

Detail Analysis for Energy Transfer and Pigment Assembling in C-Phycocyanin through Time-Resolved Spectroscopy and AlphaFold2

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Supplementary Figures:

C-PC α subunit	1-30	MKTPLTEAVS	VADSQGRFLS	STEIQVAFGR
	31-60	FRQAKAGLEA	AKALTSKADS	LISGAAQAVY
	61-90	NKFPYTTQMQ	GPNYAADQRG	KDKCARDIGY
	91-120	YLRMVTYCLI	AGGTGPMDEY	LIAGIDEINR
	121-150	TFELSPSWYI	EALKYIKANH	GLSGDAAVEA
	151-162	NSYLDYAINA	LS	
C-PC β subunit	1-30	MFDAFTKVVS	QADTRGEMLS	TAQIDALSQM
	31-60	VAESNKRLDV	VNRITSNAST	IVSNAARSLF
	61-90	AEQPQLIAPG	GNAYTSRRMA	ACLRLDMEIIL
	91-120	RYVTYAVFAG	DASVLEDRLCL	NGLRETYLAL
	121-150	GTPGSSVAVG	VGKMKEAALA	IVNDPAGITP
	151-172	GDLSALASEI	AGYFDRAAAA	VS

Figure S1. Alignment of the C-PC amino-acid sequences of the α -subunit and β -subunit from *S. platensis* (Protein Data Bank in Europe No. P13530 & P06539).

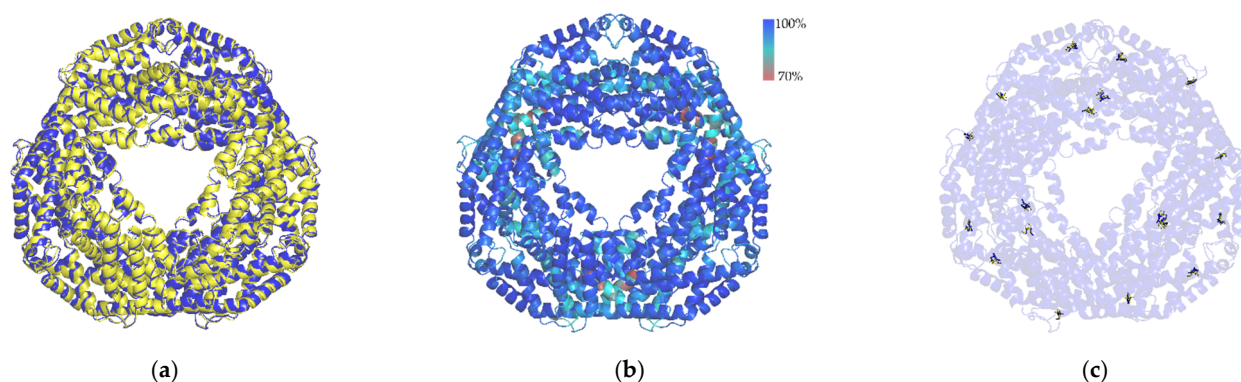


Figure S2. Comparison between computational structure and crystallographic structure based on AlphaFold2. (a) the AlphaFold2 model was aligned with the crystallographic model, (b) C-PC hexamer structure stained with pLDDT (confidence level), (c) the position and overlap of cysteine in crystallography and AlphaFold2.

Supplementary Tables:

Table S1. The deconvolution results of C-PC hexamer. Excitation was done at 570nm.

E_{em}/nm	τ_1/ps	A₁/%	τ_2/ps	A₂/%	τ_3/ps	A₃/%	τ_4/ps	A₄/%
630	5.3	40	16	46.7	197	11.2	1799	2
640	10.8	32.6	24.2	42.9	299.3	22.1	1980	2.4
650	8.7	-22.7	21	4.3	204	53.5	1040	42
660	6.1	-26	24	-5.7	331.8	43.5	1850	56.5
670	4.5	-18	27.7	-5.4	251.7	32.2	1498	67.8
680	4.6	-21.2	26.4	-4.7	232.8	43	1559.7	57
690	6.3	-26.6	17.3	-4.8	215.9	53.7	1231.5	46.3
	7		22		250		1560	

The component (A%) with a negative pre-exponential factor corresponds to the rising process of the fluorescence which indicate an energy acceptor, and the component with a positive pre-exponential corresponds to the decay process of the fluorescence which indicate an energy donor.