

Computational Chemistry

Work shop is designed to empower participants with the fundamental knowledge and practical training needed to stimulate chemical properties accurately using modern quantum mechanical soft wares. The core objective of the work shop is to bridge the gap between abstract theoretical concept and real world research applications, providing a solid foundation in molecular Quantum Chemistry. Participants will gain intensive hands on experience in building molecules, optimizing geometry and performing different types of computational calculations. Work shop will help to interpret complex outputs including IR, NMR and UV-Visible spectra as well as visualizing MO diagrams.

Molecular Docking

Molecular Docking is a powerful computational tool to predict molecular interaction level. The key applications are in drug designing, Virtual Screening of large libraries of compounds investigating the fundamental process of enzyme-substrate or drug receptor interactions. Modifying a drug structure, bio remediation, drug repurposing are some other important applications

MAJLIS COLLEGE (AUTONOMOUS)

Affiliated to University of Calicut and Approved by AICTE
Accredited by NAAC with Grade A

ABOUT THE COLLEGE

Majlis Arts and Science College is a multidisciplinary institution affiliated to the University of Calicut, approved by the Government of Kerala and recognized under Section 2(f) of the UGC Act 1956. The institution is accredited by NAAC with grade "A" in the first cycle in the year 2022. College is upgraded to Autonomous Status by UGC in 2023. Majlis Educational Complex comprises a group of educational institutions at different levels, where more than 4500 students of various age groups are being educated. Presently, the College is catering to 3200 students from across the state, in 19 undergraduate and 7 postgraduate programmes. Beginning with a minimum of four programmes in 1995, it has grown to the prestigious position as one of the largest self-financing colleges in the state. The college has all the state of the art infrastructural facilities such as well-equipped laboratories and classrooms, Multimedia studio, e-Content Development Centre. The College also provides ample facility for cultural, sports and games activities. It has sustained the long-term commitment towards the society and unswerving stand to universal human values by adhering to the vision of culture-oriented and value-based quality education.

ABOUT THE DEPARTMENT

The Department of Chemistry, incepted in the year 2005 is functioning with the declared objective of imparting knowledge in the field of Chemical Science and to help the development of student community, especially from the socially, economically and educationally backward areas of the society. The Department offers Undergraduate and Post Graduate programmes in Chemistry and also Certificate Courses in advanced areas of Chemistry every year. We have Memorandum of Understanding and Collaborations with other academic institutions and Chemistry related industries which help the students to have a better exposure in to advanced laboratory techniques and instruments.



Highlighting The centennial of quantum mechanics

INNOVATIONS IN CHEMICAL
RESEARCH: ICR-2025
**MOLECULAR
SIMULATIONS**

05

06

JAN
2026

Organized by the **PG Department of Chemistry**
in association with **IQAC**

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Dear Students and Colleagues,

We cordially invite you to the Two Day National Workshop on "Innovations in Chemical Research, ICR 2024: molecular simulations" to be held on 5th & 6th January 2026, Organized by Post Graduate Department of Chemistry. We look forward to your esteemed presence.

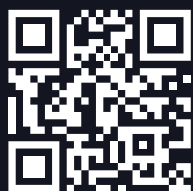
WITH BEST REGARDS,



Dr. Mohamed Kutty Kakkakunnan
(Principal)

Prof. Santhakumari P
(Head of the Department)

Mr. HARIMOHAN C S
(Co-ordinator)



For registration Scan
Registration Fee 300/-
Limited seats only

PROGRAMME CHART

DAY 1 - 5/01/2026

- Registration 09:15 AM-

- PRAYER -

Welcome Address : **Mrs. Santhakumari P**
(HoD, Dept. of Chemistry)

Presidential Address : **Dr. Mohamed Kutty Kakkakunnan**
(Principal, Majlis Arts & Science College)

Inauguration & Keynote Address : **Dr. V C Saheer**
(Assistant Professor, Govt. Brennen College, Dharmadam)

Address By : **Mr. CP Hamza**
(Secretary, MASC)
Mr. Saleem Kuruvambalam
(Chairman, MASC)
Dr. Mohamed Ali. P
(Chairman, Majlis Academic Board)

Felicitations : **Prof. K. Mohamed Haneefa**
(Controller of Examination)
Mr. Noushad. N
(Academic Director)
Mr. Rafeeq P
(IQAC Coordinator)
Mr. Muhammed Rafi. N
(NAAC Coordinator)
Dr. Geetha nambiar
(Prof., Dept. of Chemistry)
Mr. Amjadali
(Chairman, College Union)

Vote of Thanks : **Mr. Harimohan C S**
(Coordinator, ICR-2025)

- TEA BREAK -

Day I - 5/01/2026

TECHNICAL SESSION- I : **Dr. V C Saheer**
(Assistant Professor, Govt. Brennen College, Dharmadam)

Chair **Workshop on Computational Chemistry : Mrs. Santhakumari P**

- LUNCH BREAK -
(1.30-3.30pm)

Workshop on Computational Chemistry continues

Vote of Thanks : **Fathwima Shahna P.H**

Day 2 - 6/01/2026

Technical Session- II 9.30-11Am : **Dr. Anuroopa G Nadh**

Chair **MOLECULAR DOCKING : Dr. Drisya Sasidharan**

- Tea break -
11.15-12.30 Pm

Technical Session- II continues

- Lunch Break -
1.30-3.30pm

Technical Session- II continues

Vote of Thanks : **Naimah Jasmin V**

Valedictory Session

Distribution of Certificates