



Conference (ITDDD-2018) Schedule Nov 1-3,2018

Date	Technical session	Time	Title of Activity / Talk	Speaker
01-11-2018	-	9:30 – 10:30	Inauguration	-
	Keynote address	10:30-11:30	Three Decades of PASS (Prediction of Activity Spectra for Substances): Development and Application in Drug Discovery	V.V. Poriokov
	Networking with Tea Break			
	Technical session I 12:00 -13:00		Disease Specific Web Portal Development and Drug Repurposing for Metabolic Disorders	G. N Sastry
			Eigen Value ANaysiS (EVANS): an <i>in silico</i> tool to address pharmacodynamics, pharmacokinetics and toxicity issues	Evans Coutinho
	Lunch			
	Technical session II 14:00 – 15:45		Drug-Drug Interactions for FDA Approved Drugs Estimated on the Basis of Known “Mechanism-Effect” Relationships on Drug Repositioning Way2Drug Platform	Alexey A Lagunin
			Prediction of antiviral activity spectrum for small molecules based on well curated data	Dmitry Osolodkin



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			Computer-aided finding of new pharmaceutical agents with multitargeted action	Athina Geronikaki	
Networking with Tea Break					
	Technical Session III	16:00 – 17:00	As per displayed Schedule on website	Oral Presentations (5)	
02-11-2018	Technical session IV	9:30 – 10:30	Ultra-large library docking for potent unprecedented chemotypes	John Irwin	
	Technical session V	10:30 - 11:30	Molecular Calculations on the Activity and Development of Anti-Cancer Agents	Thanyada Rungrotmongkol	
			Role of ADME/T in Drug Discovery and Drug Candidate Selection	Girinath Pillai	
	Networking with Tea Break				
	Technical session VI	12:00 – 13:00	Electrostatic Complementarity as a New Approach to Visualise and Predict Activity.	Sunil Kumar	
			Way2drug Platform – Approach to Drug Repurposing for Socially Significant Diseases	Dmitry Druzhilovskiy	
	Lunch				
Technical session VII	14:00 – 15:45	Effect of Water-Restructuring Mutations on Ligand Binding to Human Carbonic Anhydrase: A theoretical study	Madhavi Sastry		
		Electronic-Structure Informatics for Discovery of Bio- Functional Molecules	Manabu Sugimoto		



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			Looking Beyond Ethnopharmacology of Medicinal Plants Through In silico approach	Alexey Lagunin
			Networking with Tea Break	
	16:00-17:00		As per displayed Schedule on website	Oral Presentations (5)
03-11-2018	Technical Session VIII	9:30-11:00	Revolutionizing Target Discovery and Lead Generation with Genome-wide DNA Shape Prediction and Reverse Transcriptome Matching	Shandar Ahmad
			Therapeutic validation of in silico study of flavonoids in Parkinson's disease	Pravir Kumar
			Computationally Driven Drug Discovery In Structure-Enabled Programs: Free Energy Calculations	Pritish Bhat
		11:00-12:00	Panel Discussion Dry lab vs wet lab and in Drug discovery <i>Moderator : Dr Sandeep Arora, Director, CCP, CU, Rajpura.</i>	Panellist Dr Rashmi K Ambasta Dr. Milind Umekar Dr G N Sastry Dr Vladimir V Poroikov Dr Pravir Kumar
		12:00-13:00	Valedictory address Dr MPS Ishar VC MRSPTU, Bathinda Prof V K Kapoor Guest of Honour Distribution of Certificates Feedback of participants	Valedictory