



**SRI G.V.G VISALAKSHI COLLEGE FOR WOMEN**  
Udumalpet, Tamilnadu, India  
Autonomous - Affiliated to Bharathiar University  
Accredited at 'A+' Grade by NAAC (Fourth Cycle)  
An ISO 9001:2015 Certified Institution  
**DEPARTMENT OF CHEMISTRY**



## Report

### Guest Lecture on

### Molecular Docking and Cheminformatics

Date: 25.09.2021

Time: 02.00 pm-03.00pm

Mode: Online Platform

Google Meet: <https://meet.google.com/ime-cbhv-tno>

No. of Beneficiaries: 84

**Resource Person : Dr. P. Lalitha**  
Associate Professor  
Department of Chemistry  
Avinashilingam Institute for Homescience and Higher  
Education for Women, Coimbatore



The Programme started with Welcome address and resource person introduction delivered by Dr.S.Umadevi, Assistant Professor of chemistry. The resource person Dr.P Lalitha, Associate

Professor, Avinashilingam Institute for Homescience and higher Education for Women, Coimbatore gave an excellent lecture on “Molecular Docking and Cheminformatics”. Some of the topics discussed under this lecture Programme includes

- i) Development of anti-inflammatory drug Piroxicom
- ii) Bioinformatics and Cheminformatics
- iii) Insilico methods of drug discovery
- iv) Molecular Docking
- v) Computer representations of chemical structures
- vi) Wiswesser line notation
- vii) Molinspiration software

The concepts were well explained with case study reports and students cleared their doubts with vibrant interactions. The programme came to an end with Vote thanks by Dr.M Indrani, Assistant Professor, Department of Chemistry.

The screenshot displays a Google Meet window with a shared screen of the Molinspiration website. The website shows the calculation of bioactivity scores for the molecule O-Terphenyl (SMILES: c3ccc(c1ccccc1c2ccccc2)cc3). The interface includes a chemical structure diagram and a table of bioactivity scores.

Molinspiration bioactivity score v2018.03	
GPCR ligand	0.02
Ion channel modulator	-0.90
Kinase inhibitor	0.04
Nuclear receptor ligand	-0.06
Protease inhibitor	-0.06
Enzyme inhibitor	0.12

The meeting interface shows Dr. P. Lalitha Chemistry Avinashilingam as the presenter. The participant list includes K.Ranjitha III C..., Dr. P. Lalitha C..., J.SIVASELVI III ..., Nandhini G III B..., Bhavana.A III c..., Chitradevi R, Kalai Nevi, 52 others, and You. The meeting time is 3:07 PM on 25-09-2021.

Meet - ime-cbhv-tno

meet.google.com/ime-cbhv-tno?pli=1&authuser=0

Dr. P. Lalitha Chemistry Avinashilingam

3:16 PM | ime-cbhv-tno

34°C Mostly sunny 15:16 25-09-2021

Meet - ime-cbhv-tno

meet.google.com/ime-cbhv-tno?pli=1&authuser=0

Dr. P. Lalitha Chemistry Avinashilingam is presenting

## Molecular Docking

- Docking is the computational determination of binding affinity between molecules (protein structure and ligand).
- Given a protein and a ligand find out the binding free energy of the complex formed by docking them.

2:51 PM | ime-cbhv-tno

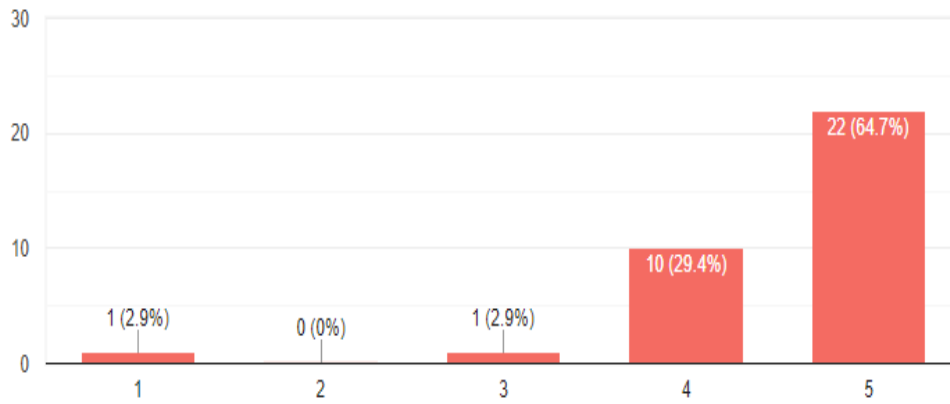
35°C Partly sunny 14:51 25-09-2021

## Feedback

Feedback Link : <https://forms.gle/vFdqFWgzLuefFzjE6>

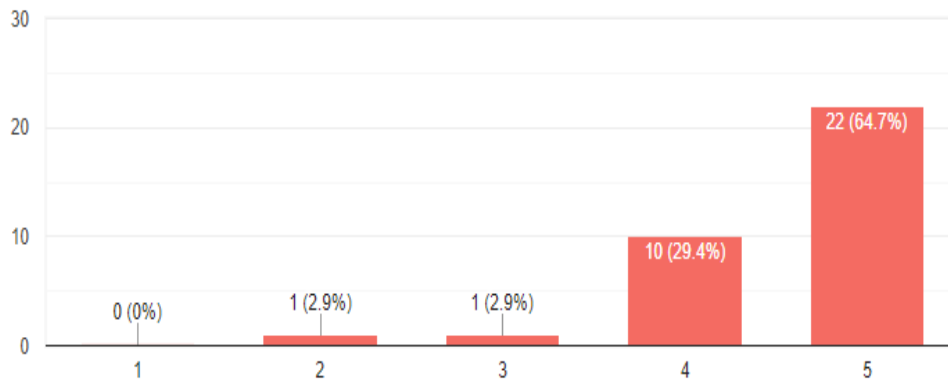
### Content Covered useful material

34 responses



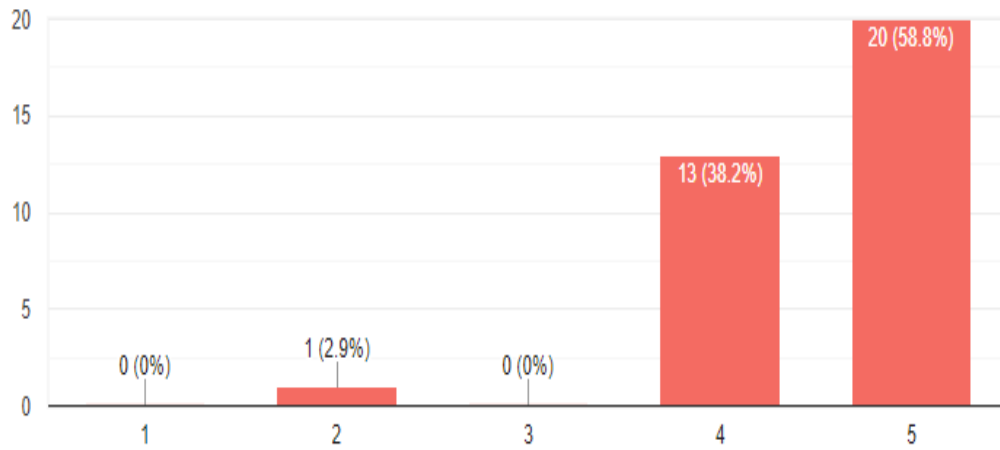
### Well organized content

34 responses



### Instructor facilitated interactions among participants well

34 responses



### Overall, how would you rate this Guest Lecture?

34 responses

