

Detection of Structural Differences around Specific Atoms in Biomolecules

The research groups at the Japan Synchrotron Radiation Research Institute (JASRI), Kobe University, and Japan Atomic Energy Agency (JAEA), in collaboration with the National Institute of Advanced Industrial Science and Technology, succeeded to detect local structural differences in the vicinity of oxygen atoms in several biomolecular amino acids using soft X-ray natural circular dichroism spectroscopy.

Soft X-ray absorption spectroscopy has been commonly used to analyze chemical bonding states. In contrast, although soft X-ray natural circular dichroism has been expected to obtain the structural information of biomolecules, research on it has made slow progress due mainly to the extreme difficulty of measurement.

In this research, high-speed switching between right and left circularly polarized soft X-rays—generated by the twin helical undulators installed in the beamline BL25SU at

SPring-8— was fully exploited to reduce the noise level down to 0.1% or less of absorption intensity, leading to drastically enhanced accuracy of the soft X-ray natural circular dichroic spectrum. The measurement technique enables high sensitivity detection of small differences in types of steric conformations that have been hitherto inaccessible by conventional absorption spectroscopy. Subtle differences in a variety of amino acid side chains were detected by using soft X-ray natural circular dichroism spectroscopy. The measurement technique places expectations on developing a range of applications in a variety of fields, e.g. detailed structural elucidation of proteins and biomolecules, and applications in drug discovery.

The research results were published in the *Journal of Chemical Physics*, a journal published by the American Institute of Physics, on February 21, 2012 (EST).

Reference: "Characteristic oxygen K-edge circular dichroism spectra of amino acid films by improved measurement technique" Yudai Izumi, Maiko Tanabe, Akiko Imazu, Aki Mimoto, Masahito Tanaka, Akane Agui, Takayuki Muro, and Kazumichi Nakagawa *The Journal of Chemical Physics* **138**, 074305 (2013)

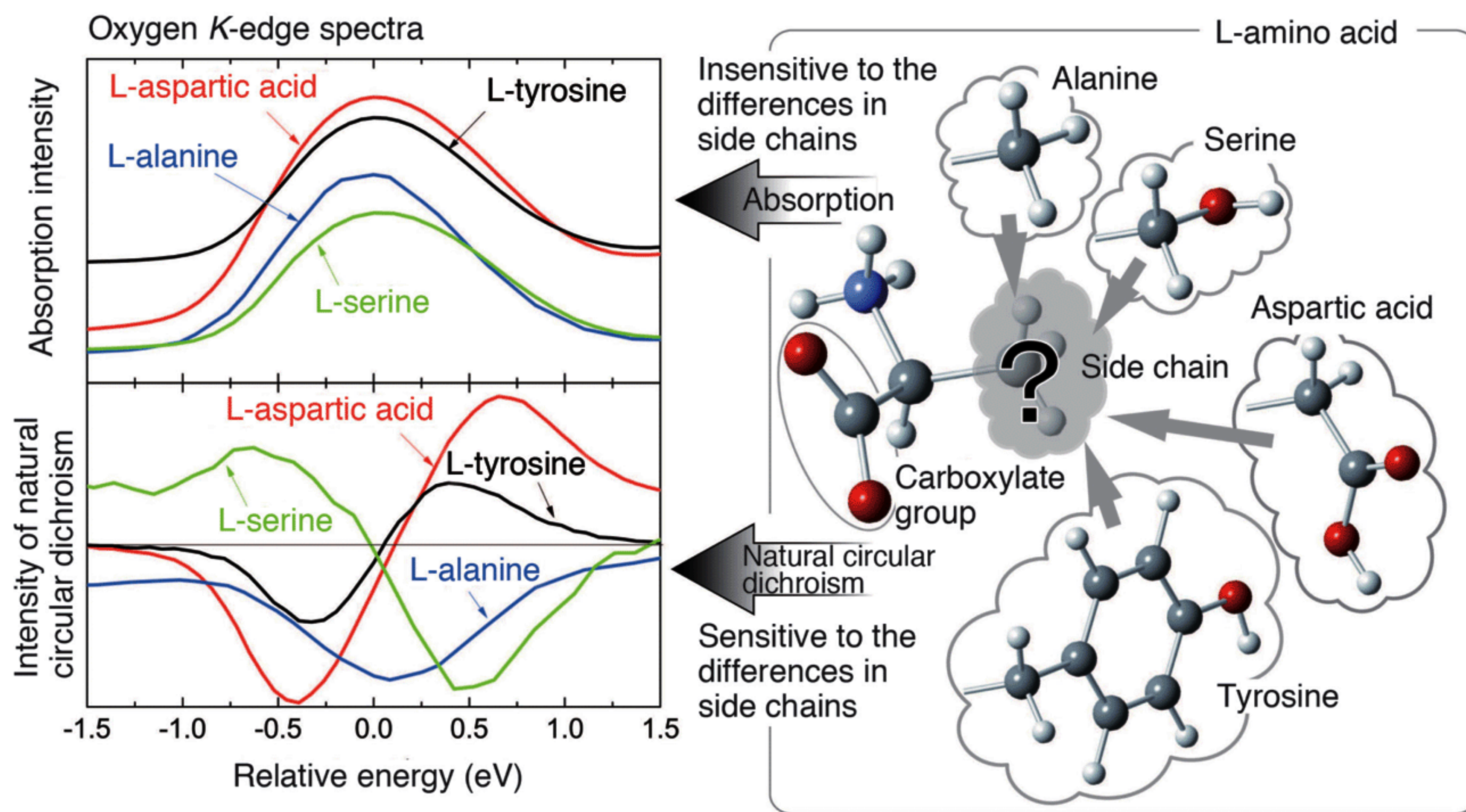


Fig.1. (Right) The structure of L amino acid. Its side chain varies depending on the type of the amino acid. Absorption spectra (upper left), and natural circular dichroism spectra (lower left) of the carboxylate oxygen (common part in all amino acids). The horizontal axis represents relative energy in reference to the value at the peak of the absorption spectra (defined as 0eV). Actual energy at the peak is equivalent to approximately 532eV.