
NIRMALA COLLEGE OF PHARMACY MUVATTUPUZHA
Seminar On
COMPUTER AIDED
DRUG DESIGN
Resource Person
Tuesday
27 JUNE 2023
Time:9.30 am -4.30 pm
Dr.P.V Krishnan Namboori
Associate Professor
Amrita Vishwa Vidya Peetham
CEO Bio Pharma Solutions
Organised By
DEPT. OF PHARMACEUTICAL CHEMISTRY
IN ASSOCIATION WITH KSCSTE AND IMAG


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Date: 10/2/2023

COURSE TITLE: ADVANCED COMPUTATIONAL DRUG DESIGN

Credit: 3 Theory & 2 Practical

AIM:
The purpose of this course is to help students to understand the Advanced Computational Drug Design is to expedite and improve the process of discovering new drugs or optimizing the existing ones.

OBJECTIVE:
The objective of the training course on "Advanced Computational Drug Design" is to bring up the development of advanced tools specifically tailored for the pharmaceutical sector.

Course Outcomes

Upon completion of the course, the student shall be able to understand and apply

Course outcome 1 (CO1): Design and discovery of lead molecules

Course outcome 2 (CO2): The role of drug design in drug discovery process

Course outcome 3 (CO3): The concept of QSAR and docking

Course outcome 4 (CO4): Various strategies to develop new drug like molecules.

Course outcome 5 (CO5): Illustrative example of designing an active biomolecule against any target

Sl no	Content	Hours
1	Introduction to drug design, Ligand based and target bases approaches, Mechanism based drug design, Principles and mechanisms of drug action, Natural substances as drugs, Target and potential molecules screening using SAR/Biomolecular networking, Evolutionary molecules, drug likeness screening, concept of pharmacophore mapping and pharmacophore-based screening, Docking based screening.	5
2	Modeling and simulation for drug design, Deep drug design, Development Stages of drug discovery and development, Molecular view of diseases and drug-target molecules, Software tools used to retrieve Drug targets, Ligands and Ligand databases, Software tools used to process molecular data files, Drug absorption, distribution, Receptor-Drug interactions	5

3	Protein modeling, Molecular docking and drug receptor interactions, Dinding site identification, Structure based drug designing, Molecular Dynamics and binding free energy methods, Homology Model Building, QSAR, 3D-QSAR, Deep learning for active screening, Evaluation of docking using MD simulation, MMPBSA, MMGBSA, Structural and dynamic aspects of protein-ligand complexes.	8
4	Target identification, Target characterization, The Drug Design Process for a Known Protein target, The Drug Design Process for an Unknown target, Drug Design for Other targets.	7
5	Illustration and hands-on training with the modeling and simulation tools and platforms, Google cloud-based modeling and simulation, use of Jupyter notebooks, Repurposing of drugs, Computational research in the area of Cancer, Life-style diseases and degenerative disorders.	7

REFERENCES:

1. Burger's Medicinal Chemistry and Drug Discovery

2. Comprehensive Medicinal Chemistry. Vol IV.

3. G. Patrick. (2013) An Introduction to Medicinal Chemistry. Oxford University Press, UK.

4. D. C. Young. (2009) Computational Drug Design – A Guide for Computational and Medicinal Chemist. John Wiley & Sons, Inc., Hoboken, New Jersey.

5. A. Hinchliffe. (2008) Molecular Modelling for Beginners. John Wiley & Sons Ltd, England.

Admission eligibility: Candidates studying in B Pharm / Pharm D/M Pharm course at Nirmala College of Pharmacy, Muvattupuzha, Emakulam are eligible to apply.

Assessment mode: Theory Exam -Multiple choice questions

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Passing criteria: Candidate must have at least 80% attendance in both theory and practical sessions and must score at least 50% marks in the examination to pass the course.

Prepared by :Mrs. Saranya TS,
Assistant Professor,
Department of Pharmaceutical Chemistry,
Nirmala College of Pharmacy.

NIRMALA
COLLEGE OF PHARMACY
Nirmala Hills, Muvattupuzha P.O,
Ernakulam district, Kerala, India - 686 661

Date : 08|03|2023

ADDON COURSE SYLLABUS VETTING FORM

NAME OF ADDON COURSE: ADVANCED COMPUTATIONAL DRUG DESIGN (ACDD5)

S.NO	Parameters	Remarks
1	Whether the content of syllabus is sufficient to meet the outcome	Yes
2	Whether the number of hours mentioned for each unit is appropriate for achieving the outcome.	Yes
3	Is there any gap in the syllabus based on outcome mentioned?	No
4	Whether the assignment /activities sufficient to inculcate the outcome in the students.	Yes
5	Suggestion if any	Nil

DECLARATION

I hereby recommended/recommended with modification, the above add on course.

Name: Dr P K Krishnan Namboori

Designation: CEO-Biopharma Solutions

Signature:

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info@nirmalacp.org
www.nirmalacp.org

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NBA NATIONAL BOARD OF ACCREDITATION

NIRMALA
COLLEGE OF PHARMACY
Nirmala Hills, Muvattupuzha P.O,
Ernakulam district, Kerala, India - 686 661

Date : 10/05/2023

ADD- ON COURSE SYLLABUS APPROVAL FORM

NAME OF THE COURSE: ADVANCED COMPUTATIONAL DRUG DESIGN (ACDD5)

S No.	Name	Designation	Signature
1	Rev.Fr. Jose Pullopillil	Administrator	
2	Prof.Dr. Badmanaban R	Principal	
3	Prof.Dr.Deepa Jose	ARC Head	
4	Dr. Dhanish Joseph	IQAC Head	

DECLARATION :

I hereby approve/approve with modification, the above add on course.

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NIRMALA COLLEGE OF PHARMACY, MUVATTUPUZHA

DEPARTMENT OF PHARMACEUTICAL CHEMISTRY

OFFERING ADD-ON COURSE ON

ADVANCED COMPUTATIONAL DRUG DESIGN

BIOPHARMA SOLUTIONS
The R&D solution to academic needs

In association with

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A6-B Staff Quarters Amrita VishwaVidyapeetham, 641112 Coimbatore

AIM:

The purpose of this course is to help students to understand the Advanced Computer Aided Drug Design is to expedite and improve the process of discovering new drugs or optimizing the existing ones.

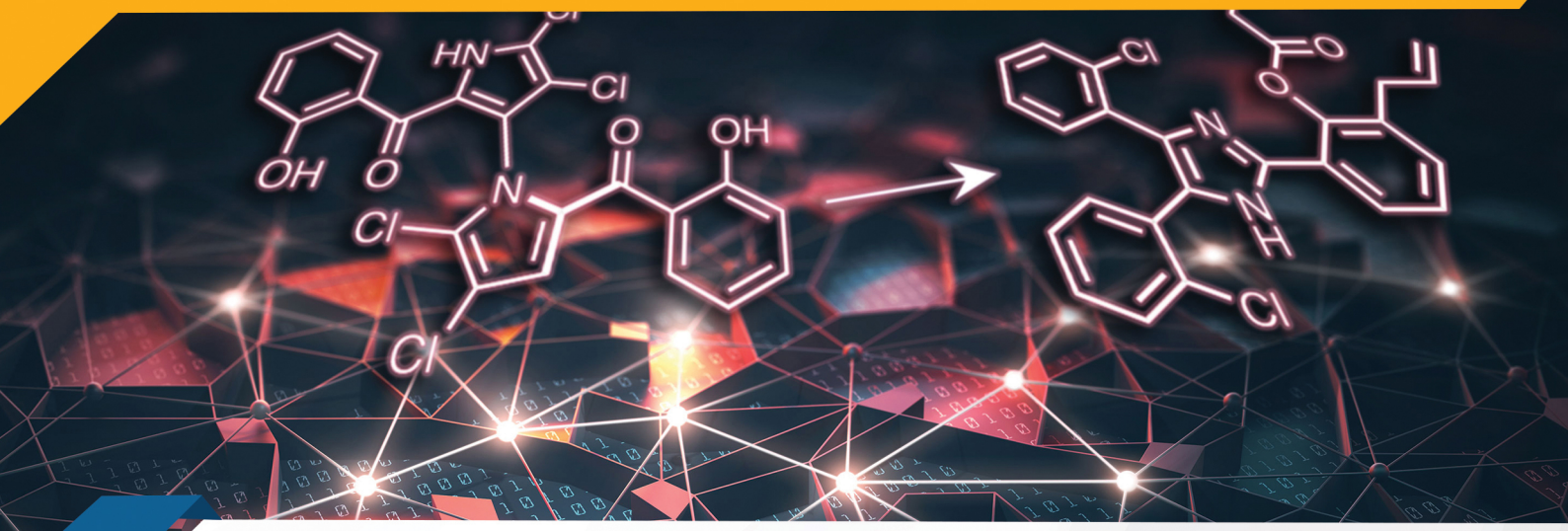
OBJECTIVE:

The objective of the training course on "Advanced Computer-Aided Drug Design" is to bring up the development of advanced tools specifically tailored for the pharmaceutical sector.

COURSE OUTCOMES

- Upon completion of the course, the student shall be able to understand and apply
- Course outcome 1: Design and discovery of lead molecules
- Course outcome 2: The role of drug design in drug discovery process
- Course outcome 3: The concept of QSAR and docking
- Course outcome 4: Various strategies to develop new drug like molecules.
- Course outcome 5: Illustrative example of designing an active biomolecule against any target

START DATE :05/06/2023



ADMISSION ELIGIBILITY:

Candidates studying in B Pharm / Pharm D/M Pharm course at Nirmala College of Pharmacy, Muvattupuzha, Ernakulam

ASSESSMENT MODE:

Exam –Theory (Multiple choice questions) &Practical Section

PASSING CRITERIA:

Candidate must have at least 80% attendance in both theory and practical sessions and must score at least 50% marks in the examination

COURSE COORDINATOR

MRS. SARANYA T S
ASSISTANT PROFESSOR
DEPT. OF
PHARMACEUTICAL CHEMISTRY

NIRMALA COLLEGE OF PHARMACY

Muvattupuzha P.O., Ernakulam District, Kerala - 686 661, India.
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(Approved by PCI, NewDelhi, Govt. of Kerala and affilliated to Kerala University of Health Sciences, Thrissur)

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ADD ON COURSE ENROLLMENT REGISTER

NIRMALA COLLEGE OF PHARMACY
Muvattupuzha

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ADD ON COURSE ENROLLMENT REGISTER

Name of Course : ADVANCED COMPUTATIONAL BIOCHEMISTRY. **Course Code :** ACBOG

Duration : 35 Hrs **Academic Year :** 2022-2023 **Period of Course :** 1 month

Sl. No.	College Admission Number	Name of the Student	Program of Study	Batch	Semester / Year of Study	Student Signature
1	1393	Aboobakkar Sidhik Sunil	PharmD	2020-2026	3rd Year	
2	1389	Anas Muhammed Azad	PharmD	2020-2026	3rd Year	
3	1224	Anjana Raj	PharmD	2020-2026	3rd Year	
4	1394	Aparna S Biju	PharmD	2020-2026	3rd Year	
5	1385	Ashly Mary Mathew	PharmD	2020-2026	3rd Year	
6	1386	Ayona Elezabeth	PharmD	2020-2026	3rd Year	
7	1370	Edwin Sam	PharmD	2020-2026	3rd Year	
8	1397	Eveena Sara Binny	PharmD	2020-2026	3rd Year	
9	1373	Freddy Alappatt	PharmD	2020-2026	3rd Year	
10	1376	Gouri Ganesh	PharmD	2020-2026	3rd Year	
11	1380	Hanna Mathew	PharmD	2020-2026	3rd Year	
12	1388	Hila A.D	PharmD	2020-2026	3rd Year	
13	1387	Jannath Parwin K I	PharmD	2020-2026	3rd Year	
14	1371	Jeevan Joseph Jaison	PharmD	2020-2026	3rd Year	
15	1244	Mabel Angustine	PharmD	2020-2026	3rd Year	
16	1396	Megha Shaji	PharmD	2020-2026	3rd Year	
17	1378	Nadheem Muhammed Shajee	PharmD	2020-2026	3rd Year	
18	1369	Nandhana Shibu	PharmD	2020-2026	3rd Year	
19	1374	Nancy Joseph	PharmD	2020-2026	3rd Year	
20	1368	Naveen K Biju	PharmD	2020-2026	3rd Year	
21	1384	Sana Fathima	PharmD	2020-2026	3rd Year	
22	1375	Sandra Baby	PharmD	2020-2026	3rd Year	

NIRMALA COLLEGE OF PHARMACY

Muvattupuzha

ADD ON COURSE ENROLLMENT REGISTER

Name of Course : ADVANCED COMPUTATIONAL BIOCHEMISTRY Course Code : ACBOG

Duration : 36 Hrs Academic Year : 2022-2023 Period of Course : 1 months

Sl. No.	College Admission Number	Name of the Student	Program of Study	Batch	Semester / Year of Study	Student Signature
23	1391	Sneha Susan Samuel	PharmD	2020-2026	3rd year	
24	1381	Tania Sibi	PharmD	2020-2026	3rd year	
25	1372	Teresa Mary Sabi	PharmD	2020-2026	3rd year	
26	1390	Vaishnavi Vijay	PharmD	2020-2026	3rd year	
-						

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Muvattupuzha

ADD ON COURSE ENROLLMENT REGISTER

Name of Course : ADVANCED COMPUTATIONAL-DRUG DESIGN. Course Code : ACDD05

Duration : 32 Hrs Academic Year : 2022-2023 Period of Course : 1 Month

Sl. No.	College Admission Number	Name of the Student	Program of Study	Batch	Semester / Year of Study	Student Signature
1	1542	ANJANA BABY	(PHARMACOLOGY) M.PHARM	2021-2023	II SEM	
2	1544	JESNA THANKAM JOHN	(PHARMACOLOGY) M PHARM	2021-2023	II SEM	
3	1541	THASNI PM	(PHARMACOLOGY) M.PHARM	2021-2023	II SEM	