8th INDO-US WORKSHOP ON MATHEMATICAL CHEMISTRY 2022 (SEPTEMBER 13-17, 2022)

DAY -1, SEPTEMBER 13, 2022

INAUGURATION- IST 6:00 PM - 6:45 PM

SESSION-1

S. No	Name	Affiliation	Country	Abstract Title	Timing
1	**Plenary lecture by Dr Milan Randic**	Former President, International Academy of Mathematical Chemistry & Emeritus Ellis and Nelle Levitt Professor of Mathematics and Computer Science, Drake University, Des Moines, IA 50010, USA	USA	Graph theory and chemistry	IST 6:55 PM - 7:40 PM
2	**Keynote lecture by Dr Claudiu N. Lungu**	Department of Chemistry, Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University, 400028 Cluj, Romania	Romania	Molecular descriptors in shaping the retrosynthetic space	IST 7:45 PM - 8:15 PM

DAY -1, SEPTEMBER 13, 2022
SESSION-2

S. No	Name	Affiliation	Country	Abstract Title	Timing
1	**Plenary lecture by Dr Paul Mezey**	Chair, Department of Chemistry, Memorial University of Newfoundland, St. John's, Canada & Editor, Journal of Mathematical Chemistry	Canada	Awaited	IST 8:30 PM - 9:15 PM
2	**Keynote lecture by Dr Emilio Benfenati**	Department of Environmental Health Sciences, Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy	Italy	Identifying risks related to cosmetic products, and finding safer alternatives: new programs	IST 9:20 PM - 9:50 PM

3	**Plenary lecture by Dr Ramon Carbó-Dorca**	Head, Section of Quantum and Mathematical Chemistry, Institute of Computational Chemistry, Universitat de Girona, Girona, Spain	Spain	Determination of Unknown Molecular Properties in Molecular Spaces	IST 10:00 PM - 10:40 PM
DAY -2, SEPTEMBER 14, 2022					
SESSION-1: PART A					
S. No	**Name**	**Affiliation**	**Country**	**Abstract Title**	**Timing**
1	**Keynote lecture by Dr Smarajit Manna**	Centre for Interdisciplinary Research and Education, Jodhpur Park, Kolkata 700068, India	India	Computational approach and analysis of Anti-viral vaccine design with significant tolerance against random mutations	IST 12:45 PM - 1:15 PM
2	**Plenary lecture by Dr Xueliang Li**	Vice-President of the International Academy of Mathematical Chemistry & Professor and Co-Director Center for Combinatorics, Nankai University, Tianjin, China	China	Extermal problems for graphical function-indices and f-weighted adjacency matrix	IST 1:30 PM - 2:10 PM
3	**Keynote lecture by Dr Anil Kumar Saxena**	Department of Pharmaceutical Chemistry, Global Institute of Pharmaceutical Education and Research, Kashipur, INDIA	India	Physicochemical significance of ChemDraw and Dragon computed parameters: Correlation studies in the sets with aliphatic and aromatic substituents	IST 2:15 PM - 2:45 PM
DAY -2, SEPTEMBER 14, 2022 SESSION-1: PART B					
1	**Oral Presentation by Mainak Chatterjee**	Jadavpur University, India	India	Use of 2D-QSAR and read-across approaches for the prediction of aquatic toxicity of binary and multicomponent pharmaceutical mixtures against *Aliivibrio fischeri*	IST 2:50 PM - 3:00 PM
2	**Oral Presentation by Priyanaka De**	Jadavpur University, India	India	Repurposing FDA approved drugs as antiviral drugs candidates against SARS-CoV-2: an *in silico* -based approach	IST 3:05 PM - 3:15 PM
3	**Oral Presentation by Tathagata Dey**	Centre for Interdisciplinary Research and Education, India	India	Computational analysis to characterize the mutational changes of any viral sequences	IST 3:20 PM - 3:30 PM

4	**Keynote lecture by Dr Chandan Raychaudhury and Dr Debnath Pal**	Department of Computational and Data Sciences, Indian Institute of Science Bangalore, India	India	Identification of Potential Oral Cancer Drugs as Bcl-2 inhibitors from Known Anti-Neoplastic Agents Through Docking Studies	IST 3:45 PM - 4:15 PM
5	**Oral Presentation by Joyita Roy**	Jadavpur University, India	India	Risk assessment and data gap filling of toxicity of metal oxide nanoparticles (Me_{Ox}NPs) used in nanomedicines: A QSTR approach	IST 4:20 PM - 4:30 PM
6	**Oral Presentation by Vinay Kumar**	Jadavpur University, India	India	Identification of promising antivirals against COVID-19 3CLpro enzyme through multiple virtual screening approach	IST 4:35 PM - 4:45 PM
DAY -2, SEPTEMBER 14, 2022 SESSION-2: PART A This session is dedicated to Late Dr Mircea Diudea					
S. No	**Name**	**Affiliation**	**Country**	**Abstract Title**	**Timing**
1	**Plenary lecture by Dr Pratim Kumar Chattaraj**	Department of Chemistry, IIT, Kharagpur and IIT Bombay, Powai, Mumbai, India	India	Global optimization and toxicity prediction : A soft computing perspective	IST 5:00 PM - 5:40 PM
2	**Keynote lecture by Dr Mihai V. PUTZ**	West University of Timisoara, Romania	Romania	The Multiplex Networking of Molecules. The Chemical Reactivity Reloaded	IST 5:45 PM - 6:15 PM
3	**Keynote lecture by Dr R. Natarajan, Dr C Lungu and Dr Subhash Basak**	Saranathan College of Engineering, Tiruchirappalli, India	India, Romania and USA	Development and use of chirality indices.	IST 6:20 PM : 6:50 PM
4	**Keynote lecture by Dr Matthias Dehmer**	Swiss Distance University of Applied Science, Depart of Computer Science, 3900 Brig, Switzerland	Switzerland	Aspects of Network Complexity Measures	IST 6:55 PM - 7:25 PM
DAY -2, SEPTEMBER 14, 2022 SESSION-2: PART B					
1	**Keynote lecture by Dr Constanza Cárdenas C**	Núcleo Biotecnología Curauma, Pontificia Universidad Católica de Valparaíso, Fono: 56322274826, Av. Universidad 330 Curauma, Valparaíso-Chile	Chile	In the search of bioactive peptides, a little help from mathematical chemistry	IST 7:30 PM - 8:00 PM

2	**Oral presentation by Sisir Nandi**	Global Institute of Pharmaceutical Education and Research	India	Exploring the biochemical mechanisms of indazole compounds against SAH/MTAN-mediated quorum sensing utilizing QSAR and docking	IST 8:10 PM - 8:20 PM
3	**Oral presentation by Arkaprava Banerjee**	Jadavpur University, India	India	Ligand- and Structure-based Modeling of Androgen Receptor Binding Affinity of Endocrine Disruptor Chemicals	IST 8:25 PM - 8:35 PM
4	**Oral presentation by Dr Asish Mitra**	College of Engineering and Management, Kolaghat, India	India	Simulation of drug concentrations over time for a one-compartment model	IST 8:40 PM - 8:50 PM
5	**Oral presentation by Laxmi Sule**	SGSITS Indore	India	Effect of mutation on ligand-protein interactions: A computational modeling study	IST 8:55 PM -9:05 PM
6	**Keynote lecture by Dr Rama K Mishra**	Biochemistry and Molecular Genetics, Feinberg School of Medicine, Northwestern University, Chicago, IL, USA	USA	Can We Accurately Predict the Binding Energy of the Drug Molecules Using In-Silico Methods?	IST 9:10 PM - 9:40 PM
7	**Keynote lecture by Dr Sagar M Goyal**	Professor of Virology, College of Veterinary Medicine, University of Minnesota, 1333 Gortner Ave, St. Paul, MN 55108-1098, USA	USA	Method to determine in vitro antiviral activity of a compound	IST 9:45 PM- 10:15 PM

DAY -3, SEPTEMBER 15, 2022

SESSION-1: PART A
This sesson is dedicated to Late Dr Dilip K Sinha

S. No	Name	Affiliation	Country	Abstract Title	Timing
1	**Keynote lecture by Dr Kunal Roy**	Drug Theoretics and Cheminformatics Laboratory, Department of Pharmaceutical Technology, Jadavpur University, Kolkata, India	India	Chemical Read-Across: Quantitative Predictions and Their Reliability Measures	IST 1:30 PM - 2:00 PM
2	**Keynote lecture by Dr Jinwei Duan**	Associate Professor, School of Sciences, Chang'an University, Xi'an 710064, China	China	Molecular design of DNA polyhedral structures based on graph theory	IST 2:05 PM- 2:35 PM

3	**Keynote lecture by Dr Lim Soon**	Institute for Research in Molecular Medicine, Universiti Sains Malaysia	Malaysia	Approaches towards the refinement of recombinant antibody properties	IST 2:40 PM - 3:10 PM
4	**Keynote lecture by Dr Guillermo Restrepo**	Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany	Germany	The evolution and history of chemistry: an interplay of chemical data and mathematics	IST 3:15 PM - 3:45 PM
DAY -3, SEPTEMBER 15, 2022 SESSION-1: PART B					
1	**Oral presentation by Dr Harishchandra S Ramane**	Karnataka University, India	India	Terminal Eccentricity Indices of Graphs	IST 4:00 PM -4:10 PM
2	**Oral presentation by Abhay Rajpoot**	IIT, Varanasi	India	Predictive ability of physicochemical properties of PCB molecules using symmetric division degree index	IST 4:15 PM -4:25 PM
3	**Oral presentation by Dr S K Ray**	Former Professor, Amity University, Gurgaon	India	Organ based adult stem cell ,OBASC induced cellular therapy for universal vaccine	IST 4:30 PM -4:40 PM
4	**Oral presentation by Dr Swagata Gupta**	Bherulal Patidar Govt. P G College, MHOW, MP, India	India	A Novel application of Kier- Hall electrotopological Descriptors in determining new HIV-1 Non Nucleoside Reverse Transcriptase Inhibitors(NNRTIs) on the basis ofcChemical similarity	IST 4:45 PM -4:55 PM
5	**Oral presentation by Shayeri Das**	Manipal University Jaipur	India	A DFT study of X3O4 (X- Ti, Fe and Zn) based clusters	IST 5:00 PM - 5:10 PM
6	**Oral presentation by Dr Subhabrata Majumdar**	Applied ML Research, Splunk	USA	Beware of External Validation! When and How to use Proper Validation in QSAR	IST 5:15 PM -5:35 PM
7	**Oral presentation by Subhash Ajmani**	Citadel Precision Medicine LLC,	USA	Computational Framework for Discovering Potential Drug Similarities in Multi-omics Era and its Application	IST 5:40 PM - 6:00 PM
8	**Oral presentation by Sumanta Dey**	Centre for Interdisciplinary Research and Education, Kolkata, India	India	A novel in-silico approach for peptide vaccine design for any emerging pathogen	IST 6:05 PM - 6:15 PM

9	**Oral presentation by Sutanu Mukhopadhyay**	Ramakrishna Mission Vivekananda Ceneterary College, Rahara, India	India	Topological indices study of Nirmatrelvir 9PF-07321332), an antiviral drug against SARS-CoV-2 main protease	IST 6:20 PM - 6:30 PM
DAY -3, SEPTEMBER 15, 2022 SESSION-2					
S. No	**Name**	**Affiliation**	**Country**	**Abstract Title**	**Timing**
1	**Keynote lecture by Dr Snigdhansu Chatterjee**	Institute for Research in Statistics and its Applications (IRSA) Professor, School of Statistics, University of Minnesota, 313 Ford Hall, 224 Church Street S. E., Minneapolis, MN 55455, USA	USA	Supervised learning methods for discovery of chemical properties and bio-activities	IST 6:45 PM - 7:15 PM
2	**Plenary lecture by Dr Krishnan Balasubramanian**	Professor, School of Molecular Sciences, Arizona State University, Tempe AZ 85287-1604, USA	USA	Combinatorics, Big Data & Artificial Intelligence pertinent to molecules & Drug Discovery	IST 7:20 PM - 8:00 PM
3	**Keynote lecture by Dr Wieslaw Nowak**	Director of Doctoral School of Exact Science and Head of Department of Biophysics, Institute of Physics, N. Copernicus University in Torun, Poland	Poland	Bioinformatics, computer modeling and photoactived proteins	IST 8:05 PM - 8:35 PM
4	**Keynote lecture by Dr Marjana Novic**	National Institute of Chemistry, Ljubljana, Slovenia	Slovenia	Efflux of Chemicals through the Cell Membrane: Human P-glycoprotein protein Structure-Function Relationships	IST 8:40 PM - 9:10 PM
5	**Keynote lecture by Dr Suman Chakravarti**	VC MultiCase Inc., USA	USA	FlexFilters: A modular and flexible framework for implementing (Q)SAR approaches to meet the needs of rapidly evolving field of computational toxicology	IST 9:15 PM - 9:45 PM
DAY -4, SEPTEMBER 16, 2022					
SESSION-1					
S. No	**Name**	**Affiliation**	**Country**	**Abstract Title**	**Timing**

1	**Plenary lecture by Dr Vladimir Palyulin**	Department of Chemistry, Moscow State University, Moscow, Russia	Russia	Artificial intelligence in drug discovery	IST 3:00 PM - 3:40 PM
2	**Keynote lecture by Dr Prasad V. Bharatam**	Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research (NIPER), Sector-67, S.A.S. Nagar (Mohali) – 160 062, Punjab, India	India	3D thinking in anti-cancer agent discovery	IST 3:45 PM - 4:15 PM
3	**Keynote lecture by Dr Indira Ghosh**	School of Computational & Integrative Sciences, Jawaharlal Nehru University, New Delhi	India	Deep look into the antimalarial drive – Resistance ,Novel compound search & Novel target(s)	IST 4:20 PM - 4:50 PM
4	**Keynote lecture by Dr Gung Hu**	School of Biology and Basic Medical Sciences, Soochow University, Suzhou 215123, China	China	Applications of graph theory in studying protein structure, dynamics, interactions	IST 4:55 PM - 5:25 PM
5	**Keynote lecture by Dr Lavanya Selvaganesh**	IIT, Varanasi	India	Potential Application of Novel AL indices as Molecular Descriptors	IST 5:30 PM - 6:00 PM

DAY -4, SEPTEMBER 16, 2022
SESSION-2: PART A
This session is dedicated to Late Dr Nenad Trinajstic

S. No	Name	Affiliation	Country	Abstract Title	Timing
1	**Plenary lecture by Dr Douglas Klein**	Texas A&M University at Galveston, Galveston, Texas	USA	Partial Orderings in Chemistry	IST 6:15 PM - 6:55 PM
2	**Keynote lecture by Dr Bono Lucic**	The Rugjer Boskovic Institute, P. O. Box 1016, 41001 Zagreb, Croatia	Croatia	Zagreb indices: an overview and development of new variants	IST 7:00 PM - 7:30 PM
3	**Keynote lecture by Dr Ajit Basak**	Department of Crystallography, Birkbeck College, Malet Street, London WC1E 7HX, United Kingdom	UK	Structural investigation of pore-forming toxins from Clostridium perfringens	IST 7:35 PM - 8:05 PM

DAY -4, SEPTEMBER 16, 2022 SESSION-2: PART B This session is dedicated to Late Dr Ashesh Nandy					
1	**Plenary lecture by Dr Subhash Basak**	University of Minnesota Duluth, USA	USA	Mathematical chemodescriptors and proteomics-based biodescriptors: Development and applications in quantitative structure-activity/toxicity relationship (QSAR/ QSTR) studies	IST 8:10 PM - 8:50 PM
2	**Keynote lecture by Dr Andres Fernando Bernal Escobar**	Departamento de Ciencias Básicas, Universidad de Bogotá Jorge Tadeo Lozano	Colombia	Lipinski's rule of 5 and the base rate fallacy	IST 8:55 PM - 9:25 PM
3	**Keynote lecture by Dr Nitin Sapre**	G S Institute of Technology and Science, Indore	India	Computational modeling studies inducing missense mutation in NNRTI protein: Design of modelled proteins and their stability studies	IST 9:30 PM - 10:00 PM

DAY -5, SEPTEMBER 17, 2022					
SESSION-1					
S. No	**Name**	**Affiliation**	**Country**	**Abstract Title**	**Timing**
1	**Plenary lecture by Dr David A. Winkler**	Medicinal Chemistry, Monash Institute of Pharmaceutical Sciences (MIPS), Australia	Australia	Species susceptibilities to, and possible origin of the SARS-CoV-2 virus	IST 3:00 PM-3:40 PM
2	**Keynote lecture by Dr Kinkar Chandra Das**	Department of Mathematics, Sungkyunkwan University,Republic of Korea	Korea	On Modified First Zagreb Connection Index of molecular graphs with chemical significance	IST 3:45 PM - 4:15 PM
3	**Plenary lecture by Dr Tanmoy Chakraborty**	Department of Chemistry and Biochemistry, Sharda University, Greater Noida, India	India		IST 4:20 PM - 5:00 PM
4	**Keynote lecture by Dr Prabhat Ranjan**	Department of Mechatronics Engineering, Manipal University Jaipur	India	Computational analysis of chalcopyrite-type semiconductors	IST 5:05 PM - 5:35 PM

DAY -5, SEPTEMBER 17, 2022 SESSION-2: PART A					
S. No	**Name**	**Affiliation**	**Country**	**Abstract Title**	**Timing**
1	**Plenary lecture by Dr G. Narahari Sastry**	Director, CSIR - North East Institute of Science & Technology (CSIR-NEIST), Jorhat-785006, Assam, India	India	A Comparison of Molecular Modeling, Mathematical Modeling and Machine Learning Approaches to predict Toxicity	IST 5:45 PM - 6:25 PM
2	**Oral presentation by Poonam Yadav**	Department of Chemistry, Manipal University Jaipur	India	A study of 5lipoxygenase inhibitors invoking DFTbased descriptor nucleophilicity index	IST 6:30 PM - 6:40 PM
3	**Oral presentation by Saloni**	Department of Chemistry and Biochemistry, Sharda University, Greater Noida, India	India	A computational approach to study transition metal-based chalcopyrite having potential application as intermediate band solar cell	IST 6:45 PM - 6:55 PM
4	**Oral Presentation by Dimple and Pooja**	Department of Chemistry and Biochemistry, Sharda University, Greater Noida, India	India	Variation of electrophilicity index of elements under different pressures: A theoretical study	IST 7:00 PM - 7:10 PM
DAY -5, SEPTEMBER 17, 2022 SESSION-2: PART B					
1	**Keynote lecture by Dr Denis Sabirov**	Director of the Institute of Petrochemistry and Catalysis, UFRC, Russian Academy of Sciences, 450075 Ufa, Russia	Russia	Information entropy of chemical objects: an interplay between structural, digital, and physical chemistry	IST 7:15 PM - 7:45 PM
2	**keynote lecture by Dr Marjan Vracko**	Research Associate Professor, National Institute of chemistry, Ljubljana, Slovenia	Slovenia	How to use chemometrics in analysis and merging of the ‘small and big’ data	IST 7:50 PM - 8:20 PM
3	**Keynote lecture by Dr Shahul H. Nilar**	Director, Computational Chemistry, Global Blood Therapeutics, South San Francisco, CA 94080, USA	USA	Application of Artificial Intelligence techniques in the Deconvolution of Covid-19 hits into Fragments	IST 8:25 PM - 8:55 PM
4	**Keynote lecture by Dr Apurba Bhattacharjee**	Department of Microbiology and Immunology, School of Medicine, Georgetown University, Washington, DC 20057, USA	USA	Discovery of potential anti-Covid-19 compounds using QM based interaction pharmacophore profiling	IST 9:00 PM - 9:30 PM
VALEDICTORY: IST 9:35 PM - 10:00 PM					

In case of any queries, you may contact:

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