

**STATE LEVEL FDP**  
**ON**  
**“MOLECULAR DOCKING STUDIES IN DRUG DISCOVERY”**  
**ON 10-03-23**

**Organized by**  
**Department of Chemistry (Under Graduate & Post Graduate)**  
**&**  
**Department of Biotechnology**  
**Government Degree College for Women (A), Begumpet,Hyd**

The department of Chemistry and Biotechnology of Government Degree College for Women (A), Begumpet, Hyd organized a one day State level Faculty Development Programme on Molecular Docking studies in Drug Discovery on 10-03-2023. Total 75 faculty members from various colleges of Telangana have been registered and participated in the programme.

**About the FDP**

This FDP is a capacity building for science lecturers in computational applications of Chemistry & Biochemistry using Molecular modeling to obtain a new approach in drug design processes. Drawing and visualizing three dimensional structure of molecules and calculating their Physico-Chemical & Biological properties are the most valuable information to the pre-experimental work. Present FDP will provide a basic platform to the faculty and postgraduate students to attain an immense knowledge in the field of Drug discovery using molecular docking approaches, which can be disseminated to the students by the trained lecturers.

**Objectives of FDP**

- ✓ Introduction to Computer aided drug discovery.
- ✓ Introduction to Molecular Docking.
- ✓ Introduction to Biological databases (PUBMED, RCSB)
- ✓ Working with MGL Tools
- ✓ Molecular docking with Autodock
- ✓ Visualizations & Docking Analysis (PYMOL).
- ✓ Hands on session on Molecular Docking.

- ✓ Demonstration of UV-VIS Spectrophotometer

### Program Schedule

9:00am-9:30am	<b>Registration</b>
<i>Session-1: 9.30am-10:15am</i>	<i>Inaugural session</i>
10:15-10.30am	Tea break
<i>Session-2: 10:30am-11:45 pm</i>	<b>Introduction on Molecular Docking and Databases</b> Speaker: Dr. <u>Purushotham Uppula, Director, Qstatix Pvt.Ltd.</u>
<i>Session-3: 11:45-1:00pm</i>	<b>Demonstration on Molecular docking using <u>Autodock</u></b> Speaker: Dr. <u>Karunakar Tanneeru, Director, Qstatix Pvt.Ltd.</u>
<b>1:00-1:45pm</b>	<b>Lunch Break</b>
1.45-2.00pm	Demonstration on UV-VIS Spectrophotometer
<i>Session-4: 2:00-3:30pm</i>	<b>Hands-on session on Molecular docking with <u>Autodock</u></b> By Dr. <u>Purushotham Uppula, Director, Qstatix Pvt.Ltd.</u>
3:30pm-3:45pm	Tea Break
<i>Session-5: 3:45-5.00pm</i>	<b>Hands-on session on Molecular docking with <u>Autodock</u></b> By Dr. <u>Karunakar Tanneeru, Director, Qstatix Pvt.Ltd.</u>
5:00-5.15pm	Valedictory

#### RESOURCE PERSONS

- 1.Dr. Purushotham Uppula, Director, Qstatix Pvt.Ltd.,Hyd
- 2.Dr. Karunakar Tanneeru, Director, Qstatix Pvt.Ltd.,Hyd

**Inaugural session:**

Principal, Prof.K.Padmavathi, Chief Guest and keynote speaker **Prof. Vijjulatha, Principal and First Incharge Vice Chancellor of Telangana Mahila Viswavidyalayam,** Vice principal Dr.Vasuda, PGcoordinator Dr.katoori sreenivas , Convener Dr.G.Pranitha, Resource persons from Qstatix Pvt.Ltd Dr.karunakar and Dr. purushotham and faculty members of various colleges of telangana have graced the occasion.



**Principal, Convener and faculty of GDCW,Begumpet were receiving the chief Guest**



**Inviting all the Guests to the Dias**

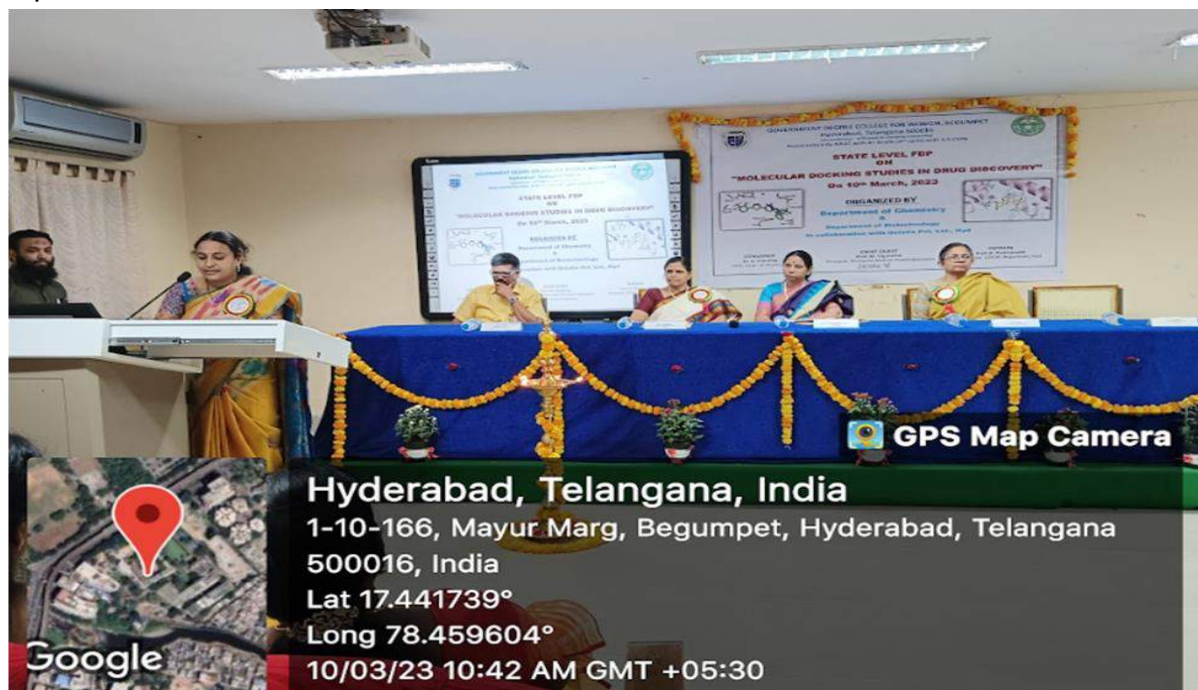




**Lightening of the lamp by the Dignitaries and followed by prayer song by P.Sowmya,B.Sc MPC III year**



Welcome Address by the Program Convener, HOD of the Department of Chemistry Dr. G. Pranitha about the importance of Faculty development programme on Molecular Docking Studies in recent trends in Drug Discovery and gave a brief introduction of College and department and also addressed achievements of the college and department.



Principal addressed the gathering



**Prof. Vijjulatha** , Principal and First incharge Vice Chancellor of Telangana Mahila Viswavidyalayam delivered keynote address on importance of molecular docking in computational design and synthesis of novel drug like molecules having high potency towards inhibition of disease causing proteins and finding drug-receptor interactions using Molecular Docking studies. Madam also discussed the selection process of ligand and receptors and docking applications by taking one example.



Felicitation was done to the Chief Guest Prof. Vijjulatha , Principal and First incharge Vice Chancellor of Telangana Mahila Visvavidyalayam by Principal and Chemistry faculty of GDCW(A), Begumpet, Hyd.







**Session-1:** Dr. Purushotham was delivering lecture on Introduction on Molecular Docking and Databases



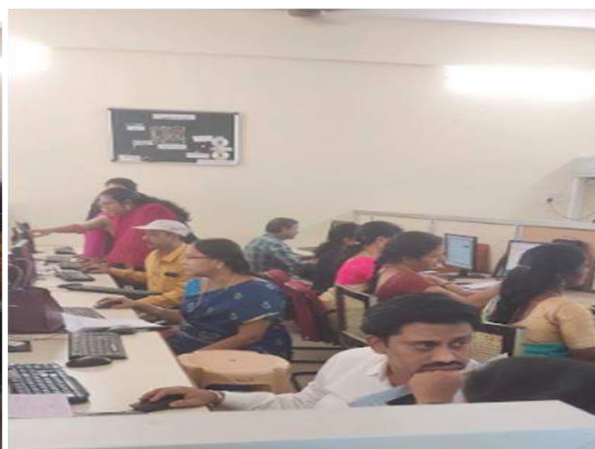


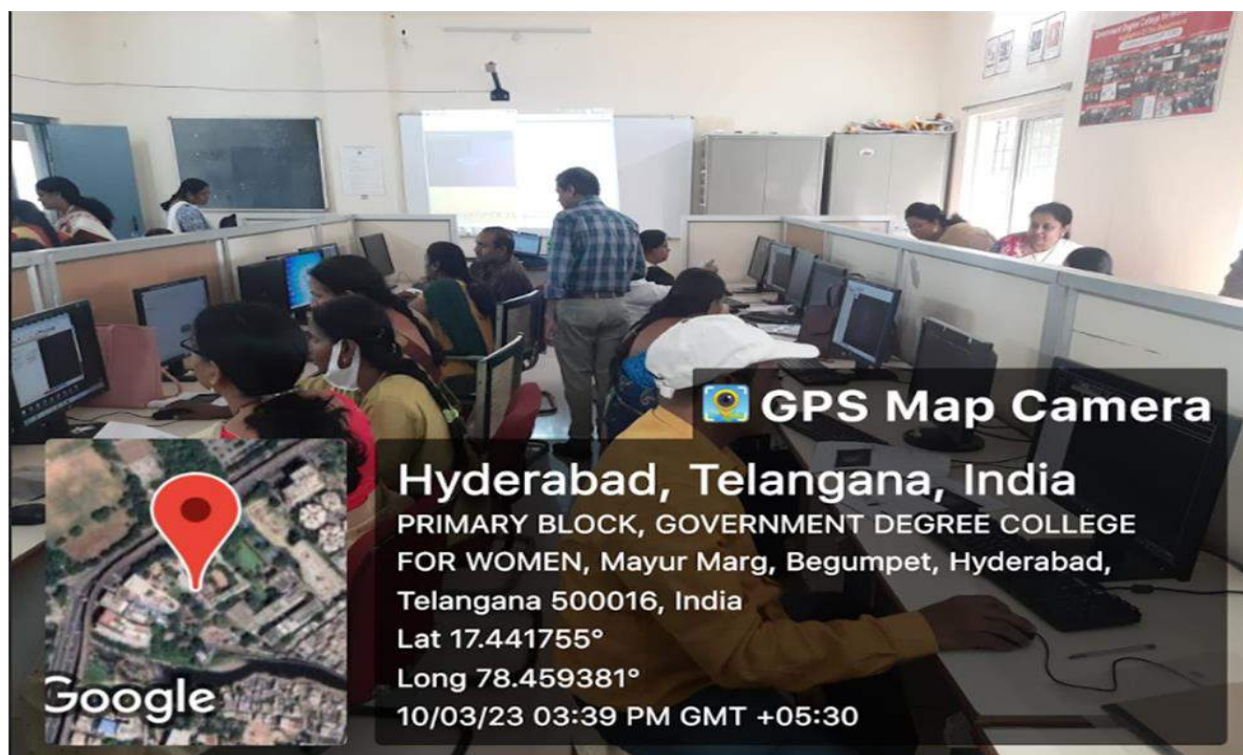
**Session-2:** Dr. Karunakar Tanneeru was demonstrating on Molecular Docking and Databases using Autodock and MGL Tool.



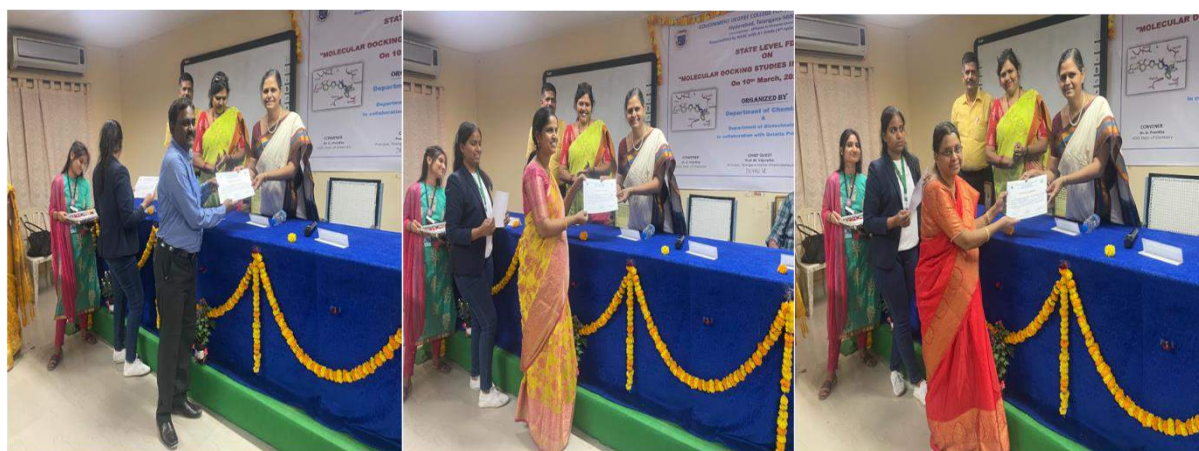


**Session 3:** Demonstration on UV-VIS Spectrophotometer by B.Sc Final Year students and faculty interacting with the students and appreciated for their way of demonstration.





**Session 4 & 5:** Hands-on session on Molecular docking with Autodock (Hands-outs provided to the participants for Hands-on training on Molecular docking with Autodock) By Dr. Purushotham & Dr. Karunakar. All the participants very actively participated in Hands on session, cleared their doubts by interacting with resource persons and submitted given assigned tasks.



**Valedictory:** Distribution of certificates to the participants by Principal, IQAC Coordinator, PG Coordinator and Convenor.



N.Shravani, Asst. Prof. of Chemistry, Tara Government College (A), Sangareddy gave very good feedback about the FDP, learning tools during the hands-on session. Overall very good feedback received from participants.



**Participants with principal**

## డ్రగ్స్ డిస్కవరీపై శాస్త్రీయ చర్య వేదిక

బేగంపేట, న్యూసెంటుడే: బేగంపేట లోని ప్రభుత్వ మహిళా డిగ్రీ కళాశాలలో శుక్రవారం తెమిస్ట్రీ, బయో టెక్నాలజీ విభాగాల ఆధ్వర్యంలో 'మాలిక్యులర్ డాకింగ్ స్పెషిస్ ఇన్ డ్రగ్ డిస్కవరీ' అంశంపై శాస్త్రీయ చర్యవేదిక నిర్వహించారు. తెలంగాణ మహిళా విశ్వవిద్యాలయం డన్ ఛార్జి వైస్ ఛాన్సలర్ ప్రొఫెసర్ విజ్జలత కార్యక్రమానికి ముఖ్యఅతిథిగా హాజరయ్యారు. ఆమె మాట్లాడుతూ మానవాళికి ఉపయోగపడేలా ఔషధ తయారీ రంగంలో మరిన్ని పరిశోధనలు, శాస్త్రీయ చర్యలు అవసరమన్నారు. టార్గెట్ మాలిక్యులర్, సింథసిస్ పేటెంట్ మాలిక్యులర్స్ అంశాలపై కళాశాల విద్యార్థినులకు అవగాహన కల్పించారు. డాకింగ్ స్పెషిస్ ప్రాముఖ్యత వివరించారు. ఈ కార్యక్రమంలో కళాశాల ప్రెసిడెంట్ డా.కె.పద్మావతి, డా.వి.ప్రదీప్, డా.కె.వెంకటేశ్వర్లు, వి.రోహిణి తదితరులు పాల్గొన్నారు.



**చర్య వేదికను జ్యోతి వెలిగించి ప్రారంభిస్తున్న విజ్జలత, చిత్రంలో డా.కె.పద్మావతి తదితరులు**



(c) eenad

## Registered participants list

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