Scientific Program

XXXI Symposium on Bioinformatics and Computer-Aided Drug Discovery (BCADD-2025)

Scheduled time - Moscow (UTC+3)

Monday October 20, 2025

Chairpersons: Vladimir Poroikov and Roman Efremov

08:30	*Opening of the Symposium*

Plenary lecture	
09:00	AI-ASSISTANT, AI-ANALYST AND AI-RESEARCHER: THREE LEVELS OF DIGITAL TECHNOLOGIES IN CHEMISTRY **Valentine Ananikov** Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, Russia

Oral presentations	
10:00	TRANSCRIPTOMIC PROFILING OF T CELLS IN 4T1 TNBC TUMORS **Md. Iftehimul** Institute of Biotechnology, Bangladesh Agricultural University, Mymensingh, Bangladesh
10:20	TRANSCRIPTOMICS-BASED DRUG REPURPOSING OF SP600125 TO TARGET PRONEURAL-MESENCHYMAL TRANSITION IN GLIOBLASTOMA **Kirill Odarenko** Institute of Chemical Biology and Fundamental Medicine, Novosibirsk, Russia
10:40	DO-NO-HARM MOLECULAR GENERATION 12-MODEL BENCHMARK AND KRAS G12D CASE STUDY **Daria Ryabchenko** Skolkovo Institute of Science and Technology, Moscow, Russia

Keynote lectures	
11:00	ON OUR UNDERSTANDING OF AGING, PERSONALIZED MEDICINE AND GERIATRIC CARE **G. Narahari Sastry** Department of Biotechnology, Indian Institute of Technology Hyderabad, Kandi, Telangana, India
11:30	FRAGMENT-BASED NMR SCREENING FOR INHIBITORS OF BACTERIAL ENZYMES **Vladimir Polshakov** Chemical Department, Lomonosov Moscow State University, Russia

Oral presentations

12:00	HARNESSING BIOINFORMATICS FOR HPV THERAPEUTICS ENHANCED DRUG REPURPOSING, PROTEIN HOMOLOGY, AND COMPREHENSIVE DATA MINING FOR TARGETED TREATMENT DEVELOPMENT **Arli Aditya Parikesit** Department of Biotechnology, School of Life Sciences, Indonesia International Institute for Life Sciences, Jakarta, Indonesia
12:20	SEARCH FOR MONKEYPOX VIRUS 2-O-METHYLTRANSFERASE INHIBITORS BY MOLECULAR MODELING **Ekaterina Mandrygina** Research Computing Center, Lomonosov Moscow State University, Moscow, Russia
12:40	STRUCTURE-BASED DISCOVERY OF INHIBITORS TARGETING NIPAH VIRUS RNA-DEPENDENT RNA POLYMERASE THROUGH VIRTUAL SCREENING AND MOLECULAR DYNAMICS SIMULATIONS **Manos Vlasiou** University of Nicosia, School of Veterinary Medicine, Nicosia, Cyprus

lunch break 13:00-15:00

Chairpersons: Jose Medina-Franco and Vladimir Palyulin

Keynote lectures	
15:00	COMBINING COMPUTATIONAL METHODS AND EPR SPECTROSCOPY FOR PROTEIN–LIGAND BINDING SITE ANALYSIS **Olesya Krumkacheva** International Tomography Center SB RAS, Novosibirsk, Russia
15:30	NEXT-GENERATION COMPUTATIONAL MODELS OF THE BLOOD-BRAIN BARRIER **Christian Jorgensen** University of Portsmouth, Portsmouth, United Kingdom

Oral presentations	
16:00	DEVELOPMENT OF A VIRTUAL SCREENING PIPELINE FOR THE DISCOVERY OF NOVEL SARS-COV-2 MPRO INHIBITORS **Daniel Malikin** Lomonosov Moscow State University, Moscow, Russia
16:20	ROLE OF INTERACTION FINGERPRINTS IN MACHINE LEARNING MODELS FOR SARS-COV-2 MPRO INHIBITORS **Anastasiia Fomina** Chumakov FSC R&D IBP RAS (Institute of Poliomyelitis), Moscow, Russia
16:40	IN SILICO SCREENING OF PROBIOTIC-DERIVED METABOLITES AS LUXS QUORUM SENSING INHIBITORS IN OTITIS MEDIA PATHOGENS **Samir Zergat** University of Pisa, Pisa, Italy
17:00	AN INTEGRATED COMPUTATIONAL STRATEGY FOR PROFILING TERPENOID FOR DUAL-TARGET LEADS AGAINST KLEBSIELLA PNEUMONIAE PENICILLIN-BINDING PROTEIN 3 AND BETA-LACTAMASE **Gideon Gyebi** Department of Biotechnology and Food Science, Faculty of Applied Sciences, Durban University of Technology, Durban, South Africa

17:20	CONSENSUS METHODOLOGY FOR DIRECTED SEARCH OF COMPOUNDS WITH ANTIMICROBIAL ACTIVITY AGAINST S. AUREUS **Arina Golubeva** Volgograd State Medical University, Volgograd, Russia
17:40	A CHEMINFORMATICS APPROACHES FOR THE IDENTIFICATION OF INHIBITORS AGAINST MACROLIDE 2'-PHOSPHOTRANSFERASE TYPE I **Carlos Alberto Lobato-Tapia** Universidad Politécnica Metropolitana de Puebla, Puebla, Mexico

Keynote lectures	
18:00	MACHINE LEARNING METHODOLOGIES AND THE FUTURE OF DRUG DISCOVERY **Rachelle Bienstock** RJB Computational Modeling LLC, Chapel Hill, NC, USA
18:30	COMBINING MACHINE LEARNING AND STRUCTURE-BASED APPROACHES FOR THE EFFICIENT IDENTIFICATION OF NOVEL BIOACTIVE SCAFFOLDS **Alan Talevi** National University of La Plata (UNLP), La Plata; Argentinean National Council of Scientific and Technical Research, La Plata; Boolzi SA, Buenos Aires, Argentina

Tuesday October 21, 2025

Chairpersons: Kunal Roy and Dmitry Shulga

Keynote lectures	
09:00	A NOVEL DRUG DESIGN APPROACH: QUANTITATIVE STRUCTURE-INTERACTION ACTIVITY RELATIONSHIP (QSIAR) IN ANTI-TUBERCULAR AGENTS **Anil Saxena** Global Institute of Pharmaceutical Education and Research, Kashipur, Uttarakhand, India
09:30	MULTI-AGENT DRUG DISCOVERY ORCHESTRA **Andrei Dmitrenko** ITMO University, St. Petersburg, Russia; D ONE AG, Zurich, Switzerland

Oral presentations	
10:00	TOXAI ASSISTANT - AN IN SILICO ALTERNATIVE TO RATS TESTING FOR ACUTE TOXICITY **Oleg Tinkov** Ligand Pro, Moscow, Russia
10:20	REVOLUTIONIZING DRUG SAFETY ASSESSMENT VIA QSAR AND Q-RASAR BASED TOXICITY PREDICTION TO PROTECT HUMAN HEALTH **Shubha Das** Drug Discovery and Development Laboratory, Department of Pharmaceutical Technology, Jadavpur University, Kolkata, India
10:40	ADVERSE REACTIONS OF WORLD-WIDE APPROVED DRUGS **Polina Savosina** Institute of Biomedical Chemistry, Moscow, Russia

11:00	CONSENSUS QSAR APPROACHES FOR PREDICTING PLACENTAL BARRIER PERMEABILITY IN REPRODUCTIVE TOXICOLOGY **Pabitra Samanta** Drug Discovery and Development Laboratory, Department of Pharmaceutical Technology, Jadavpur University, Kolkata, India
11:20	FULLY-CONNECTED CONVOLUTIONAL NEURAL NETWORKS BASED ON MULTIPLE DOCKING A NEW MACHINE LEARNING METHOD FOR SEARCHING BIOLOGICAL ACTIVE COMPOUNDS **Pavel Vassiliev** Volgograd State Medical University, Volgograd, Russia
11:40	DEEP LEARNING CONVOLUTIONAL CORRELATION NEURAL NETWORK BASED ON MULTIPLE DOCKING FOR IDENTIFYING PHARMACOLOGICALLY ACTIVE COMPOUNDS **Maksim Perfilev** Volgograd State Medical University, Volgograd, Russia

Keynote lectures	
12:00	STRUCTURE AND FUNCTIONING OF TRPV CHANNELS: INSIGHTS FROM MOLECULAR MODELING **Yuri Trofimov** Shemyakin-Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences; Research Institute for Systems Biology and Medicine, Moscow, Russia
12:30	MOLECULAR DYNAMICS AND PHARMACOPHORE MODELING OF THE INACTIVE MINERALOCORTICOID RECEPTOR FOR ANTAGONIST DISCOVERY **Carlos Lagos** Universidad San Sebastián, Centro Basal Ciencia & Vida, Santiago, Chile

lunch break 13:00-16:00

Chairpersons: Athina Geronikaki and Alexey Lagunin

Young Scientists flash presentations	
15:10	IN SILICO–GUIDED IDENTIFICATION AND BIOLOGICAL EVALUATION OF TRITERPENOID-TYPE P-GLYCOPROTEIN INHIBITORS **Arsenii Moralev** Institute of Chemical Biology and Fundamental Medicine, Novosibirsk, Russia
15:20	COMPUTATIONAL MODELING OF BIOACCUMULATION POTENTIAL OF PER- & POLY-FLUOROALKYL SUBSTANCES: MACHINE LEARNING BASED QUANTITATIVE READ-ACROSS STRUCTURE-PROPERTY RELATIONSHIP APPROACH **Akash Chandra** Drug Theoretics and Cheminformatics Laboratory, Jadavpur University, Kolkata, India
15:30	MAGNESIUM BINDING TO TRPV6 ION CHANNEL: INSIGHTS FROM MOLECULAR MODELING **Irina Veretenenko** Shemyakin–Ovchinnikov Institute of bioorganic chemistry RAS, Moscow, Russia
15:40	COMPUTATIONAL WORKFLOW FOR PREDICTING DRUG METABOLISM BY GUT MICROBIOTA **Anton Kolodnitsky**

	Institute of Biomedical Chemistry, Moscow, Russia
15:50	TIP: WEB APPLICATION FOR PREDICTING DRUG–TRANSPORTER INTERACTIONS **George Khodos** Pirogov Russian National Research Medical University, Moscow, Russia
16:00	DENR+POL: THEORETICALLY CONSISTENT POLARIZABLE EMPIRICAL CHARGES FOR DRUG-LIKE AND BIOLOGICAL MOLECULES **Vitaly Frolov** Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia
16:10	X-RAY CRYSTALLOGRAPHIC ANALYSIS OF 17-PYRIDIN-2-YL ESTRANE DERIVATIVES: LEAD-LIKE COMPOUNDS AGAINST BREAST AND CERVICAL CANCER **Nikola Radnović** University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Novi Sad, Serbia
16:20	IMPLEMENTATION OF HIGH-THROUGHPUT SCREENING DATA FOR DRUG SYNERGY PREDICTION IN ONCOLOGY **Vladislav Sukhachev** Institute of Biomedical Chemistry, Moscow, Russia
16:30	COMPARATIVE EVALUATION OF LSTM AND GRAPH NEURAL NETWORKS FOR ADVERSE DRUG REACTION PREDICTION **Nsikan Udo** Moscow Institute of Physics and Technology, Dolgoprudny, Russia
16:40	FROM IN SILICO DESIGN TO EXPERIMENTAL IMPLEMENTATION: DEVELOPMENT OF A NOVEL GLUCOKINASE ACTIVATOR **Kira Inzhevatkina** National Research Mordovia State University, Saransk, Russia
16:50	DEVELOPMENT OF A PROBABILITY FACTOR BASED ON BLIND AND TARGET-SITE DOCKING ANALYSIS FOR IMPROVED IC_{50} PREDICTION OF CANDIDATE COMPETITIVE ENZYME INHIBITORS **Dionysia Amanatidou** Department of Biomedical Sciences, School of Health, International Hellenic University, Thessaloniki, Greece
17:00	COMPARATIVE EFFICIENCY OF STRUCTURE ACTIVITY RELATIONSHIP AND PROTEOCHEMOMETRIC MODELLING **Georgii Malakhov** Department of Bioinformatics, Institute of Biomedical Chemistry, Moscow, Russia
17:10	A LARGE-SCALE DATASET OF QUANTUM CHEMICAL PROPERTIES OF DRUG-LIKE MOLECULES FOR Δ-LEARNING MODELS **Dmitry Frolov** Sirius University of Science and Technology, Sirius, Russia
17:20	THE POLAR PATCH IN THE HYDROPHOBIC GATE OF THE TRPV1 CHANNEL AND ITS FUNCTIONAL ROLE **Ivan Lazarev** Shemyakin–Ovchinnikov Institute of Bioorganic chemistry RAS, Moscow, Russia
17:30	AMIACTIVE (AIA): A LARGE-SCALE QSAR BASED TARGET FISHING AND POLYPHARMACOLOGY PREDICTIVE WEB TOOL **Luis Felipe Melo** Federal University of Paraiba, João Pessoa, Brazil

17:40	CHEMECAL PROFILE EVALUATION AND ACTIVITY OF TAMARINDUS INDICA L. SEEDS ON HELICOBACTER PYLORI AND UREASE **Ester Tonini** Department of Pharmaceutical Sciences, Health Center Sciences, Federal University of Espírito Santo, Vitória, Brazil
17:50	DESIGN AND SYNTHESIS OF PEPTIDE INHIBITORS TARGETING HER2 AS A THERAPEUTIC STRATEGY IN BREAST CANCER **Luis Angel Gil Ruiz** Laboratory for the Design and Development of New Drugs and Biotechnological Innovation, Escuela Superior de Medicina, Instituto Politécnico Nacional, Mexico

Keynote lectures	
18:00	ULTRA-LARGE LIBRARIES AND CHEMICAL SPACES OF VIRTUAL SCREENING SAMPLES WITH PROPOSED SYNTHETIC ROUTES **Marc C. Nicklaus** Actyon Discovery, Inc., San Diego/Catonsville, United States
18:30	COMPUTER-AIDED ANTIMICROBIAL DISCOVERY: STRUCTURE–ANTIMICROBIAL ACTIVITY RELATIONSHIPS OF RECOMBINANT HOST DEFENSE PEPTIDES AGAINST DRUG-RESISTANT BACTERIA **William J. Zamora** University of Costa Rica, San Pedro, San José, Costa Rica; 4National Advanced Computing Collaboratory (CNCA), National High Technology Center (CeNAT), Costa Rica

Wednesday October 22, 2025

Chairpersons: Rajesh Goel and Dmitry Osolodkin

Keynote lectures	
09:00	AN IMPROVED Q-RASAR MODELING FRAMEWORK FOR ENVIRONMENTAL TOXICITY ENDPOINTS **Kunal Roy** Jadavpur University, Kolkata, India
09:30	PROTEIN ENGINEERING METHODS FOR CHALLENGING MEMBRANE-BOUND DRUG TARGETS **Ivan Gushchin** Moscow Institute of Physics and Technology (National Research University), Dolgoprudny, Russia

Oral presentations	
10:00	THE NATURE OF ENTROPY-ENTHALPY COMPENSATION, EXOTIC ARRHENIUS PARAMETER AND KINETIC ISOTOPE EFFECT IN THE DENATURATION KINETICS OF PROTEINS **Alexey Baklanov** Institute of Chemical Kinetics and Combustion SB RAS, Novosibirsk, Russia
10:20	COMPUTER MODELING OF SUPRAMOLECULAR CHEMICAL SYSTEMS PROPERTIES AND REACTIVITY AND ITS POTENTIAL IMPACT IN COMPUTER-AIDED DRUG DISCOVERY **Alexander Novikov**

	Saint Petersburg State University, Saint Petersburg, Russia
10:40	HOW FLAVONOID PARAMETERIZATION DETERMINES DRUG-INDECED MEMBRANE BIOPHYSICAL OUTCOMES **Anna Malykhina** Laboratory of Membrane and Ion Channel Modeling, Institute of Cytology of Russian Academy of Sciences, Saint Petersburg, Russian Federation

Keynote lectures	
11:00	A LONG, HARD ROAD TO PHYSICALLY CORRECT CALCULATION OF PROTEIN–PROTEIN BINDING FREE ENERGIES **Anton Chugunov** Shemyakin-Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences; Research Institute for Systems Biology and Medicine, Moscow, Russia
11:30	STATE-OF-THE-ART COVALENT VIRTUAL SCREENING WITH ALPHAFOLD3 **Nir London** The Weizmann Institute of Science, Rehovot, Israel

Oral presentations	
12:00	TOOL FOR DIVERSITY VISUALIZATION ON THE LEVEL OF MOLECULAR SCAFFOLDS, TDV CHEMICAL DATA AT GLANCE **Pavel Pogodin** Institute of Biomedical Chemistry, Moscow, Russia
12:20	STUDYING THE ALLOSTERIC COMMUNICATION IN BIOMOLECULES USING INFORMATION THEORY **Ruslan Mallaev** M.M. Shemyakin and Yu.A. Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences, Moscow, Russia
12:40	IN SILICO REVERSE FRAGMENT BASED DRUG DISCOVERY APPROACH (R-FBDD) CORE IDEAS, CURRENT STATUS AND FUTURE DIRECTIONS **Dmitry Shulga** Department of Chemistry at Moscow State University, Moscow, Russia

lunch break 13:00-16:00

Chairpersons: Alexander Kel and Olga Tarasova

Oral presentations	
16:00	A NOVEL STRATEGY TO OVERCOME PARPI RESISTANCE TARGETING UBE2N WITH NON-COVALENT INHIBITORS **Shafi Ullah Khan** Université de Caen Normandie, INSERM U1086 ANTICIPE (Interdisciplinary Research Unit for Cancers Prevention and Treatment), BioTICLA laboratory (Precision medicine for ovarian cancers), Caen, France
16:20	STEROIDAL PREGNANES AS NOVEL 11-HSD1 INHIBITORS INSIGHTS FROM MACHINE LEARNINGBASED QSAR AND MOLECULAR MODELING **Oludare Ogunyemi** Structural and Computational Biology Group, Nutritional and Industrial Biochemistry Research Unit, Department of Biochemistry, College of Medicine, University of Ibadan, Ibadan, Nigeria

16:40	IRACEMA, A DATABASE MANAGEMENT SYSTEM FOR BIOACTIVE COMPOUNDS ISOLATED AND CHARACTERIZED BY BRAZILIAN RESEARCHERS **Thais Lourenco** University of São Paulo, São Paulo, Brazil

Keynote lectures	
17:00	A COMPUTATIONAL PIPELINE FOR ACCELERATING THE DESIGN OF GLYCOMIMETICS **Robert J. Woods** Complex Carbohydrate Research Center, University of Georgia, Athens, GA, USA
17:30	IN SILICO SMALL MOLECULE DRUG DISCOVERY FROM THE PHARMA COMPANY POINT OF VIEW **Germes Chilov** JSC "Valenta Pharm", Shchelkovo, Moscow Region, Russia

Plenary lectures

18:00	ON THE USE OF MACHINE LEARNING MODELS FOR NEW APPROACH METHODOLOGIES **Tudor I. Oprea** Expert Systems Inc., San Diego, California, USA

19:00	*Closure of the XXXI Symposium on Bioinformatics and Computer-Aided Drug Discovery*