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REF/MSRCASC/CHEM/BIOCHEM/2025

Date 15.03.25

CIRCULAR

Department of Chemistry and Biochemistry (UG)

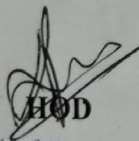Department of Chemistry and Biochemistry (UG) is organizing Value added programme on **"Drug Design Active Site Prediction"** Invitro and Insilico approach Under **DBT star college scheme for IV sem BSc students C sec** on 24/03/25 to 27/03/25,in collaboration with **Insearch laboratory ,Kammanahalli, Bengaluru.**

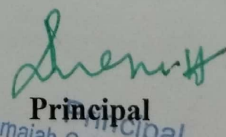**Attendance is Mandatory for all students**

Time: 11:00AM to 2:00PM

Venu: Kuvempu Seminar Hall

Coordinator: Mrs Ramya Kumari B S

HOD
Head of the Department
CHEMISTRY / BIO-CHEMISTRY
M.S. Ramaiah College of Arts,
Science & Commerce
Bangalore - 560 054

Principal
M.S.Ramaiah College of Arts, Science &
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MSRIT POST, MSR Nagar
Bengaluru - 560 054

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Date: 15/03/25

To

The Principal
M S Ramaiah College of Arts Science and Commerce
Bengaluru-54

From
Ramya Kumari B S
Assistant Professor & HOD (UG)
Department of Chemistry and Biochemistry
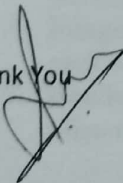M S Ramaiah College of Arts Science and Commerce
Bengaluru-54

Respected Madam

Sub: Seeking permission to conduct Value Added Programme for IV sem C sec Students from 24/03/25 to 27/03/25
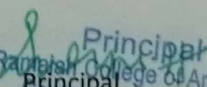
With reference to subject mentioned above requesting you to give permission to conduct Value added programme on **Drug Design Active Site Prediction" Invitro and Insilico approach** for IV sem BSc Biochemistry students(C Sec) from 24/03/25 to 27/03/25.The programme schedule is mentioned below

Sl.No	Date	Time	Programme	Venu
1	24/03/25	11:00am to 02:00pm	Inauguration and Theoretical Knowledge to students	Kuvempu seminar hall
2	25/03/25	9:30am to 3:30pm	Hands on training	Insearch Lab Kammanahalli
3	26/03/25	9:30am to 3:30pm	Hands On training	Insearch Lab Kammanahalli
4	27/03/25	10:00am to 1:00pm	In silicon work hands on	Digital Lab-Library
5	27/03/25	2:00pm to 3:30pm	Valedictory	Viswesvaraiaya Auditorium

Note: Transportation is booked for two days that is on 25/03/25 and 26/03/25

Thank You

Principal
M.S.Ramaiah College of Arts, Science &
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Bengaluru - 560 054

Department of Chemistry and Biochemistry

Report on

Value Added Programme   "Drug Design Active Site Prediction:

In Vitro and In Silico Approaches"

Date: 24/03/25 to 27/03/25

Duration: 30hrs

Paticipants: IV sem BSc Students C Sec -40students

Introduction

Drug design and discovery are integral processes in modern medicine, aimed at identifying novel therapeutic agents to combat various diseases. A crucial step in drug design is the identification and analysis of the active site of a protein, as the drug must interact with this site to exert its therapeutic effects. This Value Added Programme (VAP) focuses on two major approaches for active site prediction and drug design: **In Vitro** and **In Silico** methods.

- **In Vitro**: Refers to experimental techniques performed in a controlled environment outside a living organism.
- **In Silico**: Refers to computational methods used to simulate biological processes, predicting the structure and function of biological molecules.

The combination of these two approaches allows for a comprehensive and efficient strategy in drug discovery, significantly reducing the time and cost involved in the process.

Programme Objectives

1. **Understand Drug Design Fundamentals**: To provide students with a fundamental understanding of drug design and the significance of active sites in drug interactions.
2. **Explore In Vitro Techniques**: Introduce experimental laboratory-based methods used to predict and study protein active sites.
3. **Explore In Silico Approaches**: Train students in using computational tools and techniques to predict active sites and drug-binding interactions.
4. **Integrate Both Approaches**: Show how in vitro and in silico techniques complement each other in the drug design process.
5. **Hands-On Learning**: Provide students with practical exposure to both in vitro and in silico methods through demonstrations, case studies, and exercises.

Program Structure

The programme was divided into two major parts: theoretical learning and practical exposure, with a blend of laboratory and computational activities.

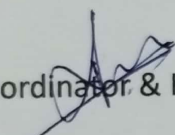# Part 1: Introduction to Drug Design and Active Site Prediction

1. **What is Drug Design?**
   - Drug design involves the identification of a molecule that interacts with a specific biological target, usually a protein or receptor, to elicit a desired biological effect.
   - The active site of a protein is the specific region where the drug molecule binds. Predicting this site is essential for effective drug design.
2. **Importance of Active Site Prediction**
   - Active site prediction allows scientists to identify potential drug targets by locating binding sites where drug molecules can interact with proteins.
   - Knowing the structure of the active site helps in designing drugs with higher specificity and efficacy while reducing side effects.
3. **In Vitro Techniques for Active Site Prediction**
   - **X-ray Crystallography**: Provides high-resolution 3D structures of proteins and their binding sites.
   - **NMR Spectroscopy**: Used to determine the structure of proteins in solution and their interactions with ligands.
   - **Enzyme Activity Assays**: Measures the biological activity of enzymes to infer the functional regions, including active sites.
4. **In Silico Techniques for Active Site Prediction**
   - **Molecular Docking**: A computational method that simulates the interaction between a drug molecule and its target protein, predicting binding affinity and active site.
   - **Molecular Dynamics (MD) Simulations**: Used to study the conformational changes in proteins and to predict binding sites through the simulation of protein-ligand interactions.
   - **Homology Modeling**: Predicts the 3D structure of a protein based on the known structure of a homologous protein and is useful in predicting active sites.
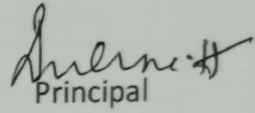
Part 2: In Vitro Approach - Practical Exposure

1. **Laboratory Session 1: Protein Purification**
   - Objective: To purify a target protein and identify its potential active site.
   - Methods: Students were introduced to protein extraction, purification, and confirmation through SDS-PAGE.

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The Value Added Programme on "Drug Design Active Site Prediction: In Vitro and In Silico Approaches" was successful in providing BSc students with a comprehensive understanding of drug discovery techniques. By integrating both experimental and computational methods, students gained a holistic view of how drug design processes work in real-world settings. The programme encouraged students to appreciate the significance of active site prediction in the design of effective drugs and equipped them with essential skills for future academic and professional endeavors in the field of pharmacology, biochemistry, and computational biology.

This report summarizes the key components and outcomes of the programme, ensuring that the students were well-prepared to explore the rapidly evolving field of drug design.

Coordinator & HOD

Ramya Kumari B S

Principal

Principal
M.S.Ramaiah College of Arts, Science &
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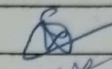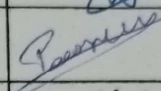MSRIT POST, MSR Nagar
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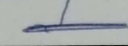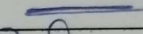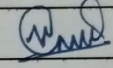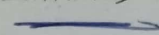Recognized by UGC under 2F & 12B of UGC act 1956

Department of Chemistry and Biochemistry

Value Added Programme on **Drug Design Active Site Prediction"** Invitro and Insilico **approach** for IV sem BSc students **("C" Sec) from 24/03/25 to 27/03/25.**

Attendance Sheet (24/03/25)

Sl.No	Register Number	Students Names	Signature
1.	U18EV23S0066	PRIYA.N	Priya.N
2.	U18EV23S152	KOKILA .G	Kokila G.
3.	U18EV23S0080	S HAREESH BALAJI	Hareesh
4.	U18EV23S0187	ANAQHA PRAVIN	Anagha
5.	U18EV23S0383	PAVITHRA R	Pravi
6.	U18EV23S0060	KUSHI D B	
7.	U18EV23S0392	K M CHINNAMBIKHA	Chinnambikha
8.	U18EV23S0069	MONIKA	Monika .P
9.	U18EV23S0068	TEJASHREE S	T
10.	U18EV23S0067	INDHUJA U	Indhuja.U
11.	U18EV23S0065	DEVIKA V	Vevka.
12.	U18EV23S0088	BHANUSHREE H R	
13.	U18EV23S0134	AKKA MAHADEVI D	madhu
14.	U18EV23S0053	SHAILAJA ANANDA KUMAR	Shijsk
15.	U18EV23S0058	SUFYAN AHMED K	Sufyan
16.	U18EV23S0102	KALLURI SURYA SRIKAR	K.Surya Srikar
17.	U18EV23S0086	YUVIKA SARIN	yuvika
18.	U18EV23S0380	MOHITHA SUSHMA SRI K	Sushma.
19.	U18EV23S0061	BHUSHAN B	Bludy
20.	U18EV23S0131	ARKAPRABHA DEB	Arley
21.	U18EV23S0184	C THANUJA	Thanuja
22.	U18EV23S0077	AISHWARYA S V	AishyaSV
23.	U18EV23S0078	BIDHISHA DAS	
24.	U18EV23S0085	VAISHNAVI	Vaishnavi

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		GANAPATI HEGDE	
25.	U18EV23S0087	TANUSHREE R	Tanushree . R
26.	U18EV23S0084	SHRIYA GEJJEHALLI	
27.	U18EV23S0079	H M POORNA CHANDRA	
28.	U18EV23S0081	ARTHI S	Arthi S
29.	U18EV23S0083	GAUTHAM KUMAR GUPTA	
30.	U18EV23S0117	RAKSHITHA B R	Raku
31.	U18EV23S0151	SANJANA	Sanjana.L
32.	U18EV23S0062	AMINA NAUSHAD	
33.	U18EV23S0185	NAKSHATHRA K S	
34.	U18EV23S0057	VIBHASHREE M V SS	
35.	U18EV23S0059	SMAKSHI DAS	Smakshi Das
36.	U18EV23S0150	SHRUTHISEN GUPTA	

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Department of Chemistry and Biochemistry

Value Added Programme on **Drug Design Active Site Prediction"** Invitro and Insilico **approach** for IV sem BSc students(C Sec) from 24/03/25 to 27/03/25.

Attendance Sheet (25/03/25)   Batch-I

Sl.No	Register Number	Students Names	Signature
1.	U18EV23S0066	PRIYA.N	Priya.N
2.	U18EV23S152	KOKILA .G	Kokila G
3.	U18EV23S0080	S HAREESH BALAJI	Hareesh Balaji
4.	U18EV23S0187	ANAQHA PRAVIN	Anagha
5.	U18EV23S0383	PAVITHRA R	Papu
6.	U18EV23S0060	KUSHI D B	Kushi
7.	U18EV23S0392	K M CHINNAMBIKHA	Chinnam
8.	U18EV23S0069	MONIKA	Monika
9.	U18EV23S0068	TEJASHREE S	TJ
10.	U18EV23S0067	INDHUJA U	Indhujav
11.	U18EV23S0065	DEVIKA V	Vevika
12.	U18EV23S0088	BHANUSHREE H R	Bhanu.R
13.	U18EV23S0134	AKKA MAHADEVI D	Madhu
14.	U18EV23S0053	SHAILAJA ANANDA KUMAR	Shailaja
15.	U18EV23S0058	SUFYAN AHMED K	Sufyan
16.	U18EV23S0102	KALLURI SURYA SRIKAR	K.Surya Srikar
17.	U18EV23S0086	YUVIKA SARIN	Yuvika Sarin
18.	U18EV23S0380	MOHITHA SUSHMA SRI K	Sushma

Department of Chemistry and Biochemistry

Value Added Programme on **Drug Design Active Site Prediction"** Invitro and Insilico approach for IV sem BSc students(C Sec) from 24/03/25 to 27/03/25.

Attendance Sheet (26/03/25)   Batch-II

Sl.No	Register Number	Student Names	Signature
1.	U18EV23S0061	BHUSHAN B	Bhu
2.	U18EV23S0131	ARKAPRABHA DEB	Arkaprabha
3.	U18EV23S0184	C THANUJA	Thanuja
4.	U18EV23S0077	AISHWARYA S V	
5.	U18EV23S0078	BIDHISHA DAS	
6.	U18EV23S0085	VAISHNAVI GANAPATI HEGDE	Vaishnavi
7.	U18EV23S0087	TANUSHREE R	Tanushree.R
8.	U18EV23S0084	SHRIYA GEJJEHALLI	Shrija.
9.	U18EV23S0079	H M POORNA CHANDRA	Poorna
10.	U18EV23S0081	ARTHI S	Arthi
11.	U18EV23S0083	GAUTHAM KUMAR GUPTA	—
12.	U18EV23S0117	RAKSHITHA B R	Rakshitha
13.	U18EV23S0151	SANJANA	Sanja
14.	U18EV23S0062	AMINA NAUSHAD	—
15.	U18EV23S0185	NAKSHATHRA K S	—
16.	U18EV23S0057	VIBHASHREE M V SS	Vibhi
17.	U18EV23S0059	SMAKSHI DAS	Smaksh
18.	U18EV23S0150	SHRUTHISEN GUPTA	

U18EV23S0066   PRIYA N   Priya.N

U18EV23S0152   KOKILA G   Kokila.G.

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Department of Chemistry and Biochemistry

Value Added Programme on **Drug Design Active Site Prediction"** Invitro and Insilico approach for IV sem BSc students(C Sec) from 24/03/25 to 27/03/25.

Attendance Sheet (27/03/25)

Sl.No	Register Number	Students Names	Signature	Afternoon session
✓ 1.	U18EV23S0066	PRIYA.N	Priya N	Priya.N
✓ 2.	U18EV23S152	KOKILA .G	Kokila	kiku
3.	U18EV23S0080	S HAREESH BALAJI	S.H-tull	V.Haull
4.	U18EV23S0187	ANAQHA PRAVIN	Anaghy	Anaghu
5.	U18EV23S0383	PAVITHRA R	Ppari	Ppari
6.	U18EV23S0060	KUSHI D B	Kushi DB	Kushi
7.	U18EV23S0392	K M CHINNAMBIKHA	Chatube	Chatia
8.	U18EV23S0069	MONIKA	Monika	Monika
9.	U18EV23S0068	TEJASHREE S	Tet	If
10.	U18EV23S0067	INDHUJA U	Indhuja.U	Indhuja.U
11.	U18EV23S0065	DEVIKA V	Vevika	Vevika
12.	U18EV23S0088	BHANUSHREE H R	Bhanush R	Bhanush-R
13.	U18EV23S0134	AKKA MAHADEVI D	madhu	madhu
14.	U18EV23S0053	SHAILAJA ANANDA KUMAR	Selijak	Selijak
15.	U18EV23S0058	SUFYAN AHMED K	Sufyan	Sufyan
16.	U18EV23S0102	KALLURI SURYA SRIKAR	K.Surya Srikar	k. surya srikar
• 17.	U18EV23S0086	YUVIKA SARIN	yuvika	—
• 18.	U18EV23S0380	MOHITHA SUSHMA SRI K	—	—
• 19.	U18EV23S0061	BHUSHAN B	—	—
20.	U18EV23S0131	ARKAPRABHA DEB	Arkaprabha Deb.	Arkaprabha Deb
21.	U18EV23S0184	C THANUJA	Thanuja	Thanuja
22.	U18EV23S0077	AISHWARYA S V	Aishwarya SV	Aish SV
23.	U18EV23S0078	BIDHISHA DAS	Bidhisa Das	Bidhisa Das
24.	U18EV23S0085	VAISHNAVI	vaishnavi	vaishnavi

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Afternoon

		GANAPATI HEGDE	—	
✓ 25.	U18EV23S0087	TANUSHREE R	Tanushree	Tanushree
✓ 26.	U18EV23S0084	SHRIYA GEJJEHALLI		
✓ 27.	U18EV23S0079	H M POORNA CHANDRA	Poornachandra	Poornachandra
✓ 28.	U18EV23S0081	ARTHI S	Arthi S	Arthi S
✗ 29.	U18EV23S0083	GAUTHAM KUMAR GUPTA	—	—
▪ 30.	U18EV23S0117	RAKSHITHA B R	—	—
✓ 31.	U18EV23S0151	SANJANA	Sanjana .L	Sanjana.L
✗ 32.	U18EV23S0062	AMINA NAUSHAD	—	—
✗ 33.	U18EV23S0185	NAKSHATHRA K S	—	
✓ 34.	U18EV23S0057	VIBHASHREE M V SS		
✓ 35.	U18EV23S0059	SMAKSHI DAS		Smakshi Das
✗ 36.	U18EV23S0150	SHRUTHISEN GUPTA	—	—