

Stereochemical Structural Elucidation Methods

Schedule:

Week 1: The significance of asymmetry and chirality.

Week 2: Basic concepts of stereochemistry: isomers.

Week 3: Types of chirality. Conformational and configurational enantiomers and diastereomers.

Week 4: Descriptors for absolute configuration: use of R/S and D/L descriptors, Cahn–Ingold–Prelog system.

Week 5: Compounds containing multiple stereogenic centers. Axial chirality.

Week 6: Optical rotation. Separation of enantiomers.

Week 7: Chiral drugs.

Week 8: Methods for determining absolute and relative configuration. Chemical correlation and kinetic resolution.

Week 9: NMR methods for determining absolute configuration. Mosher method and its modifications.

Week 10: Interaction between light and matter. Circular dichroism and circular birefringence. Chiroptical methods.

Week 11: Semi-empirical ECD rules and exciton-coupled circular dichroism.

Week 12: TDDFT-ECD calculations for determining the configuration of natural compounds I.

Week 13: TDDFT-ECD calculations for determining the configuration of natural compounds II.