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

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

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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Dt: 05.12.2022

NOTICE

We are delighted to announce that like previous years, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India is again going to conduct the Add-on Course on **"Computational Drug Design using QSAR/ Cheminformatics and Bioinformatics"** for the Academic year **2022-23**. The Add on course will be a hands-on workshop and will be conducted on both theoretical and practical basis. The theoretical demonstration will be in smart classroom based course delivery while hands on practice sessions would be performed in computer laboratory.

The course will commence from 21st February, 2023 and will be conducted every week on Tuesday and Thursday. The class timing is 6:00-8:00 pm on each assigned day. The total course would be conducted for M. Pharm 1st year students for a total duration of 08 weeks and will be free of cost. Certificates would be issued upon completion of the course based on attendance greater than or equal to 85%.

The soft copy of the Enrolment/ Registration form is available with the Course Coordinator Dr. Souvik Basak, Associate Professor and Divisional-In-Charge, Department of Pharmaceutical Chemistry. Interested students are requested to submit the filled up printed copy of the registration form after duly signing the form.

The deadline of Registration is 11th January, 2023.

Prof. Subhabrata Ray
Principal

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