Dr. B.C. Roy College of Pharmacy and Allied Health Sciences

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Approved by PCI & Affiliated to MAKAUT, WB and WBSCT&VE&SD
Dr. Meghnad Saha Sarani, Bidhannagar, Durgapur-713206, West Bengal (India)

ADD ON COURSE: COMPUTATIONAL DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND BIOINFORMATICS

COURSE CONTENT/ STRUCTURE

No. of Chapter	Name of the Chapter	Theory (h)	Lab (h)
1	Brief Introduction of QSAR and its workflow	1	1
2	Structure drawing with ACD Lab Chemsketch/ Chem Office, download, installation, creating new molecules and playing with various parameters to edit the molecule, switch between 2D and 3D parameters	1	1
3	Concept of molecular mechanics and semi-empirical methods of energy minimization, Use of AVOGADRO, CORINA, ORCA, MOPAC, GAMESS etc., concept of Molecular Modeling	1	1
4	Building up 2D QSAR model equation with biological acitivity (predicted) and molecular descriptors, using REGRESSION ANALYSIS and ARRAY FORMULA	1	1
5	Validating QSAR model, comparison between OBA and PBA by ANOVA (Student t-test)	1	1
6	Use of genetic algorithm in QSAR model development- Use of DTC-QSAR and QSARIN, Use of Q2, Williams plot and other validations	1	1
7	*In silico* drug likeliness testing, application of Lipinski Rule of Five, Using Molinspiration server, in silico toxicity testing, using admetSAR, to screen drug molecules	1	1

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Prof. (Dr.) Samir Kumar Samanta
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8	Concept of Docking	1	1
9	Working with PDB, protein structure search, downloading protein structure in PDB format	1	1
10	Working protein structure in UCSF chimera, add hydrogens, delete native water molecules, preparation of final protein structure in .pdb format	1	1
11	Predicting biological activity of selected compounds by molecular docking with SWISSDOCK or PARDOCK, counting the docking scores, analysing protein-ligand binding interactions with UCSF Chimera	1	1
12	Basic Bioinformatics Working with gene and protein sequences from NCBI, downloading gene and protein sequences	1	1
13	BLAST, Multiple sequence alignment (MSA) by CLUSTALW/OMEGA, structure and functional analysis from MSA, finding active sites of proteins by bioinformatics with DISCOVERY STUDIO VISUALIZER, mapping ligand-protein interactions	1	1
14	Phylogenetic analysis by MEGA, TREE construction	1	1
15	Basic concept of Homology modeling, Introduction to SWISS MODEL and MODELLER	1	1
Total contact hours = 30			

Sourav Barua 31/1/23

SIGNATURE OF THE COURSE COORDINATOR

SIGNATURE OF THE PRINCIPAL

Dr. B. C. Roy College of Pharmacy & AHS, Durgapur

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