

JKK MUNIRAJAH MEDICAL RESEARCH FOUNDATION'S

ANNAI JKK SAMPOORANI AMMAL COLLEGE OF PHARMACY



Approved by: Pharmacy Council of India, New Delhi &

Affiliated to The Tamilnadu Dr. M.G.R Medical University, Chennai.

Accredited by NAAC "A" Grade and ISO Certified

Ethirmedu, B. Komarapalayam - 638183, Namakkal Dist. Tamilnadu, India.

Website: www.jkkmmrfpharmacy.edu.in / e.mail : principal@jkkmmrfpharmacy.edu.in

Contact No : +919789456750, +919943066944, +919943069944

Dr. N. SENTHILKUMAR, Ph.D.,
Principal

ADD ON COURSE	COMPUTATIONAL METHODS IN DRUG DISCOVERY
DEPARTMENT	PHARMACEUTICAL CHEMISTRY
ACADEMIC YEAR	2023-2024
DATE	07.08.2023 to 11.08.2023
VENUE	SEMINAR HALL

REPORT SUMMARY

No of Students Enrolled:60

No of Students Certified:59

No of student absent:01

Course Overview:

The Department of Pharmaceutical Chemistry at JKKMMRF's Annai JKK Sampoorani Ammal College of Pharmacy conducted an Add-On Course titled "**Computational Methods in Drug Discovery**" from **7th August to 11th August 2023**. The course aimed to provide students with in-depth knowledge and hands-on experience with computational techniques crucial for modern drug discovery.

Key Details:

- ❖ **Duration:** 30 Hours
- ❖ **Venue:** Seminar Hall, JKKMMRF's Annai JKK Sampoorani Ammal College of Pharmacy
- ❖ **Resource Persons:**

Dr. T. Venkatachalam, Professor and Head, Dept. of Pharmaceutical Chemistry,
JKKMMRF's Annai JKK Sampoorani Ammal College of Pharmacy,
Komarapalayam (Molecular Docking, MD Simulations)

Dr. N. SENTHILKUMAR,
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- ✓ Dr. M. Chitra, Associate Professor, Dept. of Pharmaceutical Chemistry, Pharmacy, Komarapalayam (Machine Learning, AI in Drug Discovery, Computational Toxicology)
- ✓ Dr. A. Chitra, Associate Professor, Dept. of Pharmaceutical Chemistry, JKKMMRF's Annai JKK Sampoorani Ammal College of Pharmacy, Komarapalayam (Systems Biology, HTS Data Analysis)

Course Content:

1. **Molecular Docking** – Studying interactions between drug candidates and target proteins.
2. **Molecular Dynamics (MD) Simulations** – Examining atomic movements in drug interactions.
3. **Machine Learning & AI** – Application in predicting biological activity of compounds.
4. **Computational Toxicology** – Predicting potential drug side effects.
5. **Systems Biology & Network Analysis** – Understanding complex biological interactions.
6. **High-Throughput Screening (HTS) Data Analysis** – Screening large compound libraries for drug candidates.

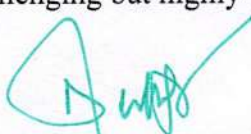
Student Participation:

A total of **60 students** across **Pharm.D., Pharm., and M. Pharm.** courses enrolled in the program. The course had active participation with students assessed through multiple-choice exams. Performance ranged from **50% to 100%**, with certificates awarded upon successful completion.

Outcome & Feedback:

- **Feedback:** Students rated the course highly for relevance, quality of instruction, and practical application. The course content was considered challenging but highly beneficial.




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Dr. N. SENTHILKUMAR, Ph.D.,

- **Evaluation:** Students were evaluated based on their knowledge in topics like molecular docking, machine learning, and HTS, scoring well on average.


PROGRAMME COORDINATOR


HOD


PRINCIPAL




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Dr. N. SENTHILKUMAR, Ph.D.,

Principal

Date: 01.08.2023

REF.NO: JKKM/PG-PHARM.CHEM/REQ/2023/001

From

Department of Pharmaceutical chemistry,

JKKMMRF'S Annai JKK Sampoorani Ammal College of Pharmacy.

Komarapalayam, Namakkal [Dist.]

Tamil Nadu, PIN:638183.

To

The Principal,

JKKMMRF'S Annai JKK Sampoorani Ammal College of Pharmacy.

Komarapalayam, Namakkal [Dist.]

Tamil Nadu, PIN:638183.

Respected Sir,

Subject: Letter for requesting Permission to Conduct an **ADD ON COURSE** regarding: -

We Are writing this letter to request permission to conduct an Add on Course in the Seminar Hall on **07.08.2023 to 11.08.2023**. We wish to conduct an add on course regarding the **COMPUTATIONAL METHODS IN DRUG DISCOVERY**. We believe this will be a very informative session that many students will wish to attend.

We request you to kindly permit to conduct training program as this would be a great opportunity for Students to learn all about **COMPUTATIONAL METHODS IN DRUG DISCOVERY** that would help a great deal to shape the students.

Looking forward to hearing from you.


Thank you,

Yours sincerely,




Dr. N.SENTHILKUMAR,
PRINCIPAL,

JKK MUNIRAJAH MEDICAL RESEARCH FOUNDATION
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ETHIRMEDU, KOMARAPALAYAM - 638 183,
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PROGRAMME CO-ORDINATOR

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Date: 04.08.2023

CIRCULAR

This is inform to the all PHARM.D, M. PHARM, B. PHARM Students that the following value added course titled on **COMPUTATIONAL METHODS IN DRUG DISCOVERY** can be conducted by the Department of Pharmaceutical Chemistry, JKKMMRF'S- ANNAL JKK SAMPOORANI AMMAL COLLEGE OF PHARMACY, KOMARAPALAYAM and it will be commenced as per the schedule:


Course Name	Schedule	Duration	Venue	Resource Person
COMPUTATIONAL METHODS IN DRUG DISCOVERY	07.08.2023 TO 11.08.2023	30 HRS	SEMINAR HALL	Dr. Venkatachalam Dr. M. Chitra Dr. A. Chitra

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

NOTE: Certificates should be issued to all the students after completion of the course and examination.


PROGRAMME CO-ORDINATOR


HOD


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SYLLABUS

DATE	HOURS	TOPIC	SUB TOPICS	RESOURCE PERSON
07.08.2023	6 Hrs	COMPUTATIONAL METHODS IN DRUG DISCOVERY	Molecular Docking	Dr. Venkatachalam
08.08.2023	6 Hrs		Molecular Dynamics (MD) Simulations	
09.08.2023	6 Hrs		Machine Learning and Artificial Intelligence & Computational Toxicology	Dr. M. Chitra
10.08.2023	6 Hrs		Systems Biology and Network Analysis	Dr. A. Chitra
11.08.2023	6 Hrs		High-Throughput Screening (HTS) Data Analysis	



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**JKKMMRF's ANNAI JKK SAMPOORANI AMMAL COLLEGE OF
PHARMACY, KOMARAPALAYAM.**

**ADD-ON COURSE ENTITLED ON
COMPUTATIONAL METHODS IN DRUG DISCOVERY**

Organized by:
Department of Pharmaceutical Chemistry

**Duration: 7th August 2023 –
11th August 2023 (30 hours)
Venue: Seminar Hall.**

Resource Persons:

- Dr. T. Venkatachalam
- Dr. M. Chitra
- Dr. A. Chitra

Organising secretary:

Mr. R. Vijay Amirtharaj

Organising members:

- Dr. K. Sumathi
- Dr. P. Kalaiselvi
- Mr. V. Suresh Kannan
- Ms. P. Gayathri
- Mrs. P. Ragavi

Course Highlights:

- *Interactive Sessions*
- *Hands-on Training*
- *Certificate of Completion for all participants*

Registration:

All Pharm.D, M.Pharm, and B.Pharm students are required to enroll for this course and actively participate.

Note: Certificates will be awarded upon successful completion of the course and the examination.



Dr. N. Senthil Kumar
PRINCIPAL

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Topics Covered:

Date	Hours	Topics	Resource Person
07.08.2023	6 Hrs	Molecular Docking	Dr. T. Venkatachalam
08.08.2023	6 Hrs	Molecular Dynamics (MD) Simulations	Dr. T. Venkatachalam
09.08.2023	6 Hrs	Machine Learning and Artificial Intelligence in Computational Toxicology	Dr. M. Chitra
10.08.2023	6 Hrs	Systems Biology and Network Analysis	Dr. A. Chitra
11.08.2023	6 Hrs	High-Throughput Screening (HTS) Data Analysis	Dr. A. Chitra

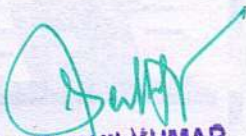
Contact Information:

For further details, please contact the Course Coordinator at clnaac2020@gmail.com.

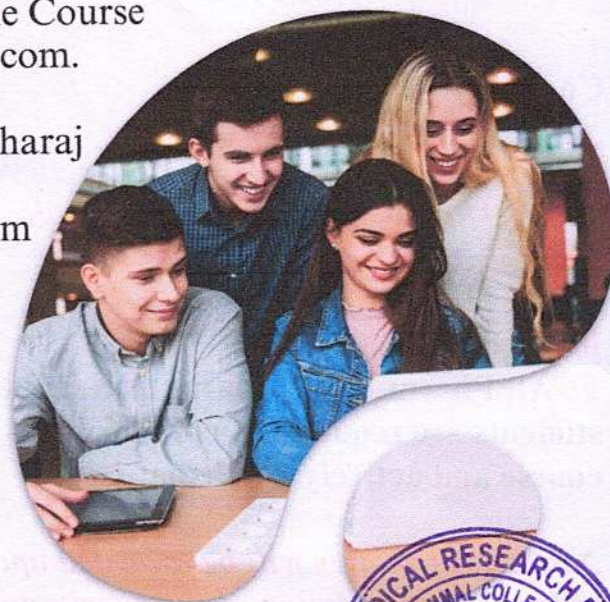
Program Coordinator: Mr. R. Vijay Amirtharaj

Head of Department: Dr. T. Venkatachalam

Principal: Dr. N. Senthilkumar


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Join us for an enriching learning experience!



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RESOURCE PERSON DETAILS



Dr. T. Venkatachalam

Dr. T. Venkatachalam is a Professor in the Department of Pharmaceutical Chemistry, specializing in Phytochemistry, Phytopharmacology, synthesis of organic molecules, drug design, and impurities profiling. With 16 years of experience in academia, he has published 45 international and 19 national papers, guided numerous undergraduate and postgraduate projects, and holds 6 patents, including innovative methods for evaluating anticonvulsant activities and preparing transdermal patches. He has also authored 5 books and received two prestigious awards, including the Dr. Abdul Kalam Gold Medal from the Global Economic Research Association. Dr. Venkatachalam is also actively involved in conferences, having attended over 60 events and acted as a resource person in 5 workshops. He is a life member of both APTI (TNLM-510) and IPGA (LM-549).




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RESOURCE PERSON DETAILS



Dr. M. Chitra

Dr. M. Chitra, an Associate Professor in the Department of Pharmaceutical Chemistry, has 22 years of experience. She holds an M. Pharm and Ph.D., focusing on natural and synthetic pharmaceutical chemistry and analysis. She has published 15 international and 18 national papers and has guided numerous undergraduate and postgraduate research projects. One of her notable patents is the development of a stability-indicating method for Ribavirin by RP-HPLC. Dr. M. Chitra has been an active participant in conferences, having attended 13 and conducted 3 such events. Additionally, she has served as a resource person in 5 workshops. Like her peers, she is a life member of the Association of Pharmaceutical Teachers of India (APTI), TN/LM-509.



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RESOURCE PERSON DETAILS



Dr. A. Chitra

Dr. A. Chitra is an Associate Professor in the Department of Pharmaceutical Chemistry. She holds an M. Pharm and a Ph.D., specializing in Pharmaceutical Chemistry with a focus on both natural and synthetic compounds. Her research extends to Pharmaceutical Analysis, particularly in method development and validation. With over 20 years of experience, she has published 14 international and 18 national research papers and has also guided 14 undergraduate and 7 postgraduate projects. Dr. Chitra has obtained a patent for a method to extract *Spondias pinnata* fruit extract, showcasing her contribution to innovative research. She has attended 14 conferences, workshops, and seminars, and has served as a resource person in 5 such events. She is a life member of the Association of Pharmaceutical Teachers of India (APTI), TN/LM-507.



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LIST OF STUDENTS ENROLLED FOR THE COURSE

S.NO	REG.NO	NAME OF THE STUDENTS	COURSES	SIGNATURE OF THE STUDENTS
1	380022507503	DANISHA T	II PHARM D	T. Danisha
2	380022507504	DHARANIKA S	II PHARM D	Dharanika S
3	380021507525	SREESANTHEYA S G	III PHARM D	S G Sreesanth
4	380021507526	SUBASH B	III PHARM D	B. Subash
5	381810409	BIBIN RIJO W	VI PHARM D	W. Binji
6	381810410	DIVIKA S	VI PHARM D	S. Divika
7	381810411	EZILKKAVIA S	VI PHARM D	S. Ezilkkavia
8	560023507505	ANANDHAKUMAR V	SEM-I B.PHARM	V. Anand
9	560023507506	ARAVIND S	SEM-I B.PHARM	S. Aravind
10	560023507507	ARAVINDH R	SEM-I B.PHARM	R. Aravind
11	560023507508	ARIYA A K	SEM-I B.PHARM	K. Ariya
12	560023507509	BALAGURUNATHAN V	SEM-I B.PHARM	V. Balagurunathan
13	560023507510	BAVANYA S	SEM-I B.PHARM	S. Bavanya



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14	560023507596	VINOTHA S	SEM-I B.PHARM	Principal
15	560023507597	VISHAL K	SEM-I B.PHARM	V. Vishal
16	560023507598	YAMUNA N	SEM-I B.PHARM	K. Thiruv
17	560023507599	YUVARAJ M	SEM-I B.PHARM	Yamuna
18	560022507509	ARUN K S	SEM-III B.PHARM	M. Yuvaraj
19	560022507510	ASWINI D	SEM-III B.PHARM	Arun K S
20	560022507511	APPYAPPAN P	SEM-III B.PHARM	Aswini D
21	560022507512	BALAJI V	SEM-III B.PHARM	P. Appy
22	560022507513	BALAKRISHNAN S	SEM-III B.PHARM	V. Balaji
23	560021507534	HARIDHARSHINI M	SEM-IV B.PHARM	Balakrishnan S
24	560021507535	HEMA DIVYA R	SEM-IV B.PHARM	M. Haridharshini
25	560021507536	HIRUTHIKA S	SEM-IV B.PHARM	Hema Divya R
26	560021507537	INDHUMATHI A	SEM-IV B.PHARM	S. Hiruthika
27	560021507538	ISAIMOZHI M	SEM-IV B.PHARM	A. Indhumathi
28	560021507539	IYYAPPAN M	SEM-IV B.PHARM	M. Isaimozhi
29	560021507540	JAGATHISHVARAN P	SEM-IV B.PHARM	M. Iyyappan
30	560021507541	JEEVA N R	SEM-IV B.PHARM	P. Jagathish
31	560020507527	GOKULAKANNAN P	SEM-VI B.PHARM	R. Jeeva
32	560020507529	GOWTHAM J	SEM-VI B.PHARM	P. Gokulakannan
33	560020507530	GOWTHAMAN K	SEM-VI B.PHARM	Gowtham J
34	560020507531	HARIHARAN K	SEM-VI B.PHARM	K. Gowthaman
35	560020507532	HARISHRAGUL G	SEM-VI B.PHARM	Harihara
36	560020507533	HARITHRA P S	SEM-VI B.PHARM	G. Harishragul
37	560020507534	HARIVARMAN P	SEM-VI B.PHARM	P. Harithra
38	560020507535	HEMANATH N	SEM-VI B.PHARM	P. Harivarma
39	560020507536	HEMANTH KUMAR K	SEM-VI B.PHARM	N. Hemanath
40	560020507567	PRABHAKARAN P	SEM-VI B.PHARM	K. Hemant Kumar
41	560020507568	PRAKASH S R	SEM-VI B.PHARM	P. Prabhakar
				S. Prakash



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42	560020507569	PRIYADHARSHINI P	SEM-VI B.PHARM	P. Priyadharshini
43	560020507570	RAJESHKUMAR R	SEM-VI B.PHARM	R. Rajesh Kumar
44	560020507571	RANJITH R	SEM-VI B.PHARM	R. Ranjith
45	560020507572	SABARINATHAN M	SEM-VI B.PHARM	M. Sabarinathan
46	560020507573	SANTHOSH S	SEM-VI B.PHARM	Santhosh S.
47	560020507574	SARAN S	SEM-VI B.PHARM	
48	560020507575	SARANYA S	SEM-VI B.PHARM	S. Saranya
49	560020507576	SATHIYANARAYANAN M	SEM-VI B.PHARM	Sathiyaraj
50	560020507577	SHIVA G	SEM-VI B.PHARM	S. Shiva
51	261123507511	RASIGA S	SEM-I M.PHARM (PHARMACEUTICS)	S. Rasiga
52	261123507512	RENUGA R	SEM-I M.PHARM (PHARMACEUTICS)	R. Renuka
53	261223507505	LOGANANTHAM P	SEM-I M.PHARM (P'CEUTICAL CHEM)	P. Loganathan
54	261523507508	MOHAMED IRSHAD T	SEM-I M.PHARM (PHARMACY PRACTICE)	T. Mohamed Irshad
55	261523507509	NARMATHA S	SEM-I M.PHARM (PHARMACY PRACTICE)	Narmatha S.
56	261523507510	PRAMESHWARI V	SEM-I M.PHARM (PHARMACY PRACTICE)	V. Parameshwari
57	261523507511	PRAVEEN M	SEM-I M.PHARM (PHARMACY PRACTICE)	M. Praveen



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58	261522507501	AMEER SUHAIL A K	SEM-III M.PHARM (PHARMACY PRACTICE)	<i>Amersuhail AK</i>
59	261522507502	ASHROOK AHAMED E K	SEM-III M.PHARM (PHARMACY PRACTICE)	<i>Ek Ashrook</i>
60	261522507503	HEMA R	SEM-III M.PHARM (PHARMACY PRACTICE)	<i>P. Hema</i>

PROGRAMME COORDINATOR

HOD

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ADD ON COURSE	COMPUTATIONAL METHODS IN DRUG DISCOVERY
DEPARTMENT	PHARMACEUTICAL CHEMISTRY
ACADEMIC YEAR	2023-2024
DATE	07.08.2023 to 11.08.2023
VENUE	SEMINAR HALL

LIST OF STUDENTS ATTENDENCE FOR THE COURSE

S.NO	REG.NO	NAME OF THE STUDENTS	COURSES	7/8	8/8	9/8	10/8	11/8
1	380022507503	DANISHA T	II PHARM D	/	/	/	/	/
2	380022507504	DHARANIKA S	II PHARM D	/	/	/	/	/
3	380021507525	SREESANTHEYA S G	III PHARM D	/	/	/	/	/
4	380021507526	SUBASH B	III PHARM D	/	/	/	/	/
5	381810409	BIBIN RIJO W	VI PHARM D	/	/	/	/	/
6	381810410	DIVIKA S	VI PHARM D	/	/	/	/	/
7	381810411	EZILKKAVIA S	VI PHARM D	/	/	/	/	/
8	560023507505	ANANDHAKUMAR V	SEM-I B.PHARM	/	/	/	/	/
9	560023507506	ARAVIND S	SEM-I B.PHARM	/	/	/	/	/
10	560023507507	ARAVINDH R	SEM-I B.PHARM	Ab	Ab	Ab	Ab	Ab
11	560023507508	ARIYA A K	SEM-I B.PHARM	/	/	/	/	/
12	560023507509	BALAGURUNATHA N V	SEM-I B.PHARM	/	/	/	/	/
13	560023507510	BAVANYA S	SEM-I B.PHARM	/	/	/	/	/



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14	560023507596	VINOTHA S	SEM-I B.PHARM	/	/	/	/	/
15	560023507596	VISHAL K	SEM-I B.PHARM	/	/	/	/	/
16	560023507597	YAMUNA N	SEM-I B.PHARM	/	/	/	/	/
17	560023507598	YUVARAJ M	SEM-I B.PHARM	/	/	/	/	/
18	560022507509	ARUN K S	SEM-III B.PHARM	/	/	/	/	/
19	560022507510	ASWINI D	SEM-III B.PHARM	/	/	/	/	/
20	560022507511	AYYAPPAN P	SEM-III B.PHARM	/	/	/	/	/
21	560022507512	BALAJI V	SEM-III B.PHARM	/	/	/	/	/
22	560022507513	BALAKRISHNAN S	SEM-III B.PHARM	/	/	/	/	/
23	560021507534	HARIDHARSHINI M	SEM-IV B.PHARM	/	/	/	/	/
24	560021507535	HEMA DIVYA R	SEM-IV B.PHARM	/	/	/	/	/
25	560021507536	HIRUTHIKA S	SEM-IV B.PHARM	/	/	/	/	/
26	560021507537	INDHUMATHI A	SEM-IV B.PHARM	/	/	/	/	/
27	560021507538	ISAIMOZHI M	SEM-IV B.PHARM	/	/	/	/	/
28	560021507539	IYYAPPAN M	SEM-IV B.PHARM	/	/	/	/	/
29	560021507540	JAGATHISHVARAN P	SEM-IV B.PHARM	/	/	/	/	/
30	560021507541	JEEVA N R	SEM-IV B.PHARM	/	/	/	/	/
31	560020507527	GOKULAKANNAN P	SEM-VI B.PHARM	/	/	/	/	/
32	560020507529	GOWTHAM J	SEM-VI B.PHARM	/	/	/	/	/
33	560020507530	GOWTHAMAN K	SEM-VI B.PHARM	/	/	/	/	/
34	560020507531	HARIHARAN K	SEM-VI B.PHARM	/	/	/	/	/
35	560020507532	HARISHRAGUL G	SEM-VI B.PHARM	/	/	/	/	/
36	560020507533	HARITHRA P S	SEM-VI B.PHARM	/	/	/	/	/
37	560020507534	HARIVARMAN P	SEM-VI B.PHARM	/	/	/	/	/
38	560020507535	HEMANATH N	SEM-VI B.PHARM	/	/	/	/	/



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39	560020507536	HEMANTH KUMAR K	SEM-VI B.PHARM	/	/	/	/	/
40	560020507567	PRABHAKARAN P	SEM-VI B.PHARM	/	/	/	/	/
41	560020507568	PRAKASH S R	SEM-VI B.PHARM	/	/	/	/	/
42	560020507569	PRIYADHARSHINI P	SEM-VI B.PHARM	/	/	/	/	/
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54	261523507508	MOHAMED IRSHAD T	SEM-I M.PHARM (PHARMACY PRACTICE)	/	/	/	/	/
55	261523507509	NARMATHA S	SEM-I M.PHARM (PHARMACY PRACTICE)	/	/	/	/	/



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56	261523507510	PRAMESHWARI V	SEM-I M.PHARM (PHARMACY PRACTICE)	/	/	/	/	/
57	261523507511	PRAVEEN M	SEM-I M.PHARM (PHARMACY PRACTICE)	/	/	/	/	/
58	261522507501	AMEER SUHAIL A K	SEM-III M.PHARM (PHARMACY PRACTICE)	/	/	/	/	/
59	261522507502	ASHROOK AHAMED E K	SEM-III M.PHARM (PHARMACY PRACTICE)	/	/	/	/	/
60	261522507503	HEMA R	SEM-III M.PHARM (PHARMACY PRACTICE)	/	/	/	/	/



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ADD ON COURSE – STUDENT ANSWER SHEET

ADD – ON COURSE TITLE	COMPUTATIONAL METHODS IN DRUG DISCOVERY	
NAME OF THE STUDENT	P. PRIYADHARSHINI	
DATE	11/08/2023	
REGISTER NO	560020507569	
COURSE/ YEAR/ SEM	B.Pharm / IV Year / VII sem	MARKS OBTAINED: 15
SIGNATURE:	STUDENT:	STAFF:

ANSWER ALL THE QUESTIONS:

MULTIPLE CHOICE QUESTION

MARKS:20

1. What is the primary purpose of molecular docking in drug discovery?
 - A) To design new chemical compounds from scratch
 - ☒ B) To simulate the interaction between a drug candidate and a target protein
 - C) To predict the toxicity of a drug
 - D) To analyze biological data like genomics
2. Which computational method involves studying the movement of atoms and molecules over time?
 - A) Molecular Docking
 - B) Pharmacophore Modeling
 - ☒ C) Molecular Dynamics Simulations
 - D) QSAR Modeling
3. In QSAR modeling, what is the relationship that is being studied?
 - ☒ A) The chemical structure of a drug and its biological activity
 - B) The chemical structure of a drug and its market value
 - C) The chemical structure of a drug and its regulatory status
 - D) The chemical structure of a drug and its regulatory status



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4. Which method is used for the virtual screening of large compound libraries to identify potential drug candidates?

- A) De Novo Drug Design
- B) Molecular Dynamics Simulations
- ☒ C) Virtual Screening
- D) Systems Biology

5. Pharmacophore modeling is primarily used to:

- A) Predict the toxicity of compounds
- ☒ B) Identify the essential features of a molecule required for biological activity
- C) Simulate the physical movements of atoms
- D) Analyze genomic data to find drug targets

6. Which of the following methods is best suited for designing new drug molecules from scratch?

- A) QSAR Modeling
- B) Molecular Docking
- ☒ C) De Novo Drug Design
- D) Chemoinformatics

7. What is the main advantage of using machine learning in drug discovery? **

- ☒ A) It reduces the need for laboratory experiments
- B) It allows for the real-time analysis of patient data
- C) It can predict the biological activity of new compounds based on large datasets
- D) It is primarily used for regulatory approval processes

8. Which computational method is used to predict potential side effects of drug candidates?

- A) Pharmacophore Modeling
- B) Molecular Docking
- ☒ C) Computational Toxicology
- D) High-Throughput Screening



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9. Systems biology in drug discovery is primarily concerned with:

- A) Modeling the physical movements of molecules
- B) Analyzing the cost-effectiveness of drug production
- ☒ C) Understanding the complex interactions within biological systems
- D) Designing new chemical compounds

10. In which computational method is a chemical compound library screened to identify those most likely to bind to a drug target?

- A) De Novo Drug Design
- B) Molecular Dynamics Simulations
- ☒ C) Virtual Screening
- D) QSAR Modeling




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ADD ON COURSE	COMPUTATIONAL METHODS IN DRUG DISCOVERY
DEPARTMENT	PHARMACEUTICAL CHEMISTRY
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ANSWER KEY: ANSWER

ALL THE QUESTIONS:

1. What is the primary purpose of molecular docking in drug discovery?

- A) To design new chemical compounds from scratch
- B) To simulate the interaction between a drug candidate and a target protein
- C) To predict the toxicity of a drug
- D) To analyze biological data like genomics

Answer: B) To simulate the interaction between a drug candidate and a target protein

2. Which computational method involves studying the movement of atoms and molecules over time?

- A) Molecular Docking
- B) Pharmacophore Modeling
- C) Molecular Dynamics Simulations
- D) QSAR Modeling

Answer: C) Molecular Dynamics Simulations

3. In QSAR modeling, what is the relationship that is being studied?

- A) The chemical structure of a drug and its manufacturing cost
- B) The chemical structure of a drug and its biological activity



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- C) The chemical structure of a drug and its market value
- D) The chemical structure of a drug and its regulatory status

Answer: B) The chemical structure of a drug and its biological activity

4. Which method is used for the virtual screening of large compound libraries to identify potential drug candidates?

- A) De Novo Drug Design
- B) Molecular Dynamics Simulations
- C) Virtual Screening
- D) Systems Biology

Answer: C) Virtual Screening

5. Pharmacophore modeling is primarily used to:

- A) Predict the toxicity of compounds
- B) Identify the essential features of a molecule required for biological Activity
- C) Simulate the physical movements of atoms
- D) Analyze genomic data to find drug targets

Answer: B) Identify the essential features of a molecule required for biological activity

6. Which of the following methods is best suited for designing new drug molecules from scratch?

- A) QSAR Modeling
- B) Molecular Docking
- C) De Novo Drug Design
- D) Chemoinformatics

Answer: C) De Novo Drug Design

7. What is the main advantage of using machine learning in drug discovery? **

- A) It reduces the need for laboratory experiments
- B) It allows for the real-time analysis of patient data
- C) It can predict the biological activity of new compounds based on large datasets



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D) It is primarily used for regulatory approval processes

8. Which computational method is used to predict potential side effects of drug candidates?

- A) Pharmacophore Modeling
- B) Molecular Docking
- C) Computational Toxicology
- D) High-Throughput Screening

Answer: C) Computational Toxicology

9. Systems biology in drug discovery is primarily concerned with:

- A) Modeling the physical movements of molecules
- B) Analyzing the cost-effectiveness of drug production
- C) Understanding the complex interactions within biological systems
- D) Designing new chemical compounds

Answer: C) Understanding the complex interactions within biological systems

10. In which computational method is a chemical compound library screened to identify those most likely to bind to a drug target?

- A) De Novo Drug Design
- B) Molecular Dynamics Simulations
- C) Virtual Screening
- D) QSAR Modeling

Answer: C) Virtual Screening




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VENUE	SEMINAR HALL

STUDENTS MARKSHEETS

S.NO	REG.NO	NAME OF THE STUDENTS	COURSES	MARKS SCORED	% MARKS
1	380022507503	DANISHA T	II PHARM D	18	90%
2	380022507504	DHARANIKA S	II PHARM D	16	80%
3	380021507525	SREESANTHEYA S G	III PHARM D	17	85%
4	380021507526	SUBASH B	III PHARM D	18	90%
5	381810409	BIBIN RIJO W	VI PHARM D	15	75%
6	381810410	DIVIKA S	VI PHARM D	14	70%
7	381810411	EZILKKAVIA S	VI PHARM D	18	90%
8	560023507505	ANANDHAKUMAR V	SEM-I B.PHARM	19	95%
9	560023507506	ARAVIND S	SEM-I B.PHARM	20	100%
10	560023507507	ARAVINDH R	SEM-I B.PHARM	AB	AB
11	560023507508	ARIYA A K	SEM-I B.PHARM	19	95%
12	560023507509	BALAGURUNATHA N V	SEM-I B.PHARM	16	80%



Dr. N.SENTHILKUMAR,
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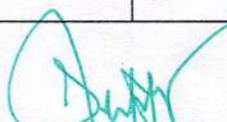
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Dr. N. SENTHILKUMAR, Ph.D.,
Principal

13	560023507510	BAVANYA S	SEM-I B.PHARM	17	85%
14	560023507596	VINOTHA S	SEM-I B.PHARM	16	80%
15	560023507597	VISHAL K	SEM-I B.PHARM	14	70%
16	560023507598	YAMUNA N	SEM-I B.PHARM	13	65%
17	560023507599	YUVARAJ M	SEM-I B.PHARM	12	60%
18	560022507509	ARUN K S	SEM-III B.PHARM	19	95%
19	560022507510	ASWINI D	SEM-III B.PHARM	18	90%
20	560022507511	AYYAPPAN P	SEM-III B.PHARM	17	85%
21	560022507512	BALAJI V	SEM-III B.PHARM	16	80%
22	560022507513	BALAKRISHNAN S	SEM-III B.PHARM	15	75%
23	560021507534	HARIDHARSHINI M	SEM-IV B.PHARM	14	70%
24	560021507535	HEMA DIVYA R	SEM-IV B.PHARM	13	65%
25	560021507536	HIRUTHIKA S	SEM-IV B.PHARM	12	60%
26	560021507537	INDHUMATHI A	SEM-IV B.PHARM	18	90%
27	560021507538	ISAIMOZHI M	SEM-IV B.PHARM	19	95%
28	560021507539	IYYAPPAN M	SEM-IV B.PHARM	15	75%
29	560021507540	JAGATHISHVARAN P	SEM-IV B.PHARM	14	70%
30	560021507541	JEEVA N R	SEM-IV B.PHARM	17	85%
31	560020507527	GOKULAKANNAN P	SEM-VI B.PHARM	16	80%
32	560020507529	GOWTHAM J	SEM-VI B.PHARM	18	90%
33	560020507530	GOWTHAMAN K	SEM-VI B.PHARM	17	85%
34	560020507531	HARIHARAN K	SEM-VI B.PHARM	14	70%
35	560020507532	HARISHRAGUL G	SEM-VI B.PHARM	15	75%
36	560020507533	HARITHRA P S	SEM-VI B.PHARM	18	90%
37	560020507534	HARIVARMAN P	SEM-VI B.PHARM	19	95%




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38	560020507535	HEMANATH N	SEM-VI B.PHARM	18	90%
39	560020507536	HEMANATH KUMAR K	SEM-VI B.PHARM	19	95%
40	560020507567	PRABHAKARAN P	SEM-VI B.PHARM	16	80%
41	560020507568	PRAKASH S R	SEM-VI B.PHARM	14	70%
42	560020507569	PRIYADHARSHINI P	SEM-VI B.PHARM	15	75%
43	560020507570	RAJESHKUMAR R	SEM-VI B.PHARM	10	50%
44	560020507571	RANJITH R	SEM-VI B.PHARM	15	75%
45	560020507572	SABARINATHAN M	SEM-VI B.PHARM	12	60%
46	560020507573	SANTHOSH S	SEM-VI B.PHARM	19	95%
47	560020507574	SARAN S	SEM-VI B.PHARM	14	70%
48	560020507575	SARANYA S	SEM-VI B.PHARM	15	75%
49	560020507576	SATHIYANARAYAN AN M	SEM-VI B.PHARM	16	80%
50	560020507577	SHIVA G	SEM-VI B.PHARM	16	80%
51	261123507511	RASIGA S	SEM-I M.PHARM (PHARMACEUTICS)	16	80%
52	261123507512	RENUGA R	SEM-I M.PHARM (PHARMACEUTICS)	18	90%
53	261223507505	LOGANANTHAM P	SEM-I M.PHARM (P'CEUTICAL CHEM)	18	90%
54	261523507508	MOHAMED IRSHAD T	SEM-I M.PHARM (PHARMACY PRACTICE)	19	95%
55	261523507509	NARMATHA S	SEM-I M.PHARM (PHARMACY PRACTICE)	18	90%
56	261523507510	PRAMESHWARI V	SEM-I M.PHARM (PHARMACY PRACTICE)	19	95%
57	261523507511	PRAVEEN M	SEM-I M.PHARM (PHARMACY PRACTICE)	18	90%



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58	261522507501	AMEER SUHAIL A K	SEM-III M.PHARM (PHARMACY PRACTICE)	19	95%
59	261522507502	ASHROOK AHAMED E K	SEM-III M.PHARM (PHARMACY PRACTICE)	18	90%
60	261522507503	HEMA R	SEM-III M.PHARM (PHARMACY PRACTICE)	17	85%

PROGRAMME CO-ORDINATOR

HOD

PRINCIPAL



Dr. N.SENTHILKUMAR,
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ADD ON COURSE	COMPUTATIONAL METHODS IN DRUG DISCOVERY
DEPARTMENT	PHARMACEUTICAL CHEMISTRY
ACADEMIC YEAR	2023-2024
DATE	07.08.2023 to 11.08.2023
VENUE	SEMINAR HALL

STUDENT NAME: V. BALAJI

DATE: 11/08/2023

YEAR/ COURSE: SEM-III . B-PHARM

COURSE CODE: —

DURATION: —

EVALUATE HONESTLY:

Questions	Excellent	Good	Fair	Poor
The objectives of the training were	<input checked="" type="checkbox"/>			
The instructor's contribution to the course was:	<input checked="" type="checkbox"/>			
The presentation materials were relevant	<input checked="" type="checkbox"/>			
The instructor's effectiveness in teaching the subject matter was:	<input checked="" type="checkbox"/>			
Answers to the students questions by the instructor		<input checked="" type="checkbox"/>		
The venue was appropriate for the event	<input checked="" type="checkbox"/>			
Course organisation was:	<input checked="" type="checkbox"/>			
Level of course was		<input checked="" type="checkbox"/>		
Course content was:	<input checked="" type="checkbox"/>			

Student Participation

- On average, how many hours a week did you spend on this course (in and out of class)?
A)0-2 B) 2-5 C)6-10 D)11-14 E)15-16
- What grade do you expect in this course?
A) BELOW 50% B) 50-60% C) 60-70% D) 70-80% E) ABOVE 80%



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V. Balaji
SIGNATURE

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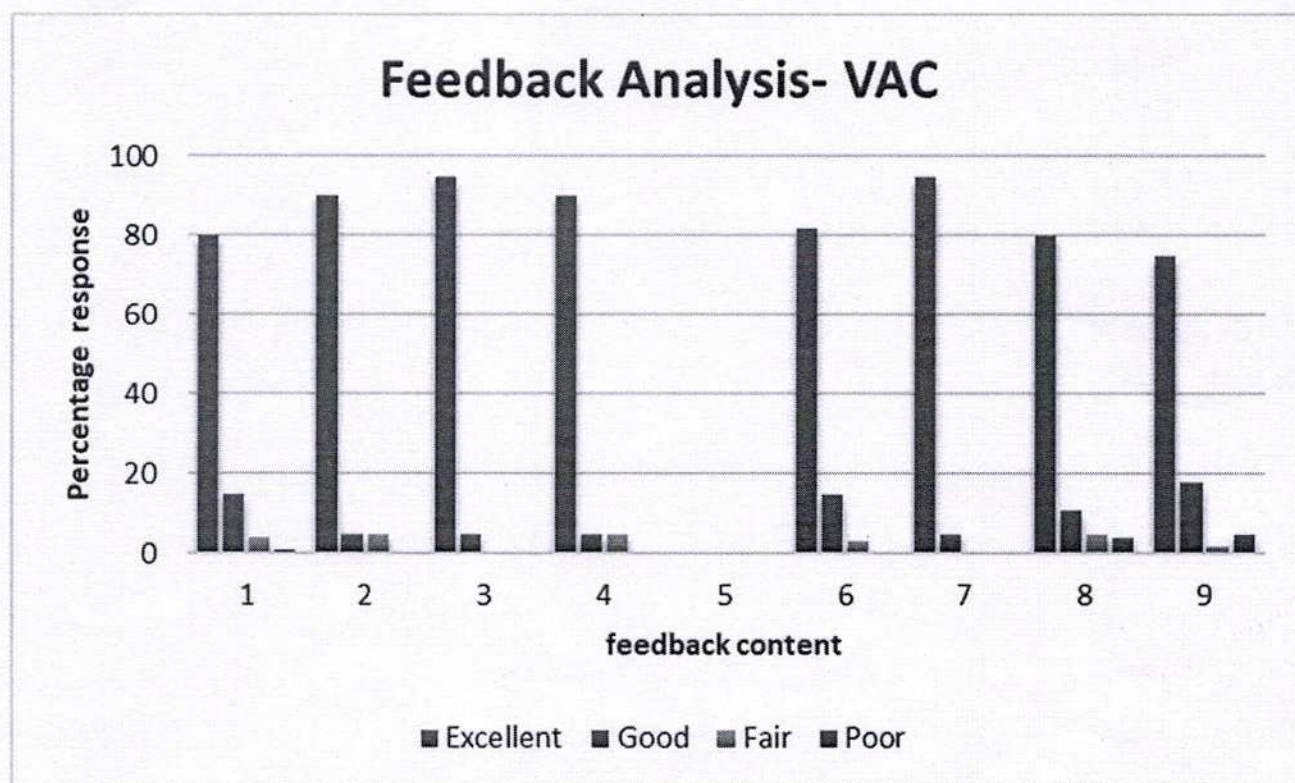
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DEPARTMENT	PHARMACEUTICAL CHEMISTRY
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STUDENTS FEEDBACK ANALYSIS




Dr. N. SENTHILKUMAR,
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Presentation was given by Dr.T. Venkatachalam, Professor & Head, Dept of Pharmaceutical Chemistry on 08.08.2023.



The Presentation was given by Dr.M. Chitra, Associate Professor, Dept of Pharmaceutical Chemistry on 09.08.2023.



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The Presentation was given by Dr.A. Chitra, Associate Professor, Dept of Pharmaceutical Chemistry on 10.08.2023.




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JKKMMRF'S ANNAI JKK SAMPOORANI AMMAL COLLEGE OF PHARMACY

CERTIFICATE OF PARTICIPATION

This is to certify that MR./MS./MRS.

M. PRAVEEN

Has appreciated for his/ her participation in Value Added Course-

COMPUTATIONAL METHODS IN DRUG DISCOVERY

Organized by the Department of Pharmaceutical Chemistry

on 7.8.2023 to 11.8.2023

P. Senthil Kumar

COORDINATOR



Dr. N. Senthil Kumar

CONVENOR

Dr. N. Senthil Kumar

Dr. N. SENTHILKUMAR,
PRINCIPAL,

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