Abstract Submitted
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2D IR measurements of the coupling in transmembrane helix dimers[1] CHONG FANG, Department of Chemistry, University of Pennsylvania, LIDIA CRISTIAN, ALESSANDRO SENES, WILLIAM DEGRADO, Department of Biochemistry & Biophysics, University of Pennsylvania, ROBIN HOCHSTRASSER, Department of Chemistry, University of Pennsylvania — Ultrafast 2D IR photon echo spectroscopy has been adapted to the study of transmembrane helix dimers. Residues Gly-79 on each of the two helical strands of Glycophorin A (GpA) dimers in sodium dodecyl sulfate (SDS) micelles were isotopically selected. The 2D IR spectra reveal the tertiary interaction between the helices. The waiting time dependence of the echo informs on the conformational dynamics of different regions of the GpA dimer. Both the ^{13}C and ^{13}C=^{18}O labeled homodimers showed elongated diagonal peaks in the 2D IR correlation spectra. The cross peaks in the heterodimer spectrum indicated an off-diagonal anharmonicity of $\sim$3.8 cm^{-1}. This anharmonicity is caused by through-space interactions between amide units on different strands. The angle between the two Gly-79 amide-I transition dipoles was estimated to be $\sim$35° from the polarization of the 2D IR signal in the cross-peak region. The method also identifies residues that are exposed to water.

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