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Affiliated to the Tamilnadu Dr. M.G.R. Medical University,
and The Directorate of Medical Education, Chennai.

REF.NO:SSIP/ REQ/2023/007 Date: 17/10/2023

From

Department of Pharmaceutical Analysis,

SS institute of pharmacy,

Sankari, Salem (DIST) - 637301.

To

The principal,

SS institute of pharmacy,

Sankari, Salem (DIST) – 637301.

Subject: Letter for requesting permission to conduct **ADD ON COURSE** -Reg.

Respected sir,

We are requesting you to grand permission to conduct add-on course in the seminar hall on **01/11/2023 to 08/11/2023**. We wish to conduct add on course on the title "**Computational Protein Modeling And Analytics".** This add-on course program would be a great opportunity for students to learn and that would help to shape the students.

Thanking you,

Yours truly,

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KUPPANUR (PO), SANKARI (TK).
SALEM - 637301

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KUPPANUR (PO), SANKARI (TK).
SALEM - 637301

JOTHIMANIVANNAN ESAVALU
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Date: 2024.10.01 11:14:53+05'30'

NH-544, Kuppanur (Po), Sankari (Tk), Salem (Dt) – 637301, Tamilnadu, India
Phone : 04283 241080 | E-mail : SSIPHARM@gmail.com | Website : www.ssip.edu.in

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33

DATE: 17/10/2023

CIRCULAR

This is to inform that will B.PHARM students have the schedule of following value - added course to be conducted by our SS Institute of Pharmacy and it as mentioned below.

COURSE NAME	SCHEDULE	DURATION	VENUE	RESOURCE PERSON
COMPUTATIONAL PROTEIN MODELING AND ANALYTICS	01/11/2023 to 08/11/2023	35 HOURS	SEMINAR HALL	ANITHA. B

All the above-mentioned students must enroll and actively participate in the course without fail.

Note: Certificates will be issued for the eligible students after completion of the course and examination.

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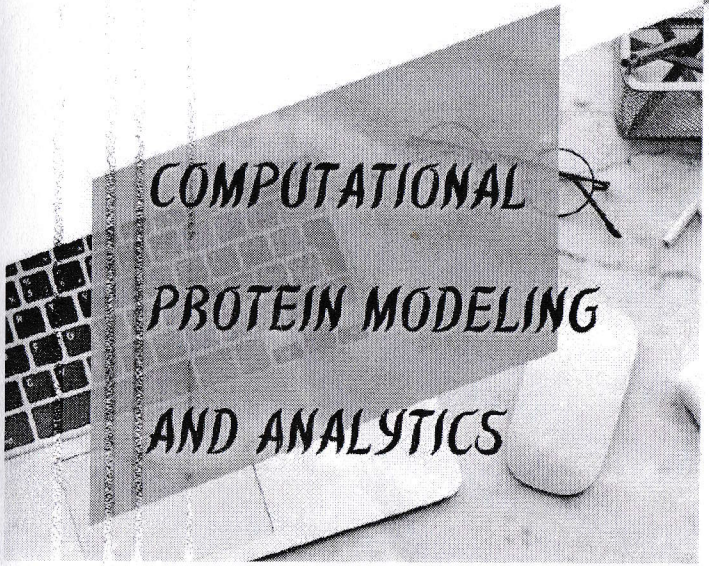
Phone : 04283 241080 | E-mail : [illegible]@gmail.com | Website : www.ssip.edu.in

- Protein Structure Prediction
- Molecular Dynamics(MD) Simulations
- Docking Studies
- Computational Mutagenesis
- Software and Algorithms
- Structural Bioinformatics
- MachineLearning in Protein Modeling



SS institute of pharmacy

Sankari, Salem

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RESOURCE PERSON

Mrs.B.Anitha. M.Pharm.,
Assistant professor,
Department of Chemistry

Contact Us

Phone:
9443026056

Email:
ssip1718@gmail.com

Address:
Manjakkalpatty, Sankari,
Salem - 637301.

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KUPPANUR (PO), SANKARI (TK),
SALEM - 637301

SS INSTITUTE OF PHARMACY ★ SANKARI

Venue : SSIP Seminar hall
Date :01/11/23-08/11/23
Time : 01.30pm - 04.30pm

SYLLABUS

COMPUTATIONAL PROTEIN MODELING AND ANALYSIS

Sl. No.	TOPIC	DATE
1	**Fundamentals of Protein Structure and Computational Methods** - Overview of Protein Structure and Function - Key Concepts: Primary, Secondary, Tertiary, and Quaternary Structures - Importance of Computational Methods in Protein Modeling	**1/11/2023**
2	**Techniques in Protein Structure Prediction** - Homology Modeling - Ab Initio Modeling - Threading and Fold Recognition - Comparative Modeling Techniques	**2/11/2023**
3	**Molecular Dynamics and Simulations** - Principles and Setup of Molecular Dynamics (MD) Simulations - Analyzing MD Simulation Data - Applications of MD in Protein Dynamics	**3/11/2023-4/11/2023**
4	**Protein Interactionand Docking Methods** - Techniques for Protein-Ligand Docking - Predicting Protein-Protein Interactions - Rigid and Flexible Docking Approaches - Scoring Functions and Validation	**6/11/2023-7/11/2023**
5	**Tools, Refinement, and Validation** - Structural Bioinformatics Tools and Databases - Protein Structure Refinement Techniques (Energy Minimization, Rosetta) - Validation and Quality Assessment Metrics (RMSD, Ramachandran Plot)	**8/11/2023**

RESOURCE PERSON:B.Anitha

TOTAL HOURS:35Hrs

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ADD ON / CERTIFICATE VALUE ADDED COURSES
ACADEMIC YEAR 2023-2024

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ACADAMIC YEAR 2023-2024

S.NO	NAME OF ADD ON CERTIFICATES PROGRAMS	COURSE CODE	NO OF STUDENTS ENROLLED	TYPE OF ADD ON CERTIFICATE PROGRAMS
1.	Advanced therapy topics in immunotherapy	23ATTI01	55	Self-framed course
2.	Green cell factories	23GCF02	58	Self-framed course
3.	Advanced techniques in enzymology .	23ATE03	70	Self-framed course
4.	Biomechanics and orthopaedic implants	23BOI04	58	Self-framed course
5.	Blockchain technology in pharmaceuticals	23BTP05	30	Self-framed course
6.	Cell designer modeling tool for gene-regulatory & biomedical networks	23CDMTGRBN06	27	Self-framed course
7.	Computational protein modeling and analytics	23CPMA07	59	Self-framed course
8.	Scientific writing in health research	24SWHR08	54	Self-framed course
9.	Systematic reviews for pharmacy health professionals	24SRPHP09	57	Self-framed course
10.	Advanced bioinformatics: Tools & applications	24ABTA10	111	Self-framed course
11.	Telemedicine: Principles & practices	24TPP11	58	Self-framed course

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ADD ON COURSE – ENROLLMENT LIST

NAME OF ADD ON COURSE : COMPUTATIONAL PROTIEN MODELING AND ANALYSIS

COURSE INSTRUCTORS : ANITHA.B

YEAR OFFERED : 3rd SEM B.PHARM

COURSE DURATION : 35 hrs

S.NO	NAME OF THE STUDENT	REGISTER NO	COURSE
1.	ABINESH. S	560021523501	2nd B.PHARM
2.	ABISHEK.B	560021523502	2nd B.PHARM
3.	ABISURYA .C	560021523503	2nd B.PHARM
4.	ANANDASIVAM.T	560021523504	2nd B.PHARM
5.	ANBU .R	560021523505	2nd B.PHARM
6.	ARAVINTH.M	560021523506	2nd B.PHARM
7.	ARCHANA.A	560021523507	2nd B.PHARM
8.	ARIVILKUMAR.P	560021523508	2nd B.PHARM
9.	ARUN .A	560021523509	2nd B.PHARM
10.	ARUN KUMAR .K	560021523510	2nd B.PHARM
11.	ARUNKUMAR.M	560021523511	2nd B.PHARM
12.	BALAMURUGAN.B	560021523512	2nd B.PHARM
13.	BATHRINATH.A	560021523513	2nd B.PHARM
14.	BOOPATHI.G	560021523514	2nd B.PHARM
15.	BOOPATHI.P	560021523515	2nd B.PHARM
16.	CHITHARTHA.M	560021523516	2nd B.PHARM
17.	DEVIPRIYA.K	560021523517	2nd B.PHARM
18.	DHATCHNAMOORTHI.K	560021523518	2nd B.PHARM
19.	DHIVYA.N	560021523519	2nd B.PHARM
20.	GAYATHRI.S	560021523521	2nd B.PHARM
21.	GOPIKA.K	560021523522	2nd B.PHARM
22.	GOPI.K	560021523523	2nd B.PHARM
23.	GURUMOORTHI.M	560021523524	2nd B.PHARM
24.	HARIPRIYA.K	560021523525	2nd B.PHARM
25.	JOTHIPRAKASH.P	560021523526	2nd B.PHARM
26.	KARTHICK KANNAN.J	560021523527	2nd B.PHARM
27.	KARTHICK.K	560021523528	2nd B.PHARM

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28.	KARTHIKEYAN.M	560021523529	2nd B.PHARM
29.	KAVIBHARATHI.S	560021523530	2nd B.PHARM
30.	KAVIYA .S	560021523531	2nd B.PHARM
31.	KESAVAN.P	560021523532	2nd B.PHARM
32.	KIRUBANIDHI.R	560021523533	2nd B.PHARM
33.	KIRUTHIKA.P	560021523534	2nd B.PHARM
34.	MEGALA.G	560021523535	2nd B.PHARM
35.	MOHAMMED KABEER.A	560021523536	2nd B.PHARM
36.	RANISH.G	560021523537	2nd B.PHARM
37.	SARAN MOHAN.R	560021523538	2nd B.PHARM
38.	SASIKALA.G	560021523539	2nd B.PHARM
39.	SATHYA JASMINE.A	560021523540	2nd B.PHARM
40.	SETHURAMAN.P	560021523541	2nd B.PHARM
41.	SOWMIYA.D	560021523542	2nd B.PHARM
42.	SRIGANTH.K	560021523543	2nd B.PHARM
43.	SUGASHINI.M	560021523544	2nd B.PHARM
44.	SUNDHAR.S	560021523545	2nd B.PHARM
45.	SURIYA.M	560021523546	2nd B.PHARM
46.	SYED ABDULLA.A	560021523547	2nd B.PHARM
47.	TAMILMANI.P	560021523548	2nd B.PHARM
48.	THIRUMALAI.R	560021523549	2nd B.PHARM
49.	THIRUMENINATHAN.M	560021523550	2nd B.PHARM
50.	UMA SHANKARI.E	560021523551	2nd B.PHARM
51.	VAITHEESWARI.V	560021523552	2nd B.PHARM
52.	VIGNESH.C	560021523553	2nd B.PHARM
53.	VIGNESH.S	560021523554	2nd B.PHARM
54.	VIJAYASARATHI.S	560021523555	2nd B.PHARM
55.	VIMAL.R	560021523556	2nd B.PHARM
56.	VINOTHINI.A	560021523557	2nd B.PHARM
57.	VISHALATCHI.K	560021523558	2nd B.PHARM
58.	YAZHINI.B	560021523559	2nd B.PHARM
59.	S.YUVAKIRUTHIGA	560021523560	2nd B.PHARM

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COURSE INSTRUCTORS : ANITHA.B

YEAR OFFERED : 3rd SEM B.PHARM

COURSE DURATION : 35 hrs

S.NO	NAME OF THE STUDENT	REGISTER NO	ATTENDANCE						
			1/11/23	2/11/23	3/11/23	4/11/23	6/11/23	7/11/23	8/11/23
1.	ABINESH. S	560021523501							
2.	ABISHEK.B	560021523502							
3.	ABISURYA .C	560021523503							
4.	ANANDASIVAM.T	560021523504							
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6.	ARAVINTH.M	560021523506							
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11.	ARUNKUMAR.M	560021523511							
12.	BALAMURUGAN.B	560021523512							
13.	BATHRINATH.A	560021523513							
14.	BOOPATHI.G	560021523514							
15.	BOOPATHI.P	560021523515							
16.	CHITHARTHA.M	560021523516							
17.	DEVIPRIYA.K	560021523517							
18.	DHATCHNAMOORTHI.K	560021523518							
19.	DHIVYA.N	560021523519							
20.	GAYATHRI.S	560021523521							
21.	GOPIKA.K	560021523522							
22.	GOPI.K	560021523523							
23.	GURUMOORTHI.M	560021523524							
24.	HARIPRIYA.K	560021523525							
25.	JOTHIPRAKASH.P	560021523526							

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26.	KARTHICK KANNAN.S	560021523527							
27.	KARTHICK.K	560021523528							
28.	KARTHIKEYAN.M	560021523529							
29.	KAVIBHARATHI.S	560021523530							
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32.	KIRUBANIDHI.R	560021523533							
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34.	MEGALA.G	560021523535							
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ADD ON COURSE	COMPUTATIONAL PROTIEN MODELING AND ANALYTICS
DEPARTMENT	PHARMACEUTICAL ANYALSIS
ACADEMIC YEAR	2023-2024
DATE	01/11/2023 to08/11/2023
VENUE	SEMINAR HALL
NAME: DHATCHANAMOORTHI .K	COURSE: D-YEAR

ANSWER ALL THE QUESTIONS: **DATE:08/11/2023**

MULTIPLE CHOICE QUESTIONS **MARKS:15**

13

1. Which technique is commonly used to predict the three-dimensional structure of a protein from its amino acid sequence?
   A) NMR Spectroscopy
   B) X-ray Crystallography
   C) Homology Modeling
   D) Mass Spectrometry

2. Which software tool is popular for protein structure prediction and refinement based on homology modeling?
   A) GROMACS
   B) SWISS-MODEL
   C) PyMOL
   D) Chimera

3. What is the primary goal of molecular docking in computational protein modeling?
   A) To predict the secondary structure of proteins
   B) To determine the interaction between proteins and potential ligands
   C) To analyze protein stability
   D) To visualize protein dynamics

4. Which computational approach uses energy minimization to refine protein structures and reduce steric clashes?
   A) Molecular Dynamics (MD)
   B) Homology Modeling
   C) Quantum Mechanics
   D) Energy Minimization

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5. Which database provides a comprehensive collection of experimentally determined protein structures?
   A) UniProt
   B) PDB (Protein Data Bank)
   C) SWISS-MODEL
   D) KEGG

6. What is the purpose of using molecular dynamics simulations in protein modeling?
   A) To predict protein sequence
   B) To observe the protein's behavior over time and under different conditions
   C) To determine the protein's crystal structure
   D) To identify protein-ligand binding sites

7. Which tool is widely used for visualizing and analyzing protein structures and their interactions?
   A) BLAST
   B) RCSB PDB
   C) PyMOL
   D) NCBI

8. In protein modeling, what does the term "secondary structure" refer to?
   A) The sequence of amino acids in a protein
   B) The 3D folding pattern of a protein
   C) Local structures like alpha-helices and beta-sheets
   D) The interaction between different protein subunits

9. Which software is used for performing energy calculations and molecular dynamics simulations?
   A) SWISS-MODEL
   B) AutoDock
   C) GROMACS
   D) BLAST

10. What does the term "homology modeling" refer to in computational protein modeling?
    A) Predicting protein structure from genetic data
    B) Predicting protein structure based on known structures of similar proteins
    C) Analyzing the interaction between proteins
    D) Visualizing protein-ligand interactions

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11. Which technique provides high-resolution structural information by determining the electron density of protein crystals?
    A) NMR Spectroscopy
    B) Cryo-EM
    C) X-ray Crystallography
    D) Mass Spectrometry

12. What does "protein-ligand docking" aim to achieve in computational studies?
    A) To determine the protein's tertiary structure
    B) To predict how a small molecule (ligand) binds to a protein
    C) To model protein-protein interactions
    D) To analyze protein sequence data

13. Which approach involves simulating the physical movements of atoms and molecules over time?
    A) Molecular Docking
    B) Homology Modeling
    C) Molecular Dynamics (MD)
    D) Energy Minimization

14. In computational protein modeling, what does the term "tertiary structure" refer to?
    A) The sequence of amino acids in a protein
    B) The folding pattern of alpha-helices and beta-sheets
    C) The overall 3D structure of a single polypeptide chain
    D) The interaction between different protein chains

15. Which method is used to determine the interaction and binding affinity between proteins and small molecules?
    A) Energy Minimization
    B) Molecular Dynamics Simulation
    C) Molecular Docking
    D) Homology Modeling

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DEPARTMENT	PHARMACEUTICAL ANYALSIS
ACADEMIC YEAR	2023-2024
DATE	01/11/2023 to08/11/2023

ANSWER KEY: **DATE:08/11/2023**

MULTIPLE CHOICE QUESTIONS **MARKS:15**

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   C) To analyze protein stability
   D) To visualize protein dynamics

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   C) Quantum Mechanics
   D) Energy Minimization

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   C) PyMOL
   D) NCBI

8. In protein modeling, what does the term "secondary structure" refer to?
   A) The sequence of amino acids in a protein
   B) The 3D folding pattern of a protein
   C) Local structures like alpha-helices and beta-sheets
   D) The interaction between different protein subunits

9. Which software is used for performing energy calculations and molecular dynamics simulations?
   A) SWISS-MODEL
   B) AutoDock
   C) GROMACS
   D) BLAST

10. What does the term "homology modeling" refer to in computational protein modeling?
    A) Predicting protein structure from genetic data
    B) Predicting protein structure based on known structures of similar proteins
    C) Analyzing the interaction between proteins
    D) Visualizing protein-ligand interactions

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11. Which technique provides high-resolution structural information by determining the electron density of protein crystals?
    A) NMR Spectroscopy
    B) Cryo-EM
    C) X-ray Crystallography
    D) Mass Spectrometry

12. What does "protein-ligand docking" aim to achieve in computational studies?
    A) To determine the protein's tertiary structure
    B) To predict how a small molecule (ligand) binds to a protein
    C) To model protein-protein interactions
    D) To analyze protein sequence data

13. Which approach involves simulating the physical movements of atoms and molecules over time?
    A) Molecular Docking
    B) Homology Modeling
    C) Molecular Dynamics (MD)
    D) Energy Minimization

14. In computational protein modeling, what does the term "tertiary structure" refer to?
    A) The sequence of amino acids in a protein
    B) The folding pattern of alpha-helices and beta-sheets
    C) The overall 3D structure of a single polypeptide chain
    D) The interaction between different protein chains

15. Which method is used to determine the interaction and binding affinity between proteins and small molecules?
    A) Energy Minimization
    B) Molecular Dynamics Simulation
    C) Molecular Docking
    D) Homology Modeling

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ADD ON COURSE – MARK LIST

NAME OF ADD ON COURSE : COMPUTATIONAL PROTIEN MODELING AND ANALYSIS

COURSE INSTRUCTORS : ANITHA.B

YEAR OFFERED : 3rd SEM B.PHARM

COURSE DURATION : 35hrs

S.NO	NAME OF STUDENT	REGISTER NO	MARKS (15)	PERCENTAGE (%)
1.	ABINESH. S	560021523501	12	80%
2.	ABISHEK.B	560021523502	12	80%
3.	ABISURYA .C	560021523503	14	93%
4.	ANANDASIVAM.T	560021523504	13	86%
5.	ANBU .R	560021523505	13	86%
6.	ARAVINTH.M	560021523506	15	100%
7.	ARCHANA.A	560021523507	14	93%
8.	ARIVILKUMAR.P	560021523508	15	100%
9.	ARUN .A	560021523509	13	86%
10.	ARUN KUMAR .K	560021523510	13	86%
11.	ARUNKUMAR.M	560021523511	13	86%
12.	BALAMURUGAN.B	560021523512	13	86%
13.	BATHRINATH.A	560021523513	15	100%
14.	BOOPATHI.G	560021523514	15	100%
15.	BOOPATHI.P	560021523515	14	93%
16.	CHITHARTHA.M	560021523516	15	100%
17.	DEVIPRIYA.K	560021523517	13	86%
18.	DHATCHNAMOORTHI.K	560021523518	13	86%
19.	DHIVYA.N	560021523519	12	80%
20.	GAYATHRI.S	560021523521	13	86%
21.	GOPIKA.K	560021523522	14	93%
22.	GOPI.K	560021523523	12	80%
23.	GURUMOORTHI.M	560021523524	13	86%
24.	HARIPRIYA.K	560021523525	14	93%
25.	JOTHIPRAKASH.P	560021523526	12	80%
26.	KARTHICK KANNAN.S	560021523527	14	93%
27.	KARTHICK.K	560021523528	15	100%
28.	KARTHIKEYAN.M	560021523529	13	86%

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NH-544, Kuppanur (Po), Sankari (Tk), Salem(Dt) – 637301 Tamilnadu, India
Phone : 04283 241080 | E-mail : ssip1718@gmail.com | Website : www.ssip.edu.in

29.	KAVIBHARATHI.S	560021523530	13	86%
30.	KAVIYA .S	560021523531	13	86%
31.	KESAVAN.P	560021523532	14	93%
32.	KIRUBANIDHI.R	560021523533	15	100%
33.	KIRUTHIKA.P	560021523534	13	86%
34.	MEGALA.G	560021523535	13	86%
35.	MOHAMMED KABEER.A	560021523536	13	86%
36.	RANISH.G	560021523537	13	86%
37.	SARAN MOHAN.R	560021523538	15	100%
38.	SASIKALA.G	560021523539	13	86%
39.	SATHYA JASMINE.A	560021523540	14	93%
40.	SETHURAMAN.P	560021523541	15	100%
41.	SOWMIYA.D	560021523542	13	86%
42.	SRIGANTH.K	560021523543	13	86%
43.	SUGASHINI.M	560021523544	12	80%
44.	SUNDHAR.S	560021523545	13	86%
45.	SURIYA.M	560021523546	12	80%
46.	SYED ABDULLA.A	560021523547	15	100%
47.	TAMILMANI.P	560021523548	15	100%
48.	THIRUMALAI.R	560021523549	13	86%
49.	THIRUMENINATHAN.M	560021523550	13	86%
50.	UMA SHANKARI.E	560021523551	14	93%
51.	VAITHEESWARI.V	560021523552	14	93%
52.	VIGNESH.C	560021523553	13	86%
53.	VIGNESH.S	560021523554	13	86%
54.	VIJAYASARATHI.S	560021523555	13	86%
55.	VIMAL.R	560021523556	13	86%
56.	VINOTHINI.A	560021523557	13	86%
57.	VISHALATCHI.K	560021523558	15	100%
58.	YAZHINI.B	560021523559	13	86%
59.	S.YUVAKIRUTHIGA	560021523560	12	80%

TOTAL NUMBER OF STUDENT : 59

TOTAL NUMBER OF PERCENTAGE : 89.6%

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ADD ON COURSE : SUMMARY REPORT

Course code and Name : 23CPMA07/ Computational Protein Modeling And Analytics

Date Of Add On Programme : 01/11/2023 to 08/11/2023

Course Duration : 35 Hours

Year Offered : 3rd Sem B.Pharm

Course Instructors : B.Anitha.,M.Pharm.

Course Outcomes :

- **Molecular Dynamics Simulation**: Gain experience in running and analyzing molecular dynamics (MD) simulations to study protein dynamics, stability, and conformational changes. Learn about simulation parameters, analysis methods, and interpretation of results.
- **Docking and Protein-Protein Interactions**: Understand how to use computational docking techniques to predict and analyze protein-protein interactions, as well as protein-ligand interactions. Learn to evaluate binding affinities and predict complex formation.

Course Type : Add on Course

Assessment Mode:

Total Duration : 35 Hours

Number of Participants : 59

Scheme of Exam : MCQ type, offline Mode

Date of Exam : 08/11/2023

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Course Coordinator

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R. SARAN MOHAN

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PARTICIPATION IN ONE DAY SEMINAR ON

COMPUTATIONAL PROTEIN MODELING

AND ANALYTICS

01/11/2023 TO 08/11/2023

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01/11/2023 TO 08/11/2023

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HAS APPRICATED FOR HIS / HER

PARTICIPATION IN ONE DAY SEMINAR ON

COMPUTATIONAL PROTEIN MODELING

AND ANALYTICS

01/11/2023 TO 08/11/2023

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STUDENT FEEDBACK FORM

STUDENT NAME: Vimal .R. DATE: 08/11/2023.

YEAR/COURSE: B. pharm - IV Sem.

NAME OF THE ADD ON COURSE: Computational protein modeling & analytics.

COURSE CODE: 23CPMA07. DURATION: 35hrs.

EVALUATE HONESTLY:

Questions	Excellent	Good	Fair	Poor
How was the objectives of the training	✓			
How satisfied are you with our seminar	✓			
How would you rate the clarity and effectiveness of the presenter's delivery		✓		
Was the seminar duration appropriate	✓			
How engaging and interactive was the seminar		✓		
Usefulness of the information provided	✓			
Overall quality of session			✓	

R. Vimal
SIGNATURE

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PHOTOGRAPH **DATE :** 1/11/23

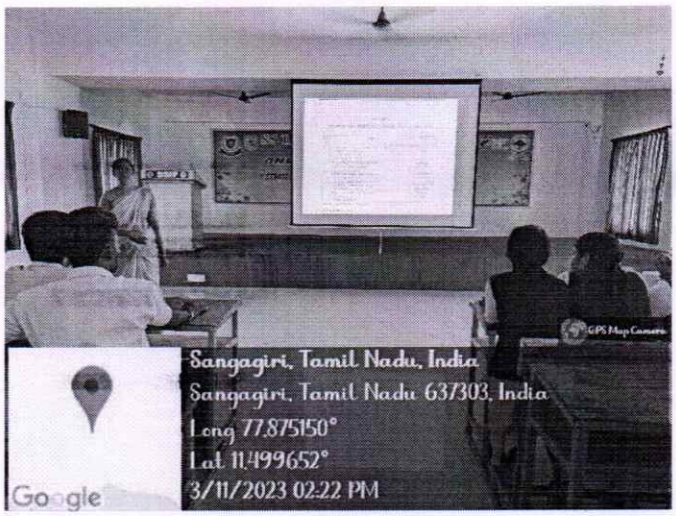
COMPUTATIONAL PROTIEN MODELING AND ANALYSIS

NAME OF ADD ON COURSE : COMPUTATIONAL PROTIEN MODELING AND ANALYSIS

COURSE INSTRUCTORS : ANITHA.B

YEAR OFFERED : 3rd SEM B.PHARM

COURSE DURATION : 35 hrs



Add-on course regarding the Topic Application Computational Protien Modeling And Analysis 1/11/23, the speech delivered By **B.Anitha.,M.Pharm..** which was an interactive session and students could able to understand the Application of Computational Protien Modeling And Analysis in the fields of pharmaceutical sciences

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