### 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.



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

# DEPARTMENT OF PHARMACEUTICAL CHEMISTRY REPORT

# SEMINAR ON COMPUTATIONAL CHEMISTRY IN DRUG DESIGN: SIMULATING SUCCESS

VENUE: Seminar Hall Date: 24-11-2023

#### **RESOURCE PERSONS**

1. Dr. T. Venkatachalam, M. Pharm, Ph.D.

Associate Professor, Department of Pharmaceutical chemistry,

JKKMMRF'S Annai JKK Sampoorani Ammal College of Pharmacy, Komarapalayam

2. Mr.V.Suresh kannan, M.Pharm.

Associate Professor, Department of Pharmaceutical chemistry,

JKKMMRF'S Annai JKK Sampoorani Ammal College of Pharmacy, Komarapalayam

No. of Students enrolled: 59

No. of Students attented: 59

#### Overview:

This seminar emphasized the role of computational chemistry in modern drug discovery, focusing on efficiency and precision in drug design.

#### **Key Highlights:**

- Molecular Modelling: Understanding drug-target interactions.
- Virtual Screening: Identifying and optimizing lead compounds.
- Case Studies: Real-world examples of computational techniques in drug development.

#### Schedule:

- Session 1 (10:00 AM 11:30 AM): *Molecular Modelling and Simulation Techniques* by Dr. T. Venkatachalam
- Session 2 (02:00 PM 03:30 PM): Structure-Based Drug Design by Mr. V. Suresh Kannan

#### Outcome:

The seminar provided practical knowledge of computational tools, empowering researchers and students to drive innovation in pharmaceutical development. Certificates were distributed to participants.

Impact: Enhanced understanding of emerging pharmaceutical trends and computational tools.

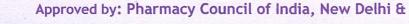
These seminars collectively aimed at bridging academia and industry to prepare students for challenges in pharmaceutical sciences.

Programme Co-ordinator HOD

Principal

Dr. N.SENTHILKUMAR, PRINCIPAL,

ANNAI JKK SAMPOORANI AMMAL COLLEGE OF PHARMACY



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



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

> > Date: 14.11.2023

REF.NO:JKKM/PG-PHARM.CHEM/REQ/2023/005

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 a **SEMINAR** regarding: -

We Are writing this letter to request permission to conduct a seminar in the **SEMINAR HALL** on **24.11.2023.** We wish to conduct a seminar regarding the "**Computational Chemistry in Drug Design: Simulating Success**". 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 Chemistry in Drug Design: Simulating Success" that would help a great deal to shape the students. Looking forward to hearing from you.

Thank you,

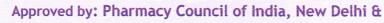
Yours sincerely,

Programme Co-ordinator.

Dr. N.SENTHILKUMAR, PRINCIPAL.











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**

# **CIRCULAR**

This is inform to the all PHARM.D, M.PHARM, B.PHARM Students that the following seminar titled on: "Computational Chemistry in Drug Design: Simulating Success'can be conducted by the Department of Pharmaceutical Chemistry, JKKMMRF'S- ANNAI JKK SAMPOORANI AMMAL COLLEGE OF PHARMACY, KOMARAPALAYAM and it will be commenced as per the schedule:

Course Name	Schedule	Duration	Venue	Resource Person
"COMPUTATIONAL CHEMISTRY IN DRUG DESIGN: SIMULATING SUCCESS"	24.11.2023	3 Hrs	SEMINAR HALL	Dr. T. VENKATACHALAM Mr. V. SURESH KANNAN

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

NOTE: Certificates should be issued to all the delegates.

rogramme Cb-ordinate

Dr. N.SENTHILKUMAR, PRINCIPAL.







# JKKMMRF'S ANNAI JKK SAMPOORANI AMMAL COLLEGE OF PHARMACY, KOMARAPALAYAM.

**ONE DAY Seminar on** 

"Computational Chemistry in Drug Design: Simulating Success"

Organized by:
Department of Pharmaceutical
Chemistry & INTERNAL QUALITY
ASSURANCE CELL (IQAC)

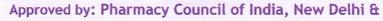
Date: 24.11.2023

**Duration: 3 hours** 

Dr. N.SENTHILKUMAR,
PRINCIPAL,
JAH MEDICAL RESEARCH FOUNDATION
CORANI AMMAL COLLEGE OF PHARMACY
LL OMAR A PALL OVAN 629 192

Venue: Seminar Hall MARAPALAYAM - 638 183,









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

We bsite: www.jkkmmrfpharmacy.edu.in/e.mail:principal@jkkmmacy.edu.in/e.mail:principal@jkkmmrfpharmacy.edu.in/e.mail:principal@jkkmmrfpharmacy.edu.in/e.mail:principal@jkkmmrfpharmacy.edu.in/e.mail:principal@jkkmmrfpharmacy.edu.in/e.mail:principal@jkkmmrfpharmacy.edu.in/e.mail:principal@jkkmmrfpharmacy.edu.in/e.mail:principal@jkkmmrfpharmacy.edu.in/e.mail:principal@jkkmmrfpharmacy.edu.in/e.mail:principal@jkkmmrfpharmacy.edu.in/e.mail:princip

Contact No: +919789456750, +919943066944, +919943069944

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

#### **SYLLABUS**

DATE	TIME	TOPIC	SESSION TITLE	RESOURCE PERSON
			Molecular Modeling	
	10.00 am -	"COMPUTATIONAL	and Simulation	
	11.30 am	CHEMISTRY IN	Techniques in Drug	Dr. T. VENKATACHALAM
		DRUG DESIGN:	Design	
24.11.2023		SIMULATING	Structure-Based Drug	
	02.00 pm –	SUCCESS"	Design: From Virtual	
	03.30 pm		Screening to Lead	Mr. V. SURESH KANNAN
			Optimization	

Programme Co-ordinator

HOD

Principal

Dr. N.SENTHILKUMAR, PRINCIPAL.



# 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.



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** 

# **DEPARTMENT OF PHARMACEUTICAL CHEMISTRY** SEMINAR FEEDBACK FORM

STUDENT NAME:

DATE:

YEAR/ COURSE:

NAME OF THE SEMINAR:

**DURATION:** 

E	1	1/	VI	LI	JA	T	E	H	0	N	E	S	r	L	Y	

Questions	Excellent	Good	Fair	Poor
The objectives of the training were				
The instructor's contribution to the course was:				
The presentation materials were relevant				
The instructor's effectiveness in teaching the subject matter was:			•	
Answers to the students questions by the instructor				
The venue was appropriate for the event			ı	
Course organisation was:				
Level of course was				
Course content was:				

#### **Student Participation**

- 1. 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)15UP
- 2. What grade do you expect in this course? A)BELOW 50% B) 50-60% C) 60-70% D) 70-80% E) ABOVE 80%

PRINCIPAL

JKK MUNIRAJAH MEDICAL RESEARCH FOUNDATION ANNAI JKK SAMPOORANI AMMAL COLLEGE OF PHARMACY. ETHIRMEDU, KOMARAPALAYAM - 638 183, NAMAKKAL DISTRICT, TAMILNADU.

Signature of the Student

### 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.



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

# ABOUT THE ONE DAY SEMINAR TITLED ON: "COMPUTATIONAL CHEMISTRY IN DRUG DESIGN: SIMULATING SUCCESS"

This one-day seminar, titled "Computational Chemistry in Drug Design: Simulating Success", is aimed at shedding light on the pivotal role of computational chemistry in the modern drug discovery process. As pharmaceutical research continues to evolve, the use of computational tools has become indispensable in the design, simulation, and optimization of drug molecules.

The seminar will focus on how advanced computational techniques are transforming the traditional approaches to drug design by reducing time, cost, and resources. It will provide attendees with insights into the latest innovations in molecular modeling, quantum chemistry, and simulation techniques, all of which are crucial in predicting molecular interactions and improving the efficacy of potential drug candidates.

#### Key Highlights of the Seminar:

- Introduction to Computational Drug Design: A foundational overview of how computational chemistry accelerates drug discovery.
- Molecular Modeling and Dynamics: How simulations aid in understanding drug-target interactions at the molecular level.
- Structure-Based Drug Design and Virtual Screening: Using computational approaches to identify and optimize lead compounds.
- Case Studies: Success stories of drugs developed using computational chemistry techniques.

• Challenges and Future Trends: Analyzing the current limitations of computational chemistry and exploring future trends in the field.

This seminar is designed for pharmaceutical researchers, students, and professionals who wish to deepen their understanding of how computational techniques are driving innovation in drug discovery. Participants will gain practical knowledge of the tools and methodologies that are shaping the future of the pharmaceutical industry.

Programme Co-ordinator He

Principal

ANNAI JKK SAMPOORANI AMMAL COLLEGE OF PHARMACY

Approved by: Pharmacy Council of India, New Delhi &



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

#### **DEPARTMENT OF PHARMACEUTICAL CHEMISTRY**

#### STUDENT FEEDBACK FORM NAME OF STUDENT: **REGISTRATION NO:** COURSE: YEAR & SEMESTER: **SEMINAR TOPIC:** DATE & TIME: Overall, how satisfied were you with this seminar? Very satisfied Satisfied 0 Neutral Dissatisfied Very dissatisfied How clear were the ideas and concepts we presented? 2. Extremely clear Very clear Moderately clear Not very clear Not at all clear What percentage of the information was new to you? 3. 100% 0 75% C 50% 25% How informative did you find our seminar? 4. **Extremely Informative** Very Informative Moderately Informative Not very informative

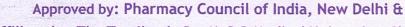
	ဝ	Not informative at all
5.	We	ere there any technical issues that prevented you from seeing or hearing the
semi	nar?	
		Yes
	0	No
6. W	ould ;	you like to learn more about this topic?
		Yes
	_0	No
7.		te the content of the slides/virtual aid?
	0	Extremely clear
312	0	Very clear
	ಂ	Moderately clear
	0	Not very clear
	0	Not at all clear
8.		w accurate was the session description?
	ಂ	Extremely clear
	C	Very clear
	o	Moderately clear
	0	Not very clear
	0	Not at all clear
9.	Ho	w did the session compare to your expectations?
	-0	Excellent
	0	Good
	0	
	0	Fair
811	0	Poor Not at all clear
10.		w would you rate the content of the seminar?
	C	
	0	
	C	
	C	3
	_	



Student Name with Signature

Dr. N.SENTHILKUMAR, PRINCIPAL,

# ANNAI JKK SAMPOORANI AMMAL COLLEGE OF PHARMACY



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



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

#### STUDENTS FEEDBACK ANALYSIS

DATE: 25/11/2023

s.No	QUESTION DESCRIPTION	ANSWERS	MARKS	TOTAL MARKS
		Very satisfied	5	
	Control of Manager 19 Control of	Satisfied	3	
1	Satisfaction	Neutral	2	5
		Dissatisfied	1	
		Very dissatisfied	0	
		Extremely clear	5	
		Very clear	4	
2	Clarity	Moderately clear	2	5
		Not very clear	1	
A British Mark Company		Not at all clear	0	
The House of the Control of the Cont		100%	5	
		75%	4	
3	Percentage of the information was new	50%	3	5
	imormation was new	25%	2	
		0%	1	
	0.2 % And Co.	Extremely Informative	5	
		Very Informative	3	
4	Informative	Moderately Informative	2	5
		Not very informative	1	
		Not informative at all	0	
5	Technical issues	Yes	5	<b>F</b>
	recimical issues	No	0	5

6	Like to learn more about	Yes	5	5
O The Control of the	this topic	No	0	3
	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Extremely clear	5	
		Very clear	3	
7	Rate the content of the	Moderately clear	2	5
	slides/virtual aid	Not very clear	1	
	Company of the compan	Not at all clear	0	
		Extremely clear	5	
		Very clear	3	
8	Accuracy of the sessions	Moderately clear	2	5
		Not very clear	1	
And the second s		Not at all clear	0	
	- Historian	Excellent	5	
		Good	3	
9	Session expectations	Fair	2	5
		Poor	1	
	Cast the same	Not at all clear	0	
		1	1	
		2	2	
10	Rate the content of the seminar	3	3	5
	Schillar	4	4	
1 - 1		5	5	

Head of the Department

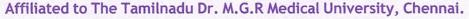
Principal

Dr. N.SENTHILKUMAR, PRINCIPAL,



## ANNAI JKK SAMPOORANI AMMAL COLLEGE OF PHARMACY

Approved by: Pharmacy Council of India, New Delhi &





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

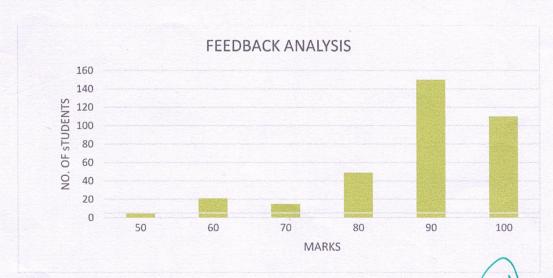
Website: www.jkkmmrfpharmacy.edu.in/e.mail: principal@jkkmmrfpharmacy.edu.in Contact No: +919789456750, +919943066944, +919943069944

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

#### REPORT SUMMARY

#### Feedback Question Analysis - Question Asked-Feedback Rating

1.Satisfaction	6.Like to learn more about this topic
2.Clarity	7.Rate the content of the slides/virtual aid
3. Percentage of the information was new	8.Accuracy of the sessions
4.Informative	9.Session expectations
5.Technical issues	10.Rate the content of the seminar





Dr. N.SENTHILKUMAR, PRINCIPAL.

# 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.



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

#### LIST OF STUDENTS ENROLLED FOR THE SEMINAR

S.NO	REG.NO	NAME OF THE STUDENTS	COURSES
5.110	KEG.NO	NAME OF THE STUDENTS	COURSES
1	560022507551	PALANISAMY P	II B.PHARM III SEM
2	560022507552	PAVISH V	II B.PHARM III SEM
3	560022507553	PRADHAP E	II B.PHARM III SEM
4	560022507554	PRAGADEESWARAN S D	II B.PHARM III SEM
5	560022507555	PRAVEEN K S	II B.PHARM III SEM
6	560022507556	PREM L	II B.PHARM III SEM
7	560022507557	PRITHA R	II B.PHARM III SEM
8	560022507558	PRITHIKA M	II B.PHARM III SEM
9	560022507559	PRIYADHARSHINI S	II B.PHARM III SEM
10	560022507560	RAGAPRIYA R	II B.PHARM III SEM
11	560022507561	RAHUL R	II B.PHARM III SEM
12	560022507563	RAMESH V	II B.PHARM III SEM
13	560022507564	RANJITHKUMAR M	II B.PHARM III SEM
14	560022507565	RASIKA R S	II B.PHARM III SEM
15	560022507566	RITHIKA S	II B.PHARM III SEM
16	560022507567	SACHIN G	II B.PHARM III SEM
17	560022507568	SADAKHATH W	II B.PHARM III SEM
18	560022507569	SANJAY M	II B.PHARM III SEM



Dr. N.SENTHILKUMAR, PRINCIPAL,

19.	560022507570	SANJAY KUMAR S	II B.PHARM III SEM
20	560022507571	SARATH P	II B.PHARM III SEM
21	560022507572	SARATHYLINGAM S R	II B.PHARM III SEM
22	560022507573	SARAVANAN K	II B.PHARM III SEM
23	560022507574	SARAVANESH M	II B.PHARM III SEM
24	560022507575	SARIGASRI K	II B.PHARM III SEM
25	560022507576	SATHISH A	II B.PHARM III SEM
26	560022507577	SEKAR G	
27	560022507578	SHEIK ABDULLA M	II B.PHARM III SEM
28	560022507579	SHOMESHWARAN P	II B.PHARM III SEM
29	560022507580	SIVANI C	II B.PHARM III SEM
30	560022507581		II B.PHARM III SEM
31		SRIRAM S	II B.PHARM III SEM
	560022507582	SUBAN M	II B.PHARM III SEM
32	560022507583	SUBASH K	II B.PHARM III SEM
33	560022507584	SUJITH S	II B.PHARM III SEM
34	560022507585	SUNDARRAJ T	II B.PHARM III SEM
35	560022507586	SURESH C	II B.PHARM III SEM
36	560022507587	TAMILSELVAN M	II B.PHARM III SEM
37	560022507588	VAISHNAVI P	II B.PHARM III SEM
38	560022507589	VASANTH R	II B.PHARM III SEM
39_	560022507590	VENKATESHWARI K	II B.PHARM III SEM
40	560022507591	VIGNESHWARAN K	II B.PHARM III SEM
41	560022507592	VIJAYANANTH A	II B.PHARM III SEM
42	560022507594	YESWANTH V	II B.PHARM III SEM
43	560022507595	YUVARAJ C	II B.PHARM III SEM
44	560023507600	DEEPAK B	II B.PHARM III SEM
45	560023507601	DINESH R	II B.PHARM III SEM
46	560023507602	HARIKISHORE P	II B.PHARM III SEM
47	560023507603	HARIPRASANTH M	II B.PHARM III SEM
48	560023507604	JAYASRI R	II B.PHARM III SÉM



Dr. N.SENTHILKIMAR,
PRINCIPAL,

49	560023507605	MAHESHBOOPATHI G	II B.PHARM III SEM
50	560023507606	MANIKANDAN S	II B.PHARM III SEM
51	560023507607	MOHAN RAJ R	II B.PHARM III SEM
	560023507608	NISHA POONGODI	II B.PHARM III SEM
52	300023307008	KUMARAVEL	
53	560023507609	PUGAZH K	II B.PHARM III SEM
54	560023507610	SARAVANAN S	II B.PHARM III SEM
55	560023507611	SELVAMURUGAN C G	II B.PHARM III SEM
56	560023507612	SUNDARAPANDIYAN D	II B.PHARM III SEM
57_	560023507613	UDHAYACHANDRAN M	II B.PHARM III SEM
58	560023507614	VIDHYABHARATHI J	II B.PHARM III SEM
59	560023507615	YUVARAJ M	II B.PHARM III SEM

Programme Co-ordinator Nob

Principal



# 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.



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

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

Contact No: +919789456750, +919943066944, +919943069944

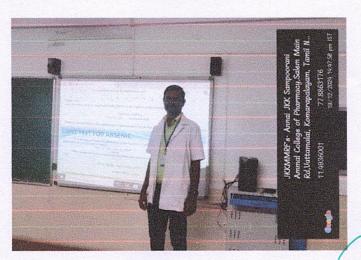
Dr. N. SENTHILKUMAR, Ph.D.,
Principal

#### Seminar photos

**Title:** Structure-Based Drug Design: From Virtual Screening to Lead Optimization **Date:**24/11/23

Resource person interact with students





Dr. N.SENTHILKUMAR, PRINCIPAL,





# JKKMMRF'S ANNAI JKK SAMPOORANT AMMAL COLLEGE OF PHARMACY, KOMARAPALAYAM. Certificate of Participation

This certificate is proudly awarded to

HAS PARTICIPATED AS A DELEGATE IN THE SEMINAR TITLED ON "Computational Chemistry in Drug Design: Simulating Success" IN THE JKKMMRF'S ANNAI JKK SAMPOORANI AMMAL COLLEGE OF PHARMACY, KOMARAPALAYAM ON 24.11.2023.

COORDINATOR



PRINCIPAL