

Date: 18<sup>th</sup> June, 2020

## DEPARTMENT OF PHARMACEUTICAL ANALYSIS

### National Webinar on - "Molecular Docking and In – Silico ADMET Prediction: An Overview"

**Resource Person** : **Dr. S. Jubie, Assistant Professor,**  
**Department of Pharmaceutical Chemistry,**  
**J.S.S. College of Pharmacy, Ootacamund, Tamil Nadu**

**Faculty Convener** : **Dr. Anna Balaji**

**Faculty Organizing Secretary** : **Dr. R. Shanmugam**

**Faculty Co-ordinator** : **Dr. B. Poornima**

**Department of Pharmaceutical Analysis** of Sree Vidyanikethan College of Pharmacy, Tirupati organized an National webinar on "**Molecular Docking and In-Silico ADMET Prediction: An Overview**" to the faculty, Research scholars and students members of various institutions, on 18<sup>th</sup> June, 2020.

Welcoming the delegates for the national webinar, **Dr. Anna Balaji, Principal** and the **Convener** of the event, explained the importance of New Drug Discovery and relevance of Molecular Docking studies. **Dr. R. Shanmugam**, the Organizing Secretary, introduced the speaker. He thanked the resource person **Dr. S. Jubie** for accepting to deliberate on her research for this occasion.

#### **YouTube link of National Webinar:**

<https://www.youtube.com/watch?v=6IAO2-RTDcM&t=295s>



National **Webinar** on  
**Molecular Docking and In-Silico  
ADMET prediction: An Overview**

**18.06.2020 | 11.00- 12.30pm**



Organized by  
Department of Pharmaceutical Analysis  
**SREE VIDYANIKETHAN COLLEGE OF PHARMACY**

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## About College:

Sree Vidyanikethan College of Pharmacy stands tall magnificently facing the Tirumala hills of the temple town of Tirupati. The College is approved by the All India Council for Technical Education (AICTE), New Delhi and Pharmacy Council of India (PCI) New Delhi, the institution took shape in the year 2004. It is affiliated to Jawaharlal Nehru Technological University, Anantapur, Anantapuramu.

The college offers B. Pharmacy program for an intake of 100 students, M. Pharmacy program (Pharmaceutics and Pharmaceutical analysis), Pharm D for an intake of 30 students and Pharm D (PB) for a 10 students intake. Infrastructure, state-of-the-art laboratories and eminent teaching faculty are exclusive strengths of the institution. The basic degree course of Pharmacy education is designed to ensure that the newly qualified pharmacist has the necessary knowledge and skills to commence practicing competently in a variety of settings including community pharmacy, hospital pharmacy and pharmaceutical industry. Continuing professional development must then be a lifelong commitment for every practicing pharmacist. The education, which a pharmacy student receives, knowledge gained, the skills learned and the attitudes taken.

## About Webinar:

In modern drug design, molecular docking and In Silico screening of ADMET profiles provide useful information about drug-receptor interactions and are often used to predict the binding orientation of small molecule drug candidates to their protein targets to determine the affinity and activity of small predict molecules. New computer predictions of pharmacokinetics such as absorption, distribution, metabolism and excretion (ADME) and toxicity studies have become increasingly important in the drug selection and promotion process and are promising tools for the early detection of potential drug candidates.



## Speaker

**Dr. S. Jubie**, Asst. Professor, Department of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty, Tamil Nadu, India.

**Convener-** Dr. Anna Balaji

**Organizing Secretary-** Dr. R. Shanmugam

**Co-Ordinator-** Dr. B. Poornima

## Key Take Away

- Gains knowledge about the molecular docking and In-Silico ADMET prediction in research area.
- Free Registration.
- e-Certificate can be downloaded after submitting the feedback form.

## Webinar Registration link:

<https://docs.google.com/forms/d/1AEPsTdkdp0GA8l60BrdARbxJM09z7kGEDPh6WjcyncA/edit>



## Molecular docking and *in-silico* ADMET prediction: an overview

**Dr. Jubie Selvaraj**

Asst. Professor

Department of Pharmaceutical Chemistry

JSS College of Pharmacy, Ootacamund-643 001

JSS Academy of Higher Education & Research (Deemed to be University)

Accredited A+ Grade by NAAC

zoom

### **Dr. S. Jubie, Resource person while delivering the session**

The resource person, **Dr. S. Jubie** discussed different types of docking methodologies, various software's used in docking studies, crucial role of molecular docking & *in-silico* screening of ADMET profiles, drug- receptor interactions in designing a drug molecule. She also enlighten her deliver with criteria for selection of protein target. She also discussed *in-silico* predictions of pharmacokinetic parameter such as absorption, distribution, metabolism, excretion and toxicity (ADMET) which play a key role in the drug selection & promotion process. She emphasized that Molecular Docking is a popular tool for the early detection of potential drug candidates.

**Dr. B. Poornima**, Faculty, co-ordinator of this event proposed the vote of thanks for the occasion. She mentioned that the delegates were immensely benefitted and thanked the Resource person, and the organizers who contributed for the success of the national webinar.

**Principal**