



VIT-AP
UNIVERSITY

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One-Week Workshop on
Computational Chemistry

GROMACS | GAUSSIAN | AutoDock |

Organized by

Department of Chemistry, School of Advanced Sciences, VIT-AP University

"June 23-27, 2023 (Friday-Tuesday)"



Registration link:

<https://vtop1.vitap.ac.in/CCS/Conferenceinitial>



About the Program:

This one-week program offers a unique opportunity for participants to delve into the world of computational chemistry and gain hands-on experience with some of the most widely used software tools, such as Gaussian, Gromacs, and AutoDock, etc in the field. Whether you are a beginner or an experienced researcher looking to enhance your skills, this workshop will provide you with valuable insights and practical knowledge.

About the Department:

The Department of Chemistry offers M. Sc. Programme with the specialization in Analytical Chemistry and Pharmaceutical Chemistry. The students will have the scope to pursue their post-graduation thesis work at various national and international institutions and industries. Overall, through an approach of integrating the in-depth core and elective courses, and research work, instructed and guided by highly qualified and well experienced faculty members, students will gain the foundation and skill in advancing their career in higher studies as well as in industry.

<https://vitap.ac.in/departement-of-chemistry/>

About the School :

The School of Advanced Sciences (SAS) is one of the seven Schools of VIT-AP University and it houses the Departments of Mathematics, Physics, and Chemistry. SAS earnestly pursues a vision of providing local, regional, national and International leadership in the research and technology development. We believe in quality of education and research with ethical and professional standards for better tomorrow. Here, students make their choices based on their preferences and requirements that equips them with a balance of logical-thinking and problem-solving skills.

<https://vitap.ac.in/school-of-advanced-sciences/>

What You Can Learn:

- Basics of molecular dynamics simulations
- Running the MD simulation and analysis of basic results
- Training on molecular visualization software
- DFT calculations using Gaussian Software
- Analysis of electronic properties

Limited capacity with only 40 seats available. Participants will be selected on a first-come, first-served basis.

campus accommodation for selected out-of-town participants.

Registration Fee: Rs. 2000

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More Information:

<https://sites.google.com/vitap.ac.in/computat-chemistry-workshop/home>

Faculty Coordinators :

Dr. Bibhab Bandhu Majumdar

Dr. Sabeel M Basheer