



POPULAR SCIENCE LECTURE

On

Computational Pharmaceutics: Can It Help Understand Drug Targeting?



**SUNANDAN DIVATIA
SCHOOL OF SCIENCE**

Organized by

Indian Women Scientists' Association

Vashi, Navi Mumbai

Supported by BRNS-DAE

In association with

Sunandan Divatia School of Science

SVKM's NMIMS (Deemed-to-be) University

Vile Parle (W), Mumbai



**Dr. VANDANA
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Professor of Pharmaceutics
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Research Interests:

- Development of nanocarriers with major emphasis on malaria, cancer and neurodegenerative disorders
- Medical device development
- Nanodiagnostics
- Nanovaccines



7th January, 2021 at 5:30 pm

Session will be held through MS Teams

Register online to participate in the webinar

Link: <https://bit.ly/3a89AfM>

Last date for registration- 31st Dec, 2020

e-Certificate will be provided to the attendees

Computational Pharmaceutics: Can It Help Understand Drug Targeting?

Dr. VANDANA PATRAVALE

Abstract

The advent of computers revolutionized the world but their entry in pharmaceutical science has uplifted its significance to another level. Artificial intelligence (AI) is on its way to break all barriers that were posed to humans through several centuries. Pharmaceutical science is equally and positively impacted by the inclusion of numerous emerging concepts based out of AI, in regular practice. The importance of computational science has been well established in the field of drug discovery and is a continually growing field, even today. However, use of computational tools in the field of formulation design and development is still a nascent but dynamic concept. Scientists are always on a lookout for tools which can aid in rational design of formulations but also curb the extensive loss of man and materials in the process. Computational tools can bridge this gap and offer a highly cost and time effective approach in this direction. These tools can be utilized right from pre-formulation up to *in vivo* activity prediction with a sound correlation if applied with prior knowledge of their key concepts. Study of molecular aspects of formulation and all of its components would help in understanding the formulation in simulation conditions. Excipients screening, drug excipient interactions, drug receptor interactions, solubility predictions, enzyme inhibition, protein-peptide interactions, bio-membrane permeation, etc are some of the prime applications of these tools. The increasing market of biopharmaceuticals has driven this industry to take utmost interest in this upcoming computational trend.