Small molecule and protein crystallography in drug design.

J.Wouters

Both fundamentals aspects of crystallography and examples/case studies will be covered. Following items will be covered: fundamental aspects of crystallography, symmetry and space groups, crystal structure determination by single crystal X-ray diffraction, powder diffraction. Applications in small molecule and proteins crystallography (including structure-based drug design, pharmaceutical salts and co-crystals, polymorphism).

Lectures :

Day 1 Principles of crystallography (symmetry and space groups, principle of X-ray diffraction)

Day 2 Principles of powder diffraction techniques and crystal structure determination by single crystal X-ray diffraction

Day 3 Applications in small molecule (pharmaceutical salts and co-crystals, polymorphism).

Day 4 Applications proteins crystallography (structure-based drug design).