Supplementary material

Conformational changes in light-harvesting complex II trimer depending on its binding location

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Table S1. Information of molecular structures of photosystem supercomplexes from a green alga used in this study.

Label	PSII C_2S_2	PSII $C_2S_2M_2L_2$	PSI–LHCI–LHCII
PDB ID	6kac	6kad	7dz7
Organism	*C. reinhardtii 137c*	*C. reinhardtii 137c*	*C. reinhardtii pph1;pbcp*
Analyzed LHCII (Orange / purple / yellow)	S-trimer: LhcbM1/2/3	S-trimer: LhcbM1/2/3	LHCII-1: LhcbM1/2/3
Method	EM	EM	EM
Resolution	2.70 Å	3.40 Å	2.84 Å
Aggregation state	Particle	Particle	Particle
Detergent	α-DDM	α-DDM → A8–35	α-DDM
Buffer conditions	25 mM MES-KOH, pH 6.5	25 mM MES-NaOH, pH 6.5	25 mM MES pH 6.5
References	Sheng et al. Nat. Plants (2019)	Sheng et al. Nat. Plants (2019)	Pan et al. Nat. Plants (2020)

Table S2. Information of molecular structures of photosystem supercomplexes from vascular plants.

Label	LHCII	Plant C_2S_2	Plant $C_2S_2M_2$	Plant PSI–LHCI–LHCII
PDB ID	1rwt	3jcu	5xnl	5zji
Organism	*Spinacia oleracea*	*Spinacia oleracea*	*Pisum sativum*	*Zea mays*
Analyzed LHCII (Orange / purple / yellow)	Lhcb1/2(?)	S-trimer: 1RWT	S-trimer: 1RWT	LhcbM2/1/1
Method	X-ray Diffraction	EM	EM	EM
Resolution	2.72 Å	3.20 Å	2.70 Å	3.30 Å
Aggregation state	Crystal	Particle	Particle	Particle
Detergent	β-DDM	α-DDM	α-DDM	α-DDM
Buffer conditions	50 mM HEPES-NaOH, pH 7.5	10 mM HEPES, pH 7.5	25 mM MES 5 mM CaCl2, pH 5.7	10 mM HEPES, pH 7.5
References	Liu et al. Nature (2004)	Wei et al. Nature (2016)	Su et al. Science (2017)	Pan et al. Science (2018)

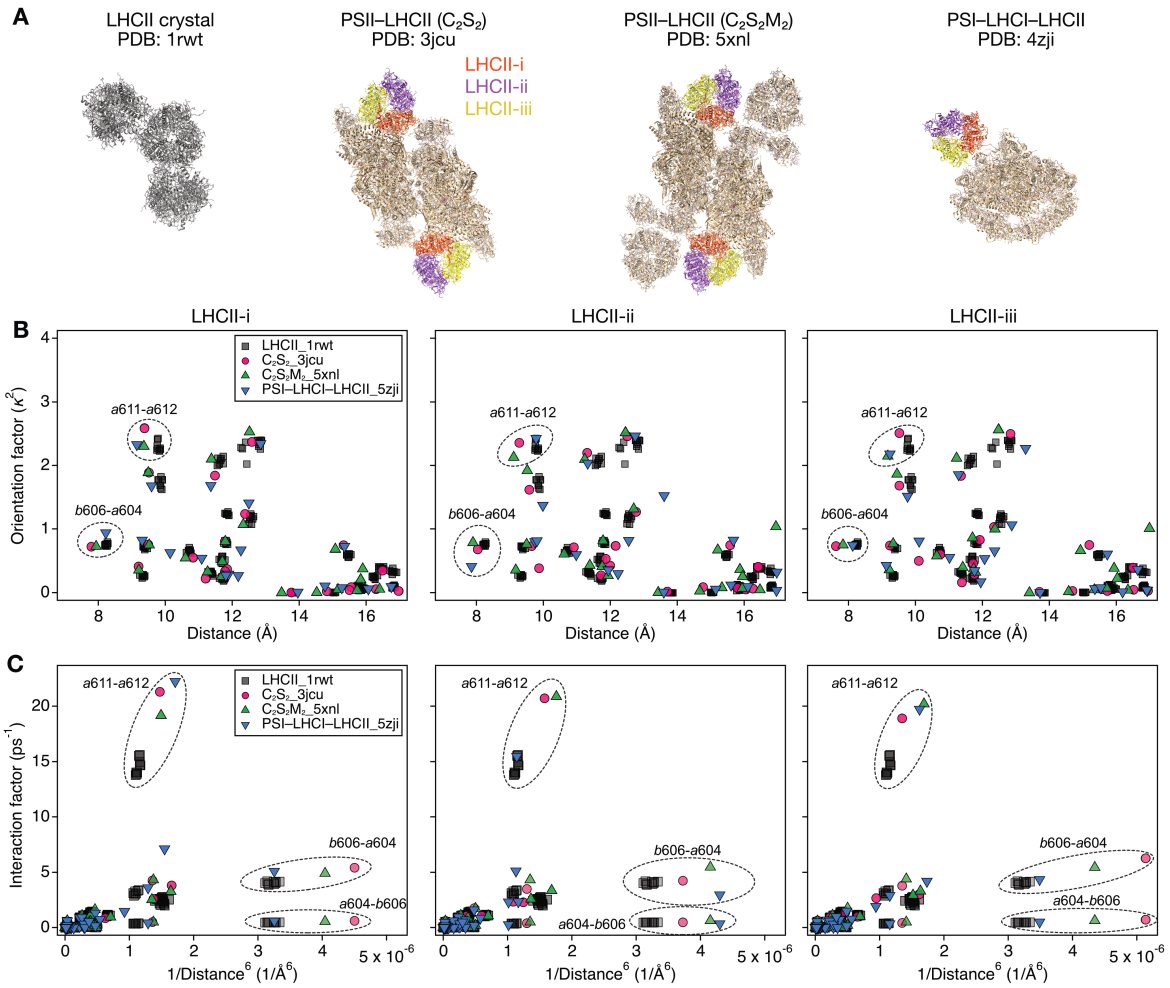

Figure S1. Chl configurations in LHCII trimers of crystal structures and three different photosystem supercomplexes from vascular plants. (A) Crystalized LHCII trimers (pdb.1rwt) and tentative labels of LHCII subunit of LHCII trimers in PSII–LHCII supercomplexes—C_2S_2 (pdb.3jcu) and $C_2S_2M_2$ (pdb.5xnl)—and a PSI–LHCI–LHCII supercomplex (pdb.5zji) from vascular plants. LHCII-i, LHCII-ii, and LHCII-iii are represented by orange, purple, and yellow colors, respectively, whereas LHCII subunits of crystalized LHCII trimers are not classified due to its uncertainty. **(B)** Scatter plots of configuration factors (Orientation factor and distance) between all Chls in the crystallized LHCII trimers and each LHCII subunit of each photosystem supercomplex. **(C)** Scatter plots of interaction factor (Energy transfer rate constant based on FRET principle) and 1/distance^6 derived from (B). 1rwt, 6kac, 6kad, and 7dz7 were represented by gray, pink, green, and cyan colors, respectively.