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Network Analyses with Quantum Dynamic Calculations on Energy Flow in the Photosystem II Supercomplex

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In green plants, chlorophyll-*a* and chlorophyll-*b* are the predominant pigments bound to light-harvesting proteins. While the individual characteristics of these chlorophylls are well understood, the advantages of their coexistence remain unclear. In this study, we investigated a method to simulate excitation energy transfer within the entire photosystem II supercomplex by employing network analysis integrated with quantum dynamic calculations. We then investigated the effects of the coexistence of chlorophyll-*a* and chlorophyll-*b* by comparing various chlorophyll compositions. Our results reveal that the natural chlorophyll composition allows the excited energy to preferentially flow through specific domains that act as safety valves, preventing downstream overflow. Our findings suggest that the light-harvesting proteins in a photosystem II supercomplex achieve evolutionary advantages with the natural chlorophyll-*a*/*b* ratio, capturing light energy efficiently and safely across various light intensities. Using our framework, one can better understand how green plants harvest light energy and adapt to changing environmental conditions.