



**JSS Academy of Higher Education & Research,  
Mysuru**  
(Deemed to be University)  
Accredited 'A+' Grade by NAAC  
**JSS COLLEGE OF PHARMACY, OOTACAMUND**  
**(An ISO 9001:2015 Certified Institution)**

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**A Report on**  
**JSS AHER, Mysuru, sponsored one day Virtual Symposium**  
**on**  
**“Building an innovation platform through artificial intelligence in**  
**drug discovery”**  
(11<sup>th</sup> December 2020)

Organized by  
Department of Pharmaceutical Chemistry  
JSS College of Pharmacy, Ooty

**11<sup>th</sup> December 2020**

**Submitted By**  
**Dr. Gomathy S**

Assistant Professor, Dept. of Pharmaceutical Chemistry  
JSS College of Pharmacy, Ooty

Department of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty, has organized JSS Academy of Higher Education & Research, Mysuru Sponsored one day Virtual Symposium on “**Building an innovation platform through artificial intelligence in drug discovery**” during 11<sup>th</sup> December, 2020.

### **Importance of the symposium**

- Artificial Intelligence (AI) can help academic researchers to identify drug targets, find good molecules from data libraries, suggest chemical modifications, and identify candidates for repurposing and so on. Imaging-based information can be used as an additional source of information for existing virtual screening methods, thereby making drug discovery more efficient. Integrative computational biology and AI help improve treatment of complex disease by building explainable models. These models use different mathematical methods, and help to predict new targets for known compounds, repurpose to new indications, search for compounds with specific multi-target profile, or identify potential liabilities. AI will also significantly reduce the probability of human error and study historical data to cut costs.
- In the early process of drug discovery, machine learning has many potential uses, from initial screening of drug compounds to prediction of the success rate of a drug. More specifically, AI may play a role in drug target identification and validation, target-based, phenotypic and multi-target drug discoveries, drug repurposing and biomarker identification.
- Collaboration with academia: Industry-academia partnership are expected to keep growing as pharma is starting to embrace AI.
- The chemical entities are likely to enter higher phases of the drug development process. This had resulted in paradigm shift in identifying the drug likeness properties of lead molecules early in the drug discovery process. Hence, *in-silico* approaches are now

widely used to investigate the ADME properties as a tool to optimize the selection of the most suitable candidates for drug development

### **Inauguration**

One day virtual symposium was inaugurated by Dr. S.P. Dhanabal, Principal, JSS College of Pharmacy, Ooty, and all faculties of the department of Pharmaceutical chemistry were present. Dr. Gomathy S, Organizing secretary, welcomed the gathering and Dr. Md. Afzal Azam, Convener, briefed about the genesis of the symposium. Dr. S.P. Dhanabal, Principal, delivered his presidential address and highlighted the activities of JSS College of Pharmacy, Ooty, during this pandemic situation. He also stressed about the importance of the symposium in worldwide scenario.

### **SCIENTIFIC SESSION**

#### **Session 1: 10.00 AM-11.30 AM**

Topic : Drug Discovery in the age of AI: Automation of the ML/DL for end-to-end (E2E) application in drug discovery and development

Speaker: Dr. M. Ravikumar, Senior Scientist & founder, Immunocure, Hyderabad.

#### **Session 2: 11.30 AM-1.00 PM**

Topic : Application of Artificial Intelligence in drug design of Anti-cancer agents

Speaker: Dr. M. Karthikeyan, Senior Principal Scientist, CSIR-NCL, Pune

#### **E-Presentation Session: 2.00 PM – 4.30 PM**

We have received about 53 abstracts from over all India, based on the merit and three stage screening 28 abstracts were categorized and have been shortlisted for e- presentation. The following evaluators have been nominated for poster presentation under three category.

The e-presentation evaluation team was composed of all the subject experts in it. External experts were also included in the panel to confirm the fair evaluation.

#### **Valedictory Function: 4.30 PM – 5.00 PM**

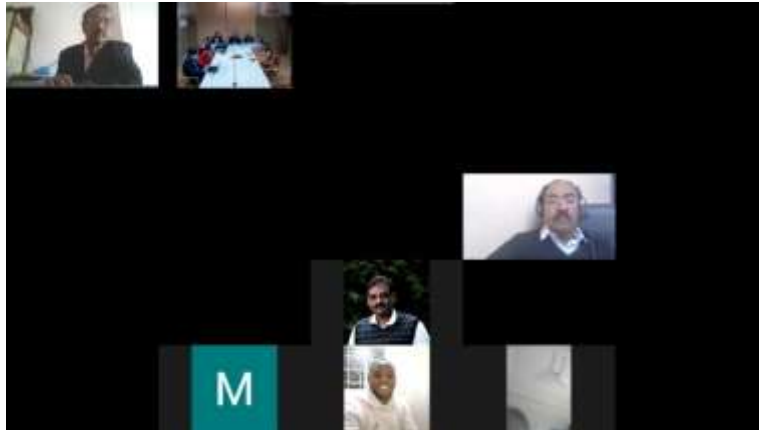
The evaluator's details are as follows.

<b>S.NO</b>	<b>NAME OF THE EVALUATOR</b>	<b>CATEGORY</b>
1	Dr Uma Maheshwari, Professor, College of Pharmacy, Sri Ramakrishna Institute of Paramedical Sciences, Coimbatore	Formulation development & Screening Techniques
2.	Dr V Senthil, Professor, Dept. of Pharmaceutics, JSS College of Pharmacy, Ooty	Formulation development & Screening Techniques
3.	Dr Bijo Mathew, Associate Professor, Dept. of Pharmaceutical Chemistry, Amrita School of Pharmacy, Amrita Vishwa Vidyapeetham, Kochi	<i>In silico</i> drug design & development
4.	Dr T.K.Praveen, Professor & Head, Dept. of Pharmacology, JSS College of Pharmacy, Ooty	<i>In silico</i> drug design & development
5.	Dr Ashish Wadhvani, Faculty, JSS Academy of Higher Education & Research, Mauritius	Phytochemistry & Analytical method development
6.	Dr Suresh Mohan Kumar, Professor & Research Director, JSS College of Pharmacy, Ooty	Phytochemistry & Analytical method development

The e-Presentation results are as follows,

<b>S. No</b>	<b>Name of the Presenter and Institute</b>	<b>Category</b>
1	Mr.Podila Naresh, Research Scholar, JSS College of Pharmacy,Ooty	<i>In silico</i> drug design & development
2	Ms. M.Gnana Ruba Priya, College of Pharmaceutical Sciences, Dayananda Sagar University, Bangalore	<i>In silico</i> drug design & development
3	Ms. S.K.Janani, Research Scholar, JSS College of Pharmacy,Ooty	Formulation development & Screening Techniques
4	Aakash Kumar S, PG Student, JSS College of Pharmacy,Ooty	Formulation development & Screening Techniques
5	Feroze Ahamed. A, Department of Microbial Technology, School of Biological Sciences, Madurai Kamaraj University, Palkalai Nagar, Madurai	Phytochemistry & Analytical method development
6	Mr. Gouru Santhosh Reddy, Research Scholar, JSS College of Pharmacy,Ooty	Phytochemistry & Analytical method development

## Glimpses of the symposium



# Drug Design of Anti-Cancer Agents



**Dr. M. Karthikeyan**  
Senior Principal Scientist  
CSIR-National Chemical Laboratory, Pune

Anti-Cancer  
Drugs






Personalized  
Medicine

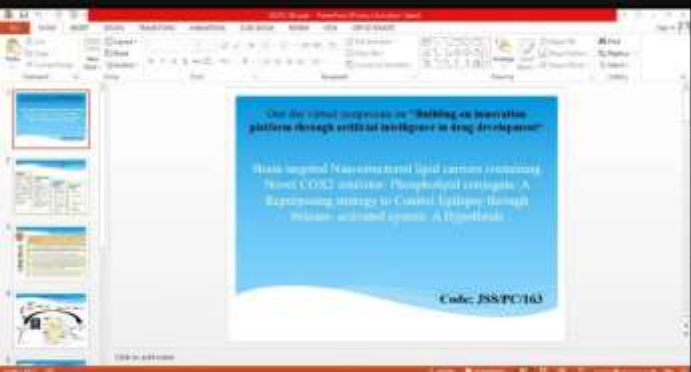


National Virtual Symposium on "Building an Innovation Platform through Artificial Intelligence in Drug Discovery" 11 Dec 2020 (Online)


## Artificial Intelligence

- what is this Artificial Intelligence?
- First coined in 1956 by John McCarthy, AI involves machines that can perform tasks that are characteristic of human intelligence.
- It includes things like planning, understanding language, recognizing objects and sounds, learning, and problem solving.



Code: JS8/PC/163



# BROCHURE



**JSS COLLEGE OF PHARMACY,  
OOTY**


JSS AHER, Mysuru Sponsored  
**One Day Virtual Symposium on**  
*"Building an Innovation Platform through  
 Artificial Intelligence in Drug Discovery"*  
 Organized by Department of Pharmaceutical Chemistry

📅 11 Dec. 2020 | 10 AM - 5 PM




JSS College of Pharmacy, Ooty, is one of the pioneering research institutions in the country imparting quality pharmaceutical education at diploma, graduate, post graduate and doctorate levels. The college is affiliated to JSS Academy of Higher Education & Research, Mysuru, which is accredited "A" Grade by NAAC. The college is certified by ISO 9001:2015. Our broad research areas are Drug delivery, Green chemistry, Drug design and Discovery, Stability, profiling, Pharmacokinetics, Neuropharmacology, Medicinal plants research, Compendry and Clinical pharmacy research etc. We have good number of research funding from Government agencies like DST, DBT, ICMR, CSIR, AYUSH, AICTE and DRDO and research publications in peer reviewed journals.

**SPEAKERS**



**DR. M. KARTHIKEYAN**  
 SENIOR PRINCIPAL SCIENTIST  
 CHEMICAL LABORATORY,  
 PUNE



**DR. M. RAVI KUMAR**  
 SENIOR SCIENTIST  
 & FOUNDER  
 (NANOCLUSTERS, HYDERABAD)

EVENT SCHEDULE

TIME	TOPIC	SPEAKER
10:30 - 11:30 AM	Drug Discovery in the age of AI: Automation of the ML/DL for real time (2D) applications in drug discovery and development	Dr. M. Karthikeyan
11:45 - 1:30 PM	Application of Artificial Intelligence in drug design of Anti-cancer agents	Dr. M. Karthikeyan
2:30 - 4:00 PM	Oral Poster Presentation	

Call for Abstracts:

Green Synthesis	Quality control evaluation of herbal drug
In silico Drug Design & Development	Next-Gen Delivery Technology
Nanobiotechnology Studies	Formulation Development & Technology transfer
Nanopharmaceutical & Technological studies	Stability studies & Analytical Methods

Level of Participants:

Academicians, Research Scholars & Post Graduate from Universities and Colleges can participate. Enrollment is restricted to **40 participants** on first come first serve basis.

Registration Link: <https://forms.gle/Tyapob6shZ2DwDw5>

<b>Patron</b>	<b>Convener</b>	<b>Organizing Secretary</b>
Dr. S.P. Dharsidhal Principal JSS College of Pharmacy, Ooty	Dr. M.L. Alal Azam Prof. & Head, Dept. of Pharmaceutical Chemistry JSS College of Pharmacy, Ooty	Dr. Ganesh Subramanian Assistant Professor Dept. of Pharmaceutical Chemistry JSS College of Pharmacy, Ooty

Organizing Committee Members

Dr. R. Karthiyan, Assistant Professor	Dr. S. Ganesh, Lecturer
Dr. S. Jothi, Assistant Professor	Dr. Srivani Lakshmi, Lecturer
Dr. B. Ganapathi, Assistant Professor	

NAME OF THE ACCOUNT - THE PRINCIPAL,  
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ACCOUNT NO. - 42800208999542

NAME OF THE BANK - PUNJAB NATIONAL BANK, COOY

BIC/SWIFT CODE - PUNB0330000

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₹100  
REGISTRATION  
FEE

Abstract Entry: From Nov 15/2020 to Dec. 10, 2020 (Last Date: 09)

Title: From Nov 15/2020 to Dec. 10, 2020 (Last Date: 09)

Abstracts: From Dec 10/2020 to Dec. 10, 2020 (Last Date: 09)

Abstract may be submitted to [chemistry@jssophoty@jssuni.ac.in](mailto:chemistry@jssophoty@jssuni.ac.in)

Last date for abstract submission: 09-12-2020

Declaration of abstract acceptance: 07-12-2020

Last date for registration: 09-12-2020

### List of External Participants

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20	Bua Bobson	PG student	JSS Academy OEP-PGDIB

My Humble Pranams to the lotus feet of His Holiness Swamiji, for his blessings. As an organizing Secretary of this symposium, Firstly, I would like to extend my heartfelt thanks to JSS Academy of Higher Education & Research, Mysuru, for their continuous support and sponsoring a seminar grant of Rs. 70, 000/- to conduct this symposium in a smoother way. I take this opportunity to express my special thanks to all the resource persons and all the participants. I sincerely thank our beloved Principal, Dr S P Dhanabal, Dr Md.Afzal Azam, Convener, for their moral support. In addition, my thanks to Administrative officer, Mr C Jayakumar, Asst Professor and Mr Gautham, System Analyst and Mr Mahesha, Grant Section. Last but not the least, I thank all the teaching and supportive staff of Department of Pharmaceutical Chemistry for their valuable support throughout the symposium.

**Dr. Gomathy S**

Organizing Secretary