF GLYCOMIMETIC DRUGS**
	18:00	**Keykavous Parang**	**AMPHIPHILIC MEMBRANE-ACTIVE PEPTIDES: BROAD-SPECTRUM ANTIBACTERIAL ACTIVITY ALONE AND IN COMBINATION WITH ANTIBIOTICS AND STRUCTURAL INSIGHTS**
18:30		**Closure of the XXIX Symposium on Bioinformatics and Computer-Aided Drug Discovery**	

Scheduled time - Moscow (CEST+1).