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Electronic Supplementary Information

A Theoretical Study on the Dynamics of Light Reaction in the Photosystem II Core Dimer: Regulation and Robustness of Energy Transfer Pathways

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In this Electronic Supplementary Information we include additional tables and figures to supplement our paper.

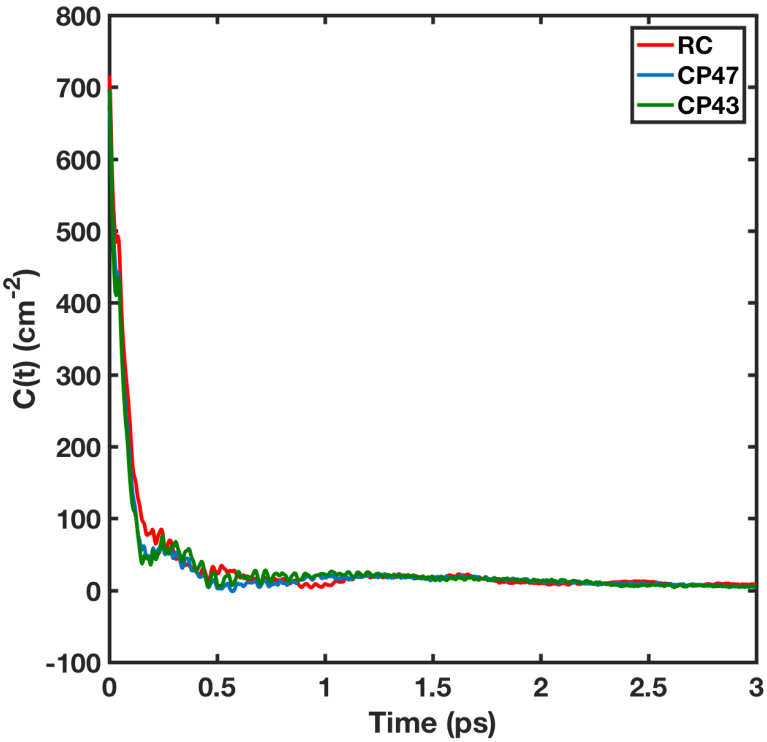

Figure S1: The time-correlation of site energy fluctuations calculated from the MD rajectories for CP47, CP43 and RC. The time-correlation functions were first calculated for each single CLA and then averaged among CLAs within each subunit of PSII-cc.

Table S1: Excitonic Hamiltonian of the PSII-cc system derived from the MD structures (Part 1). The model includeds 16 CLAs in a CP47, 13 CLAs in a CP43, 6 CLAs and 2 PHEs in a RC, a total of 74 pigments. The site labelings in the RC: P_{D1}, P_{D2}, Chl_{D1}, Chl_{D2}, $Chlz_{D1}$, $Chlz_{D2}$, Phe_{D1}, and Phe_{D2} are 604, 605, 606, 607, 610, 611, 608, and 609, respectively

P_{D1}	P_{D2}	Chl_{D1}	Chl_{D2}	$Chlz_{D1}$	$Chlz_{D2}$	Phe_{D1}	Phe_{D2}	612	613	614	615	616	617	618	619	620	621	622	623	624	625	626	627	628	629	630	631	632	633	634	635	636	637	638	639	640
15061	100	-54	-61	0	0	-7	16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	-4	0	0	0	-2	0	0	0	0	0
100	15289	-67	-43	0	0	19	-6	0	0	0	1	0	0	-3	-3	0	0	-2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-54	-67	14673	6	2	0	73	-4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7	0	0	0	0	0	0	0	0
-61	-43	6	14936	0	2	-4	0	0	0	0	0	0	0	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	2	0	14790	0	-4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7	0	0	0	0	0	0	0	0
0	0	0	2	0	14862	0	-4	4	-4	0	0	0	0	0	7	-0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-7	19	73	-4	-4	0	15070	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-6	0	0	5	0	0	0	0	0
16	-6	-4	0	0	-4	3	14940	0	0	0	0	0	0	0	-8	0	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	4	0	0	14802	71	17	-5	0	4	0	-4	6	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	-4	0	0	71	15122	-126	20	5	-6	-5	4	-18	-13	-4	5	-9	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	17	-126	14840	7	-3	0	-2	-6	24	14	1	-9	3	0	-1	-4	0	0	0	0	0	0	0	0	0	0	0	0	0
0	1	0	0	0	0	0	0	-5	20	7	14990	0	-14	77	5	-10	-3	-1	20	0	0	-3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	5	-3	0	15039	89	-19	-2	-0	-5	-3	-5	-7	-3	10	11	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	4	-6	0	-14	89	14905	6	0	7	-5	0	-3	8	0	-0	8	0	0	0	0	0	0	0	0	0	0	0	0	0
0	-3	0	0	0	0	0	0	0	-5	-2	77	-19	6	14826	0	0	1	5	-1	17	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	-3	0	7	0	7	0	-8	-4	4	-6	5	-2	0	0	14975	0	-100	-16	20	-5	-3	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	-0	0	0	6	-18	24	-10	-0	7	0	0	14964	86	8	-15	9	0	-3	5	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	3	-13	14	-3	-5	-5	1	-100	86	14861	-13	50	-1	-6	0	-7	0	0	0	0	0	0	0	0	0	0	0	0	0
0	-2	0	0	0	0	0	5	0	-4	1	-1	-3	0	5	-16	8	-13	15073	0	64	39	-17	7	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	5	-9	20	-5	-3	-1	20	-15	50	0	14808	-78	119	21	3	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	-9	3	0	-7	8	17	-5	9	-1	64	-78	14946	0	-3	2	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	-3	0	3	-3	0	-6	39	119	0	14991	-13	11	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	4	-1	-3	10	-0	0	3	-3	0	-17	21	-3	-13	14870	-8	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	-4	0	11	8	0	0	5	-7	7	3	2	11	-8	14791	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	14896	-11	-3	-1	-1	7	12	1	-7	3	0	-0	0
2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-11	14883	-36	62	0	-5	-6	4	18	-12	10	-6	-1
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-3	-36	14937	-21	-2	-1	-4	-4	-4	-12	-5	14	3
-4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	62	-21	14969	0	0	1	5	-2	20	2	-3	0
0	0	7	0	7	0	-6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	0	-2	0	14941	-13	0	-10	16	-2	-0	1	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7	-5	-1	0	-13	15018	32	10	-27	10	0	-7	7
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	12	-6	-4	1	0	32	14948	-12	59	-1	-5	20	-18
-2	0	0	0	0	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	4	-4	5	-10	10	-12	15032	22	62	39	-20	9
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0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	-12	-12	20	-2	10	-1	62	-66	14914	-63	-8	7
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0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	-0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table S2: Excitonic Hamiltonian of the PSII-cc system (Part 2).

P_{D1}	P_{D2}	Chl_{D1}	Chl_{D2}	$Chlz_{D1}$	$Chlz_{D2}$	Phe_{D1}	Phe_{D2}	612	613	614	615	616	617	618	619	620	621	622	623	624	625	626	627	628	629	630	631	632	633	634	635	636	637	638	639	640
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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0	0	0	0	0	0	0	0	0	0	0	0	-0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	-0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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15098	100	-55	-62	0	0	-7	16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	-4	0	0	0	-2	0	0	0	0	0
100	15304	-66	-46	0	0	19	-6	0	0	0	1	0	0	-3	-3	0	0	-2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-55	-66	14655	6	2	0	75	-4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7	0	0	0	0	0	0	0	0
-62	-46	6	14923	0	2	-4	0	0	0	0	0	0	0	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	2	0	14819	0	-4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7	0	0	0	0	0	0	0	0
0	0	0	2	0	14793	0	-4	0	-4	0	0	0	0	0	7	-0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-7	19	75	-4	-4	0	15090	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-6	0	0	5	0	0	0	0	0
16	-6	-4	0	0	-4	3	14960	0	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	14797	67	18	-5	0	4	0	-4	6	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	-4	0	0	67	15112	-125	20	5	-6	-5	4	-17	-13	-4	5	-9	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	18	-125	14840	7	-4	-70	-2	-6	23	15	1	-9	3	0	-1	-4	0	0	0	0	0	0	0	0	0	0	0	0	0
0	1	0	0	0	0	0	0	-5	20	7	14998	-52	-14	74	4	-9	-3	-1	20	-44	0	-3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	5	-4	-52	15057	92	-19	-2	0	-5	-3	-5	-6	-3	10	11	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	4	-6	-70	-14	92	14911	6	0	7	-5	0	-3	8	0	-1	8	0	0	0	0	0	0	0	0	0	0	0	0	0
0	-3	0	0	0	0	0	0	0	-5	-2	74	-19	6	14860	0	0	0	5	-1	17	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	-3	0	7	0	7	0	0	-4	4	-6	4	-2	0	0	14953	0	0	-16	20	-5	-3	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	-0	0	0	6	-17	23	-9	0	7	0	0	14966	0	8	-15	9	0	-3	5	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	6	0	0	3	-13	15	-3	-5	-5	0	0	0	14879	-13	50	-1	-6	0	-7	0	0	0	0	0	0	0	0	0	0	0	0	0
0	-2	0	0	0	0	0	5	0	-4	1	-1	-3	0	5	-16	8	-13	15069	-4	63	39	-17	7	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	5	-9	20	-5	-3	-1	20	-15	50	-4	14807	-80	119	21	3	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	-9	3	-44	-6	8	17	-5	9	-1	63	-80	14946	0	-3	2	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	-3	0	3	-3	0	-6	39	119	0	14997	-12	11	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	4	-1	-3	10	-1	0	3	-3	0	-17	21	-3	-12	14868	-6	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	-4	0	11	8	0	0	5	-7	7	3	2	11	-6	14795	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	14892	-9	-3	-1	-1	7	12	1	-7	3	0	-0	0
2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-9	14880	-35	64	0	-5	-6	3	19	-16	10	-6	-1
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-3	-35	14932	0	-2	-1	-4	-4	-4	-11	0	14	3
-4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	64	0	14946	0	0	1	5	-2	19	3	-3	0
0	0	7	0	7	0	-6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	0	-2	0	14924	-13	0	-10	16	-2	-0	1	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7	-5	-1	0	-13	15020	32	0	-28	10	0	-8	7
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	12	-6	-4	1	0	32	14943	-12	60	-1	-5	20	-18
-2	0	0	0	0	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	3	-4	5	-10	0	-12	15022	22	62	39	-20	9
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-7	19	-4	-2	16	-28	60	22	14850	-66	0	-2	-7
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	-16	-11	19	-2	10	-1	62	-66	14919	0	-9	7
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	10	0	3	-0	0	-5	39	0	0	14935	-18	8
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-0	-6	14	-3	1	-8	20	-20	-2	-9	-18	14863	-40
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	3	0	0	7	-18	9	-7	7	8	-40	14995

Table S3: Rate matrix of the PSII-cc system (Part 1). unit: ps^{-1}.

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39
-1.55	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.06	0	0	0.07	0	0	0	0
0	-1.61	0	0	0	0	0	0	0	0.02	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.09	0	0	0	0	0.03
0	0	-8.33	0	0	0	0.12	0	1.78	0	0.08	0	0	9.20	0	0	0	0	0	0.30	0	0	0	0.22	0.04	0	1.16	0	0	0	0	0	0	0.02	0	1.44	0.03	0	0
0	0	0	-4.43	0.15	0	0	0	0	0	0	0.05	0.03	0.01	0.37	0.28	0	0	0	0	0	0	0	0	0	1.22	0	0	5.06	0	0.56	0.01	0	0	0	0.03	1.31	0	0
0	0	0	0.13	-20.44	0	0	0	0	0	0	0.03	0.02	0	24.07	0.47	0	0	0	0	0	0	0	0	0	0.14	0	0	0.72	0	3.50	0.03	0	0	0	0.03	0.73	0	0
0	0	0	0	0	-3.34	0	0	0	0	0	0	0	0	0	0	0	0	1.13	0	0	0.69	1.11	0	0	0	0	0	0	0.34	0	0	0	0	0	0	0	0.01	0.83
0	0	0.09	0	0	0	-15.58	0	0.34	0	0.46	0	0	0.23	0	0	0	0	0	20.59	0	0	0	0.08	0.16	0	0.01	0	0	0	0	0	0	0	0	0.03	0	0	0
0	0	0	0	0	0	0	-6.78	0	0	0	0	0	0	0	0	0	0.91	0	0	0.34	0	0	0	0	0	0	1.30	0	0	0	0	2.84	0	0.60	0	0	0	0
0	0	1.18	0	0	0	0.30	0	-4.31	0	0.18	0	0	0.53	0	0	0	0	0	0.42	0	0	0	0.20	0.05	0	0.27	0	0	0	0	0	0	0.02	0	0.38	0.01	0	0
0	0.01	0	0	0	0	0	0	0	-0.09	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.08
0	0	0.05	0	0	0	0.39	0	0.17	0	-6.43	0	0	0.39	0	0	0	0	0	0.69	0	0	0	1.27	0.18	0	0.22	0	0	0	0	0	0	0	0	0.52	0.01	0	0
0	0	0	0.04	0.03	0	0	0	0	0	0	-0.44	0	0	0.01	0.01	0	0	0	0	0	0	0	0	0	0.08	0	0	0.19	0	0.07	0	0	0	0	0	0.06	0	0
0	0	0	0.02	0.01	0	0	0	0	0	0	0	-0.28	0	0.02	0.01	0	0	0	0	0	0	0	0	0	0.04	0	0	0.10	0	0.03	0.01	0	0	0	0	0.02	0	0
0	0	5.27	0.01	0	0	0.18	0	0.46	0	0.34	0	0	-15.55	0	0	0	0	0	0.24	0	0	0	0.38	0.07	0	1.26	0	0	0	0	0	0	0.08	0	2.02	0.04	0	0
0	0	0	0.23	17.27	0	0	0	0	0	0	0.01	0.02	0	-29.63	0.19	0	0	0	0	0	0	0	0	0	0.07	0	0	0.88	0	4.71	0.03	0	0	0	0.04	1.12	0	0
0	0	0	0.16	0.33	0	0	0	0	0	0	0.01	0.01	0	0.18	-8.02	0	0	0	0	0	0	0	0	0	0.05	0	0	0.20	0	1.38	0.01	0	0	0	0.09	4.42	0	0
0.01	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-0.13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.01	0	0.16	0	0	0	0
0	0	0	0	0	0	0	0.73	0	0	0	0	0	0	0	0	0	-11.19	0	0	0.21	0	0	0	0	0	0	0.69	0	0	0	0	1.11	0	0.15	0	0	0	0
0	0	0	0	0	0.69	0	0	0	0	0	0	0	0	0	0	0	0	-23.27	0	0	4.40	14.30	0	0	0	0	0	0	0.48	0	0	0	0.01	0	0	0	2.85	0.17
0	0	0.15	0	0	0	14.01	0	0.33	0	0.55	0	0	0.21	0	0	0	0	0	-22.93	0	0	0	0.09	0.08	0	0.02	0	0	0	0	0	0	0	0	0.06	0	0	0
0	0	0	0	0	0	0	0.26	0	0	0	0	0	0	0	0	0	0.20	0	0	-4.08	0	0	0	0	0	0	0.07	0	0	0	0	0.36	0	0.05	0	0	0	0
0	0	0	0	0	0.39	0	0	0	0	0	0	0	0	0	0	0	0	4.05	0	0	-12.79	2.36	0	0	0	0	0	0	0.51	0	0	0	0.01	0	0	0	1.84	0.45
0	0	0	0	0	0.58	0	0	0	0	0	0	0	0	0	0	0	0	12.16	0	0	2.18	-23.59	0	0	0	0	0	0	0.42	0	0	0	0.01	0	0	0	0.56	0.39
0	0	0.10	0	0	0	0.05	0	0.14	0	0.87	0	0	0.29	0	0	0	0	0	0.07	0	0	0	-6.27	0	0	0.10	0	0	0	0	0	0	0.02	0	0.49	0.02	0	0
0	0	0.02	0	0	0	0.10	0	0.04	0	0.13	0	0	0.06	0	0	0	0	0	0.07	0	0	0	0	-1.27	0	0.24	0	0	0	0	0	0	0.02	0	0.11	0	0	0
0	0	0	0.60	0.08	0	0	0	0	0	0	0.06	0.03	0	0.06	0.04	0	0	0	0	0	0	0	0	0	-2.66	0	0	0.52	0	0.35	0	0	0	0	0	0.13	0	0
0	0	0.52	0	0	0	0.01	0	0.18	0	0.16	0	0	0.99	0	0	0	0	0	0.02	0	0	0	0.11	0.22	0	-4.29	0	0	0	0	0	0	0	0	0.74	0.03	0	0
0	0	0	0	0	0	0	0.79	0	0	0	0	0	0	0	0	0	0.53	0	0	0.05	0	0	0	0	0	0	-7.34	0	0	0	0	1.61	0	0.15	0	0	0	0
0	0	0	2.15	0.35	0	0	0	0	0	0	0.12	0.06	0	0.61	0.14	0	0	0	0	0	0	0	0	0	0.44	0	0	-10.82	0	1.01	0.02	0	0	0	0.04	1.07	0	0
0	0	0	0	0	0.17	0	0	0	0	0	0	0	0	0	0	0	0	0.39	0	0	0.45	0.41	0	0	0	0	0	0	-3.14	0	0	0	0	0	0	0	0.15	0.25
0	0	0	0.21	1.53	0	0	0	0	0	0	0.04	0.02	0	2.86	0.87	0	0	0	0	0	0	0	0	0	0.26	0	0	0.89	0	-22.47	0.01	0	0	0	0.19	6.87	0	0
0.02	0	0	0	0.02	0	0	0	0	0	0	0	0	0	0.02	0	0	0	0	0	0	0	0	0	0	0	0	0	0.02	0	0.01	-2.67	0	0	0	0	0.03	0	0
0	0	0	0	0	0	0	1.42	0	0	0	0	0	0	0	0	0	0.70	0	0	0.23	0	0	0	0	0	0	1.33	0	0	0	0	-32.43	0	0.41	0	0	0	0
0	0.02	0.01	0	0	0	0	0	0.01	0	0	0	0	0.05	0	0	0	0	0.01	0	0	0.01	0	0.01	0.02	0	0	0	0	0	0	0	0	-6.15	0	0.03	0	0.01	0.01
0.02	0	0	0	0	0	0	0.32	0	0	0	0	0	0	0	0	0.09	0.10	0	0	0.04	0	0	0	0	0	0	0.13	0	0	0	0	0.43	0	-3.29	0	0	0	0
0	0	0.47	0.01	0.01	0	0.01	0	0.19	0	0.26	0	0	1.14	0.02	0.05	0	0	0	0.04	0	0	0	0.36	0.07	0	0.53	0	0.03	0	0.18	0	0	0.03	0	-16.37	0.01	0	0
0	0	0.01	0.43	0.28	0	0	0	0	0	0.01	0.03	0.01	0.02	0.59	2.41	0	0	0	0	0	0	0	0.02	0	0.09	0.02	0	0.82	0	5.95	0.02	0	0	0	0.01	-25.34	0	0
0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0	0	0	0	1.87	0	0	1.31	0.43	0	0	0	0	0	0	0.12	0	0	0	0.01	0	0	0	-15.01	0.35
0	0.01	0	0	0	0.31	0	0	0	0.04	0	0	0	0	0	0	0	0	0.10	0	0	0.30	0.28	0	0	0	0	0	0	0.19	0	0	0	0.01	0	0	0	0.33	-25.98
0	0	0	0	0	0	0	0.69	0	0	0	0	0	0	0	0	0	1.06	0	0	0.46	0	0	0	0	0	0	1.54	0	0	0	0	14.44	0	0.45	0	0	0	0
0	0	0	0	0	0	0	0.16	0	0	0	0	0	0	0	0	0	2.89	0	0	0.30	0	0	0	0	0	0	0.30	0	0	0	0	1.65	0	0.12	0	0	0	0
0	0	0.01	0	0	0	0	0	0.01	0	0	0	0	0.07	0	0	0	0	0	0	0	0	0	0.02	0.04	0	0.01	0	0	0	0	0	0	0.35	0	0.02	0.01	0.01	0
0	0	0	0	0	0.71	0	0	0	0.02	0	0	0	0	0	0	0	0	0.40	0	0	0.43	0.66	0	0	0	0	0	0	0.33	0	0	0	0.01	0	0	0	0.44	16.10
0	0	0	0.10	0.04	0	0	0	0	0	0	0.01	0.05	0	0.09	0.04	0	0	0	0	0	0	0	0	0	0.03	0	0	0.14	0	0.23	0.12	0	0	0	0.01	0.30	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0.02	0	0	0.01	0	0	0	0	0	0	0	0	0	0	0	0	0.01	0	0.02	0.14	0	0	0	0	0.02	0	0
0	0	0	0.02	0.11	0	0	0	0	0	0	0.02	0.01	0	0.41	0.08	0	0	0	0	0	0	0	0	0	0.04	0	0	0.05	0	0.20	0.01	0	0	0	0.01	0.14	0	0
0	0	0.14	0	0	0	0.05	0	0.32	0	0.02	0	0	1.59	0	0	0	0	0	0.16	0	0	0	0.04	0.05	0	0.03	0	0	0	0	0	0	0.13	0	0.08	0.01	0	0
0	0	0	0	0	0	0	1.35	0	0	0	0	0	0	0	0	0	0.41	0	0	0.38	0	0	0	0	0	0	0.91	0	0	0	0	3.55	0	0.24	0	0	0	0
0	0	0	0	0	0	0	0.11	0	0	0	0	0	0	0	0	0	4.04	0	0	0.31	0	0	0	0	0	0	0.15	0	0	0	0	0.61	0	0.12	0	0	0	0
0	0	0	0.04	0.06	0	0	0	0	0	0	0.01	0	0	0.17	3.18	0	0	0	0	0	0	0	0	0	0.03	0	0	0.38	0	2.23	0.01	0	0	0	0.05	1.73	0	0
0	0	0	0	0	0.03	0	0	0	0	0	0	0	0	0	0	0	0	0.46	0	0	1.57	1.20	0	0	0	0	0	0	0.11	0	0	0	0	0	0	0	0.95	1.67
0	0	0	0	0	0	0	0.42	0	0	0	0	0	0	0	0	0	0.18	0	0	1.25	0	0	0	0	0	0	0.30	0	0	0	0	1.20	0	0.13	0	0	0	0
0	0	0.03	0	0	0	0.16	0	0.09	0	3.12	0	0	0.07	0	0	0	0	0.02	0.06	0	0.01	0.01	0.23	0.02	0	0.02	0	0	0	0	0	0	0	0	0.29	0.01	0.05	0.01
0	0	0	0	0	0.02	0	0	0	0	0.01	0	0	0	0	0	0	0	1.73	0	0	0.61	0.97	0	0	0	0	0	0	0.26	0	0	0	0.04	0	0	0	7.15	0.88
0	0	0	0	0	0.10	0	0	0	0	0	0	0	0	0	0	0	0	0.12	0	0	0.13	0.19	0	0	0	0	0	0	0.19	0	0	0	0.03	0	0	0	0.26	4.14
0	0	0	0	0	0	0	0.37	0	0	0	0	0	0	0	0	0	0.08	0	0	0.04	0	0	0	0	0	0	0.24	0	0	0	0	2.25	0	0.45	0	0	0	0
0	0.01	0	0	0	0	0	0	0	0	0	0	0	0.01	0	0	0	0	0.01	0	0	0	0.01	0	0.01	0	0	0	0	0.01	0	0	0	4.85	0	0.01	0	0.06	0.03
0	0	0.08	0	0	0	0.02	0	0.13	0	0.02	0	0	0.43	0	0	0	0	0	0.07	0	0	0	0.01	0.02	0	0.04	0	0	0	0	0	0	0.10	0	0.35	0.01	0	0
0	0	0.15	0.03	0	0	0.01	0	0.09	0	0.01	0	0	0.17	0	0.01	0	0	0	0.02	0	0	0	0.16	0.02	0	0.09	0	0.04	0	0.06	0	0	0.01	0	3.94	0.31	0	0
0.01	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.01	1.98	0	0	0	0	0.01	0	0
0	0	0.02	0.20	0.01	0	0	0	0.01	0	0	0.02	0	0.01	0.02	0.05	0	0	0	0	0	0	0	0.02	0	0.02	0.01	0	0.48	0	0.54	0.01	0	0	0	0.33	2.49	0	0
0	0.01	0	0	0	0.03	0	0	0	0	0	0	0	0	0	0	0	0	0.46	0	0	0.24	0.94	0	0	0	0	0	0	0.04	0	0	0	0.02	0	0	0	0.27	0.34
0	0	0	0	0	0	0	0.15	0	0	0	0	0	0	0	0	0	0.08	0	0	0.46	0	0	0	0	0	0	0.36	0	0	0	0.01	2.34	0	0.15	0	0	0	0
0	0	0.01	0	0	0	0	0	0.01	0	0.18	0	0	0.03	0	0	0	0	0	0	0	0	0	2.96	0.22	0	0.15	0	0	0	0	0	0	0	0	0.39	0.01	0	0
0	0.10	0	0	0	0.01	0	0	0	0	0	0	0	0	0	0	0	0	0.05	0	0	0.02	0.09	0	0	0	0	0	0	0	0	0	0	0.24	0	0	0	0.02	0.07
0	0	0	0	0	0.29	0	0	0	0	0	0	0	0	0	0	0	0	0.30	0	0	0.43	0.61	0	0	0	0	0	0	0.14	0	0	0	0	0	0	0	0.04	0.18
0.07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.01	0.13	0.02	0	0.02	0	0.09	0	0
0	0	0	0.02	0.01	0	0	0	0	0	0	0	0	0	0	0.03	0	0	0	0	0	0	0	0	0	0.09	0	0	0.14	0	0.36	0.01	0	0	0	0.22	3.41	0	0
0	0	0.02	0	0	0	0	0	0.01	0	0.01	0	0	0.03	0	0	0	0	0	0.01	0	0	0	0.07	0.01	0	0.10	0	0	0	0.01	0	0	0	0	4.36	0.24	0	0
0	0	0	0.01	0.02	0	0	0	0	0	0	0	0	0	0.06	0.14	0	0	0	0	0	0	0	0	0	0.02	0	0	0.12	0	0.66	0.01	0	0	0	0.01	0.49	0	0
0	0	0	0	0.14	0	0	0	0	0	0	0	0	0	0.06	0.01	0	0	0	0	0	0	0	0	0	0.02	0	0	0.02	0	0.39	0	0	0	0	0	0.13	0	0
0	0	0	0	0	0	0.17	0	0	0	0	0	0	0.01	0	0	0	0	0	0.18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.04	0	0	0
0	0.01	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.04	0	0	0	0	0
0.01	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.04	0	0	0	0	0	0	0
0	1.43	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1.43	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table S4: Rate matrix of the PSII-cc system (Part 2). unit: ps^{-1}.

40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	$RP1_{M1}$	$RP2_{M1}$	$RP1_{M2}$	$RP2_{M2}$
0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.09	0	0	0.01	0	0	0	0.71	0.01	0	0	0	0	0	0.19	0	0	0	0
0	0	0.02	0.02	0	0	0	0	0	0	0	0	0	0	0	0	0	0.11	0	0	0	0	0.05	0	0	0.93	0	0	0	0	0	0	0	0.20	0	0	0	0	0
0	0	0.03	0	0	0	0	0.52	0	0	0	0	0	0.12	0	0	0	0	0.49	0.92	0	0.10	0	0	0.09	0	0	0	0	0.11	0	0	0.03	0	0	0	0	0	0
0	0	0	0	0.29	0.01	0.07	0	0	0	0.19	0	0	0	0	0	0	0	0	0.19	0	1.25	0	0	0	0	0	0.01	0.13	0.01	0.11	0.05	0	0	0	0	0	0	0
0	0	0	0	0.12	0	0.29	0	0	0	0.22	0	0	0	0	0	0	0	0	0.01	0	0.07	0	0	0	0	0	0	0.03	0	0.13	1.16	0	0	0	0	0	0	0
0	0	0	2.04	0	0	0	0	0	0	0	0.12	0	0	0.08	0.42	0	0	0	0	0	0	0.16	0	0	0.06	1.76	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0.14	0	0	0	0	0	0.56	0	0	0	0	0.08	0.02	0	0	0	0	0.01	0	0	0	0	0.02	0	0	1.37	0	0	0	0	0	0
1.56	0.34	0	0	0	0	0	0	3.75	0.32	0	0	1.34	0	0	0	1.23	0	0	0	0	0	0	0.68	0	0	0	0.01	0	0	0	0	0	0	0	0	0	0	0
0	0	0.02	0	0	0	0	0.79	0	0	0	0	0	0.28	0	0	0	0.01	0.50	0.37	0	0.03	0	0	0.06	0	0	0	0	0.05	0	0	0.03	0	0	0	0	0	0
0	0	0	0.05	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0.06	0	0	0	0	0	9.26	0.04	0	0	0.01	0.06	0.05	0	0.01	0	0	0.78	0	0	0	0	0.05	0	0	0.03	0	0	0	0	0	0
0	0	0	0	0.03	0.01	0.05	0	0	0	0.03	0	0	0	0	0	0	0	0	0.01	0	0.08	0	0	0	0	0	0	0.02	0	0.03	0	0	0	0	0	0	0	0
0	0	0	0	0.11	0.03	0.01	0	0	0	0.01	0	0	0	0	0	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0
0	0	0.12	0	0	0	0	3.44	0	0	0	0	0	0.19	0	0	0	0.02	1.45	0.59	0	0.05	0	0	0.10	0	0	0	0	0.12	0	0	0.07	0	0	0	0	0	0
0	0	0	0	0.17	0	0.80	0	0	0	0.46	0	0	0	0	0	0	0	0	0.01	0	0.06	0	0	0	0	0	0	0.02	0	0.29	0.37	0	0	0	0	0	0	0
0	0	0	0	0.08	0.02	0.15	0	0	0	8.19	0	0	0	0	0	0	0	0	0.02	0	0.16	0	0	0	0	0	0.01	0.13	0.01	0.69	0.03	0	0	0	0	0	0	0
0.01	0.01	0	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0	0	0
1.92	4.94	0	0	0	0	0	0	0.90	9.39	0	0	0.45	0	0	0	0.23	0	0	0	0.01	0	0	0.28	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0.70	0	0	0	0	0	0	0	1.09	0	0.04	4.30	0.30	0	0.04	0	0	0	0	1.49	0	0	0.17	1.14	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0.30	0	0	0	0	0	0.15	0	0	0	0	0.20	0.06	0	0	0	0	0.01	0	0	0	0	0.02	0	0	0.96	0	0	0	0	0	0
0.80	0.48	0	0	0	0	0	0	0.79	0.68	0	0	3.04	0	0	0	0.11	0	0	0	0	0	0	1.54	0	0	0	0.01	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0.70	0	0	0	0	0	0	0	3.38	0	0.02	1.38	0.31	0	0.01	0	0	0	0	0.72	0	0	0.07	1.50	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0.99	0	0	0	0	0	0	0	2.39	0	0.02	2.05	0.40	0	0.02	0	0	0	0	2.59	0	0	0.25	1.95	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0.03	0	0	0	0	0.07	0	0	0	0	0	0.47	0	0	0	0	0.02	0.43	0	0.06	0	0	8.68	0	0	0	0.01	0.24	0	0	0.01	0	0	0	0	0	0
0	0	0.06	0	0	0	0	0.09	0	0	0	0	0	0.05	0	0	0	0.01	0.06	0.05	0	0.01	0	0	0.70	0	0	0	0	0.02	0	0	0.01	0	0	0	0	0	0
0	0	0	0	0.05	0	0.06	0	0	0	0.07	0	0	0	0	0	0	0	0	0.01	0	0.06	0	0	0	0	0	0.01	0.32	0.01	0.09	0.07	0	0	0	0	0	0	0
0	0	0.01	0	0	0	0	0.06	0	0	0	0	0	0.03	0	0	0	0	0.10	0.24	0	0.02	0	0	0.43	0	0	0	0.01	0.35	0	0	0.02	0	0	0	0	0	0
2.13	0.39	0	0	0	0	0	0	1.53	0.26	0	0	0.57	0	0	0	0.49	0	0	0	0	0	0	0.95	0	0	0	0.01	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0.18	0.01	0.06	0	0	0	0.69	0	0	0	0	0	0	0	0	0.11	0	1.25	0	0	0	0	0	0.01	0.43	0.01	0.41	0.09	0	0	0	0	0	0	0
0	0	0	0.47	0	0	0	0	0	0	0	0.21	0	0	0.52	0.39	0	0.01	0	0	0	0	0.11	0	0	0.01	0.42	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0.27	0.02	0.24	0	0	0	3.62	0	0	0	0	0	0	0	0	0.13	0.02	1.24	0	0	0	0	0	0.04	0.97	0.03	2.08	1.39	0	0	0	0	0	0	0
0	0	0	0	0.15	0.17	0.01	0	0	0	0.02	0	0	0	0	0	0	0	0	0	4.70	0.02	0	0.02	0	0	0	0.36	0.04	0	0.02	0.01	0	0	0.37	0	0	0	0
16.44	1.77	0	0	0	0	0	0	4.93	0.89	0	0	1.91	0	0	0	3.77	0	0	0	0	0	0	5.11	0	0	0	0.06	0	0	0	0	0	0	0	0	0	0	0
0	0	0.39	0.01	0	0	0	0.18	0	0	0	0.01	0	0.01	0.07	0.05	0	9.45	0.23	0.01	0	0	0.06	0	0	0.57	0	0	0	0.01	0	0	0	0.34	0	0	0	0	0	0
0.55	0.14	0	0	0	0	0	0	0.35	0.18	0	0	0.22	0	0	0	0.80	0	0	0	0.01	0	0	0.35	0	0	0	0.05	0	0	0	0	0	0	0	0	0	0	0
0	0	0.02	0	0.01	0	0.01	0.10	0	0	0.07	0	0	0.43	0.01	0	0	0.02	0.67	7.83	0	0.68	0	0	0.83	0	0	0.01	0.53	10.76	0.04	0.01	0.15	0	0	0	0	0	0
0	0	0.01	0	0.30	0.02	0.15	0.01	0	0	2.44	0	0	0.02	0	0	0	0	0.03	0.58	0.02	4.91	0	0	0.03	0	0	0.20	7.95	0.55	1.34	0.40	0	0	0	0	0	0	0
0	0	0.01	0.50	0	0	0	0	0	0	0	1.45	0	0.08	11.62	0.43	0	0.11	0	0	0	0	0.58	0	0	0.04	0.09	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	17.35	0	0	0	0	0	0	0	2.39	0	0.01	1.34	6.41	0	0.04	0	0	0	0	0.68	0	0	0.14	0.42	0	0	0	0	0	0	0	0	0	0	0	0	0
-38.62	0.72	0	0	0	0	0	0	7.16	3.04	0	0	4.23	0	0	0	2.30	0	0	0	0.01	0	0	3.03	0	0	0	0.03	0	0	0	0	0	0	0	0	0	0	0
0.76	-13.39	0	0	0	0	0	0	1.15	4.01	0	0	0.41	0	0	0	0.26	0	0	0	0.01	0	0	0.62	0	0	0	0.01	0	0	0	0	0	0	0	0	0	0	0
0	0	-1.59	0	0	0	0	0.10	0	0	0	0	0	0.02	0.01	0.01	0	0.86	0.32	0.07	0	0.01	0	0	0.01	0.03	0	0	0	0.05	0	0	0.01	0.08	0	0	0	0	0	0
0	0	0	-31.13	0	0	0	0	0	0	0	3.03	0	0.01	1.56	5.03	0	0.04	0	0	0	0	1.13	0	0	0.15	1.46	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	-2.49	0.01	0.01	0	0	0	0.09	0	0	0	0	0	0	0	0	0.03	0.14	0.31	0	0	0	0	0	0.04	0.63	0.02	0.10	0.15	0	0	0.01	0	0	0	0
0	0	0	0	0.01	-0.83	0.01	0	0	0	0.01	0	0	0	0	0	0	0	0	0	0.71	0.03	0	0	0	0	0	0.08	0.04	0	0.01	0	0	0	0.08	0	0	0	0
0	0	0	0	0.01	0.01	-2.80	0	0	0	0.18	0	0	0	0	0	0	0	0	0.03	0	0.27	0	0	0	0	0	0.01	0.31	0.01	0.19	1.03	0	0	0	0	0	0	0
0	0	0.08	0	0	0	0	-16.83	0	0	0	0	0	0.31	0	0	0	0.21	14.94	0.80	0	0.04	0	0	0.12	0.02	0	0	0.01	0.28	0	0	1.00	0.01	0	0	0	0	0
5.88	0.89	0	0	0	0	0	0	-32.95	1.24	0	0	8.61	0	0	0	1.21	0	0	0	0.01	0	0	4.22	0	0	0	0.04	0	0	0	0	0	0	0	0	0	0	0
2.38	2.95	0	0	0	0	0	0	1.18	-22.04	0	0	0.70	0	0	0	0.17	0	0	0	0.02	0	0	1.78	0	0	0	0.04	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0.06	0.01	0.14	0	0	0	-25.89	0	0	0	0	0	0	0	0	0.26	0.01	2.62	0	0	0	0	0	0.07	2.39	0.10	10.56	1.10	0	0	0	0	0	0	0
0	0	0	2.28	0	0	0	0	0	0	0	-25.10	0	0.05	1.93	1.34	0	0.05	0	0	0	0	9.45	0	0	0.66	0.95	0	0	0	0	0	0	0	0	0	0	0	0
3.02	0.28	0	0	0	0	0	0	7.49	0.64	0	0	-26.58	0	0	0	0.66	0	0	0	0.01	0	0	6.01	0	0	0	0.11	0	0	0	0	0	0	0	0	0	0	0
0	0	0.01	0.01	0	0	0	0.25	0	0	0	0.05	0	-13.37	0	0.01	0	0.01	0.23	0.32	0	0.06	0.01	0	0.70	0	0	0	0.01	0.19	0	0	0.30	0	0	0	0	0	0
0	0	0.01	1.10	0	0	0	0	0	0	0	1.82	0	0	-27.13	0.82	0	0.04	0.01	0.01	0	0	1.30	0	0.02	0.15	0.34	0	0	0	0	0	0	0.02	0	0	0	0	0
0	0	0.01	3.50	0	0	0	0	0	0	0	1.24	0	0.01	0.80	-17.34	0	0.01	0	0	0	0	1.16	0	0	0.15	0.56	0	0	0	0	0	0	0.03	0	0	0	0	0
1.56	0.17	0	0	0	0	0	0	1.00	0.15	0	0	0.63	0	0	0	-11.59	0	0	0	0	0	0	0.46	0	0	0	0.01	0	0	0	0	0	0	0	0	0	0	0
0	0	0.49	0.02	0	0	0	0.15	0	0	0	0.05	0	0.01	0.04	0.01	0	-15.05	0.03	0.01	0	0	0.60	0	0	2.07	0.03	0	0	0.01	0	0	0.02	5.72	0	0	0	0	0	0
0	0	0.16	0	0	0	0	9.45	0	0	0	0	0	0.18	0.01	0	0	0.03	-21.67	0.25	0	0.11	0	0	0.14	0.02	0	0	0.06	0.66	0	0	2.06	0.05	0	0	0	0	0
0	0	0.03	0	0.01	0	0.02	0.49	0	0	0.20	0	0	0.24	0.01	0	0	0.01	0.24	-16.96	0	0.07	0	0	0.37	0	0	0.01	0.42	2.61	0.31	0.09	0.71	0	0	0	0	0	0
0	0	0	0	0.08	0.38	0	0	0	0.01	0	0	0.01	0	0	0	0	0	0	0	-10.55	0	0	0.15	0	0	0	3.03	0.32	0.01	0.01	0	0	0	6.13	0	0	0	0
0	0	0	0	0.16	0.01	0.14	0.02	0	0	1.87	0	0	0.04	0	0	0	0	0.10	0.07	0	-18.99	0	0	0.13	0	0	0.09	2.51	0.48	2.78	0.91	0.06	0	0	0	0	0	0
0	0	0	0.61	0	0	0	0	0	0	0	6.81	0	0.01	0.99	0.91	0	0.50	0	0	0	0	-22.42	0	0	0.16	2.46	0	0	0	0	0	0	0.07	0	0	0	0	0	0
1.58	0.31	0	0	0	0	0	0	2.68	1.19	0	0	4.38	0	0	0	0.35	0	0	0	0.14	0	0	-25.31	0	0	0	0.08	0.02	0	0	0	0	0	0.03	0	0	0	0
0	0	0	0	0	0	0	0.07	0	0	0	0	0	0.49	0.02	0	0	0	0.12	0.35	0	0.13	0	0	-13.64	0	0	0	0.07	0.32	0	0	0.10	0	0	0	0	0	0
0	0	0.02	0.08	0	0	0	0.01	0	0	0	0.47	0	0	0.11	0.11	0	1.68	0.02	0	0	0	0.15	0	0	-6.14	0.27	0	0	0	0	0	0	0.73	0	0	0	0	0	0
0	0	0	0.68	0	0	0	0	0	0	0	0.60	0	0	0.22	0.38	0	0.02	0	0	0	0	2.13	0	0	0.24	-13.36	0	0	0	0	0	0	0	0	0	0	0	0	0
0.01	0	0	0	0.02	0.04	0	0	0.02	0.02	0.04	0	0.07	0	0	0	0.01	0	0	0.01	2.52	0.08	0	0.07	0	0	0	-5.63	0.01	0.06	0.04	0.04	0	0	1.18	0	0	0	0
0	0	0	0	0.27	0.02	0.14	0.01	0	0	1.44	0	0	0.01	0	0	0	0	0.04	0.34	0.25	2.13	0	0.02	0.06	0	0	0.01	-18.26	0.01	0.46	0.46	0.04	0	0.06	0	0	0	0
0	0	0.02	0	0.01	0	0.01	0.14	0	0	0.06	0	0	0.12	0	0	0	0.01	0.52	2.10	0	0.40	0	0	0.28	0	0	0.06	0.01	-17.50	0.05	0.04	0.32	0	0	0	0	0	0
0	0	0	0	0.04	0	0.07	0	0	0	5.47	0	0	0	0	0	0	0	0	0.21	0	2.02	0	0	0	0	0	0.04	0.40	0.04	-20.07	0.35	0	0	0	0	0	0	0
0	0	0	0	0.05	0	0.35	0	0	0	0.50	0	0	0	0	0	0	0	0	0.06	0	0.58	0	0	0	0	0	0.03	0.35	0.03	0.31	-7.79	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0.36	0	0	0	0	0	0.13	0	0	0	0.01	1.17	0.41	0	0.04	0	0	0.06	0	0	0	0.03	0.23	0	0	-7.29	0	0	0	0	0	0
0	0	0.01	0	0	0	0	0	0	0	0	0	0	0	0.01	0.01	0	1.36	0.01	0	0	0	0.02	0	0	0.22	0	0	0	0	0	0	0	-7.28	0	0	0	0	0
0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.51	0	0	0.01	0	0	0	0.35	0.02	0	0	0	0	0	-8.06	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.33	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.33	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

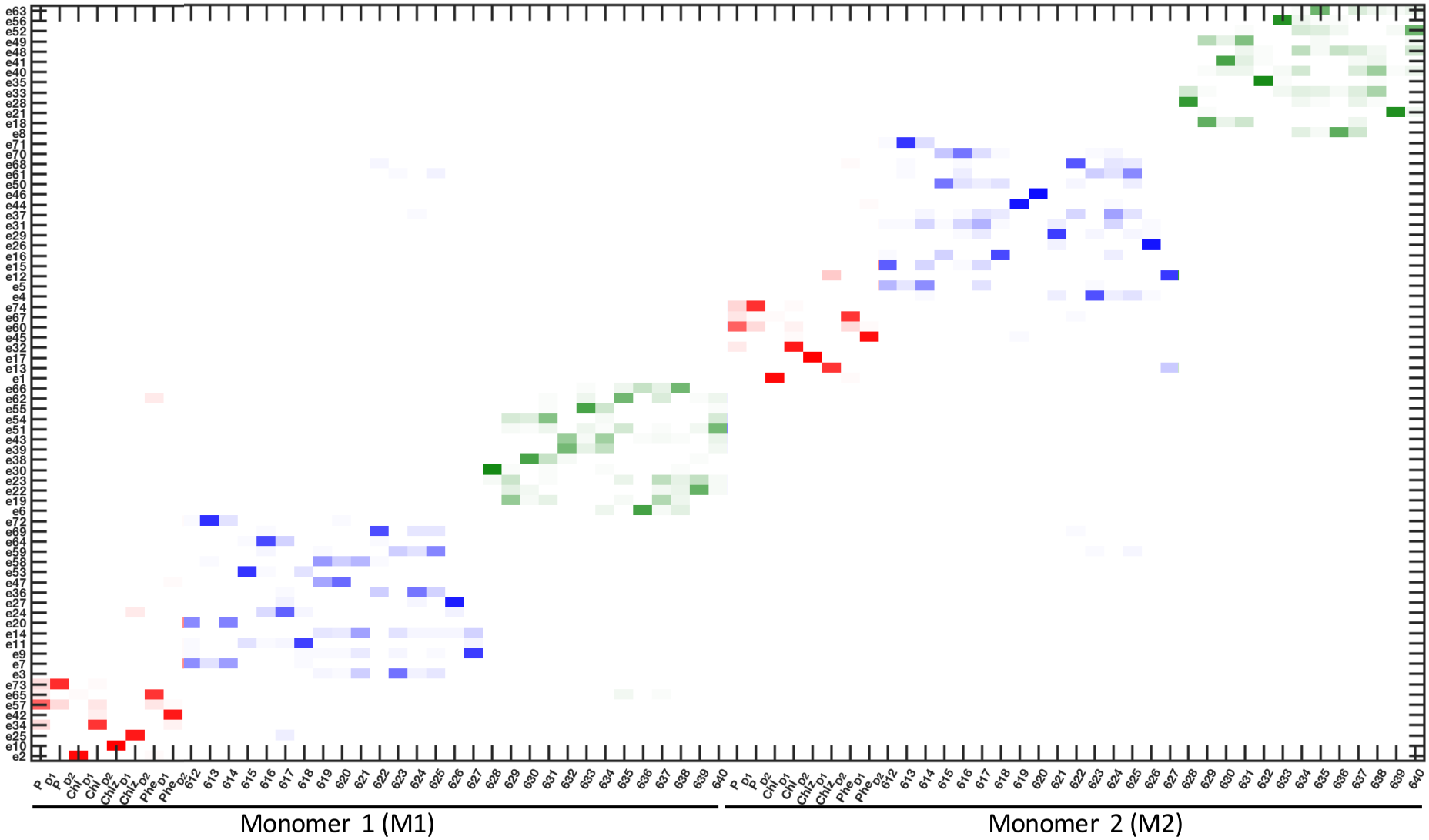

Figure S2: Illustration of the exciton states in the dimeric PSII-cc. Here, X axis labels each pigment in the PSII-cc (from left to right: pigments in RC(M1) , CP47(M1), CP43(M1), RC(M2) , CP47(M2) and CP43(M2)), and Y axis is the label of exciton states. The exciton states are labeled in ascending energy: the lowest-energy exciton state is labeled as e1 and the highest-energy state is labeled as e74. Colored map show the contribution, $|C_n^\alpha|^2$, of pigment n in exciton state α. Red color shows the contributions of pigments in the RC. Blue is the contributions of pigments in the CP47. Green is the contribution of pigments in the CP43. The scale of the contribution is from 0 to 1: the darker the color, the larger the value.

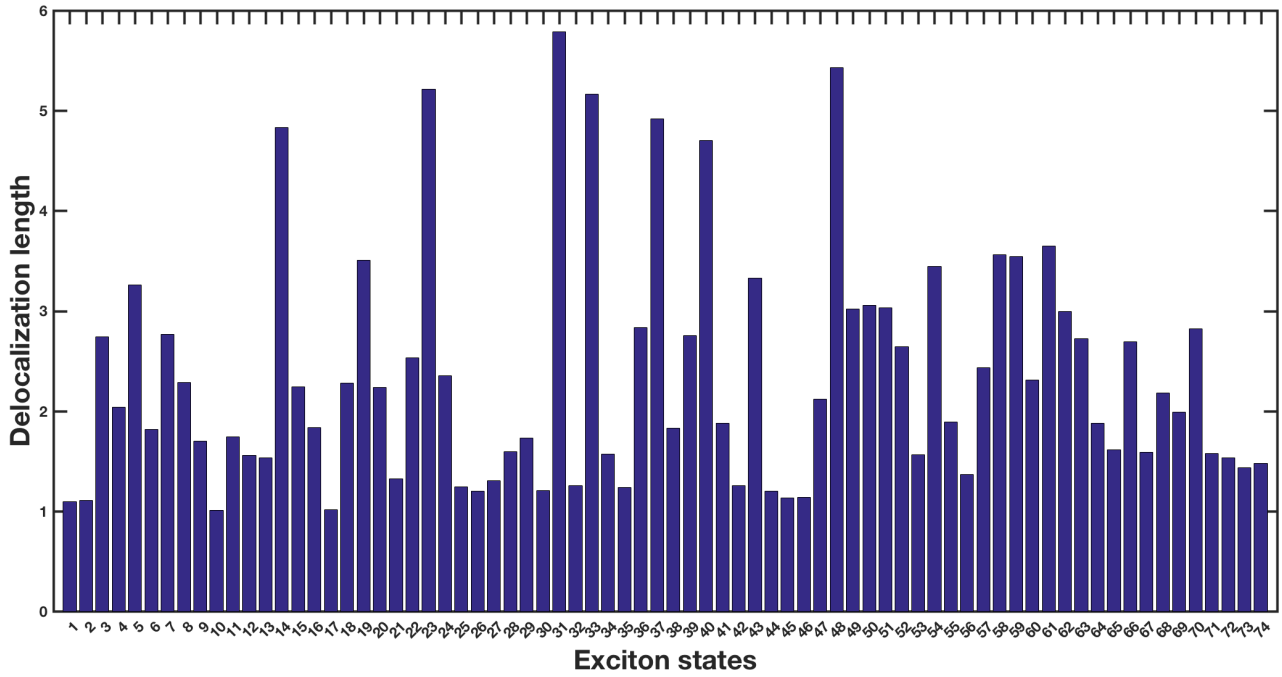

Figure S3: Delocalization length of exciton states. This bar chart shows the delocalization length of each exciton state in PSII-cc. The delocalization length is measured as the inversed participation ratio $L_\alpha = (\sum_n |C_n^\alpha|^4)^{-1}$, where C_n^α is the coefficient of the n-th pigment in the α-th exciton ($|\alpha\rangle = \sum_n C_n^\alpha |n\rangle$). The delocalization length quantifies the degree of delocalization for an exciton state.

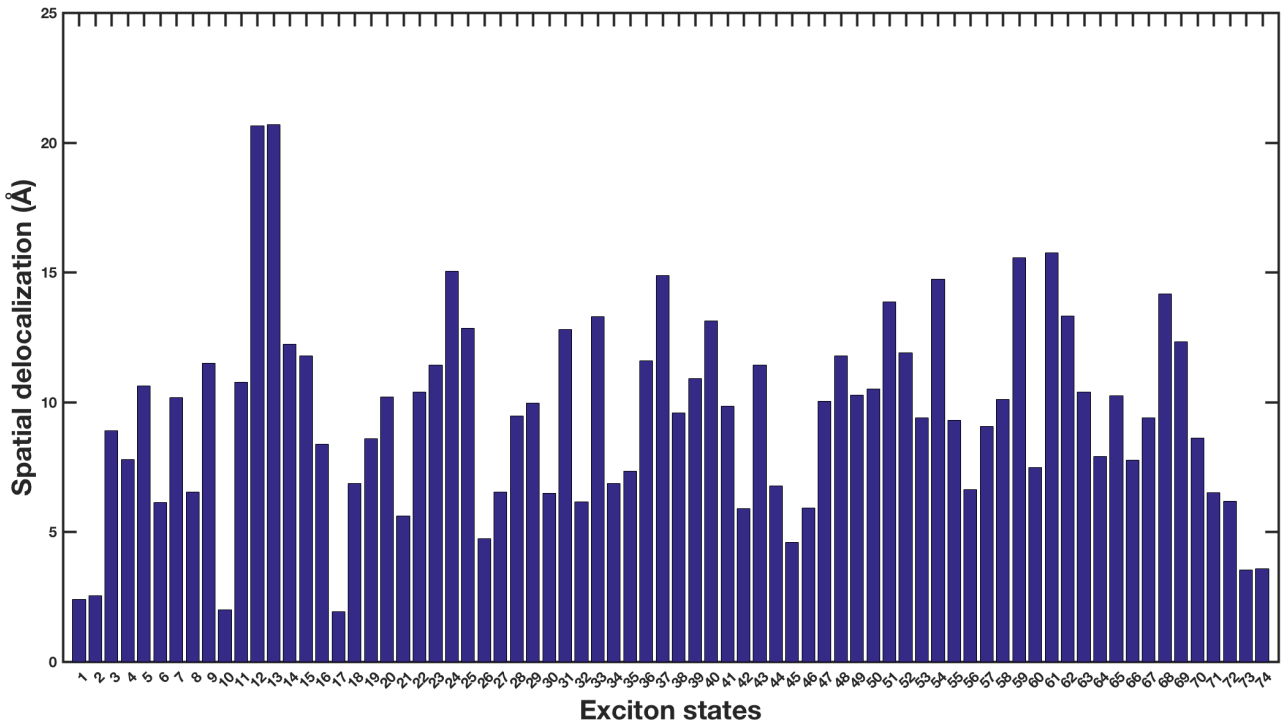

Figure S4: Spatial delocalization of exciton states. This bar chart shows the spatial delocalization distance of each exciton state in PSII-cc. The spatial delocalization for an exciton state $|\alpha\rangle = \sum_n C_n^\alpha |n\rangle$ is calculated as $\boldsymbol{\sigma}_{\boldsymbol{R}}^{\boldsymbol{\alpha}} = \sqrt{\sum_n |C_n^\alpha|^2 (\boldsymbol{R_n} - \boldsymbol{R}^{\boldsymbol{\alpha}})^2}$ where the position of the exciton state $\boldsymbol{R}^{\boldsymbol{\alpha}} = \sum_n |C_n^\alpha|^2 \boldsymbol{R_n}$, with $\boldsymbol{R_n}$ the Mg center of the n-th pigment.

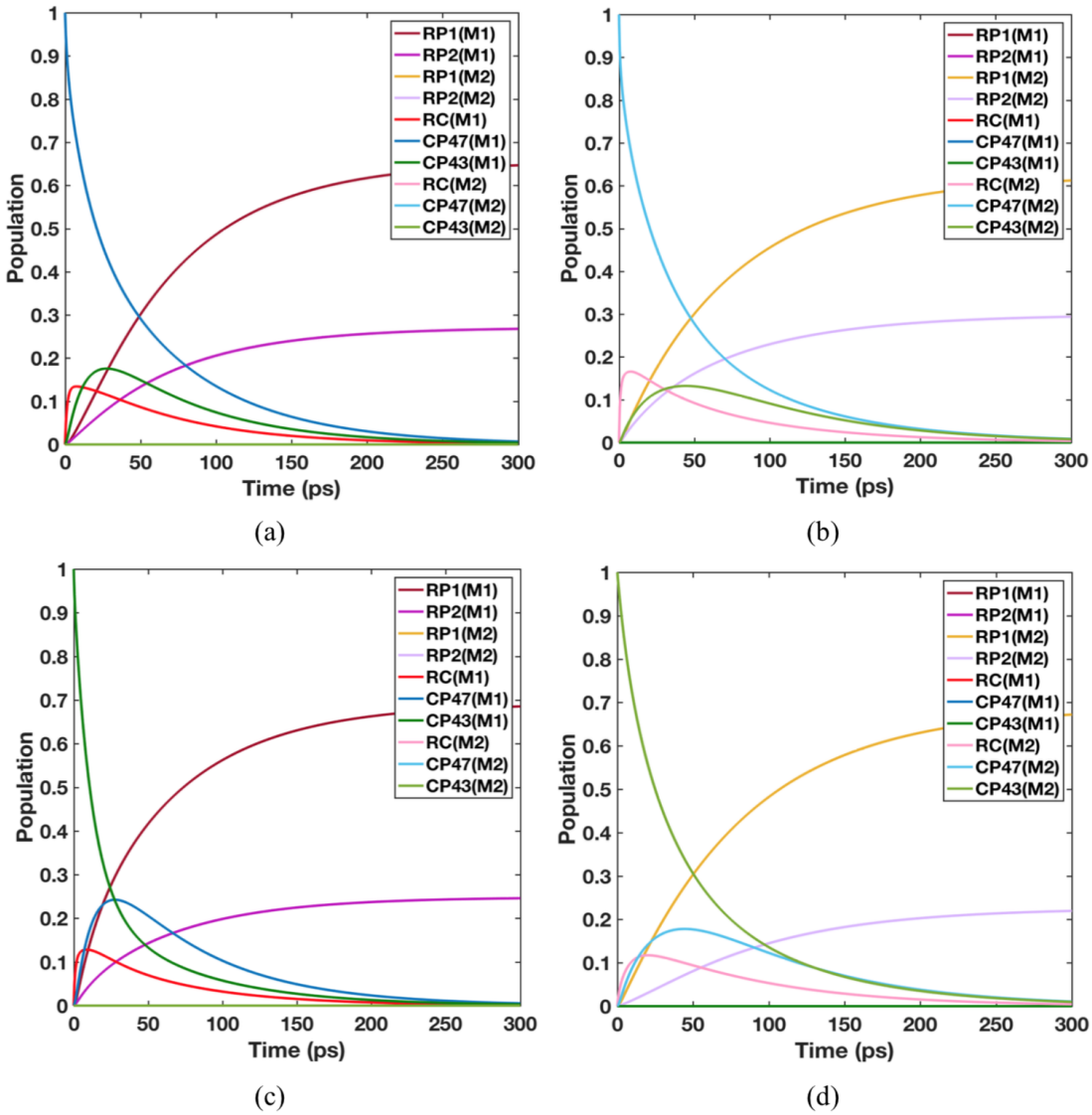

Figure S5: EET dynamics in the mutant PSII-cc without CLA625s. (a) EET dynamics with initial excitation at the CP47 of the M1. The quantum yield of charge separation: RP1(M1) is 0.66; RP2(M1) is 0.27. (b) EET dynamics with initial excitation at the CP47 of the M2. The quantum yield of charge separation: RP1(M2) is 0.63; RP2(M2) is 0.30. (c) EET dynamics with initial excitation at the CP43 of the M1. The quantum yield of charge separation: RP1(M1) is 0.69; RP2(M1) is 0.25. (d) EET dynamics with initial excitation at the CP43 of the M2. The quantum yield of charge separation: RP1(M2) is 0.69; RP2(M2) is 0.23.

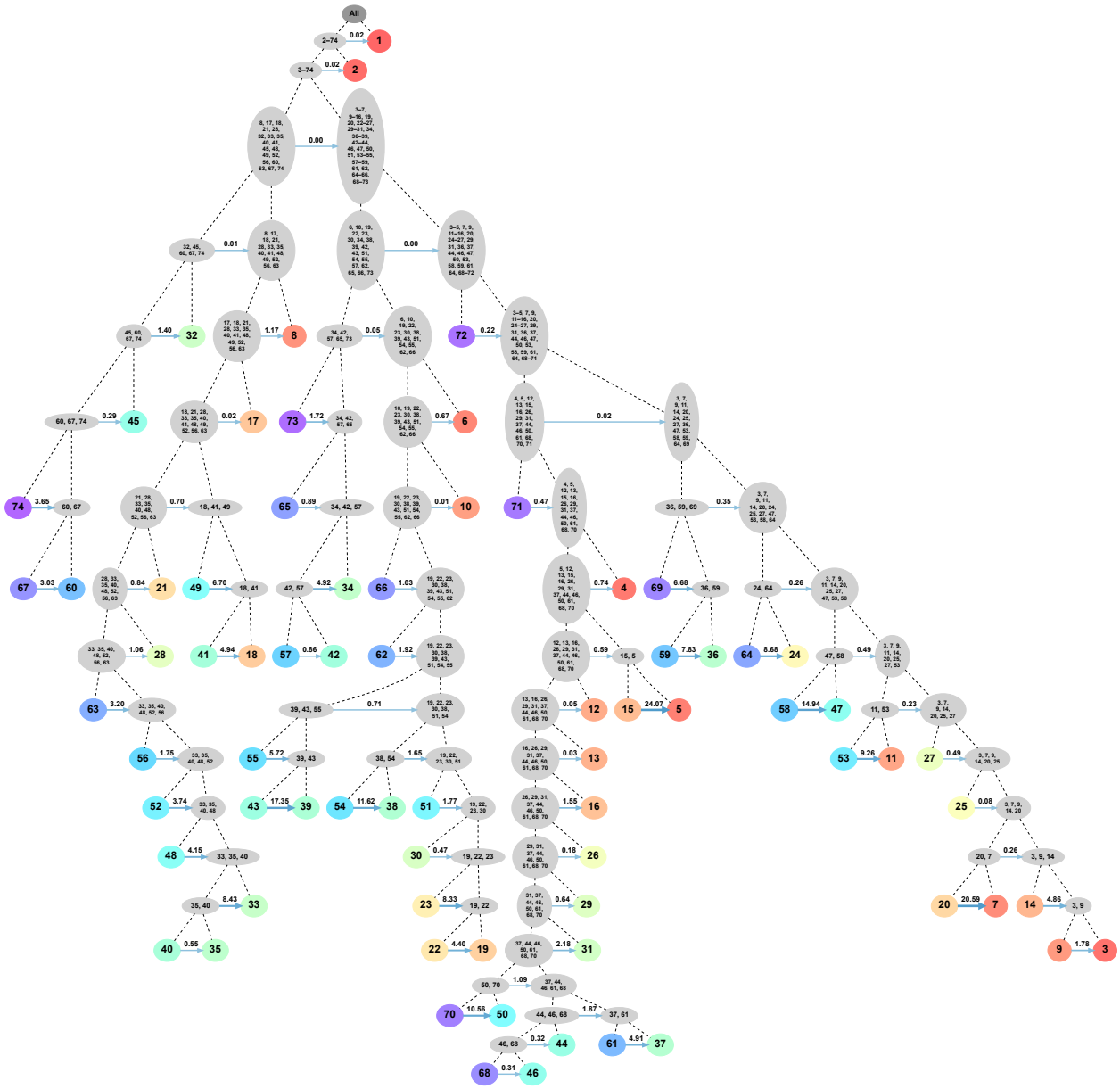

Figure S6: The minimum-cut tree for the EET dynamics in the PSII-cc. The integers inside each oval indicate the exciton states belonging to that cluster, whereas the arrows depict the maximum flow. Colored ovals emphasize the end of the division because the cluster contains only a single state. The tree is arranged such that the source side at each division is on the left and the target side is on the right.

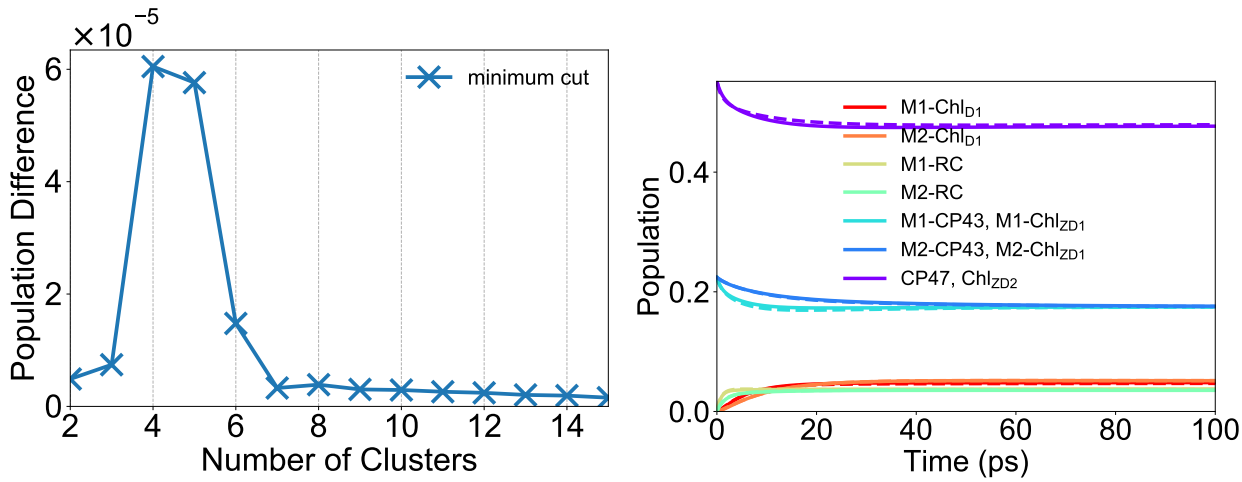

Figure S7: Validation of the coarse-grained kinetic model for the PSII-cc. (a) The integrated population difference between the CG model and the full dynamics as a function of the number of clusters employed in the CG model. (b) The comparison of the CG dynamics and the dynamicxs of the full model for the 7-cluster CG model. Both CP43 and CP47 are uniformally excited initially to mimic the dynamics in natural photosynthesis.