

# Scientific Program

XXX Symposium on Bioinformatics and Computer-Aided Drug Discovery (BCADD-2024)

## Monday September 16, 2024


Chairpersons: *Vladimir Poroikov and Roman Efremov*


8:30	Opening of the Symposium
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### Plenary lecture

9:00	COMPUTATIONAL DESIGN AND REPURPOSING OF DRUGS FOR CORONAVIRUSES AND DRUG RESISTANT PATHOGENS  <b>David Winkler</b> Monash Institute of Pharmaceutical Sciences, Melbourne, Australia
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### Oral presentations


10:00	SUCCESSFUL APPLICATION OF COMPUTING METHODS TO DEVELOPMENT SARS-COV-2 INHIBITORS  <b>Vladimir Sulimov</b> Dimonta Ltd., Research Computing Center, Lomonosov Moscow State University, Moscow, Russia
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10:20	PITFALLS OF SARS-COV2 MAIN PROTEASE COVALENT INHIBITION MODELING WITH THE COMBINED QUANTUM AND MOLECULAR MECHANICS APPROACHES  <b>Igor Polyakov</b> Lomonosov Moscow State University, Moscow, Russia
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10:40	MODELLING LETHALITY AND TERATOGENICITY OF ZEBRAFISH (DANIO RERIO) DUE TO $\beta$ -LACTAM ANTIBIOTICS EMPLOYING THE QSTR APPROACH  <b>Aniket Nath</b> Jadavpur University, Kolkata, India
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### Keynote lectures

11:00	SIXTY YEARS IN SCIENCE OF PROFESSOR NIKOLAY S. ZEFIROV: FROM ORGANIC SYNTHESIS, CONFORMATIONAL ANALYSIS AND REACTION DESIGN - TO MEDICINAL CHEMISTRY AND CADD  <b>Vladimir Palyulin</b> Faculty of Chemistry, Lomonosov Moscow State University, Moscow, Russia
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11:30	EXTENDED SIMILARITY INDICES: BENEFITS OF COMPARING MORE THAN TWO OBJECTS SIMULTANEOUSLY. THEORY, SPEED, CONSISTENCY, AND DIVERSITY SELECTION  <b>Károly Héberger</b> HUN-REN Research Centre for Natural Sciences, Budapest, Hungary
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### Oral presentations

12:00	MOLECULAR MODELING OF BACTERIAL RESISTANCE. THE ROLE OF DYNAMIC BEHAVIOR OF PROTEIN COMPLEXES WITH SUBSTRATES OR INHIBITORS  <b>Maria G. Khrenova</b> Lomonosov Moscow State University, Moscow, Russia
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12:20	DECIPHERING CAPI AS A SIGNIFICANT DRUGGABLE TARGET IN COMBATING CANDIDA ALBICANS PATHOGENESIS AND MULTIDRUG RESISTANCE  <b>Neha Jaiswal</b> National Institute of Technology Raipur, Raipur, India
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12:40	MODELING, SYNTHESIS AND IN VITRO TESTING OF PEPTIDES BASED ON UNUSUAL AMINO ACIDS AS POTENTIAL ANTIBACTERIAL AGENTS  <b>Armen Sargsyan</b> Scientific and Production Center "Armbiotechnology" NAS RA, Yerevan, Armenia
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**13:00-15:00**

**Lunch break**


*Chairpersons: Károly Héberger and Vladimir Palyulin*


**Keynote lectures**

15:00	DEVELOPMENT AND APPLICATION OF A WEB-BASED INTEGRATED PLATFORM D3CARP FOR TARGET PREDICTION AND VIRTUAL SCREENING  <b>Weiliang Zhu</b> Shanghai Institute of Materia Medica Chinese Academy of Sciences, Shanghai, China
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15:30	COMBATING CYSTIC FIBROSIS: COMPUTATIONAL STUDIES ON CFTR  <b>Hanoeh Senderowitz</b> Bar-Ilan University Faculty of Exact Sciences, Ramat-Gan, Israel
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**Oral presentations**


16:00	ESTIMATION OF RETENTION TIME OF ORGANIC PESTICIDES IN HUMAN MILK USING QSPR AND READ-ACROSS METHODS AN ALTERNATIVE APPROACH TO EXPERIMENTAL HAZARDS ASSESSMENT  <b>Ankur Kumar</b> Jadavpur University, Kolkata, India
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16:20	MULTI-TARGET NEURAL NETWORK MODEL OF ANXIOLYTIC ACTIVITY OF CHEMICAL COMPOUNDS BASED ON CORRELATION CONVOLUTION OF ENERGY SPECTRA OF MULTIPLE DOCKING  <b>Pavel Vassiliev</b> Volograd State Medical University, Volograd, Russia
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16:40	NETWORK PHARMACOLOGY REVEALED THE POTENTIAL OF BITTER HONEY IN SUPPRESSION OF CEREBRAL MALARIA-INDUCED INFLAMMASOME  <b>Michael Daniyan</b> Obafemi Awolowo University, Ile-Ife, Nigeria
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**Keynote lectures**

17:00	STRUCTURAL PHARMACOLOGY OF TRANSIENT RECEPTOR POTENTIAL CHANNELS  <b>Arthur Neuberger</b> Columbia University, New York, USA
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17:30	FINE MAPPING OF BIOMOLECULAR SURFACES USING THE NEW MOLECULAR SURFACE TOPOGRAPHY (MST) WEB TOOL  <b>Yury Trofimov</b> Shemyakin and Ovchinnikov Institute of Bioorganic Chemistry, Moscow, Russia
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### Oral presentations

18:00	UNIFIED LATIN AMERICAN NATURAL PRODUCT DATABASE LANAPDB  <b>Alejandro Gomez Garcia</b> National Autonomous University of Mexico, Mexico City, Mexico
18:20	IS CHEMICAL SPACE OF RUSSIAN VENDOR CATALOGUES SUFFICIENT FOR LEAD DISCOVERY  <b>Dmitry Osolodkin</b> Chumakov FSC RnD IBP Russian Academy of Sciences (Institute of Poliomyelitis), Moscow, Russia
18:40	LATIN AMERICAN PHYTOCHEMICAL DERIVATIVES AS PROMISING CANDIDATES FOR GALLSTONE DISEASE THERAPY INSIGHTS FROM MOLECULAR SCREENING, MOLECULAR DOCKING, DENSITY FUNCTIONAL THEORY, AND MOLECULAR DYNAMICS STUDIES  <b>Jaime Tamayo</b> Universidad Nacional Mayor de San Marcos, Lima, Peru




## Tuesday September 17, 2024

*Chairpersons: Kunal Roy and Vladimir Sulimov*


### Keynote lectures


10:00	CHRONOBIOTICSDB - WORLD FIRST DATABASE OF CIRCADIAN RHYTHM'S PHARMACOLOGICAL MODULATORS  <b>Ilya Solovov</b> Pitirim Sorokin Syktyvkar State University, Syktyvkar, Russia
10:30	COCONUT 2.0 DATABASE AND AUTOMATED LITERATURE MINING USING DECIMER.AI  <b>Kohulan Rajan</b> Friedrich Schiller University, Jena, Germany

### Oral presentations

11:00	MACHINE LEARNING ESTIMATION OF THE SMALL MOLECULE SELECTIVITY INDEX VALUE FOR INFLUENZA VIRUS STRAIN AH1N1  <b>Alexey Egorov</b> National Research Nuclear University MEPhI, Moscow, Russia
11:20	MACHINE LEARNING PREDICTIONS OF COCRYSTAL FORMATION TO ENHANCE ACTIVE PHARMACEUTICAL INGREDIENTS PROPERTIES FOR CANCER PREVENTION  <b>Nguyen Quoc Khanh Le</b> Taipei Medical University, Taipei, Taiwan
11:40	CHEMOMETRICS GUIDED LEAD IDENTIFICATION AND DESIGN OF NOVEL ANALOGS WITH TRYPANOTHIONE REDUCTASE ACTIVITY BASED ON 2-AMINOBENZIMIDAZOLE SCAFFOLDS AND MOLECULAR SIMULATIONS FOR ADDRESSING LEISHMANIASIS  <b>Arpita Biswas</b> Brainware University, Kolkata, India

### Keynote lectures

12:00	ON A SIMPLE FRAMEWORK OF DIMENSIONALITY REDUCTION FOR CLASSIFICATION MODELING OF SPARSE ENVIRONMENTAL TOXICITY DATA  <b>Kunal Roy</b> Jadavpur University, Kolkata, India
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12:30	<p>ACTIVATION OF GLYCOGENOLYSIS WITHOUT AN ACTIVATION OF ATP CONSUMPTION CAN CAUSE CELL DEATH</p> <p> <b>Victor Vitvitsky</b> Center for Theoretical Problems of Physico-Chemical Pharmacology Russian Academy of Sciences, Moscow, Russia</p>
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**13:00-15:00**


**Lunch break**


*Chairpersons: Athina Geronikaki and Alexey Lagunin*

**Young Scientists flash presentations**

15:00	<p>MOLECULAR DOCKING OF SECONDARY METABOLITE COMPOUND OF KAWISTA (Limonia acidissima) AS HUMAN EPIDERMAL GROWTH FACTOR RECEPTOR-2 (HER-2) INHIBITORS</p> <p> <b>Azka Khoirunnisa</b> Department of Pharmacy, Faculty of Health Science, University of Muhammadiyah Malang, Indonesia</p>
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15:10	<p>PREDICTION OF PROTEIN SECONDARY STRUCTURES BASED ON SUBSTRUCTURAL MNA DESCRIPTORS OF MOLECULAR FRAGMENTS</p> <p> <b>Oleg Zakharov</b> Department of Bioinformatics, Pirogov Russian National Research Medical University, Moscow, Russia</p>
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15:20	<p>STRUCTURAL AND FUNCTIONAL CHARACTERIZATION OF HYPOTHETICAL PROTEINS OF LUMPY SKIN DISEASE VIRUS TOWARD IDENTIFICATION OF VACCINE TARGETS</p> <p> <b>Bhaavikka Agarwaal</b> Mahindra University, Hyderabad, India</p>
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15:30	<p>COMPUTATIONAL EXPLORATION OF NATURAL NOVEL HYBRID MOLECULES AS RAF-1 KINASE ANTAGONISTS FOR BREAST CANCER THERAPEUTICS</p> <p> <b>Navya Aggarwal</b> Immunoncology and Molecular Theragnostics Lab, Centre for Medical Biotechnology, Amity Institute of Biotechnology, Amity University Uttar Pradesh, Noida, India</p>
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15:40	<p>FOOD CHRONOBOTICS: KEY COMPOUNDS DATABASE FOR CHRONONUTRITION</p> <p> <b>Denis Golubev</b> Pitirim Sorokin Syktyvkar State University, Syktyvkar, Russia</p>
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15:50	<p>IN-SILICO DESIGN AND STUDY OF NOVEL MANNICH BASE DERIVATIVES AGAINST THE SELECTED TARGETS FOR ITS ANTIMICROBIAL ACTIVITY</p> <p> <b>Guru Aribam Mansi Devi</b> Harsha college of pharmacy, Bengaluru, Karnataka, India</p>
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16:00	<p>QUANTITATIVE PREDICTION OF HUMAN IMMUNODEFICIENCY VIRUS DRUG RESISTANCE</p> <p> <b>Ekaterina Stolbova</b> National Research University Higher School of Economics, Moscow, Russia</p>
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16:10	<p>4'-FLUORO-5,7-DIHYDROXYFLAVONE – PIPERAZINE HYBRIDS AS VEGFR-2 INHIBITORS: DESIGN, IN-SILICO STUDY, SYNTHESIS, AND ANTICANCER ACTIVITY</p> <p> <b>Kalyani Thombre</b> Department of Pharmaceutical Science, Smt. Kishoritai Bhoyar College of Pharmacy, Kamptee, Nagpur (MS), India</p>
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16:20	<p>DRUG METABOLISM PREDICTION USING GRAPH NEURAL NETWORKS</p> <p> <b>Nikita Polomoshnov</b> Moscow State University, Moscow, Russia</p>
16:30	<p>MOLECULAR DYNAMIC SIMULATION OF SOME N-N-DISUBSTITUTED PIPERAZINE DERIVATIVES EXHIBITING ANTICHOLINESTERASE ACTIVITY</p> <p> <b>Viktor Ghamaryan</b> Russian-Armenian University, Institute of Biomedicine &amp; pharmacy, laboratory of structural bioinformatics Yerevan, Armenia</p>
16:40	<p>CREATION OF SAR MODELS FOR PREDICTION OF T-CELL EPITOPES WITH HUMAN LEUKOCYTE ANTIGENS BASED ON PROTEIN STRUCTURAL FORMULAS</p> <p> <b>Anton Smirnov</b> Department of Bioinformatics, Pirogov Russian National Research Medical University, Moscow, Russia</p>
16:50	<p>VIRTUAL SCREENING OF NEW POTENTIAL INSECT EPOXIDASE CYP15A1 INHIBITORS</p> <p> <b>Polina Yakovets</b> Research Institute for Physical Chemical Problems, Belarusian State University, Minsk, Belarus</p>
17:00	<p>LIGAND-PROTEIN BINDING SITE ANNOTATION USING GRAPH NEURAL NETWORKS</p> <p> <b>Alexey Ereshchenko</b> The Federal State Unitary Enterprise Dukhov Automatics Research Institute, Moscow, Russia</p>
17:10	<p>CASTOR OIL AND LAXATIVE ACTIVITY: VIRTUAL SCREENING OF RICINOLEIC ACID ANALOGUES</p> <p> <b>Bayouhd Sirine</b> Pharmaceutical Sciences Department B, College of Pharmacy of Monastir, University of Monastir, Monastir, 5000, Tunisia</p>
17:20	<p>WORLD WIDE APPROVED DRUGS: FROM BIG BIOMEDICAL DATA TO GLOBAL SMALL MOLECULE DRUG DATABASE</p> <p> <b>Polina Savosina</b> Institute of Biomedical Chemistry, Moscow, Russia</p>
17:30	<p>A GENERAL PROTOCOL FOR THE CONSTRUCTION OF STRUCTURE-ACTIVITY LANDSCAPES OF NON-CANONICAL PEPTIDES</p> <p> <b>Edgar López-López</b> DIFACQUIM Research Group, Department of Pharmacy, School of Chemistry, Universidad Nacional Autónoma de México, Mexico</p>
17:40	<p>POTENTIAL NEW INHIBITOR MOLECULES FOR SARS-COV-2 PLPRO: AN IN SILICO AND SYNTHETIC APPROACH</p> <p> <b>Gianfranco Sabadini</b> Organic Chemistry Laboratory, Institute of Chemistry and Biochemistry, Faculty of Sciences, University of Valparaíso. Gran Bretaña 1111, Playa Ancha, Valparaíso, Chile</p>
17:50	<p>AUTOMATED ANALYSIS OF STRUCTURE-MULTIPLE PROPERTY RELATIONSHIPS: IMPACT ON SMARTS</p> <p> <b>Jesús Israel Espinoza Castañeda</b> DIFAQUIM research group, Department of Pharmacy, School of Chemistry, National Autonomous University of Mexico</p>

### Keynote lectures

18:00	AUTOMATING THE DESIGN OF GLYCOMIMETIC AGENTS  <b>Robert J. Woods</b> University of Georgia, Athens, USA
18:30	SQUARE ANTIPRISM IS A KEY DETERMINANT FOR POTASSIUM ION SELECTIVITY  <b>Anton Chugunov</b> Shemyakin-Ovchinnikov Institute of Bioorganic Chemistry Russian Academy of Sciences, Moscow, Russia




## Wednesday September 18, 2024

*Chairpersons: Alexander Kel and Olga Tarasova*



### Keynote lectures

9:00	COMPREHENSIVE COMPUTATIONAL SYSTEMS BIOLOGY MODEL OF BLOOD PLATELET SIGNALLING: A TOOL FOR BASIC RESEARCH, DIAGNOSTICS AND PHARMACOLOGY  <b>Anastasia Sveshnikova</b> Dmitriy Rogachev National Medical Research. Center of Pediatric Hematology, Oncology, Immunology Ministry of Healthcare of Russian Federation, Moscow, Russia
9:30	ANALYSIS OF CHEMICALS-VIRUS-HOST INTERACTIONS BASED ON LARGE-SCALE BIOMEDICAL TEXT AND DATA MINING  <b>Olga Tarasova</b> Institute of Biomedical Chemistry, Moscow, Russia




### Oral presentations

10:00	EVALUATION OF NATURAL FLAVONOID COMPOUNDS N AMYLOID- (AB) INHIBITION FOR ALZHEIMER'S DISEASE TREATMENT  <b>Arli Aditya Parikesit</b> Indonesia International Institute for Life Sciences, Jakarta, Indonesia
10:20	QSAR MODELS FOR PREDICTION OF CYTOTOXIC IC50 AND GI50 VALUES OF SUBSTANCES IN RELATION TO NON-TUMOR CELL LINES  <b>Elena Lisitsa</b> Pirogov Russian National Research Medical University, Moscow, Russia
10:40	DIGEP-PRED 2.0 A WEB-SERVICE FOR PREDICTING DRUG-INDUCED CELL SIGNALING AND GENE EXPRESSION CHANGES  <b>Sergey Ivanov</b> Institute of Biomedical Chemistry, Moscow, Russia

### Keynote lectures

11:00	CHEMICAL PROTEOMICS FOR OVERCOMING DRUG RESISTANCE  <b>Roman Zubarev</b> Karolinska Institutet, Stockholm, Sweden
11:30	HOW MANY DRUG TARGETS DO WE NEED?  <b>Alexander Kel</b> geneXplain GmbH, Wolfenbuettel, Germany

### Oral presentations




12:00	MOLECULAR MODELING OF HUMAN LINE-1 ORF2 PROTEIN  <b>Anna Kulakova</b> Lomonosov Moscow State University, Moscow, Russia
12:20	THE QSAR STUDY OF THE HYDROLYSIS OF DINITROSYL IRON-SULFUR COMPLEXES  <b>Victor Luzhkov</b> Federal Research Center of Problem of Chemical Physics and Medicinal Chemistry Russian Academy of Sciences, Moscow, Russia
12:40	IN SILICO EVALUATION OF THE MUTAGENICITY, GENOTOXICITY, AND CARCINOGENICITY OF LEVETRACETAM, A NEW-GENERATION ANTIPILEPTIC  <b>Sezen Yilmaz Sarialtin</b> Ankara University, Ankara, Turkey

13:00-16:00



Lunch break

*Chairpersons: Maria Khrenova and Dmitry Shulga*


### Oral presentations

16:00	CONSTRUCTING BAYSIAN NETWORKS TO DETERMINE THE RISKS OF DRUG INTERACTIONS BASED ON INSTRUCTIONS  <b>Yurii Titov</b> Plekhanov Russian University Of Economics, Moscow, Russia
16:20	SMALL-MOLECULE ACTIVATORS FOR GLUCOSE-6-PHOSPHATE DEHYDROGENASE (G6PD) USING MACHINE LEARNING APPROACHES  <b>Madhu Sudhana Saddala</b> University of California, Irvine, USA
16:40	OLEG A. RAEVSKY - SCIENTIST, TEACHER, PERSON  <b>Oleg Tinkov</b> Shevchenko Transnistria State University, Tiraspol, Moldova

### Keynote lectures

17:00	ALPHAFOLD-LIKE MODELS FOR SMALL MOLECULE STRUCTURE PREDICTION  <b>Petr Popov</b> Constructor University, Bremen, Germany
17:30	PROTEIN 3D STRUCTURE IDENTIFICATION BY ALPHAFOLD A PHYSICS-BASED PREDICTION OR RECOGNITION USING HUGE DATABASES?  <b>Alexei Finkelstein</b> Institute of Protein Research Russian Academy of Sciences, Pushchino, Russia

### Plenary lectures

18:00	EXPLORING THE CHEMICAL SPACE AND MULTIVERSE OF FOOD CHEMICALS AND NATURAL PRODUCTS  <b>Jose Medina-Franco</b> Universidad Nacional Autonoma de Mexico, Mexico City, Mexico
18:40	<b>Closure of the XXX Symposium on Bioinformatics and Computer-Aided Drug Discovery</b>