NINTH INDO-US WORKSHOP ON MATHEMATICAL CHEMISTRY

With Applications to Drug Discovery, Computational Toxicology, Cheminformatics and Bioinformatics

Ramanathan Natarajan &

Subhash C. Basak

January 6-10, 2025

Host Institute

Saranathan College of Engineering,

Tiruchirappalli 620012, Tamil Nadu India

THE EVENT REPORT

INDO-US WORKSHOP SERIES ON MATHEMATICAL CHEMISTRY

Founder Chairman of the Workshop Series

Dr Subhash C. Basak

Retired Adjunct Professor, Department of Chemistry and Biochemistry &
Senior Scientist, Natural Resources' Research Institute, University of Minnesota
Duluth, MN, USA.

Ninth Indo-US Workshop on Mathematical Chemistry

Event Organizer

Dr Ramanathan Natarajan

Professor and Head, Research and Development, Saranathan College of
Engineering, Tiruchirappalli 620012, Tamil Nadu, India

Date: January 6-10, 2025

Host Institute

Saranathan College of Engineering, Tiruchirappalli 620 012
Tamil Nadu, India

Dedication

The Ninth edition of the workshop series is the Silver Jubilee event and we miss some of our long-time supporters. We pay our sincere prayers for these souls departed. This report is dedicated in the fond and respectful memories of the following scientists.

Dr Dilip K. Sinha
Jan 9,1940 – Apr 2, 2021

Professor Ray Hefferlin
1929 -Mar 7, 2015

Professor Nickolay Zefirov
Sep 13, 1935 – Apr 28, 2017

Professor Nenad Trinajstić
Oct 26, 1936 – Aug 27, 2021

Professor Ashesh Nandy
Apr 26, 1943- Apr 24, 2022

1 Preamble

The major objectives of the three mathematical chemistry conferences, viz. Indo-US workshop on mathematical chemistry series; Indo-US lecture series on discrete mathematical chemistry and Mathematical chemistry workshop of the Americas, were to stimulate basic and applied research in mathematical chemistry and allied subject areas. To that end, a three-pronged approach was taken consisting of a) High level presentations on basic & applied aspects of mathematical chemistry, b)publications of international quality peer-reviewed papers in top journals of the field based on presentations by speakers c) publication of books by internationally reputed researchers from India, USA, and other countries and, d) development of a *Pustika* (white paper) to inform and educate practitioners of the field regarding the advancing frontiers of mathematical chemistry.

Pustika or White paper

Subhash C. Basak and Dilip K. Sinha jointly developed a *Pustika* (white paper) describing the lessons learned from the three sets of mathematical chemistry conferences organized in India, as well of countries of North America & South Americas.

Papers Published:

High quality peer reviewed scientific papers were published in top ranked scientific Journals:

Journal Chemical Information and Computer Science (Journal Chemical Information and Modeling)

Journal of Mathematical Chemistry

Books edited:

Researchers associated with the three mathematical chemistry series published the following books:

1. Statistical and Machine Learning Approaches for Network Analysis, Matthias Dehmer and Subhash C. Basak, Editors, Wiley, Hoboken, New Jersey, USA, 2012 (11 chapters)
2. Advances in Mathematical Chemistry and Applications, Volume 1 & 2, Subhash C. Basak, Guillermo Restrepo, and Jose Luis Villaveces, Editors, Elsevier & Bentham Science Publishers, 2015 (27 chapters).
3. Zika virus: Basic biology, surveillance, vaccine design and anti-Zika drug discovery: Computer-assisted strategies to combat the menace, Subhash C. Basak, Apurba K. Bhattacharjee and Ashesh Nandy (Editors), In Press, Nova Science Publishers, Inc., Hauppauge, USA, 2019.

4. Big Data Analytics in Chemoinformatics and Bioinformatics (with applications to computer-aided drug design, cancer biology, emerging pathogens and computational toxicology), Subhash C. Basak and Marjan Vracko (Eds.), Elsevier, in press, 2022.
5. Basak, S. C. (Editor), Mathematical Descriptors of Molecules and Biomolecules: Applications in Chemistry, Drug Design, Chemical Toxicology, and Computational Biology, Series: Synthesis Lectures on Mathematics & Statistics Springer-Nature, 2024.

2 Pre-conference preparations for the 9th workshop

The discussion to organize the Ninth Indo-US Workshop on Mathematical Chemistry at Saranathan College of Engineering, Tiruchirappalli, Tamil Nadu, India started in January 2024 after a few rounds of discussion with Dr Subash C. Basak the founder chairman of the workshop Series. In the discussion it was decided to conduct it in hybrid mode so senior scientists who are unable to travel to India will be able to attend online. Dr Ramanathan Natarajan, the event organizer, got permission from the college management for financial support on 28th March 2024. Letters of invitation to be on the international advisory committee were sent via email to several internationally reputed scientists in the field. A three-tier team was formed to get the input from senior scientists from India and abroad, and to organize the event without any glitch. 1) International advisory committee, 2) Indo-US organizing committee, and 3) Local organizing committee.

2.1 International Advisory Committee

The members of the International Advisory committee are:

International Advisory Committee

1. David Winkler, Department of Biochemistry and Chemistry, La Trobe Institute for Molecular Science, La Trobe University, Melbourne, Victoria, 3086, Australia.
2. Xueling Li, Center for Combinatorics, Nankai University, Tianjin, China.
3. Tomislav Doslic, University of Zagreb Faculty of Civil Engineering, Kaciceva 26, 10000 Zagreb, Croatia.
4. Guillermo Restrepo, Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany & Interdisciplinary Center of Bioinformatics, Leipzig University, Germany
5. Pratim K. Chataraj, Distinguished Visiting Professor, Chemistry Dept., BIT Mesra, Ranchi, 835215, Jharkhand, India.
6. G. Narahari Sastry, Fifth Paradigm Lab, Department of Biotechnology, Indian Institute of Technology, Hyderabad,Telangana India.
7. Dr Emilio Benfenati, Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Via Mario Negri 2, 20156 Milano, Italy.
8. Giuseppina C. Gini, Politecnico di Milano, Department of Electronics, Informatics and Bioengineering Piazza L. Da Vinci 32, 20133 Milano, Italy.

9. 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.
10. Dr. Habil. Mihai V. Putz, West University of Timișoara, Faculty of Chemistry, Biology, Geography, Laboratory of Structural and Computational Physical Chemistry for Nanoscience and QSAR, Str. Pestalozzi 16 A, Timișoara 300115, Romania.
11. Palyulin, Department of Chemistry, Lomonosov Moscow State University, Moscow 119991 Russia.
12. Marjan Vracko, National Institute of Chemistry, Ljubljana, Slovenia
13. Ramon Carbó-Dorca, Institut de Química Computacional i Catàlisi Universitat de Girona Girona 17003 (Catalonia) Spain.
14. Shahul H Nilar, Expert Computational Chemist, retired. USA.
15. Ms Kanika Basak, Duluth, USA (Advisor to Dr. Basak)
16. Gregory Grunwald, NRRI, Duluth, USA (Technical Support)

2.2 The Indo-US organizing committee

The Indo-US organizing committee was formed mainly with Indian Scientists to take leverage their experience in organizing an international conference in India. The members of the Indo-US organizing committee are:

1. Dr Apurba Bhattacharjee, Biomedical Graduate Research Organization, Department of Microbiology and Immunology, School of Medicine, Georgetown University, Washington, DC 20057, US.
2. Dr Anil Kumar Saxena, Chairman, Global Institute of Pharmaceutical Education and Research (GIPER), Kashipur, India.
3. Dr Indra Ghosh, Ex-Professor, SCIS, Jawaharlal Nehru University (JNU), New Delhi, India.
4. Dr Sanjay Batra, Chief Scientist, Division of Medicinal and Process Chemistry, Central Drug Research Institute (CSIR-CDRI), Lucknow, India.
5. Dr A. Nagarajan, Professor, Karpagam College of Pharmacy, Othakalmadapam, Coimbatore Tamil Nadu, India.
6. Dr S. Ramanathan, Principal, P.S.G. College of Pharmacy, Peelamedu, Avinashi Rd, Coimbatore, Tamil Nadu, India.
7. Dr C. Vijayalakshmi, Professor, Department Statistics and Applied Mathematics, Central University of Tamil Nadu, Thiruvarur, Tamil Nadu, India.
8. Dr D. Saravanan, Assistant Professor, Department of Chemistry, National College, Tiruchirappalli 620012, Tamil Nadu, India.
9. Dr Asish Mitra, Associate Professor, College of Engineering & Management, Kolaghat, East Midnapur, West Bengal, India
10. Dr Tanmoy Chakraborty Additional Registrar - SVKM'S NMIMS (Deemed to be University), Mumbai - 400 056. Maharashtra, India.

11. Dr. Smarajit Manna, Senior Scientist, Jagdish Bose National Science Search (JBNSTS), 1300- Rajdanga Main Road Kasba, Kolkata - 700107, West Bengal, India
12. Suman Chakravarti, Vice President & Chief Scientific Officer, MultiCASE Inc., Cleveland, Ohio, USA.
13. Dr Lavanya Selvaganesh, Assistant Professor, Department of Mathematical Sciences, Indian Institute of Technology (BHU) Varanasi, UP, India
14. Dr. Karpagam, Shrimathi Indira Gandhi College, Tiruchirappalli 620002, Tamil Nadu, India

2.3 Local Organizing Committee

The local organizing committee was formed within the host institute. The team could take care of all local arrangements such as transportation, boarding and lodging, hall arrangement, internet and other technical support for the smooth conductance of the event.

1. Dr V. Punitha, Professor and Head, Department of Computer Science and Engineering, Saranathan College of Engineering, Tiruchirappalli 620012.
2. Dr R. Thillaikarasi, Professor and Head, Department of Information Technology, Saranathan College of Engineering, Tiruchirappalli 620012.
3. Dr L. Muruganandam, Associate Professor and Head, Department of Chemistry, Saranathan College of Engineering, Tiruchirappalli 620012.
4. Dr V. Balamurugan, Assistant Professor, Department of Chemistry, Saranathan College of Engineering, Tiruchirappalli 620012.
5. Dr S. Priyarega, Assistant Professor, Department of Chemistry, Saranathan College of Engineering, Tiruchirappalli 620012.
6. Dr G. Ravichandran, Assistant Professor and Head, Department of Mathematics, Saranathan College of Engineering, Tiruchirappalli 620012.

2.4 Workshop series website

The workshop series started in the year 1998 and eight previous events (five in India and three in USA) had been conducted. However, the workshop series does not have a separate website. The host institute websites have been used all these years. Hence, it was decided to launch a separate website for the Indo-US Workshop Series on Mathematical Chemistry. Students from the department of Computer Science and Engineering, Saranathan College of Engineering (host institute of the 9th workshop) were involved in creating the website and a domain name was also registered. The new website was launched with the URL: https://indousmathchem.com/

2.5 9IUSWMC Brochure

For sharing information regarding the 9th Edition of the workshop series with colleges in Tamil Nadu a workshop brochure was designed and printed. The brochure was designed by a student from the Department of Information Technology. The brochures were sent to about 150 colleges in Tamil Nadu by post.

3 Overview

The Ninth Indo-US workshop on Mathematical Chemistry, a flagship workshop series was hosted by Saranathan College of Engineering, Tiruchirappalli, Tamil Nadu, India from 6th January 2025 to 10th January 2025. Delegates from Russia, Croatia, Macedonia and USA came to Tiruchirappalli while several delegates attended online to deliver the lectures. Overall scientists from 15 countries covering four continents made their valuable presence in hybrid mode to energize the scholars, researchers and academicians. This 5-day workshop comprised 15 technical sessions wherein invited speakers, research scholars and students presented papers on the major conference theme, Mathematical Chemistry with Applications to Drug Discovery, Computational Toxicology, Cheminformatics and Bioinformatics.

Scientists from the following countries participated in the Ninth Indo-US Workshop:

1) India
2) Malaysia
3) China
4) Croatia
5) Slovenia
6) Bosnia
7) Italy
8) Macedonia
9) Romania
10) Poland
11) Spain
12) Germany
13) France
14) Chile
15) USA

4 The venue

Saranathan College of Engineering, Tiruchirappalli, Tamil Nadu is a self-financing engineering college. It is an autonomous institution approved by All India Council for Technical Education (AICTE), New Delhi and affiliated to Anna University, Chennai. The college offers 10 bachelor's and five master's programmes and five of the departments are approved research centers under Anna University. The enrolment is about 3000. The workshop was held in the Srinivasa Ramanujan Hall

Arrival of the Guests to the Srinivasa Ramanujan Hall

5 Inauguration

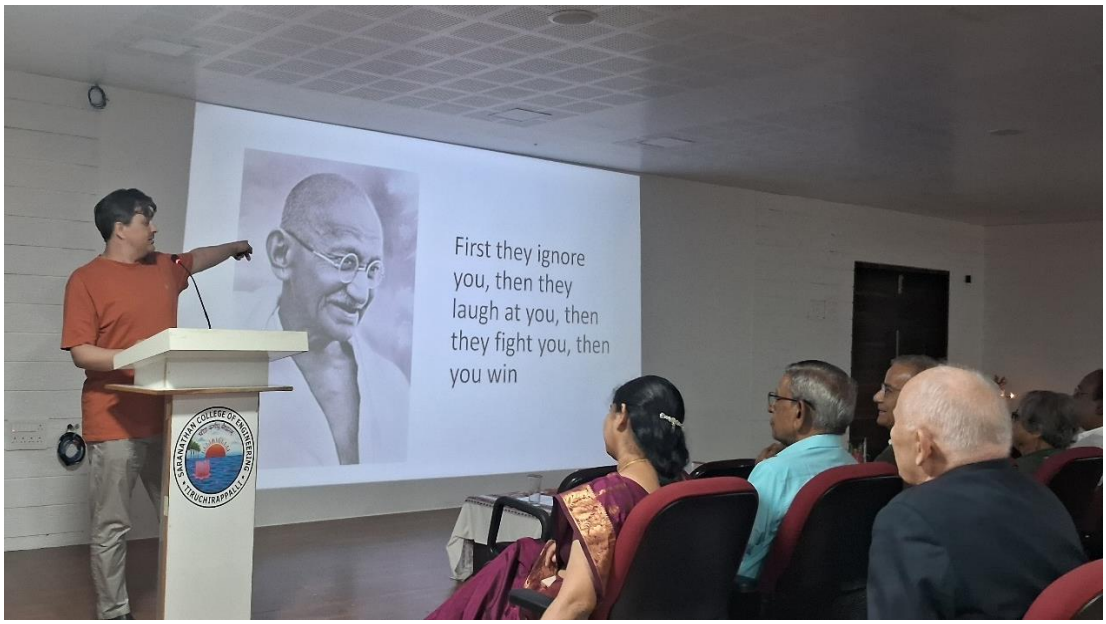
The workshop was well begun in Srinivasa Ramanuja Hall on 6th January 2025 at 8.45 A.M by invoking the blessings of the almighty through the college prayer song, followed by the Tamil Anthem which is a tribute to regional language and culture along with a Vedic hymn. Dr Michael J. Lalich, the former Director of Natural Resources Research Institute, Duluth, Minnesota, USA inaugurated the workshop. Dr R. Natarajan, the organizer of the event and Professor and Head of Research and Development welcomed the gathering. The delegates on the dais ignited the holy lamp to symbolize the ignition of knowledge among the participants. The history of the workshop series was presented by Dr Subash C. Basak, founder chairman of the workshop series. Followed by him, Dr D. Valavan, the Principal of Saranathan College of Engineering, Dr Vladimir Palyulin, a renowned chemist from Russia and Igor Kuzmanovski from Macedonia felicitated the proceeding. The inaugural ceremony concluded with the vote of thanks proposed by Dr V. Punitha, Head, Department of Computer Science and Engineering.

Dr Michael J Lalich, Former Director of NRRI, Duluth, Minnesota USA inaugurated the conference online

Dr Subhash C. Basak, Founder Chairman of the Indo-US Workshop series introduced Dr Michael J Lalich

The dignitaries lighted the Holy Lamp – A symbolic event to represent illumination of knowledge

Felicitation by Prof Vladimir A Palyulin



Felicitation by Prof. Igor Kuzmanovski

This workshop laid a platform for the communion of Indian foreign cultural ties. A group photo was taken as a memoir for unforgettable nostalgia

Group photograph of offline participants

6 Technical Sessions

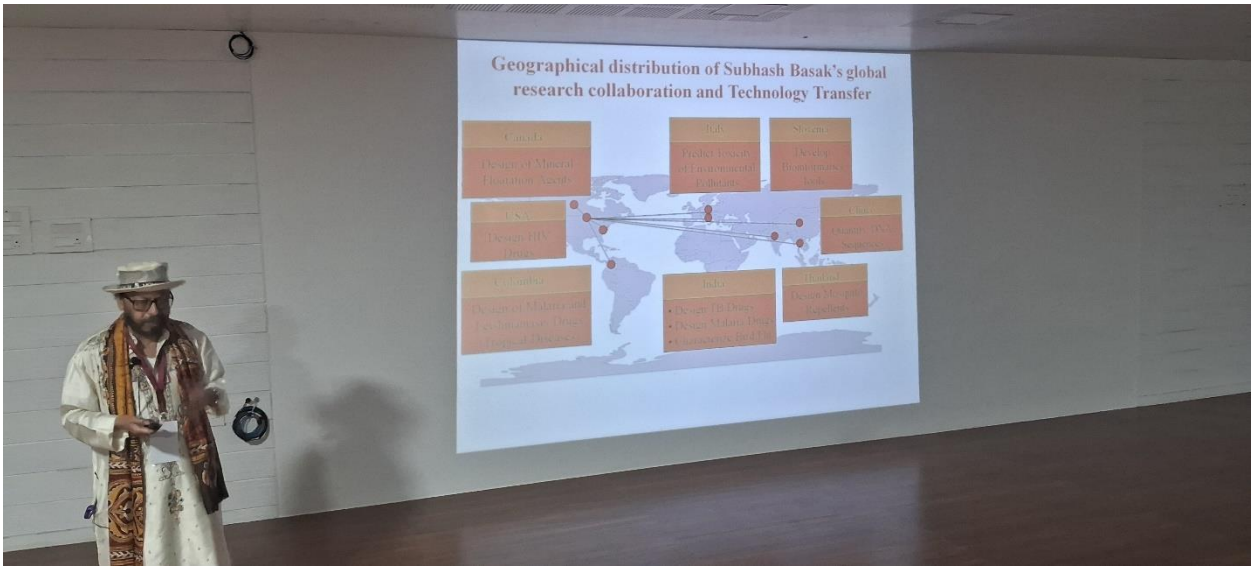
There were 15 technical sessions conducted in hybrid mode (online and offline combined) featuring 20 oral presentations and 12 poster presentations and 31 invited lectures in various domains by subject experts from 15 countries. The presentation topics and the extensive Global coverage made the workshop a historic event.

6.1 DAY-1: January 6, 2025

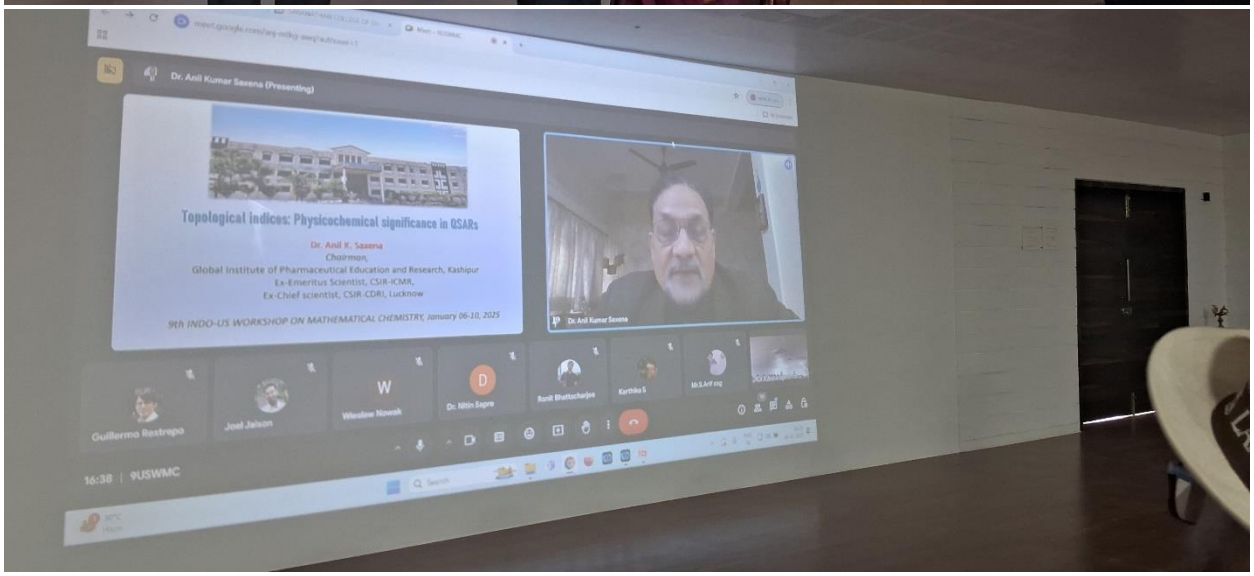
The technical sessions started after the inauguration, social mixing and group photograph session. The first presentation of the Ninth Workshop was presented by Dr Valdimir Palyulin from Moscow, Russia. The next lecture was by Dr S. C. Basak the founder chairman of the workshop series. The speakers and the titles of their presentations are given below:

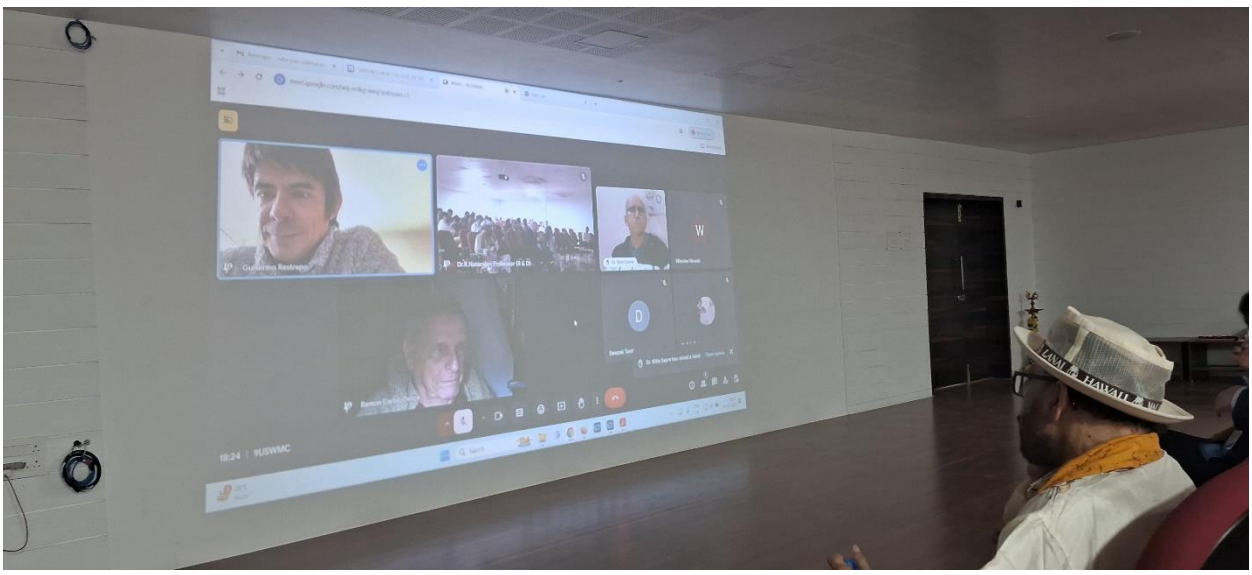
DAY-1: JAN 6, 2025	
TECHNICAL SESSION-1 GENERAL	
11.00-11.45 **Invited Lecture-1**	"*Neuroprotective AMPA receptor modulators: from computer-aided drug design to synthesis and preclinical studies*" by **Dr Valdimir A Palyulin**, **Russia.**
11.45-12.30 **Invited Lecture-2**	"*Adventures in the evolving landscape of mathematical descriptors of molecules and biomolecules: A tortuous journey of fifty years*" by **Dr Subhash C. Basak**, **USA.**
TECHNICAL SESSION-2: VECTOR CONTROL	
13.30-14.10 **Invited Lecture-3**	"*Pharmacophore recognition of bioactive molecules may aid in more efficient AI -driven database searches for discovery of potent compounds*" by **Dr Apurba K. Bhattacharjee**, **USA.**
14.15-14.45 **Invited Lecture-4**	"Bioinformatics, computer modeling and mosquitos: Insect sodium channels functioning from a theoretical perspective" by **Dr Wieslaw Nowak, Poland.**
14.45-15.00 **Oral Presentation -1**	"*Essential oils from a tropical medicinal plant, Ruta chalepensis as a potential raw material in the manufacture of vector control formulations*" by **Dharani Jayagopal.**
15.00-15.15 **Oral Presentation -2**	"*Bioactive compounds from Ocimum tenuiflorum as vector agent against Aedes albopictus*" by **Joel Jaison**
TECHNICAL SESSION-3 GENERAL	
15.45-16.15 **Invited Lecture-5**	"*Simulating optical properties of organic and biomaterials*" by **Dr Nađa Došlić**, **Croatia.**
16.15-16.45 **Invited Lecture-6**	"*Topological indices: Physicochemical significance in QSARs*" by **Dr A.K. Saxena, India**
16.45-17.30 **Invited Lecture-7**	"*Higher-dimensional structures for a better understanding of the chemical space and its evolution*" by **Dr Guillermo Restrepo, Germany.**


Metabotropic
KA receptors


Geographical distribution of Subhash Basak's global research collaboration and Technology Transfer

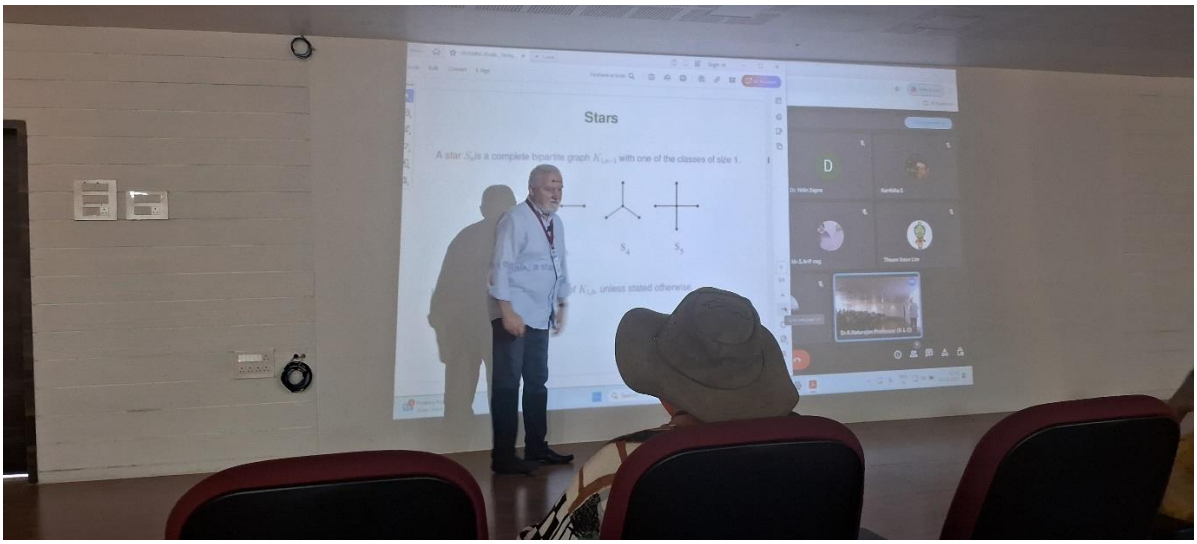

Joel Jaison
Karthika S
16:37 | 9USWMC


Dr. Anil Kumar Saxena (Presenting)
Topological indices: Physicochemical significance in QSARs
Dr. Anil K. Saxena
Chairman,
Global Institute of Pharmaceutical Education and Research, Kashipur
Ex-Emeritus Scientist, CSIR-ICMR,
Ex-Chief scientist, CSIR-CDRI, Lucknow
9th INDO-US WORKSHOP ON MATHEMATICAL CHEMISTRY, January 06-10, 2025
Dr. Anil Kumar Saxena
Guillermo Restrepo
Joel Jaison
Wieslaw Nowak
Dr. Nitin Sapre
Ronit Bhattacharjee
Karthika S
16:38 | 9USWMC

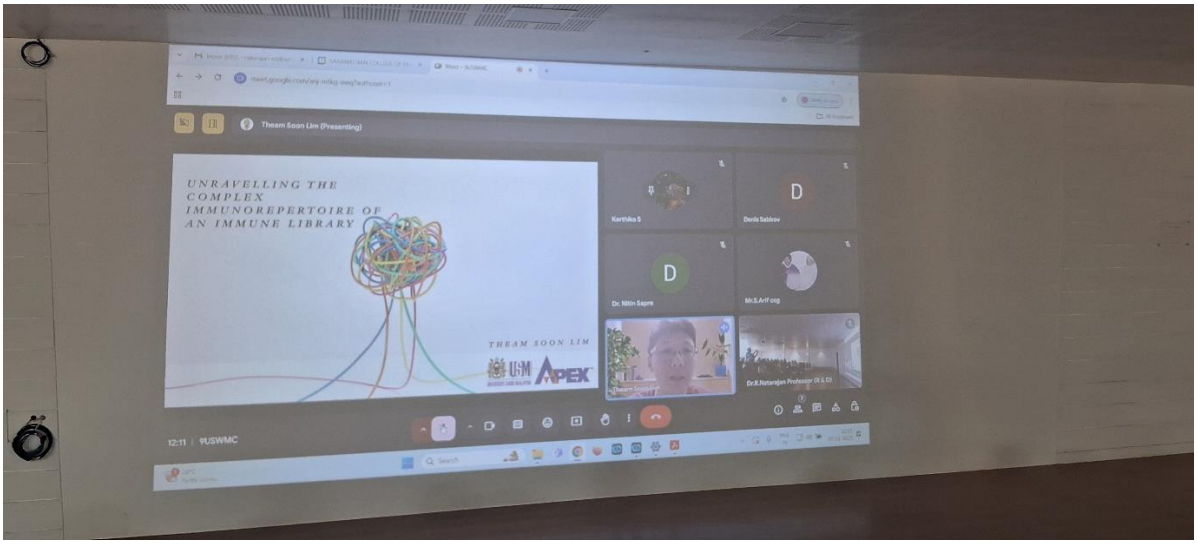

Guillermo Restrepo
18:24 | 9USWMC

6.2 DAY-2: January 7, 2025

The second day of the workshop started with presentations from USA. The first was by Dr Moumita Banerjee from John Hopkins, USA. The second was by Dr Shahul Nilar and it was a professional corporate presentation that enlightened the student participants regarding presentation skills in a professional meeting. There were three offline presentations (invited lectures) by Dr. Ramanathan, Dr. Tomislov Doslić and Lavanya Selvaganesh and an online presentation by Theom Soon from Malaysia. After these lectures lunch was served, and it was followed with the poster session wherein student participants had very good interactions with the senior professors. In the afternoon all the participants were taken for a tour to Thanjavur Brihadeeswara temple, a 1000-year-old UNESCO heritage center (Hindu temple) - an architectural marvel



DAY-2: JAN 7, 2025	
TECHNICAL SESSION-4: GENERAL	
09.30-10.00 **Oral Presentation -10**	"*Computational insights into photoactive systems: exploring photo-switching, TADF, and photosensitization*" by **Moumita Banerjee, John Hopkins, USA**
10.00-10.30 **Invited Lecture-8**	"*A novel pyruvate kinase activator - From a HTS impurity to a lead series*" by **Dr Shahul Nilar, USA**
10.30-11.00 **Invited Lecture-9**	"*Assessment of JNK3 enzyme inhibition of piceatannol - in silico and in-vitro studies*" by **Dr M. Ramanathan, India**
TECHNICAL SESSION-5: GENERAL	
11.20-11.50 **Invited Lecture-10**	*"Modelling adsorption of small structures onto fullerene graphs*" by **Dr Tomislav Doslic, Croatia**
11.50-12.20 **Invited Lecture-11**	"*Unravelling the complex immunorepertoire of an immune library*" by **Dr Theom Soon Lim, Malaysia**
12.20-13.00 **Invited Lecture-32**	"*Recent trends in the study of molecular descriptors using graph theoretic approach*" **Dr Lavanya Selvaganesh, India**
TECHNICAL SESSION-6: POSTER PRESENTATION	
" *Semi-synthetic PTP1B inhibitor from Cassia auriculata linn. by in silico method for diabetes management"* **Ezhilanbu, K.**	
"Exploring the role of revolutionizing the potential of explainable AI in drug discovery" by **Visali, K.**	
"Molecular dynamics simulations of phytochemicals from Citrullus colocynthis and Pulicaria crispa for anti-cancer potentials" by Jancy **Reena, I.M**.	
"Molecular dynamics study of afimetoran using desmond: Insights into structural dynamics and binding interactions" by **Madhu Krishna, M**.	
"Quantum mechanical analysis of the conformational and structural properties of clopidogrel bisulfate in the gas phase" by **Davis Presley, S.I.**	
"Identification of new chemical entities targeting glycogen synthase kinase-3 protein using in silico through artificial intelligence having indirubin as reference molecule" by **Manas Kumar, G**.	
"Integrative in silico framework for evaluating meridine analogues: toxicity, QSAR, and molecular dynamics insight" by **Vishnu, R.**	
"Medicinal mushrooms in cancer treatment" by **Mekala, S.**	
"Application of machine learning in drug discovery" by **Renita an Sindhiya, J.**	
"AI and ML in drug discovery" by **Aishvarya, V.**	
"Zero maintenance system for production of biofuels" by **Kanishka, S.**	
A Conference Tour was arranged to Thanjavur Temple, a UNESCO heritage site	

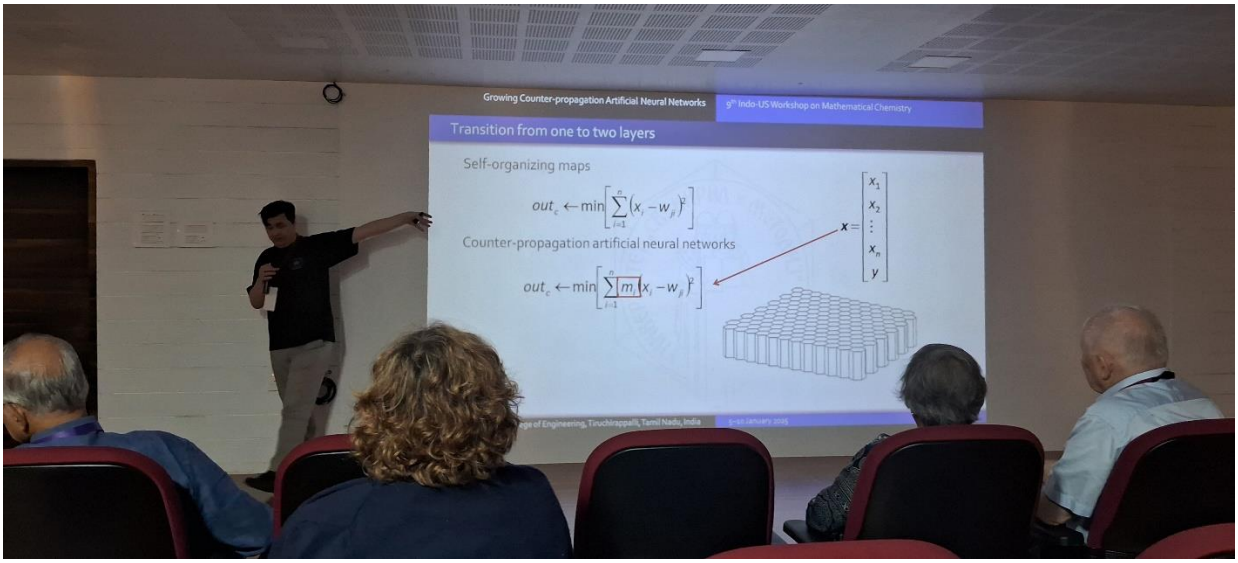

Theam Soon Lim (Presenting)
UNRAVELLING THE COMPLEX IMMUNOREPERTOIRE OF AN IMMUNE LIBRARY
THEAM SOON LIM
12:11 | 9USWMC

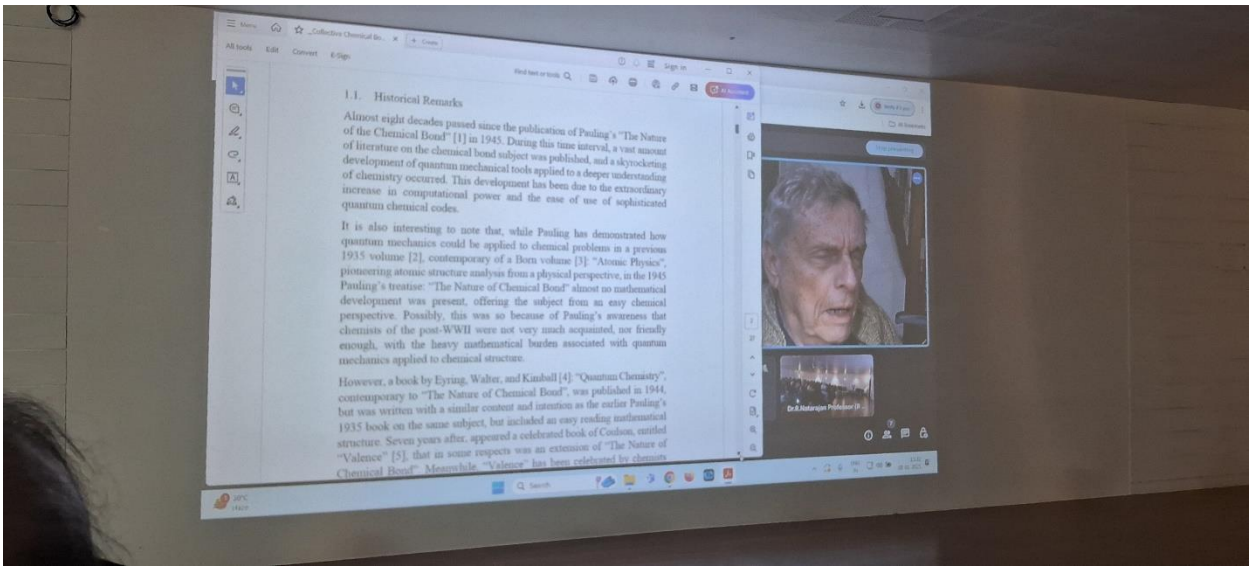
6.3 DAY-3: Jan 8, 2025

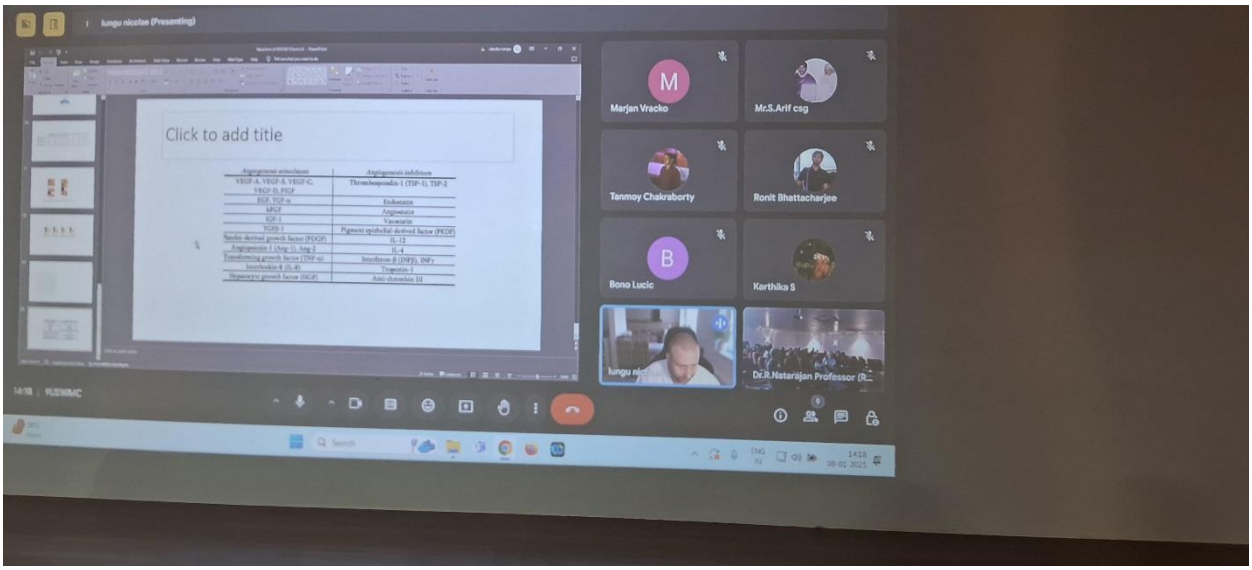
Third day was a much longer day with the afternoon sessions loaded with presentations from Europe. The first lecture in the morning was by Suman Chakravarti, USA. As he was sick the slides of his lecture were presented before the audience. There were presentations on BBB modeling and ANN. Dr C. Vijayalakshmi presented how mathematical modeling with Deep learning using CNN could help children with autism. The lecture demonstrated the advancing frontiers of ML and deep learning. After five oral presentations the afternoon witnessed lectures by Dr Claudiu Lungu, the veteran Ramon Crabo-Darca and Marjan Vračko. Marjan also had a joint presentation with Cardenas Carvajal, Chile and Tathagata Dutta, India. In the evening there was cultural programme by the college students followed by a gala dinner at Ramyas Hotels.

DAY-3: JAN 8, 2025	
TECHNICAL SESSION-7: GENERAL	
09.00-09.30 Invited Lecture-13	"*Building better computational toxicology solutions with AI and ML*" by **Dr Suman Chakravarti, USA**
09.30-10.15 Invited Lecture-14	"*Assessment of Blood-Brain Barrier entry of a structurally diverse set of chemicals using computed descriptors*" by **Dr Aritra Banerjee, USA**
10.15-10.45 Invited Lecture-15	"*Growing counter-propagation artificial neural networks*" by **Dr Igor Kuzmanovski, Macedonia**
TECHNICAL SESSION-8: GENERAL	
11.15-11.45 Invited Lecture-17	"*Emotions extraction of autism children through art using deep learning techniques*" by **Dr C. Vijayalakshmi, India.**
11.45-12.00 Oral Presentation-3	*"Exploring the phytoconstituents and therapeutic potential of Plumeria rubra flower extract for SGLT-2 receptor targeting: GC–MS and an in-silico approach" by* **Abin V Geevarghese**

DAY-3: JAN 8, 2025	
12.00-12.15 Oral Presentation-4	*"In silico evaluation of the isolates of Calotropis procera and Nigella sativa as anti-cancer potentials" by* **Renugadevi**
12.15-12.30 Oral Presentation-5	*"Molecular docking studies of phytomolecules against multi targets associated with antioxidants, anti-inflammatory and anticancer pathways" by* **Maida Engels**
12.30-12.45 Oral Presentation-6	*"Structural insights into 4-bromomandelic acid as a potent M2 muscarinic receptor antagonist: A molecular docking approach" by* **Judith Rashma**
12.45-13.00 Oral Presentation-9	*Dielectric Relaxation Spectral and molecular interaction analysis of aqueous pyrazine in ethanol using Time domain reflectometry (TDR) by* **Dr. P. Senthilkumar.**
TECHNICAL SESSION-9: GENERAL	
14.00-14.20 Invited Lecture-18	"*VEGFR2 chemical space: Stimulator and inhibitory peptides*" by **Drs Claudiu N Lungu & Gabriela Gurau, Romania.**
14.20-14.40 Invited Lecture-19	"*Rhombelane based vaccines*" by Drs **Claudiu N Lungu & Mihai V Putz, Romania.**
14.40-15.00 Invited Lecture-20	"*Mediated vasculogenesis and morphogenesis*" by **Drs Claudiu N Lungu & Mihaela C Mehedinti, Romania**
TECHNICAL SESSION-10: GENERAL	
15.30-16.00 Invited Lecture-21	*On the nature of chemical bond: Quantum molecular polyhedra and collective bond description" by* **Dr Ramon Carbo Darca, Spain (Catalonia).**
16.00-16.30 Invited Lecture-22	*"Clustering/classification of chemicals, proteomic data and emerging global viruses considering different kinds of representations"* by **Dr Marjan Vračko, Slovenia.**
16.30-16.50 Invited Lecture-22A	"*Chemometric characterization of Infectious salmon anemia (ISA) virus sequences using Alignment-free sequence descriptors Part-1*" by **Dr Cardenas Carvajal, Chile**
16.50-17.15 Invited Lecture-22B	"*Chemometric characterization of Infectious salmon anemia (ISA) virus sequences using Alignment-free sequence descriptors Part-2*" by **Dr Marjan Vračko, Slovenia**
17.15-17.45 Oral Presentation-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*" by **Tathagata Dutta**


Growing Counter-propagation Artificial Neural Networks
9th Indo-US Workshop on Mathematical Chemistry
Transition from one to two layers
Self-organizing maps
Counter-propagation artificial neural networks


1.1. Historical Remarks
Almost eight decades passed since the publication of Pauling's "The Nature of the Chemical Bond" [1] in 1945. During this time interval, a vast amount of literature on the chemical bond subject was published, and a skyrocketing development of quantum mechanical tools applied to a deeper understanding of chemistry occurred. This development has been due to the extraordinary increase in computational power and the ease of use of sophisticated quantum chemical codes.
It is also interesting to note that, while Pauling has demonstrated how quantum mechanics could be applied to chemical problems in a previous 1935 volume [2], contemporary of a Born volume [3]: "Atomic Physics", pioneering atomic structure analysis from a physical perspective, in the 1945 Pauling's treatise: "The Nature of Chemical Bond" almost no mathematical development was present, offering the subject from an easy chemical perspective. Possibly, this was so because of Pauling's awareness that chemists of the post-WWII were not very much acquainted, nor friendly enough, with the heavy mathematical burden associated with quantum mechanics applied to chemical structure.
However, a book by Eyring, Walter, and Kimball [4]: "Quantum Chemistry", contemporary to "The Nature of Chemical Bond", was published in 1944, but was written with a similar content and intention as the earlier Pauling's 1935 book on the same subject, but included an easy reading mathematical structure. Seven years after, appeared a celebrated book of Coulson, entitled "Valence" [5], that in some respects was an extension of "The Nature of Chemical Bond". Meanwhile, "Valence" has been celebrated by chemists

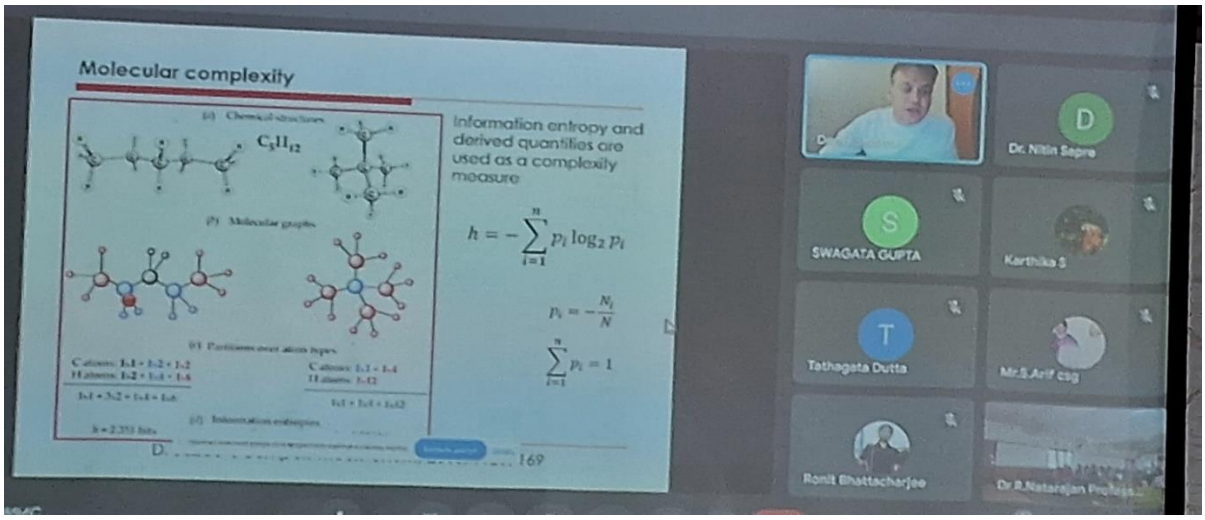

Iungu nicolae (Presenting)
Click to add title
Marjan Vracko
Mr.S.Arif csg
Tanmoy Chakraborty
Ronit Bhattacharjee
Bono Lucic
Karthika S

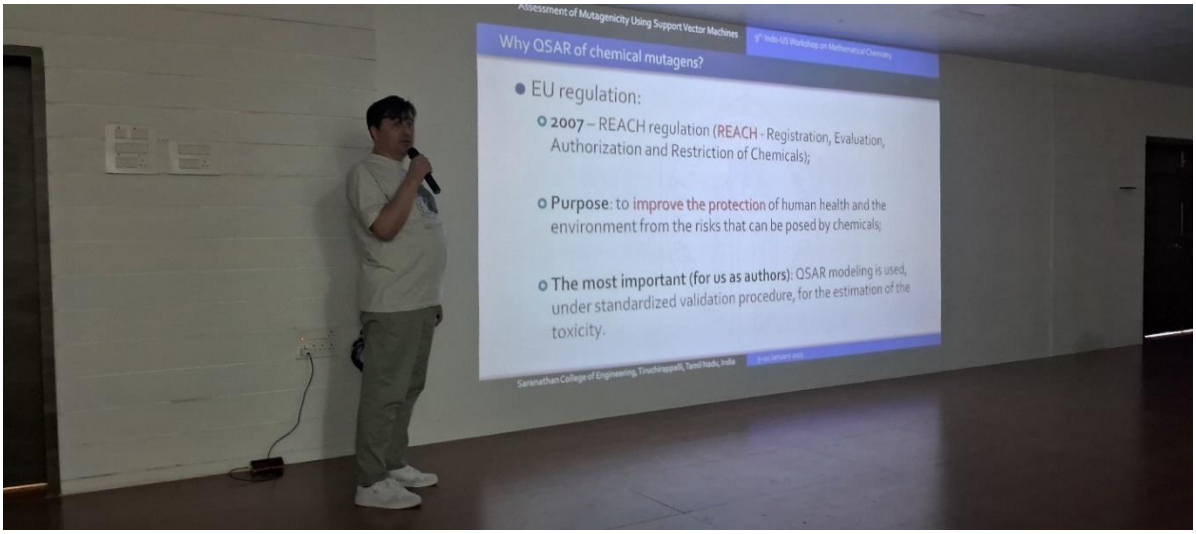
6.4 DAY-4: Jan 9, 2025

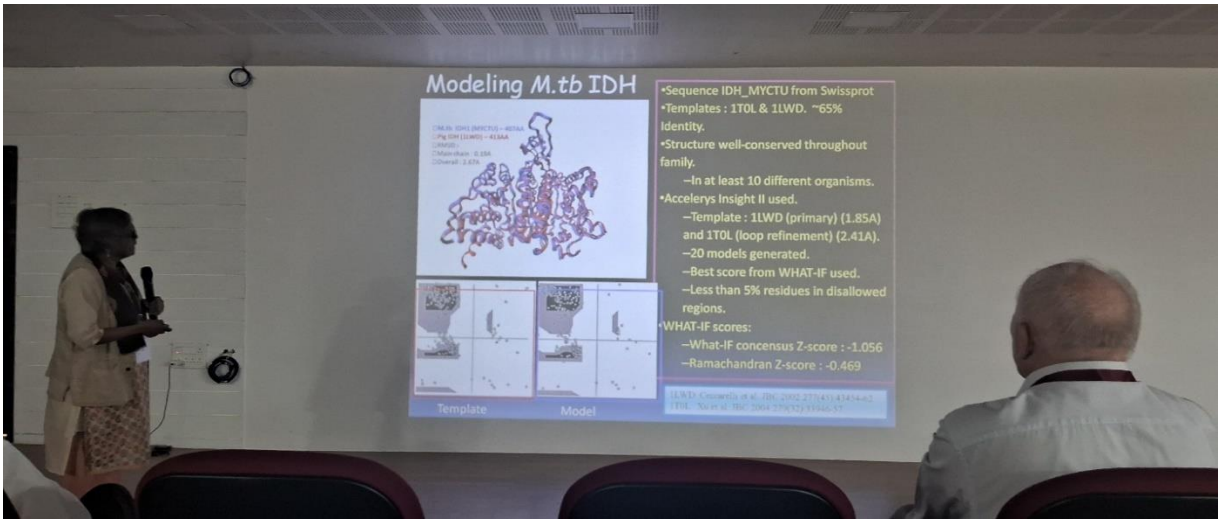
The fourth day of the workshop was along day stretching from 9.30 am to 6.00 pm. In the afternoon, there was a parallel session for Schools Students. Students from different schools participated via online and a separate link was shared with individual students, and also to schools. Unfortunately, Dr Guang Hu who was sick on that day could not present his lecture. Dr Jin-wei Duan who was indisposed also could not deliver the lecture but shared his presentation slides. There were six invited lectures and eight oral presentations on Day 4.

DAY-4: JAN 9, 2025	
TECHNICAL SESSION-11: GENERAL	
09.30-10.00 Invited Lecture-23	"*Information-entropy descriptors for chemical reactions*" by **Dr Denis Sebirov, Russia**
10.00-10.30 Invited Lecture-24	"*Topological isomers of DNA dodecahedral links*" by **Dr Jin-wei Duan, China**
10.30-11.00 Invited Lecture-25	"*Perturbation response scanning analysis for drug-target networks*" by **Dr Guang Hu, China**
TECHNICAL SESSION-12: GENERAL	
11.20-11.50 Invited Lecture-26	"*All-metal aromaticity and conceptual DFT*" by Dr **Pratim K. Chattaraj, India.**
11.35-12.15 Invited Lecture-12	"*Entrapment of flow of substrate to diversion pathway for combating persistent tuberculosis: Bioinformatics Approach*" by **Dr Indira Ghosh, India**
12.15-12.30 Oral Presentation-7	*"Optimizing large-scale molecular docking: A novel software prototype for efficient drug discovery"* by **Ravikiran**
12.30-13.00 Oral Presentation-11	*"Prosopis juliflora leaf extract assisted synthesized tin oxide nanoparticles for applications high-performance supercapacitor electrode*" by **G. Suganya**
13.00-13.15 Oral Presentation-12	"*Green synthesis of zinc oxide nanorods using Ficus benghalensis aerial root extract and enhanced antibacterial activity*" by **Princess Gracia**
TECHNICAL SESSION-13: GENRAL	
14.00-14.15 Oral Presentation-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*" by **V. Bargavi**
14.15-14.45 Oral Presentation-15	*"Predicting mutagenicity of a diverse set of chemicals using mathematical molecular descriptors and different statistical methods*" by **Ronit Bhattacharjee**
14.45-15.00 Oral Presentation-16	*"Machine learning-integrated template-guided docking: a novel approach for identifying potent HIV-1 NNRTIs*" by **Swagata Gupta**
15.00-15.15 Oral Presentation-17	*"A DFT study of lead-free halide perovskites GaMX3 (X= Sr, Ba; X= F, Cl) for solar cell applications*" by **Vinita Rohlan**

DAY-4: JAN 9, 2025	
15.15-15.30 **Oral Presentation-18**	*"Design and evaluation of quercetin-5-fluorouracil conjugates and other similar conjugates as anti-cancer agents*" by **Dr Priya Rega**
TECHNICAL SESSION-14: GENRAL	
16.00-16.30 **Invited Lecture-27**	"*The application of the QSPR methodology can help improve the prediction of protein folding rates*" by **Dr Bono Lucic, Croatia**
16.30-17.15 **Invited Lecture-28**	"*Molecular descriptors or machine-generated features? Their impact in predictive modelling and QSAR*" by **Giuseppina Gini, Italy.**
17.15-17.45 **Invited Lecture-16**	"*Assessment of mutagenicity using computed molecular descriptors and support vector machines*" by **Igor Kuzmanovski, Macedonia**
PARALLEL SESSION FOR SCHOOL STUDENTS	
14.00-14.30	S.C. Basak, USA
14.30-15.00	Apurba K. Bhattacharjee, USA
15.00-15.30	Guillermo Restrepo, Germany
15.30-16.00	Suman Chakravarty, USA






Modeling M.tb IDH
•Sequence IDH_MYCTU from Swissprot
•Templates : 1T0L & 1LWD. ~65% identity.
•Structure well-conserved throughout family.
–In at least 10 different organisms.
•Accelerys Insight II used.
–Template : 1LWD (primary) (1.85A) and 1T0L (loop refinement) (2.41A).
–20 models generated.
–Best score from WHAT-IF used.
–Less than 5% residues in disallowed regions.
•WHAT-IF scores:
–What-IF concensus Z-score : -1.056
–Ramachandran Z-score : -0.469
Template
Model


Optimizing Large
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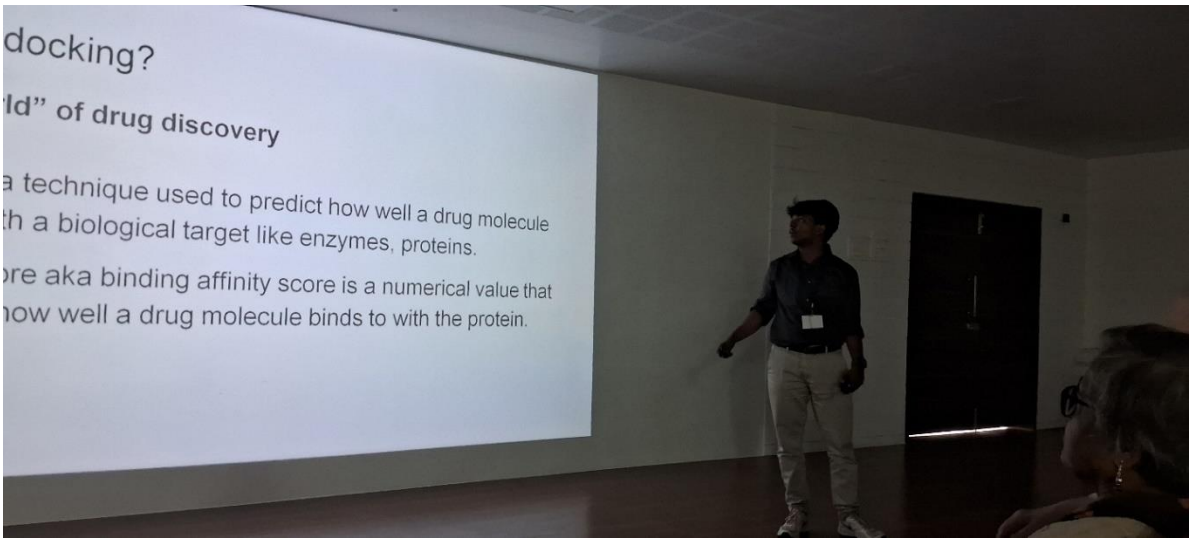
docking?
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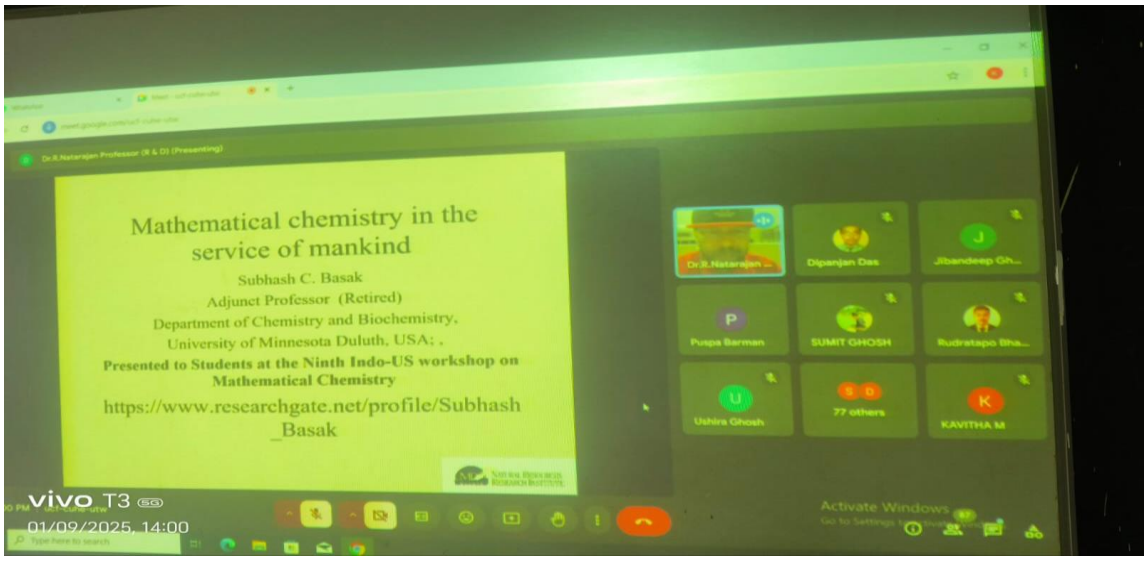
a technique used to predict how well a drug molecule
th a biological target like enzymes, proteins.
re aka binding affinity score is a numerical value that
ow well a drug molecule binds to with the protein.

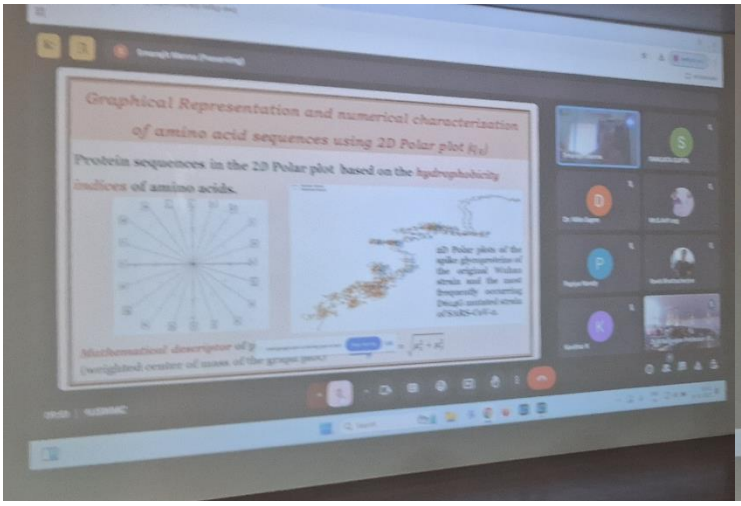


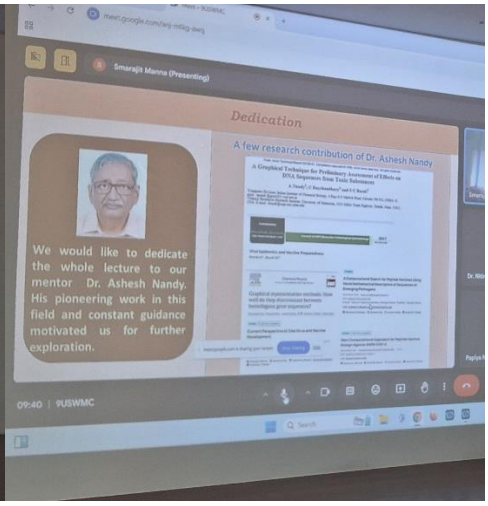
The online session for school students

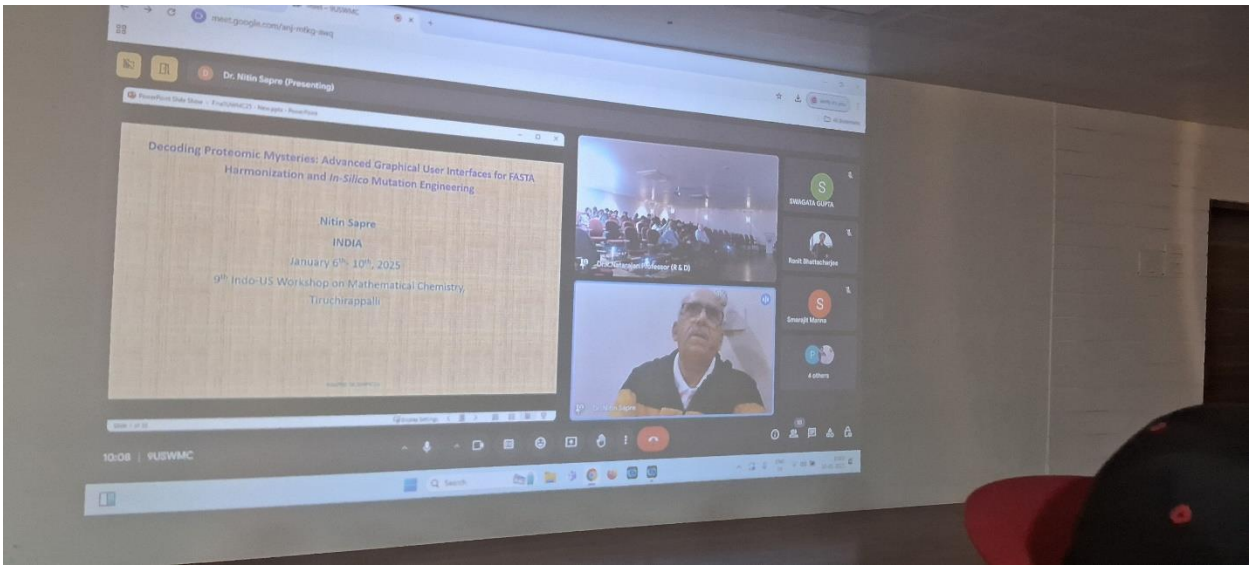
6.5 DAY-5: Jan 10, 2025

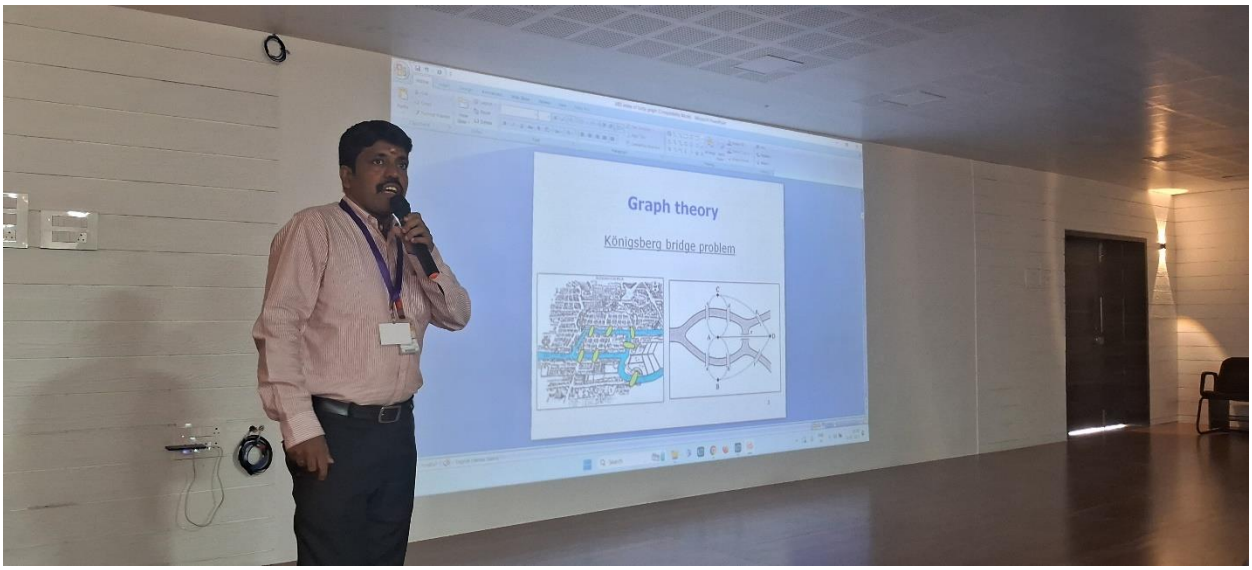
The last and the fifth day was a half-day and the technical presentations were only in the forenoon session. The last presentation was by Dr Natarajan, the convenor and organizer of the ninth edition of the IUSWMC series. All the technical presentations were completed by 12 noon

DAY-5: JAN 10, 2025	
TECHNICAL SESSION-14: GENERAL	
09.30-10.00 **Invited Lecture-29**	"*Use of alignment-free sequence descriptors (AFSDs) in the computer assisted unified vaccine design*" by **Dr Samarjit Manna, India.**
10.00-10.30 **Invited Lecture-30**	"*Decoding proteomic mysteries: advanced graphical user interfaces for FASTA harmonization and in-silico mutation engineering*" by **Dr Nitin Sapre, India**.
10.30-10.45	*"Synthesis of Schiff bases as corrosion inhibitors*" by **Dr Balamurugan**
TECHNICAL SESSION-15: GENERAL	
11.15-11.30	"Atom-bond sum connectivity index of fuzzy graphs" by **Dr Sivamani**
11.30-12.00 **Invited Lecture-31**	"*Mathematical chemodescriptors for the characterization of molecular chirality*" by **Dr R. Natarajan, India**









7 Cultural Programme

To cherish the ninth Indo-US workshop series, the participants, scholars, delegates, the Heads of various departments of Saranathan College of Engineering were entertained with cultural programmes performed by the students and faculty of the college. This was organized on the evening of Day 3, Jan 8, 2025. There was vocal music and flute recital by students while the faculty supported the students on the percussion instruments. After the cultural event, the college management hosted the gala conference Banquet dinner at the Hotel Ramyas.

8 Workshop Tour

As a token of cultural sociability, the delegates and participant s were taken for a tour to Thanjavur Brihadeeswara temple on 7th January 2025, a 1000-year-old UNESCO heritage center (Hindu temple)- an architectural marvel. The place is about 60 km from the conference venue. All the participants went there by a bus and spent the evening from 4 pm to 7 pm at the temple. Approved tour guides were arranged to explain the importance and the cultural significance of the temple. It is a complete granite structure built with about 130,000 tons of interlocking granite stones in a span of 7 years. That is about 50 tons of granites were moved everyday around the clock. As the granite pieces were interlocking no plastering material was used. The top "Vimana" is 140 tons and had been hoisted to 130 m in the days were no mechanical devices such as cranes and pulleys were not known.

The Big Temple of Thanjavur; under illumination


9 Valediction

The Valedictory function was on 10th January 2025 immediately after the technical presentations were completed. The function started gloriously with a prayer song orchestrated by Srikamakshi. Dr. Basak delivered the Valedictory address. The principal of the college made remarks about the workshop. The Workshop certificates were distributed to the participants and presenters. A special mention was made to the students of Saranathan College who created website, banner and other conference materials. The participants offered feedback. Dr R. Natarajan, the organizer of the event, proposed the vote of thanks. The programme came to an end with the rendering of the Indian National Anthem.

Distribution of participation certificates

9.1 Feedback from participants

Participants were invited to give their feedback regarding the conference arrangements, facility and the scientific sessions. Some student participants and professors came forward to give their feedback. Everyone appreciated the diverse topic covered and the high quality of the speakers. Students were very happy regarding the arrangements for their stay, food, and transportation. Several participants said that the long breaks planned in the agenda by the organizers gave them ample time to interact and discuss with senior professors. They appreciated the college management for making their stay very comfortable. Everyone felt it was an excellent conference of very high standard and went back with the satisfaction of gaining more knowledge, experience, and new relationships for future collaborations.

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