



PEOPLE'S UNIVERSITY

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ISO 9001 : 2008 Certified

SCHOOL OF PHARMACY & RESEARCH

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. (VIIIth 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 = $E_{wd} + E_{ee} + E_{hyd} + \dots$
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
- Selectivity
- Solubility
- Bioavailability
- Clearance / half-life
- Permeability
- CYP inhibition
- hERG blockade
- **Synthesizability**
- **Toxicity**

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

Lecture on Molecular Modelling and Virtual ...



REC Debanjan Sen is presenting

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

Participants: Debanjan Sen, ARNAB Pal, BISHWAJEET SINGH, Alka CA Marish Singh, shubham prajapati, 9 others

Veber Rule

- 1) Rotatable Bond Count ≤ 10
- 2) PSA ≤ 140 *AZ*

MDDR-like rules

- No. Rings ≥ 3
- No. Rigid bonds ≥ 18
- No. Rotatable bonds ≥ 6

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

$+$

RB
 $RB < 10$

\rightarrow

Good drug absorption and permeation

Oprea TI. 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

Participants: Debanjan Sen, ARNAB Pal, Ghanshyam Sahu, BISHWAJEET SINGH, Lavi Kashiv, diksha dwivedi, shubham prajapati, 9 others, You



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Mol 3	Green									
Mol 4	Green									

Hit Compounds
Lead Compounds
Drug Candidates

Virtual ...

meet.google.com/wbc-jodv-huv?authuser=0

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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

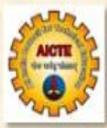
on

"MOLECULAR MODELLING AND VIRTUAL SCREENING
TECHNIQUES"

June 21, 2021 to June 22, 2021

Google Meet link:

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



COURSES

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