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Terahertz radiation as a pump and probe for studying low frequency vibrations in proteins

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Many functionally important structural changes in proteins proceed along the direction of their lowest frequency vibrations. These vibrations correspond to picosecond collective dynamics. Establishing the fundamental relationship between these vibrations and protein function remains a challenge within biophysics. Electromagnetic radiation in the terahertz frequency range (0.1-10 THz) can excite collective picosecond vibrations which makes it suitable as a probe for direct observation as well as a pump for the selection of functionally relevant vibrations for detection by other methods. The use of terahertz radiation for biological applications is hampered by several technical difficulties such as water absorption and thermal effects. For these reasons, method development is an important aspect when applying terahertz radiation to biological problems. In this work, terahertz radiation has been used to identify and characterize low frequency vibrations in three different proteins by applying both novel experimental design and analysis methods.

Terahertz absorption spectroscopy was used to identify the change in collective dynamics upon photo activation of a photosynthetic reaction centre. The collective vibrations were of non-thermal origin and localized to the chromophore containing subunits implying the involvement of collective dynamics in photosynthesis.

By combining X-ray crystallography with 0.4 THz excitation the presence of collective dynamics was detected in both lysozyme and thermolysin. In lysozyme, the vibrational mode was localized to a central α-helix. The vibrational mode had a lifetime longer than expected which most likely arise from a hypothetical Fröhlich condensation process not previously observed. The interaction of terahertz radiation with thermolysin was identified through a Bayesian statistical analysis of X-ray diffraction data.