Science Advances
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Supplementary Materials for

Structure of cyanobacterial phycobilisome core revealed by structural modeling and chemical cross-linking

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Published 6 January 2021, *Sci. Adv.* **7**, eaba5743 (2021)
DOI: 10.1126/sciadv.aba5743

This PDF file includes:

Tables S1 to S6
Figs. S1 to S6

Table S1. Structure alignment between different PBS (s, *Synechocystis* 6803) subunits and the corresponding components in PpPBS-core (PDBID: 6KGX). All predicted homology models are included. Three cylinders are evaluated independently based on the location of various subunits. The RMSD value is calculated among all Cα in the two corresponded structures given by PyMOL software.

		Alignment with PpPBS-core, (6KGX) RMSD (Å)	
		Basal Cylinder	**Cylinder B**
sApcA/B		(A) 0.621/0.725	0.59/0.608
		(A′) 0.762/0.771	
sApcC		0.665	
sApcD		0.912	-
sApcE (or α^{LCM})	**M1**	0.535	-
	M2	0.647	-
	M3	0.770	-
	M4	0.563	-
	M5	0.739	-
sApcE_LD1	**M1**	0.692	
sApcE_LD2	**M1**	1.005	-
sApcE_LD3	**M1**	-	0.473
	M2	-	0.733
	M3	-	0.724
	M4	-	0.703
	M5	-	1.833
sApcF	**M1**	0.791	-

Table S2. MS-information of the inter cross-links in WT-PBS.

Raw file scan number	Charge	Precursor_Mass	Cross-linking sites	Subunit sites	#
072815_PBS_X02_02.16890.16890.4.0.dta	4	4039.1570	AASVISANAATIVKEAVAK(14)-DITKAYSQSISYLESQVR(4)	ApcB (53)-ApcE (296)	1
072815_PBS_X02_02.16840.16840.4.0.dta	4	4051.2340			
072815_PBS_X02_02.11205.11205.4.1.dta	4	2906.6930	AASVISANAATIVKEAVAK(14)-VDKEVTPR(3)	ApcB (53)-ApcE (685)	2
072815_PBS_X02_02.11186.11186.4.0.dta	4	2894.6240			
072815_PBS_X02_01.27051.27051.3.0.dta	3	1855.0170	AITTAASR(1)-MFDVFTR(1)	cpcC1 (2)-cpcB (1)	3
072815_PBS_X02_01.27163.27163.3.1.dta	3	1842.9390			
072815_PBS_X02_01.34996.34996.3.0.dta	3	2164.2270	ALPLLNYAPK(1)-MFDVFTR(1)	cpcG1 (2)-cpcB (1)	4
072815_PBS_X02_01.35148.35148.3.0.dta	3	2152.1510			
072815_PBS_X02_01.24141.24141.4.0.dta	4	3390.8150	DAVTTLIKNYDLTGR(8)-SIVTKSIVNADAEAR(5)	ApcF (10)-ApcA (6)	5
072815_PBS_X02_01.24117.24117.4.1.dta	4	3402.8870			
072815_PBS_X02_02.5149.5149.4.0.dta	4	2197.1860	ETIVKQAGDR(5)-VDKEVTPR(3)	ApcA (52)-ApcE (685)	6
072815_PBS_X02_02.5066.5066.4.0.dta	4	2209.2510			
072815_PBS_X02_02.13696.13696.4.0.dta	4	4392.3690	GPAVNNQVGNPSAVGEFPGSLGAKVFR(24)-SIVTKSIVNADAEAR(5)	ApcE (511)-ApcA (6)	7
072815_PBS_X02_02.13739.13739.4.0.dta	4	4380.2950			
072815_PBS_X02_02.8194.8194.4.0.dta	4	2341.3990	IKAFVTGGAAR(2)-EKVLESQLR(2)	ApcA (27)-cpcG1 (64)	8
072815_PBS_X02_02.8220.8220.4.0.dta	4	2329.3260			
072815_PBS_X02_01.25344.25344.3.0.dta	3	2155.2090	IKAFVTGGAAR(2)-MFDVFTR(1)	ApcA (27)-cpcB (1)	9
072815_PBS_X02_01.25378.25378.3.0.dta	3	2143.1360			
072815_PBS_X02_02.6559.6559.4.0.dta	4	2183.2970	IKAFVTGGAAR(2)-VDKEVTPR(3)	ApcA (27)-ApcE (685)	10
072815_PBS_X02_02.6634.6634.4.0.dta	4	2171.2210			
072815_PBS_X02_01.29273.29273.3.0.dta	3	2353.2470	LGGKVASITPASLS(4)-MFDVFTR(1)	cpcC1 (281)-cpcB (1)	11
072815_PBS_X02_01.29232.29232.2.0.dta	2	2365.3180			
072815_PBS_X02_02.9576.9576.4.0.dta	4	2498.3700	LKSYFASGELR(2)-IKAFVTGGAAR(2)	ApcB (28)-ApcA (27)	12
072815_PBS_X02_02.9474.9474.4.1.dta	4	2510.4480			
072815_PBS_X02_01.30404.30404.3.0.dta	3	3057.6410	MKTPLTEAVSTADSQGR(1)-ETIVKQAGDR(5)	cpcA (1)-ApcA (52)	13
072815_PBS_X02_01.31395.31395.3.0.dta	3	3045.5670			
072815_PBS_X02_01.23741.23741.3.0.dta	3	2872.4590	MKTPLTEAVSTADSQGR(2)-MFDVFTR(1)	cpcA (2)-cpcB (1)	14
072815_PBS_X02_01.23767.23767.3.0.dta	3	2860.3860			
072815_PBS_X02_01.30665.30665.3.0.dta	3	2949.4220	MLGQSSLVGYSNTQAANR(1)-MFDVFTR(1)	cpcD (1)-cpcB (1)	15
072815_PBS_X02_01.30533.30533.3.1.dta	3	2961.5010			
072815_PBS_X02_01.22492.22492.3.0.dta	3	3825.8750	MLGQSSLVGYSNTQAANR(1)-MKTPLTEAVSTADSQGR(1)	cpcD (1)-cpcA (1)	16
072815_PBS_X02_01.22359.22359.3.0.dta	3	3837.9500			
072815_PBS_X02_01.27937.27937.3.0.dta	3	3471.8040	MQDAITAVINSADVQGK(1)-SIVTKSIVNADAEAR(5)	ApcB (1)-ApcA (6)	17
072815_PBS_X02_01.28017.28017.3.1.dta	3	3483.8780			

PBS-core related cross-links (lime)

Table S2. MS-information of the inter cross-links in WT-PBS (continued).

Raw file scan number	Charge	Precursor_Mass	Cross-linking sites	Subunit sites	#
072815_PBS_X02_02.17319.17319.4.0.dta	4	4767.4620	MQDAITAVINSADVQGKYLDGAAMDK(17)-IFTGGSPLSYLEKPVER(13)	ApcB (17)-ApcE (87)	18
072815_PBS_X02_01.30217.30217.4.0.dta	4	4755.3910			
072815_PBS_X02_01.26492.26492.3.0.dta	3	3028.5940	NAMDELKAYFESGSAR(7)-IKAFVTGGAAR(2)	ApcF (28)-ApcA (27)	19
072815_PBS_X02_01.26530.26530.3.0.dta	3	3016.5220			
072815_PBS_X02_01.24032.24032.3.0.dta	3	2101.1290	NQKTVGFSR(3)-MFDVFTR(1)	cpcC2 (161)-cpcB (1)	20
072815_PBS_X02_01.23987.23987.3.0.dta	3	2089.0530			
072815_PBS_X02_02.10300.10300.4.0.dta	4	3858.0760	SINPAANTIPKVSAQNINIEASVPR(11)-ETIVKQAGDR(5)	cpcG1 (234)-ApcA (52)	21
072815_PBS_X02_02.10268.10268.4.1.dta	4	3870.1460			
072815_PBS_X02_01.23079.23079.4.0.dta	4	4610.4860	SINPAANTIPKVSAQNINIEASVPR(11)-MKEAALDIVNDPNGITR(2)	cpcG1 (234)-cpcB (135)	22
072815_PBS_X02_01.23144.23144.4.0.dta	4	4598.4240			
072815_PBS_X02_01.15644.15644.4.0.dta	4	2475.3290	SIVTKSIVNADAEAR(5)-IMKMGGK(3)	ApcA (6)-ApcC (45)	23
072815_PBS_X02_01.15437.15437.3.0.dta	3	2487.4030			
072815_PBS_X02_01.23179.23179.3.0.dta	3	3123.6500	SIVTKSIVNADAEAR(5)-KQFFEPFINSR(1)	ApcA (6)-ApcE (331)	24
072815_PBS_X02_01.23164.23164.3.1.dta	3	3135.7200			
072815_PBS_X02_02.8790.8790.4.1.dta	4	2590.4410	SIVTKSIVNADAEAR(5)-LYNKLTK(4)	ApcA (6)-ApcE (875)	25
072815_PBS_X02_02.8778.8778.4.1.dta	4	2602.5180			
072815_PBS_X02_02.8310.8310.4.0.dta	4	2589.4240	SIVTKSIVNADAEAR(5)-QQTKVFK(4)	ApcA (6)-ApcE (722)	26
072815_PBS_X02_02.8239.8239.4.0.dta	4	2601.4980			
072815_PBS_X02_01.33620.33620.3.0.dta	3	3504.9070	SNKAVIVPFEQLNQTLQQINR(3)-MFDVFTR(1)	cpcC1 (259)-cpcB (1)	27
072815_PBS_X02_01.33652.33652.3.0.dta	3	3492.8470			
072815_PBS_X02_01.32003.32003.4.0.dta	4	5643.8230	VEGYEIGSEEKPVVFTTENILSSSDMDNLIEAAYR(11)-VEITAISAPGYPKVR(13)	cpcG1 (27)-cpcC1 (253)	28
072815_PBS_X02_01.32115.32115.4.0.dta	4	5655.8990			
072815_PBS_X02_01.26928.26928.3.0.dta	3	2653.4060	VEITAISAPGYPKVR(13)-MFDVFTR(1)	cpcC1 (253)-cpcB (1)	29
072815_PBS_X02_01.26882.26882.3.0.dta	3	2665.4800			
072815_PBS_X02_01.29488.29488.4.3.dta	4	4759.7300	VLNGLKETYNSLGVPISSTVQAIQAIK(6)-IVKVELATGRPGTNAGLA(3)	ApcB (113)-ApcC (52)	30
072815_PBS_X02_02.16899.16899.4.3.dta	4	4747.6140			
072815_PBS_X02_02.16035.16035.4.0.dta	4	3924.1670	VLNGLKETYNSLGVPISSTVQAIQAIK(6)-VDKEVTPR(3)	ApcB (113)-ApcE (685)	31
072815_PBS_X02_02.16020.16020.4.0.dta	4	3936.2400			
072815_PBS_X02_01.15130.15130.4.1.dta	4	2317.2840	YLDGAAMDKLK(9)-VDKEVTPR(3)	ApcB (26)-ApcE (685)	32
072815_PBS_X02_01.15173.15173.4.0.dta	4	2305.2090			
				FNR(69)-CpcB(1)	33*

PBS-core related cross-links (lime), **Liu et al.*, 2019, mBio Ref#27

Table S3. MS-information of the inter cross-links in CK-PBS.

Raw file scan number	Charge	Precursor_Mass	Cross-linking sites	Subunit sites	#
072815_CK_X02_01.28466.28466.4.2.dta	4	4051.232	AASVISANAATIVKEAVAK(14)-DITKAYSQSISYLESQVR(4)	**ApcB (53)-ApcE (296)**	**1***
072815_CK_X02_01.28474.28474.4.0.dta	4	4039.157			
072815_CK_X02_02.13676.13676.4.0.dta	4	3041.741	AASVISANAATIVKEAVAK(14)-IKAFVTGGAAR(2)	ApcB (53)-ApcA (27)	2
072815_CK_X02_02.13646.13646.4.2.dta	4	3053.812			
072815_CK_X02_01.20034.20034.4.0.dta	4	2894.625	AASVISANAATIVKEAVAK(14)-VDKEVTPR(3)	**ApcB (53)-ApcE (685)**	**3***
072815_CK_X02_01.19943.19943.4.0.dta	4	2906.693			
072815_CK_X02_01.27971.27971.3.0.dta	3	4282.235	APLNQKEIQQYNQILASQGLK(6)-MQDAITAVINSADVQGK(1)	ApcE (817)-ApcB (1)	4
072815_CK_X02_01.27925.27925.3.0.dta	3	4294.307			
072815_CK_X02_01.20872.20872.3.0.dta	3	4095.211	APLNQKEIQQYNQILASQGLK(6)-SIVTKSIVNADAEAR(5)	ApcE (817)-ApcA (6)	5
072815_CK_X02_01.20898.20898.3.0.dta	3	4107.287			
072815_CK_X02_01.23068.23068.3.0.dta	3	3402.881	DAVTTLIKNYDLTGR(8)-SIVTKSIVNADAEAR(5)	**ApcF (10)-ApcA (6)**	**6***
072815_CK_X02_01.23227.23227.3.0.dta	3	3390.815			
072815_CK_X02_01.24136.24136.3.1.dta	3	2767.652	ELVVPSFTPVVKVGG(12)-IKAFVTGGAAR(2)	ApcE (893)-ApcA (27)	7
072815_CK_X02_01.24193.24193.3.0.dta	3	2755.583			
072815_CK_X02_01.8063.8063.3.0.dta	3	2209.254	ETIVKQAGDR(5)-VDKEVTPR(3)	**ApcA (52)-ApcE (685)**	**8***
072815_CK_X02_01.8173.8173.3.0.dta	3	2197.181			
072815_CK_X02_01.31333.31333.3.0.dta	3	3890.911	EVASGLMSSDDAAEASAYFDFVIGKMS(25)-VDKEVTPR(3)	ApcA (159)-ApcE (685)	9
072815_CK_X02_01.31398.31398.3.0.dta	3	3878.819			
072815_CK_X02_02.13993.13993.4.3.dta	4	3909.162	GPAVNNQVGNPSAVGEFPGSLGAKVFR(24)-IKAFVTGGAAR(2)	ApcE (511)-ApcA (27)	10
072815_CK_X02_02.13996.13996.4.0.dta	4	3897.083			
072815_CK_X02_02.14524.14524.4.2.dta	4	4392.373	GPAVNNQVGNPSAVGEFPGSLGAKVFR(24)-SIVTKSIVNADAEAR(1)	ApcE (511)-ApcA (2)	11
072815_CK_X02_02.14846.14846.4.1.dta	4	4380.288			
072815_CK_X02_02.14655.14655.4.2.dta	4	4392.372	GPAVNNQVGNPSAVGEFPGSLGAKVFR(24)-SIVTKSIVNADAEAR(5)	**ApcE (511)-ApcA (6)**	**12***
072815_CK_X02_02.14627.14627.4.0.dta	4	4380.287			
072815_CK_X02_02.8677.8677.4.0.dta	4	2175.265	IKAFVTGGAAR(2)-LAKSPLYR(3)	ApcA (27)-ApcE (325)	13
072815_CK_X02_02.8629.8629.4.0.dta	4	2187.343			
072815_CK_X02_01.11543.11543.4.0.dta	4	2183.295	IKAFVTGGAAR(2)-VDKEVTPR(3)	**ApcA (27)-ApcE (685)**	**14***
072815_CK_X02_01.11395.11395.4.0.dta	4	2171.219			
072815_CK_X02_01.16550.16550.4.0.dta	4	2510.449	LKSYFASGELR(2)-IKAFVTGGAAR(2)	**ApcB (28)-ApcA (27)**	**15***
072815_CK_X02_01.16959.16959.4.0.dta	4	2498.374			
072815_CK_X02_01.26259.26259.3.0.dta	3	2988.585	MQDAITAVINSADVQGK(1)-IKAFVTGGAAR(2)	ApcB (1)-ApcA (27)	16
072815_CK_X02_01.26095.26095.3.0.dta	3	3000.638			
072815_CK_X02_01.25154.25154.3.0.dta	3	2776.459	MQDAITAVINSADVQGK(1)-QQTKVFK(4)	ApcB (1)-ApcE (722)	17
072815_CK_X02_01.25144.25144.3.0.dta	3	2788.536			

* are identified in WT-PBS

Table S3. MS-information of the inter cross-links in CK-PBS (Continued).

Raw file scan number	Charge	Precursor_Mass	Cross-linking sites	Subunit sites	#
072815_CK_X02_01.26915.26915.3.0.dta	3	3483.881	MQDAITAVINSADVQGK(1)-SIVTKSIVNADAEAR(5)	**ApcB (1)-ApcA (6)**	**18***
072815_CK_X02_01.27064.27064.3.0.dta	3	3471.804			
072815_CK_X02_01.24450.24450.3.2.dta	3	2841.475	MQDAITAVINSADVQGK(1)-VDKEVTPR(3)	ApcB (1)-ApcE (685)	19
072815_CK_X02_02.15339.15339.3.1.dta	3	2853.542			
072815_CK_X02_01.23159.23159.4.1.dta	4	3991.06	MQDAITAVINSADVQGKYLDGAAMDK(17)-ETIVKQAGDR(5)	ApcB (17)-ApcA (52)	20
072815_CK_X02_01.23177.23177.4.0.dta	4	3978.996			
072815_CK_X02_01.23209.23209.4.2.dta	4	4120.12	MQDAITAVINSADVQGKYLDGAAMDK(17)-IAETLAENEKK(10)	ApcB (17)-ApcD (48)	21
072815_CK_X02_02.14536.14536.4.0.dta	4	4108.051			
072815_CK_X02_01.29018.29018.4.0.dta	4	4755.394	MQDAITAVINSADVQGKYLDGAAMDK(17)-IFTGGSPLSYLEKPVER(13)	**ApcB (17)-ApcE (87)**	**22***
072815_CK_X02_01.29091.29091.4.1.dta	4	4767.464			
072815_CK_X02_01.25045.25045.4.0.dta	4	3965.083	MQDAITAVINSADVQGKYLDGAAMDK(17)-IKAFVTGGAAR(2)	ApcB (17)-ApcA (27)	23
072815_CK_X02_01.25076.25076.4.0.dta	4	3953.009			
072815_CK_X02_01.23178.23178.4.0.dta	4	3805.904	MQDAITAVINSADVQGKYLDGAAMDK(17)-VDKEVTPR(3)	ApcB (17)-ApcE (685)	24
072815_CK_X02_01.23156.23156.4.2.dta	4	3817.974			
072815_CK_X02_01.25575.25575.3.0.dta	3	3028.598	NAMDELKAYFESGSAR(7)-IKAFVTGGAAR(2)	**ApcF (28)-ApcA (27)**	**25***
072815_CK_X02_01.25550.25550.3.0.dta	3	3016.522			
072815_CK_X02_01.14770.14770.3.0.dta	3	2475.326	SIVTKSIVNADAEAR(5)-IMKMGGK(3)	**ApcA (6)-ApcC (45)**	**26***
072815_CK_X02_01.14689.14689.4.1.dta	4	2487.402			
072815_CK_X02_02.13643.13643.4.4.dta	4	3135.712	SIVTKSIVNADAEAR(5)-KQFFEPFINSR(1)	**ApcA (6)-ApcE (331)**	**27***
072815_CK_X02_02.14058.14058.4.3.dta	4	3123.645			
072815_CK_X02_01.15684.15684.3.0.dta	3	2602.523	SIVTKSIVNADAEAR(5)-LYNKLTK(4)	**ApcA (6)-ApcE (875)**	**28***
072815_CK_X02_01.15755.15755.3.0.dta	3	2590.44			
072815_CK_X02_01.14561.14561.3.0.dta	3	2589.422	SIVTKSIVNADAEAR(5)-QQTKVFK(4)	**ApcA (6)-ApcE (722)**	**29***
072815_CK_X02_01.14513.14513.3.0.dta	3	2601.497			
072815_CK_X02_01.13791.13791.4.1.dta	4	2654.433	SIVTKSIVNADAEAR(5)-VDKEVTPR(3)	ApcA (6)-ApcE (685)	30
072815_CK_X02_01.13832.13832.4.0.dta	4	2666.513			
072815_CK_X02_01.26917.26917.4.0.dta	4	4097.244	VLNGLKETYNSLGVPISSTVQAIQAIK(6)-ETIVKQAGDR(5)	ApcB (113)-ApcA (52)	31
072815_CK_X02_01.26934.26934.4.0.dta	4	4109.327			
072815_CK_X02_01.28355.28355.4.0.dta	4	4759.737	VLNGLKETYNSLGVPISSTVQAIQAIK(6)-IVKVELATGRPGTNAGLA(3)	**ApcB (113)-ApcC (52)**	**32***
072815_CK_X02_01.28354.28354.4.3.dta	4	4747.628			
072815_CK_X02_02.17119.17119.4.0.dta	4	3924.171	VLNGLKETYNSLGVPISSTVQAIQAIK(6)-VDKEVTPR(3)	**ApcB (113)-ApcE (685)**	**33***
072815_CK_X02_02.17138.17138.4.0.dta	4	3936.243			
072815_CK_X02_01.17514.17514.4.0.dta	4	2464.405	YLDGAAMDKLK(9)-IKAFVTGGAAR(2)	ApcB (26)-ApcA (27)	34
072815_CK_X02_01.17564.17564.4.0.dta	4	2452.33			
072815_CK_X02_01.14358.14358.3.0.dta	3	2317.286	YLDGAAMDKLK(9)-VDKEVTPR(3)	**ApcB (26)-ApcE (685)**	**35***
072815_CK_X02_01.14412.14412.3.1.dta	3	2305.212			

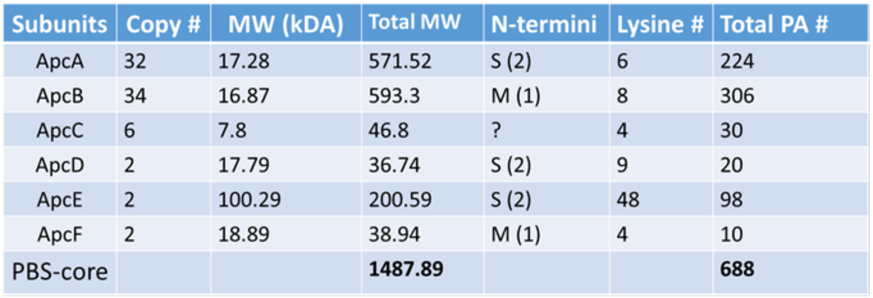
* are identified in WT-PBS

Table S4. Cross-links identified in CpcL-PBS.

Raw file scan number	Charge	Precursor_Mass	Cross-linking sites	Subunit sites	#
072815_AB_X02_01.26910.26910.2.0.dta	2	2365.315	LGGKVASITPASLS(4)-MFDVFTR(1)	cpcC1 (281)-cpcB (1)	1
072815_AB_X02_01.26941.26941.2.0.dta	2	2353.238			
072815_AB_X02_01.23420.23420.3.0.dta	3	1985.058	MGGKIVSIK(4)-MFDVFTR(1)	FNR (69)-cpcB (1)	2
072815_AB_X02_01.23411.23411.3.2.dta	3	1997.137			
072815_AB_X02_02.9991.9991.4.0.dta	4	3030.568	MKEAALDIVNDPNGITR(2)-NQKTVGFSR(3)	cpcB (135)-cpcC2 (161)	3
072815_AB_X02_02.9965.9965.4.0.dta	4	3042.642			
072815_AB_X02_02.12000.12000.4.2.dta	4	3594.918	MKEAALDIVNDPNGITR(2)-VEITAISAPGYPKVR(13)	cpcB (135)-cpcC1 (253)	4
072815_AB_X02_02.11973.11973.4.0.dta	4	3606.992			
072815_AB_X02_01.24579.24579.3.1.dta	3	2856.462	MKTPLTEAVSTADSQGR(1)-MFDVFTR(1)	cpcA (1)-cpcB (1)	5
072815_AB_X02_01.30916.30916.3.1.dta	3	2844.411			
072815_AB_X02_01.24767.24767.3.0.dta	3	2856.465	MKTPLTEAVSTADSQGR(2)-MFDVFTR(1)	cpcA (2)-cpcB (1)	6
072815_AB_X02_01.24704.24704.3.0.dta	3	2844.393			
072815_AB_X02_01.28305.28305.3.0.dta	3	2949.424	MLGQSSLVGYSNTQAANR(1)-MFDVFTR(1)	cpcD (1)-cpcB (1)	7
072815_AB_X02_01.28303.28303.3.0.dta	3	2961.502			
072815_AB_X02_01.20517.20517.3.0.dta	3	3837.95	MLGQSSLVGYSNTQAANR(1)-MKTPLTEAVSTADSQGR(2)	cpcD (1)-cpcA (2)	8
072815_AB_X02_01.20532.20532.3.0.dta	3	3825.877			
072815_AB_X02_01.21994.21994.3.0.dta	3	2089.055	NQKTVGFSR(3)-MFDVFTR(1)	cpcC2 (161)-cpcB (1)	9
072815_AB_X02_01.21845.21845.3.0.dta	3	2101.129			
072815_AB_X02_02.15746.15746.4.1.dta	4	4369.279	SNKAVIVPFEQLNQTLQQINR(3)-MKTPLTEAVSTADSQGR(1)	cpcC1 (259)-cpcA (1)	10
072815_AB_X02_02.15757.15757.4.1.dta	4	4381.363			
072815_AB_X02_01.31132.31132.3.0.dta	3	2735.501	TLPLIAYAPVSQNQR(1)-MFDVFTR(1)	cpcG2 (2)-cpcB (1)	11
072815_AB_X02_01.31152.31152.3.0.dta	3	2723.425			
072815_AB_X02_01.29833.29833.3.0.dta	3	3490.985	TLPLIAYAPVSQNQR(1)-TLPLIAYAPVSQNQR(1)	cpcG2 (2)-cpcG2 (2)	12
072815_AB_X02_01.30065.30065.3.0.dta	3	3478.906			
072815_AB_X02_01.24799.24799.3.0.dta	3	2665.482	VEITAISAPGYPKVR(13)-MFDVFTR(1)	cpcC1 (253)-cpcB (1)	13
072815_AB_X02_01.24859.24859.3.0.dta	3	2653.408			
				FNR (1)-cpcB (1)	14*

**Liu et al.,* 2019 mBio Ref#27

Table S5. Composition of sPBS-core and N-terminal modifications, primary amine # (PA).

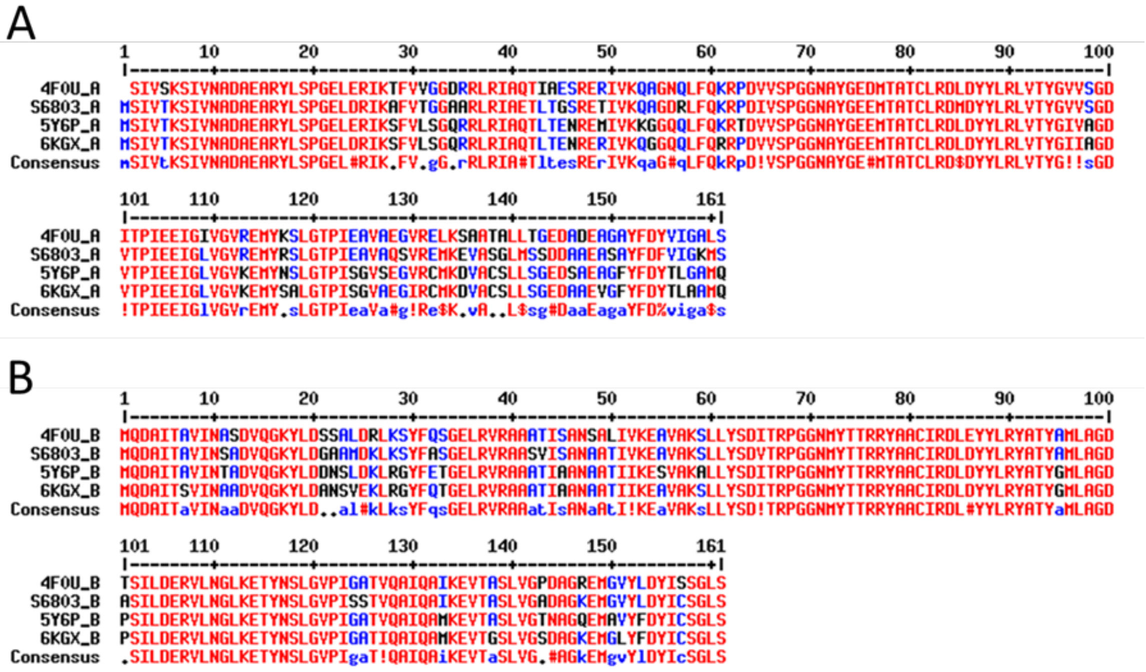


Subunits	Copy #	MW (kDA)	Total MW	N-termini	Lysine #	Total PA #
ApcA	32	17.28	571.52	S (2)	6	224
ApcB	34	16.87	593.3	M (1)	8	306
ApcC	6	7.8	46.8	?	4	30
ApcD	2	17.79	36.74	S (2)	9	20
ApcE	2	100.29	200.59	S (2)	48	98
ApcF	2	18.89	38.94	M (1)	4	10
PBS-core			**1487.89**			**688**

Table S6. Cross-links originally annotated as Intralinks.

Raw file scan number	Charge	Precursor_Mass	Cross-linking sites	Subunit sites	#*
072815_CK_X02_02.14460.14460.4.2.dta	4	3175.725	AASVISANAATIVKEAVAK(14)-YLDGAAMDKLK(9)	ApcB (53)-ApcB (26)	1
072815_CK_X02_02.14458.14458.4.0.dta	4	3187.799			
072815_CK_X02_01.11898.11898.4.0.dta	4	2344.299	IKAFVTGGAAR(2)-ETIVKQAGDR(5)	ApcA (27)-ApcA (52)	2
072815_CK_X02_01.11570.11570.4.1.dta	4	2356.372			
072815_CK_X02_02.16481.16481.4.0.dta	4	4145.137	MQDAITAVINSADVQGKYLDGAAMDK(17)-LKSYFASGELR(2)	ApcB (17)-ApcB (28)	3
072815_CK_X02_01.25953.25953.4.0.dta	4	4133.06			
072815_CK_X02_01.16476.16476.3.1.dta	3	2813.624	SIVTKSIVNADAEAR(5)-IKAFVTGGAAR(2)	ApcA (6)-ApcA (27)	4
072815_CK_X02_01.16396.16396.3.0.dta	3	2801.55			

*from 19 intralinks



A

```
           1        10        20        30        40        50        60        70        80        90        100
           |--------+---------+---------+---------+---------+---------+---------+---------+---------+---------|
   4F0U_A   SIVSKSIVNADAEARYLSPGELERIKTFVVGGDRRLRIAQTIAESRERIVKQAGNQLFQKRPDVVSPGGNAYGEDMTATCLRDLDYYLRLVTYGVVSGD
  S6803_A  MSIVTKSIVNADAEARYLSPGELDRIKAFVTGGAARLRIAETLTGSRETIVKQAGDRLFQKRPDIVSPGGNAYGEEMTATCLRDMDYYLRLVTYGVVSGD
   5Y6P_A  MSIVTKSIVNADAEARYLSPGELERIKSFVLSGQRRLRIAQTLTENREMIVKKGGQQLFQKRTDVVSPGGNAYGEEMTATCLRDLDYYLRLVTYGIVAGD
   6KGX_A  MSIVTKSIVNADAEARYLSPGELDRIKSFVLSGQRRLRIAQTLTENRERIVKQGGQQLFQRRPDVVSPGGNAYGEEMTATCLRDLDYYLRLVTYGIIAGD
Consensus  mSIVtKSIVNADAEARYLSPGEL#RIK.FV.gG.rRLRIA#TltesREr IVKqaG#qLFQkRpD!VSPGGNAYGE#MTATCLRD$DYYLRLVTYG!!sGD

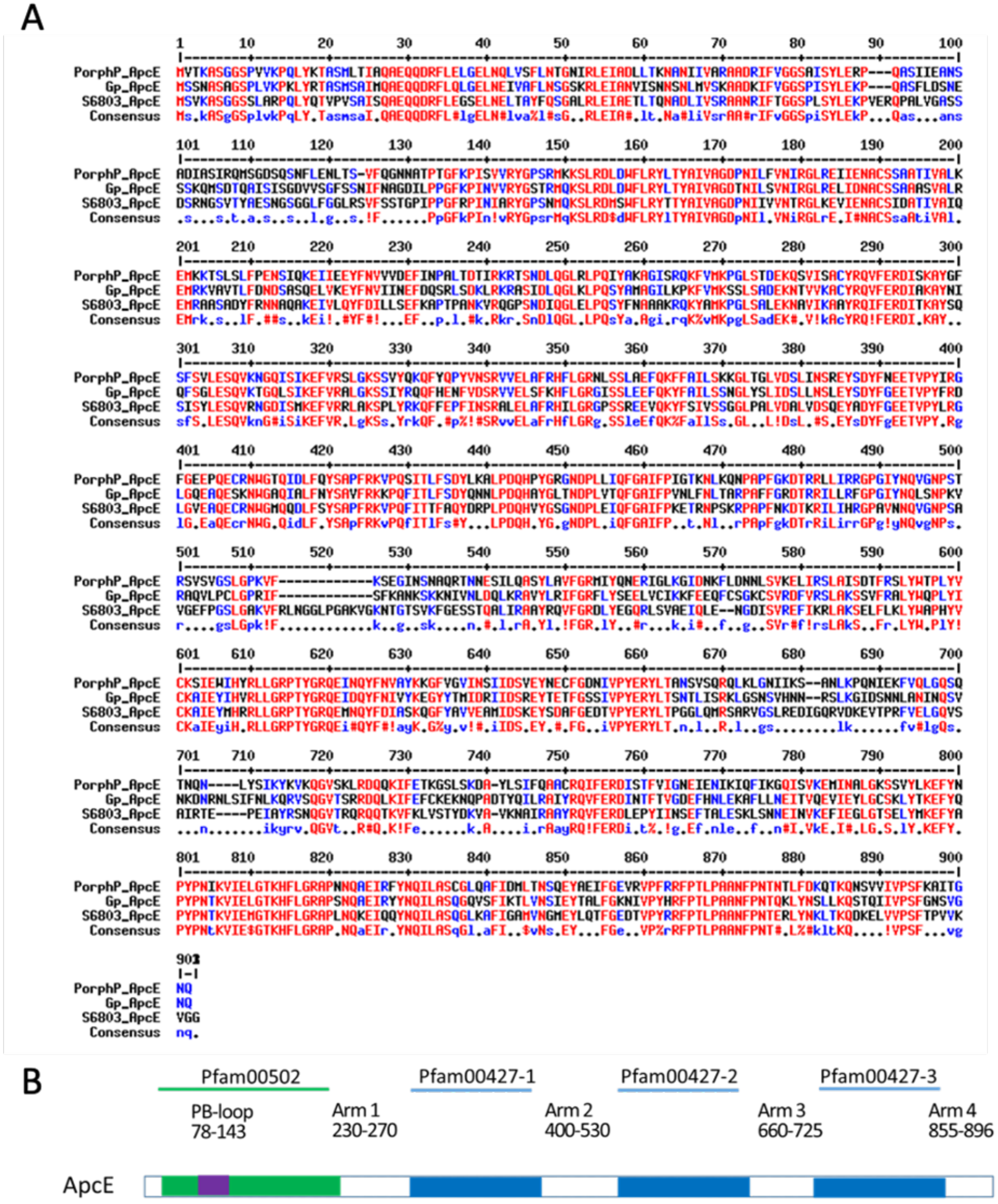
           101      110       120       130       140       150       161
           |--------+---------+---------+---------+---------+---------+|
   4F0U_A  ITPIEEIGIVGVREMYKSLGTPIEAVAEGVRELKSAATALLTGEDADEAGAYFDYVIGALS
  S6803_A  VTPIEEIGLVGVREMYRSLGTPIEAVAQSVREMKEVASGLMSSDDAAEASAYFDFVIGKMS
   5Y6P_A  VTPIEEIGLVGVKEMYNSLGTPISGVSEGVRCMKDVACSLLSGEDSAEAGFYFDYTLGAMQ
   6KGX_A  VTPIEEIGLVGVKEMYSALGTPISGVAEGIRCMKDVACSLLSGEDAAEVGFYFDYTLAAMQ
Consensus  !TPIEEIGlVGVrEMY.sLGTPIeaVa#g!Re$K.vA..L$sg#DaaEagaYFD%viga$s
```

B

```
           1        10        20        30        40        50        60        70        80        90        100
           |--------+---------+---------+---------+---------+---------+---------+---------+---------+---------|
   4F0U_B  MQDAITAVINASDVQGKYLDSSALDRLKSYFQSGELRVRAAATISANSALIVKEAVAKSLLYSDITRPGGNMYTTRRYAACIRDLEYYLRYATYAMLAGD
  S6803_B  MQDAITAVINSADVQGKYLDGAAMDKLKSYFASGELRVRAASVISANAATIVKEAVAKSLLYSDVTRPGGNMYTTRRYAACIRDLDYYLRYATYAMLAGD
   5Y6P_B  MQDAITAVINTADVQGKYLDDNSLDKLRGYFETGELRVRAAATIAANAATIIKESVAKALLYSDITRPGGNMYTTRRYAACIRDLDYYLRYATYGMLAGD
   6KGX_B  MQDAITSVINAADVQGKYLDANSVEKLRGYFQTGELRVRAAATIAANAATIIKEAVAKSLLYSDITRPGGNMYTTRRYAACIRDLDYYLRYATYGMLAGD
Consensus  MQDAITaVINaaDVQGKYLD..al#kLksYFqsGELRVRAAatIsANaAtI!KEaVAKsLLYSD!TRPGGNMYTTRRYAACIRDL#YYLRYATYaMLAGD

           101      110       120       130       140       150       161
           |--------+---------+---------+---------+---------+---------+|
   4F0U_B  TSILDERVLNGLKETYNSLGVPIGATVQAIQAIKEVTASLVGPDAGREMGVYLDYISSGLS
  S6803_B  ASILDERVLNGLKETYNSLGVPISSTVQAIQAIKEVTASLVGADAGKEMGVYLDYICSGLS
   5Y6P_B  PSILDERVLNGLKETYNSLGVPIGATVQAIQAMKEVTASLVGTNAGQEMAVYFDYICSGLS
   6KGX_B  PSILDERVLNGLKETYNSLGVPIGATIQAIQAMKEVTGSLVGSDAGKEMGLYFDYICSGLS
Consensus  .SILDERVLNGLKETYNSLGVPIgaT!QAIQAiKEVTaSLVG.#AGkEMgvYlDYIcSGLS
```

Fig. S1. Sequence homology analysis of ApcA and ApcB. (A) ApcA and (B) ApcB from 4F0U (PDBID), *Synechocystis* 6803 (S6803), GpPBS (PDBID: 5Y6P), and PpPBS (6KGX).



```
               1        10        20        30        40        50        60        70        80        90       100
               |--------+---------+---------+---------+---------+---------+---------+---------+---------+---------|
  PorphP_ApcE  MVTKASGGSPVVKPQLYKTASMLTIAQAEQQDRFLELGELNQLVSFLNTGNIRLEIADLLTKNANIIVARAADRIFVGGSAISYLERP---QASIIEANS
      Gp_ApcE  MSSNASAGSPLVKPKLYRTASMSAIMQAEQQDRFLQLGELNEIVAFLNSGSKRLEIANVISNNSNLMVSKAADKIFVGGSPISYLEKP---QASFLDSNE
   S6803_ApcE  MSVKASGGSSLARPQLYQTVPVSAISQAEQQDRFLEGSELNELTAYFQSGALRLEIAETLTQNADLIVSRAANRIFTGGSPLSYLEKPVERQPALVGASS
    Consensus  Ms.kASgGSplvkPqLY.TasmsaI.QAEQQDRFL#lgELN#lva%l#sG..RLEIA#.lt.Na#liVsrAA#rIFvGGSpiSYLEkP...Qas...ans

             101      110       120       130       140       150       160       170       180       190       200
               |--------+---------+---------+---------+---------+---------+---------+---------+---------+---------|
  PorphP_ApcE  ADIASIRQMSGDSQSNFLENLTS-VFQGNNATPTGFKPISVVRYGPSRMKKSLRDLDWFLRYLTYAIVAGDPNILFVNIRGLREIIENACSSAATIVALK
      Gp_ApcE  SSKQMSDTQAISISGDVVSGFSSNIFNAGDILPPGFKPINVVRYGSTRMQKSLRDLDWFLRYLTYAIVAGDTNILSVNIRGLRELIDNACSSAAASVALR
   S6803_ApcE  DSRNGSVTYAESNGSGGLFGGLRSVFSSTGPIPPGFRPINIARYGPSNMQKSLRDMSWFLRYTTYAIVAGDPNIIVVNTRGLKEVIENACSIDATIVAIQ
    Consensus  .s...s.t.a.s..s..l.g..s.!F......PpGFkPIn!vRYGpsrMqKSLRD$dWFLRYlTYAIVAGDpNIl.VNiRGLrE.I#NACSsaAtiVAl.

             201      210       220       230       240       250       260       270       280       290       300
               |--------+---------+---------+---------+---------+---------+---------+---------+---------+---------|
  PorphP_ApcE  EMKKTSLSLFPENSIQKEIIEEYFNVVVDEFINPALTDTIRKRTSNDLQGLRLPQIYAKAGISRQKFVMKPGLSTDEKQSVISACYRQVFERDISKAYGF
      Gp_ApcE  EMRKVAVTLFDNDSASQELVKEYFNVIINEFDQSRLSDKLRKRASIDLQGLKLPQSYAMAGILKPKFVMKSSLSADEKNTVVKACYRQVFERDIAKAYNI
   S6803_ApcE  EMRAASADYFRNNAQAKEIVLQYFDILLSEFKAPTPANKVRQGPSNDIQGLELPQSYFNAAAKRQKYAMKPGLSALEKNAVIKAAYRQIFERDITKAYSQ
    Consensus  EMrk.s..lF.##s..kEi!.#YF#!...EF..p.l.#k.Rkr.SnDlQGL.LPQsYa.Agi.rqK%vMKpgLSadEK#.V!kAcYRQ!FERDI.KAY..

             301      310       320       330       340       350       360       370       380       390       400
               |--------+---------+---------+---------+---------+---------+---------+---------+---------+---------|
  PorphP_ApcE  SFSVLESQVKNGQISIKEFVRSLGKSSVYQKQFYQPYVNSRVVELAFRHFLGRNLSSLAEFQKFFAILSKKGLTGLVDSLINSREYSDYFNEETVPYIRG
      Gp_ApcE  QFSGLESQVKTGQLSIKEFVRALGKSSIYRQQFHENFVDSRVVELSFKHFLGRGISSLEEFQKYFAILSSNGLYSLIDSLLNSLEYSDYFGEETVPYFRD
   S6803_ApcE  SISYLESQVRNGDISMKEFVRRLAKSPLYRKQFFEPFINSRALELAFRHILGRGPSSREEVQKYFSIVSSGGLPALVDALVDSQEYADYFGEETVPYLRG
    Consensus  sfS.LESQVknG#iSiKEFVR.LgKSs.YrkQF.#p%!#SRvvELaFrHfLGRg.SSleEfQK%FaIlSs.GL..L!DsL.#S.EYsDYFgEETVPY.Rg

             401      410       420       430       440       450       460       470       480       490       500
               |--------+---------+---------+---------+---------+---------+---------+---------+---------+---------|
  PorphP_ApcE  FGEEPQECRNWGTQIDLFQYSAPFRKVPQSITLFSDYLKALPDQHPYGRGNDPLLIQFGAIFPIGTKNLKQNPAPFGKDTRRLLIRRGPGIYNQVGNPST
      Gp_ApcE  LGQEAQESKNWGAQIALFNYSAVFRKKPQFITLFSDYQNNLPDQHAYGLTNDPLVTQFGAIFPVNLFNLTARPAFFGRDTRRILLRFGPGIYNQLSNPKV
   S6803_ApcE  LGVEAQECRNWGMQQDLFSYSAPFRKVPQFITTFAQYDRPLPDQHVYGSGNDPLEIQFGAIFPKETRNPSKRPAPFNKDTKRILIHRGPAVNNQVGNPSA
    Consensus  lG.EaQEcrNWG.QidLF.YSApFRKvPQfITlFs#Y...LPDQH.YG.gNDPL.iQFGAIFP..t.Nl..rPApFgkDTrRiLirrGPg!yNQvgNPs.

             501      510       520       530       540       550       560       570       580       590       600
               |--------+---------+---------+---------+---------+---------+---------+---------+---------+---------|
  PorphP_ApcE  RSVSVGSLGPKVF------------KSEGINSNAQRTNNESILQASYLAVFGRMIYQNERIGLKGIDNKFLDNNLSVKELIRSLAISDTFRSLYWTPLYV
      Gp_ApcE  RAQVLPCLGPRIF------------SFKANKSKKNIVNLDQLKRAVYLRIFGRFLYSEELVCIKKFEEQFCSGKCSVRDFVRSLAKSSVFRALYWQPLYI
   S6803_ApcE  VGEFPGSLGAKVFRLNGGLPGAKVGKNTGTSVKFGESSTQALIRAAYRQVFGRDLYEGQRLSVAEIQLE--NGDISVREFIKRLAKSELFLKLYWAPHYV
    Consensus  r....gsLGpk!F............k..g..sk....n.#.l.rA.Yl.!FGR.lY..#r...k.i#..f..g..SVr#f!rsLAkS..Fr.LYW.PlY!

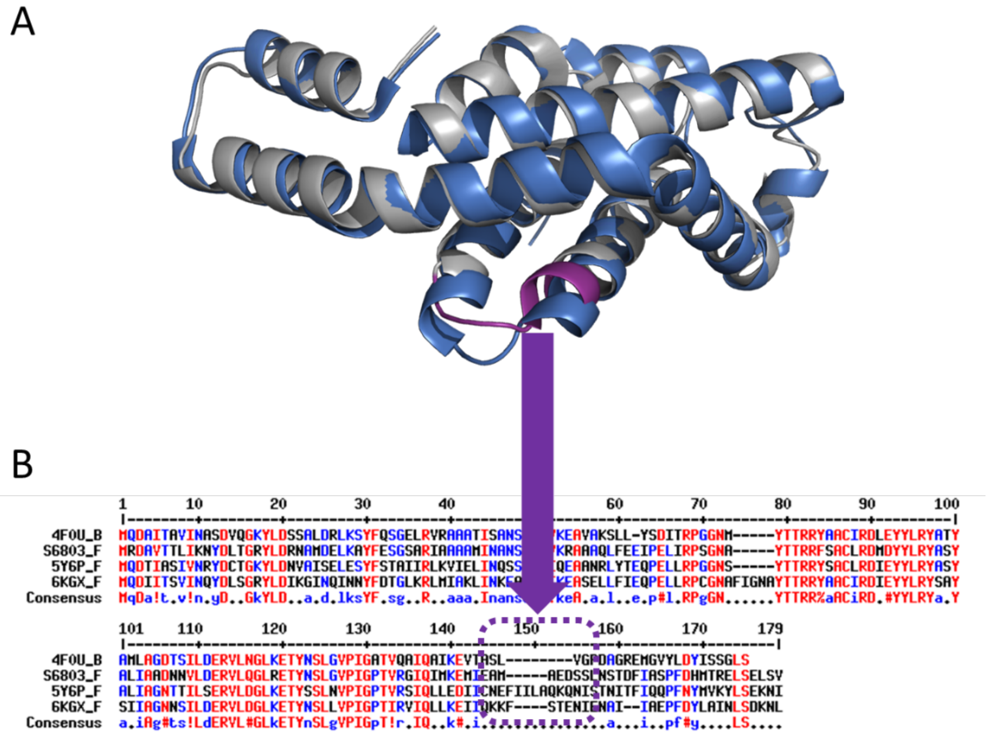
             601      610       620       630       640       650       660       670       680       690       700
               |--------+---------+---------+---------+---------+---------+---------+---------+---------+---------|
  PorphP_ApcE  CKSIEWIHYRLLGRPTYGRQEINQYFNVAYKKGFVGVINSIIDSVEYNECFGDNIVPYERYLTANSVSQRQLKLGNIIKS--ANLKPQNIEKFVQLGQSQ
      Gp_ApcE  CKAIEYIHVRLLGRPTYGRQEIDQYFNIVYKEGYYTMIDRIIDSREYTETFGSSIVPYERYLTSNTLISRKLGSNSVHNN--RSLKGIDSNNLANINQSV
   S6803_ApcE  CKAIEYMHRRLLGRPTYGRQEMNQYFDIASKQGFYAVVEAMIDSKEYSDAFGEDTVPYERYLTPGGLQMRSARVGSLREDIGQRVDKEVTPRFVELGQVS
    Consensus  CKaIEyiH.RLLGRPTYGRQEi#QYF#!ayK.G%y.v!#.iIDS.EY.#.FG..iVPYERYLT.n.l..R.l..gs........lk......fv#lgQs.

             701      710       720       730       740       750       760       770       780       790       800
               |--------+---------+---------+---------+---------+---------+---------+---------+---------+---------|
  PorphP_ApcE  TNQN----LYSIKYKVKQGVSKLRDQQKIFETKGSLSKDA-YLSIFQAACRQIFERDISTFVIGNEIENIKIQFIKGQISVKEMINALGKSSVYLKEFYN
      Gp_ApcE  NKDNRNLSIFNLKQRVSQGVTSRRDQLKIFEFCKEKNQPADTYQILRAIYRQVFERDINTFTVGDEFHNLEKAFLLNEITVQEVIEYLGCSKLYTKEFYQ
   S6803_ApcE  AIRTE----PEIAYRSNQGVTRQRQQTKVFKLVSTYDKVA-VKNAIRAAYRQVFERDLEPYIINSEFTALESKLSNNEINVKEFIEGLGTSELYMKEFYA
    Consensus  ...n.......ikyrv.QGVt..R#Q.K!Fe......k.A....i.rAayRQ!FERDi.t%.!g.Ef.nle..f..n#I.VkE.I#.LG.S.lY.KEFY.

             801      810       820       830       840       850       860       870       880       890       900
               |--------+---------+---------+---------+---------+---------+---------+---------+---------+---------|
  PorphP_ApcE  PYPNIKVIELGTKHFLGRAPNNQAEIRFYNQILASCGLQAFIDMLTNSQEYAEIFGEVRVPFRRFPTLPAANFPNTNTLFDKQTKQNSVVIVPSFKAITG
      Gp_ApcE  PYPNTKVIELGTKHFLGRAPSNQAEIRYYNQILASQGQVSFIKTLVNSIEYTALFGKNIVPYHRFPTLPAANFPNTQKLYNSLLKQSTQIIVPSFGNSVG
   S6803_ApcE  PYPNTKVIEMGTKHFLGRAPLNQKEIQQYNQILASQGLKAFIGAMVNGMEYLQTFGEDTVPYRRFPTLPAANFPNTERLYNKLTKQDKELVVPSFTPVVK
    Consensus  PYPNtKVIE$GTKHFLGRAP.NQaEIr.YNQILASqGl.aFI..$vNs.EY...FGe..VP%rRFPTLPAANFPNT#.L%#kltKQ....!VPSF...vg

             903
               |-|
  PorphP_ApcE  NQ
      Gp_ApcE  NQ
   S6803_ApcE  VGG
    Consensus  nq.
```

Fig. S2. Sequence analysis of ApcE. (A) Sequence alignment of ApcE from *Synechocystis* 6803, GpPBS (PDBID: 5Y6P), and PpPBS (PDBID: 6KGX). (B) Functional domains of ApcE (*Synechocystis* 6803).



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4F0U_B    MQDAITAVINASDVQGKYLDSSALDRLKSYFQSGELRVRAAATISANS[illegible]KEAVAKSLL-YSDITRPGGNM-----YTTRRYAACIRDLEYYLRYATY
S6803_F   MRDAVTTLIKNYDLTGRYLDRNAMDELKAYFESGSARIAAAAMINANS[illegible]KRAAAQLFEEIPELIRPSGNA-----YTTRRFSACLRDMDYYLRYASY
5Y6P_F    MQDTIASIVNRYDCTGKYLDNVAISELESYFSTAIIRLKVIELINQSS[illegible]QEAANRLYTEQPELLRPGGNS-----YTTRRYSACLRDIEYYLRYASY
6KGX_F    MQDIITSVINQYDLSGRYLDIKGINQINNYFDTGLKRLMIAKLINK[illegible]KEASELLFIEQPELLRPCGNAFIGNAYTTRRYAACIRDIEYYLRYSAY
Consensus MqDa!t.v!n.yD..GkYLD..a.d.lksYF.sg..R..aaa.Inans[illegible]keA.a.l..e.p#l.RPgGN......YTTRR%aACiRD.#YYLRYa.Y

4F0U_B    AMLAGDTSILDERVLNGLKETYNSLGVPIGATVQAIQAIKEVTASL--------VGPDAGREMGVYLDYISSGLS
S6803_F   ALIAADNNVLDERVLQGLRETYNSLGVPIGPTVRGIQIMKEMIEAM-----AEDSSLNSTDFIASPFDHMTRELSELSV
5Y6P_F    ALIAGNTTILSERVLDGLKETYSSLNVPIGPTVRSIQLLEDIICNEFIILAQKQNISTNITFIQQPFNYMVKYLSEKNI
6KGX_F    SIIAGNNSILDERVLDGLKETYNSLLVPIGPTIRVIQLLKEIIQKKF----STENIENAI--IAEPFDYLAINLSDKNL
Consensus a.iAg#ts!LdERVL#GLkETYnSLgVPIGpT!r.IQ..k#.i..................a...i..pf#y....LS....
```

Fig. S3. Structural variation of ApcF. (A) Protein structure and sequence alignment of sApcF-M1 (S6803), grey) onto the PpApcF (marine). Highlighted region (purple) is the hypervariable region. (B) The sequence alignment of PpApcF and sApcF. Main sequence/secondary structure difference is boxed.

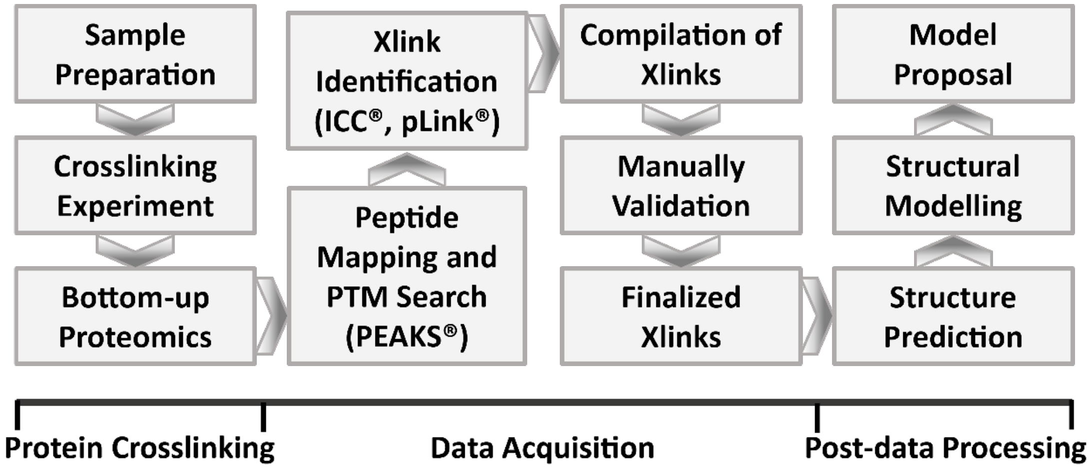

Fig. S4. Summarized workflow of this study.

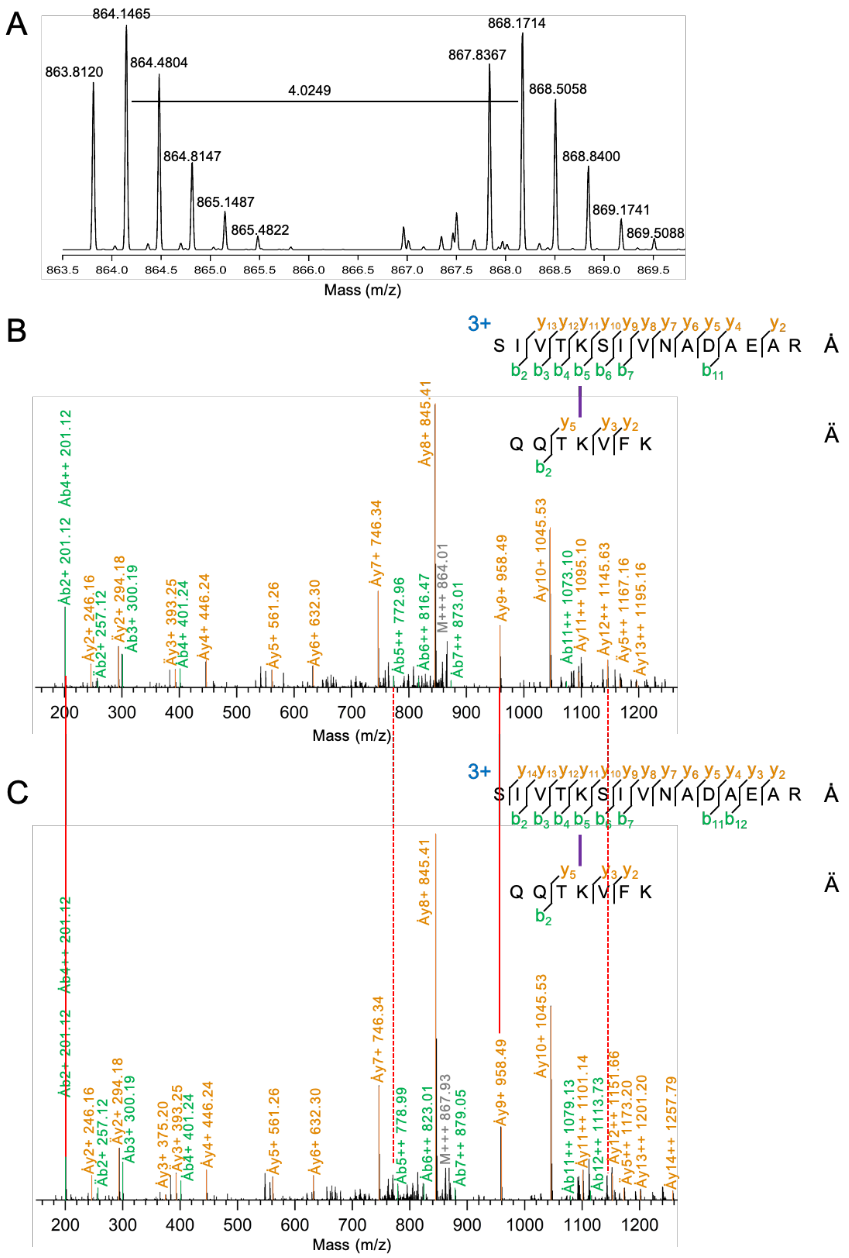

Fig. S5. MS and MS/MS spectra of cross-link ApcA-K6–ApcE-K722. (A) The MS1 spectra of the light and heavy cross-linked peptide (BS^3-H_{12}/D_{12}) which are separated by m/z 4.0249 (z=3). (B). MS/MS spectra of the cross-linked peptide (light). (C). MS/MS spectra of the cross-linked peptide (heavy). Note, e.g., m/z shift of ion Ȧb5++ (778.99) from C and ion Ȧb5++(772.96) from B is 6.03. The mass difference is 12.06 Da total. Ȧb2+ and Ȧb9+ are control ions (solid line from B to C) with identical m/z.

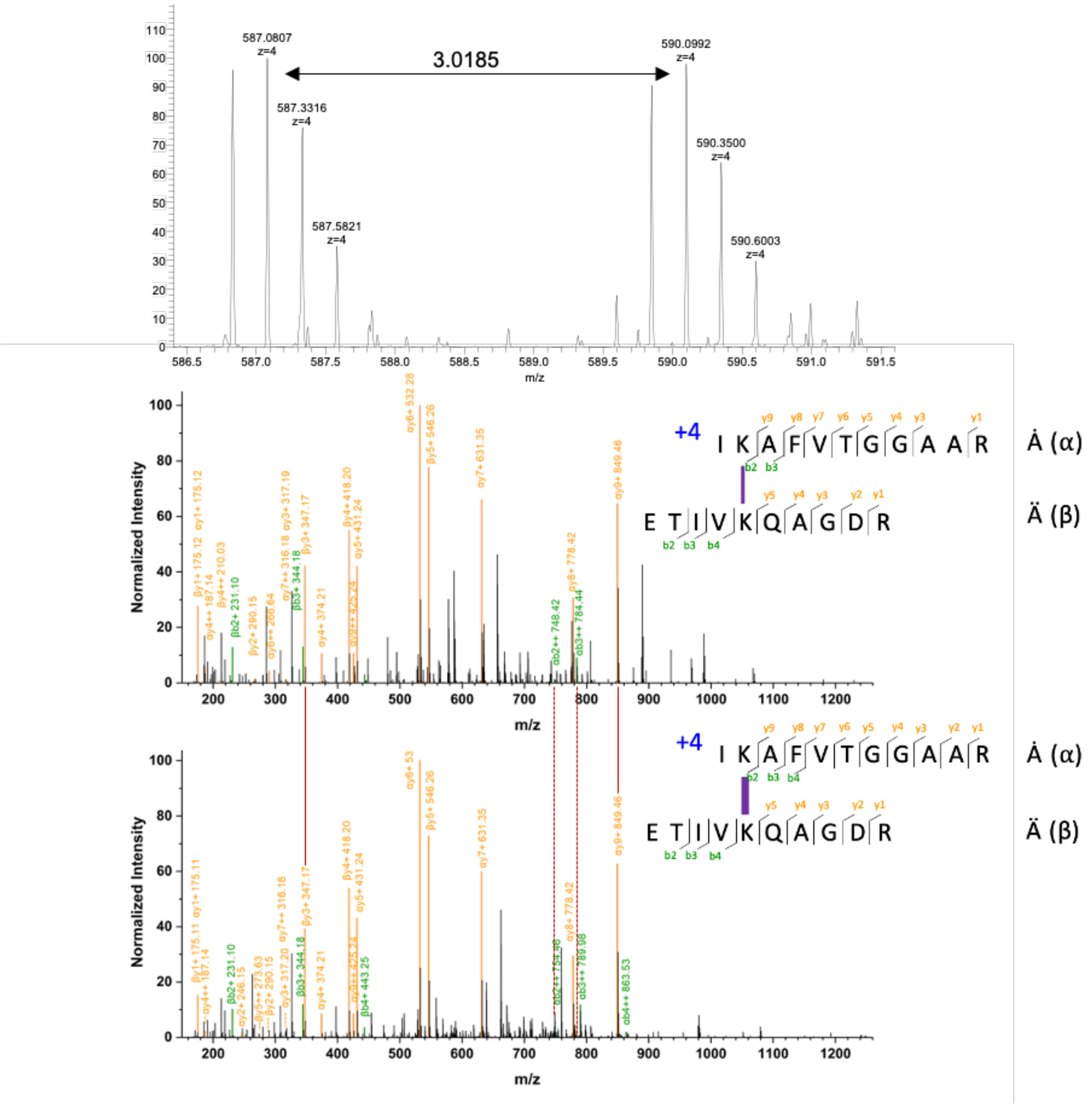

Fig. S6. MS and MS/MS spectra of cross-link ApcA-K27–ApcA-K52. (A) The MS1 spectrum of the light and heavy cross-linked peptide (BS^{3}-H$_{12}$/D$_{12}$) that are separated by m/z 3.0185 (z=4). (B). MS/MS spectrum of the cross-linked peptide (light). (C). MS/MS spectrum of the cross-linked peptide (heavy). Note, e.g., 6.04 m/z shift of fragment ion Ȧb2++ (748.42) from B to fragment ion Ȧb2++(754.46) from C is detected, indicating 12.08 Da mass difference from isotope labeling. Äy3+ and Ȧy9+ are control ions (solid line from B to C) with identical m/z.