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

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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

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.

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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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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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