This project introduces students to computational molecular modeling and quantum chemistry through a complete, research-like workflow focused on sumatriptan, a small bioactive molecule used in migraine treatment. Sumatriptan is an excellent model system: its experimental vibrational spectra (IR/Raman) and crystal structure are available, making it possible to directly compare theory with experiment and critically evaluate computational results.

The project begins with preparation of the molecular structure and computational environment. In the first week, students will install and test the required software (CREST, ORCA, Quantum ESPRESSO, Python) and examine the experimental data that will serve as a reference throughout the project.
The second stage focuses on conformational analysis. Using CREST with the GFN-xTB method, students will explore the conformational space of sumatriptan and generate an ensemble of possible geometries. With Python scripts, they will process the results and select representative low-energy conformers for further investigation.
The third and fourth weeks involve quantum-chemical refinement and spectral calculations. Selected conformers will be optimized at the DFT level (e.g., PBE0/def2-TZVP) using ORCA. Students will then compute harmonic vibrational frequencies and simulate Raman and IR spectra. These calculated spectra will be compared with experimental data.
In the fifth week, the focus shifts to solid-state modeling. Students will import the experimental crystal structure of sumatriptan and relax it using periodic DFT in Quantum ESPRESSO. They will analyze the resulting lattice parameters, visualize molecular packing, and discuss differences between calculated and experimental structures. This step highlights how computational chemistry connects molecular properties with bulk material behavior.
Finally, students will compile their findings into a mini-research report and give a short presentation. They will include conformational diagrams, overlaid theoretical and experimental spectra, and visualizations of the optimized crystal structure.

By the end of this project, students will have experienced the complete workflow of computational chemistry — from exploring conformational space, through predicting molecular spectra, to modeling a crystal structure. They will gain hands-on experience with state-of-the-art software, semiempirical and DFT methods, and Python-based data analysis. This project provides not just theoretical knowledge, but practical skills in connecting computational predictions with experimental results, an essential part of modern chemical research.