

Computational chemistry and its application in pharmacy and drug development

Wednesday, 1 December 2021 14:30 (30 minutes)

Summary:

Computational chemistry involves the use of theoretical methods and computers to solve chemistry and interdisciplinary problems. It has progressed with the explosive increase of computational power and availability of user-friendly software. Computational chemistry is also benefiting from the boom of the ICT sector.

This presentation gives an overview of the fundamentals of computational chemistry methods and their applications in pharmacy and drug development.

Objectives:

1. Collaboration with Computational Chemistry Group, Department of Chemistry, Faculty of Science, University of Mauritius.
2. Increase awareness of faculty and students about the importance of the computational chemistry and its use in all fields of science, especially in pharmacy and health sciences.
3. Possibility to do joint graduation project with Prof Ramasami.

Student?

No

Supervisor name

Supervisor email

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Session Classification: HPC Applications

Track Classification: Computational Chemistry