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

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

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.

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- The institute thus approves and gives no objection for onset of such value-added course for the students, upon completion of which the students would obtain certificates acknowledged by the institute.

- Thus, it is hereby decided that the institute, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur-713206, WB, India is going to initiate certification course on "Computational drug design using QSAR/Cheminformatics and Bioinformatics" from January, 2017.

Approved by

10/1/2017

Prof. (Dr.) Subrata Chakraborty
M. Pharm., Ph.D.
Director

Dr. Subrata Chakraborty,
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17/1/17

*Principal*
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# Basic course on computational drug design using Cheminformatics and Bioinformatics

## COURSE OBJECTIVE (COB)

1. To understand the basic workflow of Quantitative Structure Activity Relationship (QSAR)

2. To understand the methodology of structure drawing, energy minimization, descriptor calculation

3. Know the hands on technology of docking, analysis of its results, interpretation of best docking conformer

4. Knowledge of 2D QSAR model equation, understand the relationship between biological activity and descriptors

5. Understand tools of basic bioinformatics

## COURSE OUTCOME (CO)

At the end of the course, the student will be able to

1. Understand quantitative correlation between any set of medicinal compounds and their biological activities.

2. Construct chemical structures *in silico* and perform further processing on them

3. Perform, analyze and interpret manual docking working with protein and chemical structures of medicinal interest.

4. Create new QSAR model equations in the subset of medicinal compounds and biological activities

5. Utilize basic tools of bioinformatics to manipulate, engineer or design newer proteins; identify unknown receptors, delineate mutations and other parameters of active proteins of physiological systems.

**Online Course Chapters**

| No. of Chapter | Name of the Chapter | Theory (h) | Lab (h) |
|---|---|---|---|
| 1 | Brief Introduction of QSAR and its workflow | 1 | 2 |
| 2 | Structure drawing with ACD Lab Chemsketch/ ChemOffice, download, installation, creating new molecules and playing with various parameters to edit the molecule, switch between 2D and 3D parameters | 1 | 2 |
| 3 | In silico drug likeliness testing, application of Lipinski Rule of Five, Using Molinspiration server, in silico toxicity testing, using admetSAR, to screen drug molecules | 1 | 2 |
| 4 | Concept of Docking | 1 | 2 |
| 5 | Working with PDB, protein structure search, downloading protein structure in PDB format | 1 | 2 |
| 6 | Working protein structure in UCSF chimera, add hydrogens, delete native water molecules, preparation of final protein structure in .pdb format | 1 | 2 |
| 7 | Predicting biological activity of selected compounds by molecular docking with SWISSDOCK or PARDOCK, counting the docking scores, analysing protein-ligand binding interactions with UCSF Chimera | 1 | 2 |
| 8 | Building up 2D QSAR model equation with biological acitivity (predicted) and molecular descriptors, using REGRESSION ANALYSIS and ARRAY FORMULA | 1 | 2 |
| 9 | Validating QSAR model, comparison between OBA and PBA by ANOVA (Student t-test) | 1 | 2 |
| 10 | Basic Bioinformatics Working with gene and protein sequences from NCBI, downloading gene and protein sequences | 1 | 2 |
| | | **Total contact hours = 30** | |

# Quiz
# Chapter 1
# Overflow of CADD and QSAR

Full Marks: 10 Time: 10 min

1. QSAR starts from

a) Finding the lead b) Optimizing the lead c) Finding Bioactivity of the lead d) None of these

2. CADD involves

a)Varying pharmacophore and keeping substituents constant
b) Varying substituents and keeping pharmacophore constant
c) keeping both pharmacophore and substituents constant
d) All of these
e) None of these

3. Receptor in QSAR is a

a) native physiological protein b) small molecule c) native protein modified in specific positions d) protein-ligand complex

4. In QSAR, structures are depicted in terms of

a) Descriptors b) Bonds c) No. of atoms d) All of these

5. The first set of molecules under investigation can be filtered out by

a) Docking b) in vivo biological activity evaluation c) Lipinsky's rule d) toxicity evaluation

6. In QSAR biological activity is often described in

a) Log scale b) Semilog scale c) Linear scale d) Eigenvalue scale

7. BA in log scale with molecular descriptors can be correlated with

a) Regression analysis d) Addition c) Subtraction d) All of these

8. MW as per Lipinsky's rule should be

a) <200 Da b) <300 Da c) <400Da d) <500Da

9. Log P is correlated with

a) Compound's steric effect b) Compound hydrophobicity c) Compound's lipophicity d) both a and b e) both b and c

10. Ligands in protein fit in

a) Binding site b) Allosteric sites c) both of these d) None of these

# Quiz
# Chapter 2
# Structure Drawing

Full marks: 1 x 10 =10

1. Draw the structures of the following:

a) Indomethacin

b) Tolmetin

c) Ibuprofen

d) Amoxicillin

e) Penicillin-G

f) Penicillin-V

g) Procaine

h) Mitomycin C

i) Albendazole

j) Nifedipine

# Quiz
# Chapter 3
# Drug Likeliness and *in silico* Toxicity

Full Marks: 10 Time: 10 min

1. Drug likeliness can be tested by

a) OSIRIS Properties calculator b) admetSAR c) admetTOX d) None of these

2. As per Lipinsky's rule logP should be

a) < 1 b) <3 c) <5 d) None of these

3. AMES toxicity is a measure of

a) mutagenicity b) teratogenicity c) environmental toxicity d) cardiac toxity

4. Free ADMET determining software is

a) admetSAR b) MOLINSPIRATION c) MolCalc d) MOLSOFT

5. hERG gene toxicity is

a) cardiac toxicity b) nephrotoxicity c) liver toxicity d) terratogenicity

6. *Tetrahymena pyriformis* toxicity is related with

a) mutagenicity b) teratogenicity c) environmental toxicity d) cardiac toxicity

7. SMILEY is

a) Compound docking format b) compound structure writing format c) representing compound bond angles d) QSAR output format

8. CYP3A4 inhibition

a) increase drug concentration in blood b) decrease drug concentration in blood c) increase Log P of compound d) increase lipophilicity of compound

9. The full form of QSTR is _____

10. Red score in OSIRIS PROPERTIES CALCULATOR indicate result that is

a) acceptable b) not acceptable c) depends on case to case d) can not be calculated

# Quiz
# Chapter 4-7
# Docking

Full Marks: 10 Time: 10 min

1. Which one is a free tool for docking?

a) GOLD b) GLIDE c) SCHRODINGER d) SWISS DOCK

2. Which one of the following is a software to read protein?

c) UCSF Chimera b) PyMOL c) Rasmol d)All of these

3. .mol2 is a format to save

a) Protein b) Ligand c) Both of these d) None of these

4. Which one of the following is suppressed in PDB derived protein structure but required to add explicitly during docking?

a) All bonds in protein b) All Amino acid residues in protein c) All hydrogens of protein d) All –COOH terminals in protein

5. In docking, which one is true?

a) Protein-flexible, ligand-rigid b) Both protein and ligands are flexible c) Protein-rigid, ligand flexible d) All of these

6. Which one of the following is preferentially the output format of docking energy (binding energy)?

a) ΔG b) ΔH c) ΔA d) ΔG/ΔH

7. in SWISSDOCK, conformers of a specific docking generated ligand is categorized as

a) most fitting to lowest fitting b) Lowest fitting to most fitting c) Highest potential energy to lowest potential energy d) None of these

8. The favorable conformations generated by SWISS DOCK can be analyzed by

a) UCSF Chimera b) Chem Draw c) JMol d) ISIS DRAW

9. The most favorable bonding between ligand and protein is

a) Covalent bonding b) Metal Binding c) vander Waals Bonding d) Hydrogen bonding

10. The inbound ligand in PDB protein helps in

a) intiate the ligand protein interaction b) solvating the protein while docking c) helping in determining the binding pocket within the protein d) helping in determining the conformation of the interacting ligand

# Quiz
# Chapter 8-9
# QSAR model building and validation

Full Marks: 10 Time: 10 min

1. Quantitatively a structure can be depicted as

a) by its atomic number b) by its molecular weight c) by number of carbon atoms d) by a set of physic chemical properties which are known as descriptors

2. Which of the following descriptors is mostly related with compound's biological activity?

a) Molecular weight b) Molar refractivity c) Log P d) percentage atom composition in the molecule

3. In 2D QSAR model the quantitative correlation is established between

a) Biological Activity (BA) vs Descriptors b) Log BA vs Descriptors c) BA vs Log Descriptors d) Log BA bs Log Descriptors

4. Multiple Linear Regression (MLR) is possible with

a) single y and multiple x variables b) single x and multiple y c) multiple x and multiple y d) none of these

5. MLR in MS Excel can be achieved by

a) SUM function b) LINEST function c) TTEST function d) ANOVA

6. The regression coefficients by LINEST command are generated

a) in forward order b) in reverse order c) in matrix d) both a and c e) both b and c

7. To compare between observed biological activity and predicted biological activity by QSAR model, one of the simplest way is to perform

a) subtraction analysis between the two b) Analysis of standard deviation between the two c) TTEST between the two d) FTEST between the two

8. In order to find out major descriptors contributing significantly in a QSAR model, rationally one can perform

a) Trial and error technique b) Randomization technique c) MLR d) Principle Component Analysis (PCA)

9. Drug likeliness score can be calculated by

a) OSIRIS properties calculator b) admetSAR c) MOLINSPIRATION d) None of these

10. Which one of the following is true for model establishment and validation in QSAR model?

a) Test set-model development & Trainee set-model validation

b) Trainee set- model development & Test set- model validation

c) Both Test set and Trainee set- model validation

d) Both Test set and Trainee set- model development

# Quiz
# Chapter 10
# Bioinformatics

Full Marks: 10 Time: 10 min

1. The activity of a protein is related with

a) Gene sequence of the protein b) Amino acid sequence of the protein c)Both of these d) None of these

2. The amino acid sequence of a protein can be retrieved from

a) Expasy b) SWISS PDB c) PDB d) NCBI

3. Identification of a gene or protein can be retrieved by sequence alignment with known gene/ proteins. This could be done by

a) BLAST b) Homology Modeling c) SWISS-PROT d) Clustal W

4. Homology modeling of a protein may be done by the following:

a) CASTp b) LigASite c) SWISS MODEL d) PSI BLAST

5. One gene can lead to a particular protein, but a protein can lead to multiple genes- The statement is

a) TRUE b) FALSE c) Can not be said-depends on case to case

6. The sequence alignment may be done with

a) Gene Bank format b) FASTA Format c) Python format d) .txt format

7. The amino acid substitution in a protein can be tracked by

a) sequence alignment with BLAST b) sequence alignment with CLUSTAL W c) Sequence alignment with BoxShade d) All of these

8. If a receptor structure is unknown, still the docking between the receptor and ligand can be performed. The statement is true IF

a) the sequence of the protein is known b) the sequence of the protein is unknown c) the biological activity of the protein is known d) the statement can not be true

9. Homology modeling of a protein requires

a) template proteins with high percentage similarity b) template proteins with low percentage similarity c) template proteins with same binding sites d) both a and c e) both b and c

10. The hydrophathicity (hydrophobicity) of a protein can be measured by

a) GRAVY index b) $\pi$ index c) Ramachandran Plot d) $\sigma$-$\pi$ plot

LECTURE 1: Brief Introduction of QSAR and its work flow

Date: 8.2.2017

| DATE | NAME | MODULE | SIGNATURE |
|---|---|---|---|
| 8.2.2017 | BHARGAB KAR | 1 | Bhargab Kar |
| 8.2.2017 | DEBAYAN DAS | 1 | Debayan Das |
| 8.2.2017 | GAURIC BHUSHAN MANDAL | 1 | Gauric B. Mandal |
| 8.2.2017 | INDRANI SEN | 1 | Indrani Sen |
| 8.2.2017 | ISHIKA DUTTA CHOWDHURY | 1 | Ishika Dutta Chowdhury |
| 8.2.2017 | PRITAM DAS | 1 | Pritam Das |
| 8.2.2017 | RITUPARNA PARUI | 1 | Rituparna Parui |
| 8.2.2017 | RUDRA BHATTACHARJEE | 1 | Rudra Bhattacharjee |
| 8.2.2017 | RUSHAM DAS | 1 | Rusham Das |
| 8.2.2017 | SALMAN KHURSHID | 1 | Salman Khurshid |
| 8.2.2017 | SOHINI CHATTERJEE | 1 | Sohini Chatterjee |
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LECTURE 2: Structure drawing with ACD Lab/ChemSketch/ Chemoffice: download, installation, creating new molecules and playing with various parameters to edit the molecule, switch between 2D and 3D parameters

Date: 9.2.2017

| DATE | NAME | MODULE | SIGNATURE |
|---|---|---|---|
| 9.2.2017 | BHARGAB KAR | 2 | Bkar |
| 9.2.2017 | DEBAYAN DAS | 2 | Debayan Das |
| 9.2.2017 | GAURIC BHUSHAN MANDAL | 2 | Gauric B. Mandal |
| 9.2.2017 | INDRANI SEN | 2 | Indrani Sen |
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| 9.2.2017 | PRITAM DAS | 2 | Pritam Das |
| 9.2.2017 | RITUPARNA PARUI | 2 | Rituparna Parui |
| 9.2.2017 | RUDRA BHATTACHARJEE | 2 | A |
| 9.2.2017 | RUSHAM DAS | 2 | Rusham Das |
| 9.2.2017 | SALMAN KHURSHID | 2 | A |
| 9.2.2017 | SOHINI CHATTERJEE | 2 | Sohini Chatterjee |
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LECTURE 3: Insilico drug likeness testing, application of Lipinski Rule of Five, Using Molinspiration server, insilico toxicity testing - using admetSAR, to screen drug molecules

Date: 10.2.2017

| DATE | NAME | MODULE | SIGNATURE |
|---|---|---|---|
| 10.2.2017 | BHARGAB KAR | 3 | B Kar |
| 10.2.2017 | DEBAYAN DAS | 3 | Debayan Das |
| 10.2.2017 | GAIRIC BHUSHAN MANDAL | 3 | Gairic B. Mandal |
| 10.2.2017 | INDRANI SEN | 3 | Indrani Sen |
| 10.2.2017 | ISHIKA DUTTA CHOWDHURY | 3 | Ishika Dutta Chowdhury |
| 10.2.2017 | PRITAM DAS | 3 | Pritam Das |
| 10.2.2017 | RITUPARNA PARUI | 3 | Rituparna Parui |
| 10.2.2017 | RUDRA BHATTACHARJEE | 3 | Rudra Bhattacharjee |
| 10.2.2017 | RUSHAM DAS. | 3 | Rusham Das |
| 10.2.2017 | SALMAN KHURSHID | 3 | Salman Khurshid |
| 10.2.2017 | SOHINI CHATTERJEE | 3 | Sohini Chatterjee |
| 10.2.2017 | SUPARNA GARAI | 3 | Suparna Garai |

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# LECTURE 4 : CONCEPT OF DOCKING

DATE : 11.2.2017

| DATE | NAME | MODULE | SIGNATURE |
|---|---|---|---|
| 11.2.2017 | BHARGAB KAR | 4 | Bkar |
| 11.2.2017 | DEBAYAN DAS | 4 | Debayan Das. |
| 11.2.2017 | GAIRIC BHUSHAN MANDAL | 4 | Gairic B. Mandal |
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| 11.2.2017 | ISHIKA DUTTA CHOWDHURY | 4 | Ishika Dutta Chowdhury |
| 11.2.2017 | PRITAM DAS | 4 | Pritam Das |
| 11.2.2017 | RITUPARNA PARUI | 4 | Rituparna Parui |
| 11.2.2017 | RUDRA BHATTACHARJEE | 4 | Rudra Bhattacharjee |
| 11.2.2017 | RUSHAM DAS | 4 | Rusham Das |
| 11.2.2017 | SALMAN KHURSHID | 4 | Salman Khurshid |
| 11.2.2017 | SOHINI CHATTERJEE | 4 | Sohini Chatterjee |
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LECTURE 5: Working with PDB, protein structure search, downloading protein structure in PDB format.

Date: 13.2.2017

| DATE | NAME | MODULE | SIGNATURE |
|---|---|---|---|
| 13.2.2017 | BHARGAB KAR | 5 | Bhargab Kar |
| 13.2.2017 | DEBAYAN DAS | 5 | Debayan Das |
| 13.2.2017 | GAIRIC BIKRAN MANDAL | 5 | Gairic B. Mandal |
| 13.2.2017 | INDRANI SEN | 5 | Indrani Sen |
| 13.2.2017 | ISHIKA DUTTA CHOWDHURY | 5 | Ishika Dutta Chowdhury |
| 13.2.2017 | PRITAM DAS. | 5 | Pritam Das |
| 13.2.2017 | RITUPARNA RUI | 5 | Rituparna Parui |
| 13.2.2017 | RUDRA BHATTACHARJEE | 5 | Rudra Bhattacharjee |
| 13.2.2017 | RUSHAM DAS. | 5 | Rusham Das |
| 13.2.2017 | SALMAN KHURSHID | 5 | Salman Khurshid |
| 13.2.2017 | SOHINI CHATTERJEE | 5 | Sohini Chatterjee |
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LECTURE 6: Working protein structure in UCF Chimera, add hydrogens, delete native water molecules preparation of final protein structure in pdb format

DATE: 13.2.2017

| DATE | NAME | MODULE | SIGNATURE |
|---|---|---|---|
| 13.2.2017 | BHARGAB KAR | 6 | Bhar |
| 13.2.2017 | DEBAYAN DAS | 6 | Debayan Das |
| 13.2.2017 | GAIRIC BHUSHAN MONDAL | 6 | Gairic B. Mondal |
| 13.2.2017 | INDRANI SEN | 6 | Indrani Sen |
| 13.2.2017 | ISHIKA DUTTA CHOWDHURY | 6 | Ishika Dutta Chowdhury |
| 13.2.2017 | PRITAM DAS | 6 | Pritam Das |
| 13.2.2017 | RITUPARNA PARUI | 6 | Rituparna Parui |
| 13.2.2017 | RUDRA BHATTACHARJEE | 6 | Rudra Bhattacharjee |
| 13.2.2017 | RUSHAM DAS | 6 | Rusham Das |
| 13.2.2017 | SALMAN KHURSHID | 6 | Salman Khurshid |
| 13.2.2017 | SOHINI CHATTERJEE | 6 | Sohini Chatterjee |
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LECTURE 7. Predicting biological activity of selected compounds by molecular docking with SWISSDOCK or PARDOCK, counting the docking SCORES, analysing the protein-ligand binding interaction with UCSF chimera

Date: 14.2.2017

| DATE | NAME | MODULE | SIGNATURE |
|---|---|---|---|
| 14.2.2017 | BHARGAB KAR | 7 | Bkar |
| 14.2.2017 | DEBAYAN DAS | 7 | Debayandas |
| 14.2.2017 | GAIRIC BHUSHAN MANDAL | 7 | Gairic B. Mandal |
| 14.2.2017 | INDRANI SEN | 7 | Indrani Sen |
| 14.2.2017 | ISHIKA DUTTA CHOWDHURY | 7 | Ishika Dutta Chowdhury |
| 14.2.2017 | PRITAM DAS. | 7 | Pritam Das |
| 14.2.2017 | RITUPARNA PARUI | 7 | A |
| 14.2.2017 | RUDRA BHATTACHARJEE | 7 | Rudra Bhattacharjee |
| 14.2.2017 | RUSHAM DAS | 7 | Rusham Das |
| 14.2.2017 | SALMAN KHURSHID | 7 | Salman Khurshid |
| 14.2.2017 | SOHINI CHATTERJEE | 7 | Sohini Chatterjee |
| 14.2.2017 | SUPARNA GARAI | 7 | Suparna Garai |

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LECTURE 8: Building up 2D QSAR model equation with biological activity (predicted) and molecular descriptors, using regression analysis and array formula

Date: 15.2.2017

| DATE | NAME | MODULE | SIGNATURE |
|---|---|---|---|
| 15.2.2017 | BHARGAB KAR | 8 | |
| 15.2.2017 | DEBAYAN DAS | 8 | Debayan Das |
| 15.2.2017 | GAIRIC BIKSHAN MANDAL | 8 | Gairic B Mandal |
| 15.2.2017 | INDRANI SEN | 8 | Indrani Sen |
| 15.2.2017 | ISHIKA DUTTA CHOWDHURY | 8 | Ishika Dutta Chowdhury |
| 15.2.2017 | PRITAM DAS | 8 | Pritam Das |
| 15.2.2017 | RITUPARNA PARUI | 8 | Rituparna Parui |
| 15.2.2017 | RUDRA BHATTACHARJEE | 8 | Rudra Bhattacharjee |
| 15.2.2017 | RUSHAM DAS | 8 | Rusham Das |
| 15.2.2017 | SALMAN KHURSHID | 8 | Salman Khurshid |
| 15.2.2017 | SOHINI CHATTERJEE | 8 | Sohini Chatterjee |
| 15-2.2017 | SUPARNA GARAI | 8 | Suparna Garai |

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16/2/17

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LECTURE 9: Validating QSAR model, comparison between OBA and PBA by ANOVA (Student t-test)

| DATE | NAME | MODULE | SIGNATURE |
|---|---|---|---|
| 16.2.2017 | BHARGAB KAR | 9 | |
| 16.2.2017 | DEBAYAN DAS | 9 | Debayan Das |
| 16.2.2017 | GAIRIC BHUSHAN MANDAL | 9 | Gairic B Mandal |
| 16.2.2017 | INDRANI SEN | 9 | Indrani Sen |
| 16.2.2017 | ISHIKA DUTTA CHOWDHURY | 9 | Ishika Dutta Chowdhury |
| 16.2.2017 | PRITAM DAS | 9 | Pritam Das |
| 16.2.2017 | RITUPARNA PARUI | 9 | Rituparna Parui |
| 16.2.2017 | RUDRA BHATTACHARJEE | 9 | Rudra Bhattacharjee |
| 16.2.2017 | RUSHAM DAS | 9 | Rusham Das |
| 16.2.2017 | SALMAN KHURSHID | 9 | Salman Khurshid |
| 16.2.2017 | SOHINI CHATTERJEE | 9 | Sohini Chatterjee |
| 16.2.2017 | SUPARNA GARAI | 9 | Suparna Garai |

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16/2/17

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Durgapur

LECTURE 10: Basic bioinformatics working with gene and protein sequences from NCBI, downloading gene and protein sequences

Date: 17.2.2017

| DATE | NAME | MODULE | SIGNATURE |
|---|---|---|---|
| 17.2.2017 | BHARGAB KAR | 10 | Bhargab Kar |
| 17.2.2017 | DEBAYAN DAS | 10 | Debayan Das |
| 17.2.2017 | GAIRIK BHUSHAN MANDAL | 10 | Gairik B Mandal |
| 17.2.2017 | INDRANI SEN | 10 | Indrani Sen |
| 17.2.2017 | ISHIKA DUTTA CHOWDHURY | 10 | Ishika Dutta Chowdhury |
| 17.2.2017 | PRITAM DAS | 10 | Pritam Das |
| 17.2.2017 | RITUPARNA PARUI | 10 | Rituparna Parui |
| 17.2.2017 | RUDRA BHATTACHARJEE | 10 | Rudra Bhattacharjee |
| 17.2.2017 | RUSHAM DAS | 10 | Rusham Das |
| 17.2.2017 | SALMAN KHURSHID | 10 | Salman Khurshid |
| 17.2.2017 | SOHINI CHATERJEE | 10 | Sohini Chatterjee |
| 17.2.2017 | SUPARNA GHARAI | 10 | Suparna Gharai |

Sourin Bera
17/2/17

Prof. (Dr.) Subhabrata Ray
Principal, M. Pharm, Ph.D.
Dr. B. C. Roy College of Pharmacy & A.H.S.
Bidhannagar, Durgapur-713206, Burdwan

Dr. B. C. Roy College of Pharmacy & A.H.S. Durgapur

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

## Durgapur - 713206, West Bengal, India

## (Approved by AICTE & PCI, Affiliated to MAKAUT)

***Certificate course***

***On***

## Procedure of Doing Computer Aided Drug Design (CADD)

This certificate is issued to *Bhargab Kar*, student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Procedure of Doing Computer Aided Drug Design (CADD)" by Dr. Souvik Basak from 8th February, 2017 to 17th February, 2017.

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

*Dr. S. Chakraborty*
*Director, BCRCP*

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

## Durgapur - 713206, West Bengal, India

## (Approved by AICTE & PCI, Affiliated to MAKAUT)

***Certificate course***

***On***

## Procedure of Doing Computer Aided Drug Design (CADD)

This certificate is issued to *Debayan Das*, student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Procedure of Doing Computer Aided Drug Design (CADD)" by Dr. Souvik Basak from 8th February, 2017 to 17th February, 2017.

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

*Dr. S. Chakraborty*
*Director, BCRCP*

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

## Durgapur - 713206, West Bengal, India

## (Approved by AICTE & PCI, Affiliated to MAKAUT)

***Certificate course***

***On***

## Procedure of Doing Computer Aided Drug Design (CADD)

This certificate is issued to *Gairik Bhushan Mandal*, student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Procedure of Doing Computer Aided Drug Design (CADD)" by Dr. Souvik Basak from 8th February, 2017 to 17th February, 2017.

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

***Dr. S. Chakraborty***
***Director, BCRCP***

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

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

**(Approved by AICTE & PCI, Affiliated to MAKAUT)**

***Certificate course***

***On***

## Procedure of Doing Computer Aided Drug Design (CADD)

This certificate is issued to *Indrani Sen*, student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Procedure of Doing Computer Aided Drug Design (CADD)" by Dr. Souvik Basak from 8th February, 2017 to 17th February, 2017.

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

*Dr. S. Chakraborty*
*Director, BCRCP*

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

## Durgapur - 713206, West Bengal, India

## (Approved by AICTE & PCI, Affiliated to MAKAUT)

***Certificate course***
***On***

**Procedure of Doing Computer Aided Drug Design (CADD)**

This certificate is issued to *Ishika Dutta Chowdhury*, student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Procedure of Doing Computer Aided Drug Design (CADD)" by Dr. Souvik Basak from 8th February, 2017 to 17th February, 2017.

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

*Dr. S. Chakraborty*
*Director, BCRCP*

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

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

**(Approved by AICTE & PCI, Affiliated to MAKAUT)**

***Certificate course***

***On***

## Procedure of Doing Computer Aided Drug Design (CADD)

This certificate is issued to *Pritam Das*, student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Procedure of Doing Computer Aided Drug Design (CADD)" by Dr. Souvik Basak from 8th February, 2017 to 17th February, 2017.

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

*Dr. S. Chakraborty*
*Director, BCRCP*

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

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

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***Certificate course***

***On***

## Procedure of Doing Computer Aided Drug Design (CADD)

This certificate is issued to *Rituparna Parui*, student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Procedure of Doing Computer Aided Drug Design (CADD)" by Dr. Souvik Basak from 8th February, 2017 to 17th February, 2017.

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

*Dr. S. Chakraborty*
*Director, BCRCP*

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

## Durgapur - 713206, West Bengal, India

## (Approved by AICTE & PCI, Affiliated to MAKAUT)

***Certificate course***
***On***

**Procedure of Doing Computer Aided Drug Design (CADD)**

This certificate is issued to *Rudra Bhattacharjee*, student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Procedure of Doing Computer Aided Drug Design (CADD)" by Dr. Souvik Basak from 8th February, 2017 to 17th February, 2017.

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

*Dr. S. Chakraborty*
*Director, BCRCP*

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

## Durgapur - 713206, West Bengal, India

## (Approved by AICTE & PCI, Affiliated to MAKAUT)

***Certificate course***

***On***

## Procedure of Doing Computer Aided Drug Design (CADD)

This certificate is issued to *Rusham Das*, student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Procedure of Doing Computer Aided Drug Design (CADD)" by Dr. Souvik Basak from 8th February, 2017 to 17th February, 2017.

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

***Dr. S. Chakraborty***
***Director, BCRCP***

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

## Durgapur - 713206, West Bengal, India

## (Approved by AICTE & PCI, Affiliated to MAKAUT)

***Certificate course***
***On***

**Procedure of Doing Computer Aided Drug Design (CADD)**

This certificate is issued to *Salman Khurshid*, student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Procedure of Doing Computer Aided Drug Design (CADD)" by Dr. Souvik Basak from 8th February, 2017 to 17th February, 2017.

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

*Dr. S. Chakraborty*
*Director, BCRCP*

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

## Durgapur - 713206, West Bengal, India

## (Approved by AICTE & PCI, Affiliated to MAKAUT)

***Certificate course***

***On***

**Procedure of Doing Computer Aided Drug Design (CADD)**

This certificate is issued to *Sohini Chatterjee*, student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Procedure of Doing Computer Aided Drug Design (CADD)" by Dr. Souvik Basak from 8th February, 2017 to 17th February, 2017.

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

*Dr. S. Chakraborty*
*Director, BCRCP*

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

## Durgapur - 713206, West Bengal, India

## (Approved by AICTE & PCI, Affiliated to MAKAUT)

***Certificate course***

***On***

## Procedure of Doing Computer Aided Drug Design (CADD)

This certificate is issued to *Suparna Garai*, student of Dr. B. C. Roy College of Pharmacy & AHS, for completing the certificate course on "Procedure of Doing Computer Aided Drug Design (CADD)" by Dr. Souvik Basak from 8th February, 2017 to 17th February, 2017.

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

*Dr. S. Chakraborty*
*Director, BCRCP*

# Lecture-1 : Brief Introduction of QSAR and its workflow

Date:- 16.01.2020

| DATE | NAME | ROLL NO. | MODULE NO. | SIGNATURE |
|---|---|---|---|---|
| 16.01.2020 | Pronay Mondal | 62 | 1 | Pronay |
| 16.01.2020 | Roundk Ghosh | 54 | 1 | R.Gh |
| 16.01.20 | Soshanta Ata | 12 | 1 | SA |
| 16/01/20 | Pritam Kundu | 66 | 1 | P.K. |
| 16/1/20 | Anwab Purkait | 105 | 1 | Anwab. |
| 16/1/20 | Wasim Rahman | 02 | 1 | |
| 16/1/20 | Anupam Maity | 108 | 1 | |
| 16/1/20 | Subhendu Ghosh | 21 | 1 | |
| 16/1/20 | Saurov Das | 50 | 1 | Das. |
| 16/1/20 | Tanuj GhoshDastidar | 06 | 1 | TGD |
| 16/1/20 | Sudipto Chaurabarti | 17 | 1 | Schaurabarti |

Soniya Barua
16/1/20

Prof. (Dr.) Subhabrata Ray
Principal
Dr. B. C. Roy College of Pharmacy & AHS
Durgapur-713206

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

Lecture 2: Structure drawing with ACD Lab/Chemsketch/Chemoffice

Date- 17.01.2020 download, installation, creating new molecules and playing with various parameters to edit the molecule, switch between 2D and 3D parameters

Lecture 3 In

Date- 18.01.2020 of Li

| DATE | NAME | ROLL NO. | MODULE NO | SIGNATURE |
|---|---|---|---|---|
| 17/01/20 | Dritam Kundu | 66 | 2 | |
| 17/1/20 | Sushanta Ata | 12 | 2 | |
| 17/01/20 | Pranay Mandal | 62 | 2 | |
| 17/01/2020 | Rounak Ghosh | 54 | 2 | |
| 17/01/20 | Subhendu Ghosh | 21 | 2 | |
| 17/1/20 | Anwab Purkait | 105 | 2 | |
| 17/1/20 | Saurov Das | 50 | 2 | |
| 17/1/20 | Wasim Rahman | 02 | 2 | |
| 17/1/20 | Anupam Maity | 146 | 2 | |
| 17/1/20 | Sudipta Chowdhury | 17 | 2 | |
| 17/1/20 | Tanuj Ghosh Dastidar | 06 | 2 | |

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Durgapur

| DATE | NAME |
|---|---|
| 18/1/20 | Sudipta Chow |
| 18/1/20 | Jahnavi Ba |
| 18/1/20 | Rounak Ghosh |
| 18/1/20 | Saurov D |
| 18/1/20 | Anwab Purkait |
| 18/1/20 | Pranay Mandal |
| 18/1/20 | Subhendu Ghosh |
| 18.1.20 | Sushanta Ata |
| 18.1.20 | Anupam Maity |
| 18/1/20 | Dritam Kundu |
| 18/1/20 | Tanuj Ghosh Dastidar |

# Lecture-1 : Brief Introduction of QSAR and its workflow

Date:- 16.01.2020

| DATE | NAME | ROLL NO. | MODULE NO. | SIGNATURE |
|---|---|---|---|---|
| 16.01.2020 | Pronay Mondal | 62 | 1 | Pronay |
| 16.01.2020 | Roundk Golwch | 54 | 1 | Rdg |
| 16.01.20 | Soshanta Ata | 12 | 1 | SA |
| 16/01/20 | Pritam Kundu | 66 | 1 | P.K. |
| 16/1/20 | Anwab Purkait | 105 | 1 | Anwab |
| 16/1/20 | Wasim Rahman | 02 | 1 | |
| 16/1/20 | Anupam Maity | 108 | 1 | |
| 16/1/20 | Subhendu Ghosh | 21 | 1 | |
| 16/1/20 | Saurov Das | 50 | 1 | |
| 16/1/20 | Tanuj GhoshDastidar | 06 | 1 | TGD |
| 16/1/20 | Sudipto Chaurabarti | 17 | 1 | |

Sourav Das
16/1/20

Prof. (Dr.) Subhabrata Ray
Principal
Dr. B. C. Roy College of Pharmacy & AHS
Durgapur-713206

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

Lecture 2: Structure drawing with ACD Lab / Chemsketch / Chemoffice
Date: 17.01.2020 download, installation, creating new molecules and playing with various parameters to edit the molecule, switch between 2D and 3D parameters

| DATE | NAME | ROLL NO. | MODULE NO | SIGNATURE |
|---|---|---|---|---|
| 17/01/20 | Pritam Kundu | 66 | 2 | P.K. |
| 17/1/20 | Soshanta Ata | 12 | 2 | SA |
| 17/01/20 | Pranay Mondal | 62 | 2 | Pranay |
| 17/01/2020 | Rounak Ghosh | 54 | 2 | RG |
| 17/01/20 | Subhendu Ghosh | 21 | 2 | SG |
| 17/1/20 | Anwab Purkait | 105 | 2 | Anwab. |
| 17/1/20 | Saurov Das | 50 | 2 | |
| 17/1/20 | Wasim Rahman | 02 | 2 | |
| 17/1/20 | Anupam Maity | 106 | 2 | Anu |
| 17/1/20 | Sudipto Chowdhury | 17 | 2 | SChowdhury |
| 17/1/20 | Tanuj Ghosh Dastidar | 06 | 2 | TGD |

Saurov Das
17/1/20

Prof. (Dr.) Subhabrata Ray
Principal

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

Lecture 3: In silico Drug likeliness testing, application of Lipinsky Rule of Five, Using Molinspiration server, in silico toxicity testing. Using admetSAR to screen Drug molecules

Date: 18-01-2020

(3)

| DATE | NAME | ROLL NO. | MODULE NO | SIGNATUR |
|---|---|---|---|---|
| 18/1/20 | Sudipti Chowdhury | 17 | 3 | S Chowdhury |
| 18/1/20 | Wasim Rahman | 02 | 3 | |
| 18/1/2020 | Roynak Ghosh. | 54 | 3 | Roy |
| 18/1/20 | Saurov Das | 50 | 3 | |
| 18/1/20 | Anwab Purkait | 105 | 3 | Anwab. |
| 18/1/20 | Pronay Mondal | 62 | 3 | Pronay |
| 18/1/20 | Sukhendu Ghosh | 21 | 3 | SG |
| 18.1.20 | Sushanta Ata | 12 | 3 | SA |
| 18.1.20 | Anupam Maity | 106 | 3 | |
| 18/01/20 | Pritam Kundu | 66 | 3 | P.K. |
| 18/1/20 | Tanuj GhoshDastidar | 66 | 3 | TGD |

Sourin Bera
18/1/20

Prof. (Dr.) Subhabrata Ray
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B.C. Roy College of Pharmacy & AHS
Durgapur

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

Lecture 4: Concept of Docking

Date:- 21.01.2020

| DATE | NAME | ROLL NO | MODULE No | SIGNATURE |
|---|---|---|---|---|
| 21/1/20 | Anupam Maity | 106 | 4 | |
| 21/1/20 | Sudipto Chowdhury | 17 | 4 | |
| 21/1/20 | Wasim Rahman | 02 | 4 | |
| 21/01/2020 | Kounak Ghosh | 54 | 4 | |
| 21/01/20 | Subhendu Ghosh | 21 | 4 | |
| 21/1/20 | Sushanta Ata | 12 | 4 | |
| 21/1/20 | Pranay Mondal | 62 | 4 | |
| 21/1/20 | Sadrov Das | 50 | 4 | |
| 21/01/20 | Pritam Kundu | 66 | 4 | |
| 21/01/20 | Tanmoy Ghosh Dastidar | 06 | 4 | |

Sourav Barua
21/1/20

Prof. (Dr.) Subhabrata Ray
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Durgapur

Lecture 5: Working with PDB, protein structure
Date: 22.01.2020 search, downloading protein structure in PDB format

| DATE | NAME ~~ROLL NO~~ | ROLL NO | MODULE NO | SIGNATURE |
|---|---|---|---|---|
| 22/1/20 | Tanuj Ghosh Dastidar | 06 | 5 | |
| 22/1/20 | Pronay Mondal | 62 | 5 | Pronay |
| 22/1/20 | Anwesha Purkait | 105 | 5 | Anwesha |
| 22/01/2020 | Rounak Ghosh | 54 | 5 | R.G |
| 22/01/20 | Sushanta Ata | 12 | 5 | SA |
| 22/01/20 | Subhendu Ghosh | 21 | 5 | |
| 22/1/20 | Wasim Rahman | 02 | 5 | |
| 22/1/20 | Anupam Maity | 106 | 5 | |
| 22/1/20 | Saurov Das | 50 | 5 | |
| 22/01/20 | Pritam Kundu | 66 | 5 | P.K |
| 22/1/20 | Sudipta Chowdhury | 17 | 5 | Sudipta |

Saurav Basu
22/1/20

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Durgapur-713206

Dr. B. C. Roy College of Pharmacy & A.H.S. Durgapur

Lecture 6: Working protein structure in UCSF chimera, add hydrogens, delete native water molecules, preparation of final protein structure in pdb format

Date:- 24.01.2020

| DATE | NAME | ROLL NO | MODULE No | SIGNATURE |
|---|---|---|---|---|
| 24/01/20 | Pritam Kundu | 66 | 6 | P.K. |
| 24/01/2020 | Roynak Ghosh. | 54 | 6 | R.G |
| 24/1/20 | Anupam Maity | 106 | 6 | |
| 24/01/20 | Pranay Mondal | 62 | 6 | Pranay |
| 24/1/20 | Anwab Purkait | 105 | 6 | Anwab. |
| 24/1/20 | Sushanta Ata | 12 | 6 | |
| 24/1/20 | Subhendu Ghosh | 21 | 6 | |
| 24/1/20 | Wasim Rahman | 02 | 6 | |
| 24/1/20 | Sudipta Chowdhury | 17 | 8 | S Chowdhury. |
| 24/1/20 | Tanuj GhoshDastidar | 06 | 6 | TGD |

Sonia Bora
24/1/20

Prof. (Dr.) Subhabrata Ray
Principal
Dr. B. C. Roy College of Pharmacy & AHS
Durgapur-713206

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Durgapur

Lecture 7: Predicting biological activity of selected compounds by molecular docking with SWISSDOCK or PARDOCK, counting the docking scores, analysing protein-ligand binding interactions with UCSF chimera

Date:- 25.01.2020

| DATE | NAME | ROLL NO | MODULE | SIGNATURE |
|---|---|---|---|---|
| 25/1/20 | Anupam Maity | 105 | 7 | |
| 25/1/20 | Saurov Das | 30 | 7 | |
| 25/01/2020 | Rounak Ghosh | 54 | 7 | R.G |
| 25/01/20 | Pritam Kundu | 66 | 7 | P.K. |
| 25/1/20 | Pranay Mondal | 62 | 7 | Pranay |
| 25/1/20 | Subhendu Ghosh | 21 | 7 | |
| 25/1/20 | Anwab Purkait | 105 | 7 | Anwab |
| 25/1/20 | Sushanta Ata | 12 | 7 | SA |
| 25/1/20 | Sudipta Chaudhuri | 17 | 7 | Sudipta |
| 25/1/20 | Wasim Rahman | 02 | 7 | |

Soumen Basu
25/1/20

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

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

Lecture 8:- Building up QSAR model equation with biological activity (predicted) and molecular descriptors, using REGRESSION ANALYSIS and ARRAY FORMULA

Date:- 28.01.2020

| DATE | NAME | ROLL NO. | MODULE NO | SIGNATURE |
|---|---|---|---|---|
| 28/1/20 | Tanmoy Ghosh Dastidar | 06 | 8 | |
| 28/1/20 | Anwab Purkait | 105 | 8 | |
| 28/1/20 | Sudipta Chamuah | 17 | 8 | |
| 28/1/20 | Pranay Mondal | 62 | 8 | |
| 28/1/20 | Anupam Maity | 106 | 8 | |
| 28/01/2020 | Raunak Ghosh | 54 | 8 | |
| 28/1/20 | Sushanta Ata | 12 | 8 | |
| 28/1/20 | Wasim Rahman | 02 | 8 | |
| 28/1/20 | Subhendu Ghosh | 21 | 8 | |
| 28/1/20 | Saurov Das | 50 | 8 | |
| 28/01/20 | Pritam Kundu | 66 | 8 | |

Prof. (Dr.) Subhabrata Ray
Principal
Dr. B. C. Roy College of Pharmacy & AHS
Durgapur-713206

Sonia Bam
28/1/20

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

Lecture 9: Validating QSAR model, comparison between OBA and PBA by ANOVA (Student t-test)

Date: 30.01.2020

| DATE | NAME | ROLL NO | MODULE No | SIGNATURE |
|---|---|---|---|---|
| 30/1/20 | Anupam Maity | 106 | 9 | Anu |
| 30/1/20 | Pronay Mondal | 62 | 9 | Pronay |
| 30/01/20 | Pritha Kundu | 66 | 9 | P.K. |
| 30/1/20 | Wasim Rahman | 02 | 9 | WR |
| 30/01/2020 | Rounak Ghosh | 54 | 9 | R.G. |
| 30/01/20 | Saurov Das | 50 | 9 | Das. |
| 30/1/20 | Anwab Purkait | 105 | 9 | Anwab. |
| 30/1/20 | Sushanta Ata | 12 | 9 | SA |
| 30/1/20 | Subhendu Ghosh | 21 | 9 | SG |
| 30/1/20 | Sudipta Chakraborty | 17 | 9 | S Chakraborty |
| 20/1/20 | Tanuj Ghoshdastidar | 06 | 9 | TG |

Soumi Bera
30/1/20

Prof. (Dr.) Subhabrata Ray
Principal
Dr. B. C. Roy College of Pharmacy & AHS
Durgapur-713206

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

Lecture 10: Basic Bioinformatics Working with gene and protein sequences from NCBI, downloading gene and protein sequences

Date:- 31.01.2020

10

| DATE | NAME | ROLL NO | MODULE NO | SIGNATURE |
|---|---|---|---|---|
| 31/1/20 | Anuvab Pwikait | 105 | 10 | Anuvab. |
| 31/01/20 | Pritam Kundu | 66 | 10 | P.K. |
| 31/1/20 | Wasim Rahman | 02 | 10 | |
| 31/1/20 | Punay Mondal | 62 | 10 | Punay |
| 31/1/2020 | Anupam Maity | 106 | 10 | |
| 31/01/2020 | Rounak Ghosh | 54 | 10 | R.G. |
| 31/1/20 | Sushanta Ata | 02 | 10 | |
| 31/1/20 | Subhendu Ghosh | 21 | 10 | |
| 31/1/20 | Saurav Das | 50 | 10 | |
| 31/1/20 | Sudipto Chowdhury | 17 | 10 | SChowdhury |
| 31/1/20 | Tanuj Ghoshbastidar | 06 | 10 | |

Prof. (Dr.) Subhabrata Ray
*Principal*
Dr. B. C. Roy College of Pharmacy & AHS
Durgapur-713206

Saurav Barua
31/1/20

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

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

## Durgapur - 713206, West Bengal, India

***Certificate course***
***On***

## Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics

**Course coordinator**
***Dr. Souvik Basak***
*Associate Professor, Department of Pharmaceutical Chemistry*
*Dr. B. C. Roy College of Pharmacy & AHS*

*This certificate is issued to* **Anupam Maity**, *student of Dr. B. C. Roy College of Pharmacy & AHS, for completing* **"Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics"** *by* **Dr. Souvik Basak** *from 16th January, 2020 to 31st January, 2020 .*

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

*Dr. S. Chakraborty*
*Director, BCRCP*

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

## Durgapur - 713206, West Bengal, India

***Certificate course***
***On***

## Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics

**Course coordinator**
***Dr. Souvik Basak***
*Associate Professor, Department of Pharmaceutical Chemistry*
*Dr. B. C. Roy College of Pharmacy & AHS*

*This certificate is issued to* **Anuvab Purkait**, *student of Dr. B. C. Roy College of Pharmacy & AHS, for completing* "**Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics**" *by* **Dr. Souvik Basak** *from 16th January, 2020 to 31st January, 2020 .*

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

*Dr. S. Chakraborty*
*Director, BCRCP*

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

## Durgapur - 713206, West Bengal, India

**Certificate course**
**On**

## Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics

**Course coordinator**
***Dr. Souvik Basak***
*Associate Professor, Department of Pharmaceutical Chemistry*
*Dr. B. C. Roy College of Pharmacy & AHS*

*This certificate is issued to* **Pritam Kundu**, *student of Dr. B. C. Roy College of Pharmacy & AHS, for completing* **"Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics"** *by* **Dr. Souvik Basak** *from 16th January, 2020 to 31st January, 2020 .*

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

*Dr. S. Chakraborty*
*Director, BCRCP*

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

## Durgapur - 713206, West Bengal, India

***Certificate course***
***On***

## Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics

**Course coordinator**
***Dr. Souvik Basak***
*Associate Professor, Department of Pharmaceutical Chemistry*
*Dr. B. C. Roy College of Pharmacy & AHS*

*This certificate is issued to* **Pronay Mondal**, *student of Dr. B. C. Roy College of Pharmacy & AHS, for completing* **"Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics"** *by* **Dr. Souvik Basak** *from 16th January, 2020 to 31st January, 2020 .*

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

*Dr. S. Chakraborty*
*Director, BCRCP*

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

## Durgapur - 713206, West Bengal, India

***Certificate course***
***On***

## Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics

**Course coordinator**
***Dr. Souvik Basak***
*Associate Professor, Department of Pharmaceutical Chemistry*
*Dr. B. C. Roy College of Pharmacy & AHS*

*This certificate is issued to* **Rounak Ghosh**, *student of Dr. B. C. Roy College of Pharmacy & AHS, for completing* **"Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics"** *by* **Dr. Souvik Basak** *from 16th January, 2020 to 31st January, 2020 .*

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

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

## Durgapur - 713206, West Bengal, India

***Certificate course***
***On***

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**Course coordinator**
***Dr. Souvik Basak***
*Associate Professor, Department of Pharmaceutical Chemistry*
*Dr. B. C. Roy College of Pharmacy & AHS*

*This certificate is issued to* **Saurov Ghosh**, *student of Dr. B. C. Roy College of Pharmacy & AHS, for completing* **"Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics"** *by* **Dr. Souvik Basak** *from 16th January, 2020 to 31st January, 2020 .*

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

## Durgapur - 713206, West Bengal, India

***Certificate course***
***On***

## Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics

**Course coordinator**
***Dr. Souvik Basak***
*Associate Professor, Department of Pharmaceutical Chemistry*
*Dr. B. C. Roy College of Pharmacy & AHS*

*This certificate is issued to* **Subhendu Ghosh**, *student of Dr. B. C. Roy College of Pharmacy & AHS, for completing* **"Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics"** *by* **Dr. Souvik Basak** *from 16th January, 2020 to 31st January, 2020 .*

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

## Durgapur - 713206, West Bengal, India

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***On***

## Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics

**Course coordinator**
***Dr. Souvik Basak***
*Associate Professor, Department of Pharmaceutical Chemistry*
*Dr. B. C. Roy College of Pharmacy & AHS*

*This certificate is issued to* **Sudipto Chakraborty**, *student of Dr. B. C. Roy College of Pharmacy & AHS, for completing* "**Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics**" *by* **Dr. Souvik Basak** *from 16th January, 2020 to 31st January, 2020 .*

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

*Dr. S. Chakraborty*
*Director, BCRCP*

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

## Durgapur - 713206, West Bengal, India

**Certificate course**
**On**

## Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics

**Course coordinator**
***Dr. Souvik Basak***
*Associate Professor, Department of Pharmaceutical Chemistry*
*Dr. B. C. Roy College of Pharmacy & AHS*

*This certificate is issued to* **Susanta Ata**, *student of Dr. B. C. Roy College of Pharmacy & AHS, for completing* **"Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics"** *by* **Dr. Souvik Basak** *from 16th January, 2020 to 31st January, 2020 .*

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

*Dr. S. Chakraborty*
*Director, BCRCP*

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

## Durgapur - 713206, West Bengal, India

***Certificate course***
***On***

## Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics

**Course coordinator**
***Dr. Souvik Basak***
*Associate Professor, Department of Pharmaceutical Chemistry*
*Dr. B. C. Roy College of Pharmacy & AHS*

*This certificate is issued to* **Tanuj Ghosh Dastidar**, *student of Dr. B. C. Roy College of Pharmacy & AHS, for completing* "**Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics**" *by* **Dr. Souvik Basak** *from 16th January, 2020 to 31st January, 2020 .*

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

*Dr. S. Chakraborty*
*Director, BCRCP*

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## Durgapur - 713206, West Bengal, India

**Certificate course**
**On**

## Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics

**Course coordinator**
***Dr. Souvik Basak***
*Associate Professor, Department of Pharmaceutical Chemistry*
*Dr. B. C. Roy College of Pharmacy & AHS*

*This certificate is issued to* **Wasim Rahaman**, *student of Dr. B. C. Roy College of Pharmacy & AHS, for completing* **"Basic course on Computational Drug Design using Chemoinformatics and Bioinformatics"** *by* **Dr. Souvik Basak** *from 16th January, 2020 to 31st January, 2020 .*

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

*Dr. S. Chakraborty*
*Director, BCRCP*

# COMPUTER-AIDED DRUG DESIGN WITH QSAR/ BIOINFORMATICS

## A JOINT COLLABORATION OF

LSSSDC | SHRM biotechnologies

**COURSE HIGHLIGHTS**

- STRUCTURE DRAWING FOR QSAR, ISOMER GENERATION
- MOLECULAR MECHANICS, ENERGY OPTIMISATION, 3D REPRESENTATION
- DESCRIPTOR GENERATION, HANSCH, FREE-WILSON, TAFT, FUJITA-BAN, TOPLISS, BRANCHING, ETSA, WEINER ANALYSIS
- 3D QSAR, COMFA- THEORY TO HANDS ON
- CLUSTER ANALYSIS, MLR, PCA, ANOVA, Q2 VALIDATION
- IN-SILICO TOXICITY, STATISTICAL ANALYSIS, DRUG PATHWAY PREDICTION
- BIOINFORMATICS, PDB AND NCBI HANDLING, HOMOLOGY MODELLING
- ANALYSIS OF MODELLED PROTEIN WITH PROCHECK, MODELLER
- AUTODOCK/ CASE STUDIES
- DISCOVERY STUDIO VISUALIZER, PDBSUM, PYMOL

## WHAT STUDENTS WILL GAIN

- CERTIFICATION BY 3 STATUTORY BODIES:

LSSSDC, GOVT. OF INDIA,
DR. B.C.ROY COLLEGE OF PHARMACY & AHS
SHRM BIOTECHNOLOGIES PVT. LTD.

- DIRECT INTERACTION WITH SOME INDUSTRY AND ACADEMIC EXPERTS
- ASSIGNMENT AFTER EACH SESSION FOR PRACTICE, RELATED TO DRUG DISCOVERY

## FUTURE BENEFITS/ JOB OPPORTUNITIES

- AID IN B.PHARM/B.TECH/B.SC/M.PHARM /M.TECH/M.SC PROJECTS AND DISSERTATIONS ON CADD, BIOINFORMATICS (EXTRA CHARGES INVOLVED)
- ASSIST IN HIGHER STUDIES RELATED TO DRUG DISCOVERY
- JOB OPPORTUNITIES IN COMPANIES LIKE- SYNGENE INTERNATIONAL, SAI LIFESCIENCES, TCG LIFESCIENCES, ANTHEM BIOSCIENCES, VITAS PHARMA, GVK, AURIGENE DISCOVERY TECHNOLOGIES, JUBILIANT BIOSYS LTD. AND MANY OTHER DRUG ENTERPRISES ACROSS INDIA

**ANY LIFE SCIENCE STUDENT FROM B.SC/B.PHARM/B.TECH/M.SC/M.PHARM/M.TECH /PHD/RESEARCH SCHOLAR IS ELIGIBLE FOR THE COURSE**

**ONE MONTH E-COURSE**
**HANDS-ON TRAINING**

**COURSE FEES: 5000 INR**

## REGISTER SOON !!

**Dr. SOUVIK BASAK, PhD**
**TRAINER-ONLINE VERTICAL**

## ABOUT US:

### LIFE SCIENCE SECTOR SKILL DEVELOPMENT COUNCIL, GOVT. OF INDIA

LSSSDC is a not-for-profit, Non-statutory Certification Body under the mandate of GOVT. OF INDIA, the Ministry of Skill Development and Entrepreneurship and is registered under the Societies Act, 1860. It has been setup by National Skill Development Corporation (NSDC) and is a PCI-Approved Training partner.

### SHRM BIOTECHNOLOGIES PVT.LTD, KOLKATA

SHRM BIOTECHNOLOGIES IS A 15-YEAR ORGANISATION, WHICH IS ALSO AN ISO CERTIFIED, MSME CERTIFIED, AND DBT RECOGNISED COMPANY. IT IS HONORARY ACCREDITED BY LSSSDC, GOVT OF INDIA. IT HAS TRAINED OVER 8000 STUDENTS ACROSS PAN INDIA.

### DR B.C.ROY COLLEGE OF PHARMACY & AHS, DURGAPUR

DR B.C.ROY COLLEGE OF PHARMACY & AHS, DURGAPUR IS AN AICTE AND PCI-APPROVED INSTITUTION. IT IS AFFILIATED TO MAKAUT, NBA ACCREDITED AND NIRF RANKED WITHIN TOP 100 COLLEGES (2020).

## FOR REGISTRATION CONTACT:

OR
+91 8697718140
+91 8981003215
info@shrmbio.com

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Life Sciences Sector Skill Development Council
9h ·

Amity University Galgotias University WBUT WBUT AICTE Pharmaceutical group

To Dated: 02-06-2021

The Authority,

**Life Sciences Sector Skill Development Council (LSSSDC),**

**C/o Ministry of Skill Development and Entrepreneurship,**

**Govt. of India**

**Through**

Mr. Kunal Vora,

Director & CEO,

SHRM Biotechnologies Pvt Ltd., Kolkata, WB, India.

**Sub: Soliciting approval/affiliation of "Virtual Skill Development Programme: a learning companion for students"** comprising two online training courses **"Computer Aided Drug design with QSAR and Bioinformatics: from theory to hands-on training" & "Organic Spectroscopy-a detailed understanding, practical interpretations and industrial applications".**

**Affiliating Partner (Proposed): Life Sciences Sector Skill Development Council (LSSSDC), C/o Ministry of Skill Development and Entrepreneurship, Govt. of India**

**Knowledge Partner:** Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India (AICTE/PCI Approved, affiliated to MAKAUT, WB, NBA Accredited (B. Pharm. 2020-23), NIRF ranked within top 100 (2020))

**Marketing and Promotion Partner:** SHRM Biotechnologies Pvt Ltd., Kolkata, WB, India. An ISO and MSME Certified organization, DBT

recognized, **Honorary accredited to LSSSDC**, National award winner in Skill development and training

**Course proposal with synopsis and layout:**

**Why Virtual Skill Development Program?**

The reason behind that during past one year especially during pandemic situation worldwide, virtual platform (online) has been an important role in every sector like school, colleges, Universities and even in Industry for teaching as well as skill development. Many of the professional development programs that are currently offered to students fail to provide the kind of ongoing skill development process students need to make effective use of their knowledge for their profession, and as a result, only few students are in a position to integrate new technologies or knowledge into their skill for obtaining their desired job. **Thus, Me, Dr. Souvik Basak (Associate Professor and Division-In-Charge, Division of Pharmaceutical Chemistry, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India)** and **Dr. Parthasarathi Panda, (Assistant Professor, Division of Pharmaceutical Chemistry, Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India) would like to initiate the Virtual Skill Development Programme Jointly with SHRM Biotechnologies Pvt. Ltd., Kolkata as our collaborating partner in different industrially viable courses/programmes.**

**Why us?**

**1. Reaching and helping out to students.**

**2. Different modes of learning (Audio-visual, Life demonstration, Interactive session, Dissemination of course materials to registered candidates for life long benefit).**

**3. Best quality of teaching and study material.**

**4. Hands on training to various software analysis and interpretation of various case studies solving Industrial problems.**

**5. In special cases, direct introduction to the industrially experienced personnel.**

**6. Providing platform for knowledge growth relevant to various job opportunities and Industrial sectors.**

**7. Establishing Institute-Industry partnership.**

**Proposed candidates for the course:**

Our proposed programme is not only designed for Pharmacy students but also for other Science students such as BSc and MSc in chemistry, Microbiology, Biochemistry, Physiology, Biotechnology, etc. those are interested to work on Drug Design and Discovery or in Pharma Industries. Virtual Skill Development Programme contains various courses as per current suitability and requirement for acquiring knowledge so that students can apply their knowledge for working in Pharmaceuticals, Nutraceuticals and chemical Industries as well as their higher studies.

**Projected Financial benefits:**

***We expect, thus, a considerable revenue generation for the college in future.***

**Allocation of the Revenue Generated: The generated revenue will be shared with the following three partners, on mutual discussions.**

**Relevance with NBA and NAAC:**

Besides, this programme can be presented as a teaching method under **"Self Learning" or "Remedial Teaching" or "Gap Teaching" as per NBA nomenclature. Another prima face of the course is that the course teaches the students on hands-on basis the contents which are part of their theoretical curriculum**. Consequently, it may be considered as outreach activities of the college as per important criteria for NAAC, NBA. The detailed course structure is given here.

**Relevance with Mandatory Additional Requirement (MAR) activities in compliance with MAKAUT, WB**

The certificates will be helpful for them to fulfill the "MAR" activities as proposed by our university (MAKAUT) together with their future benefits. THE DURATION OF THE COURSE IS AROUND 6 WEEKS FOR ONE BATCH WHICH WILL RUN AFTER COLLEGE HOURS. These courses may be beneficial to get their future jobs in various industries or institutes or will help them to carry their projects in this field during higher studies.

**Duration:** 1 month for each course, classes would be scheduled preferably after college hours on week days

**COURSE-1**

**Name of the course**: **Computer Aided Drug design with QSAR and Bioinformatics: from theory to hands-on training**

**Unique Selling Proposition (USP)/ Industrial relevance:**

Drug design is always a thrust area in industrial and research based chemistry since a lot of candidate molecules fail in clinical trial per year and no therapeutically active molecule is present in the market with optimum activity and zero toxicity. Thus rational drug design is always a thrust area

to a pharmaceutical or chemistry student through which he/ she can design a drug/lead with all checkboxes ticked. Moreover, biostatistics, either in pharmacology, bioassays, process design or in chemometrics play an important role to excavate the significant outcome of the results in order to assign the crucial variables of the project. In this course we offer both in theoretical as well as in hands-on training upon completion of which a student should be an independent worker at least for basic demands of these fields. The relevant theories would be dealt with here with basic understandings and above all the student would be introduced with various relevant softwares that he needs to encounter in his future domain/s. A lot of practical examples would be solved, systematic approach would be inculcated and a few case studies would be given as realistic assignments. Various bioinformatics tools would be accompanied with, and after the completion of the course, the student should be confident enough to tackle such kind of problems in industries/academic fields.

**N.B.** Especially for B. Pharm and M. Pharm students, although theoretical aspects of drug design and bioinformatics are dealt in theoretical curriculum, the recipient also lacks the application of the same in actual practice due to lack of practical or hands on training during his curriculum. Also the essence of the subject is partially lost to the student/s due to lack of understanding of what actually occurs during drug design or QSAR or molecular docking. This course is aimed to fill this gap/s and hope this course would help all level of students to comprehend the actual essence, significance and architecture of drug design and QSAR

**Total Number of Chapter**: 12

**Total Number of Classes**: 12

| No. of Chapters | Name of the chapter |
|---|---|
| 1 | Brief Introduction to CADD, Structure based drug design (SBDD), Ligand based drug design (LBDD), QSAR and its workflow |
| 2 | Structure drawing with ACD Lab Chemsketch, 3D structure transition (Avogadro/Corina, Chem 3D), Molecular Mechanics, Energy Minimization, Geometry optimization, descriptor generation |
| 3 | A brief introduction to other descriptors (sigma, pi, Es, ETSA, MR, Branching index), a brief introduction to Dragon |
| 4 | *In silico* drug likeliness testing, application of Lipinsky Rule of Five, Ghose-Crippen Rule, Veber rule, Blood Brain Barrier rule, Using Molinspiration server, SWISS ADME, Raddar plot, Boiled EGG Diagram, using MolSoft, in silico toxicity testing, using admetSAR, to screen drug molecules |
| 5 | Development of 2D QSAR model with descriptors and Biological Activity, application of Multiple Linear Regression (MLR), calculation of $R^2$, ANOVA, F-test and T-test between Observed and Predicted Biological Activity (significance test) |
| 6 | Introduction to 3D-QSAR, basic concept of COMFA and COMSiA |
| 7 | Basic Practical demonstration on COMFA, QSAR model build up in 3D-interface between 3D descriptors and Biological Activity |
| 8 | QSAR model validation, Part-I: Leave one out method (LOO), |

| | |
|---|---|
| | Principle Component Analysis (PCA), Partial Least Square (PLS) method |
| 9 | QSAR Model validation Part II: Cluster analysis, Hierarchical and K-means Clustering |
| 10 | Introduction to Bioinformatics, its importance in **structure based drug design**, database mining, NCBI, BLAST, searching PDB, checking protein structures, PDBsum, PROCHECK, Ramachandran Plot, ERRAT Plot, protein binding site prediction (Discovery Studio), MGL Tools |
| 11 | Docking: basic docking protocol with AutoDock/Vina, **Results interpretation and use in drug design** |
| 12 | Homology Modelling: a case demonstration in MODELLER, **importance in structure based drug design** |

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

## COURSE-2

**Name of the course**: **Organic Spectroscopy-a detailed understanding, practical interpretations and industrial applications.**

**Preamble:** Characterization of organic spectra such as UV, IR, NMR, MS has always been a prime important task to chemists working in R&D, F&D, Active Pharmaceutical Ingradients (API), synthetic chemistry plant and such relevant places. The spectral array is not only required to assign chemical

structure in core synthetic field, but is also required to assign precise changes in polymer grafting, drug-polymer and polymer-polymer interaction, drug-drug interaction, serum metabolomics and other chemo-fingerprinting etc. However, the theoretical corrigendum of our syllabus provide little opportunities to learn interpretations of these spectroscopy and demands extensive training and application of the same. This course offers all these training and applications, a lots of practice problems, examples of realistic case studies. We hope this course would help students deliver better in their future endeavours both in industry as well as higher studies.

**Total Number of Chapters**: 12

**Total Number of Classes**: 12

| No. of Chapters | Name of the chapter |
|---|---|
| 1 | Brief Introduction to Organic Spectroscopic Analysis and its importance in Pharmaceutical and Chemical fields. |
| 2 | UV-visible Spectroscopy |
| 3 | IR Spectroscopy, Basic principle, concept about IR peaks |
| 4 | IR Spectroscopy, interpretation to various structures and functional groups |
| 5 | NMR Spectroscopy-I: Introduction to 1D NMR and its application |
| 6 | NMR Spectroscopy-II: Introduction to 2D NMR and its application |
| 7 | Mass Spectroscopy-I: Introduction to MS, different techniques |

| | |
|---|---|
| 8 | Mass Spectroscopy-II: Mass fragmentation and application of MS in structure elucidation, metabolomics, Bioequivalence study |
| 9 | XRD: Introduction to XRD, different methods and its application |
| 10 | Structure Determination based on IR, UV-Vis, MS, 1H and 13C NMR spectroscopic data- Part I |
| 11 | Structure Determination based on IR, UV-Vis, MS, 1H and 13C NMR spectroscopic data- Part II |
| 12 | Hand on practice for structure elucidation |

**Course Instructor: Dr. Parthasarathi Panda,**
**Assistant Professor,**
**Division of Pharmaceutical Chemistry,**
**Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB**

It is also proposed that Course Co-instructor will take examinations in due times of the course, passing which, students will acquire certificates **Endorsed by all three course partners.**

**Addendum:**

**Proposed Course Fees structure**:

Rs 5000/-. Per course Per candidate

THE FEE MAY BE REVISED BASED ON SUBSEQUENT FEEBACK AND RESPONSE. **The course also offers the opportunities to internal and external students for carrying out the project work in this field for which they need to pay additional registration fee (to be decided by the authority).**

Therefore, I would like to request to your Good Self for your kind affiliation and approval for initiation of these skill development course programs in National Level. Thanking you,

Best Regards,

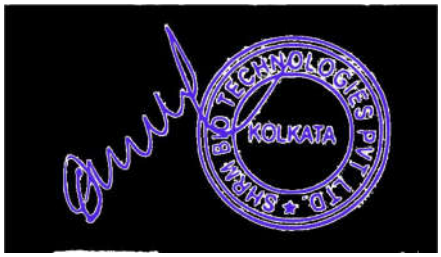
**Dr. Souvik Basak,**

**Associate Professor & Division-In-Charge,**
**Division of Pharmaceutical Chemistry,**
**Dr. B.C. Roy College of Pharmacy & Allied Health Sciences,**
**Durgapur, WB, India**

**Dr. Parthasarathi Panda,**

**Assistant Professor,**
**Division of Pharmaceutical Chemistry,**
**Dr. B.C. Roy College of Pharmacy & Allied Health Sciences,**
**Durgapur, WB, India**

**Endorsed By:**




**Mr. Kunal Vora,**

**Director & CEO,**
**SHRM Biotechnologies Pvt. Ltd,**
**Kolkata, WB, India**

**SHRM Bio-technologies Pvt Ltd**
CIN NO – U40107WB2006PTC110903 MSME No – WB14D0013023
Honorary Recognization From LSSSDC, NSDC, Govt. of India.
An ISO 9001:2015 Certified Organisation

Humaipur .PO: Abdalpur
Madhyamgram Kolkata 700155
Phone: +91 89810 03215
Email: info@shrmbio.com
www.shrmbio.com

**Ref:- SHRM / WB/ BCR/ TR / 001** **Date:- 16th April, 2021**

To,
Dr. Souvik Basak,
Associate Professor,
Dr. B.C. Roy College of Pharmacy & Allied Health Sciences.
Durgapur, India

**Sub: Joint Collaboration for launching vocational online certification course**

Dear Sir,

We refer to your email dated 13th April, 2021, herewith we agree to launch the two vocational online certification programmes as below:

**Course I**
Computer Aided Drug design with QSAR and biostatistics: from theory to hands-on training

**Course II**
Organic Spectroscopy-a detailed understanding, practical interpretations and industrial applications.

**Course III**
Chromatography: understanding, detailed applications and trouble shooting

**The other details are mentioned herewith:-**

**Duration of the course:** 1-1.5 months (12 classes both on theory and online practical training)

Course structure: theory, online training, quiz, assignments, marking, Joint Certification

Expected Start of the Online Programme :- Mid May, 2021

**Tentative sharing of revenue generation:**

Dr. B.C. Roy College of Pharmacy & Allied Health Sciences (BCRCP): 50% (inclusive of course instructor fee 15~20%)

SHRM Biotechnologies Pvt Ltd.: 50%

The payment would be collected by SHRM Biotechnologies Pvt Ltd, and would be divided in the ratio mentioed above.

**Key Job Role**

BCRCP: Knowledge Partner, Technical Course Delivery Partner

SHRM Biotech: Marketing and Promotion Partner

Both Entities would market the said course in their respetive websites, bothe entities have rights to use their logo solely for the promotion and certification of the said course and programes.

We look forward for our esteemed partnership in this regard, we would also request a detailed MoU in the said prespective to be signed.

Thanking you,

Sincerely,


Kunal Vora
Director

Awarded the Best Biotech Training provider in Eastern India- 2018 by Union Minister of Agriculture
Awarded Training Excellence Award on Life Sciences by Hon'ble governors of Orissa & Tripura in 2017

**SHRM Bio-technologies Pvt Ltd**
CIN NO – U40107WB2006PTC110903 MSME No – WB14D0013023
Honorary Recognization From LSSSDC, NSDC, Govt. of India.
An ISO 9001:2015 Certified Organisation

Humaipur .PO: Abdalpur
Madhyamgram Kolkata 700155
Phone: +91 89810 03215
Email: info@shrmbio.com
www.shrmbio.com

**Ref:- SHRM / WB/ BCR/ TR / 001** **Date:- 16th April, 2021**

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

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Director

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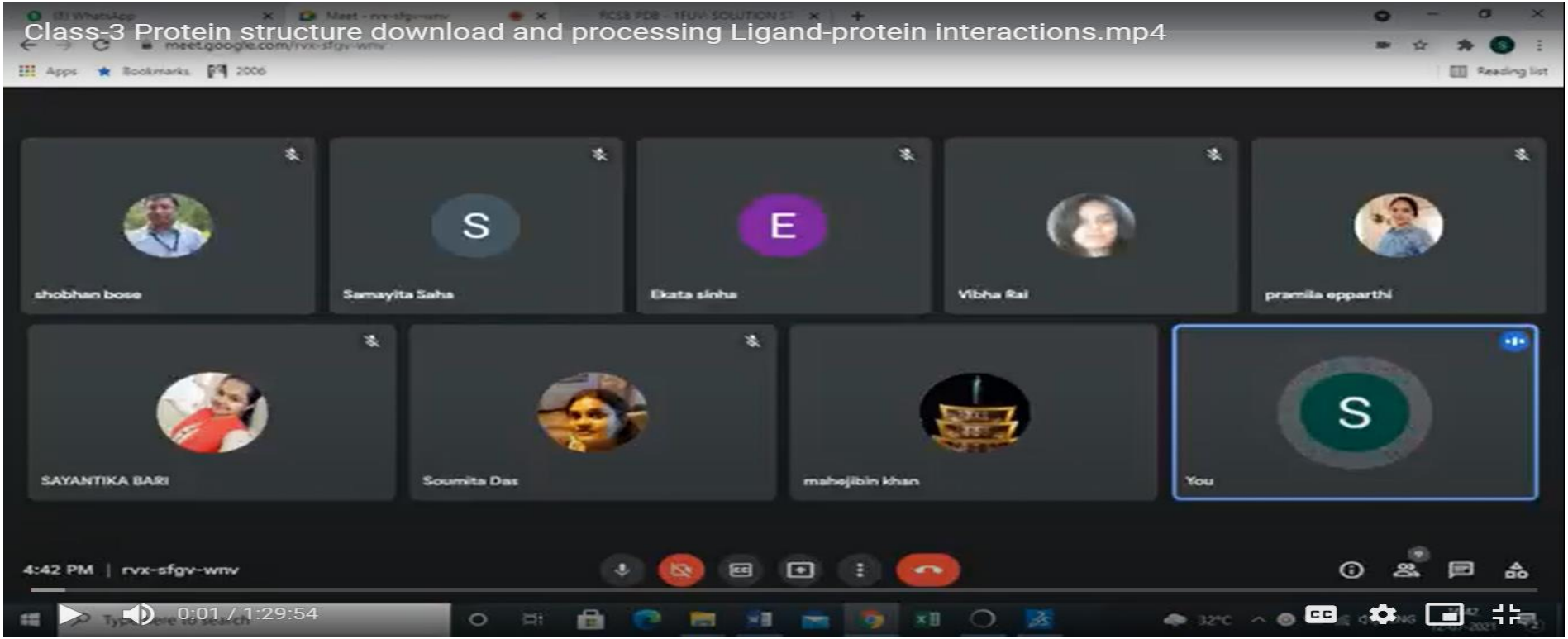
Awarded Training Excellence Award on Life Sciences by Hon'ble governors of Orissa & Tripura in 2017

# Computer Aided Drug Design with QSAR and Bioinformatics

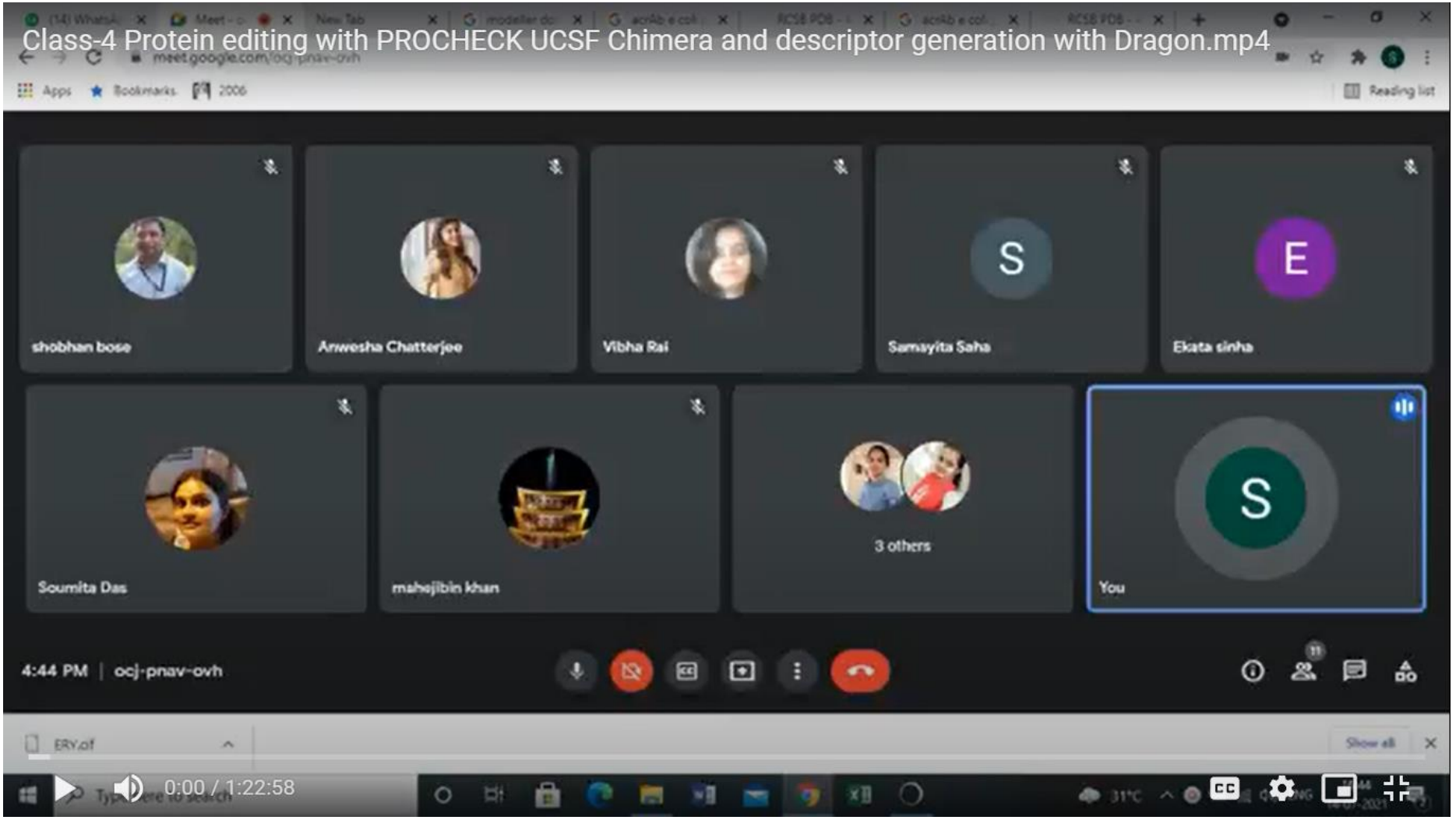
Students' attendance

Since this Add on/ certificate course has been conducted during the pandemic (Covid-19) season, online mode of teaching learning was adopted. Each class (1.5-2.0 h) audio-visual was posted in Google classroom and the tutorial was taken in form of assignments in the same Google classroom. Hence, the attendance of students was recorded as follows:

**12/07/2021**



**14/07/2021**


Class-4 Protein editing with PROCHECK UCSF Chimera and descriptor generation with Dragon.mp4
shobhan bose
Anwesha Chatterjee
Vibha Rai
Samayita Saha
Ekata sinha
Soumita Das
mahejibin khan
3 others
You
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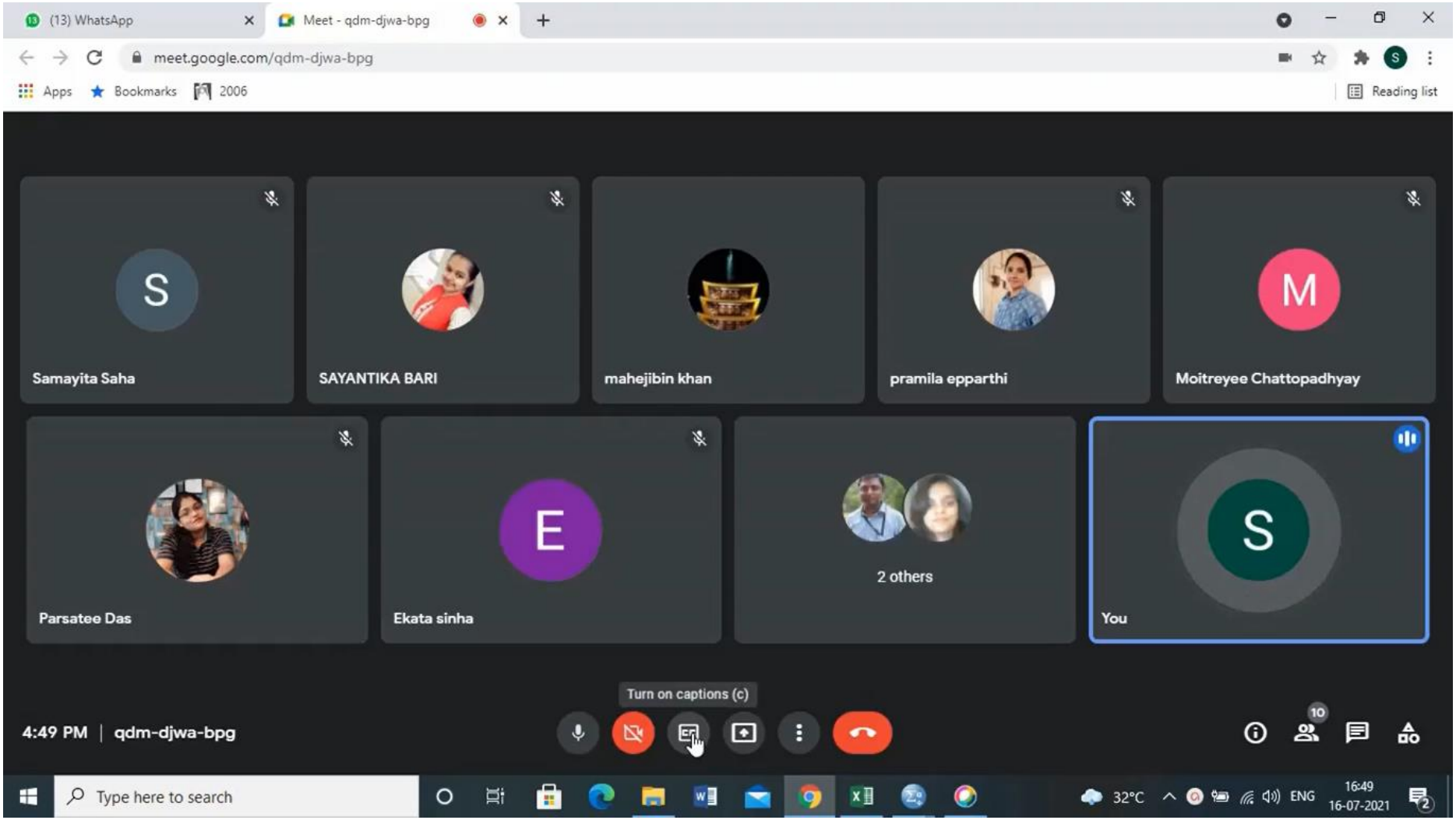
**16/07/2021**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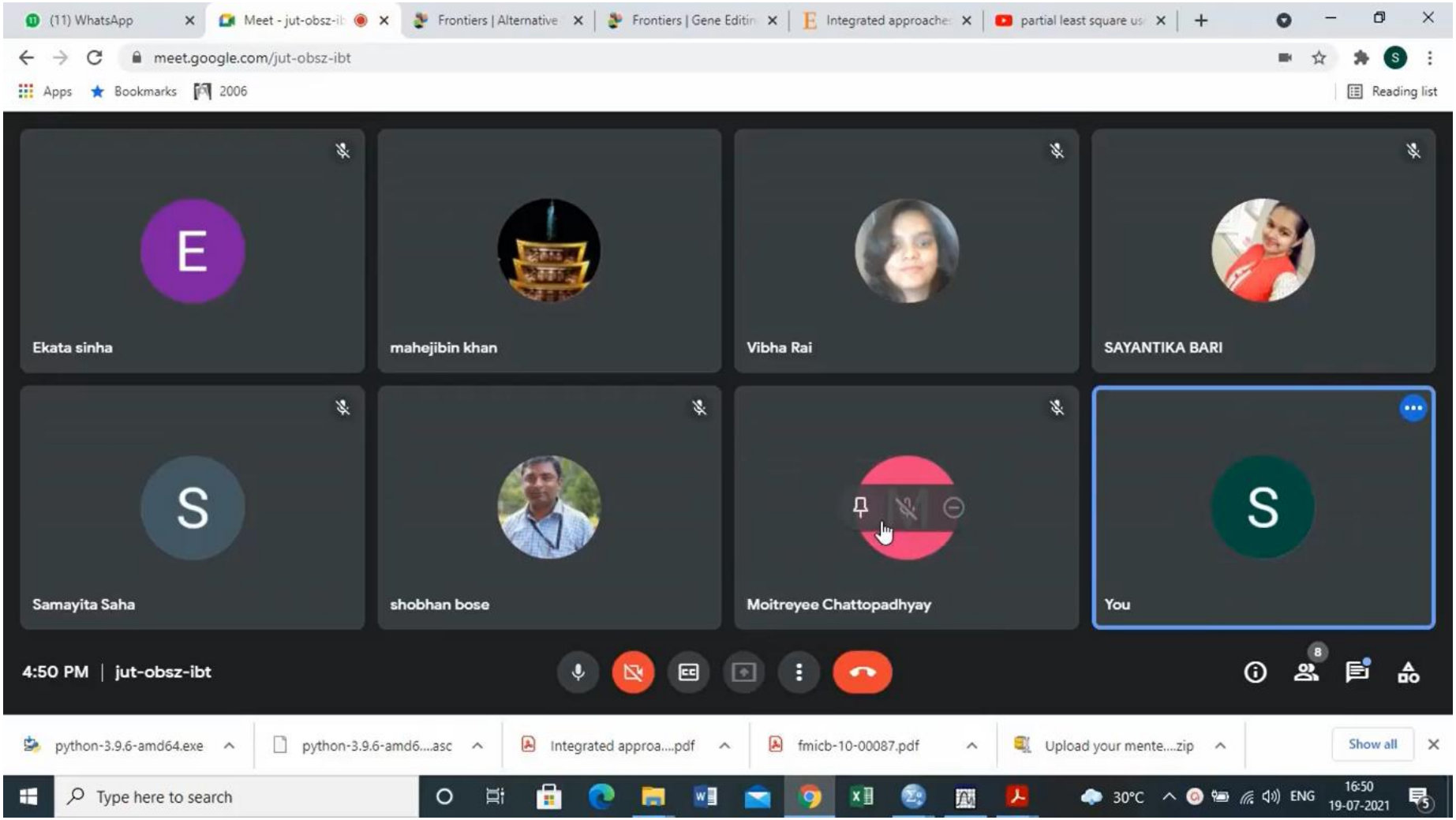
**19/07/2021**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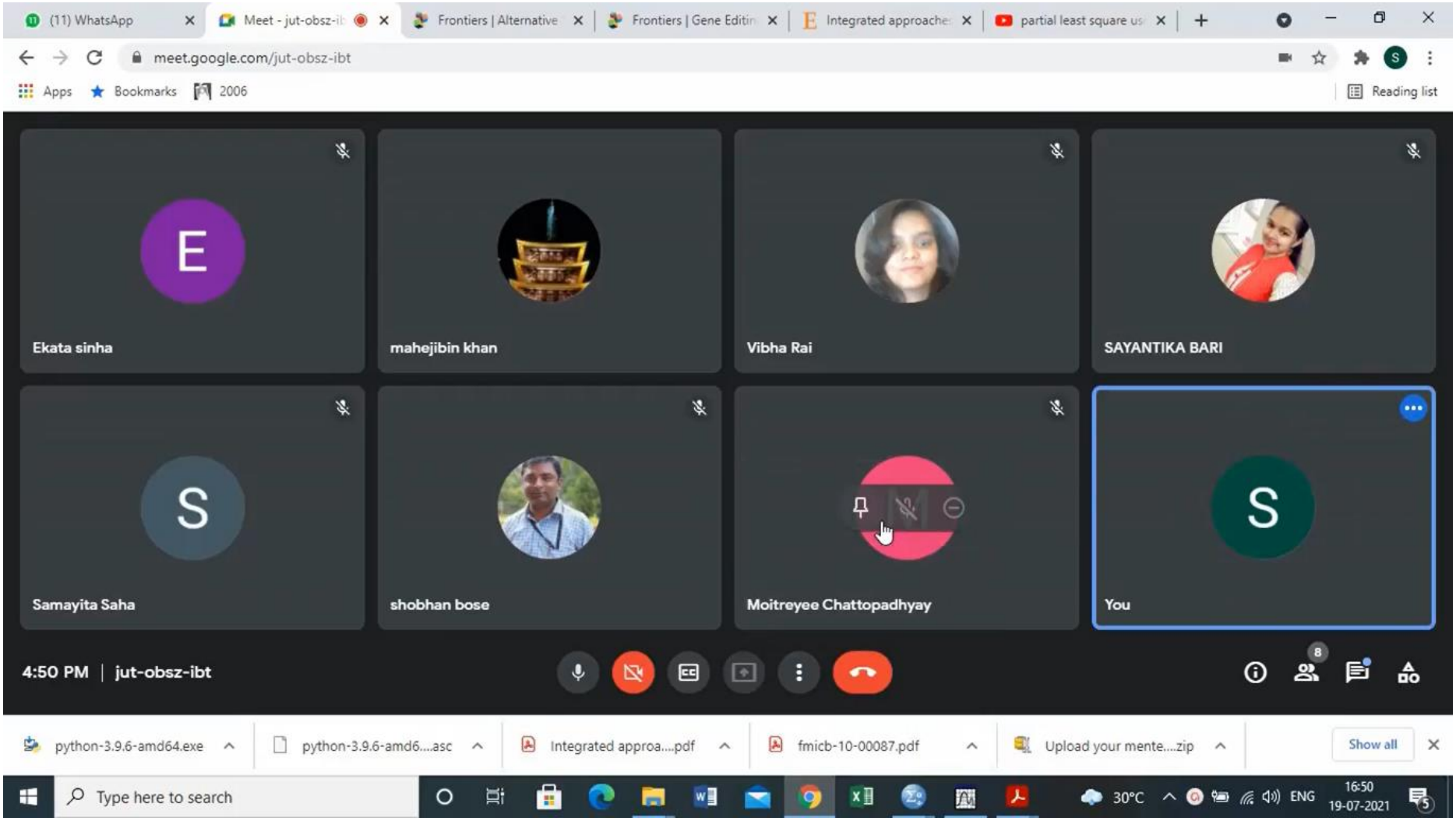
**21/07/2021**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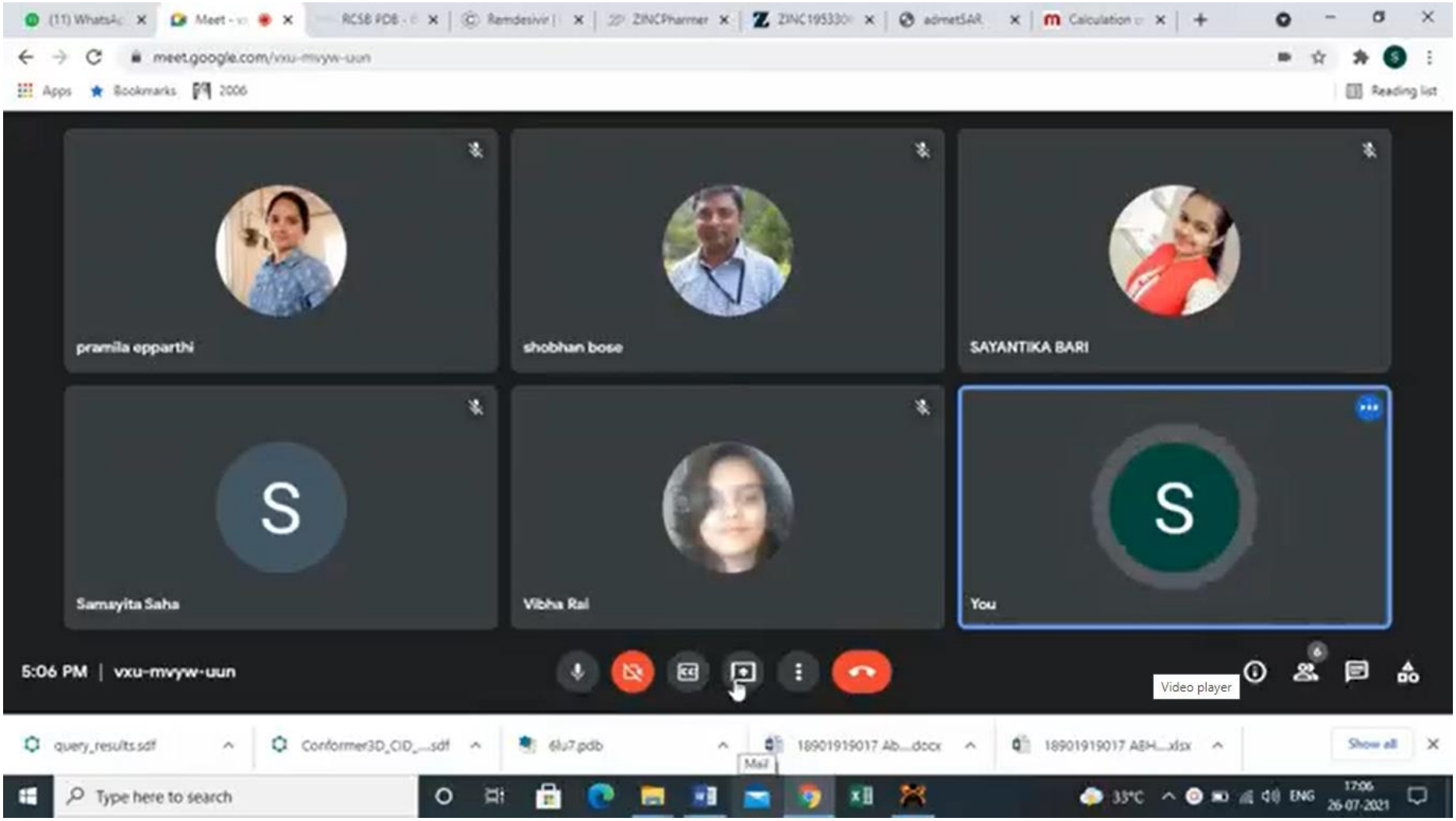
**26/07/2021**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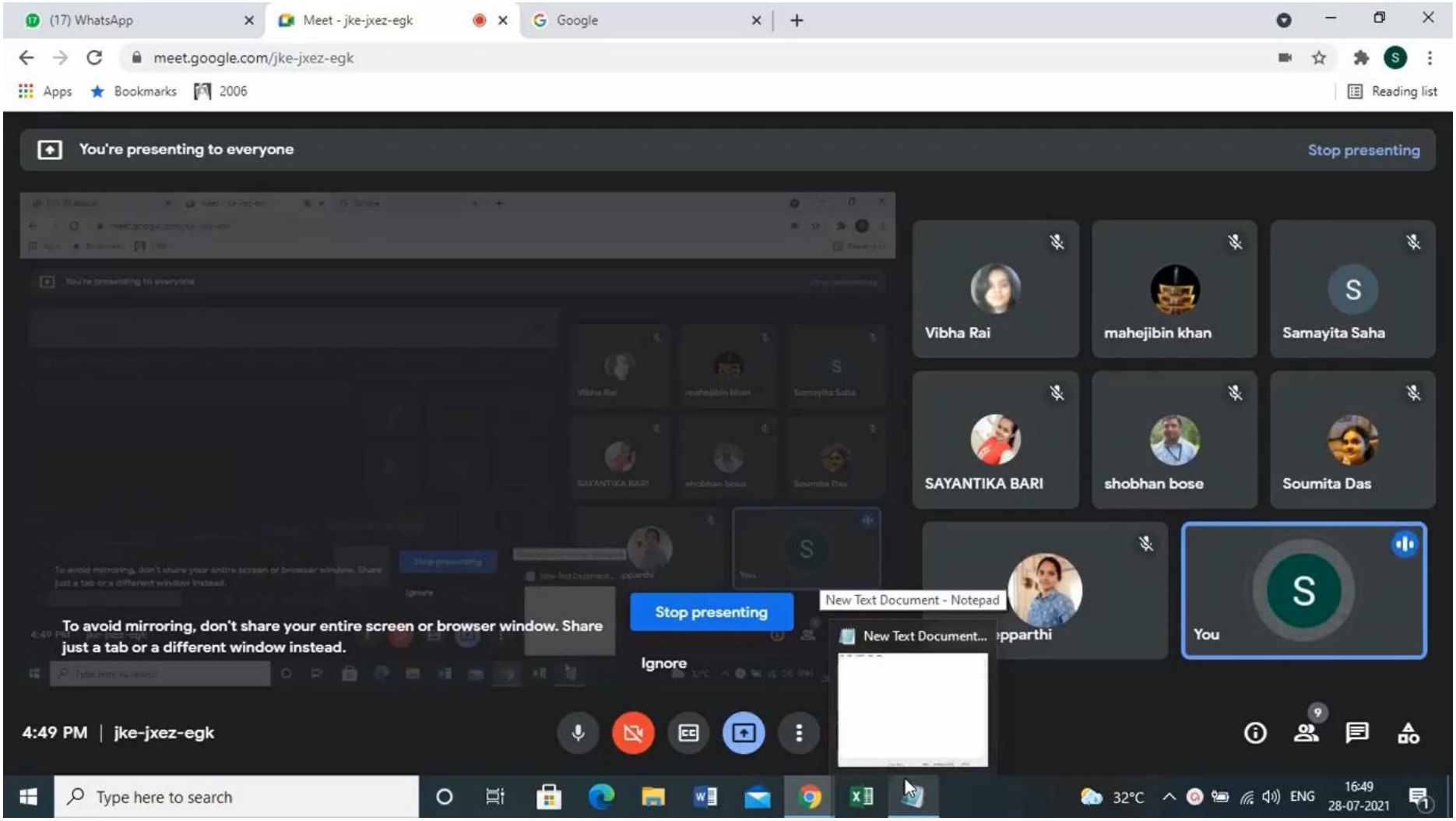
**28/07/2021**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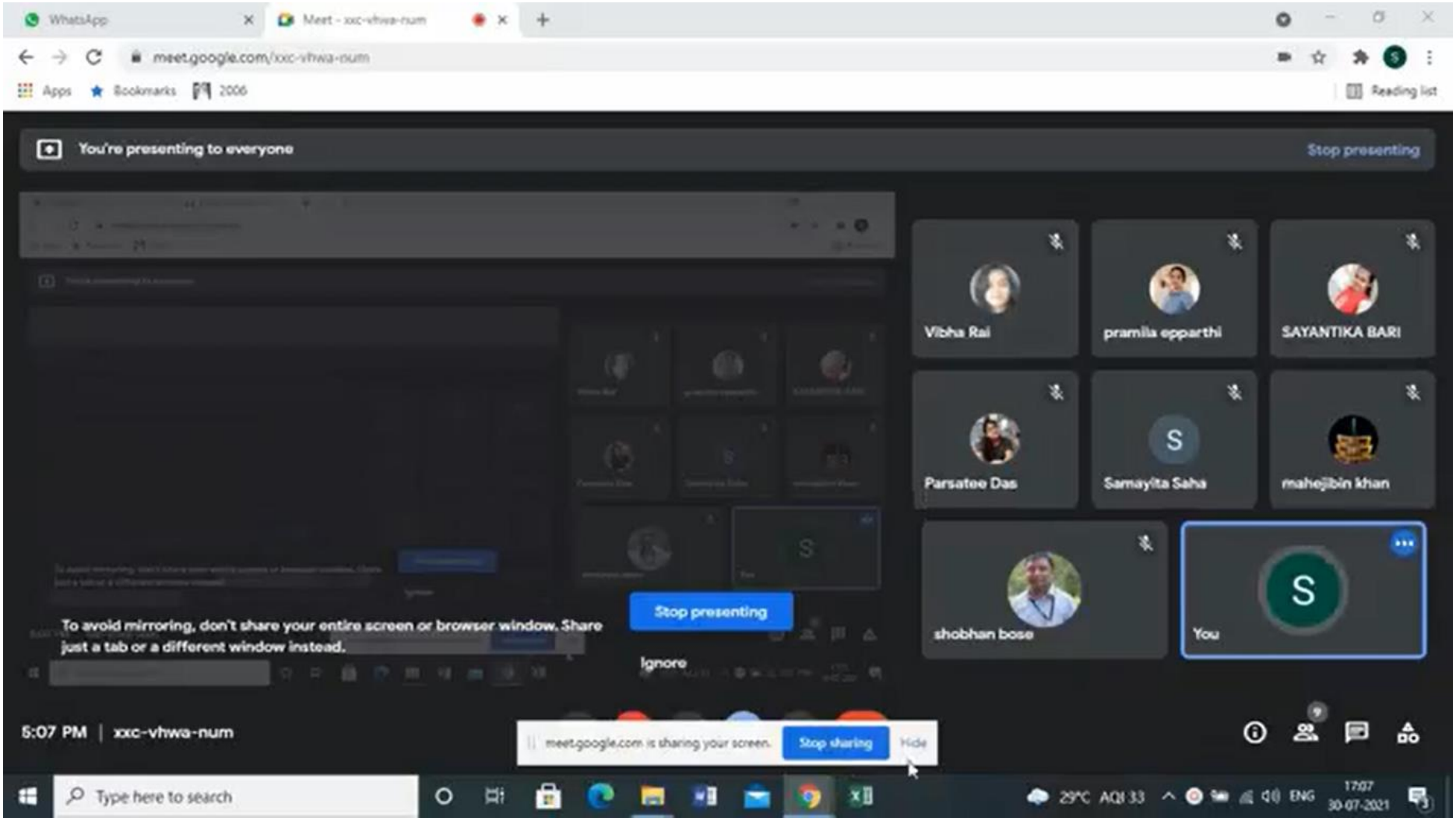
**30/07/2021**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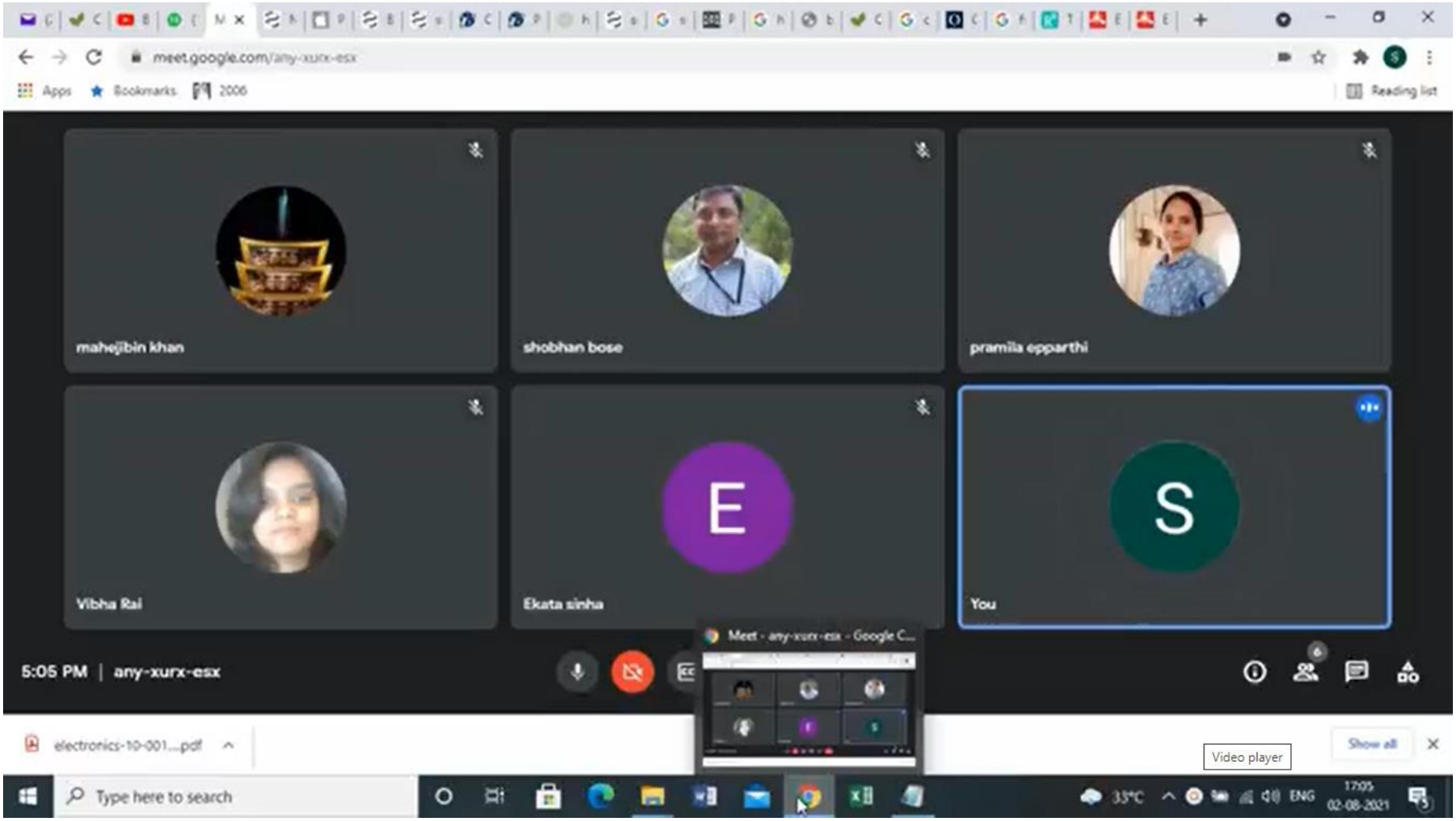
**02/08/2021**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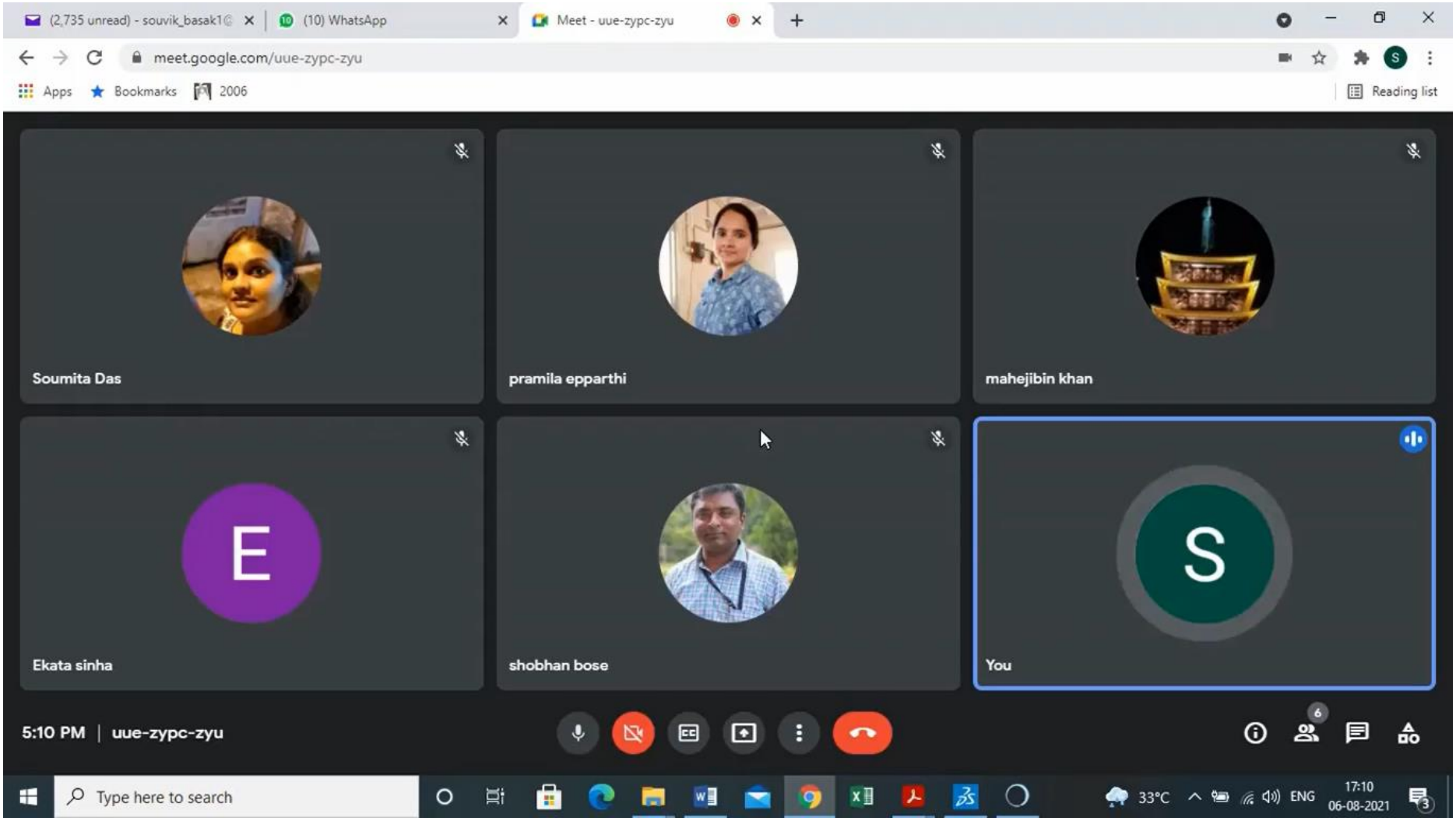
**06/08/2021**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06-08-2021

# Proposal to LSSSDC for becoming the Certification Partner for E-Vocational Training Programmes.

From: Kunal Vora (kunal.vora@shrmbio.com)

To: sachin.sachdeva@lsssdc.in

Cc: aniruddha@lsssdc.in; souvik_basak1@yahoo.com; trishamicrobiologist@gmail.com

Date: Friday, April 23, 2021, 04:57 AM PDT

Dear Sir,

Warm Greetings !!!

We hope that you and your family are keeping in best of your health, and are safe with the said pandemic.

As discussed in the telecon, herewith we would like your Esteemed Organization "***LSSSDC" to become our Certification Partner*** for the vocational online certification programmes as mentioned below:

**Course I**
Computer Aided Drug design with QSAR and biostatistics: from theory to hands-on training

**Course II**

Organic Spectroscopy-a detailed understanding, practical interpretations and industrial applications.

**Course III**

Chromatography: understanding, detailed applications and trouble shooting

**The details structure of the course, is attached for your kind perusal.**

**The other details are mentioned herewith:-**

**Duration of the course:** 1 months (12 classes both on theory and online practical training)

Course structure: Theory, Online Training, Quiz, Assignments, Marking, Certification

Expected Start of the Online Programme :- Mid May, 2021 (Expected to start – 20th May, 2021 – 1st batch)

**Tentative sharing of Revenue Generation:**

**KNOWLEDGE PARTNER :-** Dr. B.C. Roy College of Pharmacy & Allied Health Sciences (BCRCP)

**INDUSTRY PARTNER** :- SHRM Biotechnologies Pvt Ltd.(SHRM Biotech)

**CERTIFICATION PARTNER :-** Life Science Sector Skill Development Council (LSSSDC)

Tentative Fees from each Student :- Rs 5000/-

Tentative Revenue to LSSSDC :- Rs 1000/- per certification.

The Fees collection and payments would be collected by SHRM Biotechnologies Pvt Ltd, and would be segregated to all the 3 partners.

**Key Job Role**

BCRCP: Knowledge Partner, and Technical Course Delivery Partner

SHRM Biotech: Marketing and Promotion Partner

LSSSDC :- Certification and Promotional Partner

All the Entities would market the said course in their respective websites, all entities have rights to use their logo solely for the promotion and certification of the said course and programmes.

We look forward for our esteemed partnership in this regard, we would also request a detailed collaboration Letter in the said perspective to be signed among all the entities, once you approve the same.

Thanking You

Regards,

Mr. Kunal Vora
Founder & CEO
SHRM Biotechnologies Pvt Ltd
Kolkata
(M) +91 98300 19234
(O) +91 89810 03215
www.shrmbio.com

3 Vocational Training Courses .pdf
161.6kB

SHRM/1404-03/855

# CERTIFICATE OF COMPLETION

This is to certify that

# Anwesha Chatterjee

Has Successfully Completed The One month Online
Training in Computer Aided Drug Design With QSAR

Souvik Basak

DR. SOUVIK BASAK
ASSOCIATE PROFESSOR,
DR. B. C ROY COLLEGE OF PHARMECY &AHS

Date : 28/09/2021.

KUNAL VORA
DIRECTOR,
SHRM BIOTECHNOLOGIES PVT. LTD

SHRM/1404-03/857

# CERTIFICATE OF COMPLETION

This is to certify that

## *Dr Moitreyee Chattopadhyay*

Has Successfully Completed The One month Online
Training in Computer Aided Drug Design With QSAR

DR. SOUVIK BASAK
ASSOCIATE PROFESSOR,
DR. B. C ROY COLLEGE OF PHARMECY &AHS

Date : 28/09/2021.

KUNAL VORA
DIRECTOR,
SHRM BIOTECHNOLOGIES PVT. LTD

SHRM/1404-03/854

# CERTIFICATE OF COMPLETION

This is to certify that

# *Mahejibin Khan*

Has Successfully Completed The One month Online
Training in Computer Aided Drug Design With QSAR

DR. SOUVIK BASAK
ASSOCIATE PROFESSOR,
DR. B. C ROY COLLEGE OF PHARMECY &AHS

Date : 28/09/2021.

KUNAL VORA
DIRECTOR,
SHRM BIOTECHNOLOGIES PVT. LTD

SHRM/1404-03/850

# CERTIFICATE OF COMPLETION

This is to certify that

# *Parastee Das*

Has Successfully Completed The One month Online
Training in Computer Aided Drug Design With QSAR

DR. SOUVIK BASAK
ASSOCIATE PROFESSOR,
DR. B. C ROY COLLEGE OF PHARMECY &AHS

Date : 28/09/2021.


KUNAL VORA
DIRECTOR,
SHRM BIOTECHNOLOGIES PVT. LTD

SHRM/1404-03/851

# CERTIFICATE OF COMPLETION

This is to certify that

# *Pramila Epparti*

Has Successfully Completed The One month Online
Training in Computer Aided Drug Design With QSAR

DR. SOUVIK BASAK
ASSOCIATE PROFESSOR,
DR. B. C ROY COLLEGE OF PHARMECY &AHS

Date : 28/09/2021.

KUNAL VORA
DIRECTOR,
SHRM BIOTECHNOLOGIES PVT. LTD

SHRM/1404-03/849

# CERTIFICATE OF COMPLETION

This is to certify that

# *Samayita Saha*

Has Successfully Completed The One month Online
Training in Computer Aided Drug Design With QSAR

DR. SOUVIK BASAK
ASSOCIATE PROFESSOR,
DR. B. C ROY COLLEGE OF PHARMECY &AHS

Date : 28/09/2021.

KUNAL VORA
DIRECTOR,
SHRM BIOTECHNOLOGIES PVT. LTD

SHRM/1404-03/852

# CERTIFICATE OF COMPLETION

This is to certify that

# *Shobhan Bose*

Has Successfully Completed The One month Online
Training in Computer Aided Drug Design With QSAR

DR. SOUVIK BASAK
ASSOCIATE PROFESSOR,
DR. B. C ROY COLLEGE OF PHARMECY &AHS

Date : 28/09/2021.

KUNAL VORA
DIRECTOR,
SHRM BIOTECHNOLOGIES PVT. LTD

SHRM/1404-03/853

# CERTIFICATE OF COMPLETION

This is to certify that

# Soumita Das

Has Successfully Completed The One month Online
Training in Computer Aided Drug Design With QSAR

DR. SOUVIK BASAK
ASSOCIATE PROFESSOR,
DR. B. C ROY COLLEGE OF PHARMECY &AHS

Date : 28/09/2021.

KUNAL VORA
DIRECTOR,
SHRM BIOTECHNOLOGIES PVT. LTD