Department of Chemistry, Providence Women's College

Two-day hands-on workshop on molecular modelling and drug designing software

(Under DBT STAR college scheme)

Resource Persons: Kavya C S, Hariprasad C. K., SERAH ZINES LLP, Kozhikode. (Incubated at AIC-SEED Foundation, IISER Pune, Maharashtra)

No. of Participants: 40

Computerized techniques for molecular visualization and 3D simulations plays an important role in the training portfolios of students learning chemistry. In order to promote the conceptual understanding and spatial ability of students, it is essential to use dynamic tools and visual representations of interactions between individual atoms and molecules. Students' understanding of many unobservable phenomena could be enhanced when computerized molecular models, simulations, and animations are integrated into the teaching -learning process.

Department of Chemistry, Providence Women's College, Calicut, conducted a two-day hands-on workshop to develop skills and expertise of undergraduate chemistry students. The 2-day workshop on 'Molecular modelling and drug designing software' was successfully conducted on 14/02/24 and 22/02/24. The workshop aimed at motivating students and improving their attitude toward science in general, and toward chemistry in particular. The objective of the

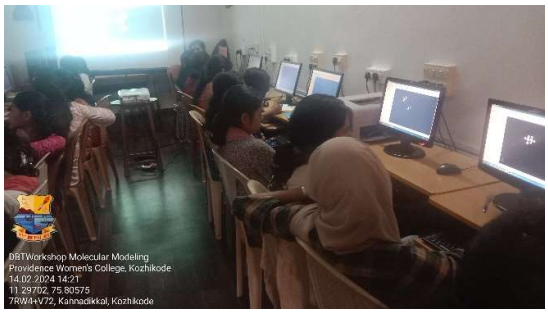
workshop is to develop skills in molecular dynamics and to enrich skills in structural and spatial analysis. The workshop was specially crafted to improvise the practical skills of the students by providing a hands-on experience on molecular visualization and three-dimensional simulation in general, and the 'Avogadro' program in particular. The course is expected to broaden the foundational knowledge and introduce the students to diverse research opportunities. The course would further enable the students visualize and understand complex molecular structures; thus, facilitating a deeper comprehension of chemical principles and molecular bonding.

Day 1: The session stated with an informal introduction of the resource speakers to the participants by Dr. Deepthi Jose, Asst. Professor, Providence Women's College.

In the first session, Mr. Hari Prasad C. K. (Serah Zines LLP, Kozhikode) introduced the concept of Molecular Modelling to the participants. He further elaborated on Molecular descriptors, Coordinate System, Chemical structure formats, Molecular graphics, Potential energy surface etc. citing various examples. Session 2 stated with a hand-on session on creating and editing 3D molecular structures using the molecule editor and visualizer 'Avogadro'. Visualization in Wireframe, Ball & Stick and Space fill models, creating molecules with different functional groups, optimization of molecules using molecular mechanics, prediction of molecular properties, exporting of molecules in different file formats were also explained in detail.

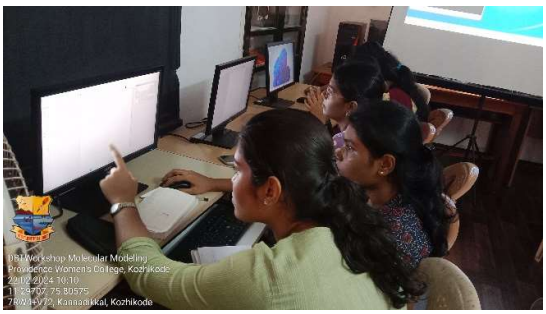
The afternoon session was handled by Ms. Kavya C. S. (Serah Zines LLP, Kozhikode) where elaborated sessions on measurement of bond length, bond angles and dihedral angles; conformer Search, Hydrogen Bond, importing molecules by name, building with SMILES, Image rendering using 'Avogadro' were taken. Further, the hand on session continued with Structure of protein, Understanding PDB file, introduction to Jmol, importing structures from Protein Data Bank, demonstration of interactive image of protein in Jmol, manipulation of images of a protein, usage of Jmol menus for the protein display, modification and display of hydrogen bonds.

Towards the concluding session, the students were segregated into groups and tasks were assigned for completion based on the learning they received from the session.



Day 2: The forenoon session was kicked off with a detailed session on 'Avogadro'. Building a Peptide, DNA & RNA, Carbon Nanotubes, Supercell, Polymer unit cell, viewing electrostatic potential maps etc were demonstrated. This was followed by a comprehensive session on 'Jmol'. Students were educated on visualization of atomic and molecular orbitals, geometric and conformational isomers, creation and visualization of animations for various symmetry operations, generation gif files, incorporation of Jmol in PowerPoint slides, introduction to drug databases and retrieval of drug molecules.

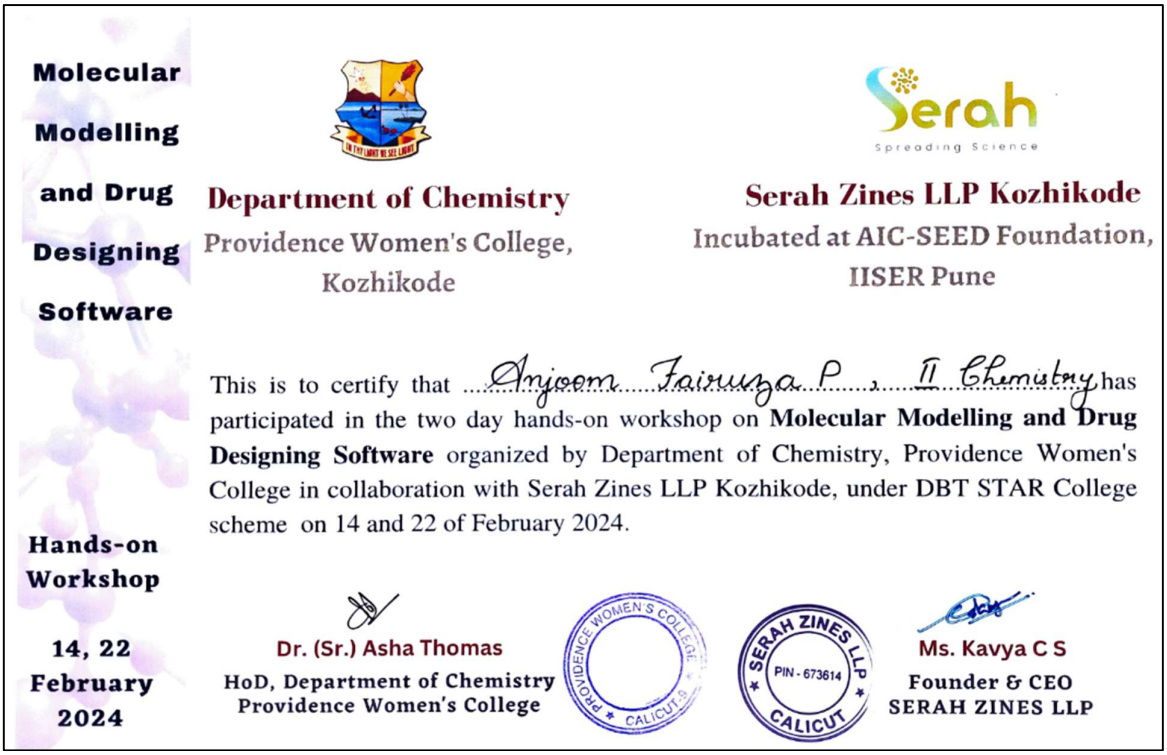
In the afternoon session, students were directed to present their assignment work; where they proudly exhibited the insights, they gained from the two-day workshop. The assignments were evaluated and feedback was provided.

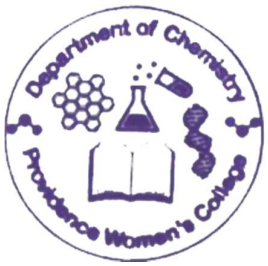


Feedback/Conclusion: The students agreed that workshop was very helpful in good understanding of conceptual terms and visualisation of molecules. Many students indicated that learning chemistry with Avogadro and Jmol was extremely helpful, bringing the microscopic world of molecules closer to them. The integration of computerized techniques and modelling tools into traditional face-to-face instruction thus produced a better hybrid model of teaching-learning.

Course Plan		
DAY 1	Session 1 9.30 am -10.30 am	Back ground of Molecular Modelling: Molecular descriptors, Coordinate System, Chemical Structure formats, Molecular graphics, Potential energy surface
	Session 2 10.45 am – 12.45 pm	Creating and editing 3D molecular structures using Avogadro; Visualization in Wireframe, Ball and Stick and Space fill models; Create molecules with different functional groups, optimize molecules using molecular mechanics, Predict molecular properties, Export molecules in different file formats.
	Session 3 1.30 pm – 3.00	Avogadro: Making Selections, Coloring Part of a Molecule, Measurement of bond length, bond angles and dihedral angles; Conformer Search, Hydrogen Bond, importing molecules by name, building with SMILES, Image rendering

	Session 4 3.15 – 4.45 pm	Structure of protein, Understanding PDB file, Jmol: Import structures from the Protein Data Bank, display an interactive image of the protein in Jmol, manipulate images of a protein with mouse, use the Jmol menus to change the way the protein is displayed, change the display style of selected parts of a protein, display hydrogen bonds.
Assignment		
Day 2	Session 1 9.30 am -10.30 am	Avogadro: Building a Peptide, DNA & RNA, Carbon Nanotubes, Supercell, Polymer unit cell, viewing electrostatic potential maps
	Session 2 10.45 am – 12.45 pm	Jmol: Visualizing atomic and molecular orbitals, geometric and conformational isomers
	Session 3 1.30 pm – 3.00	Create and visualize the animations for various symmetry operations, generating gif files, incorporate Jmol views in powerpoint slides, Introduction to different drug databases and retrieving structure of drug molecules
	Session 4 3.15 – 4.45 pm	Presentation and Assignment Evaluation





WORKSHOP CONTENTS

- Back ground of molecular modelling and drug biomolecular interactions
- Create and edit 3D molecular structures using Avogadro
- Measurement of bond length, bond angles and dihedral angles
- Create and visualize atomic and molecular orbitals
- Generate the animations for various symmetry operations
- Understand crystal structure and unit cell parameters
- Understand structure of proteins and enzymes using JMOL
- Generate GIF files and incorporate in powerpoint

RESOURCE PERSON

Kavya C S

Hariprasad C. K.

SERAH ZINES LLP, Kozhikode.
(Incubated at AIC-SEED Foundation, IISER Pune, Maharashtra)

Serah

Spreading Science

Objectives of the Workshop

- Improvise Practical Skills: Enhance the practical skills through hands-on experience in molecular modeling.
- Broaden Foundational Skills: Expand the foundational skills in the field of molecular modeling and drug designing software.
- Introduce to Diverse Research Opportunities: Familiarize with various research opportunities in the domain of molecular modeling and drug design.
- Enable Visualization of Complex Molecular Structures: Equip students with the ability to visualize and comprehend intricate molecular structures.
- Facilitate Deeper Understanding of Chemical Principles: Foster a deeper understanding of chemical principles and molecular bonding through practical applications

4 QUALITY EDUCATION

17 PARTNERSHIPS FOR THE GOALS

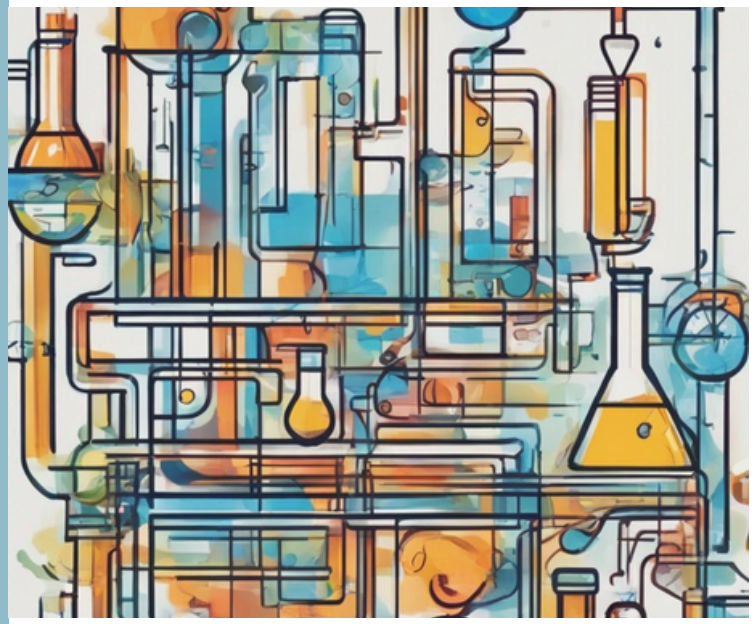
IN THY LIGHT WE SEE LIGHT

सत्यमेव जयते
DEPARTMENT OF BIOTECHNOLOGY
GOVERNMENT OF INDIA

Under DBT STAR COLLEGE Scheme

Two Day Hands-on Workshop

Molecular Modelling and Drug Designing Software



14, 22 February 2024
Cheminformatics Lab

Department of Chemistry
Providence Women's College,
Kozhikode 673009, Kerala
www.providencecollegecalicut.ac.in

Hands-On Workshop on Molecular Modelling and Drug Designing Softwares

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14, 22 February 2024
Under PBG Star College Scheme

	Name of student	Class of study	14/02/24	22/02/24
1.	Anaina Azeez K T	II Chemistry		
2.	Jains Bobby	II Chemistry		
3.	Krishna Chandra T	II Chemistry		
4.	Saganga Surendran K	II Chemistry		
5.	Adhithya Saji	II Chemistry		
6.	Anjalikrishna T C	II Chemistry		
7.	Ajisha Liba T K	II Chemistry		
8.	Fathima Hamna P	II Chemistry		
9.	Liya K. P	II Chemistry		
10.	Megha K P	II Chemistry		
11.	Shradha K Devadas	II Chemistry		
12.	Adra S	II Chemistry		
13.	Akhina K Kushnan	II Chemistry		
14.	Ananya Jayaprakash	II Chemistry		
15	Arya K R	II Chemistry		
16.	Avani Rajeev	II Chemistry		
17	Jasmine K M	II Chemistry	Jasmine	Jasmine
18.	Krishna Priya V	II Chemistry		
19.	Linda S Babu	II Chemistry		
20	Liya Denny	II Chemistry		
21	Megha V	II Chemistry		
22	Mufeeda Mashiyam	II Chemistry		
23	Nandana Vinod	II Chemistry		
24	Nandhana T K	II Chemistry		
25	Sanika Sunil N K	II Chemistry		
26	Shijnia V	II Chemistry		
27	Srilakshmi S	II Chemistry		
28	Sruja Santhosh	II Chemistry		
29	Yadhika M	II Chemistry		
30	Adeesha O	II Chemistry		
31	Anjoon Fairuza P	II Chemistry		
32	Aiswarya T	II Chemistry		
33	Arathi Rajesh K P	II Chemistry		
34	Devananda M	II Chemistry		

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35	Akshara P	II Chemistry		
36	Ansila Nasrin	II Chemistry		
37	Arathi Sathyan	II Chemistry		
38	Diya R	II Chemistry		
39	Shahala A K	II Chemistry		
40	Thrithya Krishnan	II Chemistry		
41	Minha Fathima	I Chemistry		

For SERAH ZINES LLP
Kavya CS
Designated Partner

SERAH ZINES LLP PIN - 673614 CALICUT

Sr. ASHA
Assistant Pr
Dept. of
Providence

Serah
Spreading science

SERAH ZINES LLP

C/o AIC-SEED IISER Pune

Date : 05/02/2024

Invoice with Cost Breakdown for the Workshop on molecular modelling and drug designing software

Dear Madam,

Greetings of the day.

This is to inform you that the total cost for the conduct of upcoming 12-hour workshop on molecular modelling and drug designing software for 40 students at Dept of Chemistry, Providence Women's College by SERAH ZINES LLP is **Rs. 20,000/-**. The workshop is aimed at improvising the practical skills of the students by providing a hands-on experience on molecular modelling. The course is expected to broaden the foundational skills and introduce the audience to diverse research opportunities. The course would further enable the students visualize and understand complex molecular structures thus facilitating a deeper comprehension of chemical principles and molecular bonding.

Kindly find below the detailed cost breakdown for the workshop which provide a clear understanding of how the fund is utilized for various components of the workshop.

1. Training Materials and Resources: Rs. 3500/-
2. Instructor Fees: Rs. 8000/- (4000 per day)
3. Software installation Costs: Rs. 5000/-
4. Contigency: Rs. 3500/-

Total Cost: Rs. 20,000/-

Account Name	: SERAH ZINES LLP
Account Number	: 50200081990221
Bank	: HDFC Bank
IFSC Code	: HDFC0008743

Please make the payment to the provided bank account.

Thank you for choosing us for the skill training and workshop needs. If you have any questions or concerns, please don't hesitate to contact us at *infoteamserah@gmail.com*.

Sincerely,

Kavya C S
Founder and CEO

SERAH ZINES LLP PIN - 673614 CALICUT

SERAH ZINES LLP

C/o AIC-SEED IISER Pune

Date : 05/02/2024

12-hour workshop on molecular modelling and drug designing software

Course Plan		
Day 1	Session 1 9.30 am -10.30 am	Back ground of Molecular Modelling: Molecular descriptors, Coordinate System, Chemical Structure formats, Molecular graphics, Potential energy surface
	Session 2 10.45 am – 12.45 pm	Creating and editing 3D molecular structures using Avogadro; Visualization in Wireframe, Ball and Stick and Space fill models; Create molecules with different functional groups, optimize molecules using molecular mechanics, Predict molecular properties, Export molecules in different file formats.
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	Assignment	

For SERAH ZINES LLP

Kavya CS

Designated Partner

SERAH ZINES LLP

C/o AIC-SEED IISER Pune

Date : 05/02/24

Course Plan		
Day 2	Session 1 9.30 am -10.30 am	Avogadro: Building a Peptide, DNA & RNA, Carbon Nanotubes, Supercell, Polymer unit cell, viewing electrostatic potential maps
	Session 2 10.45 am – 12.45 pm	Jmol: Visualizing atomic and molecular orbitals, geometric and conformational isomers
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For SERAH ZINES LLP

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