

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



Keynote lectures

18:00	<p>MACHINE LEARNING METHODOLOGIES AND THE FUTURE OF DRUG DISCOVERY</p> <p> Rachelle Bienstock RJB Computational Modeling LLC, Chapel Hill, NC, USA</p>
18:30	<p>COMBINING MACHINE LEARNING AND STRUCTURE-BASED APPROACHES FOR THE EFFICIENT IDENTIFICATION OF NOVEL BIOACTIVE SCAFFOLDS</p> <p> 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</p>




Tuesday October 21, 2025




Chairpersons: Kunal Roy and Dmitry Shulga

Keynote lectures



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

Oral presentations

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

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

Keynote lectures

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



lunch break 13:00-16:00

Chairpersons: Athina Geronikaki and Alexey Lagunin

Young Scientists flash presentations



16:00	TBA
16:10	TBA
16:20	TBA
16:30	TBA
16:40	TBA
16:50	TBA
17:00	TBA
17:10	TBA
17:20	TBA
17:30	TBA
17:40	TBA
17:50	TBA




Keynote lectures


18:00	<p>ULTRA-LARGE LIBRARIES AND CHEMICAL SPACES OF VIRTUAL SCREENING SAMPLES WITH PROPOSED SYNTHETIC ROUTES</p> <p> Marc C. Nicklaus Actyon Discovery, Inc., San Diego/Catonsville, United States</p>
18:30	<p>COMPUTER-AIDED ANTIMICROBIAL DISCOVERY: STRUCTURE–ANTIMICROBIAL ACTIVITY RELATIONSHIPS OF RECOMBINANT HOST DEFENSE PEPTIDES AGAINST DRUG-RESISTANT BACTERIA</p> <p> 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</p>


Wednesday October 22, 2025

Chairpersons: Rajesh Goel and Dmitry Osolodkin




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

Oral presentations	
10:00	<p>THE NATURE OF ENTROPY-ENTHALPY COMPENSATION, EXOTIC ARRHENIUS PARAMETER AND KINETIC ISOTOPE EFFECT IN THE DENATURATION KINETICS OF PROTEINS</p> <p> Alexey Baklanov Institute of Chemical Kinetics and Combustion SB RAS, Novosibirsk, Russia</p>
10:20	<p>COMPUTER MODELING OF SUPRAMOLECULAR CHEMICAL SYSTEMS PROPERTIES AND REACTIVITY AND ITS POTENTIAL IMPACT IN COMPUTER-AIDED DRUG DISCOVERY</p> <p> Alexander Novikov Saint Petersburg State University, Saint Petersburg, Russia</p>
10:40	<p>HOW FLAVONOID PARAMETERIZATION DETERMINES DRUG-INDECEDED MEMBRANE BIOPHYSICAL OUTCOMES</p> <p> Anna Malykhina Laboratory of Membrane and Ion Channel Modeling, Institute of Cytology of Russian Academy of Sciences, Saint Petersburg, Russian Federation</p>

Keynote lectures	
11:00	<p>A LONG, HARD ROAD TO PHYSICALLY CORRECT CALCULATION OF PROTEIN–PROTEIN BINDING FREE ENERGIES</p> <p> Anton Chugunov</p>

	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
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17:30	IN SILICO SMALL MOLECULE DRUG DISCOVERY FROM THE PHARMA COMPANY POINT OF VIEW  Germes Chilov JSC "Valenta Pharm", Shchelkovo, Moscow Region, Russia
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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
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19:00 *Closure of the XXXI Symposium on Bioinformatics and Computer-Aided Drug
Discovery*