School of Chemistry

Module Aims: Session 2023-2024, Semester 1

Module CH3717: Computational Chemistry

Course Title: Computational Chemistry

Duration: 7 hours

Lecturer: Dr T. van Mourik

Aims: The aim of this part of the module is to become familiar with computational chemistry techniques that are used in modern drug design processes, covering force field calculations, molecular dynamics, molecular docking, QSAR and virtual screening.

Objectives:

1. Introduction to computational chemistry for medicinal chemists, covering its use in the design and development of drugs, with practical examples.

2. To learn how molecular mechanics force fields are used in modelling.

3. To learn the basic concepts of molecular dynamics, including the calculation of thermodynamic properties.

4. To learn how molecular docking is used to predict whether a drug candidate will bind to its target receptor.

5. To understand the basics of QSAR (Quantitative Structure Activity Relationships), and how it is used to correlate chemical structure with biological activity.

6. To understand what pharmacophores are and how they can be used to identify lead compounds.