Decipher three-dimensional structures of molecules and molecular complexes using two-dimensional IR spectroscopy

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First Project

Soluble amyloid-β peptides (Aβ) are found in all biological fluids of the human body as well as in amyloid plaques in brain, which are considered to be neurological indicators of Alzheimer's Disease (AD). Despite significant progress in understanding the mechanisms associated with the disease on a molecular level,[1] the physiological roles of β-amyloid precursor protein (APP) and especially of Aβ are not well understood. Recent experimental data indicate that binding of metal ions, such as Cu^{2+}, Cu^{+}, and Zn^{2+}, modifies the Aβ properties significantly affecting the Aβ oligomerization rates, modulating therefore the physiological function of Aβ, and affecting the Aβ fibrilization pathways. The data on the structures of Aβ complexes with ions are contradictory. The first aim is to investigate the binding sites of Aβ with Cu^{2+} and Zn^{2+} ions and study how the structure of Aβ changes due to the binding. A set of specifically labeled synthetic Aβ peptides and their mutant modifications, will be used to clarify the binding structures using 2DIR, linear IR and optical spectroscopies.

Second Project

Molecular systems which exhibit reversible photo-induced isomerization can potentially serve as photo triggers, memory devices, sensors, etc. Working in collaboration with Prof. Jeffrey Rack of Ohio University, who synthesized a family of ruthenium-polypyridine complexes that undergo photo-induced isomerization, we are trying to understand mechanisms of the processes occurring and the structures forming in such compounds under illumination with light. The project involves using triggered 2DIR spectroscopy for understanding the structural changes occurring during the photo isomerization.

Research Overview

Protein structure and structural dynamics determine their functioning. We are developing new spectroscopic methods of two-dimensional infrared spectroscopy (2DIR) and use them for deciphering three-dimensional structures of molecules, including peptides, proteins, inorganic complexes, and model compounds.

Prerequisites and Experience

The two projects are highly interdisciplinary and involve intensive use of analytical spectroscopic techniques and require basic knowledge in organic (1st project) and inorganic (2nd project) chemistry.