

## **Report of molecular docking dynamics in the drug discovery process workshop.**

Molecular docking dynamics in the drug discovery process workshop was organized by the Department of Biochemistry in Mount Carmel College on 11th and 12th November 2021. The speaker was Mr. Poojith N Rajendran, he is working as an assistant professor in the field PG diploma in Bioinformatics in JSS Academy of Higher Education and Research in Mysuru. It was a two day workshop where sir spoke about the introduction of Bioinformatics and drug discovery.

On day one sir explained that Drug discovery is a method of finding the treatment or cure of a disease or condition by knowing its origin, causes, symptoms, mode of transmission, incubation period. The two molecules which are required for drug discovery are Target and Drug molecules and the region of an enzyme where the substrate bind is determined by CASTp. Molecular docking is a key tool for drug design and study of how two or more molecules fit together by predicting the structure database of a target by other tools like Homology Modeling, Protein data bank, and Uniprot. The Ligand is designed by following rules like octet rule, valence electron, valency, atoms and electronic configuration by using Chem Sketch and ZINC15 database. After designing, ligand must undergo an ADMET testing to investigate all of the properties of a potential drug.

On day two sir explained about molecular docking, dynamics and interpretation of Hexokinase - 2 Deoxy D Glucose interaction studies Autodock, Pymol discovery with respect to cancer cells. 2 Deoxy D Glucose competes with glucose and can competitively inhibit glycolysis by binding to hexokinase and converts to 2 deoxy d glucose 6 phosphate which inhibits cell growth and death of cancer cells and the tool used for docking is Autodock database which shows the crystal structure with active site amino acid sequence was visualized. The physical movements of atoms and molecules can be analyzed to give a view of dynamic evolution of a system which can be represented in a graphical view by using RMSD, RMSF.



**Mount Carmel College, Autonomous**  
No.58 Palace Road, Bengaluru – 560 052.  
(Re-accredited with a A+ Grade (4<sup>th</sup> cycle) by NAAC)



**WORKSHOP**  
Organized by  
Department of Biochemistry

**Topic : Molecular Docking, Dynamics In Drug Discovery Process**

**SPEAKER :**

**Mr. Poojith Rajendran**

Assistant Professor, Online Learning- PG Diploma in Bioinformatics  
(eVBAB, MEA, Govt. of India)  
Centre for Distance and Online Education  
JSS Academy of Higher Education and Research  
Mysuru-570015  
Karnataka, INDIA




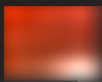
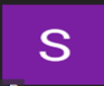
**Patronised  
by  
Dr. Sr. Arpana  
Principal,  
Mount Carmel College.**

**Date : 11<sup>th</sup> & 12<sup>th</sup> Oct 2021**  
**Time: 11.00am – 1.00pm**

Joining link :  
<https://us02web.zoom.us/j/84122117046?pwd=VWthaCtzZlVsQ3Rhbk55ak5uWVhSQ09>

Zoom Meeting

Recording

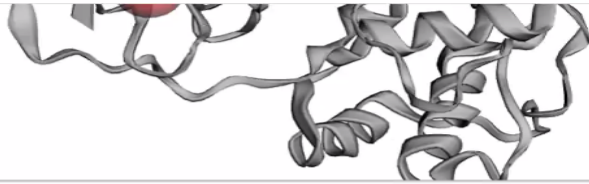
 Poojith N Rajendran	shlini p shlini p	 MANSI M JAIN	Shruti Shruti
Aditi Jain Aditi Aditi Jain Aditi	BHAVYA.M BHAVYA.M	Meghna Oraganti Meghna Oraganti	Gayathri K S Gayathri K S
Sahana Kamaraj Sahana Kamaraj	Raksha Harish Raksha Harish	Navya Navya	Gayathri KM Gayathri KM
Sheetal k Sheetal k	 Shilpa R	Viola Pinto Viola Pinto	sowmya sowmya
Rebecca Finny Rebecca Finny	Apeksha Rao H Apeksha Rao H	Devangna Paul Devangna Paul	Amrutha Shastr... Amrutha Shastry Padaru

You are viewing Amrutha Shastry Padaru's screen

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Chain	Residue	Sequence
1	A	
1	A	
1	A	
1	A	

### Sequence ?

Chain A

SGFRKMAFPSPGKVEGCMVQVTCGTTTLNGLWLDDDVVYCPRHVICTSED  
 RKSNNHNFVLQAGNVQLRVIGHSMQNCVLKLLKVDATANPKTPKYKFVRIQ  
 NGSPSGVYQCAMRPNFTIKGSFLNGSCGSGVGFNIDYDCVSFCYMHME  
 EGNFYGPFDVDRQTAQAAGTDTTITVNVLAWLAAVINGDRWFLNRFIT  
 YNYEPLTQDHVDILGPLSAQTGIAVLDMCASLKEELLQNGMNGRTILGS  
 VVRQCSCSGVTTFQ

Chain C

AVL

Zoom Meeting

Recording

1/2

Participants: 31

Chat: 42

Share Screen

Record

Reactions

Mute My Audio (Alt+A)

Participants:

- Poojith N Rajendran
- shlini p
- Rebecca Finny
- Shilpa R
- Hamsa
- Meghna Oraganti
- Apeksha Rao
- Sheetal k
- sowmya
- Maryam Arif
- Shruti
- Gayathri K S
- Aditi Jain Aditi
- Devangna Paul
- Sahana Kamaraj
- BHAVYA.M
- Medeline Joseph
- Bibi Hajira
- Indhu Sakthi
- Navya