

JSS Academy of Higher Education & Research, Mysuru

(Deemed to be University, Accredited 'A+' Grade by NAAC)

2-DAY NATIONAL CONFERENCE

ON

SUSTAINABLE DEVELOPMENT WITH PHARMACOLOGICAL RESEARCH AND INNOVATIONS

September 28-29, 2018

&

2-DAY WORKSHOP

ON

COMPUTATIONAL METHODS IN DRUG DISCOVERY

September 28-29, 2018

Department of Pharmacology

JSS COLLEGE OF PHARMACY, Ootacamund, Tamil Nadu

(An ISO 9001:2015 Certified Institution)

(Ranked 15th by NIRF-MHRD, Govt. of India)

CONFERENCE SPONSORED BY



Two-day national conference entitled "2-DAY National Conference on Sustainable Development with Pharmacological Research and Innovations" and two day workshop entitled "2-DAY Workshop on Computational Methods in Drug Discovery" was organized by Department of Pharmacology, JSS College of Pharmacy Ooty during 28 -29 September 2018. The conference was sponsored by Science and Engineering Research Board (SERB), Department of Science and Technology (DST), Govt. of India.

The Inaugural function was held on 28th September 2018, 9.45 am in the presence **Dr. Rajkumar Banerjee, Principal Scientist, IICT- Hyderabad** as the chief guest, **Dr. Girinath G Pillai, CEO, Zastra Innovations Pvt. Ltd., Bengaluru** as the guest of honour with the august presence of all the speakers and delegates. The organizing secretary **Dr. T.K. Praveen,** of both **National Conference and Workshop** welcomed the gathering and addressed on the genesis of the conference and workshop to the gathering. The conference and workshop was inaugurated by a prayer song and traditional way of lightning the lamp. The Scientific Abstract as a CD of 2-Day National Conference was released during the Inauguration program and it was provided to the speakers and the delegates.

In his chief guest address, Dr. Rajkumar Banerjee, Principal Scientist, IICT- Hyderabad emphasized on the importance of research towards drug discovery by advanced and newer strategies. The **Conveners of the workshop- Mr. B. Shivaramakrishnan & Mr. J. Saravanan** released the learning & resource materials to the workshop participants and it was conducted in the Pharm. Regulatory Lab. JSS College of Pharmacy, Ooty.

Dr. Md. Afzal Azam, Vice principal, JSS College of Pharmacy, Ooty presided the function and Dr. R. Vadivelan; Convener, National Conference delivered the vote of thanks. Mr. Basavalinga Devaru, Admin. Officer JSS College of Pharmacy Ooty, Dr. P.R. Anand Vijayakumar & Dr. A. Justin- Organising Members, Press and Media were also present.

Report on 2 Day National Conference

A total of 150 delegates from various parts of India had participated in the 2 Day National Conference conducted in the Auditorium, JSS College of Pharmacy, Ooty. The nine eminent speakers from the scientific community across the country had shared their research expertise and promoted innovative research strategies against diseases. Eminent Scientists and Academicians from Manipal Academy of Higher Education-Manipal, CSIR-Indian Institute of Chemical Technology (IICT)- Hyderabad, CSIR- Central Food Technology Research Institute (CFTRI)-Mysuru, Zastra Innovations Pvt. Ltd. Bengaluru, Royal Care Hospitals Coimbatore, Central Research Laboratory-MS Ramaiah Medical College and Hospitals- Bengaluru and JSS Academy

of Higher Education & Research (JSS AHER)-Mysuru had delivered their talks on various aspects and newer innovative approaches to sustainable pharmacological research in drug discovery. The Conference was divided into 9 lecture sessions spread across two days along with e-poster presentation session held on 28th November 2018.

The lecture sessions of the Conference were organised over two days during which the invited speakers emphasised on the need for employing newer & current approaches for drug discovery. These lecture sessions with the respective highlights are as follows:

DAY-1, September 28, 2018

- 1) Role of Computational Methods and Data for Drug Candidate selection By Dr. Girinath G Pillai, CEO, Zastra Innovations Pvt. Ltd., Bengaluru
- 2) Glucocorticoid Receptor: A Potent Drug-Sensitizing, Nano-therapeutic Delivery Target for Cancer
 - By Dr. Rajkumar Banerjee, Principal Scientist, CSIR-IICT, Hyderabad
- 3) Computer Aided Drug Design
 - By Dr. K. Sreedhara Ranganath Pai, Professor & Head, department of Pharmacology, MAHE, Manipal
- 4) A Novel Approach in Delivery of Nutraceuticals for Obesity By Dr. S P Muthukumar, Principal Scientist & Associate professor, Central Food Technological Research Institute, Mysuru
- 5) In Vitro cell culture models for high-throughput drug screening and toxicity By Dr. Ashish Wadhwani, Asst. Professor & Head, Dept. of Pharm. Biotechnology, JSSCP, Ooty

DAY-2, September 29, 2018

- 6) Bioequivalence
 - By Dr. K.T. Manisenthil Kumar, Administrator-Pharmacy and Quality Control, Royal Care Hospitals, Coimbatore.
- Ligand based virtual screening: Basics and applications in drug discovery
 By Dr. B.R. Prashantha Kumar, Asst. Professor, Department of Pharmaceutical Chemistry,
 JSSCP, Mysuru
- 8) Zebra fish A potential alternate vertebrate model for preclinical research

 By Dr. S. N. Manjula, Professor & Head, Department of Pharmacology, JSSCP, Mysuru
- 9) Cell model for Pharmacology Research: Best alternate or Incidental Alternate By Dr. Kotamballi N Chidambara Murthy, Principal Scientist, Central Research Laboratory, MS Ramaiah Medical College and Hospitals, Bengaluru

An e-poster presentation session was conducted under three classifications based on the nature of the work carried out. They are synthesis & biological research, phyto-pharmaceutical research and clinical cases. Selected 30 Abstracts and its' posters were evaluated by a panel of 3 judges per session. Overall, 5 best posters were awarded on the valedictory function.

Report on 2 Day Workshop

A total of 50 participants from various parts of India had participated in the 2 Day workshop entitled "Computational Methods in Drug Discovery" was organized by Department of Pharmacology, JSS College of Pharmacy Ooty during 28 -29 September 2018. The venue was Pharmaceutical Regulatory Lab where the necessary technical facilities were arranged for the participants to have an up-close interaction with the Resource person- **Dr. Girinath G Pillai, CEO, Zastra Innovations Pvt. Ltd., Bengaluru.**

The workshop entailed 'hands-on' experiences using the <u>StarDrop and other softwares</u> with practical experience under the following modules:

- 1. Introduction to databases, file formats and existing knowledge resources.
- 2. Introduction to StarDrop- Software
 - Getting started & Gaining familiarity with the StarDrop
 - Importing compound data
 - Calculating simple properties for compounds
 - Visualising data, Using Card View
- 3. Multi-Parameter Optimization in Drug Discovery- Probabilistic Scoring
- 4. Lead Optimisation I: Guiding the Design of Balanced Compounds- 2D and 3D SAR Analysis, Interactive Design and the Glowing Molecule
- 5. Lead Optimisation II: Guiding the Design of Balanced Compounds- Running 3D docking and alignment models with the Pose Generation Interface
- 6. API-Co-crystal screening

The participants had access to all the information and databases with a learning period of one month free license.

Overall, 2-day workshop covered the computational methods that would guide researchers on compound selection, design & identify lead candidates. This course has enabled and guided the participants a good understanding of the importance of drug design and drug delivery properties including the latest methods for multi-parameter lead optimization and decision analysis, which help to quickly target compounds for a drug discovery process.

The valedictory function was held on 29th September 2018 between 3.00 to 4.00 pm. **Dr. Praveen T.K.,** Organizing secretary gave a brief report on the conference and workshop, followed by oral and written feedback from the participants. The **Patron, Dr. S.P. Dhanabal,** Principal JSS College of Pharmacy, Ooty gave away the best poster awards and participation certificates of the Conference and Workshop. The conference & workshop ended with vote of thanks given by the Organising Secretary.

I express my sincere gratitude to Science and Engineering Research Board (SERB), Department of Science and Technology (DST), Govt. of India, for the financial support for conducting this National Conference. I also profusely thank JSS Academy of Higher Education and Research, Mysuru at this juncture and its constant support to successfully conduct this conference and workshop in a grand manner.

Signature of Organizing Secretary (with rubber stamp)

Signature of Head of Organization/Institute (with rubber stamp)

INAUGURAL FUNCTION





GLIMPSES OF CONFERENCE













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