SARVAJANIK UNIVERSITY
INCLUSIVE | INTEGRATED | INNOVATIVE

SARVAJANIK UNIVERSITY
Sarvajanik College of Engineering and Technology
Department of Computer Engineering / Information Technology

PhD, Semester 1
Course Work

Subject Name: AI and ML for Drug Discovery **Subject Code:** PTCO13102
Type of course: Self Study Course
Prerequisite (if any): AI & ML
List of Courses where this course will be prerequisite: --

Rationale: Classical drug discovery process is a time consuming and expensive process. It takes roughly 12 years for drug to reach marketplace and it costs around US 1.0 B dollars. Several candidates that enter clinical trials fail because of several reasons. Computer assisted drug design can speed up the process, reduce surprises and predict the properties, thereby reduce the cost of R&D

Teaching and Examination Scheme:

TEACHING SCHEME				Theory Marks			Practical Marks		Total
L	T	P	C	TEE	CA1	CA2	TEP	CA3	
0	0	0	4	60	25	15	0	0	100

CA1: Continuous Assessment (assignments/projects/open book tests/closed book tests CA2: timely submissions of assignments/self-learning attitude/solving advanced problems TEE: Term End Examination TEP: Term End Practical Exam (Performance and viva on practical skills learned in course) CA3: Regular submission of Lab work/Quality of work submitted/Active participation in lab sessions/viva on practical skills learned in course

Content:

No.	Description	No. of Hours
1	Introduction: Introduction to drug discovery, Drug discovery process, Drug targets, Applications of AI and ML at different stages of drug discovery, Benefits and drawbacks of AI in drug discovery, Current available solutions in drug discovery based on AI and ML techniques	8
2	Drug Discovery: Proteomics, Genomics, Drug discovery issues, Drug databases, Compound selection & preclinical studies, Target and lead identification, Drug properties: SMILES, solubility, permeability, ADME.	12
3	AI and ML for Drug Discovery: Introduction to artificial neural networks and their applications in drug discovery, Molecule properties prediction	10

	using supervised, semi-supervised and self-supervised learning, Convolutional neural networks, Recurrent neural networks.	
4	Genome in Drug Discovery: Comparing Genome sequences, Principal component analysis on Genome sequences, cluster the genome sequences using the K-means algorithm, Predicting bit score to find sequence matches	8
5	Deep Learning for Genomics: Applications of deep learning to regulatory genomics, variant scoring and population genetics, Applications of deep learning to predicting protein structure and pharmacogenomics	11
6	Advanced Concepts: De novo Molecule Generation and optimization, Rection prediction and retro synthesis, Multiomics and Clinical Data-based Drug Repurposing, Case Studies from the Literature.	11

Reference Books:

Sr No	Title of book /article	Author(s)	Publisher and details like ISBN	Year of publication	Publication Edition
1.	Molecular Modelling: Principles and Applications -	Andrew R. Leach	Pearson Higher Education	2001	-
2.	Genomics in Drug Discovery and Development	Dimitri Semizarov, Eri c Blomme	Wiley	2008	-
3.	Artificial Intelligence In Drug Discovery by Edited by Nathan Brown, Royal Society Of Chemistry	Nathan Brown	Royal Society Of Chemistry	2020	
4.	Artificial Intelligence in Drug Design	Alexander Heif etz	Humana, New York	2022	1st edition

Course Outcomes:

Sr. No.	CO statement	Marks % weightage
CO-1	Acquire information on the state-of-the art AI methods applied in computer aided drug discovery	15

CO-2	Aanalyze genome sequences to find similarities and identify target subsequences using predictive models.	25
CO-3	Identify various Drug-Target Interactions using various machine learning and deep learning techniques	30
CO-4	Apply different machine learning and deep learning algorithms for various stages of drug discovery process	30

List of Open learning website:

1. NPTEL Course on Computer Aided Drug Design: https://nptel.ac.in/courses/102/106/102106070/
2. Udemy course on Introduction to AI & ML techniques in drug discovery: https://www.udemy.com/course/introduction-to-artificial-intelligence-techniques-in-drug-discovery/

List of Open Source Software:

1. Open Source Python Libraries : NumPy, SciPy, Pandas, SCIKIT-Learn, TensorFlow, BeautifulSoup, Matplotlib, Seaborn
2. IDEs: Jupyter Notebook, Spyder, WIDE -Google Colab

FOR LAB SESSIONS:

List of Experiments: