

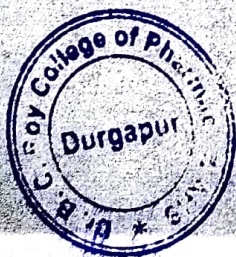


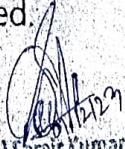
BASIC POLICY

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.



  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

An ISO 9001:2008 Institution Conducting UG & PG Courses

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



Ph (0343) 263 2678/79  
Telefax (0343) 263 2679  
e-mail bcrp\_dgp@yahoo.co.in  
www.bcrp.org/www.bcrp.ac.in

Approved by AICTE & PCI and Affiliated to Maulana Abul Kalam Azad University of Technology (Formerly known as WBUT) Dr. Meghnad Saha Sarani, Bidhannagar, Durgapur - 713208, 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

*Subrata Chakraborty* 10/1/2017

Dr. Subrata Chakraborty,  
Director,

Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur-713206, WB, India

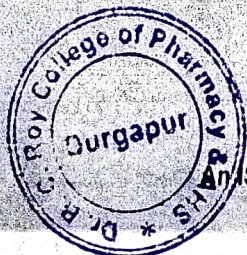
*Samir Kumar Samanta*  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal 713206

*Subhadrata Ray*

Dr. Subhadrata Ray,  
Principal,

Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur-713206, WB, India

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



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Dt: 05.12.2022


## NOTICE

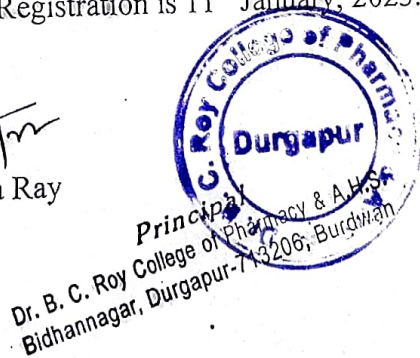
We are delighted to announce that like previous years, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India is again going to conduct the Add-on Course on **“Computational Drug Design using QSAR/Cheminformatics and Bioinformatics”** for the Academic year 2022-23. The Add on 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 21<sup>st</sup> 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 1<sup>st</sup> 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 11<sup>th</sup> January, 2023.

  
Prof. Subhabrata Ray  
Principal



  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206



Dt: 11.01.2023

## NOTICE

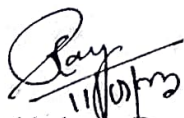
In persuasion of the previous notice dated 05.12.2023 regarding resuming the Add-on course **“Computational Drug Design using QSAR/Cheminformatics and Bioinformatics”** for the Academic year 2022-23, it has been noticed that only 13 students (M. Pharm 1<sup>st</sup> year) have submitted their enrolment form for getting admission of the course. As mentioned earlier, the course will commence from 21<sup>st</sup> February, 2023 and will be conducted every week on Tuesday and Thursday, 6:00-8:00 pm.


We again want to mention that this course would be of great opportunity for the students (M. Pharm 1<sup>st</sup> year for this batch) since this course would let the students learn various CADD and Bioinformatics related techniques together with problem solutions by theoretical as well as hands-on basis. Certificates of accomplishment would also be provided after due completion of the course that would be of great help for students for their future jobs as well as higher studies.


Hence we encourage the M. Pharm 1<sup>st</sup> year students to enrol more in this course and avail this great opportunity for their career purpose.

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

The extended deadline of Registration is 20<sup>th</sup> January, 2023.

  
Prof. Subhabrata Ray  
Principal

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

  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206




Dt: 20.01.2023

## NOTICE

In persuasion of the previous notice dated 11.01.2023 regarding resuming the Add-on course "Computational Drug Design using QSAR/Cheminformatics and Bioinformatics" for the Academic year 2022-23, we are pleased that total 23 students (M. Pharm 1<sup>st</sup> year) have submitted their enrolment form till now. As mentioned earlier, the course will commence from 21<sup>st</sup> February, 2023 and will be conducted every week on Tuesday and Thursday, 6:00-8:00 pm. As a final call, we are extending the last round of registration upto 31.01.2023 to accommodate more students of target batch and help them to avail the opportunities of enrolling in the course.


Please collect the soft copy of the Enrolment/ Registration form from the Course Coordinator Dr. Souvik Basak, Associate Professor and Divisional-In-Charge, Department of Pharmaceutical Chemistry. You are requested to submit the filled up printed copy of the registration form to the course coordinator after duly signing the form.

The final deadline of Registration is 31<sup>st</sup> January, 2023. The final enrolment/ registration of all the entrants will be duly approved by the undersigned, and once done, no more enrolment would be entertained.

  
Prof. Subhabrata Ray  
Principal

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



  
Prof. (Dr.) Sanku Kumar Samanta  
M. Pharm., Ph.D. (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206



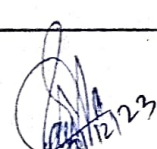
**ADD ON COURSE: COMPUTATIONAL DRUG DESIGN USING QSAR/  
CHEMINFORMATICS AND BIOINFORMATICS**

**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 Chems sketch/ 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 activity (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 Q <sub>2</sub> , Williams plot and other validations	1	1
7	<i>In silico</i> drug likeliness testing, application of Lipinski Rule of Five, Using Molinspiration server, <i>in silico</i> toxicity testing, using admetSAR, to screen drug molecules	1	1



ACCREDITED BY NAAC (B++) & NBA (FOR UG PHARMACY)

  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206



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

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
<b>Total contact hours = 30</b>			

SIGNATURE OF THE COURSE COORDINATOR

SIGNATURE OF THE PRINCIPAL



ACCREDITED BY NAAC (B++) & NBA (FOR UG PHARMACY)

Principal  
Dr. B. C. Roy College of Pharmacy,  
Bidhannagar, Durgapur-713206, Burdwan

Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206





**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 Chems sketch/ 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 activity (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 Q <sub>2</sub> , Williams plot and other validations	1	1
7	<i>In silico</i> drug likeliness testing, application of Lipinski Rule of Five, Using Molinspiration server, <i>in silico</i> toxicity testing, using admetSAR, to screen drug molecules	1	1



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M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206





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

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
<b>Total contact hours = 30</b>			

SIGNATURE OF THE COURSE COORDINATOR

SIGNATURE OF THE PRINCIPAL



ACCREDITED BY NAAC (B++) & NBA (FOR UG PHARMACY)

Principal  
Dr. B. C. Roy College of Pharmacy,  
Bidhannagar, Durgapur-713206, Burdwan

Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206





Dt: 05.12.2022


## NOTICE

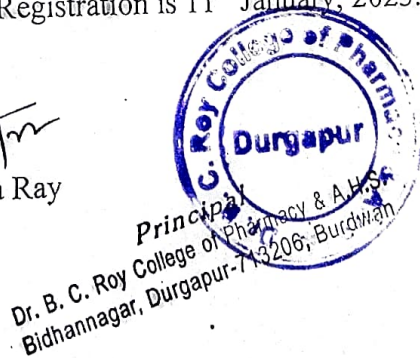
We are delighted to announce that like previous years, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India is again going to conduct the Add-on Course on “**Computational Drug Design using QSAR/Cheminformatics and Bioinformatics**” for the Academic year 2022-23. The Add on 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 21<sup>st</sup> 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 1<sup>st</sup> 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 11<sup>th</sup> January, 2023.

  
Prof. Subhabrata Ray  
Principal



  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**

**ENROLMENT FORM FOR ADD ON COURSE ON "COMPUTATIONAL**  
**DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND**  
**BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

Name of the student : ANUSKA CHATTERJEE

University Roll no.: 2214009

Program: M. Pharm

Division: Pharmaceutics

Ph : 9382039854

e-mail: anuskachat0609@gmail.com

Why opted for this course? : Interested in Molecular modelling, Docking, PDB,  
Protein structures

*A. Chatterjee*  
Signature of the student with date 20/1/23

*Soumi Banerjee*  
Signature of the course coordinator with date 20/1/23



*Ray*  
Signature of the Principal with date 20/1/23



*Prof. (Dr.) Samir Kumar Samanta*  
Principal  
Dr. B. C. Roy College of Pharmacy & A.H.S.  
Bidhannagar, Durgapur-713206, Burdwan  
20/1/23

Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**

**ENROLMENT FORM FOR ADD ON COURSE ON "COMPUTATIONAL**  
**DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND**  
**BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

Name of the student : ANANYA DEY

University Roll no.: 2214011

Program: M. Pharm

Division: Pharmaceutics

Ph : 9382375258

e-mail: ananyadey1694@gmail.com

Why opted for this course? : Drug Design hands on learning, Machine learning in drug delivery design, job interview

*Adey 11/1/2023*

Signature of the student with date

*Souci Baner 11/1/23*

Signature of the course coordinator with date



Signature of the Principal with date

*[Signature]*  
11/1/23

*[Signature]*  
11/1/23

Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D. (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & A.H.S.  
Durgapur, West Bengal-713206

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

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**DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND**  
**BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

Name of the student : PARTHA PRATIM BEZ

University Roll no.: 2214013

Program: M. Pharm

Division: Pharmaceutics

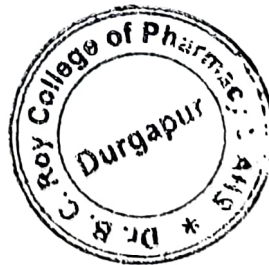
Ph : 6296265214

e-mail: parthabez37@gmail.com

Why opted for this course? : CADD, Statistical analysis in biology

Signature of the student with date *P. Bez* 20/1/23

Signature of the course coordinator with date *Somen Baner* 20/1/23



Signature of the Principal with date



*Ray*  
20/1/23

*[Signature]*  
20/1/23  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)

Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Bldhannagar, Durgapur-713206  
West Bengal

**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH  
SCIENCES  
DURGAPUR, WB, INDIA**

**ENROLMENT FORM FOR ADD ON COURSE ON "COMPUTATIONAL  
DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND  
BIOINFORMATICS"  
ACADEMIC YEAR: 2022-23**

Name of the student : AKASH MONDAL

University Roll no.: 2214014

Program: M. Pharm

Division: Pharmaceutics

Ph : 7001622920

e-mail: tdas92848@gmail.com

Why opted for this course? : CADD, docking, modeling, project purpose

Signature of the student with date *Akash Mondal* 31/1/23

Signature of the course coordinator with date *Soumi Banerjee* 31/1/23

Signature of the Principal with date *Samir Kumar Samanta* 31/1/23

Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal

Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

Principal  
Dr. B. C. Roy College of Pharmacy & AHS,  
Bidhannagar, Durgapur-713206, West Bengal

**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**

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**DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND**  
**BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

Name of the student : ANUPAM BERA

University Roll no.: 2214017

Program: M. Pharm

Division: Pharmaceutics

Ph : 8170085609

e-mail: anupamb601@gmail.com

Why opted for this course? : Interested in Drug Design (CADD), Applicable for Drug delivery

*Anupam Bera*

Signature of the student with date

*20/01/23*

*Soumi Banerjee*  
*20/1/23*

Signature of the course coordinator with date



Signature of the Principal with date

*Ray*  
*21/1/23*

*[Signature]*  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS

Principal  
Dr. B. C. Roy College of Pharmacy & A.H.S.,  
Bidhanagar, Durgapur-713208, B.W.India

**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**

**ENROLMENT FORM FOR ADD ON COURSE ON "COMPUTATIONAL**  
**DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND**  
**BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

Name of the student : SAYANTAN NAG

University Roll no.: 2214006

Program: M. Pharm

Division: Pharmaceutics

Ph : 9064762623

e-mail: sayantannag6@gmail.com

Why opted for this course? : CADD in drug delivery and molecule design

*Sayantana Nag*

Signature of the student with date 11.01.23

*Soumitra Das*  
11/1/23

Signature of the course coordinator with date



Signature of the Principal with date



*Princip*  
31/01/23

Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Bidhannagar, Durgapur-713206, India



**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**

**ENROLMENT FORM FOR ADD ON COURSE ON "COMPUTATIONAL**  
**DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND**  
**BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

Name of the student : NURUL HASSAN MONDAL

University Roll no.: 2214081

Program: M. Pharm

Division: Pharmacology

Ph : 8017733722

e-mail: nurulmondalhasan@gmail.com

Why opted for this course? : Computational pharmacology, docking, drug activity

*N. H. Mondal*

Signature of the student with date 20.01.23

*Soumit Banerjee*  
20/1/23

Signature of the course coordinator with date



Signature of the Principal with date

*Samir Kumar Samanta*  
21/1/23

Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal

Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

Principal  
Dr. B. C. Roy College of Pharmacy & Allied H.S.,  
Bidhannagar, Durgapur-713206, West Bengal

**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**

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**DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND**  
**BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

Name of the student : PAYEL GHOSH

University Roll no.: 2214082

Program: M. Pharm

Division: Pharmacology

Ph : 8910743013

e-mail: payelpharma009@gmail.com

Why opted for this course? : Interested in Drug Design (CADD), Applicable for Drug delivery

Signature of the student with date

*Payel Ghosh*  
20/01/23

Signature of the course coordinator with date

*Samir Kumar*  
20/01/23



Signature of the Principal with date

*Payel*  
20/01/23



*Samir Kumar*  
20/01/23  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Bldhannagar, Durgapur-713206, West Bengal

**ENROLMENT FORM FOR ADD ON COURSE ON "COMPUTATIONAL  
DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND  
BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

Name of the student : SANJUKTA DAS

University Roll no.: 2214083

Program: M. Pharm

Division: Pharmacology

Ph : 7031531845

e-mail: dassanjukta099@gmail.com

Why opted for this course? : Docking, Proteins, activity prediction

Signature of the student with date

*Sanjukta Das*  
11/1/23

Signature of the course coordinator with date

*Soumi Banerjee*  
11/1/23



Signature of the Principal with date

*Ray*  
31/6/23



*Samir Kumar Samanta*  
11/1/23  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Bidhannagar, Durgapur-713206, Burdwan

**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH  
SCIENCES  
DURGAPUR, WB, INDIA**

**ENROLMENT FORM FOR ADD ON COURSE ON "COMPUTATIONAL  
DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND  
BIOINFORMATICS"  
ACADEMIC YEAR: 2022-23**

Name of the student : SNEHA GHOSH

University Roll no.: 2214085

Program: M. Pharm

Division: Pharmacology

Ph : 9564802501

e-mail: snehaghosh0705@gmail.com

Why opted for this course? : Interested in Drug Design (CADD), drug activity prediction, project work, job purpose

Signature of the student with date

*Sneha Ghosh*  
11/1/23

Signature of the course coordinator with date

*Soumi Ban*  
11/1/23



Signature of the Principal with date

*Ray*  
31/1/23

*Samir Kumar Samanta*  
11/1/23  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal

Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal 713240

**Principal**  
Dr. B. C. Roy College of Pharmacy & A.H.S.  
Bidhanagar, Durgapur-713240, Burdwan

**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**

**ENROLMENT FORM FOR ADD ON COURSE ON "COMPUTATIONAL**  
**DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND**  
**BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

Name of the student : TANMOY DAS

University Roll no.: 2214086


Program: M. Pharm

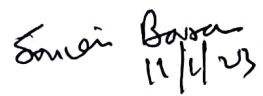
Division: Pharmacology

Ph : 7001622908

e-mail: tdas92848@gmail.com


Why opted for this course? : CADD, docking, modeling, project purpose

  
Signature of the student with date

  
Signature of the course coordinator with date

  
Signature of the Principal with date



  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH  
SCIENCES  
DURGAPUR, WB, INDIA**

**ENROLMENT FORM FOR ADD ON COURSE ON "COMPUTATIONAL  
DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND  
BIOINFORMATICS"  
ACADEMIC YEAR: 2022-23**

Name of the student : SANDIPAN SAU

University Roll no.: 2214089

Program: M. Pharm

Division: Pharmacology

Ph : 6297538780

e-mail: sandipansau0@gmail.com

Why opted for this course? : Docking, Bioinformatics, toxicological testing of drugs

*Sandipan Sau (11/1/23)*

Signature of the student with date

*Soumi Barua  
11/1/23*

Signature of the course coordinator with date



Signature of the Principal with date

*Prof. (Dr.) Samir Kumar Samanta  
11/1/23*

Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal

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**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**

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**DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND**  
**BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

Name of the student : PALLABI PRADHAN

University Roll no.: 2214090

Program: M. Pharm

Division: Pharmacology

Ph : 6294106882

e-mail: pallabipradhan9@gmail.com

Why opted for this course? : Computational bioactivity prediction, docking,  
protein-ligand interactions

Pallabi Pradhan 20-01-23  
Signature of the student with date

Signature of the course coordinator with date



Somen Banerjee  
20/1/23



Signature of the Principal with date

Signature of the Principal

Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

Signature of the Principal  
20/1/23

Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Bidhanagar, Durgapur-713203, WB, India

**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**

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**DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND**  
**BIOINFORMATICS”**  
**ACADEMIC YEAR: 2022-23**

Name of the student : RAJIB DE

University Roll no.: 2214092

Program: M. Pharm

Division: Pharmacology

Ph : 6295791626

e-mail: rajibde2001@gmail.com

Why opted for this course? : Docking, protein design, homology modeling,  
project and job purpose

*Rajib De 20/1/23*

Signature of the student with date

*Soumi Banerjee  
20/1/23*

Signature of the course coordinator with date



Signature of the Principal with date

*Rajib De  
20/1/23*

*Rajib De 20/1/23*  
Prof. (Dr.) Sainir Kumar Samanta  
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Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

Principal  
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**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
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**DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND**  
**BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

Name of the student : DISHA DAS

University Roll no.: 2214094

Program: M. Pharm

Division: Pharmacology

Ph : 7098759807

e-mail: disha.das.kir@gmail.com

Why opted for this course? : Drug Design (DD), Toxicological QSAR, Protein handling, Application in pharmacology

Disha Das 31/1/2023

Signature of the student with date

Sandeep Barua  
31/1/23

Signature of the course coordinator with date



Signature of the Principal with date



Ray  
31/01/23

Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal

Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, Bidhannagar, Durgapur-713206, Burdwan District, West Bengal-713206

**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**

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**DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND**  
**BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

Name of the student : TAMAL PAL

University Roll no.: 2214096

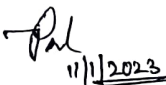
Program: M. Pharm

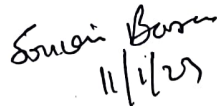
Division: Pharmacology

Ph : 8145967493

e-mail: tamal21pal@gmail.com

Why opted for this course? : CADD, Biostatistics in CADD, Docking,  
Homology modeling, application in project and future job purpose

  
Signature of the student with date 11/1/2023

  
Signature of the course coordinator with date 11/1/23



Signature of the Principal with date



Prof. (Dr.) Saikat Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal

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Principal  
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**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
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**DURGAPUR, WB, INDIA**

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**BIOINFORMATICS”**  
**ACADEMIC YEAR: 2022-23**

**Name of the student : AYAN MAHATA**

**University Roll no.: 2214097**

**Program: M. Pharm**

**Division: Pharmacology**

**Ph : 9091588335**

**e-mail: mahataayan007@gmail.com**

**Why opted for this course? : Docking, Bioinformatics, statistical modelling**

*Ayan Mahata*  
**Signature of the student with date** 20/01/23

*Soumi Banerjee*  
**Signature of the course coordinator with date** 20/1/23



*[Signature]*  
**Signature of the Principal with date** 20/01/23

*[Signature]*  
Prof. (Dr.) Semir Kumar San  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

*[Signature]*  
Principal  
Dr. B. C. Roy College of Pharmacy & A.H.S,  
Bidhannagar, Durgapur-713206, Burdwan

**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**

**ENROLMENT FORM FOR ADD ON COURSE ON "COMPUTATIONAL**  
**DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND**  
**BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

Name of the student : RIKU ROY

University Roll no.: 2214098

Program: M. Pharm

Division: Pharmacology

Ph : 7003224189

e-mail: rikuroy51@gmail.com

Why opted for this course? : Computer Aided Drug Design (CADD), Docking,  
Molecular pharmacology and modelling

*Riku Roy 21/01/23*  
Signature of the student with date

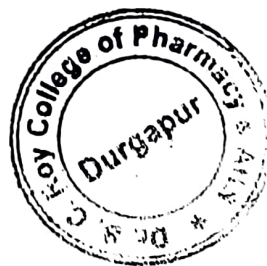
*Souain Barua 31/1/23*  
Signature of the course coordinator with date



Signature of the Principal with date

*[Signature]*  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph D (J.U.)  
Principal

Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206



*[Signature]*  
21/01/23

Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
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**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH  
SCIENCES  
DURGAPUR, WB, INDIA**

**ENROLMENT FORM FOR ADD ON COURSE ON "COMPUTATIONAL  
DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND  
BIOINFORMATICS"  
ACADEMIC YEAR: 2022-23**

Name of the student : SRIJITA CHATTERJEE

University Roll no.: 2214051

Program: M. Pharm

Division: PHARMACEUTICAL ANALYSIS

Ph : 8597634519

e-mail: srijitachatterjee.rim@gmail.com

Why opted for this course? : QSAR, Docking

*Srijita Chatterjee*  
Signature of the student with date 11/01/23

*Soumi Banerjee*  
Signature of the course coordinator with date 11/1/23



*Samir Kumar Samanta*  
Signature of the Principal with date 21/01/23

*Samir Kumar Samanta*  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

*Samir Kumar Samanta*  
Principal  
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Bidhannagar, Durgapur-713206, Burdwan

**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**

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**BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

Name of the student : ARUP KOLEY

University Roll no.: 2214052

Program: M. Pharm

Division: Pharmaceutical Analysis

Ph : 7001622920

e-mail: arup.koley1@gmail.com

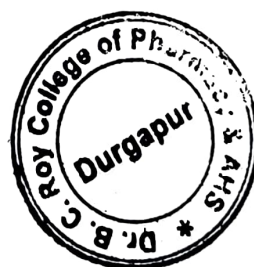
Why opted for this course? : CADD, docking, modeling, project purpose

*Arup Koley* 31/1/23

Signature of the student with date

*Soumi Banerjee*  
31/1/23

Signature of the course coordinator with date



Signature of the Principal with date

*Arup Koley*  
31/1/23

Prof. (Dr.) Sanku Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

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

**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH  
SCIENCES  
DURGAPUR, WB, INDIA**

**ENROLMENT FORM FOR ADD ON COURSE ON "COMPUTATIONAL  
DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND  
BIOINFORMATICS"  
ACADEMIC YEAR: 2022-23**

Name of the student : SUVROJYOTI GHOSH ROY

University Roll no.: 2214053

Program: M. Pharm

Division: PHARMACEUTICAL ANALYSIS

Ph : 9475362417

e-mail: suvrojyotighoshroy@gmail.com

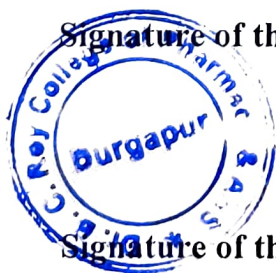
Why opted for this course? : QSAR, docking, application of the CADD in job

*S. Ghosh Roy* 11/1/23

Signature of the student with date

*Soumi Barua*  
11/1/23

Signature of the course coordinator with date



Signature of the Principal with date



*Roy*  
11/1/23

*[Signature]*  
11/1/23

Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal

Principal  
Dr. B. C. Roy College of Pharmacy & AHS,  
Bidhannagar, Durgapur-713206, Burdwan

**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**

**ENROLMENT FORM FOR ADD ON COURSE ON "COMPUTATIONAL**  
**DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND**  
**BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

Name of the student : SOUVIK BHANDARY

University Roll no.: 2214058

Program: M. Pharm

Division: PHARMACEUTICAL ANALYSIS

Ph : 9734958292

e-mail: souvikbhandary1@gmail.com

Why opted for this course? CADD, Molecular modeling, analysis of drug-protein interaction, docking

*Souvik Bhandary 11/1/23*  
Signature of the student with date

*Souvik Bhandary*  
11/1/23

Signature of the course coordinator with date



Signature of the Principal with date

*[Signature]*  
21/1/23  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

*[Signature]*  
31/1/23  
Principal  
Dr. B. C. Roy College of Pharmacy & A.H.S.  
Bidhannagar, Durgapur-713206, West Bengal



**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH  
SCIENCES  
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DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND  
BIOINFORMATICS"  
ACADEMIC YEAR: 2022-23**

Name of the student : SUSMITA AFTAB

University Roll no.: 2214060

Program: M. Pharm

Division: PHARMACEUTICAL ANALYSIS

Ph : 7047892004

e-mail: susmitaafstab@gmail.com

Why opted for this course? : QSAR, docking, protein structures

*Susmita Aftab*  
11/1/23

Signature of the student with date

*Soumi Banerjee*  
11/1/23

Signature of the course coordinator with date



Signature of the Principal with date

*[Signature]*  
11/1/23

Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

*[Signature]*  
31/01/23

Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
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**DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND**  
**BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

Name of the student : DIPANWITA BERA

University Roll no.: 2214061

Program: M. Pharm

Division: PHARMACEUTICAL ANALYSIS

Ph : 7980227719

e-mail: dipabera.haldia@gmail.com

Why opted for this course? : CADD, Computational modeling, application in job purpose

*Dipansita Bera*  
20/1/23

Signature of the student with date

*Soumi Bera*  
20/1/23



Signature of the course coordinator with date

Signature of the Principal with date

*[Signature]*  
20/1/23  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

*[Signature]*  
20/1/23

Principal  
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**BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

Name of the student : SUSMITA MALLICK

University Roll no.: 2214062

Program: M. Pharm

Division: PHARMACEUTICAL ANALYSIS

Ph : 7908982516

e-mail: susmitamallick00@gmail.com

Why opted for this course? : Interested in Drug Design (CADD), Applicable for Drug delivery

*Susmita Mallick*  
11/11/23

Signature of the student with date

*Soumita Baner*  
11/11/23

Signature of the course coordinator with date



Signature of the Principal with date

*Samir Kumar Samanta*  
11/11/23

Prof. (Dr.) Samir Kumar Samanta  
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**DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND**  
**BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

Name of the student : MOLOY ROY

University Roll no.: 2214063

Program: M. Pharm

Division: PHARMACEUTICAL ANALYSIS

Ph : 8145330950

e-mail moloy.ayan@gmail.com

Why opted for this course? : CADD, Docking, Bioinformatics, job purpose,  
project application

*M Roy 31/1/23*

Signature of the student with date

*Somen Barua  
31/1/23*

Signature of the course coordinator with date



Signature of the Principal with date

*Samir Kumar Samanta  
31/1/23*

*Samir Kumar Samanta  
31/1/23*  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
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Durgapur, West Bengal-713206

Principal  
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Bidhannagar, Durgapur-713206, Burdwan



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**DRUG DESIGN USING QSAR/ CHEMINFORMATICS AND**  
**BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

Name of the student : PIU GHOSH

University Roll no.: 2214034

Program: M. Pharm

Division: INDUSTRIAL PHARMACY

Ph : 8617658886

e-mail - pujaplu123@gmail.com

Why opted for this course? : Application in Polymer design, drug-polymer docking, for job purpose

*Piu Ghosh 20.1.23*  
Signature of the student with date

*Sandeep Bora 20/1/23*  
Signature of the course coordinator with date



Signature of the Principal with date

*Prof. (Dr.) Samir Kumar Samanta 20/1/23*

*Prof. (Dr.) Samir Kumar Samanta 20/1/23*  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
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Principal  
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BIOINFORMATICS"  
ACADEMIC YEAR: 2022-23**

Name of the student : NABYENDU MANDAL

University Roll no.: 2214033

Program: M. Pharm

Division: INDUSTRIAL PHARMACY

Ph : 8250159066

e-mail - pharmanabyendu09@gmail.com

Why opted for this course? : Application in polymer design, industrial pharmacy

*N. Mandal*  
11/1/23

Signature of the student with date

*Soumi Banerjee*  
11/1/23

Signature of the course coordinator with date



Signature of the Principal with date

*Ray*  
28/10/22

*[Signature]*  
28/10/22  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
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Durgapur, West Bengal-713206

Principal  
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**BIOINFORMATICS"**  
**ACADEMIC YEAR: 2022-23**

**Name of the student : ADARSHA DUTTA**

**University Roll no.: 2214026**

**Program: M. Pharm**

**Division: Industrial Pharmacy**

**Ph : 7001275374**

**e-mail: ad.2@gmail.com**

**Why opted for this course? : CADD, docking, modeling, project purpose**

*A Dutta*  
*31/1/23*

**Signature of the student with date**

*Soumi Ban*  
*31/1/23*

**Signature of the course coordinator with date**



**Signature of the Principal with date**

*Ray*  
*31/1/23*

*Samir Kumar Samanta*  
*31/1/23*  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

*Principal*  
Dr. B. C. Roy College of Pharmacy & A.H.S.  
Bidhannagar, Durgapur-713206, Burdwan  
*31/1/23*



1.2.2. Add on/ Certification program offered during 2022-23

List of Students Enrolled

**TITLE OF COURSE: COMPUTATIONAL DRUG DESIGN  
(USING SOFTWARE)**

SL NO.	UNIVERSITY ROLL NO.	NAME OF THE STUDENT	PROGR AM	DIVISION
1	2214009	ANUSKA CHATTERJEE	M. PHARM.	PHARMACEUTICS
2	2214011	ANANYA DEY	M. PHARM.	PHARMACEUTICS
3	2214013	PARTHA PRATIM BEZ	M. PHARM.	PHARMACEUTICS
4	2214014	AKASH MONDAL	M. PHARM.	PHARMACEUTICS
5	2214017	ANUPAM BERA	M. PHARM.	PHARMACEUTICS
6	2214006	SAYANTAN NAG	M. PHARM.	PHARMACEUTICS
7	2214081	NURUL HASSAN MONDAL	M. PHARM.	PHARMACOLOGY
8	2214082	PAYEL GHOSH	M. PHARM.	PHARMACOLOGY
9	2214083	SANJUKTA DAS	M. PHARM.	PHARMACOLOGY
10	2214085	SNEHA GHOSH	M. PHARM.	PHARMACOLOGY
11	2214086	TANMOY DAS	M. PHARM.	PHARMACOLOGY
12	2214089	SANDIPAN SAU	M. PHARM.	PHARMACOLOGY
13	2214090	PALLABI PRADHAN	M. PHARM.	PHARMACOLOGY
14	2214092	RAJIB DE	M. PHARM.	PHARMACOLOGY
15	2214094	DISHA DAS	M. PHARM.	PHARMACOLOGY
16	2214096	TAMAL PAL	M. PHARM.	PHARMACOLOGY
17	2214097	AYAN MAHATA	M. PHARM.	PHARMACOLOGY
18	2214098	RIKU ROY	M. PHARM.	PHARMACOLOGY
19	2214051	SRIJITA CHATTERJEE	M. PHARM.	PHARMACEUTICAL ANALYSIS








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

20				
21	2214052	ARUP KOLEY	M. PHARM.	PHARMACEUTICAL ANALYSIS
22	2214053	SUVROJYOTI GHOSH ROY	M. PHARM.	PHARMACEUTICAL ANALYSIS
23	2214058	SOUVIK BHANDARY	M. PHARM.	PHARMACEUTICAL ANALYSIS
24	2214060	SUSMITA AFTAB	M. PHARM.	PHARMACEUTICAL ANALYSIS
25	2214061	DIPANWITA BERA	M. PHARM.	PHARMACEUTICAL ANALYSIS
26	2214062	SUSMITA MALLICK	M. PHARM.	PHARMACEUTICAL ANALYSIS
27	2214063	MOLOY ROY	M. PHARM.	PHARMACEUTICAL ANALYSIS
28	2214034	PIU GHOSH	M. PHARM.	INDUSTRIAL PHARMACY
29	2214033	NABYENDU MANDAL	M. PHARM.	INDUSTRIAL PHARMACY
29	2214026	ADARSHA DUTTA	M. PHARM.	INDUSTRIAL PHARMACY



  
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**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**  
**Academic Year: 2022-23**  
**Attendance**

Course name: COMPUTATIONAL DRUG DESIGN USING QSAR/CHEMINFORMATICS AND BIOINFORMATICS

Course Instructor: Dr. Souvik Basak, Associate Professor & DIC, Division of Pharmaceutical Chemistry, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India

Class no.:1

Date: 21/02/2023


Topic: Brief introduction of QSAR and its workflow

Duration: 2h

**ATTENDANCE**

SL NO.	UNIVERSITY ROLL NO.	NAME OF THE STUDENT	Signature
1	2214009	ANUSKA CHATTERJEE	A. Chatterjee
2	2214011	ANANYA DEY	A. Dey
3	2214013	PARTHA PRATIM BEZ	P. Bez
4	2214014	AKASH MONDAL	Akash Mondal
5	2214017	ANUPAM BERA	Anupam Bera
6	2214006	SAYANTAN NAG	Sayantana
7	2214081	NURUL HASSAN MONDAL	N. H. Mondal
8	2214082	PAYEL GHOSH	Payel Ghosh
9	2214083	SANJUKTA DAS	Sanjukta Das
10	2214085	SNEHA GHOSH	Sneha Ghosh
11	2214086	TANMOY DAS	T. Das
12	2214089	SANDIPAN SAU	S. Sau
13	2214090	PALLABI PRADHAN	Pallabi Pradhan
14	2214092	RAJIB DE	Rajib De
15	2214094	DISHA DAS	Disha Das
16	2214096	TAMAL PAL	Tal
17	2214097	AYAN MAHATA	Ayan Mahata



  
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 Durgapur, West Bengal-713206

18	2214098	RIKU ROY	Riku Roy
19	2214051	SRIJITA CHATTERJEE	Srijita Chatterjee
20	2214052	ARUP KOLEY	A Koley
21	2214053	SUVROJYOTI GHOSH ROY	S. Ghosh Roy
22	2214058	SOUVIK BHANDARY	Souvik Bhandary
23	2214060	SUSMITA AFTAB	Susmita Aftab
24	2214061	DIPANWITA BERA	Dipansita Bera
25	2214062	SUSMITA MALLICK	Susmita Mallick
26	2214063	MOLOY ROY	M Roy
27	2214034	PIU GHOSH	Piu Ghosh
28	2214033	NABYENDU MANDAL	N. Mandal
29	2214026	ADARSHA DUTTA	A Dutta

Sonai Bara  
21/4/2023

Signature of the Course Coordinator



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**DURGAPUR, WB, INDIA**  
**Academic Year: 2022-23**  
**Attendance**

Course name: COMPUTATIONAL DRUG DESIGN USING QSAR/CHEMINFORMATICS AND BIOINFORMATICS

Course Instructor: Dr. Souvik Basak, Associate Professor & DIC, Division of Pharmaceutical Chemistry, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India

Class no.: 2

Date: 23/02/2023

Topic: Structure Drawing, parametrization, interplay between 2D & 3D structures

Duration: 2h

**ATTENDANCE**

SL NO.	UNIVERSITY ROLL NO.	NAME OF THE STUDENT	Signature
1	2214009	ANUSKA CHATTERJEE	A. Chatterjee
2	2214011	ANANYA DEY	Ananya
3	2214013	PARTHA PRATIM BEZ	P. Bez
4	2214014	AKASH MONDAL	Akash Mondal
5	2214017	ANUPAM BERA	Anupam Bera
6	2214006	"SAYANTAN NAG"	Sayantana
7	2214081	NURUL HASSAN MONDAL	N.M. Mondal
8	2214082	PAYEL GHOSH	Payel Ghosh
9	2214083	SANJUKTA DAS	Sanjukta Das
10	2214085	SNEHA GHOSH	Sneha Ghosh
11	2214086	TANMOY DAS	T. Das
12	2214089	SANDIPAN SAU	S. Sau
13	2214090	PALLABI PRADHAN	Pallabi Pradhan
14	2214092	RAJIB DE	Rajib De
15	2214094	DISHA DAS	Disha Das
16	2214096	TAMAL PAL	Tal
17	2214097	AYAN MAHATA	Ayan Mahata

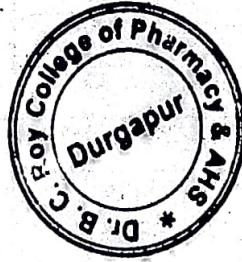


Prof. (Dr.) Samir Kumar Samanta  
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18			
	2214098	RIKU ROY	Riku Roy
19	2214051	SRIJITA CHATTERJEE	Srijita Chatterjee
20	2214052	ARUP KOLEY	Akoley
21	2214053	SUVROJYOTI GHOSH ROY	S. Ghosh Roy
22	2214058	SOUVIK BHANDARY	Souvik Bhandary
23	2214060	SUSMITA AFTAB	Susmita Aftab
24	2214061	DIPANWITA BERA	Dipanjita Bera
25	2214062	SUSMITA MALLICK	Susmita Mallik
26	2214063	MOLOY ROY	M Roy
27	2214034	PIU GHOSH	Piu Ghosh
28	2214033	NABYENDU MANDAL	N Mandal
29	2214026	ADARSHA DUTTA	A Dutta

Soumi Banna  
23/2/23

Signature of the Course Coordinator



Prof. (Dr.) Soumi Kumar Samanta  
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**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**  
**Academic Year: 2022-23**  
**Attendance**

Course name: COMPUTATIONAL DRUG DESIGN USING QSAR/CHEMINFORMATICS AND BIOINFORMATICS

Course Instructor: Dr. Souvik Basak, Associate Professor & DIC, Division of Pharmaceutical Chemistry, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India

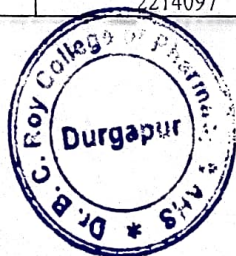
Class no.:3

Date: 28/02/2023

Topic: Molecular Mechanics, energy minimization, semi empirical methods,  
 Duration: 2h Molecular Modelling

**ATTENDANCE**

SL NO.	UNIVERSITY ROLL NO.	NAME OF THE STUDENT	Signature
1	2214009	ANUSKA CHATTERJEE	A. Chatterjee
2	2214011	ANANYA DEY	A. Dey
3	2214013	PARTHA PRATIM BEZ	P. Bez
4	2214014	AKASH MONDAL	Akash Mondal
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12	2214089	SANDIPAN SAU	S. Sau
13	2214090	PALLABI PRADHAN	Pallabi Pradhan
14	2214092	RAJIB DE	Rajib De
15	2214094	DISHA DAS	Disha Das
16	2214096	TAMAL PAL	Tal
17	2214097	AYAN MAHATA	Ayan Mahata

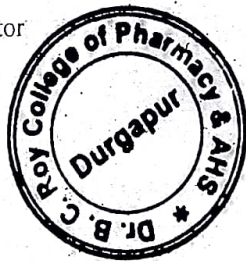


Prof. (Dr.) Sanvir Kumar Samanta  
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18	2214098	RIKU ROY	Riku Roy
19	2214051	SRIJITA CHATTERJEE	Srijita Chatterjee
20	2214052	ARUP KOLEY	Akoley
21	2214053	SUVROJYOTI GHOSH ROY	S. Ghosh Roy
22	2214058	SOUVIK BHANDARY	Souvik Bhandary
23	2214060	SUSMITA AFTAB	Susmita Aftab
24	2214061	DIPANWITA BERA	Dipansita Bera
25	2214062	SUSMITA MALICK	Susmita Mallick
26	2214063	MOLOY ROY	M Roy
27	2214034	PIU GHOSH	Piu Ghosh
28	2214033	NABYENDU MANDAL	N. Mandal
29	2214026	ADARSHA DUTTA	A Dutta

Soumi Basu  
28/1/23

Signature of the Course Coordinator



*[Handwritten Signature]*  
28/1/23

Prof. (Dr.) Samir Kumar Samanta  
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**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
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**DURGAPUR, WB, INDIA**  
**Academic Year: 2022-23**  
**Attendance**

Course name: COMPUTATIONAL DRUG DESIGN USING QSAR/CHEMINFORMATICS AND BIOINFORMATICS

Course Instructor: Dr. Souvik Basak, Associate Professor & DIC, Division of Pharmaceutical Chemistry, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India

Class no.:4

Date: 09/03/2023


Topic: MLR to build up 2D QSAR model, descriptor generation, feature selection

Duration: 2h

**ATTENDANCE**

SL NO.	UNIVERSITY ROLL NO.	NAME OF THE STUDENT	Signature
1	2214009	ANUSKA CHATTERJEE	A. Chatterjee
2	2214011	ANANYA DEY	A. Deay
3	2214013	PARTHA PRATIM BEZ	P. Bez
4	2214014	AKASH MONDAL	Akash Mondal
5	2214017	ANUPAM BERA	Anupam Bera
6	2214006	SAYANTAN NAG	Sayantana
7	2214081	NURUL HASSAN MONDAL	N.M. Mondal
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11	2214086	TANMOY DAS	T. Das
12	2214089	SANDIPAN SAU	S. Sau
13	2214090	PALLABI PRADHAN	Pallabi Pradhan
14	2214092	RAJIB DE	Rajib De
15	2214094	DISHA DAS	Disha Das
16	2214096	TAMAL PAL	Pal
17	2214097	AYAN MAHATA	Ayan Mahata



  
 Prof. (Dr.) Samir Kumar Samanta  
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18	2214098	RIKU ROY	Riku Roy
19	2214051	SRIJITA CHATTERJEE	Srijita Chatterjee
20	2214052	ARUP KOLEY	Arup Koley
21	2214053	SUVROJYOTI GHOSH ROY	Souvik Bhandary S. Ghosh Roy
22	2214058	SOUVIK BHANDARY	Souvik Bhandary
23	2214060	SUSMITA AFTAB	Susmita Aftab
24	2214061	DIPANWITA BERA	Dipanita Bera
25	2214062	SUSMITA MALLICK	Susmita Mallik
26	2214063	MOLOY ROY	M Roy
27	2214034	PIU GHOSH	Piu Ghosh
28	2214033	NABYENDU MANDAL	N. Mandal
29	2214026	ADARSHA DUTTA	A Dutta

Souci Bera  
9/3/23

Signature of the Course Coordinator



  
Prof. (Dr.) Samir Kumar Samanta  
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Durgapur, West Bengal-713206

**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH  
SCIENCES  
DURGAPUR, WB, INDIA  
Academic Year: 2022-23  
Attendance**

Course name: COMPUTATIONAL DRUG DESIGN USING QSAR/CHEMINFORMATICS AND BIOINFORMATICS

Course Instructor: Dr. Souvik Basak, Associate Professor & DIC, Division of Pharmaceutical Chemistry, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India

Class no.: 5

Date: 14/03/2023

Topic: Validating QSAR by OBA/PBD plot, ANOVA, t-test.

Duration: 2h

**ATTENDANCE**

SL NO.	UNIVERSITY ROLL NO.	NAME OF THE STUDENT	Signature
1	2214009	ANUSKA CHATTERJEE	A. Chatterjee
2	2214011	ANANYA DEY	A. Dey
3	2214013	PARTHA PRATIM BEZ	P. Bez
4	2214014	AKASH MONDAL	Akash Mondal
5	2214017	ANUPAM BERA	Anupam Bera
6	2214006	SAYANTAN NAG	Sayantana
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14	2214092	RAJIB DE	Rajib De
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16	2214096	TAMAL PAL	T. Pal
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Durgapur, West Bengal-713206

18	2214098	RIKU ROY	Riku Roy
19	2214051	SRIJITA CHATTERJEE	Srijita Chatterjee
20	2214052	ARUP KOLEY	A. Koley
21	2214053	SUVROJYOTI GHOSH ROY	S. Ghosh Roy
22	2214058	SOUVIK BHANDARY	Souvik Bhandary
23	2214060	SUSMITA AFTAB	Susmita Aftab
24	2214061	DIPANWITA BERA	Dipansita Bera
25	2214062	SUSMITA MALLICK	Susmita Mallick
26	2214063	MOLOY ROY	M. Roy
27	2214034	PIU GHOSH	Piu Ghosh
28	2214033	NABYENDU MANDAL	N. Mandal
29	2214026	ADARSHA DUTTA	A. Dutta

Soumi Basu  
14/3/23

Signature of the Course Coordinator



*[Handwritten Signature]*  
14/3/23

Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D. (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**  
**Academic Year: 2022-23**  
**Attendance**

Course name: COMPUTATIONAL DRUG DESIGN USING QSAR/CHEMINFORMATICS AND BIOINFORMATICS

Course Instructor: Dr. Souvik Basak, Associate Professor & DIC, Division of Pharmaceutical Chemistry, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India

Class no.:6

Date: 16/03/2023

Topic: Use of genetic algorithm in QSAR model development - use of DTC-QSAR & SARIN,  $Q^2$ , Williams plot

Duration: 2h

**ATTENDANCE**

SL NO.	UNIVERSITY ROLL NO.	NAME OF THE STUDENT	Signature
1	2214009	ANUSKA CHATTERJEE	A. Chatterjee
2	2214011	ANANYA DEY	A. Dey
3	2214013	PARTHA PRATIM BEZ	P. Bez
4	2214014	AKASH MONDAL	Akash Mondal
5	2214017	ANUPAM BERA	Anupam Bera
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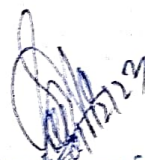
Prof. (Dr.) Samir Kumar Samanta  
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Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713205

18	2214098	RIKU ROY	Riku Roy
19	2214051	SRIJITA CHATTERJEE	Srijita Chatterjee
20	2214052	ARUP KOLEY	Akoley
21	2214053	SUVROJYOTI GHOSH ROY	S. Ghosh Roy
22	2214058	SOUVIK BHANDARY	Souvik Bhandary
23	2214060	SUSMITA AFTAB	Susmita Aftab
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27	2214034	PIU GHOSH	Piu Ghosh
28	2214033	NABYENDU MANDAL	N. Mandal
29	2214026	ADARSHA DUTTA	A Dutta

Soumi Banerjee  
16/3/23

Signature of the Course Coordinator



  
Prof. (Dr.) Samir Kumar Samanta  
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**DURGAPUR, WB, INDIA**  
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Course name: COMPUTATIONAL DRUG DESIGN USING QSAR/CHEMINFORMATICS AND BIOINFORMATICS

Course Instructor: Dr. Souvik Basak, Associate Professor & DIC, Division of Pharmaceutical Chemistry, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India

Class no.:7

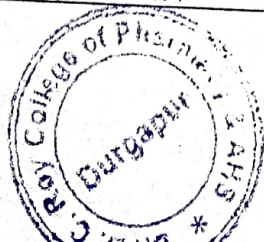
Date: 21/03/2023

Topic: Drug-likeness, Lipinski Rule of five, Molinspiration, admetSAR

Duration: 2h

**ATTENDANCE**

SL NO.	UNIVERSITY ROLL NO.	NAME OF THE STUDENT	Signature
1	2214009	ANUSKA CHATTERJEE	A. Chatterjee
2	2214011	ANANYA DEY	A. Dey
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M. Pharm., Ph.D (J.U.)  
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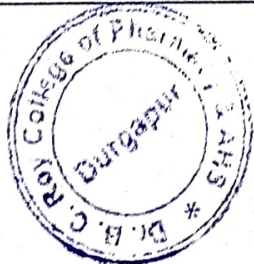
Date: 21/03/2023


Topic: Drug Uneliness, Lipinski Rule of five, MOInspiration, admetSAR

Duration: 2h

**ATTENDANCE**

SL NO.	UNIVERSITY ROLL NO.	NAME OF THE STUDENT	Signature
1	2214009	ANUSKA CHATTERJEE	A. Chatterjee
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3	2214013	PARTHA PRATIM BEZ	P. Bez
4	2214014	AKASH MONDAL	Akash Mondal
5	2214017	ANUPAM BERA	Anupam Bera
6	2214006	SAYANTAN NAG	Sayantana
7	2214081	NURUL HASSAN MONDAL	N.M. Mondal
8	2214082	PAYEL GHOSH	Payel Ghosh
9	2214083	SANJUKTA DAS	Sanjukta Das
10	2214085	SNEHA GHOSH	Sneha Ghosh
11	2214086	TANMOY DAS	T. Das
12	2214089	SANDIPAN SAU	S. Sau
13	2214090	PALLABI PRADHAN	Pallabi Pradhan
14	2214092	RAJIB DE	Rajib De
15	2214094	DISHA DAS	Disha Das
16	2214096	TAMAL PAL	Pal
17	2214097	AYAN MAHATA	Ayan Mahata




  
 Prof. (Dr.) Samir Kumar Samanta  
 M. Pharm., Ph.D (J.U.)  
 Principal  
 Dr. B. C. Roy College of Pharmacy & AHS  
 Durgapur, West Bengal-713206

18	2214098	RIKU ROY	Riku Roy
19	2214051	SRIJITA CHATTERJEE	Srijita Chatterjee
20	2214052	ARUP KOLEY	Akoley
21	2214053	SUVROJYOTI GHOSH ROY	S. Ghosh Roy
22	2214058	SOUVIK BHANDARY	Souvik Bhandary
23	2214060	SUSMITA AFTAB	Susmita Aftab
24	2214061	DIPANWITA BERA	Dipanita Bera
25	2214062	SUSMITA MALLICK	Susmita Aftab Susmita Mallik
26	2214063	MOLOY ROY	M Roy
27	2214034	PIU GHOSH	Piu Ghosh
28	2214033	NABYENDU MANDAL	N. Mandal
29	2214026	ADARSHA DUTTA	Adulta

Souain Basu  
21/3/2023  
Signature of the Course Coordinator



  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
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**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**  
**Academic Year: 2022-23**  
**Attendance**

Course name: COMPUTATIONAL DRUG DESIGN USING QSAR/CHEMINFORMATICS AND BIOINFORMATICS

Course Instructor: Dr. Souvik Basak, Associate Professor & DIC, Division of Pharmaceutical Chemistry, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India

Class no.8

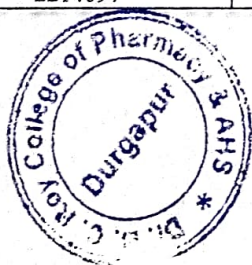
Date: 28/03/2023


Topic: Docking, Theory, software, Basic command line of AutoDocu-Vina

Duration: 2h

**ATTENDANCE**

SL NO.	UNIVERSITY ROLL NO.	NAME OF THE STUDENT	Signature
1	2214009	ANUSKA CHATTERJEE	A.Chatterjee
2	2214011	ANANYA DEY	A.dey
3	2214013	PARTHA PRATIM BEZ	P. Bez
4	2214014	AKASH MONDAL	Akash Mondal
5	2214017	ANUPAM BERA	Anupam Bera
6	2214006	SAYANTAN NAG	Sayantana
7	2214081	NURUL HASSAN MONDAL	N.M. Mondal
8	2214082	PAYEL GHOSH	Payel Ghosh
9	2214083	SANJUKTA DAS	Sanjukta Das
10	2214085	SNEHA GHOSH	Sneha Ghosh
11	2214086	TANMOY DAS	T.Das
12	2214089	SANDIPAN SAU	S.Sau
13	2214090	PALLABI PRADHAN	Pallabi Pradhan
14	2214092	RAJIB DE	Rajib De
15	2214094	DISHA DAS	Disha Das
16	2214096	TAMAL PAL	Tal
17	2214097	AYAN MAHATA	Ayan Mahata



  
 Dr. Samir Kumar Samanta  
 M. Pharm., Ph.D (J.U.)  
 Principal  
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 Durgapur, West Bengal-713206

18			
	2214098	RIKU ROY	Riku Roy
19			
	2214051	SRIJITA CHATTERJEE	Srijita Chatterjee
20			
	2214052	ARUP KOLEY	A Koley
21			
	2214053	SUVROJYOTI GHOSH ROY	S. Ghosh Roy
22			
	2214058	SOUVIK BHANDARY	Souvik Bhandary
23			
	2214060	SUSMITA AFTAB	Susmita Aftab
24			
	2214061	DIPANWITA BERA	Dipanjita Bera
25			
	2214062	SUSMITA MALLICK	Susmita Mallik
26			
	2214063	MOLOY ROY	M Roy
27			
	2214034	PIU GHOSH	Piugosh
28			
	2214033	NABYENDU MANDAL	N. Mandal
29			
	2214026	ADARSHA DUTTA	A Dutta

Souvi Bera  
28/3/25

Signature of the Course Coordinator



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**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
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**DURGAPUR, WB, INDIA**  
**Academic Year: 2022-23**  
**Attendance**

Course name: COMPUTATIONAL DRUG DESIGN USING QSAR/CHEMINFORMATICS AND BIOINFORMATICS

Course Instructor: Dr. Souvik Basak, Associate Professor & DIC, Division of Pharmaceutical Chemistry, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India

Class no.9

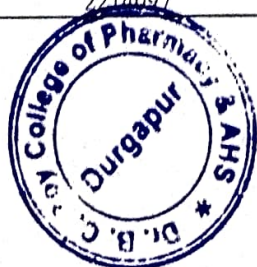
Date: 30/03/2023

Topic: PDB, Analysis, Interactions

Duration: 2h

**ATTENDANCE**

SL NO.	UNIVERSITY ROLL NO.	NAME OF THE STUDENT	Signature
1	2214009	ANUSKA CHATTERJEE	A. Chatterjee
2	2214011	ANANYA DEY	A. Dey
3	2214013	PARTHA PRATIM BEZ	P. Bez
4	2214014	AKASH MONDAL	Akash Mondal
5	2214017	ANUPAM BERA	Anupam Bera
6	2214006	SAYANTAN NAG	Sayantana
7	2214081	NURUL HASSAN MONDAL	N.M. Mondal
8	2214082	PAYEL GHOSH	Payel Ghosh
9	2214083	SANJUKTA DAS	Sanjukta Das
10	2214085	SNEHA GHOSH	Sneha Ghosh
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14	2214092	RAJIB DE	Rajib De
15	2214094	DISHA DAS	Disha Das
16	2214096	TAMAL PAL	Tal
17	2214097	AYAN MAHATA	Ayan Mahata

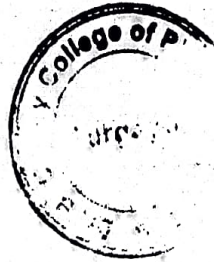



30/3/23

Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
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Durgapur, West Bengal-713205

18	2214098	RIKU ROY	Riku Roy
19	2214051	SRIJITA CHATTERJEE	Srijita Chatterjee
20	2214052	ARUP KOLEY	Akoley
21	2214053	SUVROJYOTI GHOSH ROY	S. Ghosh Roy
22	2214058	SOUVIK BHANDARY	Souvik Bhandary
23	2214060	SUSMITA AFTAB	Susmita Aftab
24	2214061	DIPANWITA BERA	Dipanjita Bera
25	2214062	SUSMITA MALLICK	Susmita Mallick
26	2214063	MOLOY ROY	M Roy
27	2214034	PIU GHOSH	Piu Ghosh
28	2214033	NABYENDU MANDAL	N. Mandal
29	2214026	ADARSHA DUTTA	A Dutta

Soumi Banerjee  
30/3/23  
Signature of the Course Coordinator



  
Prof. (Dr.) Sanku Kumar Samanta  
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**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**  
**Academic Year: 2022-23**  
**Attendance**

Course name: COMPUTATIONAL DRUG DESIGN USING QSAR/CHEMINFORMATICS AND BIOINFORMATICS

Course Instructor: Dr. Souvik Basak, Associate Professor & DIC, Division of Pharmaceutical Chemistry, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India

Class no.10

Date: 04/04/2023

Topic: UCSF Chimera, Discovery studio visualizer, Analysis & Processing of Protein structures

Duration: 2h

**ATTENDANCE**

SL NO.	UNIVERSITY ROLL NO.	NAME OF THE STUDENT	Signature
1	2214009	ANUSKA CHATTERJEE	A. Chatterjee
2	2214011	ANANYA DEY	A. Dey
3	2214013	PARTHA PRATIM BEZ	P. Bez
4	2214014	AKASH MONDAL	Akash Mondal
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14	2214092	RAJIB DE	Rajib De
15	2214094	DISHA DAS	Disha Das
16	2214096	TAMAL PAL	T. Pal
17	2214097	AYAN MAHATA	Ayan Mahata



Prof. (Dr.) Samir Kumar Samanta  
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Dr. B. C. Roy College of Pharmacy & AHS  
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*(Handwritten signature)*  
04/04/23

Dr. B. C. Roy College of Pharmacy & Allied Health Sciences  
Durgapur, West Bengal-713206  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (I.U.)  
Principal

18	2214098	RIKU ROY	Riku Roy
19	2214051	SRIJITA CHATTERJEE	Srijita Chatterjee
20	2214052	ARUP KOLEY	Akoley
21	2214053	SUVROJYOTI GHOSH ROY	S. Ghosh Roy
22	2214058	SOUVIK BHANDARY	Souvik Bhandary
23	2214060	SUSMITA AFTAB	Susmita Aftab
24	2214061	DIPANWITA BERA	Dipanjita Bera
25	2214062	SUSMITA MALLICK	Susmita Mallik
26	2214063	MOLOY ROY	M Roy
27	2214034	PIU GHOSH	Piu Ghosh
28	2214033	NABYENDU MANDAL	N. Mandal
29	2214026	ADARSHA DUTTA	A. Dutta

Sonovic Baner  
4/4/23

Signature of the Course Coordinator



Prof. (Dr.) Samir Kumar Samanta  
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**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**  
**Academic Year: 2022-23**  
**Attendance**

Course name: COMPUTATIONAL DRUG DESIGN USING QSAR/CHEMINFORMATICS AND BIOINFORMATICS

Course Instructor: Dr. Souvik Basak, Associate Professor & DIC, Division of Pharmaceutical Chemistry, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India

Class no.11

Date: 06/04/2023

Topic: SWISSDOC, PARDOC, Result Analysis

Duration: 2h

**ATTENDANCE**

SL NO.	UNIVERSITY ROLL NO.	NAME OF THE STUDENT	Signature
1	2214009	ANUSKA CHATTERJEE	A. Chatterjee
2	2214011	ANANYA DEY	A. Dey
3	2214013	PARTHA PRATIM BEZ	P. Bez
4	2214014	AKASH MONDAL	Akash Mondal
5	2214017	ANUPAM BERA	Anupam Bera
6	2214006	SAYANTAN NAG	Sayantana
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9	2214083	SANJUKTA DAS	Sanjukta Das
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11	2214086	TANMOY DAS	T. Das
12	2214089	SANDIPAN SAU	S. Sau
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14	2214092	RAJIB DE	Rajib De
15	2214094	DISHA DAS	Disha Das
16	2214096	TAMAL PAL	Tal
17	2214097	AYAN MAHATA	Ayan Mahata



  
 06/04/23


Prof. (Dr.) Samir Kumar Samanta  
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 Durgapur, West Bengal-713206

18	2214098	RIKU ROY	Riku Roy
19	2214051	SRIJITA CHATTERJEE	Srijita Chatterjee
20	2214052	ARUP KOLEY	Akoley
21	2214053	SUVROJYOTI GHOSH ROY	Sujoyoti Roy
22	2214058	SOUVIK BHANDARY	Souvik Bhandary
23	2214060	SUSMITA AFTAB	Susmita Aftab
24	2214061	DIPANWITA BERA	Dipanjita Bera
25	2214062	SUSMITA MALLICK	Susmita Mallik
26	2214063	MOLOY ROY	M Roy
27	2214034	PIU GHOSH	Piu Ghosh
28	2214033	NABYENDU MANDAL	N. Mandal
29	2214026	ADARSHA DUTTA	ADutta

Samir Barua  
6/4/21

Signature of the Course Coordinator



  
Prof. (Dr.) Samir Kumar Samanta  
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Dr. B. C. Roy College of Pharmacy & AHS  
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**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**  
**Academic Year: 2022-23**  
**Attendance**

Course name: COMPUTATIONAL DRUG DESIGN USING QSAR/CHEMINFORMATICS AND BIOINFORMATICS

Course Instructor: Dr. Souvik Basak, Associate Professor & DIC, Division of Pharmaceutical Chemistry, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India

Class no.12

Date: 11/04/2023


Topic: Basic Bioinformatics, NCBI, gene & protein sequence

Duration: 2h

**ATTENDANCE**

SL NO.	UNIVERSITY ROLL NO.	NAME OF THE STUDENT	Signature
1	2214009	ANUSKA CHATTERJEE	A. Chatterjee
2	2214011	ANANYA DEY	A. Dey
3	2214013	PARTHA PRATIM BEZ	P. Bez
4	2214014	AKASH MONDAL	Akash Mondal
5	2214017	ANUPAM BERA	Anupam
6	2214006	SAYANTAN NAG	Sayantana
7	2214081	NURUL HASSAN MONDAL	N.M. Mondal
8	2214082	PAYEL GHOSH	Payel Ghosh
9	2214083	SANJUKTA DAS	Sanjukta Das
10	2214085	SNEHA GHOSH	Sneha Ghosh
11	2214086	TANMOY DAS	Tan
12	2214089	SANDIPAN SAU	S. Sau
13	2214090	PALLABI PRADHAN	Pallabi Pradhan
14	2214092	RAJIB DE	Rajib De
15	2214094	DISHA DAS	Disha Das
16	2214096	TAMAL PAL	Tam
17	2214097	AYAN MAHATA	Ayan Mahata




  
 Prof. (Dr.) Samir Kumar Samanta  
 M. Pharm., Ph.D (J.U.)  
 Principal  
 Dr. B. C. Roy College of Pharmacy & AHS  
 Durgapur, West Bengal-713205

18	2214098	RIKU ROY	Riku Roy
19	2214051	SRIJITA CHATTERJEE	Srijita Chatterjee
20	2214052	ARUP KOLEY	Arup Koley
21	2214053	SUVROJYOTI GHOSH ROY	S. Ghosh Roy
22	2214058	SOUVIK BHANDARY	Souvik Bhandary
23	2214060	SUSMITA AFTAB	Susmita Aftab
24	2214061	DIPANWITA BERA	Dipankrita Bera
25	2214062	SUSMITA MALLICK	Susmita Mallik
26	2214063	MOLOY ROY	M Roy
27	2214034	PIU GHOSH	Piu Ghosh
28	2214033	NABYENDU MANDAL	N. Mandal
29	2214026	ADARSHA DUTTA	A. Dutta

Samir Barua  
11/4/23

Signature of the Course Coordinator



  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**  
**Academic Year: 2022-23**  
**Attendance**

Course name: COMPUTATIONAL DRUG DESIGN USING QSAR/CHEMINFORMATICS AND BIOINFORMATICS

Course Instructor: Dr. Souvik Basak, Associate Professor & DIC, Division of Pharmaceutical Chemistry, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India

Class no.13

Date: 13/04/2023

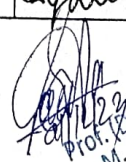
Topic: BLAST, MSA, CLUSTAL W/CLUSTAL OMEGA, active site Analysis

Duration: 2h

**ATTENDANCE**

SL NO.	UNIVERSITY ROLL NO.	NAME OF THE STUDENT	Signature
1	2214009	ANUSKA CHATTERJEE	A. Chatterjee
2	2214011	ANANYA DEY	A. Dey
3	2214013	PARTHA PRATIM BEZ	P. Bez
4	2214014	AKASH MONDAL	Akash Mondal
5	2214017	ANUPAM BERA	Anupam
6	2214006	SAYANTAN NAG	Sayantana
7	2214081	NURUL HASSAN MONDAL	N.M. Mondal
8	2214082	PAYEL GHOSH	Payel Ghosh
9	2214083	SANJUKTA DAS	Sanjukta Das
10	2214085	SNEHA GHOSH	Sneha Ghosh
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12	2214089	SANDIPAN SAU	S. Sau
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15	2214094	DISHA DAS	Disha Das
16	2214096	TAMAL PAL	Tal
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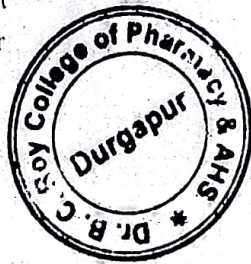



  
 Prof. (Dr.) Samir Kumar Ghosh  
 M. Pharm., Ph.D. (I.U.)  
 Principal  
 Dr. B.C. Roy College of Pharmacy & Allied Health Sciences  
 Durgapur, West Bengal-713206

18	2214098	RIKU ROY	Riku Roy
19	2214051	SRIJITA CHATTERJEE	Srijita Chatterjee
20	2214052	ARUP KOLEY	Akoley
21	2214053	SUVROJYOTI GHOSH ROY	S. Ghosh Roy
22	2214058	SOUVIK BHANDARY	Souvik Bhandary
23	2214060	SUSMITA AFTAB	Susmita Aftab
24	2214061	DIPANWITA BERA	Dipanjita Bera
25	2214062	SUSMITA MALLICK	Susmita Mallick
26	2214063	MOLOY ROY	M Roy
27	2214034	PIU GHOSH	Piu Ghosh
28	2214033	NABYENDU MANDAL	N. Mandal
29	2214026	ADARSHA DUTTA	A Dutta

Samir Banerjee  
13/4/23

Signature of the Course Coordinator



  
Prof. (Dr.) Samir Kumar Samanta  
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**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
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**DURGAPUR, WB, INDIA**  
**Academic Year: 2022-23**  
**Attendance**

Course name: COMPUTATIONAL DRUG DESIGN USING QSAR/CHEMINFORMATICS AND BIOINFORMATICS

Course Instructor: Dr. Souvik Basak, Associate Professor & DIC, Division of Pharmaceutical Chemistry, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India

Class no.14

Date: 20/04/2023

Topic: Phylogenetic Analysis by MEGA, Tree Construction

Duration: 2h

**ATTENDANCE**

SL NO.	UNIVERSITY ROLL NO.	NAME OF THE STUDENT	Signature
1	2214009	ANUSKA CHATTERJEE	A. Chatterjee
2	2214011	ANANYA DEY	A. Dey
3	2214013	PARTHA PRATIM BEZ	P. Bez
4	2214014	AKASH MONDAL	Akash Mondal
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17	2214097	AYAN MAHATA	Ayan Mahata




*(Signature)*  
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 M. Pharm., Ph.D. (I.U.)  
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 Subansiri, West Bengal-713206

18	2214098	RIKU ROY	Riku Roy
19	2214051	SRIJITA CHATTERJEE	Srijita Chatterjee
20	2214052	ARUP KOLEY	Akoley
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27	2214034	PIU GHOSH	Piu Ghosh
28	2214033	NABYENDU MANDAL	N. Mandal
29	2214026	ADARSHA DUTTA	A. Dutta

Samir Kumar  
20/4/23

Signature of the Course Coordinator



  
 Prof. (Dr.) Samir Kumar Samanta  
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**DR. B.C ROY COLLEGE OF PHARMACY AND ALLIED HEALTH**  
**SCIENCES**  
**DURGAPUR, WB, INDIA**  
**Academic Year: 2022-23**  
**Attendance**

Course name: COMPUTATIONAL DRUG DESIGN USING QSAR/CHEMINFORMATICS AND BIOINFORMATICS

Course Instructor: Dr. Souvik Basak, Associate Professor & DIC, Division of Pharmaceutical Chemistry, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India

Class no.15

Date: 25/04/2023

Topic: Homology modelling, Steps, SWISS MODEL, VIDEO DEMONSTRATION OF MODELLER

**ATTENDANCE**

SL NO.	UNIVERSITY ROLL NO.	NAME OF THE STUDENT	Signature
1	2214009	ANUSKA CHATTERJEE	A. Chatterjee
2	2214011	ANANYA DEY	A. Dey
3	2214013	PARTHA PRATIM BEZ	P. Bez
4	2214014	AKASH MONDAL	Akash Mondal
5	2214017	ANUPAM BERA	Anupam Bera
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9	2214083	SANJUKTA DAS	Sanjukta Das
10	2214085	SNEHA GHOSH	Sneha Ghosh
11	2214086	TANMOY DAS	T Das
12	2214089	SANDIPAN SAU	S. Sau
13	2214090	PALLABI PRADHAN	Pallabi Pradhan
14	2214092	RAJIB DE	Rajib De
15	2214094	DISHA DAS	Disha Das
16	2214096	TAMAL PAL	Tal
17	2214097	AYAN MAHATA	Ayan Mahata

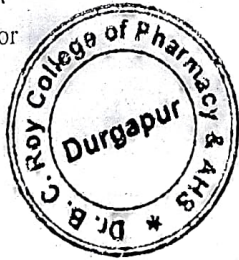



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18	2214098	RIKU ROY	Riku Roy
19	2214051	SRIJITA CHATTERJEE	Srijita Chatterjee
20	2214052	ARUP KOLEY	Akoley
21	2214053	SUVROJYOTI GHOSH ROY	S. Ghosh Roy
22	2214058	SOUVIK BHANDARY	Souvik Bhandary
23	2214060	SUSMITA AFTAB	Susmita Aftab
24	2214061	DIPANWITA BERA	Dipanjwita Bera
25	2214062	SUSMITA MALLICK	Susmita Aftab Susmita Mallik
26	2214063	MOLOY ROY	M Roy
27	2214034	PIU GHOSH	Piu Ghosh
28	2214033	NABYENDU MANDAL	N. Mandal
29	2214026	ADARSHA DUTTA	A Dutta

Souvi Bera  
25/4/23

Signature of the Course Coordinator



  
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**Dr. B. C. Roy College of Pharmacy & Allied Health Sciences, Durgapur-713206**

**Add on Course Continuous Assessment-I**

**Paper – Computational Drug Design using QSAR/Cheminformatics & Bioinformatics**

**Time – 1 hour**

**Full Marks – 50**

**MCQs (Answer all)**

**[50x1=50]**

- 1) Which of the following approach is considered under the ‘Ligand based drug designing’?**
  - a) Molecular docking
  - b) QSAR Modeling
  - c) Pharmacophore modeling
  - d) b and c both
- 2) Which of the following software is used for Phylogenetic analysis?**
  - a) LUDI
  - b) MEGA
  - c) CHEM3D
  - d) CoMFA
- 3) Which of these is gene prediction algorithm?**
  - a) UPGMA
  - b) Maximum parsimony
  - c) Hidden Markov Model
  - d) None
- 4) Procheck tool is use for**
  - a) Alignment
  - b) Protein Validation
  - c) Simulation
  - d) None of these
- 5) ARSA is search engine of**
  - a) DDBJ
  - b) GENBANK
  - c) EMBL
  - d) UNIPROT
- 6) Which one is the application of bioinformatics**
  - a) Design of primers
  - b) Grouping of proteins into families
  - c) Reconstructing genes from EST sequences
  - d) All
- 7) Which of the following method used for virtual screening**
  - a) ADMET analyses
  - b) QSAR modeling
  - c) Pharmacophore modeling
  - d) All of them
- 8) Lipinski’s rule of five is used for**
  - a) Dynamics simulation
  - b) Similarity search
  - c) Drug likeness
  - d) Docking
- 9) CoMFA method is used for**
  - a) 4D-QSAR
  - b) 3D-QSAR
  - c) 5D-QSAR
  - d) 6D-QSAR
- 10) Periodic table window in ChemDraw can appear using ..... toolbar**
  - a) File
  - b) Object
  - c) Structure
  - d) View
- 11) How is permeability predicted in Molinspiration software?**
  - a) ClogP
  - b) LlogP
  - c) KlogP
  - d) TlogP

**12) Which of the following function is not observed in ChemDraw Professional?**

- a) Convert structure to name
- b) Shows enhanced geometry
- c) Convert name to structure
- d) Show analysis window

**13) Symbol A -A in ChemDraw toolbar refers to**

- a) letter
- b) Query tool
- c) Addition
- d) None

**14) Which of the following tool is not present in ChemDraw toolbar?**

- a) Query tools
- b) Arrow tool
- c) Chromatography tool
- d) Reaction Tool

**15) Fragmentation tool is present in ChemDraw software**

- a) True
- b) False
- c) May be correct
- d) None

**16) Marquee section in ChemDraw helps to**

- a) Erase the drawing
- b) Draw double bonds
- c) Select the structures
- d) Draw phenyl rings

**17) Convert structure to name icon is present in which of the following toolbars**

- a) File
- b) Edit
- c) View
- d) Structure

**18) Chromatography tool is present in ChemDraw software**

- a) True
- b) False
- c) May be correct
- d) None

**19) Which of the following template is not present in ChemDraw toolbar?**

- a) Microorganisms
- b) Bioinstruments
- c) Shapes
- d) Walls

**20) Choose the incorrect statement about the SMILES generation of compound**

- a) Drawing the compound in the Molinspiration software
- b) Directly from Google
- c) Copy paste from the chemical drawing software
- d) Typing the SMILES of the compound on your own

**21) Which of the following are not chemical drawing softwares?**

- a) ChemDraw
- b) ChemDraw 3D
- c) Chem sketch
- d) Chem Art

**22) Which of the following would NOT be regarded as part of the science of informatics?**

- a) Storage of information about chemical properties
- b) Storage of information about physical properties
- c) Storage of information about synthetic methods
- d) Storage of information about chemical structures

23) Which of the following SMILES codes does NOT represent a cyclic structure?

- a) C1CCCCC1
- b) CC(=O)OC(C)(C)C
- c) O1CCOCC1
- d) n1CCCCC1

24) Which of the following databases CANNOT be used to store 3D structures?

- a) SMILES
- b) Alchemy
- c) Sybyl
- d) Chem3D

25) A QSAR study is only valid if

- a) It comprises of two inputs: biological data and physicochemical parameters
- b) It involves a group of closely related structures
- c) It involves an appropriate number of structures
- d) It predicts the activity of new molecules, not within the original data set

26) In order to be used in a QSAR study, biological data must

- a) Use information from the same biological test system
- b) Have been obtained in the same laboratory
- c) Have been produced by the same operator
- d) Use a quantitative measure of potency

27) Which of the following is NOT a hydrophobic parameter?

- a) Partition coefficient ( $P$ )
- b) Molecular connectivity
- c) Substituent constant ( $\Pi$ )
- d) Log  $P$

28) Which of the following is NOT an electronic parameter?

- a) Hammett substituent constant
- b) Dipole moment
- c) Molecular connectivity
- d) HOMO/LUMO

29) Which of the following is NOT used by molecular modelling software packages?

- a) Relative molecular mass
- b) Bond angles
- c) Bond lengths
- d) Torsion angles

30) Which of the following is NOT a useful statistical indicator of the goodness of fit of a regression analysis equation?

- a) Regression coefficient ( $r$ )
- b)  $r^2$
- c) Standard error ( $s$ )
- d) F tests

31) Which of the following is NOT usually used as a steric parameter?

- a) Molecular surface area
- b) Molar volume
- c) Relative molecular mass
- d) Taft's steric parameter

- 32) Which of the following scientists created the first Bioinformatics database?**  
a) Dayhoff      b) Pearson      c) Richard Durbin      d) Michael.J.Dunn
- 33) What is the deposition of cDNA into the inert structure called?**  
a) DNA probes      b) DNA fingerprinting      c) DNA polymerase      d) DNA microarrays
- 34) The identification of drugs through the genomic study is called \_\_\_\_\_.**  
a) Genomics      c) Pharmacogenetics  
b) Pharmacogenomics      d) Cheminformatics
- 35) Which of the following compounds has desirable properties to become a drug?**  
a) Fit drug      b) Lead      c) Fit compound      d) All of the above
- 36) Proteomics refers to the study of \_\_\_\_\_.**  
a) Set of proteins in a specific region of the cell      c) Biomolecules  
b) The entire set of expressed proteins in the cell      d) Set of proteins
- 37) The process of finding the relative location of genes on a chromosome is called**  
a) Gene tracking      c) Genome mapping  
b) Chromosome walking      d) Genome walking
- 38) The computational methodology that tries to find the best matching between two molecules, a receptor and ligand are called \_\_\_\_\_.**  
a) Molecular fitting      b) Molecular matching  
c) Molecule affinity checking      d) Molecular docking
- 39) Which of the following is not the application of bioinformatics?**  
a) Understand the relationships between organisms      c) Drug designing  
b) Data storage and management      d) None of the above
- 40) The term “*in vivo*” is the Latin word which refers to \_\_\_\_\_.**  
a) Within the lab      c) Within the glass  
b) Outside the lab      d) Outside the glass
- 41) The stepwise method for solving problems in computer science is**  
a) Flowchart      b) Algorithm      c) Procedure      d) Sequential design
- 42) The laboratory work using computers and associated with web-based analysis generally**  
a) In silico      b) Dry lab      c) Wet lab      d) All of the above

- 43) The computer simulation refers to**  
a) In silico                      b) Dry lab                      c) Wet lab                      d) All of the above
- 44) Which of the following tools is used for the identification of motifs?**  
a) BLAST                      b) COPIA                      c) PROSPECT                      d) Pattern hunter
- 45) Which of the following tools is used for the identification of motifs?**  
a) BLAST                      b) COPIA                      c) PROSPECT                      d) Pattern hunter
- 46) The term Bioinformatics was coined by \_\_\_\_\_.**  
a) J.D Watson                      b) Pauline Hogeweg  
c) Margaret Dayhoff                      d) Frederic Sanger
- 47) The human genome contains approximately \_\_\_\_\_ base pairs**  
a) 6 billion                      b) 5 billion                      c) 3 billion                      d) 4 billion
- 48) Which of the following is analogous to  $\sigma$  constant?**  
a) logP                      b) Rf                      c) pKa                      d) Es
- 49) Which of the following is analogous to  $\pi$  constant?**  
a) MW                      b) k'                      c) pKa                      d) Es
- 50) Which QSAR technique is performed manually?**  
a) Hansch approach                      c) Free Wilson approach  
b) Fujita Ban approach                      d) Topliss approach

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**Add on Course Continuous Assessment-II**

**Paper – Computational Drug Design using QSAR/Cheminformatics & Bioinformatics**

**Time – 1 hour**

**Full Marks – 50**

**MCQs (Answer all)**

**[25x2=50]**

**1. Lipinski rule of 5 includes**

- a) Molecular weight less than 300 daltons
- b) logP value can exceed 5
- c) All nitrogen and oxygen atoms may be more than 10
- d) Hydrogen bond donors must not be more than 5

**2. Drug likeliness means**

- a) How drug like a substance is with respect to factors like bioavailability
- b) How a drug likes the receptor
- c) Property of drug similar to receptor
- d) Affinity of drug to become a lead

**3. ADME of a drug does not include**

- a) Adsorption
- b) Distribution
- c) Metabolism
- d) Excretion

**4. Molinspiration software provides details like**

- a) Drug likeliness
- b) Bioactivity score
- c) Bioavailability
- d) All of these

**5. Chemical drawing softwares are**

- a) ChemDraw
- b) Chemical draw
- c) Chem academy
- d) ChemMaster

**6. Which of the following template is not present in ChemDraw toolbar?**

- a) Microorganisms
- b) Bioinstruments
- c) Shapes
- d) Walls

- 7. In 3D QSAR blue regions indicate favorable points for**
- Bulky groups
  - Electron rich groups
  - Electron deficient groups
  - Smaller groups
- 8. In 3D QSAR green regions indicate favorable points for**
- Bulky groups
  - Electron rich groups
  - Electron deficient groups
  - Smaller groups
- 9. In 3D QSAR yellow regions indicate favorable points for**
- Bulky groups
  - Electron rich groups
  - Electron deficient groups
  - Smaller groups
- 10. One of the following is a quantum chemical parameter**
- STERIMOL
  - Taft c constant
  - HOMO
  - Hammett's constant
- 11. One of the following is not used in QSAR**
- Molecular connectivity index
  - Molecular similarity index
  - Topological Polar surface area
  - Partition Coefficient
- 12. Which of the following are not bioisosteres of -NH<sub>2</sub>**
- OH
  - SH
  - CH<sub>3</sub>
  - H<sub>2</sub>S
- 13. Choose the compound which can be drug like with respect to their molecular weight**
- Naphthalene
  - Anthracene
  - Phenanthrene
  - All of these

**14. The chem draw files can be renamed to pdb file using .....software**

- a) Pymol
- b) Discovery Studio Visualizer
- c) Protein Data Bank
- d) ChemSketch

**15. The structures in the Auto Dock file can be opened using**

- a) Load structure
- b) Ligand-Input
- c) Load molecule
- d) Upload structure

**16. The features like ‘add Kollman charges’ and ‘compute gasteiger’ are used for**

- a) Ligand
- b) Protein
- c) Both a and b
- d) None

**17. What is the principle of AutoDock?**

- a) A tool designed to predict how small molecules and drug candidates bind to a receptor
- b) Helps to find syntax errors, spelling mistakes, missing code, and other issues in your Python code
- c) An interactive source code debugger for Python programs
- d) Identification of new protein structures via in silico approaches or can be used in protein nucleic acid interaction studies.

**18. Why are protein databases important?**

- a) It can be used in sequence analysis
- b) It identifies homologous sequences of programs
- c) It predicts protein functions based on non-sequence similarity
- d) None of the above

**19. Lead optimization helps in**

- a) Enhancing the most promising compound to improve the toxicity
- b) Obtaining lower RMSD values
- c) Building the target protein model
- d) Generating the Pharmacophore models

**20. Choose the compound with best docking score**

- a) Compound 47- Score -5.5
- b) Compound 45- Score -6.8
- c) Compound 46- Score -7.1
- d) Compound 48- Score -4.3



**21. Select the wrong pair**

- a) **MOL INSPIRATION** - Lipinsky Rule of 5
- b) **MOL SOFT**- Drug Likeliness
- c) **ADMET SAR**- Toxicity evaluation
- d) **CANIMOTO INDEX**- Dissimilarity index

**22. Choose the incorrect statement**

- a) The grid box includes the entire protein in blind docking
- b) The docking result is analyzed using Discovery Studio Visualizer software
- c) The desired protein can be easily downloaded from Protein Data Bank
- d) Binding Energy and Docking score are same parameters to determine binding

**23. The file must be converted to pdbqt before using command in .....**

- a) CHEMDRAW
- b) AUTODOCK VINA
- c) MOL INSPIRATION
- d) PYMOL

**24. nON and nOHNH refers to ..... respectively**

- a) Hydrogen bond donors and acceptors
- b) Hydrogen bond acceptors and donors
- c) Virtual screening and ligand design
- d) Ligand design and virtual screening

**25. Choose the correct statement**

- a) A compound with 1.34 milogP passes Lipinski rule of 5
- b) Human oral bioavailability can be determined by *in silico* toxicity study
- c) Ligand energy minimization is essential before docking
- d) Development of protein is not required for running AUTODOCK

**Dr. B. C. Roy College of Pharmacy & Allied Health Sciences, Durgapur-713206**

**Add on Course Continuous Assessment-III**

**Paper – Computational Drug Design using QSAR/Cheminformatics & Bioinformatics**

**Time – 1 hour**

**Full Marks – 50**

**Fill in the Blanks: - (Answer all)**

**[4x1=4]**

1. Full form of MEGA .....
2. In ..... to complete an analysis the user is not required to move between different subprograms while keeping modifying names of the intermediate output files.
3. .... deals with the interaction between computers and humans using the natural language
4. .... model were developed and incorporated in machines which mimicked the functionalities of human origin.

**Short Answer Questions: - (Answer all)**

**[23x2=46]**

1. Define Free Wilson Analysis with examples.
2. Write the applications of QSAR.
3. Enlist two ADME databases.
4. Mention two Biochemical databases.
5. Define Lead molecule with examples.
6. Define Random screening for lead optimization.
7. Define COMFA and COMSIA.
8. Write applications of pharmaceutical databases.
9. Mention any two lead optimization techniques.
10. Define bioisosteres with examples.
11. Explain Hansch analysis.
12. Compare SAR and QSAR.
13. Define COMSIA with its two applications.
14. Explain Lipinski rule of 5.
15. Protein processing for Docking in AutoDock Vina.
16. Enlist any two pharmaceutical databases.
17. How binding sites are located in PDB and Discovery studio Visualizer
18. Importance of Grid Box in docking
19. Docking in Virtual screening of compounds.
20. BLAST and gene ontology finding.
21. Multiple Sequence Alignment and protein function assessment
22. Homology modelling and use of MODELLER.
23. Semi empirical methods and energy minimization.

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Durgapur - 713206, West Bengal, India

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Certificate course  
On

## Computational Drug Design using QSAR/ Cheminformatics and Bioinformatics

This certificate is issued to *ADARSHA DUTTA*, M. PHARM. (INDUSTRIAL PHARMACY) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Computational Drug Design using QSAR/Cheminformatics and Bioinformatics" by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

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Dr. Souvik Basak  
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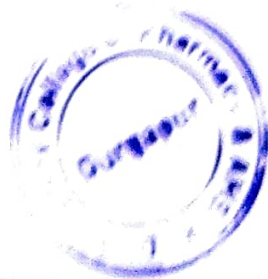
Computational Drug Design using QSAR/  
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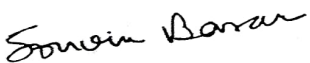
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**Computational Drug Design using QSAR/  
Cheminformatics and Bioinformatics**



This certificate is issued to *MOLOY ROY*, M. PHARM. (PHARMACEUTICAL ANALYSIS) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Computational Drug Design using QSAR/Cheminformatics and Bioinformatics" by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

*Souvik Basak*

Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRCP



*S. Ray*

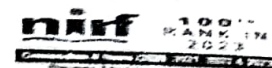
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

Prof. (Dr.) S. Ray  
Principal, BCRCP

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

**Durgapur - 713206, West Bengal, India**

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Certificate course  
On

**Computational Drug Design using QSAR/  
Cheminformatics and Bioinformatics**

This certificate is issued to *NABYENDU MANDAL*, M. PHARM. (INDUSTRIAL PHARMACY) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Computational Drug Design using QSAR/Cheminformatics and Bioinformatics" by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

*Souvik Basak*

**Dr. Souvik Basak**  
Course coordinator  
Associate Professor, BCRCP



*S. Ray*

**Prof. (Dr.) S. Ray**  
Principal, BCRCP

*S. Ray*  
Prof. (Dr.) S. Ray  
M. Pharm., Ph.D. (U.S.A.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal

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

Durgapur - 713206, West Bengal, India

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Certificate course  
On



## Computational Drug Design using QSAR/ Cheminformatics and Bioinformatics



This certificate is issued to **NURUL HASSAN MONDAL, M. PHARM.** (PHARMACOLOGY) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Computational Drug Design using QSAR/Cheminformatics and Bioinformatics" by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

*Souvik Basak*

Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRC



*S. Ray*

Prof. (Dr.) S. Ray  
Principal, BCRC

*S. Samanta*  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal 713206

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

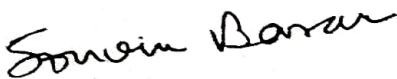
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Certificate course  
On


## Computational Drug Design using QSAR/ Cheminformatics and Bioinformatics

This certificate is issued to **NURUL HASSAN MONDAL, M. PHARM.** (PHARMACOLOGY) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Computational Drug Design using QSAR/Cheminformatics and Bioinformatics" by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

  
**Dr. Souvik Basak**  
Course coordinator  
Associate Professor, BCRCP



  
**Prof. (Dr.) S. Ray**  
Principal, BCRCP

  
**Prof. (Dr.) Sankar Kumar Samanta**  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206



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


Durgapur - 713206, West Bengal, India

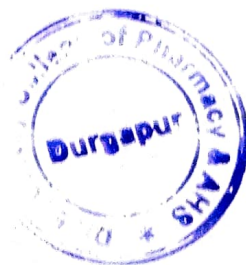
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Certificate course  
On


## Computational Drug Design using QSAR/ Cheminformatics and Bioinformatics

This certificate is issued to *PALLABI PRADHAN*, M. PHARM. (PHARMACOLOGY) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Computational Drug Design using QSAR/Cheminformatics and Bioinformatics" by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

  
Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRCP



  
Prof. (Dr.) S. Ray  
Principal, BCRCP

  
Prof. (Dr.) S. Ray  
M. Pharm., Ph.D. (Ph.D.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206





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

Durgapur - 713206, West Bengal, India

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Certificate course  
On

**Computational Drug Design using QSAR/  
Cheminformatics and Bioinformatics**

This certificate is issued to *PARTHA PRATIM BEZ*, M. PHARM. (PHARM) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the course on "Computational Drug Design using QSAR/Cheminformatics and Bioinformatics" by *Souvik Basak* from 21st February, 2023 for a duration of 8 weeks (30 hours).

*Souvik Basak*  
Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRC



*S. Ray*  
Prof. (Dr.) S. Ray  
Principal, BCRC

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

Durgapur - 713206, West Bengal, India

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Certificate course  
On

Computational Drug Design using QSAR/  
Cheminformatics and Bioinformatics



This certificate is issued to *PARTHA PRATIM BEZ*, M. PHARM. (PHARMACEUTICS) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on “Computational Drug Design using QSAR/Cheminformatics and Bioinformatics” by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

*Souvik Basak*

Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRC



*S. Ray*  
21/2/23

*S. Ray*  
Prof. (Dr.) Saimi Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206  
Prof. (Dr.) S. Ray  
Principal, BCRC

Dr. S. C. Ray College of Pharmacy and Allied Health Sciences

Barasat, West Bengal, India

Barasat, West Bengal, India

Barasat, West Bengal, India

Barasat, West Bengal, India



This certificate is issued to Mr. S. C. Ray, student of Dr. S. C. Ray College of Pharmacy & Allied Health Sciences, for completing the certificate course on "Computational Drug Design using PK/PD pharmacokinetics and Pharmacodynamics" by Dr. Souvik Prasad from 21st February, 2023 for a duration of 8 weeks (40 hours).

Dr. Souvik Prasad  
Course coordinator  
Associate Professor, BCRCP



Prof. (Dr.) S. Ray  
Principal, BCRCP

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

Durgapur - 713206, West Bengal, India

ACCREDITED BY NAAC (B++), NBA (UG)

Certificate course  
On

Computational Drug Design using QSAR/  
Cheminformatics and Bioinformatics

This certificate is issued to *PAYEL GHOSH*, M. PHARM. (PHARMACOLOGY) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on “Computational Drug Design using QSAR/Cheminformatics and Bioinformatics” by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

*Souvik Basak*  
Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRC



*S. Ray*  
Prof. (Dr.) S. Ray  
Principal, BCRC

*Samir Kumar Samanta*  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206



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

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Certificate course  
On

Computational Drug Design using QSAR/  
Cheminformatics and Bioinformatics

This certificate is issued to *PIU GHOSH*, M. PHARM. (INDUSTRIAL PHARMACY) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Computational Drug Design using QSAR/Cheminformatics and Bioinformatics" by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

*Souvik Basak*

Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRCP



*S. Ray*

Prof. (Dr.) S. Ray  
Principal, BCRCP

*Samir Kumar Samanta*  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D. (J.U.)

Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur - 713206



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Certificate course  
On

## Computational Drug Design using QSAR/ Cheminformatics and Bioinformatics



This certificate is issued to *RAJIB DE*, M. PHARM. (PHARMACOLOGY) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on “Computational Drug Design using QSAR/Cheminformatics and Bioinformatics” by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

*Souvik Basak*

Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRCP



*S. Ray*

Prof. (Dr.) S. Ray  
Principal, BCRCP

*S. Ray*  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

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

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Certificate course  
On

**Computational Drug Design using QSAR/  
Cheminformatics and Bioinformatics**



This certificate is issued to *RIKU ROY*, M. PHARM. (PHARMACOLOGY) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on “Computational Drug Design using QSAR/Cheminformatics and Bioinformatics” by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

*Souvik Basak*

Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRCP



*S. Ray*

Prof. (Dr.) S. Ray  
Principal, BCRCP

*Samita Kumar Samanta*  
Prof. (Dr.) Samita Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

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Durgapur - 713206, West Bengal, India

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Certificate course  
On

## Computational Drug Design using QSAR/ Cheminformatics and Bioinformatics



This certificate is issued to *SANDIPAN SAU*, M. PHARM. (PHARMACOLOGY) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on “Computational Drug Design using QSAR/Cheminformatics and Bioinformatics” by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

*Souvik Basak*

Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRC



*S. Ray*

Prof. (Dr.) S. Ray  
Principal, BCRC

*S. Ray*  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
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Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206



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Durgapur - 713206, West Bengal, India

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Certificate course  
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## Computational Drug Design using QSAR/ Cheminformatics and Bioinformatics



This certificate is issued to *SANJUKTA DAS*, M. PHARM. (PHARMACOLOGY) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on “Computational Drug Design using QSAR/Cheminformatics and Bioinformatics” by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

*Souvik Basak*

Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRCP



*S. Ray*

Prof. (Dr.) Samy Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

Prof. (Dr.) S. Ray  
Principal, BCRCP

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

Durgapur - 713206, West Bengal, India

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Certificate course  
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## Computational Drug Design using QSAR/ Cheminformatics and Bioinformatics

This certificate is issued to **SAYANTAN NAG**, M. PHARM. (PHARMACEUTICS) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on “Computational Drug Design using QSAR/Cheminformatics and Bioinformatics” by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

*Souvik Basak*

Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRCP



*S. Ray*

Prof. (Dr.) S. Ray  
Principal, BCRCP

*Samir Kumar Samanta*  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

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

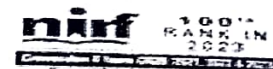
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Certificate course  
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**Computational Drug Design using QSAR/  
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*Souvik Basak*

**Dr. Souvik Basak**  
Course coordinator  
Associate Professor, BCRCP



*S. Ray*

**Prof. (Dr.) S. Ray**  
Principal, BCRCP

*Sanku Kumar Samanta*  
Prof. (Dr.) Sanku Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

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

Durgapur - 713206, West Bengal, India

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Certificate course  
On

**Computational Drug Design using QSAR/  
Cheminformatics and Bioinformatics**



This certificate is issued to *SOUVIK BHANDARY*, M. PHARM. (PHARMACEUTICAL ANALYSIS) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on “Computational Drug Design using QSAR/Cheminformatics and Bioinformatics” by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

*Souvik Basak*

**Dr. Souvik Basak**  
Course coordinator  
Associate Professor, BCRC



*S. Ray*

**Prof. (Dr.) S. Ray**  
Principal, BCRC

*S. Ray*  
**Prof. (Dr.) Samir Kumar Samanta**  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal - 713206

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

Durgapur - 713206, West Bengal, India

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Certificate course  
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## Computational Drug Design using QSAR/ Cheminformatics and Bioinformatics



This certificate is issued to *SRIJITA CHATTERJEE*, M. PHARM. (PHARMACEUTICAL ANALYSIS) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on “Computational Drug Design using QSAR/Cheminformatics and Bioinformatics” by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

*Souvik Basak*

Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRCP



*S. Ray*

Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal 713206  
Principal, BCRCP

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

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*Souvik Basak*

Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRCP



*S. Roy* Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal

Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206  
Prof. (Dr.) S. Roy  
Principal, BCRCP

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

Durgapur - 713206, West Bengal, India

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Certificate course  
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## Computational Drug Design using QSAR/ Cheminformatics and Bioinformatics

This certificate is issued to *SUSMITA AFTAB*, M. PHARM. (PHARMACEUTICAL ANALYSIS) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Computational Drug Design using QSAR/Cheminformatics and Bioinformatics" by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

*Souvik Basak*

Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRCP



*S. Ray*

Prof. (Dr.) S. Ray  
Principal, BCRCP

*S. Ray*  
Prof. (Dr.) Sanku Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206



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

Durgapur - 713206, West Bengal, India

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Certificate course  
On

## Computational Drug Design using QSAR/ Cheminformatics and Bioinformatics



This certificate is issued to *SUSMITA MALLICK*, M. PHARM. (PHARMACEUTICAL ANALYSIS) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on “Computational Drug Design using QSAR/Cheminformatics and Bioinformatics” by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

*Souvik Basak*

Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRCP



*S. Ray*

Prof. (Dr.) S. Ray  
Principal, BCRCP

*Samir Kumar Samanta*  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206



# C. Roy College of Pharmacy and Allied Health Sciences

Durgapur - 713206, West Bengal, India

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Certificate course  
On

## Computational Drug Design using QSAR/ Cheminformatics and Bioinformatics

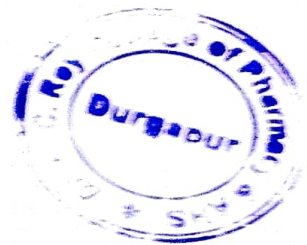


certificate is issued to **SUVROJYOTI GHOSH ROY, M. PHARM.**  
(PHARMACEUTICAL ANALYSIS) student of Dr. B. C. Roy College of Pharmacy & AHS,  
completing the certificate course on "Computational Drug Design using  
Cheminformatics and Bioinformatics" by Dr. Souvik Basak from 21st February, 2023 for

Duration

*Souvik Basak*

Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRCF



*S. Roy*  
Prof. (Dr.) S. Roy  
Principal, BCRCF  
C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

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

Durgapur - 713206, West Bengal, India  
ACCREDITED BY NAAC (B++), NBA (UG)



Certificate course  
On

## Computational Drug Design using QSAR/ Cheminformatics and Bioinformatics

This certificate is issued to **SUVROJYOTI GHOSH ROY, M. PHARM.**  
(**PHARMACEUTICAL ANALYSIS**) student of **Dr. B. C. Roy College of Pharmacy & AHS,**  
for completing the certificate course on "Computational Drug Design using  
QSAR/Cheminformatics and Bioinformatics" by **Dr. Souvik Basak** from 21st February, 2023 for  
a duration of **01 month**.



*Souvik Basak*  
**Dr. Souvik Basak**  
Course coordinator  
Associate Professor, BCRCP

*S. Roy*  
Prof. (Dr.) S. Roy, M. Pharm., Ph.D. (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206  
**Principal, BCRCP**

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

Durgapur - 713206, West Bengal, India

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Certificate course  
On

## Computational Drug Design using QSAR/ Cheminformatics and Bioinformatics



This certificate is issued to *TAMAL PAL*, M. PHARM. (PHARMACOLOGY) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on “Computational Drug Design using QSAR/Cheminformatics and Bioinformatics” by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

*Souvik Basak*

Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRCP



*S. Ray*

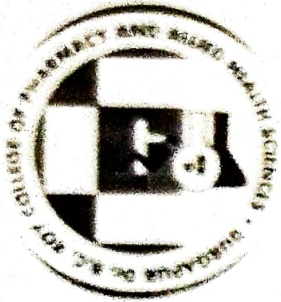
Prof. (Dr.) S. Ray  
Principal, BCRCP

*Sanku Kumar Samanta*  
Prof. (Dr.) Sanku Kumar Samanta  
M. Pharm., Ph.D. (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur, West Bengal-713206

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

Durgapur - 713206, West Bengal, India

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Certificate course  
On

**Computational Drug Design using QSAR/  
Cheminformatics and Bioinformatics**



This certificate is issued to *TANMOY DAS*, M. PHARM. (PHARMACOLOGY) student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on “Computational Drug Design using QSAR/Cheminformatics and Bioinformatics” by Dr. Souvik Basak from 21st February, 2023 for a duration of 8 weeks (30 hours).

Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRC



Prof. (Dr.) S. Ray  
Principal, BCRC

Prof. (Dr.) S. Ray  
M. Pharm  
Dr. B. C. Roy College of Pharmacy

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

Durgapur - 713206, West Bengal, India

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*Souvik Basak*

Dr. Souvik Basak  
Course coordinator  
Associate Professor, BCRCP



*S. Ray*

Prof. (Dr.) S. Ray  
Principal, BCRCP

*Samir Kumar Samanta*  
Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
Principal  
Dr. B. C. Roy College of Pharmacy & AHS  
Durgapur



## SUMMARY REPORT AND OUTCOME

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

**Start date:** 21.02.2023

**End date:** 25.04.2023

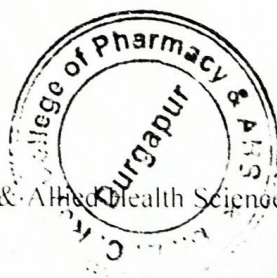
**Total Course Duration:** 30 h

**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.



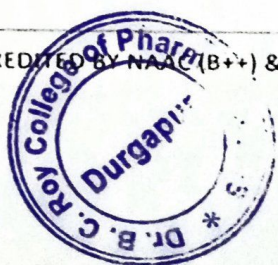
Souvik Basak  
25/4/23

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Prof. (Dr.) Samir Kumar Samanta  
M. Pharm., Ph.D (J.U.)  
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ACCREDITED BY NAAC (B++) & NBA (FOR UG PHARMACY)





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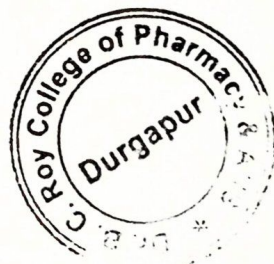
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### OUTCOME

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



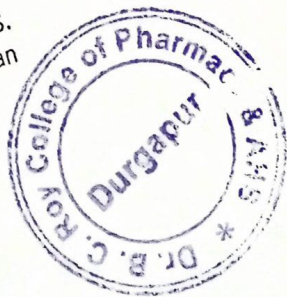
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