List of Speakers with Titles of Presentations

S. No	Title of the presentation	Presenting author
INVITED LECTURES		
I-1	Neuroprotective AMPA receptor modulators: from computer-aided drug design to synthesis and preclinical studies	Vladimir A. Palyulin
I-2	Adventures in the evolving landscape of mathematical descriptors of molecules and biomolecules: A tortuous journey of fifty years	Subhash C. Basak
I-3	Pharmacophore recognition of bioactive molecules may aid in more efficient AI -driven database searches for discovery of potent compounds	Apurba K. Bhattacharjee
I-4	Bioinformatics, computer 1olyhedra and mosquitos: Insect sodium channels functioning from a theoretical perspective	Wieslaw Nowak
I-5	Simulating optical properties of organic and biomaterials	Nađa Došlić
I-6	Topological indices: Physicochemical significance in QSARS	Anil Kumar Saxena
I-7	Higher-dimensional structures for a better understanding of the chemical space and its evolution	Guillermo Restrepo
I-8	A novel pyruvate kinase activator – From a HTS impurity to a lead series	Shahul H. Nilar
I-9	Assessment of JNK3 enzyme inhibition of piceatannol - in silico & in-vitro studies	Ramanathan, M.
I-10	Modelling adsorption of small structures onto fullerene graphs	Tomislav Došlić
I-11	Unravelling the complex immunorepertoire of an immune library	Theam Soon Lim
I-12	Entrapment of flow of substrate to diversion pathway for combating persistent tuberculosis: Bioinformatics Approach	Indira Ghosh
I-13	Building better computational toxicology solutions with AI and ML	Suman Chakravarti
I-14	Assessment of Blood-Brain Barrier entry of a structurally diverse set of chemicals using computed descriptors	Aritra Banerjee
I-15	Growing counter-propagation artificial neural networks	Igor Kuzmanovski
I-16	Assessment of mutagenicity using computed molecular descriptors and support vector machines	Igor Kuzmanovski
I-17	Emotions extraction of autism children through art using deep learning techniques	C. Vijayalakshmi
I-18	VEGFR2 chemical space: Stimulator and inhibitory peptides	Claudiu N Lungu
I-19	Rhombelane based vaccines	Claudiu N Lungu
I-20	Mediated vasculogenesis and morphogenesis	Claudiu N Lungu

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I-21	On the nature of chemical bond: Quantum molecular polyhedra and collective bond description	Ramon Carbó-Dorca
I-22	Clustering/classification of chemicals, proteomic data and emerging global viruses considering different kinds of representations	Marjan Vračko
I-23	Information-entropy descriptors for chemical reactions	Denis Sabirov
I-24	Topological isomers of DNA dodecahedral links	Jin-wei Duan
I-25	Perturbation response scanning analysis for drug-target networks	Guang Hu
I-26	All-metal aromaticity and conceptual DFT	Pratim K. Chattaraj
I-27	The application of the QSPR methodology can help improve the prediction of protein folding rates	Bono Lučić
I-28	Molecular descriptors or machine-generated features? Their impact in predictive modelling and QSAR	Giuseppina Gini
I-29	Use of alignment-free sequence descriptors (AFSDs) in the computer assisted unified vaccine design.	Smarajit Manna
I-30	Decoding proteomic mysteries: advanced graphical user interfaces for FASTA harmonization and in-silico mutation engineering	Nitin Sapre
I-31	Mathematical chemodescriptors for the characterization of molecular chirality	Natarajan, R.
I-32	Recent trends in the study of molecular descriptors using graph theoretic approach	Lavanya Selvaganesh
ORAL PRESENTATIONS		
O-1	Essential oils from a tropical medicinal plant, *Ruta chalepensis* as a potential raw material in the manufacture of vector control formulations	Dharani Jayagopal
O-2	Bioactive compounds from *Ocimum tenuiflorum* as vector agent against Aedes albopictus	Joel Jaison
O-3	Exploring the phytoconstituents and therapeutic potential of Plumeria rubra flower extract for SGLT-2 receptor targeting: GC–MS and an *in silico* approach	Abin V Geevarghese
O-4	In silico evaluation of the isolates of *Calotropis procera* and *Nigella sativa* as anti-cancer potentials	Renugadevi, T.
O-5	Molecular docking studies of phytomolecules against multi targets associated with antioxidants, anti-inflammatory and anticancer pathways	Maida Engels, S.E.
O-6	Structural insights into 4-bromomandelic acid as a potent M2 muscarinic receptor antagonist: A molecular docking approach	Judith Rashma, L.

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O-7	Optimizing large-scale molecular docking: A novel software prototype for efficient drug discovery	Ravikiran, R.
O-8	Inter- and intra-molecular interactions and dielectric dispersion studies of amino acid solubilized in anionic surfactant solution	Ganesh, T.
O-9	Dielectric Relaxation Spectral and molecular interaction analysis of aqueous pyrazine in ethanol using Time domain reflectometry (TDR)	Senthilkumar, P.
O-10	Computational insights into photoactive systems: exploring photoswitching, TADF, and photosensitization	Moumita Banerjee
O-11	*Prosopis juliflora* leaf extract assisted synthesized tin oxide nanoparticles for applications high-performance supercapacitor electrode	Suganya, G.
O-12	Green synthesis of zinc oxide nanorods using *Ficus benghalensis* aerial root extract and enhanced antibacterial activity	Princess Gracia, J.
O-13	One-pot bioinspired synthesis of PbO/CuO/FeO trimetallic oxide nanocomposite using *Vitis vinifera* fruit juice for highly sensitive electrochemical detection of 4-nitrotoluene	Bargavi, V.
O-14	Characterization of sequence similarity using BLAST versus novel alignment-free information theoretic sequence descriptors: A case study with Infectious Salmon Anemia Virus (ISAV) sequences	Tathagata Dutta & Constanza C. Carvajal
O-15	Predicting mutagenicity of a diverse set of chemicals using mathematical molecular descriptors and different statistical methods	Ronit Bhattacharjee
O-16	Machine learning-integrated template-guided docking: a novel approach for identifying potent HIV-1 NNRTIs	Swagata Gupta
O-17	A DFT study of lead-free halide perovskites GaMX3 (X= Sr, Ba; X= F, Cl) for solar cell applications	Vinita Rohlan
O-18	Design and evaluation of quercetin-5-fluorouracil conjugates and other similar conjugates as anti-cancer agents	Priyarega, S.
O-19	A novel bio-indicator of soil fertility	Nithyatharani, R.
O-20	Synthesis of Schiff bases as corrosion inhibitors	Balamurugan, V.
O-21	Atom bond sum connectivity index of fuzzy graphs	Sivamani, S.
POSTER PRESENTATIONS		
P-1	Semi-synthetic PTP1B inhibitor from Cassia auriculata linn. by in silico method for diabetes management	Ezhilanbu, K.
P-2	Exploring the role of revolutionizing the potential of explainable AI in drug discovery	Visali, K.

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P-3	Molecular dynamics simulations of phytochemicals from *Citrullus colocynthis* and *Pulicaria crispa* for anti-cancer potentials	Jancy Reen, I.M.
P-4	Molecular dynamics study of afimetoran using desmond: Insights into structural dynamics and binding interactions	Madhu Krishna, M.
P-5	Quantum mechanical analysis of the conformational and structural properties of clopidogrel bisulfate in the gas phase	Davis Presley, S.I.
P-6	Identification of new chemical entities targeting glycogen synthase kinase-3 protein using in silico through artificial intelligence having indirubin as reference molecule	Manas Kumar, G.
P-7	Integrative in silico framework for evaluating meridine analogues: toxicity, QSAR, and molecular dynamics insight	Vishnu, R.
P-8	Medicinal mushrooms in cancer treatment	Mekala, S.
P-9	Application of machine learning in drug discovery	Renita an Sindhiya, J.
P-10	AI and ML in drug discovery	Aishvarya, V.
P-11	Zero maintenance system for production of biofuels	Kanishka, S