

Report on ICT/COMPUTATION

AY:2016-2021

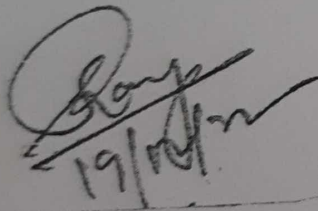
Dr. B.C. Roy College of Pharmacy & Allied Health Sciences (BCRCPAHS), Durgapur, WB started the **ICT/computational drug design** using Cheminformatics and Bioinformatics from 2017, with twelve students. The programme was not only designed for Pharmacy students but also for other Science students such as BSc and MSc in chemistry, Microbiology, Biochemistry, Physiology, Biotechnology, etc. Reaching and helping out to students with different mode of learning. Later, in 2019-20, eleven students enrolled in the course. All students attending the course received certificate. With the purpose was to start revenue generation, publicity the name of our esteemed college, direct introduction to the industrially experienced personnel and to establishing Institute-Industry partnership, SRM-Biotech also agreed to be a partner in launching the online course. The certificate course received preliminary approval and the course with renamed as “Virtual Skill Development Programme: a learning companion for student.” In the year 2020-21, about eight students enrolled for the course and received the certificates. The course instructor includes Dr. Souvik Basak, Associate Professor, BCRCP, Dr. Parthasarathi Panda, Assistant Professor, BCRCP and Mr. Shobhan Bose, Assistant Professor, BCRCP.

The following are the Online Course Chapters

- 1 Brief Introduction of QSAR and its workflow
- 2 Structure drawing with ACD Lab ChemsSketch/ ChemOffice, download, installation, creating new molecules and playing with various parameters to edit the molecule, switch between 2D and 3D parameters
- 3 In silico drug likeliness testing, application of Lipinsky Rule of Five, Using Molinspiration server, in silico toxicity testing, using admetSAR, to screen drug molecules
- 4 Concept of Docking

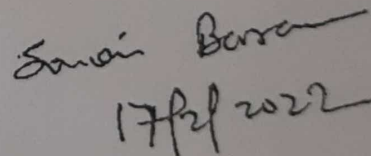


- 5 Working with PDB, protein structure search, downloading protein structure in PDB format
- 6 Working protein structure in UCSF chimera, add hydrogens, delete native water molecules, preparation of final protein structure in .pdb format
- 7 Predicting biological activity of selected compounds by molecular docking with SWISSDOCK or PARDOCK, counting the docking scores, analysing protein-ligand binding interactions with UCSF Chimera
- 8 Building up 2D QSAR model equation with biological activity (predicted) and molecular descriptors, using REGRESSION ANALYSIS and ARRAY FORMULA
- 9 Validating QSAR model, comparison between OBA and PBA by ANOVA (Student t-test)
- 10 Basic Bioinformatics Working with gene and protein sequences from NCBI, downloading gene and protein sequences


19/11/22

Principal

Dr. B. C. Roy College of Pharmacy & A.H.S.
Sidhannagar, Durgapur-713206, Burdwan


17/12/2022





Date: 10/01/2017

Implementation of Certification course on “Computational drug design using QSAR/Cheminformatics and Bioinformatics”

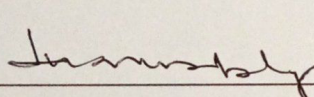
- From the theoretical classes on Medicinal Chemistry involving QSAR it has seemed that special emphasis should be provided on drug design-based components which often included additional concepts on applied physics, chemistry, mathematics, statistics, biology, protein structures *vis a vis* computational software to understand, learn and apply their knowledge in this particular domain. In addition, hands on training may be provided to the students for their understanding benefits and application-oriented training.
- Also, it may be perceived that the certificate obtained via theoretical and hands on training may help students to fit in relevant jobs in pharmaceutical and biomedical domain, guide them for relevant competitive examinations such as GPAT, GATE, NET etc. as well as helping them in various project works in both B. Pharm. and M. Pharm. Level.
- The course content may be available in institutional website or *vis a vis* may be disseminated through specific brochures among the students. Along with internal candidates, the institute may spread this course in national and international level either single or by collaboration with other industries/institutes keeping the main essence/value of the course integrated and undisturbed.



Approved by AICTE & PCI and Affiliated to Maulana Abul Kalam Azad University of Technology
(Formerly known as WBUT) Dr. Meghnad Saha Sarani, Bidhannagar, Durgapur - 713206, West Bengal

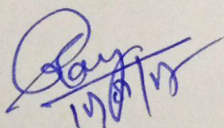
- The institute thus approves and gives no objection for onset of such value-added course for the students, upon completion of which the students would obtain certificates acknowledged by the institute.
- Thus, it is hereby decided that the institute, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur-713206, WB, India is going to initiate certification course on “Computational drug design using QSAR/Cheminformatics and Bioinformatics” from January, 2017.

Approved by

 10/11/2017

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