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2D IR Spectroscopy of Nucleic Acid Bases and the Folding of DNA Aptamers CHUNTE SAM PENG, KEVIN C. JONES, CARLOS BAIZ, MICHAEL E. REPPERT, HELENA DE PUIG GUIXE, KIMBERLY HAMAD-SCHIFFERLI, ANDREI TOKMAKOFF, MIT, TOKMAKOFF COLLABORATION, HAMAD-SCHIFFERLI COLLABORATION — DNA can adopt a wide variety of conformations that have important roles in their biological functions, such as DNA packaging, replication, and protein recognition. Vibrational spectroscopy is known to reflect DNA conformation, and basic assignments of resonances in the IR and Raman spectra of nucleic acids have existed for decades. However, traditional spectral assignments are based on simple local vibrational mode basis such as C=O and C=N double bond stretches, although computational studies describe highly delocalized vibrations. We acquired polarization dependent 2D IR spectra of the base vibrations of five nucleotide monophosphates (NMPs) as the building blocks for developing a model of DNA and RNA vibrational spectroscopy. The distinctive cross-peaks between the vibrational modes of NMPs, such as ring vibrations and C=O stretches, indicate that these vibrational modes are strongly coupled anharmonic oscillators. We have characterized the eigenstate energies, vibrational anharmonicities, transition dipole strengths, and their relative orientations through the analysis and modeling of the experimental 2D IR spectra. We are currently applying this knowledge to study the folding of some G-rich DNA aptamers.

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