

# 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	<i>Opening of the Symposium</i>
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## Plenary lecture

09:00	AI-ASSISTANT, AI-ANALYST AND AI-RESEARCHER: THREE LEVELS OF DIGITAL TECHNOLOGIES IN CHEMISTRY 👤 <b>Valentine Ananikov</b> 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 👤 <b>Md. Iftehimul</b> Institute of Biotechnology, Bangladesh Agricultural University, Mymensingh, Bangladesh
10:20	TRANSCRIPTOMICS-BASED DRUG REPURPOSING OF SP600125 TO TARGET PRONEURAL-MESENCHYMAL TRANSITION IN GLIOBLASTOMA 👤 <b>Kirill Odarenko</b> Institute of Chemical Biology and Fundamental Medicine, Novosibirsk, Russia
10:40	DO-NO-HARM MOLECULAR GENERATION 12-MODEL BENCHMARK AND KRAS G12D CASE STUDY 👤 <b>Daria Ryabchenko</b> Skolkovo Institute of Science and Technology, Moscow, Russia

## Keynote lectures

11:00	ON OUR UNDERSTANDING OF AGING, PERSONALIZED MEDICINE AND GERIATRIC CARE 👤 <b>G. Narahari Sastry</b> Department of Biotechnology, Indian Institute of Technology Hyderabad, Kandi, Telangana, India
11:30	FRAGMENT-BASED NMR SCREENING FOR INHIBITORS OF BACTERIAL ENZYMES 👤 <b>Vladimir Polshakov</b> 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  <b>Arli Aditya Parikesit</b> 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  <b>Ekaterina Mandrygina</b> Research Computing Center, Lomonosov Moscow State University, Moscow, Russia
12:40	CHRONOBOTICSDB AS THE FORERUNNER DATABASE OF AI-POWERED PERSONALISED CHRONOPHARMACOLOGY  <b>Ilya Solovev</b> Pitirim Sorokin Syktyvkar State University, Syktyvkar, Russia





**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  <b>Olesya Krumkacheva</b> International Tomography Center SB RAS, Novosibirsk, Russia
15:30	NEXT-GENERATION COMPUTATIONAL MODELS OF THE BLOOD-BRAIN BARRIER  <b>Christian Jorgensen</b> 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  <b>Daniel Malikin</b> Lomonosov Moscow State University, Moscow, Russia
16:20	ROLE OF INTERACTION FINGERPRINTS IN MACHINE LEARNING MODELS FOR SARS-COV-2 MPRO INHIBITORS  <b>Anastasiia Fomina</b> 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  <b>Samir Zergat</b> 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  <b>Gideon Gyebi</b> 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> <b>Arina Golubeva</b> 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> <b>Carlos Alberto Lobato-Tapia</b> Universidad Politécnica Metropolitana de Puebla, Puebla, Mexico</p>



#### Keynote lectures

18:00	<p>MACHINE LEARNING METHODOLOGIES AND THE FUTURE OF DRUG DISCOVERY</p> <p> <b>Rachelle Bienstock</b> 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> <b>Alan Talevi</b> 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> <b>Anil Saxena</b> Global Institute of Pharmaceutical Education and Research, Kashipur, Uttarakhand, India</p>
09:30	<p>MULTI-AGENT DRUG DISCOVERY ORCHESTRA</p> <p> <b>Andrei Dmitrenko</b> 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> <b>Oleg Tinkov</b> Pridnestrovian State University, Tiraspol, Moldova</p>
10:20	<p>REVOLUTIONIZING DRUG SAFETY ASSESSMENT VIA QSAR AND Q-RASAR BASED TOXICITY PREDICTION TO PROTECT HUMAN HEALTH</p> <p> <b>Shubha Das</b> 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> <b>Polina Savosina</b> Institute of Biomedical Chemistry, Moscow, Russia</p>

11:00	<p>CONSENSUS QSAR APPROACHES FOR PREDICTING PLACENTAL BARRIER PERMEABILITY IN REPRODUCTIVE TOXICOLOGY</p> <p> <b>Pabitra Samanta</b> 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> <b>Pavel Vassiliev</b> 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> <b>Maksim Perfilev</b> Volgograd State Medical University, Volgograd, Russia</p>





### Keynote lectures

12:00	<p>STRUCTURE AND FUNCTIONING OF TRPV CHANNELS: INSIGHTS FROM MOLECULAR MODELING</p> <p> <b>Yuri Trofimov</b> 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> <b>Carlos Lagos</b> Universidad San Sebastián, Centro Basal Ciencia &amp; Vida, Santiago, Chile</p>



**lunch break 13:00-15:10**

*Chairpersons: Athina Geronikaki and Alexey Lagunin*



### Young Scientists flash presentations

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

	Institute of Biomedical Chemistry, Moscow, Russia
15:50	TIP: WEB APPLICATION FOR PREDICTING DRUG–TRANSPORTER INTERACTIONS  <b>George Khodos</b> Pirogov Russian National Research Medical University, Moscow, Russia
16:00	DENR+POL: THEORETICALLY CONSISTENT POLARIZABLE EMPIRICAL CHARGES FOR DRUG-LIKE AND BIOLOGICAL MOLECULES  <b>Vitaly Frolov</b> 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  <b>Nikola Radnović</b> 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  <b>Vladislav Sukhachev</b> Institute of Biomedical Chemistry, Moscow, Russia
16:30	COMPARATIVE EVALUATION OF LSTM AND GRAPH NEURAL NETWORKS FOR ADVERSE DRUG REACTION PREDICTION  <b>Nsikan Udo</b> Moscow Institute of Physics and Technology, Dolgoprudny, Russia
16:40	FROM IN SILICO DESIGN TO EXPERIMENTAL IMPLEMENTATION: DEVELOPMENT OF A NOVEL GLUCOKINASE ACTIVATOR  <b>Kira Inzhevatkina</b> 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 <sub>50</sub> PREDICTION OF CANDIDATE COMPETITIVE ENZYME INHIBITORS  <b>Dionysia Amanatidou</b> Department of Biomedical Sciences, School of Health, International Hellenic University, Thessaloniki, Greece
17:00	COMPARATIVE EFFICIENCY OF STRUCTURE ACTIVITY RELATIONSHIP AND PROTEOCHEMOMETRIC MODELLING  <b>Georgii Malakhov</b> Department of Bioinformatics, Institute of Biomedical Chemistry, Moscow, Russia
17:10	A LARGE-SCALE DATASET OF QUANTUM CHEMICAL PROPERTIES OF DRUG-LIKE MOLECULES FOR $\Delta$ -LEARNING MODELS  <b>Dmitry Frolov</b> 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  <b>Ivan Lazarev</b> 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  <b>Luis Felipe Melo</b> Federal University of Paraiba, João Pessoa, Brazil

17:40	CHEMECAL PROFILE EVALUATION AND ACTIVITY OF TAMARINDUS INDICA L. SEEDS ON HELICOBACTER PYLORI AND UREASE  <b>Ester Tonini</b> Department of Pharmaceutical Sciences, Health Center Sciences, Federal University of Espirito Santo, Vitória, Brazil
17:50	DESIGN AND SYNTHESIS OF PEPTIDE INHIBITORS TARGETING HER2 AS A THERAPEUTIC STRATEGY IN BREAST CANCER  <b>Luis Angel Gil Ruiz</b> 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  <b>Marc C. Nicklaus</b> 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  <b>William J. Zamora</b> 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  <b>Kunal Roy</b> Jadavpur University, Kolkata, India
09:30	PROTEIN ENGINEERING METHODS FOR CHALLENGING MEMBRANE-BOUND DRUG TARGETS  <b>Ivan Gushchin</b> 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  <b>Alexey Baklanov</b> 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  <b>Alexander Novikov</b>

	Saint Petersburg State University, Saint Petersburg, Russia
10:40	HOW FLAVONOID PARAMETERIZATION DETERMINES DRUG-INDECEDED MEMBRANE BIOPHYSICAL OUTCOMES  <b>Anna Malykhina</b> 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  <b>Anton Chugunov</b> 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  <b>Nir London</b> 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  <b>Pavel Pogodin</b> Institute of Biomedical Chemistry, Moscow, Russia
12:20	STUDYING THE ALLOSTERIC COMMUNICATION IN BIOMOLECULES USING INFORMATION THEORY  <b>Ruslan Mallaev</b> 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  <b>Dmitry Shulga</b> 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  <b>Shafi Ullah Khan</b> 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  <b>Oludare Ogunyemi</b> Structural and Computational Biology Group, Nutritional and Industrial Biochemistry Research Unit, Department of Biochemistry, College of Medicine, University of Ibadan, Ibadan, Nigeria

16:40	<p>IRACEMA, A DATABASE MANAGEMENT SYSTEM FOR BIOACTIVE COMPOUNDS ISOLATED AND CHARACTERIZED BY BRAZILIAN RESEARCHERS</p> <p> <b>Thais Lourenco</b> University of São Paulo, São Paulo, Brazil</p>
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### Keynote lectures

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

### Plenary lectures

18:00	<p>ON THE USE OF MACHINE LEARNING MODELS FOR NEW APPROACH METHODOLOGIES</p> <p> <b>Tudor I. Oprea</b> Expert Systems Inc., San Diego, California, USA</p>
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19:00 *Closure of the XXXI Symposium on Bioinformatics and Computer-Aided Drug Discovery*