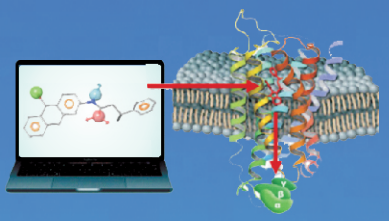

CMTPI 2017

9TH INTERNATIONAL SYMPOSIUM ON COMPUTATIONAL METHODS IN TOXICOLOGY AND PHARMACOLOGY INTEGRATING INTERNET RESOURCES

BOGMALLO BEACH RESORT, GOA, INDIA, 27-30 OCTOBER 2017

Organised By:

GLOBAL INSTITUTE OF PHARMACEUTICAL EDUCATION AND RESEARCH (GIPER), KASHIPUR (U.K.), INDIA

Web: www.giper.edu.in

CMTPI-2017

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9th International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI-2017)

Hosted by: Global Institute of Pharmaceutical Education and Research, Kashipur, India (GIPER)

From the Chairman's Desk

Dr. A. K. Saxena, *Ph.D, FRSC,*
Chairman,
Emeritus Medical Scientist (ICMR)
Ex Chief Scientist, Professor AcSIR,
Central Drug Research Institute,
Lucknow, India.

It gives me immense gratification that "9th International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI-2017)" is being organized in India by Global Institute of Pharmaceutical Education and Research, Kashipur, Uttarakhand, from 27-30 October 2017 in Goa. This symposium in continuation of previous CMPTI-2001 (Bordeaux , France), CMTPI-2003 (Thessaloniki , Greece), CMTPI-2005 (Shanghai , China), CMTPI-2007 (Moscow, Russia), CMTPI-2009 (Istanbul, Turkey), CMTPI-2011 (Maribor, Slovenia), CMTPI-2013 (Seoul, Korea) and CMTPI-2015 (Chios-Greece),will provide an international forum for bringing together leading scientists, students and young innovative minds from different parts of the globe to share a single platform to discuss the latest developments in the emerging and interdisciplinary field of Computational Methods in Toxicology and Pharmacology integrating internet resources. The invited lectures, oral and poster presentations in the symposium will broadly cover the fields viz; Internet and databases; SAR, QSPR and Molecular Modelling in Drug Discovery; SAR and QSPR in Environmental Chemistry; "OMIC"- Sciences and bioinformatics applications in pharmacology and toxicology; commercial and non-commercial computational tools and databases in the Internet and computational pharmacology and toxicology. The symposium will also help in developing collaborative relationships between participating scientists, students and organizations working in the areas pertaining to the theme of the conference in their future endeavors. I welcome you all and look forward towards your active participation to make this event a success.

I take this opportunity to thank all the International Organizing Committee members including the Chairman, Dr James Devillers, advisory board members and the local organizing committee for their untiring efforts. I also acknowledge the financial support from Indian Council of Medical Research, Themis medicare, Taylor and Francis and other sponsors for the organization of the conference.

(A. K. Saxena)

CMTPI-2017

PROGRAM SCHEDULE

27 OCTOBER 2017

Time	Program		
From 14-00	Registration		
16-00 to 17-00	Inaugural Function		
17-00 to 17-30			Coffee/Tea Break

17-30 to 19-30 (Scientific Session –I) Chairpersons: James Devillers & A. K. Saxena

17-30 to 18-00	Indira Ghosh	(IL-01)	Multiple Target based Pharmacophore designing from Active site structures.
18-00 to 18-30	Tamas Bihari	(IL-02)	The role of computational methods in toxicology and pharmacology in space chemistry.
18-30 to 19-00	Kunal Roy	(IL-03)	Is it possible to improve the quality of predictions from the use of multiple QSPR/QSAR models?
19-00 to 19-20	Sunil Kulkarni	(FL-01)	Canada's chemicals management plan: applications of *in silico* tools and approaches.
19-45 onwards			Welcome Dinner

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08-30 to 10-30Hrs (Scientific Session –II) Chairpersons: Athina Geronikaki & V.M. Kulkarni

08-30 to 9-00	Vladimir Poroikov	(IL-04)	How good are publicly available web-resources predicting bioactivity profiles for drug repurposing?
9-00 to 9-30	G. Narahari Shastry	(IL-05)	Molecular property diagnostic suite (MPDS): development of disease-specific open source web portals for drug discovery.
9-30 to 9-50	Dmitry Druzhilovskiy	(FL-02)	Way2drug platform – ligand-based approach to drug repurposing.
9-50 to 10-10	Alexander V Dmitriev	(FL-03)	Metatox-Web-Application For Predicting Structure Of Xenobiotic's Metablites.
10-10 to 10-30	Anastasiya Rudik	(FL-04)	Web Application For Prediction Of Xenobiotic's Organ-Specific Rodent Carcinogenicity.
10-30 to 11-00			Coffee/Tea Break

11-00 to 12-30Hrs (Scientific Session –III) Chairpersons: Vladimir Poroikov & Indira Ghosh

11-00 to 11-30	James Devillers	(IL-06)	Repurposing drugs for use against Zika virus infection.
11-30 to 12-00	KyoungTai No	(IL-07)	Knowledge based mass spectroscopic natural product research platform, flora genesis system.
12-00 to 12-20	Rajesh K Goel	(FL-05)	Pharmacological repurposing of Indian medicinal plants with pharmacoinformatic tools pass and pharma expert.
12-20 to 14-00			Poster Session I and LUNCH
14-00 to 20-00			Excursion and Boat Tour

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08-30 to 10-30Hrs (Scientific Session –IV) Chairpersons: KyoungTai No & Kunal Roy

8-30 to 9-00	Marjan Vracko	(IL-08)	QSAR modelling, grouping/classification and docking as tools for evaluation of chemical toxical properties.
9-00 to 9-30	Prasad V. Bharatam	(IL-09)	Quantum Chemical Studies on Drug Toxicity originating via the Mechanism Based Inhibition of Cytochromes P450.
9-30 to 9-50	Tomasz Puzyn	(FL-06)	Chemoinformatics in nanomedicine and nanotoxicology.
9-50 to 10-10	Agnieszka Gajewicz	(FL-07)	Novel in silico methods at the crossroads of "real-life" (sparse) nanotoxicity data and regulatory needs.
10-10 to 10-30	Ayako Furuhama	(FL-08)	Development of chronic aquatic toxicity models based on an interspecies relationship and molecular descriptors.
10-30 to 11-00			Coffee/Tea Break

11-00 to 13-00Hrs (Scientific Session –V) Chairpersons: Douglas W. Oliver & S.K. Puri

11-00 to 11-30	Sun Choi	(IL-10)	In Silico Classification Modeling Studies for Cytochrome P450 Inhibition Using machine-Learning Methods.
11-30 to 12-00	Anil K Saxena	(IL-11)	Molecular modeling studies in explaining the higher GPVI antago

			nistic activity of the racemic2-(4-Methoxyphenylsulfonyl)-2,3,4,9-tetrahydro-1H pyrido[3,4-b]indole-3-carboxamide than its enantiomers.
12-00 to 12-20	VibhaTandon	(IL-12)	Structure Activity Relationship OfBisbenzimidazole As *E.Coli* Topoisomerase Ia Inhibitor Targeting Mdr Bacterial Strains.
12-20 to 12-40	Shubhra G. Dastidar	(FL-09)	Inhibitors of a,ß-tubulin should be able to alter the pattern of molecular breathing.
12-40 to 13-00	Naidu Subbarao	(FL-10)	In-Silico Identification Of Novel Inhibitors Of P. Falciparum HistoneAcetyl Transferase(Gcn5) and Histone Deacetylases (Hdac1)and*In-Vitro* Validation.
13-00 to 14-30			Poster Session II and LUNCH

14-30 to 16-00Hrs (Scientific Session –VI) Chairpersons: Sun Choi & Vibha Tandon

14-30 to 15-00	Ismail Yalcin	(IL-13)	Structure-Activity Relationship Analysis Of Some New Benzothiazole Derivatives As hGST P1-1 Enzyme Inhibitors.
15-00 to 15-30	AthinaGeronikaki	(IL-14)	Docking assisted design of novel 4-adamantanyl-2-thiazolylimino-5-arylidene-4-thiazolidinones as potent NSAIDs.
15-30 to 16-00	Douglas W. Oliver	(IL-15)	Multi-Targeted Directed Ligands For Alzheimer's Disease: Design Of Novel Lead Coumarin Conjugates.
16-00 to 16-30			Coffee/Tea Break

16-30 to 18-00Hrs (Scientific Session –VII) Chairpersons: G.Narahari Sastry & Marjan Varacko

16-30 to 17-00	Esin Aki	(IL-16)	Investigation Of Binding Interactions Between TOPO IV And 1,4-Benzoxazine Derivatives In *Acinetobacter Baumannii*.
17-00 to 17-20	MridulaSaxena	(FL-11)	QSAR and Modeling of CCK2 Receptor Antagonists.
17-20 to 17-40	Eleftheriou Phaedra	(FL-12)	Docking analysis targeted to the whole enzyme molecule better predicts inhibitory action.An application on the discovery of thiomorpholine and thiazolyl derivatives with PTP1B inhibitory action.
17-40 to 18-00	Tarun Jha	(FL-13)	Multiple molecular modeling studies on some derivatives and analogs of glutamic acid as matrix.
18-30 to 19-30			Cultural Event
19-30 onwards			Banquet Dinner

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08-30 to 10-30Hrs (Scientific Session –VIII) Chairpersons: Esin Aki & P.V. Bharatam

8-30 to 8-50	Vladimir Palyulin	(FL-14)	Modeling of halogen bonding and electrostatic noncovalent sulfur interactions in drug design.
8-50 to 9-10	Minsung Kim	(SL-01)	A Priori Design of Sustainable Solvents Properties:The Dielectric Constant QSPR Predictionsfor G-SFED Solvation Free Energy MODEL.
9-10 to 9-30	Hyeon Nae JEON	(SL-02)	Solubility prediction in ionic liquids using QSAR model based on molecular descriptors.
9-30to 9-50	Debesh Ranjan Roy	(FL-15)	Group charge and inter electron transfer as the potential toxicity predictors of some ACAT inhibitors: a DFT investigation.
9-50to 10-10	Partha Pratim Roy	(FL-16)	*In silico* Bio Concentration Factor (BCF) modeling of organophosphate pesticides using online available chemometric tools.
10-10 to 10-30	Kabiruddin Khan	(SL-03)	Risk assessment of personal care products (PCPs) on aquatic organisms: QSTR models for selection of safer cosmetics.
10-30 to 11-00			Coffee/Tea Break

11-00 to 12-00Hrs (Scientific Session –IX) Chairpersons: Ismail Yalcin & Deepak Teotia

11-00 to 11-20	Sisir Nandi	(FL- 17)	Combinatorial design and virtual screening of potent anti-tubercular fluoroquinolone and isothiazoloquinolonecompoundsutilizing QSAR and pharmacophore modeling.
11-20 to 11-40	Sutapa Mondal Roy	(FL- 18)	Toxicity of aminosulfonylureasin the light of nucleic acid bases and DNA base pair interaction.
11-40 to 12-00	Aparna Shukla	(SL-04)	Development of QSAR model for anti-cancer activity prediction of potent vanilloid based derivatives against human cancercell lineMCF7
12-00 to 12-20	CS Azad	(SL-05)	Pharmacophore-based virtual screening, molecular docking and molecular dynamics studies of novel 4-aminoquinolines as a promising DNA Gyr inhibitor.
12-20 to 13-00			Valedictory Function
13-00 onwards			Lunch