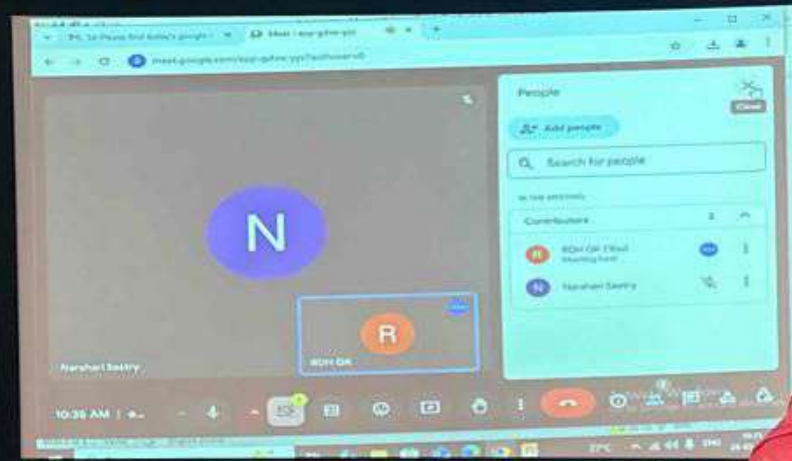


Hyderabad, Telangana, India
Street Number 8, Barkatpura, Hyderabad,
Telangana 500027, India
Lat 17.393529, Long 78.495028
03/24/2025 10:35 AM GMT+05:30
Note : Captured by GPS Map Camera



Hyderabad, Telangana, India

Street Number 8, Barkatpura, Hyderabad,
Telangana 500027, India

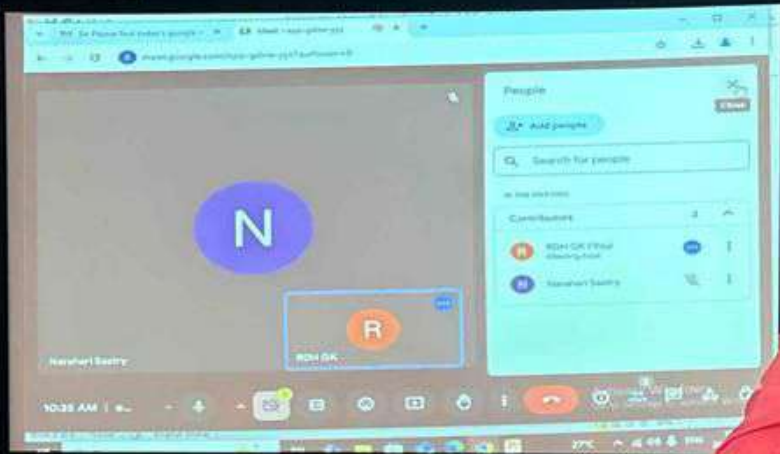
Lat 17.393490, Long 78.494982

03/24/2025 10:35 AM GMT+05:30

Note : Captured by GPS Map Camera

GPS Map Camera





Hyderabad, Telangana, India
Street Number 8, Barkatpura, Hyderabad,
Telangana 500027, India
Lat 17.393485, Long 78.494986
03/24/2025 10:35 AM GMT+05:30
Note : Captured by GPS Map Camera

GPS Map Camera



GPS Map Camera




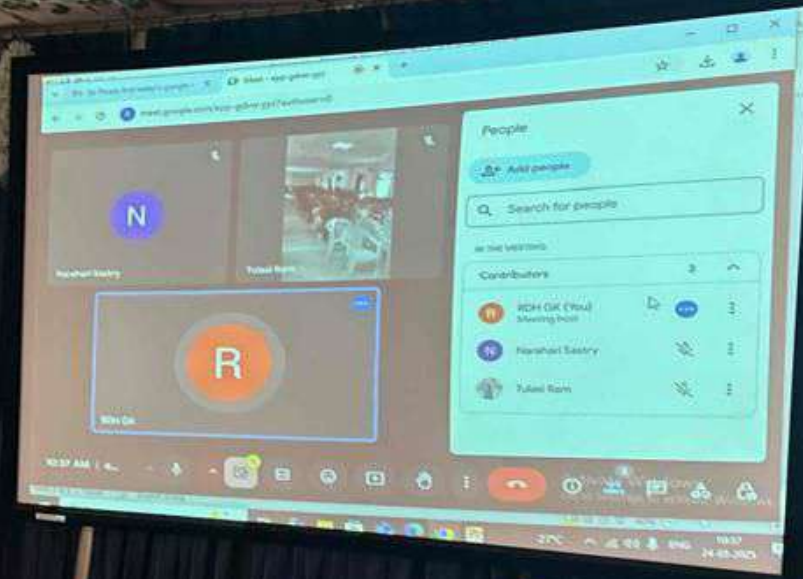
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Street Number 8, Barkatpura, Hyderabad,
Telangana 500027, India
Lat 17.393512, Long 78.494956
03/24/2025 10:36 AM GMT+05:30
Note : Captured by GPS Map Camera





Hyderabad, Telangana, India
Street Number 8, Barkatpura, Hyderabad,
Telangana 500027, India
Lat 17.393475, Long 78.494948
03/24/2025 10:36 AM GMT+05:30
Note : Captured by GPS Map Camera

 GPS Map Camera



GPS Map Camera



Hyderabad, Telangana, India

Street Number 8, Barkatpura, Hyderabad,
Telangana 500027, India

Lat 17.393554, Long 78.495029

03/24/2025 10:36 AM GMT+05:30

Note : Captured by GPS Map Camera



GPS Map Camera



Hyderabad, Telangana, India

Street Number 8, Barkatpura, Hyderabad,
Telangana 500027, India

Lat 17.393481, Long 78.494835

03/24/2025 10:41 AM GMT+05:30

Note : Captured by GPS Map Camera



GPS Map Camera



Hyderabad, Telangana, India
Street Number 8, Barkatpura, Hyderabad,
Telangana 500027, India
Lat 17.393429, Long 78.494851
03/24/2025 10:41 AM GMT+05:30
Note : Captured by GPS Map Camera




GPS Map Camera



Hyderabad, Telangana, India
Street Number 8, Barkatpura, Hyderabad,
Telangana 500027, India
Lat 17.393416, Long 78.494855
03/24/2025 10:41 AM GMT+05:30
Note : Captured by GPS Map Camera




 GPS Map Camera



Hyderabad, Telangana, India
Street Number 8, Barkatpura, Hyderabad,
Telangana 500027, India
Lat 17.393357, Long 78.494898
03/24/2025 10:41 AM GMT+05:30
Note : Captured by GPS Map Camera



 GPS Map Camera

Hyderabad, Telangana, India

Street Number 8, Barkatpura, Hyderabad,
Telangana 500027, India

Lat 17.393365, Long 78.494905

03/24/2025 10:42 AM GMT+05:30

Note : Captured by GPS Map Camera





GPS Map Camera



Hyderabad, Telangana, India
Street Number 8, Barkatpura, Hyderabad,
Telangana 500027, India
Lat 17.393453, Long 78.494651
03/24/2025 10:51 AM GMT+05:30
Note : Captured by GPS Map Camera







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GPS Map Camera



Hyderabad, Telangana, India
Street Number 8, Barkatpura, Hyderabad,
Telangana 500027, India
Lat 17.393397, Long 78.494896
03/24/2025 10:51 AM GMT+05:30
Note : Captured by GPS Map Camera



GPS Map Camera



Hyderabad, Telangana, India
Street Number 8, Barkatpura, Hyderabad,
Telangana 500027, India
Lat 17.393382, Long 78.494886
03/24/2025 10:51 AM GMT+05:30
Note : Captured by GPS Map Camera



Harshant Sastry (Presenting)

Molecular Recognition

• Substrate recognition and binding to the active site of an enzyme is a highly specific process. The substrate must fit into the active site of the enzyme, which is often described as a "lock and key" model.

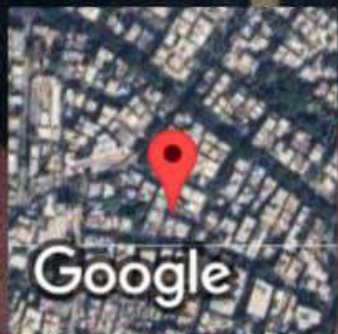
Molecular Recognition

But recognition is not an event of a process involving two dynamically changing structures.

Harshant Sastry | Chinnappa Sastry | Tubal Ram | Sushrta Peddumudi

10:53 AM | esp-9

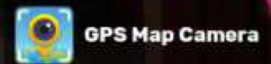
GPS Map Camera



Hyderabad, Telangana, India

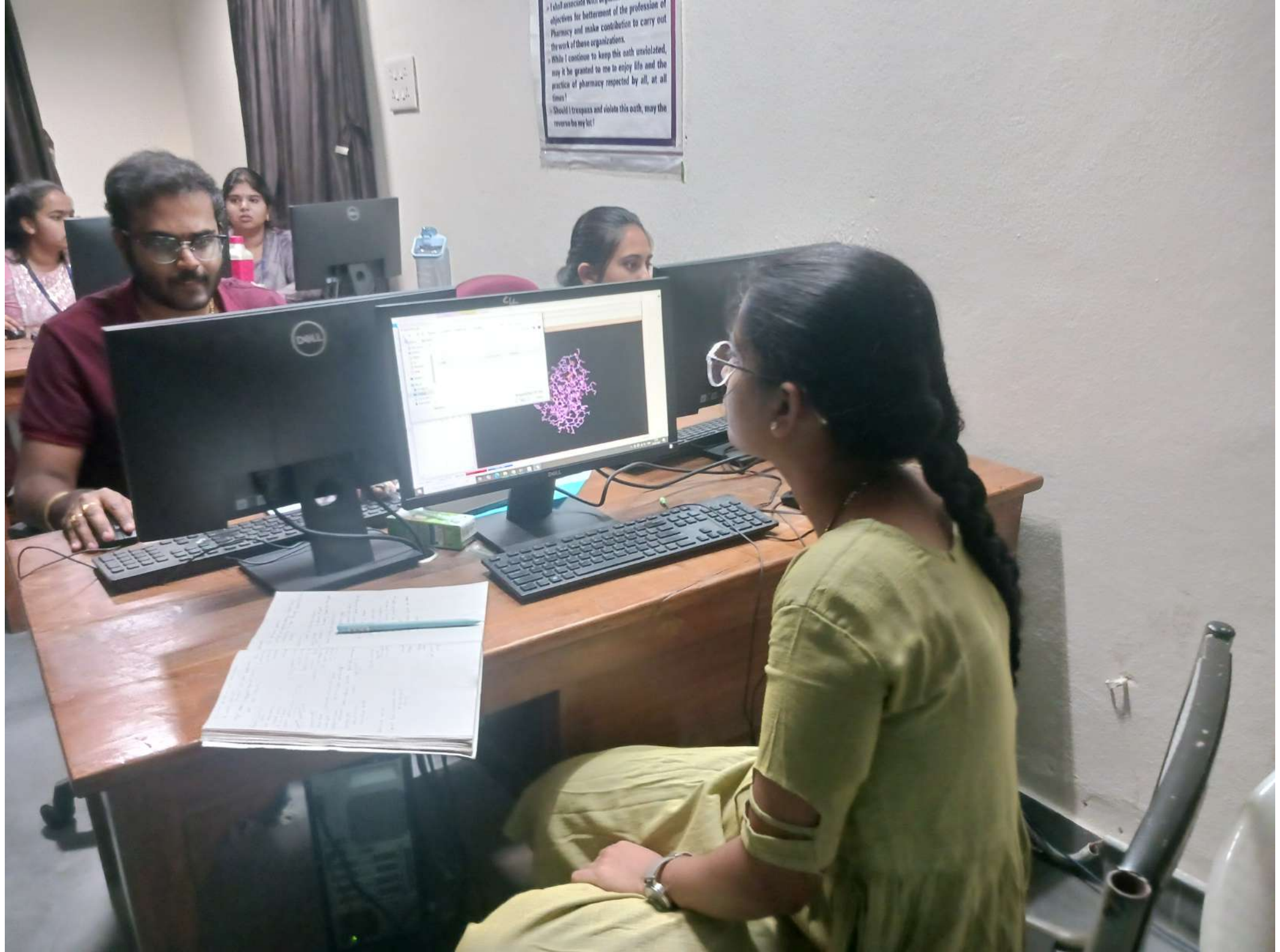
3-4-856, Barkatpura, Kachiguda, Hyderabad, Telangana 500027, India

Lat 17.3934° Long 78.494872°
24/03/2025 10:53 AM GMT +05:30



Hyderabad, Telangana, India
3-4-856, Barkatpura, Kachiguda, Hyderabad, Telangana 500027, India
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24/03/2025 10:38 AM GMT +05:30



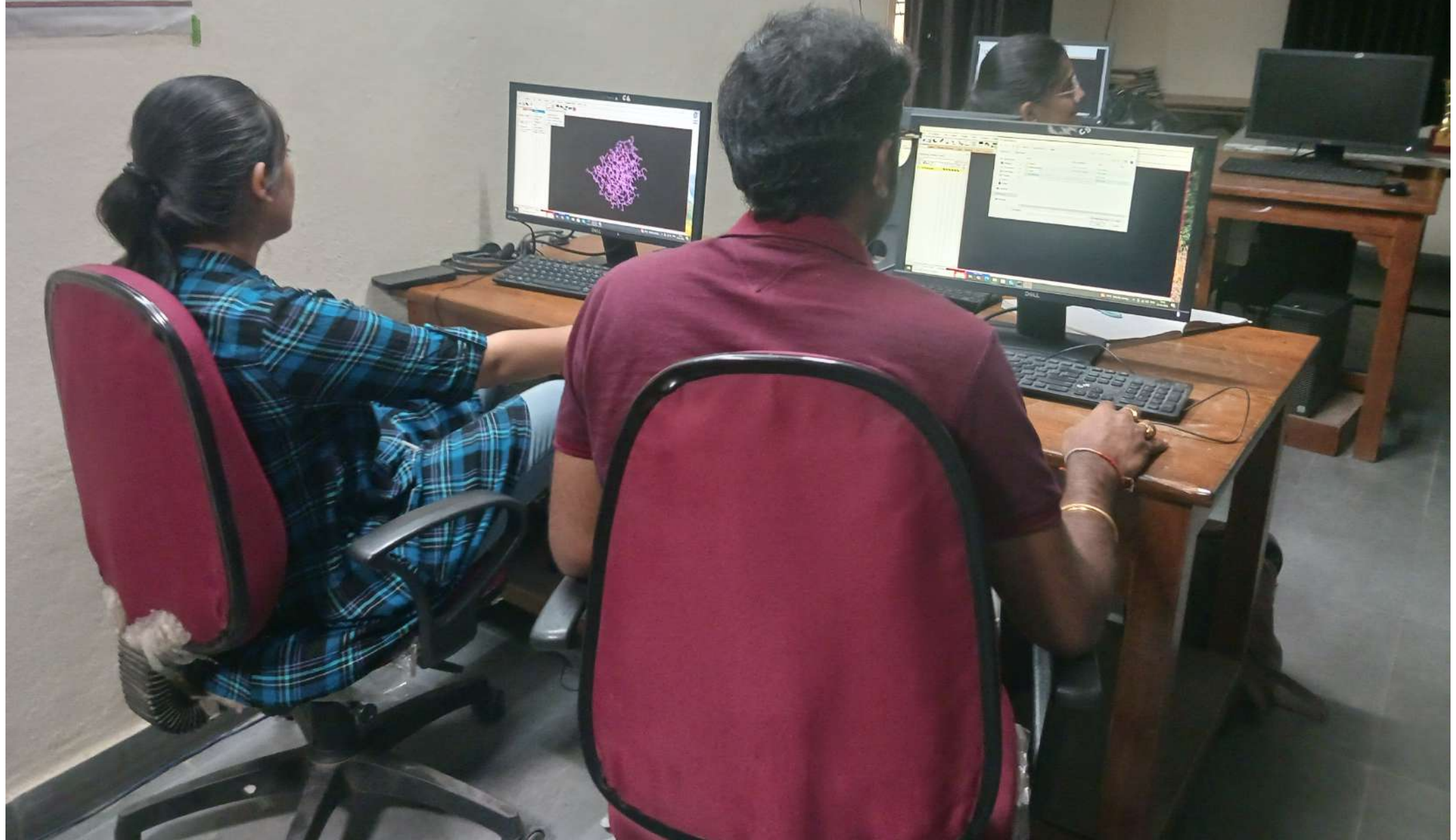


I shall associate with my colleagues
objectives for betterment of the profession of
Pharmacy and make contribution to carry out
the work of these organizations.
While I continue to keep this oath unviolated,
may it be granted to me to enjoy life and the
practice of pharmacy respected by all, at all
times!
Should I trespass and violate this oath, may the
reverse be my lot!



...sion of
on to carry out
oath unviolated,
njoy life and the
ted by all, at all
this oath, may the

THINK CLEAN AND DRINK
DUSTERS









Scoring Function

• Factors Affecting ΔG^0

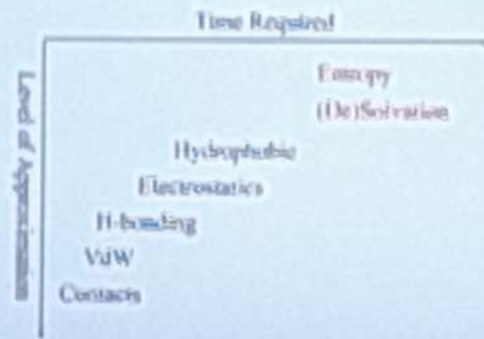
Intramolecular Forces (covalent)

- Bond lengths
- Bond angles
- Dihedral angles

Intermolecular Forces

- Electrostatics
- Dipolar interactions
- Hydrogen bonding
- Hydrophobicity
- Van der Waals

Terms in Scoring Functions



Dr. S. Kumar

28



GPS Map Camera

Check In

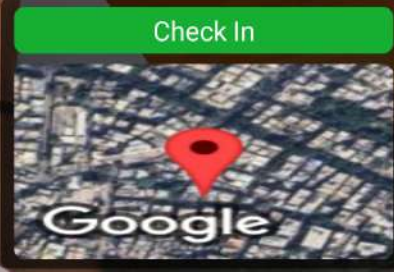


Hyderabad, Telangana, India

Lingampalli, 3-4-343, Baghlingmpally Cross Rd, Barkatpura,
Kachiguda, Hyderabad, Telangana 500027, India

Lat 17.393444° Long 78.494749°

27/03/2025 12:33 PM GMT +05:30



Check In

Hyderabad, Telangana, India

Lingampalli, 3-4-343, Baghlingmpally Cross Rd, Barkatpura, Kachiguda, Hyderabad, Telangana 500027, India

Lat 17.39343° Long 78.494733°
27/03/2025 12:32 PM GMT +05:30

Definition of problem

Defined as an optimization problem, which would describe the "best-fit" orientation of a ligand that binds to a particular protein of interest.



However, since both the ligand and the protein are flexible, a "hand-in-glove" analogy is more appropriate than "lock-and-key".

During the course of the docking process, the ligand and the protein adjust their conformation to achieve an overall 'best-fit' and this kind of conformational adjustment resulting in the overall binding is referred to as 'induced-fit'.

Dr. V. Kumar

11

Check In



Hyderabad, Telangana, India

Lingampalli, 3-4-343, Baghlingmpally Cross Rd, Barkatpura,
Kachiguda, Hyderabad, Telangana 500027, India

Lat 17.393438° Long 78.494737°

27/03/2025 11:30 AM GMT +05:30



GPS Map Camera



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Hyderabad, Telangana, India

Lingampalli, 3-4-343, Baghlingmpally Cross Rd, Barkatpura, Kachiguda, Hyderabad, Telangana 500027, India

Lat 17.393435° Long 78.494742°
27/03/2025 11:27 AM GMT +05:30





GPS Map Camera

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Hyderabad, Telangana, India

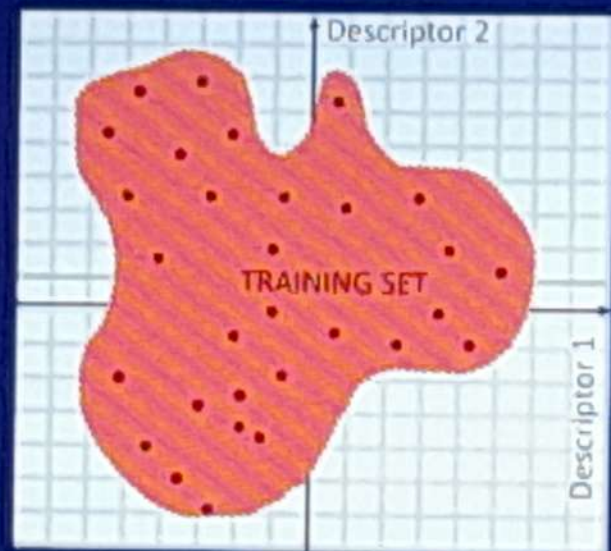
3-4-334, Barkatpura, Kachiguda, Hyderabad, Telangana 500027, India

Lat 17.393453° Long 78.494567°

27/03/2025 03:55 PM GMT +05:30

kNN (k Nearest Neighbors)

- Activity Y assessment calculating a weighted mean of the activities Y_i of its k nearest neighbors in the chemical space



$$W_i = \frac{e^{-d_j} \sum_{i=1}^K d_i}{\sum_{j=1}^K e^{-d_j} \sum_{i=1}^K d_i}$$
$$Y_{\text{unknown}} = \sum_{i=1}^K W_i Y_i$$

A. Tropsha, A. Golbraikh, 2001



GPS Map Camera

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Hyderabad, Telangana, India

Lingampalli, 3-4-343, Baghlingmpally Cross Rd, Barkatpura,
Kachiguda, Hyderabad, Telangana 500027, India

Lat 17.39343° Long 78.494723°

26/03/2025 12:18 PM GMT +05:30



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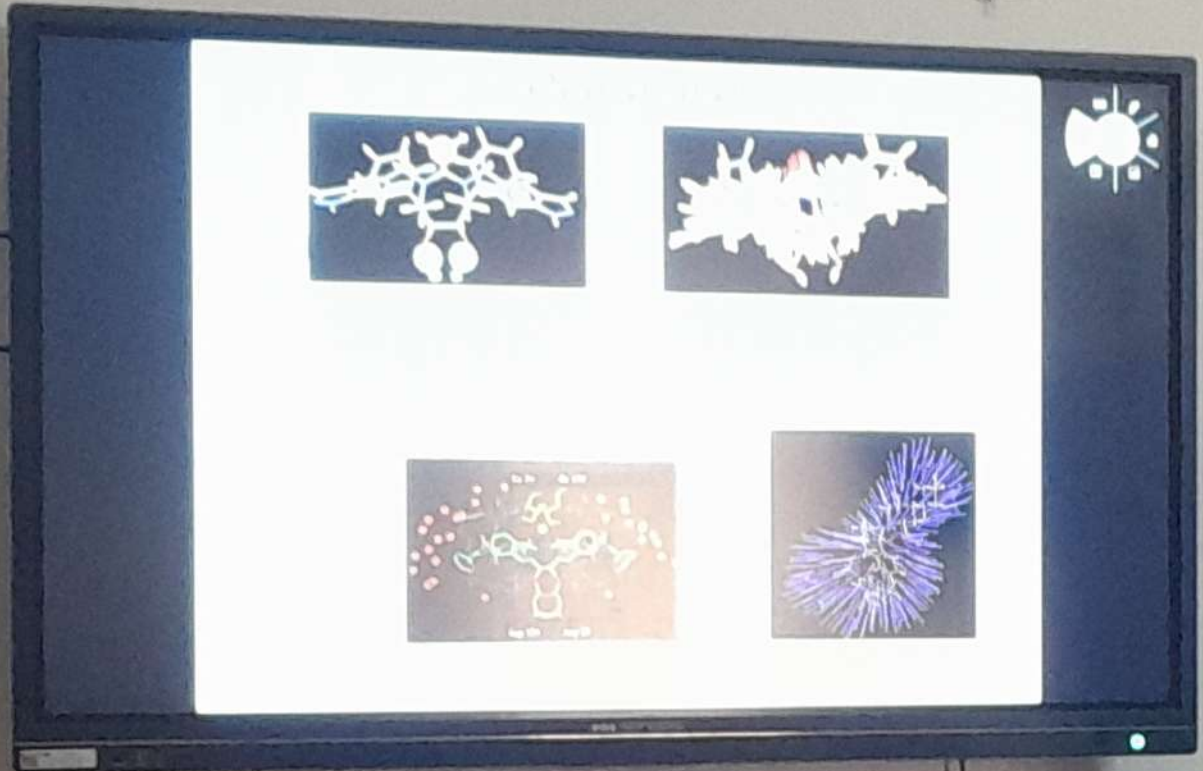


Hyderabad, Telangana, India

Lingampalli, 3-4-343, Baghlingmpally Cross Rd, Barkatpura, Kachiguda, Hyderabad, Telangana 500027, India

Lat 17.393431° Long 78.494737°
26/03/2025 11:27 AM GMT +05:30

It is very easy to defeat someone
It is very hard to win someone



Check In



Hyderabad, Telangana, India

Lingampalli, 3-4-343, Baghlingmpally Cross Rd, Barkatpura,
Kachiguda, Hyderabad, Telangana 500027, India

Lat 17.393458° Long 78.494726°
26/03/2025 01:03 PM GMT +05:30

Virtual Reality - Presenting

MOLECULAR DOCKING

Docking refers to a computational scheme that tries to find the best binding orientation between any two molecules (i.e., a receptor and a ligand where the starting point is the atomic coordinates of the two molecules). A Receptor may be a Protein, Nucleic acid, and a ligand may be a small molecule, biomolecule (peptide, polypeptides, proteins or nucleic acids) and macromolecules.

Receptor + Ligand → Ligand Bound to protein or receptor

Protein + Ligand → Protein-Ligand Complex

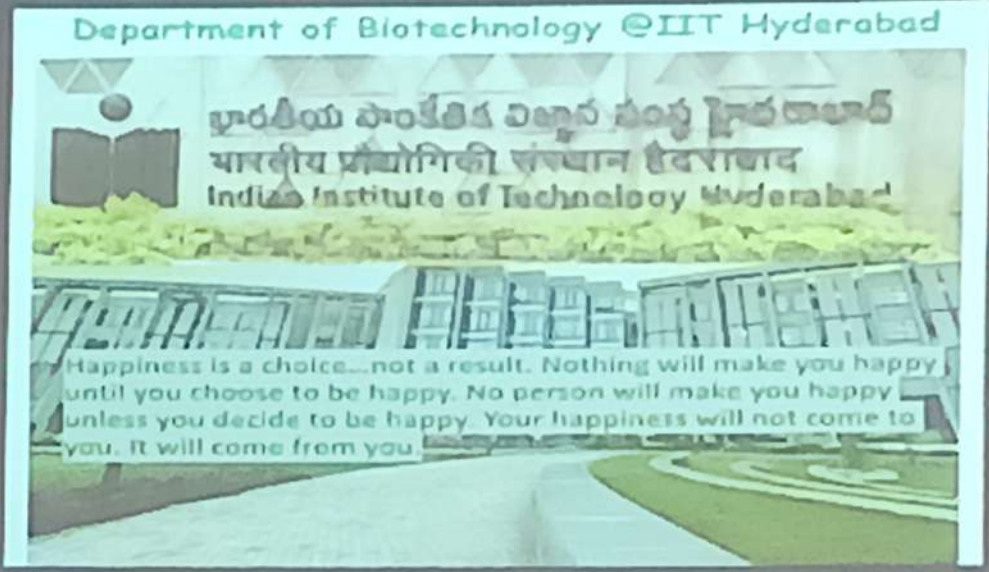


Check In

Hyderabad, Telangana, India
 Lingampalli, 3-4-343, Baghlingmpally Cross Rd, Barkatpura,
 Kachiguda, Hyderabad, Telangana 500027, India
 Lat 17.39344° Long 78.494705°
 25/03/2025 10:46 AM GMT +05:30

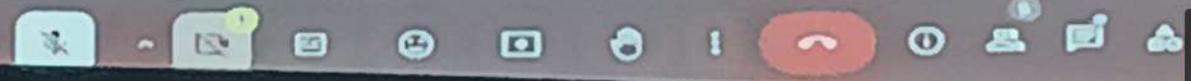


Marshari Basty (Presenting)

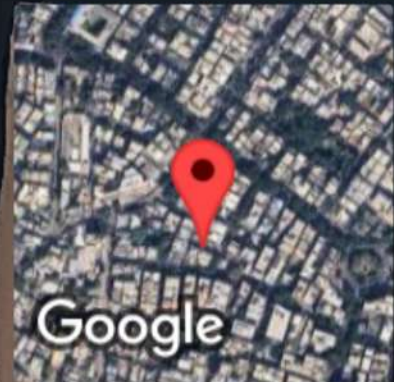


Activate Windows
Go to Settings to activate Windows.

12:39 PM | app-gd...



GPS Map Camera



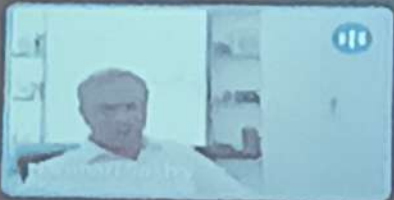
Hyderabad, Telangana, India

3-4-335, Barkatpura, Kachiguda, Hyderabad, Telangana 500027, India
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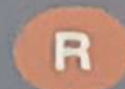


N Narehari Sastry (Presenting)

Centre for Molecular Modeling Group @CSIR-IICT



Tulasi Ram

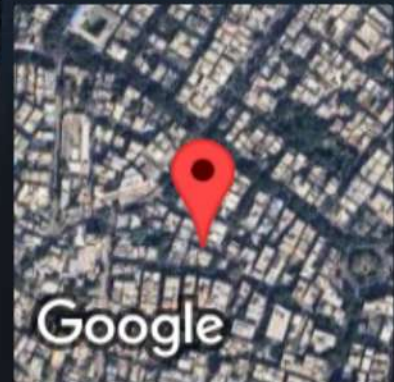


Active Windows

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Google

Hyderabad, Telangana, India

3-4-335, Barkatpura, Kachiguda, Hyderabad, Telangana 500027, India
Lat 17.393518° Long 78.494965°
24/03/2025 12:39 PM GMT +05:30



N Narehari Sastry (Presenting)

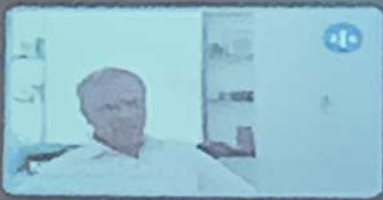
Artificial Intelligence and Industry 5.0

Fundamental

1. Genesis of Artificial Intelligence
2. Industry 3.0 and Beyond
3. Probability and Statistics
4. Artificial Neural Networks
5. Machine Learning: Principles and Concepts
6. Supervised and Unsupervised Learning
7. Deep Learning
8. CNN and RNN
9. Pattern Recognition and Feature Recognition
10. Natural Language Processing
11. Metaheuristic Algorithms

Applications

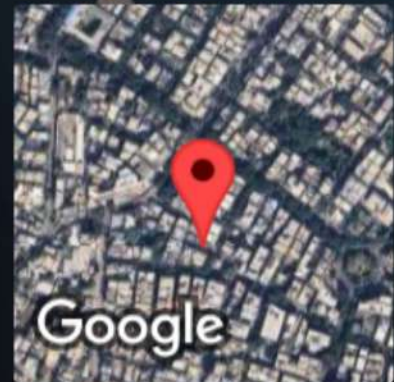
1. AI in Natural Sciences
2. AI in Cheminformatics and Bioinformatics
3. AI in Healthcare, Medicine and Pharmacy
4. AI in Drug Discovery
5. AI for Environment and Climate Change



12:37 PM | epp-gd...



GPS Map Camera



Hyderabad, Telangana, India

3-4-335, Barkatpura, Kachiguda, Hyderabad, Telangana 500027, India
 Lat 17.393523° Long 78.495018°
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