Scientific Program

Tuesday May 24, 2022			
Chairpersons: Vladimir Poroikov, Roman Efremov			
10:00	10:20	Opening of the Symposium	
Plenary lecture			
10:20	11:00	Frank Eisenhaber	THE TARGET IDENTIFICATION BOTTLENECK
Oral presentations			
11:00	11:20	Shuguang Yuan	FROM GPCR BASIC RESEARCH TO DRUG DISCOVERY VIA COMPUTATIONAL METHODS
11:20	11:40	Dmitry Shulga	THE PHILOSOPHY AND PROSPECTS OF FRAGMENT CONTRIBUTION ESTIMATIONS IN DRUG DISCOVERY
11:40	12:00	S. Balaji	INTERACTION AND INHIBITION OF ALPHA-GLUCOSIDASE WITH SELECTED MONOTERPENES
Keynote lectures			
12:00	12:30	Elena Ponomarenko	TARGETED PROTEOMICS FOR HEALTH ANALYTICS: OPPORTUNITIES AND CHALLENGES
12:30	13:00	Alexander Kel	GENE NETWORKS AND DRUGS. WHAT CAN WE LEARN USING BIO- AND CHEMOINFORMATICS?
Oral presentations			
13:00	13:20	Vladimir Ivanisenko	ANDSYSTEM AUTOMATED RECONSTRUCTION OF GENE NETWORKS FOR OMICS-DATA INTERPRETATION IN MEDICAL AND BIOLOGICAL RESEARCH
13:20	13:40	Sajjad Gharaghani	SYSTEM PHARMACOLOGY IN DRUG DISCOVERY
13:40	14:00	Eugene Radchenko	DISCOVERY OF NOVEL TANKYRASE INHIBITOR CHEMOTYPES AN INSIGHTFUL TEST CASE FOR VIRTUAL SCREENING AND MOLECULAR MODELING APPROACHES
Lunch break 14:00-16:00			

Chairpersons: Hanoch Senderowitz, Maria Khrenova			
Plenary lectures			
16:00	16:30	Hanoch Senderowitz	COMPUTATIONAL STUDIES ON GREEN PESTICIDES
16:30	17:00	Dmitry Ivankov	ALPHAFOLD: PREDICTS OR RECOGNIZES THE PROTEIN STRUCTURE?
Oral presentations			
17:00	17:20	Guzel Minibaeva	DE NOVO GENERATION OF SYNTHETICALLY FEASIBLE MOLECULES
17:20	17:40	Anna Tashchilova	SYNTHESIS, DOCKING AND IN VITRO ANTICOAGULANT ACTIVITY ASSAY OF RHODANINE DERIVATIVES OF PYRROLO3,2,1-IJQUINOLIN-2(1H)-ONE AS NEW INHIBITORS OF FACTOR XA AND FACTOR XIA
17:40	18:00	Andrey Buglak	QSPR ANALYSIS IN PHOTONICS
Keynote lectures			
18:00	18:30	Walter F. de Azevedo, Jr.	HARNESSING MACHINE LEARNING FOR DRUG DISCOVERY
18:30	19:00	Artem Cherkasov	THE USE OF DEEP DOCKING FOR AUTOMATED, CONSENSUS-BASED HIT IDENTIFICATION IN DRUG DISCOVERY
Oral presentations			
19:00	19:20	Leonid Stolbov	SELF CONSISTENT CLASSIFIER SAR APPROACH
19:20	19:40	Miguel Guerrero-Gonzalez	DEVELOPMENT OF THE "VSAfiR" METHOD AND ITS APPLICATION IN THE DEVELOPMENT OF ANTIEPILEPTICS

Wednesday May 25, 2022			
Chairpersons: Kunal Roy, Timur Madzhidov			
Plenary lectures			
10:00	10:30	Weiliang Zhu	MOLECULAR DYNAMICS STUDIES ON THE INTERACTIONS BETWEEN SARS-COV-2 SPIKE PROTEIN AND HACE2 OR MABS
10:30	11:00	Dmitry Osolodkin	COMPETITION AND COLLABORATION OF IN SILICO AND IN VITRO SCREENING IN THE SEARCH FOR NEW ANTIVIRAL COMPOUNDS
Oral presentations			
11:00	11:20	Igor Polyakov	SARS-COV-2 MAIN PROTEASE INHIBITION WITH CARMOFUR A COMPUTATIONAL STUDY
11:20	11:40	Tugba Taskin-Tok	MOLECULAR DOCKING-ASSISTED INVESTIGATION OF CU(II) COMPLEXES CARRYING “SNS” PINCER-TYPE PYRIDINE-THIOETHER LIGANDS AS POTENTIAL DRUG CANDIDATES AGAINST SARS-COV-2
11:40	12:00	Elena Aliper	A STRUCTURAL-DYNAMIC MODEL OF SARS-COV-2 SPIKE TRANSMEMBRANE DOMAIN IN CONJUNCTION WITH THE HR2 REGION. IMPLICATIONS FOR MEMBRANE FUSION
Keynote lectures			
12:00	12:30	Kyoung Tai No	DRUG DISCOVERY WITH FRAGMENT MOLECULAR ORBITAL (FMO)
12:30	13:00	Maria Khrenova	HOW DO ENZYMES RECOGNIZE SUBSTRATES AND INHIBITORS: STRUCTURAL AND ELECTRON DENSITY ASPECTS
Oral presentations			
13:00	13:20	Artem Kniga	COMPUTATIONAL CHARACTERIZATION OF N-ACETYLASPARTYLGLUTAMATE SYNTHETASE FROM THE PROTEIN PRIMARY SEQUENCE TO PLAUSIBLE CATALYTIC MECHANISM
13:20	13:40	Anastasia Fomina	ACTIVITY PREDICTION OF SARS-COV-2 MPRO INHIBITORS BASED ON ENSEMBLE DOCKING AND MACHINE LEARNING
13:40	14:00	Anton Chugunov	PHF10 THE SUBUNIT OF PBAF CHROMATIN REMODELING COMPLEX STRUCTURE AND FUNCTION PREDICTIONS

Lunch break 14:00-16:00			
Chairpersons: Pavel Polishchuk, Vladimir Palyulin			
Young scientists flash presentations			
16:00	16:10	Dessiree Allyssa Tina	UNVEILING THE POTENTIAL DRUG LIGANDS AGAINST VIRULENCE-RELATED HYPOTHETICAL PROTEIN IN CRYPTOCOCCUS NEOFORMANS AN IN SILICO ANALYSIS APPROACH
16:10	16:20	Hadiatullah Hadiatullah	VIRTUAL SCREENING OF PLANT-DERIVED COMPOUNDS TARGETING HYDROLYTIC AND LIGNIN DEGRADING ENZYMES OF GANODERMA BONINENSE
16:20	16:30	Anatoliy Bulygin	COMPUTATIONAL APPROACH FOR IMPROVING OF KNOWN PERSPECTIVE SARS-COV-2 MPRO INHIBITORS
16:30	16:40	Debanjan Saha	MULTI-TARGET APPROACH ON LEISHMANIA DONOVANI AND FINDING OUT POTENT INHIBITORS FOR ESSENTIAL ENZYMES
16:40	16:50	Alexandra Sadovskaya	SMMOLE - PIPELINE FOR SEARCHING BIOLOGICAL PROPERTIES OF SECONDARY METABOLITES BASED ON THEIR MOLECULAR STRUCTURES
16:50	17:00	Mohammed Efendi	TESTING THE ACTIVITY OF BIGUANIDES AND SOME NOVEL DESIGNED MOLECULES AGAINST SARS-COV-2 PROTEINS, IN SILICO STUDY
17:00	17:10	Egor Kozlov	DIMERIC STATES OF TRANSMEMBRANE SEGMENTS OF THE DDR1 RECEPTOR PREDICTED BY ATOMISTIC MODELING
17:10	17:20	Arkaprava Banerjee	APPLICATION OF 2D-QSAR AND CHEMICAL READ-ACROSS ALGORITHM TO PREDICT THE ANDROGEN RECEPTOR BINDING AFFINITY
17:20	17:30	Nadezhda Biziukova	NFORMATION EXTRACTION FROM TEXTS ANTIVIRAL AGENTS ACTIVE AGAINST VIRUS OR HOST PROTEINS
17:30	17:40	Aleksandra Ivanova	STRUCTURAL OPTIMIZATION OF TUBULIN INHIBITORS
17:40	17:50	Maksim Perfilev	THE CONSENSUS ENSEMBLE NEURAL NETWORK MULTITARGET MODEL OF ANXIOLYTIC ACTIVITY
17:50	18:00	Alina Kutlushina	MOLECULAR DYNAMIC PHARMACOPHORE AND ITS APPLICATION IN DESIGNING NOVEL MARK4 INHIBITORS

18:00	18:10	Ivan Kuznetsov	ALINA - A DEEP LEARNING BASED PROGRAM FOR PREDICTION OF RNA SECONDARY STRUCTURE WITHOUT SPECIFICATION OF THERMODYNAMIC PARAMETERS
18:10	18:20	Ana Luisa Chavez-Hernandez	TOWARDS THE DE NOVO DESIGN OF HIV-1 PROTEASE INHIBITORS BASED ON NATURAL PRODUCTS
18:20	18:30	Gabriela Bitencourt-Ferreira	EXPLORING THE SCORING FUNCTION SPACE FOR STRUCTURE-BASED DRUG DESIGN
18:30	18:40	Luis Heriberto Vazquez Mendoza	REPURPOSING OF FDA-DRUGS AS POTENTIAL ERB AGONISTS USING MULTICOMPLEX-BASED PHARMACOPHORE MAPS. A NEW APPROACH IN BREAST CANCER THERAPY
18:40	18:50	Alessandra Latorre	IN SILICO DESIGN OF QUERCETIN DERIVATIVES WITH POTENTIAL DUAL INHIBITORY ACTIVITY AGAINST GSK3 AND CDK5P25 FOR THE TREATMENT OF ALZHEIMER'S DISEASE
18:50	19:00	Edgar López-López	CONSENSUS VIRTUAL SCREENING OF NATURAL PRODUCT DERIVATIVES AGAINST TUBULIN

Thursday May 26, 2022			
Chairpersons: Athina Geronikaki, Dmitry Osolodkin			
Plenary lectures			
10:00	10:30	Garikapati Narahari Sastry	THE STATUS OF THE COMPUTER-AIDED DRUG DESIGN: THEN, NOW AND FUTURE
10:30	11:00	Roman Efremov	COMPUTATIONAL DRUG DESIGN FOR MEMBRANE TARGETS: DIVING INTO COMPLEX DETAILS
Oral presentations			
11:00	11:20	Petr Popov	SPATIOTEMPORAL IDENTIFICATION OF BINDING SITES WITH COMPUTER VISION
11:20	11:40	Vladimir Sulimov	NEW INHIBITORS OF THE COAGULATION FACTOR XIIA DOCKING AND EXPERIMENTAL VERIFICATION
11:40	12:00	Anastasia Borovik	AN INSIGHT INTO THE ORIGIN OF MICROTUBULE-CURLING EFFECT OF PODOPHYLLOTOXIN ESTERS MOLECULAR DYNAMICS STUDY
Keynote lectures			
12:00	12:30	Timur Madzhidov	CONDENSED GRAPH OF REACTION - SWISS-KNIFE TOOL FOR REACTION INFORMATICS
12:30	13:00	Kunal Roy	CHEMICAL READ-ACROSS PREDICTIONS OF ECOTOXICITY DATA
Oral presentations			
13:00	13:20	Yuriy Orlov	DEVELOPMENT OF BIOMEDICAL EDUCATIONAL PROGRAMS
13:20	13:40	Kuppusamy Selvam Mukunthan	A COMPREHENSIVE COMPUTATIONAL PHARMACOKINETICS IDENTIFICATION OF BIOTRANSFORMED LEADS FROM CURCUMA CAESIA ROXB
13:50	14:00	Pavel Pogodin	TCSTF, TOOL FOR CATEGORIZATION OF SHORT TEXT FRAGMENTS
Lunch break 14:00-16:00			
Chairpersons: Artem Cherkasov, Alexey Lagunin			
Keynote lectures			
16:00	16:30	Olga Bocharova	PHARMACOLOGICAL POTENTIAL OF MULTIPHYTOADAPTOGEN AS POLYVALENT MEDICATION: IN SILICO, IN VITRO, IN VIVO AND CLINICAL STUDIES

16:30	17:00	Marcus Scotti	NATURAL PRODUCTS DATABASES AS VALUABLE SOURCES OF BIOACTIVE STRUCTURES FOR VIRTUAL SCREENING
Oral presentations			
17:00	17:20	Pavel Vassiliev	THE CONSENSUS ENSEMBLE MULTIDESCRIPTOR MULTITARGET NEURAL NETWORK MODELING OF PHARMACOLOGICAL ACTIVITY OF CHEMICAL COMPOUNDS
17:20	17:40	Evgenia Alimbarashvili	DATABASE OF ANTIMICROBIAL ACTIVITY AND STRUCTURE OF PEPTIDES (DBAASP) - FINDING A WAY OUT OF MICROBIAL RESISTANCE
Keynote lectures			
17:40	18:10	Oxana Galzitskaya	AMYLOIDOGENIC PEPTIDES NEW CLASS OF ANTIMICROBIAL PEPTIDES WITH THE NOVEL MECHANISM OF ACTIVITY
18:10	18:40	Dmitry Filimonov	SIMILARITY ASSESSMENTS IN DRUG DISCOVERY
Plenary lecture			
18:40	19:20	José Medina-Franco	CHEMOINFORMATICS IN DRUG DISCOVERY AND PUBLIC HEALTH: PROGRESS AND CHALLENGES AHEAD
19:20	20:00	Closure of the XXVIII Symposium on Bioinformatics and Computer-Aided Drug Discovery	