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Correlated Protein Motion Measurements of Dihydrofolate Reductase Crystals[1] MENGYANG XU, KATHERINE NIESSEN, University at Buffalo, SUNY, JAMES PACE, VIVIAN CODY, Hauptman-Woodward Medical Research Institute - Buffalo, NY, ANDREA MARKELZ, University at Buffalo, SUNY — We report the first direct measurements of the long range structural vibrational modes in dihydrofolate reductase (DHFR). DHFR is a universal housekeeping enzyme that catalyzes the reduction of 7,8-dihydrofolate to 5,6,7,8-tetra-hydrofolate, with the aid of coenzyme nicotinamide adenine dinucleotide phosphate (NADPH). This crucial enzymatic role as the target for anti-cancer [methotrexate (MTX)], and other clinically useful drugs, has made DHFR a long-standing target of enzymological studies. The terahertz (THz) frequency range (5-100 cm^{-1}), corresponds to global correlated protein motions. In our lab we have developed Crystal Anisotropy Terahertz Microscopy (CATM), which directly measures these large scale intra-molecular protein vibrations, by removing the relaxational background of the solvent and residue side chain librational motions. We demonstrate narrowband features in the anisotropic absorbance for mouse DHFR with the ligand binding of NADPH and MTX single crystals as well as Escherichia coli DHFR with the ligand binding of NADPH and MTX single crystals.

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