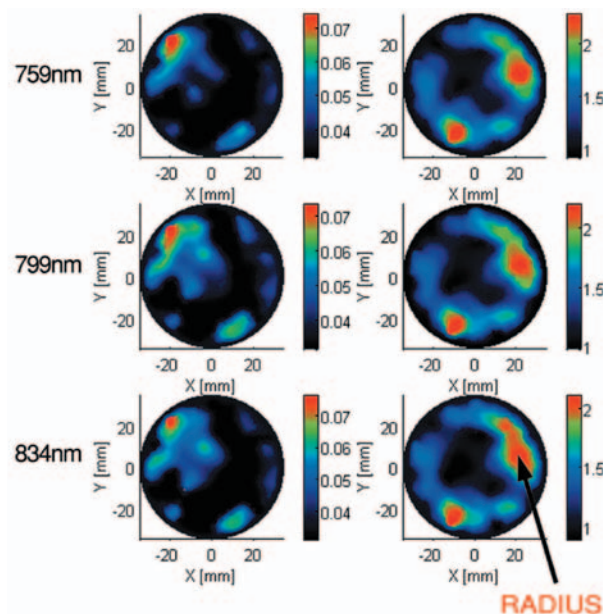


# Absolute Image Reconstruction from NIR-TR Measurement of Human Forearm

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Near infra-red (NIR) diffuse optical tomography, which aims at providing both anatomical and functional information of organs, has been increasingly receiving interests. NIR time-resolved (TR) method has ability to measure absolute absorption and scattering images. We developed modified GPST algorithm for the image reconstruction of NIR-TR data. The absolute image of absorption and scattering coefficients of human forearm were reconstructed and compared with MR image. The images revealed the inner structure of the forearm and the bones were clearly distinguished from the muscle.



Absolute absorption and scattering images of human forearm

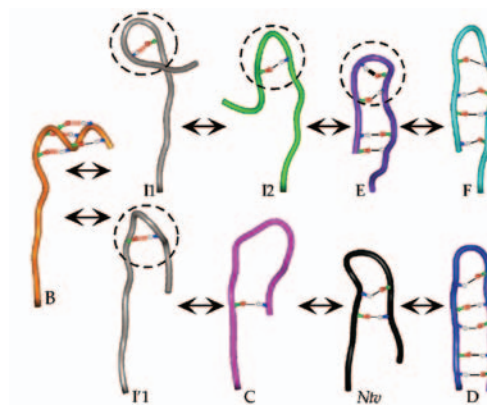
# Protein Structural Analysis by Multicanonical Molecular Dynamics

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Protein folding reaction is one of the fundamental problems in biophysics: how a protein folds into a compact native structure from unfolded random-coil conformations in a second. To calculate the free-energy landscape of a protein is an effective procedure to examine the folding process. In recent decades, the knowledge about the problem has been accumulated by not only experimental, but also theoretical means, such as Molecular Dynamics (MD) Simulation. The multicanonical MD is a novel sampling method that enables to obtain a precise free-energy landscape of a small biomolecule in explicit water. We could reveal the folding mechanism of a chameleon sequence and the stable conformations in water, by calculating the energy land-

scapes. The current study may be useful to understand the mechanism of abnormal folding that causes the diseases, such as amyloid disease.



Pathways between alpha-helix and beta-hairpin conformations