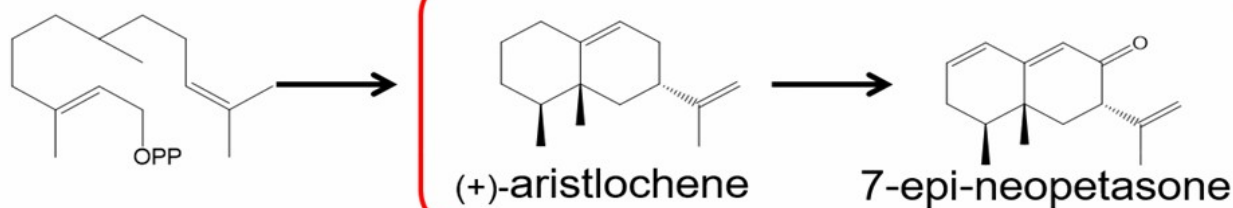
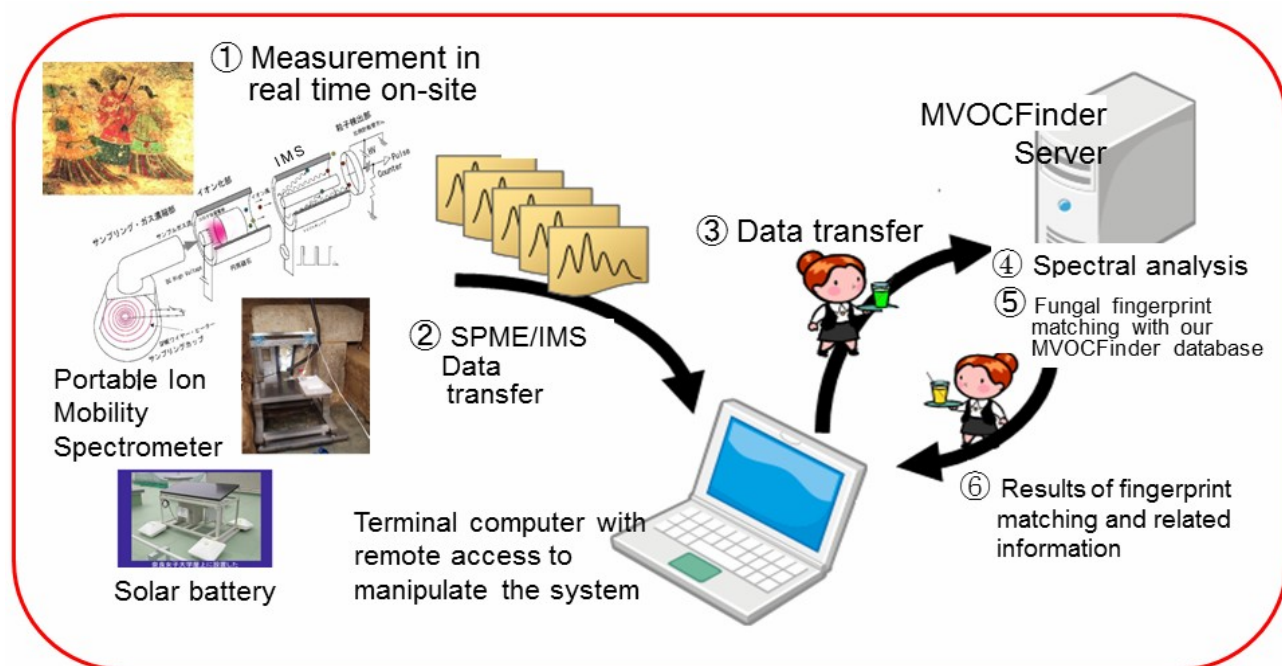


Unimolecular and Ion-Molecule Reaction Dynamics, and Applications for On-site Monitoring Mycology in Cultural Properties

Takae TAKEUCHI [Chemistry Course]



Development of a portable ion mobility spectrometer and its software to be used for on-site monitoring Mycology at cultural properties, and biosynthetic pathway for sesquiterpene such as aristlochene and its derivative

We are studying the mechanism, kinetics and dynamics for unimolecular, ion-molecule, and ion-surface reactions in gas-phases using mass spectrometry and ab initio molecular dynamics calculations. Our research focuses on constructing a theory for predicting mass spectra of various compounds, such as phosphopeptides, glycopeptides (bioactive m), and organosilicons (functional materials). By the use of this knowledge, we also isolated a new molecule which is difficult to be synthesized in solution. We are studying microbial volatile organic compounds (MVOCs) emitted from fungi for the purpose of preserving cultural properties. A portable ion mobility spectrometer and a companion software has been developed to be used for on-site monitoring of mycology. This was made possible by the theoretical calculations, using the trajectory method to predict the ion mobility spectra. This research is a new field which combined chemistry and microbiology.

Keywords : Reaction Dynamics, Quantum Chemistry, Chemical Mass Spectrometry, Cultural Property, Chemical Microbiology