MAR15-2014-020148

Abstract for an Invited Paper
for the MAR15 Meeting of
the American Physical Society

Exploring the active site structure of photoreceptor proteins by Raman optical activity

MASASHI UNNO, Saga University

Understanding protein function at the atomic level is a major challenge in a field of biophysics and requires the combined efforts of structural and functional methods. We use photoreceptor proteins as a model system to understand in atomic detail how a chromophore and a protein interact to sense light and send a biological signal. A potential technique for investigating molecular structures is Raman optical activity (ROA), which is a spectroscopic method with a high sensitivity to the structural details of chiral molecules. However, its application to photoreceptor proteins has not been reported. Thus we have constructed ROA spectrometer using near-infrared (NIR) laser excitation at 785 nm. The NIR excitation enables us to measure ROA spectra for a variety of biological samples, including photoreceptor proteins, without fluorescence from the samples. In the present study, we have applied the NIR-ROA to bacteriorhodopsin (BR) and photoactive yellow protein (PYP). BR is a light-driven proton pump and contains a protonated Schiff base of retinal as a chromophore. PYP is a blue light receptor, and this protein has the 4-hydroxycinnamyl chromophore, which is covalently linked to Cys69 through a thiolester bond. We have successfully obtained the ROA spectra of the chromophore within a protein environment. Furthermore, calculations of the ROA spectra utilizing density functional theory provide detailed structural information, such as data on out-of-plane distortions of the chromophore. The structural information obtained from the ROA spectra includes the positions of hydrogen atoms, which are usually not detected in the crystal structures of biological samples.