# Computational Chemistry and Computer Aided Drug Design

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## Overview

The course aims to take a step forward to unravel the utility of Computing Technology in Chemistry Research.

Use of computers in various fields of science is a well-known activity. However, with the advent of technology, increase in computing power and availability of efficient algorithms, use of computers in scientific research has gained a significant importance. Computational chemistry describes the use of computer modeling and simulation to study the structures and properties of molecules and materials. Computational chemistry is also used in utilizing the computational techniques aimed at understanding the structure and properties of molecules and materials. Computational chemistry has become a useful mode to explore chemical compounds that are either difficult to be found or highly expensive to be purchased. Computational chemistry even helps chemists make near accurate predictions before running the actual experiments. Computer Aided Drug Design is branch wherein efficient use of computer algorithms and computers is made for design of novel molecular entities. Prediction of Physical, Chemical and Biological properties prior to synthesis of a molecule helps in decision.

The topics in the module include use of chemistry software in drawing chemical structures, their geometry optimization, understand mathematical descriptors, their use in deriving structure-activity/property relationships, perform molecular docking and understand various ligand-protein interactions and protein modeling.

Course participants will learn these topics through lectures and hands-on practical training. Also assignments will be shared to stimulate research motivation of participants.

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| **Modules** | **Computational Chemistry and Computer Aided Drug Design : April 15th – April 19th, 2019**<br>**Number of participants for the course will be limited to fifty.** |
| **You Should Attend If…** | ▪ you are a faculty guiding research in the area of synthesis of novel molecules and need added support of computing technology.<br>▪ you are a researcher working in the area of *de novo* molecule design<br>▪ you are a student or faculty from academic institution interested in learning how to use computational chemistry in your research. |
| **Fees** | The participation fees for taking the course is as follows:<br>**Participants from abroad** : US $500<br>**Industry** : Rs. 20,000/-<br>**Research Organizations**<br>i. Outstation Participants* : Rs. 10,000/-<br>ii. Local Participants : Rs. 7,500/-<br>**Academic Institutions: a: Faculty Members/Post Docs.**<br>i. Outstation Participants* : Rs. 10,000/-<br>ii. Local Participants : Rs. 7,500/-<br>**b: Ph.D. Research Scholars :**<br>i. Outstation Participants* :Rs. 7,500/-<br>ii. Local Participants : Rs. 5,000/-<br>**c. Postgraduate Students**<br>i. Outstation Participants* :Rs. 5,000/-<br>ii. Local Participants : Rs. 2,500/-<br>The above fee includes all instructional materials, computer use for tutorials and assignments, free internet facility. The outstation participants will be provided with accommodation on sharing basis. For separate single bedded accommodation extra payment would be required. No accommodation would be provided to local participants. |

**Dr. Maria Natália Dias Soeiro Cordeiro** is an Associate Professor and Heads The group of Theoretical and Computational Chemistry of the University of Porto belonging to the Department of Chemistry of the Faculty of Sciences and is part of REQUIMTE, the associated Laboratory for green chemistry. Initially working on molecular simulations of ionic solutions and their interfaces, this being motivated by problems of heterogeneous catalysis and electrochemistry, her current scientific research mainly focuses on *in silico* tools towards the assessment of the safety of chemicals/nanomaterials as well as to be usefully applied in drug design or in property/reactivity predictions. She is an author of 250+ SCI works, of about 12 book chapters, and 90+ oral communications in international conferences.

**Dr. Nitin S. Sapre** is Professor and Head, Department of Applied Chemistry, SGSITS, Indore and is also Heading the Computational Chemistry Research group. His area of research focuses on Computational Chemistry, Computer Aided Drug Design (with an emphasis on Design of Novel Molecules as Inhibitors of HIV-1), Chem(o)-informatics, Protein Modeling.

Computational techniques in assessing the structure activity/property relationships, mode of attachment of small molecules within the protein especially the HIV-1 proteins using molecular docking methods are some of the important features. He has published and presented his work in Journals and Conferences of International repute respectively.