In silico conformational analysis and spectrum calculation of organic compounds

Schedule:

Week 1: Basic stereochemical concepts. Isomerism. Absolute and relative configuration. Central, axial, planar chirality. Methods for determining absolute and relative configuration. Chiroptical spectroscopy, interactions between light and matter, ECD, VCD.

Week 2: Molecular mechanics, ab initio methods, DFT methods. Special points of the potential energy hypersurface and their calculation. Steps of CD calculation. Conformational analysis. Examples of ECD calculation of small, rigid derivatives.

Week 3: Conformational analysis and ECD calculation of flexible systems, reduction of flexibility by truncation, reclustering, solid-state methods and chemical transformation.

Week 4: OR and VCD calculation of compounds with variable flexibility. Combined application of several chiroptical methods for determining absolute configuration.

Week 5: NMR calculation of compounds with variable flexibility for determining relative configuration. Combined application of NMR and chiroptical methods for determining absolute configuration.

Week 6: Introduction to softwares suitable for conformer generation and molecular dynamics. Performing simple searches and simulations.

Week 7: Introduction to softwares suitable for semi-empirical, DFT and ab initio calculations. Performing optimizations.

Week 8: Introduction to the Linux system. Basic Linux commands.

Week 9: Combined application of Linux commands, pipes.

Week 10: Variables, cycles. Writing simple scripts in B shell.

Week 11: Writing simple scripts in B shell for input file generation and data extraction.

Week 12: A step-by-step overview of a specific ECD calculation. Generating input files from the MM search for DFT optimization. Clustering the resulting out files. Generating ECD inputs. Extracting rotator strength and wavelength values. Generating spectra from the extracted data.

Week 13: A step-by-step overview of a specific NMR calculation. Building of possible diastereomers. Generation of input files from the MM search results for DFT optimization.

Clustering of the resulting output files. Generation of NMR inputs. Extraction of chemical shift and coupling constant values. Comparison of data with measured values.

Week 14: Discussion of stereochemical problems brought by students. Design of structure discovery strategies. Generation of input files.