Abstract Submitted
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Modifying P700, An Important Chlorophyll Species Involved In Solar Energy Conversion in Plants and Bacteria[1] GARY HASTINGS, SREEJA PARAMESWARAN, Georgia State University — P700 is the primary electron donor of photosystem I. It is an asymmetric chlorophyll *a*' (P_A)/ chlorophyll *a*(P_B) heterodimer. This asymmetry is a result hydrogen-bonding with predominantly three amino acids and a water molecule near P_A. P_B is not involved in hydrogen bonding. In an attempt to decrease this level of assymmetry, and introduce hydrogen bonds to P_B, we have changed 1, 2 or all 3 of the amino acids near P_B with the corresponding amino acids on P_A. To investigate mutation induced alteration of pigment-protein interactions we have obtained ($P700^+$-P700) FTIR difference spectra for PS I particles from wild type and all three mutants. Upon mutation, many FTIR difference bands are altered, and some of the changes are difficult to rationalize using the accepted set of assignments for bands in ($P700^+$-P700) FTIR difference spectra. To model aspects of the experimental FTIR difference spectra, density functional theory based vibrational frequency calculations of chlorophyll-*a* in the presence of solvents and H-bond interactions were undertaken. Our calculations show that mutation induced mode intensity and frequency shifts are difficult to predict *a priori*. However, via calculation many of the puzzling mutation induced alteration of bands in ($P700^+$-P700) FTIR difference spectra can be understood.

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Gary Hastings
Georgia State University

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