



## SUMMARY REPORT AND OUTCOME

**Course Name:** COMPUTATIONAL DRUG DESIGN USING QSAR/  
CHEMINFORMATICS AND BIOINFORMATICS

**Start date:** 21.02.2023

**End date:** 25.04.2023

**Total Course Duration:** 30 h

**Number of Student participants:** 29

**Assessment Procedure:** Three examinations each of 50 marks

### SUMMARY REPORT

In continuation with the previous year, the add on course "Computational Drug Design using QSAR/Cheminformatics and Bioinformatics" was launched for the in house student development for Dr. B.C. Roy College of Pharmacy & Allied Health Sciences (BCRCP), Durgapur, WB, India. This year the target audience was students enrolled in Master of Pharmacy 1<sup>st</sup> year since they are the people who are likely to use Drug design and Bioinformatics in their theory and practical papers, their practical projects as well as job opportunities. Twenty nine student participants were enrolled out of total fifty two M. Pharm.1<sup>st</sup> year enrolled students of the institute in the current academic year (AY 2022-23). By the academic support of Hon'ble Principal Prof. (Dr.) Subhabrata Ray, the course was launched and conducted by Dr. Souvik Basak, Divisional In Charge (DIC), Pharmaceutical Chemistry & Associate Professor, BCRCP. This year, five additional modules were introduced and lesson plan was modified to fifteen classes (each of 2 hours) instead of ten classes. Additional modules relating to energy minimization, semi-empirical routes of energy optimization as well as molecular modeling, phylogenetic tree construction, genetic algorithms to construct QSAR models and relevant plots were introduced. The students were trained both theoretically and practically about molecular modeling, energy minimization, QSAR model construction and validation, gene and protein search, downloads, docking, result analysis for virtual screening, drug likeliness search, *in silico* toxicity profiling, homology modeling of proteins and related bioinformatics. The hands on training were conducted on various open source drug discovery tools such as Chem Draw Ultra, AVOGADRO, DS Visualizer, MEGA, CORINA, ORCA, AutoDock Tools, VINA, UCSF Chimera and related softwares. Three assessment examinations were conducted each of 50 marks in between the examinations and at the end, certificates were issued to the students as token of acknowledgements for completing and passing the courses.



*Souvik Basak*  
25/4/23

Dr. Souvik Basak,  
Course Coordinator,

Dr. B. C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India

*[Signature]*  
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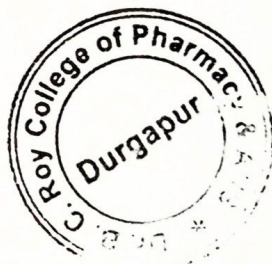
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### OUTCOME

After completion of the course, the final outcomes could be narrated as follows:

- 1) The students were able to **comprehend** the basic principles of Computation Drug Design with the help of Cheminformatics or Bioinformatics
- 2) The students were able to **analyze** various databases related to cheminformatics and bioinformatics and **apply** them in the model of drug design
- 3) The students were able to **understand** various software related to drug design using cheminformatics and bioinformatics
- 4) The students became able to **develop** their own models pertaining to their own projects or realistic problems
- 5) The students advanced towards designing newer drugs using all the trainings given in the course which might be helpful **for their future jobs, Competitive examinations or assigned projects** in relevant fields



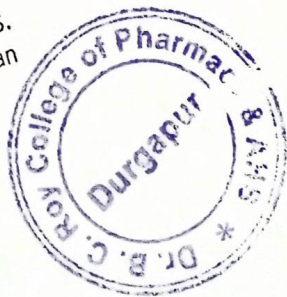
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