



# PEOPLE'S UNIVERSITY

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## SCHOOL OF PHARMACY & RESEARCH

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No: SOP&R/GL/21/175

Date: 21/05/2021

### REPORT OF THE EVENT

To sensitize students of School of Pharmacy and Research, more on Computer Aided Drug Design which has been opted as Elective subjects by some of the B. Pharm. (VIII<sup>th</sup> Sem) students, a series of guest lecture was organized virtually on 21st June to 22d June 2021. Guest speaker for this two days session was Dr. Debanjan Sen, Assistant Professor, BCDA College of Pharmacy & Technology, Hridapur, Kolkata-127. Basic objective of this Lecture was to sensitize students on “Molecular Modelling and Virtual Screening Techniques” through which students would be able to learn more about the basic techniques and different software’s used in docking. He described about virtual screening, drug likeness screening, pharmacophore mapping with suitable examples. He briefed on pharmacophore-based screening, application of pharmacophore modelling and tools related to docking experiment execution. He explained about different types on Molecular Docking on Second day of his lecture where he discussed about component of docking program with suitable examples and published research paper. He requested students to work on some free software’s available for docking and provided small hands on Training on that. At the end of Lecture series, Dr. Neeraj Upmanyu, Principal, SOPR, thanked Dr. Debanjan Sen for his untiring effort and accepted invitation to deliver the students about the nitty gritty of the subject. He appreciated the effort of Mr. Alka Singh, Assoc. Professor, SOPR and coordinator of this lecture series for this initiative and dedication towards students.



**Principal**

## IMAGES OF EVENT:

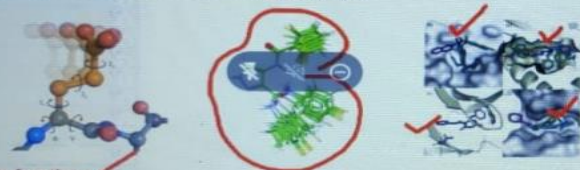
Debanjan Sen is presenting

### Components of Docking Program

Typically, protein-ligand docking software consist of two main components which work together:

- 1. Search algorithm**  
Generates a large number of poses of a molecule in the binding site
- 2. Scoring function**  
Rank orders the conformations/poses to distinguish the experimental binding pose from the rest  
Binding affinity = E<sub>vdw</sub> + E<sub>ele</sub> + E<sub>hyd</sub> + ...

*A balance between: the search space for conformational sampling, scoring function calculation and accuracy is important*




Guest Lecture on Molecular Modelling and Virtual ...

Debanjan Sen is presenting

### Designing Drugs is Hard

Need to simultaneously optimize many properties:

- Potency
- Bioavailability
- CYP inhibition
- Toxicity
- Selectivity
- Clearance / half-life
- hERG blockade
- Synthesizability
- Solubility
- Permeability



	Property 1	Property 2	Property 3	Property 4	Property 5	Property 6	Property 7	Property 8	Property 9	Property 10
Mol 1	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green
Mol 2	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green
Mol 3	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green
Mol 4	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green

• Hit Compounds  
• Lead Compounds  
• Drug Candidates

Lecture on Molecular Modelling and Virtual ...



REC Debanjan Sen is presenting

4:35 PM | Guest Lecture on Molecular Modelling and Virtual S...

Debanjan Sen

ARNAB Pal

BISHWAJEET SINGH

Alka CA Marish Singh

shubham prajapati

9 others

Veber Rule

- 1) Rotatable Bond Count  $\leq 10$
- 2)  $PSA \leq 140$

TPSA  $\leq 140 \text{ \AA}^2$

RB  $< 10$

Good drug absorption and permeation

MDDR-like rules

- No. Rings  $\geq 3$
- No. Rigid bonds  $\geq 18$
- No. Rotatable bonds  $\geq 6$

*Oprea TJ. Property distribution of drug-related chemical databases. J Comput Aided Mol Des. 2000 Mar;14(3):251-64. doi: 10.1023/a:1008130001697. PMID: 10756480*

Debanjan Sen

ARNAB Pal

Ghanshyam Sahu

BISHWAJEET SINGH

Lavi Kashiv

diksha dwivedi

shubham prajapati

9 others

You





Debanjan Sen is presenting

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Guest Lecture on Molecular Modelling and Virtual ...





**PEOPLE'S  
UNIVERSITY**

A NAAC Accredited University

# SCHOOL OF PHARMACY AND RESEARCH

People's Campus, Bhopal (M.P.)-462037 India

## Guest Speaker



**DEBANJAN SEN**

Assistant Professor,  
BCDA College of Pharmacy & Technology,  
Kolkata-127, WB, India

## Lecture Series

on

**"MOLECULAR MODELLING AND VIRTUAL SCREENING  
TECHNIQUES"**

**June 21, 2021 to June 22, 2021**

Google Meet link:

<https://meet.google.com/wbc-jodv-huv>



## COURSES

Bachelor of Pharmacy (B. Pharm) Master of Pharmacy (M. Pharm) Ph.D.  
**One Year certificate courses**

a) Clinical Research & Data Management b) Pharmacovigilance c) Medical Writing



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