# **Supporting Information**

## Zhao et al. 10.1073/pnas.1715495114

#### **SI Materials and Methods**

Cloning and Expression. All genetic manipulations are carried out according to standard protocols (1). Plasmids pACYC-ho1-pcyA for PCB and pET-cph1(1-514) have been reported (2-4). To facilitate purification via Ni<sup>2+</sup>-affinity chromatography as well as subsequent crystallization, cpcE, cpcF, and nblB from Nostoc are amplified by PCR (Table S4) and ligated into the expression vector pET30 (Novagen) via restriction sites NdeI and XhoI (Fermentas) for C-terminal fusion to a His<sub>6</sub> tag. Then  $cpcE(\Delta his-tag)$  and  $cpcF(\Delta his-tag)$ , in which the His<sub>6</sub> tag is deleted, are generated from cpcE and cpcF via PCR with primers P5-P8. cpcA and pecA from Nostoc are amplified via PCR with primers P9, P10, P11, and P12 and ligated into the expression vector pET30 (Novagen) via restriction sites NcoI and XhoI (Fermentas) for fusing an N-terminal His<sub>6</sub> tag. *cpcE* and *cpcF*, *pecE* and *pecF*, *nblB*, and *cpcF* are amplified by PCR (for primers see Table S4) and then cloned in the two cloning sites of pCDFDuet (Novagen) via restriction sites NcoI, PstI, NdeI, and XhoI (Fermentas), respectively. To analyze the structural effects on lyase activities of CpcE, CpcF, PecE, and PecF, sitedirected variants are constructed by using the MutanBEST kit (TaKaRa) with primers listed in Table S4.

For overexpression of the lyases and their variants, the respective plasmids (Table S5) are transformed into *Escherichia coli* BL21 (DE3) (Novagen). Cells are grown at 16 °C in Luria–Bertani (LB) medium supplemented with kanamycin (20  $\mu$ g/mL) and induced with isopropyl  $\beta$ -D-thiogalactoside (1 mM), and then growth is continued for an additional 12 h after induction. For chromophorylation, pET-derived expression vectors for CpcA or PecA are transformed into *E. coli* BL21 (DE3) (Novagen) containing the PCB-generating plasmid (pACYC-ho1-pcyA) and lyase-generating plasmid (pCDF-cpcE-cpcF, pCDF-pecE-pecF, or derivatives) (Table S5). The triply transformed cells are cultured at 16 °C in LB medium supplemented with kanamycin (20  $\mu$ g/mL), chloromycetin (17  $\mu$ g/mL), and streptomycin (25  $\mu$ g/mL). After induction with isopropyl  $\beta$ -D-thiogalactoside (1 mM) for 16 h, the cells are collected by centrifugation.

Cell pellets containing His-tagged CpcF and excessive CpcE( $\Delta$ his tag) lacking the His tag are resuspended in ice-cold potassium phosphate buffer (KPB; 20 mM, pH 7.3) containing 0.5 M NaCl and disrupted by five passages through a chilled French press at 1,200 bar. The suspension is centrifuged at 12,000 × g for 40 min at 4 °C. The supernatant containing crude proteins is purified via Ni<sup>2+</sup>-affinity chromatography and eluted by using KPB (20 mM, pH 7.3) containing 0.5 M NaCl and 0.5 M imidazole. After purification via Ni<sup>2+</sup>-affinity chromatography (5), the sample of the complex of CpcE and CpcF is dialyzed twice against KPB (20 mM, pH 7.3) containing 150 mM NaCl and subsequently purified further via gel filtration (HiLoad 16/600, Superdex 200; GE Healthcare) with elution of the same buffer at a flow rate of 1.0 mL/min.

**Protein Assays.** Protein concentrations are determined by the Bradford assay (6) and calibrated with BSA, and SDS/PAGE is performed with the buffer system of Laemmli (7). Proteins are stained with Coomassie brilliant blue, and those containing chromophores are identified by  $Zn^{2+}$ -induced fluorescence (8).

**Spectral Analyses.** All chromoproteins are investigated by UV-Vis absorption spectroscopy (Beckman-Coulter DU 800). Covalently bound chromophores are quantified after denaturation with acidic urea (8 M, pH 1.5) by their absorptions at 662 nm (PCB) by using an extinction coefficient of 35,500  $M^{-1}$ ·cm<sup>-1</sup> (9). Fluorescence spectra are recorded at room temperature with a F320 spectrofluorimeter (TianJin GangDong Sci and Tech Development Company).

**Oligomerization Analysis.** To determine the oligomeric state of the CpcE/F complex and its variants, the proteins are first purified by Ni<sup>2+</sup>-affinity chromatography. A total of 1.0 mL of the eluate is loaded on a Superdex 200 preparative grade column ( $60 \times 1.6$  cm) and developed (1.0 mL/min) with KPB (20 mM, pH 7.3) containing NaCl (0.15 M). The apparent molecular mass is determined by comparison with a marker set (12–443 kDa).

**Assay of Enzymatic Activities.** Relative enzymatic activities of CpcE/ F or PecE/F variants are compared with the respective wild-type lyases by a fluorescence assay, based on the fluorescence of the chromophorylated PBPs, with controls in the absence of the respective lyases and variants (5). Chromophorylated PBPs, PCB<sup>T</sup>-CpcA or PVB-PecA, were assembled in BL21(DE3) cells. After assembly, the relative amounts of the products are evaluated by their fluorescence emissions at 643 and 583 nm (10, 11), respectively.

Activity of PCB Binding to Lyases. To evaluate the relative activity of PCB binding, the purified complex of CpcE/F or its variants are incubated with PCB in KPB (0.5 M, pH 7.3) containing NaCl (0.5 M) for 1 h. The lyase is then purified by Ni<sup>2+</sup>-affinity chromatography, and the amount of bound PCB is quantitated by the fluorescence emission at 646 nm (10).

Assay of Chromophore Detachment Activities. The assay is based on chromophore transfer from covalently bound PCB<sup>T</sup>-CpcA to the apo-protein of the truncated phytochrome fragment, Cph1(1-514), of Cph1 from Synechocystis PCC 6803 (4), in the presence of NblB, CpcE, CpcF, and variants thereof (12). PCB<sup>T</sup>-CpcA (10  $\mu$ M) and Cph1(1–514) (20  $\mu$ M) are incubated at 37 °C with CpcE/F or variants (10 µM) in KPB (20 mM, pH 7.3) containing NaCl (150 mM), MgCl<sub>2</sub> (5 mM), and mercaptoethanol (5 mM). The transfer is followed by the decrease of absorption of PCB<sup>T</sup>-CpcA at 618 nm and the increase of absorption of PCB<sup>T</sup>-Cph1(1-514) at 658 nm. For measuring the related enzymatic parameters, the concentration of the donor holoprotein, PCB<sup>T</sup>-CpcA, is varied (0.5, 1.0, 2.0, 3.0, and 4.0  $\mu$ M) in a range well below that of the acceptor protein, Cph1(1-514), at 10 µM and, vice versa, by varying the concentration of the acceptor Cph1(1-514) (0.5, 1.0, 2.0, 3.0, and 4.0 µM) and maintaining the donor at 10 µM, while keeping all other conditions identical.

Crystallization and Data Collection. Initial screening for crystallization conditions of the purified CpcE/F complex is performed by using 96-well triple sitting drop plates (TTP Lab Tech; catalog no. 4150-05800) and commercial screening kits (PEGRx; Hampton Research). Crystallization droplets are prepared by mixing 200 nL of protein solution (15 mg/mL in 20 mM KPB, pH 7.3, and 0.15 M NaCl) with 200 nL of reservoir solution. They are equilibrated against 75 µL of the reservoir solution and stored at 293 K. Best diffracting crystals grow under conditions containing 0.1 M sodium acetate trihydrate (pH 4.8), 13% (wt/vol) PEG 10000 within 2 wk to a final size of  $150 \times 40 \times 20 \ \mu\text{m}^3$ . Selenomethionine-substituted CpcE/F (CpcE/F-SeMet) is prepared according to the standard protocol (13) via the CpcE/F preparation method. After purification, CpcE/F-SeMet (15 mg/mL in 20 mM KPB, pH 7.3, and 0.15 M NaCl) is crystallized similarly as described above. Best diffracting crystals grow under conditions containing 0.1 M sodium acetate trihydrate, pH 4.8, 10% (wt/vol) PEG 10000, and 20 mM spermidine within 2 wk to a final size of  $100 \times 30 \times 15 \ \mu m^3$ .

To cryoprotect CpcE/F crystals, the crystallization drops are covered with mineral oil (Sigma-Aldrich) before a single crystal is retrieved with a litho loop and flash-frozen in liquid nitrogen. Native and SAD X-ray diffraction data are collected from a single crystal in each case on beamline P11 or P13, DESY, EMBL (Hamburg, Germany). All diffraction data are processed with the XDS program package and scaled by using XSCALE (14). The crystal structure is determined by the SAD method (15) using the selenomethioninesubstituted crystals. The initial model is obtained using MRSAD on the Auto-Rickshaw server (16). The structure of native CpcE/F is determined by molecular replacement [Phaser in CCP4 (17) using CpcE/F-SeMet structure as starting model]. The structures of native CpcE/F are refined by iterative cycles of manual refinement using Coot and Refmac5 (18) from CCP4 suite (17). Data refinement statistics and model content are summarized in Table 1. The structure of complex of CpcE and CpcF from *Nostoc* is deposited at the Protein Data Bank (PDB ID code: 5N3U).

**Structure Analyses, Modeling and Docking.** Figures of protein structures are created by using PyMOL (https://pymol.org/2/) and Biovia Discovery studio (Version 16; accelrys.com/products/collaborative-science/biovia-discovery-studio/). Protein sequence alignments are created by using Clustal (www.clustal.org/).

The structures of PecE/F and of NblB from *Nostoc* are modeled by using the present crystal structure of CpcE/F from *Nostoc* as template (PDB ID code 5N3U), and those of apoproteins CpcA, CpcB, and PecA were modeled by using the respective crystal structures of holoproteins as template on the SWISS-MODEL server (19, 20). The structures were compared with the Swiss-PDBViewer (Version 4.1) (21).

For docking, the following components are used: CpcE/F (this work), PCB (ligand from the CpcT:PCB complex; PDB ID code 404S) (5), PecE/F (modeled *Nostoc* structure; this work), PCB<sup>T</sup>-CpcA [ $\alpha$ -subunit of CPC trimer from *T. elongatus* (PDB ID code 4ZIZ) (22)], and PecA modeled from holoprotein PEC from *M. laminosus* (PDB ID code 2J96) (23). The desired components (lyases and PCB) are combined for docking by using Auto-DockTools (24), and corresponding docking calculations are performed with AutoDock Vina (Version 1.1.2) (25). For the docking of CpcE/F and PCB, the center coordinates of the search box are 34, 27, -2.5 (*x*, *y*, *z*) defined from the N<sub>75</sub>Y<sub>76</sub> of CpcF, and

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the size of the box is  $20 \times 20 \times 20 \text{ Å}^3$ . For the docking of PecE/F and PCB, the center coordinates of the search box are 29.5, 30, -0.5 (*x*, *y*, *z*) defined from the H<sub>87</sub>C<sub>88</sub> of PecF, and the size of the box is  $20 \times 20 \times 20 \text{ Å}^3$ . A two-stage approach was used by first docking PCB to a lyase (CpcE/F or PecE/F), followed by docking of this complex to the respective target apoprotein, CpcA, CpcB, or PecA. The docking model of lyases (with PCB or without) and the respective target apoprotein or holoprotein are obtained by Hex (Version 8.0.0; hex.loria.fr/), and settings for docking are selected by default except correlation type (shape and electro) (26).

The docking is a fairly roundabout process. Firstly, the chromophore, PCB, is fit to the lyase, which in case of PecE/F is itself a simulated structure. We have assumed that no major structural change results in either case from chromophore binding. This complex is then docked onto empty CpcA that is modeled from the  $\alpha$ -subunit of the reported crystal structure of CPC (22). While there are many structures of chromophorylated PBPs in oligomer, there is only a single structure of an isolated subunit, PVB-PecA (23), and none of an apoprotein lacking the chromophore. The modeled CpcA seems to be slightly less structured than the holoprotein, which is in agreement with spectroscopic data (27, 28): The results of these dockings (Table S2, columns 3-5) reflect the uncertainties of the process. Besides the docking energy, several additional criteria have, therefore, been applied in selecting a likely structure of the complex formed between bilinloaded lyase and apo-PBP. First, the mutation data locate the chromophore in the cavity formed between the E and F subunits of the lyase. Therefore, the apoprotein was assumed to locate in the region of the large opening of this cavity, preferentially covering it up. Secondly, proton-donating residue(s) are close to the chromophore, thereby assisting the thiol addition. Thirdly, the chromophore is E-configured at the  $3,3^1$  double bond (5, 29). The stereochemistry of the product is then determined by which face of the chromophore locates near the binding cysteine. In no case, the best complex selected by these criteria (marked in green in Table S2) is the energetically most favorable one.

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**Fig. S1.** (*A*) The  $2F_o - F_c$  electron density maps (contoured at  $2\sigma$ ) of CpcE/F. (*B*) The electron density is clearly defined for most of the residues of CpcE (96%) and CpcF (82%). Owing to no or weak electron density for terminal or loop regions, 4% sequence of CpcE (N terminus and gap between h14 and h15) and 18% sequence of CpcF (N and C terminus) are not modeled (dashed lines). A total of 266 residues of CpcE (276 aa) and 170 residues of CpcF (208 aa; i.e., 200 aa of CpcF plus 8 aa of C-terminal His tag) of the heterodimer are resolved.



**Fig. S2.** (A) Homology between CpcE/F and PecE/F. (B) Structural comparison of CpcE/F (wheat/gray) and the modeled structure of PecE/F (chain A, cyan; chain B, blue). (C) Schematic structure, seen from the top into the cavity as in B. Curved lines indicate extended structures. The overall structures between CpcE/F and PecE/F overlap well. In the sequences, "h" marks amino acids forming helices. The isomerase motif (H<sub>87</sub>C<sub>88</sub>) is marked in red in the sequence and the structure. The motif is unique to PecF and, as verified by mutagenesis, necessary for isomerization activity of PecE/F.



**Fig. S3.** PCB chromophore transfer from PCB–CpcA to Cph1(1–514). PCB transfer from PCB–CpcA to Cph1(1–514) proceeded under the following reaction conditions: Cph1 (20  $\mu$ M) and PCB–CpcA (10  $\mu$ M) in KPB (20 mM, pH 7.3) containing NaCl (150 mM), MgCl<sub>2</sub> (5 mM), and mercaptoethanol (5 mM), in the presence of CpcE/F (solid line) or CpcE( $\Delta$ 2–10)/F (dashed line) (10  $\mu$ M) or with no lyases (dotted line). Spectra were monitored at *t* = 5 (*A*), 20 (*B*), 60 (*C*), and 100 (*D*) min, indicating nearly complete transfer in the presence of CpcE/F or CpcE( $\Delta$ 2–10)/F (*D*). The activity of CpcE( $\Delta$ 2–10)/F (dashed line) was remarkably increased compared with the wild-type lyase (solid line). Therefore, the poorly structured N terminus of CpcE may interfere with the detachment of PCB from PCB<sup>T</sup>–CpcA.



**Fig. 54.** Details of the docking complexes of CpcE/F (A–C) and PecE/F (*D*). Starting structures: CpcE/F (*Nostoc*; this work), PecE/F (*Nostoc*; modeled based on the former structure), apo-CpcA and apo-CpcB modeled from holoprotein CPC (PDB ID code 4ZIZ), and apo-PecA modeled from holoprotein PEC (PDB ID code 2J96). (*A*) Docking of PCB:CpcE/F to apo-CpcA; this corresponds to the encounter starting the chromophorylation process. CpcE, light brown; CpcF, gray; CpcA, light blue. (*B*) Docking of PCB<sup>T</sup>-CpcA (PDB ID code 4ZIZ) on CpcE/F this corresponds to the encounter starting chromophore detachment from PCB<sup>T</sup>-CpcA. Color coding is as in *A*. (*C*) Docking of PCB:CpcE/F on apo-CpcB; colors are as in *A*. (*D*) Docking of PCB:PecE/F to apo-PecA. This corresponds to the encounter starting chromophorylation of PecA. PecE, light brown; PecF, gray; PecA, purple. Numbers in black give distances (Å) indicated by the dotted lines. The detailed docking information and parameters are shown in Table S2.



Fig. S5. Simulated structure of NbIB (Alr3814) from *Nostoc*. (A) Homologies and secondary structure predictions for CpcE and NbIB. (B) Structure simulation of NbIB using CpcE from this work as template. Modeling was done by the SWISS-MODEL server (for details, see *SI Materials and Methods*). The simulated structure of NbIB (green) is generally very similar to that of CpcE (brown). It lacks, however, the N-terminal extended stretch (arm), the C-terminal helix 15, and the long loop (Val138–Pro147) between helices 7 and 8.

variants     mass (EP-nmer)     For dromo-phorylation     Por binding PCB     For detadning PCB       CpECFF     35 (1)     100     100     100       CpECF     35 (1)     0     0       CpECF     37 (1)     0     0       CpEC     37 (1)     0     0       CpECA-100/F     50 (1)     95     95     182.       CpECA-100/F     50 (1)     0     0     0       CpECA-100/F     90     5     3     0       CpECA-100/F     92     0     0     0       CpECA-100/F     92     0     0     0       CpECA-100/F     93     0     0     0       CpECA-100/F     93     0     0     0       CpECA-100/F     93     0     0     0     0		Oligomerization state		Relative activity	
CpcEFF     53 (1)     100     100     100       CpcE     37 (1)     0     0     0       CpcE     37 (1)     0     0     0       CpcE (3.2-10)/F     50 (1)     95     95     182       CpcE (3.2-10)/F)/F     33 (1)     0     33     4       NbB     45 (2)     0     51     0       NbB/CpcF     39 (2), 22 (1)     0     54     3       CpcE(83A)/F     102	Variants	mass (E/F- <i>n</i> -mer)	For chromo-phorylation	For binding PCB	For detaching PCB
CpcE/F*     53 (1)     0     0       CpcF     27 (1)     0     0       Cpcf(A2-10/n5)/F     50 (1)     95     95     182       Cpcf(A2-10/n5)/F     33 (1)     0     13     4       NbB     45 (2)     0     51     3       NbB     54 (2)     0     54     3       CpcE(BA)/F     80     2     2     2       CpcE(BA)/F     99     2     2     2       CpcE(BA)/F     99     2     2     2       CpCP(V35A)/F     98     2     2     2       CpCP(V35A)/F     99	CpcE/F	53 (1)	100	100	100
CpcE     37 (1)     0     0       CpcF     27 (1)     0     95     95     182       CpcE(2-10)F)     50 (1)     95     95     182       CpcE(2-10)F)     30 (1)     0     13     4       Nblach     45 (2)     0     51     0       Nblach     39 (2), 22 (1)     0     54     3       CpcEBAA/F     109     0     54     3       CpcEBAA/F     109     0     14     3       CpcEBAA/F     99     0     102     103     102       CpcEBAA/F     99     0     103	CpcE/F*	53 (1)	0		
CpcF     27 (1)     0     95     95     182       CpcE(22-10/n5)/F     33 (1)     0     13     4       Nbl8     45 (2)     0     51     0       Nbl8     45 (2)     0     54     3       CpcE(EA3/PF     80     3     3     3       CpcE(FA3/PF     109     2     2     3       CpcE(FA3/PF     99     2     2     3       CpcE(FA3/PF     99     2     2     2       CpcE(FA3/PF     108     2     2     2	CpcE	37 (1)	0		0
CpcE(22-10)F/SPF     50 (1)     95     95     182       Nbl8     45 (2)     0     51     0       Nbl8/CpcF     39 (2, 22 (1)     0     54     3       CpcEBA/F     109     54     3       CpcEBA/F     109     54     3       CpcEBA/F     109     54     3       CpcEBA/F     99     52     55       CpcEBA3D/F     99     52     55       CpcEPASAD/F     99     55     55       CpcEPASAD/F     99     55     55       CpcEPASAD/F     99     55     55       CpcEPASAD/F     99     56     56       CpEPASAD/F     99     56     56       CpEPASAD/F     99     57     56       CpcEPASAD/F     99     57     57       CpcEPASAD/F     99     57     57       CpcEPASAD/F     99     57     57       CpcEPASAD/F     99     57     57       CpcEPASAD/F	CpcF	27 (1)	0		0
CpcE(2A-10/h15)/F     33 (1)     0     13     4       NbB     45 (2)     0     51     0       NbB/CpcF     39 (2), 22 (1)     0     54     3       CpcE(BAN/F     109     54     3       CpcE(BAN/F     109     54     3       CpcE(M3A/A/F     99     5     5       CpcE(M3A/F     99     5     5       CpcE(M3A/F)     98     5     5       CpcE(M3A/A/F)     98     5     5       CpcE(M3A/F)     99     6     5       CpcE(M3A/F)     99     7     103     7       CpcE(M3A/F)     99     7     103     103	CpcE(∆2–10)/F	50 (1)	95	95	182
NbB     45 (2)     0     51     0       VBB/CpCF     39 (2), 22 (1)     0     54     3       CpCEBA/F     109	CpcE(∆2–10/ <i>h15</i> )/F	33 (1)	0	13	4
Nbl8(CpcF     39 (2), 22 (1)     0     54     3       CpcE(F3A)/F     109     109     100	NblB	45 (2)	0	51	0
CpcElBA//F 80 CpcElBA//F 102 CpcElBA//F 102 CpcElBA//F 99 CpcElBA//F 99 CpcElBA//F 99 CpcElBA//F 99 CpcElBA//F 98 CpcElBA//F 98 CpcElBA//F 98 CpcElBA//F 98 CpcElBA//F 99 CpcElBA//F 99 CpcElBA//F 99 CpcElBA//F 99 CpcElBA//F 99 CpcElBA//F 99 CpcElBA//F 99 CpcElBA//F 99 CpcElBA//F 99 CpcElBA//F 90 CpcElBA//F 90	NblB/CpcF	39 (2), 22 (1)	0	54	3
CpcE(H3A)/F     109       CpcE(H3A)/F     102       CpcE(H3A)/F     99       CpCE(H3A)/F     90       CpCE(H3A)/F     92       CpCE(H3A)/F     92       CpCE(H3A)/F     92       CpCE(H3A)/F     92       CpCE(H3A)/F     93       CpCE(H3A)/F     94       CpCE(H3A)/F     93       CpCE(H3A)/F     94       CpCE(H3A)/F     93       CpCE(H3A)/F     94       CpCE(H3A)/F     93       CpCE(H3A)/F     94	CpcE(E8A)/F		80		
CpcE(133K)/F     102       CpcE(133K)/F     99       CpcE(133K)/F     90       CpcE(133K)/F     92       CpcE(133K)/F     98       CpcE(133K)/F     98       CpcE(133K)/F     98       CpcE(133K)/F     99       CpcE(133K)/F     99       CpcE(133K)/F     99       CpcE(143A)/F     88       CpcE(143A)/F     99       CpcE(143A)/F     99       CpcE(143A)/F     99       CpcE(143A)/F     81       CpcE(143A)/F     99       CpcE(143A)/F     108       CpcE(143A)/F     108       CpcE(145A)/F     108       CpcE(145A)/F     101       CpcE(145A)/F     101       CpcE(145A)/F     102       CpcE(145A)/F     103       CpcE(145	CpcE(F9A)/F		109		
CµCL(%34A)/P     99       CµCL(%35A)/F     90       CµCL(%35A)/F     92       CµCL(%35A)/F     98       CµCL(%35A)/F     98       CµCL(%35A)/F     88       CµCL(%35A)/F     99       CµCL(%43A)/F     90       CµCL(%43A)/F     91       CµCL(%43A)/F     92       CµCL(%75A)/F     10       CµCL(%75A)/F     92       CµCL(%75A)/F     93       CµCL(%7A)/F     93       CµCL(%7A)/F     93       CµCL(%7A)/F	CpcE(L33R)/F		102		
CPCE(TASA)/F     90       CpCE(Y3SA)/F     92       CpCE(Y3SA)/F     98       CpCE(Y3SA)/F     98       CpCE(Y3SA)/F     86       CpCE(Y3SA)/F     86       CpCE(Y3SA)/F     99       CpCE(YASA)/F     90       CpCE(YASA)/F     90       CpCE(YASA)/F     90       CpCE(YASA)/F     90       CpCE(YASA)/F     91       CpCE(YASA)/F     103       CpCE(YASA)/F     103       CpCE(YASA)/F     91       CpCE(YASA)/F     92       CpCE(YASA)/F     93       CpCE(YASA)/F     93       CpCE(YASA)/F     93       CpCE(YASA)/F     93       CpCE(YASA)/F     104       CpCE(YASA)/F     105       CpCE(YASA)/F	CpcE(R34A)/F		99		
CPCL(1)35/W     92       CpCL(Y)35/WF     93       CpCL(Y)36/WF     95       CpCL(W)36/WF     77       DCPC(W)35/WF     47 (1)       CpCL(W)36/WF     99       CpCL(W)36/WF     99       CpCL(W)36/WF     99       CpCL(W)36/WF     99       CpCL(W)36/WF     99       CpCL(W)35/WF     99       CpCL(W)35/WF     99       CpCL(W)35/WF     99       CpCL(W)35/WF     99       CpCL(W)35/WF     99       CpCL(W)35/WF     90       CpCL(W)35/WF     90       CpCL(W)35/WF     103       CpCL(W)35/WF     91       CpCL(W)36/WF     92       CpCL(W)36/WF     92       CpCL(W)36/WF     92       CpCL(W)36/WF     93       CpCL(W)36/WF     93       CpCL(W)36/WF     93       CpCL(W)36/WF     93       CpCL(W)36/WF     93       CpCL(W)36/WF     93       CpCL(W)36/WF     94       CpCL(W)36/WF	CpcE(N34D)/F		50		
CPC1V136A)/F     25       CPC1V136A)/F     86       CPC1V136A)/F     77       CPC1V136A)/F     82       CPC1V136A)/F     82       CPC1V136A)/F     99       CPC1V136A)/F     99       CPC1V136A)/F     81       CPC1V136A)/F     99       CPC1V136A)/F     90       CPC1V136A)/F     91       CPC1V136A)/F     93       CPC1V136A)/F     93       CPC1V136A)/F     93       CPC1V13A)/F     94       CPC1V113A)/F     93       CPC1V10A)/F     9	CpcE(Y35R)/F		98		
CpcE(Y36/V)F     36       CpcE(W30A)/F     47 (1)     77     103       CpcE(W40A)/F     82     103       CpcE(W43A)/F     98     100       CpcE(W43A)/F     99     100       CpcE(W43A)/F     81     100       CpcE(W43A)/F     99     100       CpcE(W43A)/F     99     100       CpcE(W75A)/F     90     100       CpcE(W75A)/F     90     100       CpcE(W75A)/F     50 (1)     94     72       CpcE(W75A)/F     50 (1)     27     10       CpcE(W75A)/F     50 (1)     27     10       CpcE(W75A)/F     51     101     101       CpcE(W75A)/F     98     100     100       CpcE(W75A)/F     93     100     100       CpcE(W75A)/F     93     100     100       CpcE(W16A)/F     93     100     100       CpcE(W16A)/F     93     100     100       CpcE(W16A)/F     93     100     100       CpcE	CpcE(Y36A)/F		95		
CpcE(W33A)/F     47 (1)     77     103       CpcE(W43A)/F     82        CpcE(W43A)/F     99        CpcE(W43A)/F     99        CpcE(W43D)/F     108        CpcE(W75D)/F     50 (1)     27     10       CpcE(W75D)/F     52 (1)     27     10       CpcE(W75A)/F     98         CpcE(W75A)/F     93         CpcE(W75A)/F     92         CpcE(W33D)/F     93         CpcE(W75A)/F     93         CpcE(W103A)/F     93         CpcE(W103A)/F     93         CpcE(W103A)/F     93	CpcE(Y36R)/F		86		
CpcE(W40A)/F     82       CpcE(W43A)/F     98       CpcE(W43A)/F     99       CpcE(W43A)/F     81       CpcE(W43D)/F     99       CpcE(W43D)/F     99       CpcE(W45D)/F     99       CpcE(W75A)/F     99       CpcE(W75A)/F     108       CpcE(W75A)/F     50 (1)     94       CpcE(W75A)/F     50 (1)     94       CpcE(W75A)/F     50 (1)     94       CpcE(W75A)/F     50 (1)     94       CpcE(W75A)/F     51     10       CpcE(W75A)/F     98     CpcE(W75A)/F       CpcE(W75A)/F     98     CpcE(W75A)/F       CpcE(W3A)/F     93     CpcE(W3A)/F       CpcE(W3A)/F     93     CpcE(W10A)/F       CpcE(W10A)/F     93     CpcE(W11A)/F       CpcE(W11A)/F     90     Cp	CpcE(W39A)/F	47 (1)	77	103	
CpcE(K43A)/F     98       CpcE(K43A)/F     99       CpcE(K43A)/F     81       CpcE(K43A)/F     88       CpcE(K45A)/F     99       CpcE(K45A)/F     94       CpcE(K45A)/F     94       CpcE(K75A)/F     50 (1)     94       CpcE(K75A)/F     50 (1)     27       CpcE(K75A)/F     52 (1)     27       CpcE(K75A)/F     52 (1)     71       CpcE(K75A)/F     98     CpcE(K75A)/F       CpcE(K75A)/F     93     CpcE(K75A)/F       CpcE(K75A)/F     93     CpcE(K16A)/F       CpcE(C9A)/F     93     CpcE(K16A)/F       CpcE(K10A)/F     93     CpcE(K16A)/F       CpcE(K116A)/F     93     CpcE(K116A)/F       CpcE(K116A)/F     94     CpcE(K116A)/F       CpcE(K116A)/F     93     CpcE(K116A)/F       CpcE(K116A)/F     94     CpcE(K116A)/F       CpcE(K116A)/F     100     CpcE(K116A)/F       CpcE(K116A)/F     101     CpcE(K116A)/F       CpcE(K116A)/F     104     CpcE(K116A)/F<	CpcE(W40A)/F		82		
CpcE(K43D)/F     99       CpcE(K43D)/F     81       CpcE(K43D)/F     99       CpcE(K45D)/F     99       CpcE(K45D)/F     99       CpcE(K45D)/F     99       CpcE(K45D)/F     90       CpcE(K75A)/F     108       CpcE(K75A)/F     50 (1)     94       CpcE(K75A)/F     50 (1)     94       CpcE(K75A)/F     50 (1)     94       CpcE(K75A)/F     50 (1)     94       CpcE(K75A)/F     98     0       CpcE(K75A)/F     103     0       CpcE(K75A)/F     103     0       CpcE(K3B3D)/F     92     0       CpcE(K106A)/F     92     0       CpcE(K106A)/F     93     0       CpcE(K106A)/F     93     0       CpcE(K106A)/F     93     0       CpcE(K11AA)/F     100     0       CpcE(K11AA)/F     129     0       CpcE(K11AA)/F     106     0       CpcE(K11AA)/F     106     0       CpcE(K11AA)/F	CpcE(K43A)/F		98		
CpcE(P44A)/F     81       CpcE(P44A)/F     88       CpcE(P45A)/F     99       CpcE(P45A)/F     94       CpcE(P47A)/F     50 (1)     94       CpcE(P5A)/F     50 (1)     94       CpcE(P5A)/F     50 (1)     94       CpcE(P5A)/F     52 (1)     27     10       CpcE(P5A)/F     52 (1)     27     10       CpcE(P5A)/F     52 (1)     27     10       CpcE(P3A)/F     98     CpcE(P3A)/F     98       CpcE(P3A)/F     94     20     CpcE(P3A)/F       CpcE(P3A)/F     92     CpcE(P3A)/F     20       CpcE(P3A)/F     92     CpcE(P3A)/F     20       CpcE(P3A)/F     93     CpcE(P3A)/F     20       CpcE(P10A)/F     93     CpcE(P3A)/F     20       CpcE(P10A)/F     93     CpcE(P3A)/F     20       CpcE(P3A)/F     94     CpcE(P3A)/F     20       CpcE(P3A)/F     106     CpcE(P3A)/F     20       CpcE(P3A)/F     106     CpcE(P3A)/F <td< td=""><td>CpcE(K43D)/F</td><td></td><td>99</td><td></td><td></td></td<>	CpcE(K43D)/F		99		
CpcE(R45A)/F     88       CpcE(R45A)/F     99       CpcE(R45A)/F     108       CpcE(R45A)/F     108       CpcE(R45A)/F     50 (1)     94       CpcE(R45A)/F     50 (1)     97       CpcE(R45A)/F     52 (1)     27       CpcE(R45A)/F     52 (1)     27       CpcE(R45A)/F     98	CpcE(Y44A)/F		81		
CpcE(B4SD)/F     99       CpcE(B4SD)/F     94       CpcE(B7SA)/F     50 (1)     94     72       CpcE(B7SA)/F     50 (1)     27     10       CpcE(B7SA)/F     52 (1)     27     10       CpcE(B7SA)/F     98	CpcE(R45A)/F		88		
CpcE(D64R)/F     94       CpcE(R75A)/F     50 (1)     94     72       CpcE(R75D)/F     52 (1)     27     10       CpcE(R75D)/F     52 (1)     27     10       CpcE(R75D)/F     52 (1)     27     10       CpcE(R79D)/F     81	CpcE(R45D)/F		99		
CpcE(R57A)/F     50 (1)     94     72       CpcE(R75A)/F     50 (1)     27     10       CpcE(R75D)/F     52 (1)     27     10       CpcE(R75A)/F     81         CpcE(R75A)/F     98         CpcE(R79D)/F     71         CpcE(R78D)/F     94         CpcE(R58D)/F     92         CpcE(C96A)/F     93         CpcE(C106A)/F     93         CpcE(R10A)/F     93         CpcE(10A)/F     93         CpcE(R116A)/F     93         CpcE(R11A)/F     93         CpcE(R11A)/F     94         CpcE(R116A)/F     106         CpcE(R149A)/F     106         CpcE(R18AA)/F     106         CpcE(R18AA)/F     50 (1)     62	CpcE(D64R)/F		94		
CpcE(R75A)/F     50 (1)     94     72       CpcE(R75A)/F     52 (1)     27     10       CpcE(R75A)/F     81     10       CpcE(R79A)/F     98     10       CpcE(R79A)/F     98     10       CpcE(R79A)/F     103     10       CpcE(R3A)/F     92     10       CpcE(R3A)/F     92     10       CpcE(P3A)/F     93     10       CpcE(P105A)/F     94     10       CpcE(P105A)/F     129     10       CpcE(P105A)/F     129     10       CpcE(P105A)/F     100     10       CpcE(P105A)/F     89     10       CpcE(P105A)/F     50 (1)     62       CpcE(P105A)/F     50     10 <td< td=""><td>CpcE(E67A)/F</td><td></td><td>108</td><td></td><td></td></td<>	CpcE(E67A)/F		108		
CpcE(R75D)/F     52 (1)     27     10       CpcE(R75D)/F     81	CpcE(R75A)/F	50 (1)	94	72	
CpcE(R/P6A)/F   81     CpcE(R/P6A)/F   98     CpcE(R/P6A)/F   103     CpcE(K83A)/F   103     CpcE(K83D)/F   92     CpcE(C96A)/F   82     CpcE(V103A)/F   93     CpcE(V103A)/F   94     CpcE(V103A)/F   94     CpcE(V114A)/F   94     CpcE(V114A)/F   94     CpcE(V114A)/F   100     CpcE(V114A)/F   100     CpcE(V114A)/F   106     CpcE(V114A)/F   89     CpcE(V114A)/F   89     CpcE(V114A)/F   89     CpcE(V114A)/F   80     CpcE(V114A)/F   89     CpcE(V114A)/F   89     CpcE(V114A)/F   89     CpcE(V114A)/F   90     CpcE(V114A)/F   89 </td <td>CpcE(R75D)/F</td> <td>52 (1)</td> <td>27</td> <td>10</td> <td></td>	CpcE(R75D)/F	52 (1)	27	10	
CpcE(R79A)/F   98     CpcE(R79D)/F   71     CpcE(R79D)/F   103     CpcE(K83D)/F   94     CpcE(C96A)/F   92     CpcE(C96A)/F   93     CpcE(C96A)/F   93     CpcE(C106A)/F   93     CpcE(C106A)/F   93     CpcE(C10A)/F   93     CpcE(C10A)/F   93     CpcE(C10A)/F   94     CpcE(C10A)/F   129     CpcE(C10A)/F   126     CpcE(C10A)/F   106     CpcE(C18A)/F   89     CpcE(C18A)/F   89     CpcE(C120A)/F   51     CpcE(C120)/F   52 (1)     CpcE(C123A)/F   90     CpcE(C123A)/F   90     CpcE(C123A)/F   51     CpcE(C123A)/F   90     CpcE(C123A)/F   90	CpcE(N76A)/F		81		
CpcE(R/9D)/F   71     CpcE(R83A)/F   103     CpcE(R83D)/F   94     CpcE(C96A)/F   92     CpcE(C199A)/F   82     CpcE(V103A)/F   93     CpcE(E106A)/F   95     CpcE(E106A)/F   93     CpcE(E113A)/F   98     CpcE(E113A)/F   98     CpcE(E114A)/F   94     CpcE(E114A)/F   94     CpcE(E115A)/F   129     CpcE(E149A)/F   85     CpcE(E149A)/F   110     CpcE(E18AA)/F   106     CpcE(E18AA)/F   90     CpcE(E18AA)/F   90     CpcE(E12A)/F   50 (1)   65     CpcE(E12A)/F   89   51     CpcE(E12A)/F   89   51     CpcE(E12A)/F   89   51     CpcE(E12AA)/F   89   51	CpcE(R79A)/F		98		
CpcE(K83A)/F   103     CpcE(C96A)/F   92     CpcE(C96A)/F   82     CpcE(106A)/F   93     CpcE(106A)/F   93     CpcE(106A)/F   93     CpcE(106A)/F   93     CpcE(110A)/F   93     CpcE(110A)/F   93     CpcE(110A)/F   94     CpcE(116A)/F   94     CpcE(116A)/F   129     CpcE(116A)/F   129     CpcE(E149A)/F   126     CpcE(E149A)/F   110     CpcE(R177A)/F   110     CpcE(R17A)/F   106     CpcE(R184A)/F   89     CpcE(R184A)/F   90     CpcE(R184A)/F   90     CpcE(R184A)/F   90     CpcE(R12D)/F   52 (1)   18     CpcE(R12A)/F   90     CpcE(R12A)/F   9	CpcE(R/9D)/F		71		
CptE(108A)/F   94     CptE(108A)/F   92     CptE(108A)/F   93     CptE(10A)/F   94     CptE(10A)/F   104     CptE(10A)/F   89     CptE(10A)/F   89     CptE(10A)/F   80     CptE(10A)/F   90     CptE(10A)/F   51     CptE(12A)/F   90     CptE(12A)/F	CpcE(K83A)/F		103		
CpcE(C99A)/F 92   CpcE(C99A)/F 93   CpcE(P103A)/F 98   CpcE(P103A)/F 129   CpcE(P103A)/F 129   CpcE(P103A)/F 126   CpcE(P103A)/F 110   CpcE(P103A)/F 110   CpcE(P103A)/F 106   CpcE(P103A)/F 89   CpcE(P104A)/F 89   CpcE(P12A)/F 50 (1)   CpcE(P212A)/F 50 (1)   CpcE(P212A)/F 50 (1)   CpcE(P212A)/F 51   CpcE(P212A)/F 90   CpcE(P39A)/F 89   CpcE(P23A)/F 90   CpcE(P23A)/F 90   CpcE(P23A)/F 90   CpcE(P23A)/F 90   CpcE(P23A)/F 90   CpcE(P23A)/F 90   CpcE(P23A)/F 104   CpcE(P23A)/F 104   CpcE(P23A)/F 104   CpcE(P23A)/F 104	CpcE(K83D)/F		94		
CpcE(103A)/F   93     CpcE(103A)/F   93     CpcE(113A)/F   93     CpcE(113A)/F   93     CpcE(113A)/F   93     CpcE(113A)/F   98     CpcE(113A)/F   98     CpcE(114A)/F   65     CpcE(114A)/F   129     CpcE(149A)/F   126     CpcE(153A)/F   126     CpcE(1177A)/F   110     CpcE(1177A)/F   106     CpcE(18AA)/F   89     CpcE(18AA)/F   89     CpcE(18AA)/F   89     CpcE(12A)/F   50 (1)   62     CpcE(12A)/F   90   65     CpcE(12A)/F   90   6	CpcE(C90A)/F		52 87		
CpcE(E106A)/F   95     CpcE(E113A)/F   93     CpcE(E113A)/F   98     CpcE(E113A)/F   98     CpcE(E113A)/F   94     CpcE(E140F)/F   129     CpcE(E140PA)/F   85     CpcE(E140PA)/F   126     CpcE(E140A)/F   110     CpcE(E140A)/F   84     CpcE(E18AA)/F   106     CpcE(R177A)/F   106     CpcE(R18AA)/F   90     CpcE(R18AA)/F   90     CpcE(R12D)/F   50 (1)   62     CpcE(R12D)/F   50 (1)   62     CpcE(R212A)/F   50 (1)   89     CpcE(R212A)/F   50 (1)   80     CpcE(R212D)/F   52 (1)   18     CpcE(R212D)/F   52 (1)   89     CpcE(R212D)/F   90   104     CpcE(R24A)/F   90   104     CpcE(R24A)/F   104   104     CpcE(R24A)/F   104   104     CpcE(R24A)/F   104   104     CpcE(R24A)/F   104   104     CpcE(F(N44A)   93   104	CpcE(Y103A)/F		93		
CpcE(0110A)/F   93     CpcE(113A)/F   98     CpcE(M114A)/F   65     CpcE(M114A)/F   94     CpcE(G140F)/F   129     CpcE(E13A)/F   126     CpcE(R177A)/F   110     CpcE(R177A)/F   106     CpcE(R18AD)/F   89     CpcE(R18AD)/F   90     CpcE(R18AD)/F   90     CpcE(R12A)/F   50 (1)     CpcE(R12A)/F   51     CpcE(R12A)/F   51     CpcE(R212A)/F   90     CpcE(R212A)/F   52 (1)     CpcE(R212A)/F   51     CpcE(R212A)/F   90     CpcE(R212A)/F   90     CpcE(R212A)/F   51     CpcE(R212A)/F   90     CpcE(R212A)/F   90     CpcE(R212A)/F   90     CpcE(R212A)/F   104     CpcE(R212A)/F   104     CpcE(R212A)/F   104     CpcE(R212A)/F   89     CpcE(R212A)/F   104     CpcE(R212A)/F   104     CpcE(R212A)/F   104     CpcE(R212A)/F	CpcE(F106A)/F		95		
CpcE(E113A)/F   98     CpcE(M114A)/F   65     CpcE(K116A)/F   94     CpcE(G140F)/F   129     CpcE(E149A)/F   85     CpcE(E153A)/F   126     CpcE(R177A)/F   106     CpcE(R184A)/F   89     CpcE(R184A)/F   106     CpcE(R184A)/F   90     CpcE(R184A)/F   90     CpcE(R12A)/F   51     CpcE(R12A)/F   51     CpcE(R12A)/F   95     CpcE(R212A)/F   90     CpcE(R212A)/F   90     CpcE(R212A)/F   51     CpcE(R212A)/F   95     CpcE(R212A)/F   90     CpcE(L276A)/F   104     CpcE(L276A)/F   104     CpcE(L276A)/F   104     CpcE(L276A)/F   104     CpcE(L276A)/F   1	CpcE(O110A)/F		93		
CpcE(M114A)/F   65     CpcE(K116A)/F   94     CpcE(G140F)/F   129     CpcE(E149A)/F   85     CpcE(E153A)/F   126     CpcE(R177A)/F   110     CpcE(R17A)/F   106     CpcE(R184A)/F   90     CpcE(R184A)/F   90     CpcE(R184A)/F   89     CpcE(R12A)/F   50 (1)   62     CpcE(R212A)/F   50 (1)   62     CpcE(R212A)/F   50 (1)   89     CpcE(R212A)/F   50 (1)   89     CpcE(R212A)/F   50 (1)   80     CpcE(R212A)/F   50 (1)   80     CpcE(R212A)/F   90   51     CpcE(R212A)/F   90   51     CpcE(R239A)/F   89   51     CpcE(R239A)/F   89   51     CpcE(R243A)/F   90   64     CpcE(R243A)/F   90   64     CpcE(R243A)/F   104   64     CpcE(L276A)/F   89   64     CpcE(L276A)/F   120   65     CpcE/F(N4AA)   93   64	CpcE(E113A)/F		98		
CpcE(K116A)/F   94     CpcE(G140F)/F   129     CpcE(E149A)/F   85     CpcE(E153A)/F   126     CpcE(R177A)/F   110     CpcE(C180A)/F   84     CpcE(R184A)/F   06     CpcE(R184A)/F   90     CpcE(R184A)/F   90     CpcE(R184A)/F   90     CpcE(R184A)/F   65     CpcE(R212A)/F   50 (1)   62   65     CpcE(R212A)/F   50 (1)   62   65     CpcE(R212A)/F   50 (1)   89   90     CpcE(R212A)/F   50 (1)   89   51     CpcE(R212A)/F   90   51   90     CpcE(I217A)/F   90   90   90     CpcE(I217A)/F   90   90   90     CpcE(I22A)/F   90   90   90     CpcE(I24A)/F   90   90   90     CpcE(I276A)/F   89   90   90     CpcE(I276A)/F   89   90   90     CpcE(I276A)/F   89   90   90     CpcE(I276A)/F   89   9	CpcE(M114A)/F		65		
CpcE(G140F)/F   129     CpcE(E149A)/F   85     CpcE(E153A)/F   126     CpcE(R177A)/F   110     CpcE(C180A)/F   84     CpcE(R184A)/F   106     CpcE(R184D)/F   89     CpcE(R184D)/F   90     CpcE(R184D)/F   86     CpcE(R12A)/F   50 (1)   62     CpcE(R212A)/F   50 (1)   62     CpcE(R212A)/F   50 (1)   62     CpcE(R212A)/F   50 (1)   89     CpcE(R212A)/F   50 (1)   89     CpcE(R212A)/F   50 (1)   89     CpcE(L27A)/F   95   51     CpcE(F239A)/F   90   90     CpcE(I242A)/F   90   90     CpcE(I242A)/F   90   90     CpcE(I242A)/F   90   90     CpcE(I242A)/F   104   93     CpcE(L276D)/F   120   93     CpcE/F(N44A)   93   93     CpcE/F(N45A)   108   94	CpcE(K116A)/F		94		
CpcE(E149A)/F   85     CpcE(E153A)/F   126     CpcE(R177A)/F   110     CpcE(C180A)/F   84     CpcE(R184A)/F   106     CpcE(R184A)/F   90     CpcE(R184A)/F   90     CpcE(Q188A)/F   90     CpcE(R212A)/F   50 (1)   62     CpcE(R212A)/F   50 (1)   62     CpcE(R212A)/F   50 (1)   89     CpcE(R212A)/F   50 (1)   81     CpcE(R212A)/F   50 (1)   82     CpcE(R212A)/F   50 (1)   81     CpcE(R212A)/F   90   51     CpcE(R212A)/F   90   51     CpcE(F239A)/F   89   51     CpcE(I242A)/F   90   90     CpcE(I242A)/F   90   90     CpcE(K245A)/F   104   91     CpcE(L276A)/F   89   90     CpcE(L276A)/F   89   90     CpcE(L276A)/F   104   93     CpcE/F(N44A)   93   93     CpcE/F(N45A)   108   90     CpcE/F(N45A)   108	CpcE(G140F)/F		129		
CpcE(E153A)/F   126     CpcE(R177A)/F   110     CpcE(C180A)/F   84     CpcE(R184A)/F   106     CpcE(R184A)/F   90     CpcE(Q188A)/F   90     CpcE(N209A)/F   86     CpcE(R212A)/F   50 (1)   62     CpcE(R212A)/F   50 (1)   62     CpcE(R212A)/F   50 (1)   89     CpcE(R212A)/F   50 (1)   80     CpcE(R212A)/F   50 (1)   81     CpcE(R212A)/F   90   51     CpcE(R212A)/F   90   90     CpcE(F239A)/F   89   90     CpcE(I217A)/F   90   90     CpcE(I22A)/F   90   90     CpcE(I22A)/F   90   90     CpcE(I22A)/F   90   90     CpcE(I226A)/F   104     CpcE(L276A)/F   89     CpcE(L276A)/F   120     CpcE/F(N44A)   93     CpcE/F(N45A)   108     CpcE/F(N45A)   108	CpcE(E149A)/F		85		
CpcE(R177A)/F   110     CpcE(C180A)/F   84     CpcE(R184A)/F   106     CpcE(R184D)/F   89     CpcE(Q188A)/F   90     CpcE(N209A)/F   86     CpcE(R212A)/F   50 (1)   62   65     CpcE(R212A)/F   50 (1)   89   51     CpcE(D217A)/F   52 (1)   18   51     CpcE(F239A)/F   89   51   52     CpcE(I22A)/F   90   51   52     CpcE(F239A)/F   89   51   51     CpcE(I22A)/F   90   51   52     CpcE(I22A)/F   90   51   51     CpcE(I22A)/F   90   51   51     CpcE(I22A)/F   90   51   51     CpcE(I22A)/F   104   51   51     CpcE(L276A)/F   89   51   51     CpcE(I276D)/F   120   51   51     CpcE/F(N44A)   93   51   51     CpcE/F(N45A)   108   51   51     CpcE/F(N45A)   108   51   51 <td>CpcE(E153A)/F</td> <td></td> <td>126</td> <td></td> <td></td>	CpcE(E153A)/F		126		
CpcE(C180A)/F   84     CpcE(R184A)/F   106     CpcE(R184D)/F   89     CpcE(Q188A)/F   90     CpcE(Q188A)/F   90     CpcE(R209A)/F   86     CpcE(R212A)/F   50 (1)   62   65     CpcE(R212D)/F   52 (1)   18   51     CpcE(D217A)/F   95   51   51     CpcE(F239A)/F   89   51   51     CpcE(I242A)/F   90   51   51     CpcE(I276A)/F   104   51   51     CpcE(I276A)/F   104   51   51     CpcE(I276A)/F   120   51   51     CpcE/F(N44A)   93   51   51     CpcE/F(N45A)   108   51   51     CpcE/F(N45A)   51   51   51	CpcE(R177A)/F		110		
CpcE(R184A)/F   106     CpcE(R184D)/F   89     CpcE(Q188A)/F   90     CpcE(N209A)/F   86     CpcE(R212A)/F   50 (1)   62   65     CpcE(R212D)/F   52 (1)   18   51     CpcE(D217A)/F   95   52   51     CpcE(F(239A)/F   89   51   52     CpcE(I242A)/F   90   51   50     CpcE(I242A)/F   90   51   51     CpcE(L276A)/F   89   51   51     CpcE(L276A)/F   104   51   51     CpcE(L276A)/F   104   51   51     CpcE(L276A)/F   104   51   51     CpcE(L276A)/F   120   51   51     CpcE/F(N44A)   93   51   51     CpcE/F(N45A)   108   51   51	CpcE(C180A)/F		84		
CpcE(R184D)/F   89     CpcE(Q188A)/F   90     CpcE(N209A)/F   86     CpcE(R212A)/F   50 (1)   62   65     CpcE(R212D)/F   52 (1)   18   51     CpcE(D217A)/F   95   52   52     CpcE(F239A)/F   89   51     CpcE(F239A)/F   90   51     CpcE(I242A)/F   90   51     CpcE(I242A)/F   90   51     CpcE(I242A)/F   90   51     CpcE(I242A)/F   90   51     CpcE(I276A)/F   104   51     CpcE(L276A)/F   120   51     CpcE/F(N44A)   93   51     CpcE/F(N45A)   108   51	CpcE(R184A)/F		106		
CpcE(Q188A)/F   90     CpcE(N209A)/F   86     CpcE(R212A)/F   50 (1)   62   65     CpcE(R212D)/F   52 (1)   18   51     CpcE(D217A)/F   95   52   52     CpcE(F239A)/F   89   51     CpcE(I242A)/F   90   90     CpcE(I242A)/F   104   93     CpcE/F(N44A)   93   93     CpcE/F(N45A)   108   91	CpcE(R184D)/F		89		
CpcE(N209A)/F   86     CpcE(R212A)/F   50 (1)   62   65     CpcE(R212D)/F   52 (1)   18   51     CpcE(D217A)/F   95   52   52     CpcE(F239A)/F   89   51     CpcE(I242A)/F   90   50     CpcE(I242A)/F   90   50     CpcE(L276A)/F   89   50     CpcE(L276A)/F   104   50     CpcE(L276A)/F   120   50     CpcE/F(N44A)   93   50     CpcE/F(N45A)   108   50	CpcE(Q188A)/F		90		
CpcE(R212A)/F     50 (1)     62     65       CpcE(R212D)/F     52 (1)     18     51       CpcE(D217A)/F     95     95       CpcE(F239A)/F     89     90       CpcE(I242A)/F     90     90       CpcE(L276A)/F     104     92       CpcE(L276A)/F     89     90       CpcE(L276A)/F     104     93       CpcE/F(N44A)     93     93       CpcE/F(N45A)     108     91	CpcE(N209A)/F	F0 (1)	86	65	
CpcE(1212b)/r     18     51       CpcE(D217A)/F     95       CpcE(F239A)/F     89       CpcE(1242A)/F     90       CpcE(1242A)/F     104       CpcE(L276A)/F     89       CpcE(L276A)/F     89       CpcE(L276A)/F     104       CpcE(L276A)/F     93       CpcE/F(N44A)     93       CpcE/F(N45A)     108	CpcE(R212A)/F	50 (1)	02	00 51	
CpcE(F239A)/F     39       CpcE(F239A)/F     89       CpcE(I242A)/F     90       CpcE(K245A)/F     104       CpcE(L276A)/F     89       CpcE(L276A)/F     89       CpcE(L276D)/F     120       CpcE/F(N44A)     93       CpcE/F(N45A)     108	$CpcE(D217\Delta)/F$	J2 (1)	95	וכ	
CpcE(I242A)/F     90       CpcE(K245A)/F     104       CpcE(L276A)/F     89       CpcE(L276D)/F     120       CpcE/F(N44A)     93       CpcE/F(N45A)     108	CpcE(F239A)/F		89		
CpcE(K245A)/F     104       CpcE(L276A)/F     89       CpcE(L276D)/F     120       CpcE/F(N44A)     93       CpcE/F(N45A)     108	CpcE(1242A)/F		90		
CpcE(L276A)/F     89       CpcE(L276D)/F     120       CpcE/F(N44A)     93       CpcE/F(N45A)     108	CpcE(K245A)/F		104		
CpcE(L276D)/F     120       CpcE/F(N44A)     93       CpcE/F(N45A)     108	CpcE(L276A)/F		89		
CpcE/F(N44A)     93       CpcE/F(N45A)     108       CpcE/F(N45A)     108	CpcE(L276D)/F		120		
CpcE/F(N45A) 108	CpcE/F(N44A)		93		
	CpcE/F(N45A)		108		
Lpct/F(P46A) 91	CpcE/F(P46A)		91		

#### Table S1. Variants of CpcE, CpcF, PecE, and PecF, their relative activities, and oligomerization states

#### Table S1. Cont.

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	Oligomorization state	Relative activity			
Variants	mass (E/F- <i>n</i> -mer)	For chromo-phorylation	For binding PCB	For detaching PCB	
CpcE/F(D72R)	50 (1)	68	100		
CpcE/F(D73A)		87			
CpcE/F(Y74A)		80			
CpcE/F(N75A)	42 (1), 349 (7)	64	21		
CpcE/F(N75L)	47 (1)	55	54		
CpcE/F(Y76A)	53 (1)	1	91		
CpcE/F(R79A)		73			
CpcE/F(I83A)		111			
CpcE/F(R84A)		112			
CpcE/F(R93A)		89			
CpcE/F(L95A)		117			
CpcE/F(D96R)		104			
CpcE/F(D100A)		89			
CpcE/F(T104A)		75			
CpcE/F(T104R)		100			
CpcE/F(D105R)	50 (1)	59	87		
CpcE/F(F106A)	50 (1)	60	100		
CpcE/F(S109A)		109			
CpcE/F(R112D)		91			
CpcE/F(K116A)		100			
CpcE/F(K137D)		100			
CpcE/F(E140R)		97			
CpcE/F(F144D)		114			
CpcE/F(W151A)		97			
CpcE/F(Y155A)		95			
PecE/F		100			
PecE(W29A)/F		85			
PecE(R63A)/F		75			
PecE(C87A)/F		86			
PecE(C157A)/F		57			
PecE(W189A)/F		63			
PecE/F(S51A)		73			
PecE/F(Q52A)		94			
PecE/F(D53A)		78			
PecE/F(Q54A)		85			
PecE/F(Q57A)		72			
PecE/F(N86A)		120			
PecE/F(H87A)		0			
PecE/F(C88A)		1			
PecE/F(C88S)		0			
PecE/F(Q89A)		77			

The enzymatic activities of variants of CpcE, CpcF, PecE, or PecF relative to the wild-type proteins (=100%) were evaluated by chromophorylation of CpcA or PecA with PCB in *E. coli*; the PCB-binding activities of variants of CpcE, CpcF, PecE, or PecF relative to the wild-type proteins (=100%) were evaluated by the efficiency of their binding of PCB in vitro; and the PCB-detaching activities of variants of CpcE/F relative to the wild-type proteins (=100%) were evaluated by the transfer of PCB from PCB<sup>T</sup>–CpcA to Cph1(1–514) in vitro. For details, see *Materials and Methods*.

\*In this experiment, CpcA had a C-terminal his<sub>6</sub>-tag that impedes chromophorylation.

Table S2. The dockings of lyases with apo-PBPs

Model	PCB and CpcE/F <sup>a</sup>	PCB and PecE/F <sup>b</sup>	PCB/CpcE/F and CpcA <sup>c</sup>	PCB/CpcE/F and CpcB <sup>d</sup>	PCB/PecE/F and PecA <sup>e</sup>
Model 1 ∆G, R/S	-8.3	-5.6, S	-159, R	-174, R	-170, R
Model 2 ∆G, R/S	-8.1, S	-5.5	-143, R	-168, R	-164, R
Model 3 ΔG, R/S	-7.5	-5.3, S	-138, R	-166, R	-158, R
Model 4 ΔG, R/S	-7.0, S	-5.2, S	-134, R	-165, R	-157, R
Model 5 ΔG, R/S	-7.0, R	-5.1, R	-133, R	-161, R	-153, R
Model 6	-7.0, R	-5.1, R	-133, R	-160, R	-152, R

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Table S2. Cont.

∆G, R/S					
Model 7	-6.9, R	-5.1, S	-133, R	-158, R	-151, R
ΔG, R/S					
Model 8	-6.8, R	-5.1, S	-133, R	-154, R	-149, R
∆G, R/S					
Model 9	-6.8	-5.1, S	-132, R	-153, R	-148, R
∆G, R/S					
Model 10			-130, R	-153, R	-148, R
∆G, R/S					
Model 11			-130, R	-153, R	-148, R
∆G, R/S					
Model 12			-129, R	-153, R	-146, R
ΔG, R/S					
Model 13			-129, R	-152, R	-146, R
ΔG, R/S					
Model 14			-128, R	-152, R	-145, R
ΔG, R/S					
Model 15			-128, R	-151, R	-144, R
ΔG, R/S					
Model 16 ∆G, R/S			-128, R	-151, R	-144, R

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Model 17	-126, R	-150, R	-144, R
ΔG, R/S	<b>W</b>		
Model 18	-126, R	-149, R	-144, R
ΔG, R/S	<b>\$</b>	Ŵ	H.
Model 19	-126, R	-149, R	-143, R
ΔG, R/S	<b>W</b>		
Model 20	-126, R	-148, R	-143, R
ΔG, R/S			
Model 21	-126, R	-148, R	-142, R
ΔG, R/S			
Model 22	-125, R	-147, R	-141, R
ΔG, R/S			
Model 23	-125, R	-146, R	-141, R
ΔG, R/S			Ŵ
Model 24	-125, R	-146, R	-141, R
ΔG, R/S			
Model 25	-125, R	-146, R	-141, R
ΔG, R/S			

Free energy gain upon docking ( $\Delta$ G in kcal/Mol) and structures of the docked complex of the 25 best solutions. In the small figures giving an overview of the docking complex, the E and F subunits of the lyase are oriented similar as in Fig. 1, but tilted by ~30° to the front, allowing a look into the cavity. Color coding: E subunits, light brown; F subunits, gray; CpcA and CpcB, blue; PecA, purple. The models shown in bold green were the accepted ones detailed in Fig. S4. Besides the energy, the following factors were taken into consideration: (*i*) the R-configuration of C3<sup>1</sup> of PCB<sup>T</sup> after chromophorylation; (*ii*) the co-incidence of the active site (Fig. S4) with the mutation data (Table S1); and (*iii*) a position of the docked substrate near the upper opening of the cavity of the lyase. Models were discarded because (*i*) models 1–7 conflict with the mutation data; (*iii*) models 1–2 and 4–5 conflict with the mutation data, and model 3 results in S configuration; (*iii*) models 1–23 conflict with the mutation data.

Table S3. Pseud transferring the	do first-order PCB chromoj	enzyme kinetic phore from PCB <sup>T</sup>	parameters of CpcE or C -CpcA to Cph1(1-514)	pcE(∆2–10), ir	n combination w	ith CpcF, for
		Substrate PC	B <sup>T</sup> -CpcA	Substrate Cph1(1-514)		
Lyase complex	<i>K</i> <sub>m</sub> , μΜ	$k_{\rm cat}$ , min <sup>-1</sup>	$k_{cat}/K_m$ , min <sup>-1</sup> · $\mu$ M <sup>-1</sup>	<i>K</i> <sub>m</sub> , μΜ	$k_{\rm cat}$ , min <sup>-1</sup>	$k_{cat}/K_m$ , min <sup>-1</sup> ·µN

Lyase complex	<i>K</i> <sub>m</sub> , μΜ	$k_{\rm cat}$ , min <sup>-1</sup>	$k_{\rm cat}/K_{\rm m}$ , min <sup>-1</sup> · $\mu$ M <sup>-1</sup>	<i>K</i> <sub>m</sub> , μΜ	$k_{\rm cat}$ , min <sup>-1</sup>	$k_{\rm cat}/K_{\rm m}$ , min <sup>-1</sup> · $\mu$ M <sup>-1</sup>
СрсЕ/F	3.10	$2.53 \times 10^{-3}$	$0.82 \times 10^{-3}$	9.94	$6.28 \times 10^{-3}$	$0.63 \times 10^{-3}$
СрсЕ(Δ2–10)/F	26.9	$20.2 \times 10^{-3}$	$0.75 \times 10^{-3}$	1.99	$3.51 \times 10^{-3}$	$1.76 \times 10^{-3}$

Table S4. Primers for cpcA, cpcE, cpcF, pecA, pecE, pecF, and nb/B from Nostoc, and their site-directed mutants

Primer	Sequence	DNA
P1	5' CCGTCGTCATATGATAGAACCCAGT 3'	cpcE
P2	5' CTGCTCGAGCAACAATGAATCC 3'	
P3	5' CGCTCGGCATATGACTAATGAACT 3'	cpcF
P4	5' GTTCTCGAGTTGACTTTGAGCCAAT 3'	
P5	5' TAACTCGAGCACCACCACCACCACC 3'	cpcE(∆his-tag)
P6	5' caacaatgaatccataaggttcatgacc $3'$	
P7	5' TAACTCGAGCACCACCACCACCACT 3'	cpcF(∆his-tag)
P8	5' TTGACTTTGAGCCAATAGAATGCGGGCG 3'	
P9	5' ACTCCCATGGCTATGGTTAAAACCCCCATT 3'	срсА
P10	5' CAGCTCGAGCTAGCTGAGAGCGTTGATAGC 3'	
P11	5' GCACCATGGCTATGAAAACACCTTTGACCGA 3'	pecA
P12	5' CTGCTCGAGTTAACTTAAAGCGTTAATTGCA 3'	_
P13	5' GACCCATGGGCGTGACTGCTGAACCAATTCT 3'	pecE
P14	5' GACCTGCAGTTAAAGTTGAATTAATAAATCA 3'	-
P15	5' GGTTCAGCATATGAATCAAGCTTCATTGAGC 3'	pecF
P16	5' GACCTCGAGCTAACTCAAGGCGATCGCCATA 3'	
P17	5 CUTTTUUUGUAGAGAAUGGGUUAUAGUTAAU 5	<i></i> (μ(Ε(ΕδΑ)
P10 D10	5 CTTCCACACTGGGTTCTATCATTGCCATGGT 5	cpcE/EQA)
F 19 D20	5 CCCGCAGAGAACGGGCCACAGCIAACACCAG 5	CPCE(F9A)
P21		CDCE(133R)
P21	<b>5</b> ' CCCACTTATIGCTGCTTGGTGGTTAGGTAGT $5'$	CPCL(LSSN)
P23	5' GCCTATTATGCTGCTTGGTGGTTAGGTAAGT 3'	cncF(R34A)
P24	5' GAGACTTAAGTCTGATGATTGCAGATTAGCT 3'	cpc2(no n)
P25	5' GACTATTATGCTGCTTGGTGGTTAGGTAAGT 3'	cpcE(R34D)
P26	5' GAGACTTAAGTCTGATGATTGCAGATTAGCT 3'	
P27	5' GCCTATGCTGCTTGGTGGTTAGGTAAGTATCG 3'	cpcE(Y35A)
P28	5' gcggagacttaagtctgatgattgcagatta $3'$	, , , ,
P29	5' CGCTATGCTGCTTGGTGGTTAGGTAAGTATC 3'	cpcE(Y35R)
P30	5' GCGGAGACTTAAGTCTGATGATTGCAGATTA 3'	
P31	$5^{\prime}$ gctgcttggtggttaggtaagtatcgggtga $3^{\prime}$	cpcE(Y36A)
P32	5' ggcatagcggagacttaagtctgatgattgc 3'	
P33	$5^{\prime}$ gctgcttggtggttaggtagtatcgggtga $3^{\prime}$	cpcE(Y36R)
P34	$5^{\prime}$ CCGATAGCGGAGACTTAAGTCTGATGATTGC $3^{\prime}$	
P35	$5^{\prime}$ gcctggttaggtaagtatcgggtgaaagaaag $3^{\prime}$	cpcE(W39A)
P36	$5^{\prime}$ agcagcataatagcggagacttaagtctgatga $3^{\prime}$	
P37	5' gccttaggtaagtatcgggtgaaagaaagtgc 3'	cpcE(W40A)
P38	5' CCAAGCAGCATAATAGCGGAGACTTAAGTCT 3'	
P39	5' GCCTATCGGGTGAAAGAAGTGCTGCTGTTGA 3'	cpcE(K43A)
P40	5' ACCTAACCACCAAGCAGCATAATAGCGGAGA 3'	- (
P41	5' GTGACTATCGGGTGAAAGAAGTGCTGCTGT 3'	cpcE(K43D)
P42	5' CTAACCACCAAGCAGCATAATAGCGGAGACT 3'	
P43	5' CGGGTGAAAGAAAGTGCTGCTGTTGATGCTT 3'	cpcE(Y44A)
P44	5' GGCCTTACCTAACCACCAAGCAGCATAATAG 3'	cncE/DAEA)
r45 D/16		<i>τ</i> ρτε( <i>K</i> 45A)
г40 D/17	<b>J</b> UGUATAUTTAUUTAUUAAGUAGUATAA $3'$ <b>5</b> ' CTCAAACTACTACCTCCTTCTTTCATCATCATCATA	
P48		(p(L(N45D)
P49	5' CETAGAACTGAACTTGCTGCTCATTATCCTTTCC 3'	cncF(D64R)
P50	5' GGCTTCATCCTCTAACGCCGCAATTAAAGCA 3'	
P51	5' CTTGGTGGTTATCCTTTGCGGCGTAACGCAG 3'	cpcE(F67A)
P52	5' CGCAGTTCTATCGGCTTCATCCTCTAACGCC 3'	-,
P53	5' GCTAACGCAGCCAGAGCATTAGGGAAATTGG 3'	cpcE(R75A)
P54	5' CCGCAAAGGATAACCACCAAGTTCAGTTCTA 3'	
P55	5' GACAACGCAGCCAGAGCATTAGGGAAATTGG 3'	cpcE(R75D)
P56	5' CCGCAAAGGATAACCACCAAGTTCAGTTCTA 3'	
P57	5' gcagccagagcattagggaaattgggcaatc 3'	cpcE(N76A)
P58	5' ggcacgccgcaaaggataaccaccaagttca 3'	
P59	<b>5</b> ' gcagcattagggaaattgggcaatcgtaaag $3'$	cpcE(R79A)
P60	5' ggctgcgttacgccgcaaaggataaccacca 3'	
P61	<b>5</b> ' gacgcattagggaaattgggcaatcgtaaagc $3'$	cpcE(R79D)
P62	5' ggctgcgttacgccgcaaaggataaccacca 3'	

## Table S4. Cont.

Primer	Sequence	DNA
P63	5' gcattgggcaatcgtaaagccgtgccaggct 3'	cpcE(K83A)
P64	5' CCCTAATGCTCTGGCTGCGTTACGCCGCAAA 3'	
P65	5' GACTTGGGCAATCGTAAAGCCGTGCCAGGCT 3'	cpcE(K83D)
P66	$5^{\prime}$ ccctaatgctctggctgcgttacgccgcaaa $3^{\prime}$	
P67	5' GCCTTGGAGTGTCCTGACTTTTACGTGCGTG 3'	cpcE(C96A)
P68	5' GTTAATTAAGCCTGGCACGGCTTTACGATTG 3'	
P69	5' GCTCCTGACTTTTACGTGCGTGAAGCAGCAG 3'	cpcE(C99A)
P70	5' CTCCAAGCAGTTAATTAAGCCTGGCACGGCT 3'	
P/1 C70	5' GTGCGTGAAGCAGCAGCCCAATCGCTGGAAA 3'	срсе(ү 103А)
P72 D72	<b>5</b> GGLAAAGTCAGGACACTCCAAGCAGTTAATT <b>5</b> $\mathbf{E}'_{1}$ CCA CCA CCACCA A MCCCMCCA A MCCMCA A A C $2'_{1}$	cpcE(E106A)
P74	<b>5</b> ' GCAGCACCCCAATCGCTGGAAATGCTCAAAG $5'$	CPCL(LTODA)
P75	<b>5</b> ' CCATCGCTGGAAATGCTCAAAGACAAAACAG $3'$	cncE(O110A)
P76	5' GGCTGCTGCTTCACGCACGTAAAAGTCAGGA 3'	cpc2(Q1107)
P77	5' GCAATGCTCAAAGACAAAACAGCAGCACCAG 3'	cpcE(E113A)
P78	5' CAGCGATTGGGCTGCTGCTTCACGCACGTAA 3'	
P79	5' CTCAAAGACAAAACAGCAGCACCAGCACTCA 3'	cpcE(M114A)
P80	5' ggcttccagcgattgggctgctgcttcacgc 3'	
P81	$5^{\prime}$ gcagacaaaacagcagcaccagcactcatca $3^{\prime}$	cpcE(K116A)
P82	$5^\prime$ gagcatttccagcgattgggctgctgcttca $3^\prime$	
P83	$5^{\prime}$ cgacctcatttagtccaaccctacgaagcag $3^{\prime}$	cpcE(G140F)
P84	5' AAATGTTACTTGCACGGCCTGTGCGACTCCC 3'	
P85	5' GCAGCAGTATTAGAAGCGTTAGGAGCTATTG 3'	cpcE(E149A)
P86	5' GTAGGGTTGGACTAAATGAGGTCGCCCTGTT 3'	
P87	5' GCGTTAGGAGCTATTGGTGCTACTGATGCCA 3'	CPCE(E153A)
F 00 D 20	5 GGCTAATACIGCTICGTAGGGTIGGACTAAA 5	cpcE(P177A)
P90	5' GECTGAGACTGGATGCTCTAGAAATGCCTGA 3'	CPC2(N177A)
P91	5' GCCGCCGCCGCTAGGGCAATGTACCAACTGA 3'	cpcE(C180A)
P92	5' CTGCACTCGTGAGACTGGATGCTCTAGAAAT 3'	
P93	5' GCAATGTACCAACTGACACAAGAACCAGTAT 3'	cpcE(R184A)
P94	5' CGCAGCGGCGCGCACTGCACTCGTGAGACT 3'	
P95	<b>5</b> ' gcaatgtaccaactgacacaagaaccagtat $3'$	cpcE(R184D)
P96	5' gtcagcggcgcgcgcactgcactcgtgagact $3'$	
P97	5' GCACTGACACAAGAACCAGTATATGGAGAGC 3'	cpcE(Q188A)
P98	5' GTACATTGCCCTAGCGGCGCGCACTGCACT 3'	
P99	5' GCCCTACGACGCGTTGCTTTAGGTGACTTGG 3'	cpcE(N209A)
P100	5' GAGGTCGTTACCTGCTAACACTTTTACCAGC 3'	
P101 P102	5' GTTGCTTTAGGTGACTTGGGTGCAATTGGGT 3'	CPCE(R212A)
P102	<b>5</b> Generation $3$	cncE(R212D)
P104	<b>5</b> ' GTUTCGTAGGTUGACUUGGUGCAAAAGGGU $5'$	cpcL(N2T2D)
P105	5' CCTTGGGTGCAATTGGGTACTTGGCAGCAGC 3'	cpcF(D217A)
P106	5' CACCTAAAGCAACGCGTCGTAGGTTGAGGTC 3'	
P107	5' GCCAAACTCATTGCCCTCAAAGGATTGCTAG 3'	cpcE(F239A)
P108	5' GCTGTTTTCGGCTTTGGCGTTAGCGATCGCT 3'	
P109	$5^{\prime}$ gccctcaaaggattgctagaacatcagatgt $3^{\prime}$	cpcE(I242A)
P110	5' GGCGAGTTTGAAGCTGTTTTCGGCTTTGGCG 3'	
P111	5' GGATTGCTAGAACATCAGATGTCAGCAGAGT 3'	cpcE(K245A)
P112	5' GGCGAGGGCAATGAGTTTGAAGCTGTTTTCG 3'	
P113	5' GCCTAACTGCAGGTCGACAAGCTTGCGGCC 3'	CPCE(L276A)
F114 D115	5 CAAIGAAICCAIAAGGIICAIGACCCGGAI 5	cpcE(1.276D)
P116	5' CAATGAATCCATAAGGTTCATGACCCCGGAT 3'	(p(L(LZ))D)
P117	5' CAACCCAACAGCAGCCGCAATTGCCTCTACT 3'	cpcF(N44A)
P118	5' GCATAACCAAACACAGCTATTAGGGTGGGAA 3'	
P119	5' CCAACAGCAGCCGCAATTGCCTCTACTGCCT 3'	cpcF(N45A)
P120	<b>5</b> ' ggcgttataaccaaacacagctattagggtg $3'$	
P121	$5^\prime$ gcaacagcagccgcaattgcctctactgcct $3^\prime$	cpcF(P46A)
P122	<b>5</b> ' gttgttataaccaaacacagctattagggtg $3'$	
P123	$5^{\prime}$ gactacaactatggcgcacgggcttattcga $3^{\prime}$	cpcF(D72R)
P124	5' CCGTATTTGTGTGAGTAACTGGGGAACTGCT 3	

## Table S4. Cont.

Primer	Sequence	DNA
P125	5' CCTACAACTATGGCGCACGGGCTTATTCGAT 3'	cpcF(D73A)
P126	5' CATCTATTTGTGTGAGTAACTGGGGAACTGC 3'	
P127	5' GCCAACTATGGCGCACGGGCTTATTCGATTC 3'	cpcF(Y74A)
P128	5' gtcatctatttgtgtgagtaactggggaa $3'$	
P129	5' gcctatggcgcacgggcttattcgattcgca $3'$	cpcF(N75A)
P130	$5^{\prime}$ gtagtcatctatttgtgtgagtaactgggga $3^{\prime}$	
P131	$5^{\prime}$ ctctatggcgcacgggcttattcgattcgca $3^{\prime}$	cpcF(N75L)
P132	5' gtagtcatctatttgtgtgagtaactgggga 3'	
P133	5' GGCGCACGGGCTTATTCGATTCGCACTCTCG 3'	cpcF(Y76A)
P134	5' GGCGTTGTAGTCATCTATTTGTGTGAGTAAC 3'	5(570.4)
P135	5' GCTTATTCGATTCGCACTCTCGCGGCGATCG 3'	срсғ(К/9А)
P130 D127	5 CGCTGCGCCATAGTTGTAGTCATCTATTTGT 5	cncE(192A)
P138	<b>5</b> CCCCCAATAACCCCCCCCCCCCCCCCCCCCCCCCCCCC	срсг(165А)
P139	5' CACTOTOCOCCOCTOCOCCOCTOCTOCTOCT	$cncE(R84\Delta)$
P140	5' CGAATCGAATAAGCCCGTGCGCCATAGTTGT 3'	
P141	5' GCTGCTTTAGATGTATTAATCGATGCTGCTG 3'	cpcF(R93A)
P142	5' GGGGTCAGCGATCGCCGCGAGAGTGCGAATC 3'	
P143	5' GATGTATTAATCGATGCTGCTGCTACAGACT 3'	cpcF(L95A)
P144	5' ggcagcacgggggtcagcgatcgccgcgaga 3'	
P145	5' gtattaatcgatgctgctgctacagactttg $3'$	cpcF(D96R)
P146	5' CCGTAAAGCACGGGGGTCAGCGATCGCCGCG 3'	
P147	$5^{\prime}$ getgetgetacagaetttgeteceagtgtge $3^{\prime}$	cpcF(D100A)
P148	5' GGCGATTAATACATCTAAAGCACGGGGGTCA 3'	
P149	5' GACTTTGCTCCCAGTGTGCGCCGGGCTGCGG 3'	cpcF(T104A)
P150	5' TGCAGCAGCAGCATCGATTAATACATCTAAA 3'	
P151 D152	5' GACTTTGCTCCCAGTGTGCGCCGGGCTGCGG 3'	cpcF(1104R)
P153	5' CTTTCCTCCCACTCCCCCCCCCCCCCCCCCCCCCCCCC	cpcE(D105R)
P154	5' CGTGTAGCAGCAGCATCGATTAATACATCTA 3'	cpci (D1051)
P155	5' GCTCCCAGTGTGCGCCGGGCTGCGGCTAAAG 3'	cpcF(F106A)
P156	5' GGCGTCTGTAGCAGCAGCATCGATTAATACA 3'	,
P157	5' gtgcgccgggctgcggctaaaggattaggaa $3'$	cpcF(S109A)
P158	5' ggcggggggagcaaagtctgtagcagcagcatcg $3'$	
P159	<b>5</b> ' gctgcggctaaaggattaggaaacttacatt $3'$	cpcF(R112D)
P160	5' gtcgcgcacactgggagcaaagtctgtagca 3'	
P161	5' GGATTAGGAAACTTACATTGGCACAAGCTAG 3'	cpcF(K116A)
P162	5' GGCAGCCGCAGCCCGGCGCACACTGGGAGCA 3'	
P163	5' GCTTTGGAAACACTGCTGTTTATTTCTCAAG 3'	cpcF(K137D)
P104	<b>5</b> GTUTTTTGGTGUTGTTTGGTTGTUAGGAAAU <b>5</b>	cncE(E1AOP)
P166	<b>5</b> CGCACACIGCIGIIIAIIICICAAGAIGCAG $5$	CPCF(E140K)
P167	5' GACATTTCTCAAGATGCAGAATGGTCGATTC 3'	cncF(F144D)
P168	5' CAGCAGTGTTTCCAAAGCTTTTTTTGGTGCT 3'	eper (11112)
P169	5' GTCGATTCGTTATGCAGCGATCGTCGGTCTG 3'	cpcF(W151A)
P170	$5^{\prime}$ gcttctgcatcttgagaaataaacagcagtg $3^{\prime}$	
P171	<b>5</b> ' gcagcgatcgtcggtctgcaaggtttagtaa $3'$	cpcF(Y155A)
P172	$5^{\prime}$ ggcacgaatcgaccattctgcatcttgagaa $3^{\prime}$	
P173	5' CCTGGTTGGGTAAACATAACGTACAGGCTGG 3'	pecE(W29A)
P174	5' CAGCAGCATAATAACGAATTTGGTTATCCTC 3'	
P175	5' CAGGCTGCACGGGCTTTAGGATTGTTGAAAA 3'	pecE(R63A)
P1/0 D177	5' GGCACGCAGAGGATACCCTCCTGATGGGATG 3'	pacE(CQ7A)
P178	5 GAIGAGGAIIIGCGICIGAGGGAAGCAGIAA 5 5' CCCTTCCAATCCTCCAATTAACCCTCCTACA 3	pece(corA)
P179	5' GCAGCCGCTAGATATATGTATCTCCTCACCC 3'	pecF(C157A)
P180	5' GGCTTGCACACGCTCAGAATAATGCTGAAGA 3	
P181	5' GCGGCGGTATTTGATTTGGGTGCAGTTGCTC 3'	pecE(W189A)
P182	$5^{\prime}$ ggcacgtaaatacatattgtcatgattgaga $3^{\prime}$	
P183	$5^\prime$ caagatcaaggttttcaagcccagatcattc $3^\prime$	pecF(S51A)
P184	<b>5</b> ' ggcatcatcataagcagcaattaacaaatta $3'$	
P185	5' GATCAAGGTTTTCAAGCCCAGATCATTCAGG 3'	pecF(Q52A)
P186	$5^{\prime}$ ggcagaatcatcataagcagcaattaacaaa $3^{\prime}$	

### Table S4. Cont.

Primer	Sequence	DNA
P187	<b>5</b> ' caaggttttcaagcccagatcattcaggttt $3'$	pecF(D53A)
P188	<b>5</b> ' ggcttgagaatcatcataagcagcaattaac $3'$	
P189	5' ggttttcaagcccagatcattcaggttttag $3'$	pecF(Q54A)
P190	<b>5</b> ' ggcatcttgagaatcatcataagcagcaatt $3'$	
P191	5' gcccagatcattcaggttttagctcaaattg $3'$	pecF(Q57A)
P192	<b>5</b> ' ggcaaaaccttgatcttgagaatcatcataa $3'$	
P193	5' CACTGTCAAGGTAATGTCCGCCGCATTGCTG 3'	pecF(N86A)
P194	5' ggcggctacacttgtccccaccacctcggct 3'	
P195	5' CTGTCAAGGTAATGTCCGCCGCATTGCTGCA 3'	pecF(H87A)
P196	5' gcattggctacacttgtccccaccacctcgg 3'	
P197	5' gcccaaggtaatgtccgccgcattgctgcac 3'	pecF(C88A)
P198	5' gtgattggctacacttgtccccaccacctcg $3'$	
P199	5' CAAGGTAATGTCCGCCGCATTGCTGCACGAG 3'	pecF(C88S)
P200	5' cgagtgattggctacacttgtccccaccacc $3'$	
P201	5' ggtaatgtccgccgcattgctgcacgagggt 3'	pecF(Q89A)
P202	5' ggcacagtgattggctacacttgtccccacc 3'	
P203	5' CCAGATCCATATGAGTATTACTCCTGAGTCT 3'	nblB
P204	<b>5</b> ' gcactcgagaactgattgcaaagattgttga $3'$	
P205	<b>5</b> ' gcagagaacgggccacagctaacaccagaac $3'$	<i>cpcE(</i> ∆2–10)
P206	$5^\prime$ catatgtatatctccttcttaaagttaaaca $3^\prime$	
P207	5' GCTCGAGCACCACCACCACCACTGAG 3'	cpcE(∆254–276)
P208	5' gacatctgatgttctagcaatcctttgagg $3'$	i.e. cpcE(∆h15)

Antibiotic resistance	pACYCDuet derivatives	pCDFDuet derivatives	pET30 derivatives
Kanamycin			pET-histag-cpcA
			pET-cpcA-histag
			pET-pecA
			pET-cpcE
			pET-cpcE(∆his-tag)
			pET-cpcE( $\Delta 2$ –10/his-tag
			pEI-cpcE( $\Delta 2$ –10/h15)
			pEI-cpcE(W39A/Ahis-ta
			pET-cpcE(R75D/Ahis-ta)
			nFT-cncF(R212A/Ahis-t
			pET-cpcE(R212D/ $\Delta$ his-ta
			pET-cpcF
			pET-cpcF(D72R)
			pET-cpcF(N75A)
			pET-cpcF(N75L)
			pET-cpcF(Y76A)
			pET-cpcF(D105R)
			pET-cpcF(F106A)
			pET-cpcF(∆his-tag)
			pEI-nblB
Strentomycin			pe i -cpn i
sucptonyen		pCDF-cpcE( $\Delta 2$ -10)-cpcF	
		pCDF-cpcE(∆2–10/h15)-cpcF	
		pCDF-cpcE(E8A)-cpcF	
		pCDF-cpcE(F9A)-cpcF	
		pCDF-cpcE(L33R)-cpcF	
		pCDF-cpcE(R34A)-cpcF	
		pCDF-cpcE(R34D)-cpcF	
		pCDF-cpcE(Y35A)-cpcF	
		pCDF-cpCE(Y35R)-cpCF	
		pCDF-cpcE(Y36R)-cpcF	
		pCDF-cpcE(W39A)-cpcF	
		pCDF-cpcE(W40A)-cpcF	
		pCDF-cpcE(K43A)-cpcF	
		pCDF-cpcE(K43D)-cpcF	
		pCDF-cpcE(Y44A)-cpcF	
		pCDF-cpcE(R45A)-cpcF	
		pCDF-cpcE(R45D)-cpcF	
		pCDF-cpcE(D64R)-cpcF	
		pCDF-cpcE(E6/A)-cpcF	
		pCDF-cpcE(R75A)-cpcF	
		pCDF-cpcE(N76A)-cpcF	
		pCDF-cpcE(R79A)-cpcF	
		pCDF-cpcE(R79D)-cpcF	
		pCDF-cpcE(K83A)-cpcF	
		pCDF-cpcE(K83D)-cpcF	
		pCDF-cpcE(C96A)-cpcF	
		pCDF-cpcE(C99A)-cpcF	
		pCDF-cpcE(Y103A)-cpcF	
		pCDF-cpcE(E106A)-cpcF	
		$p \in DF - cp \in E(E + 12A)$	
		pCDF-cpcF(K116A)-cpcF	
		pCDF-cpcE(G140F)-cpcF	
		pCDF-cpcE(E149A)-cpcF	
		pCDF-cpcE(E153A)-cpcF	
		pCDF-cpcE(R177A)-cpcF	
		pCDF-cpcE(C180A)-cpcF	

Antibiotic resistance	pACYCDuet derivatives	pCDFDuet derivatives	pET30 derivatives
		pCDF-cpcE(R184A)-cpcF	
		pCDF-cpcE(R184D)-cpcF	
		pCDF-cpcE(Q188A)-cpcF	
		pCDF-cpcE(N209A)-cpcF	
		pCDF-cpcE(R212A)-cpcF	
		pCDF-cpcE(R212D)-cpcF	
		pCDF-cpcF(D217A)-cpcF	
		pCDF-cpcF(F239A)-cpcF	
		pCDE-cpcE(1242A)-cpcE	
		pCDF-cpcE(K245A)-cpcE	
		pCDE-cpcE(1276A)-cpcE	
		pCDF-cpcE(1276D)-cpcF	
		pCDE-cpcE-cpcE(N44A)	
		pCDE-cpcE-cpcE(N45A)	
		$pCDE_cpcE_cpcE(P46A)$	
		pCDE cpcE cpcE(D72B)	
		pCDF cpcE cpcF(D72A)	
		$p \in DF - cp (E - cp (D / SA))$	
		pCDF-cpcE-cpcF(N75A)	
		pCDF-cpcE-cpcF(N75L)	
		pCDF-cpcE-cpcF(Y76A)	
		pCDF-cpcE-cpcF(R/9A)	
		pCDF-cpcE-cpcF(I83A)	
		pCDF-cpcE-cpcF(R84A)	
		pCDF-cpcE-cpcF(R93A)	
		pCDF-cpcE-cpcF(L95A)	
		pCDF-cpcE-cpcF(D96R)	
		pCDF-cpcE-cpcF(D100A)	
		pCDF-cpcE-cpcF(T104A)	
		pCDF-cpcE-cpcF(T104R)	
		pCDF-cpcE-cpcF(D105R)	
		pCDF-cpcE-cpcF(F106A)	
		pCDF-cpcE-cpcF(S109A)	
		pCDF-cpcE-cpcF(R112D)	
		pCDF-cpcE-cpcF(K116A)	
		pCDF-cpcE-cpcF(K137D)	
		pCDF-cpcE-cpcF(E140R)	
		pCDF-cpcE-cpcF(F144D)	
		pCDF-cpcE-cpcF(W151A)	
		pCDF-cpcE-cpcF(Y155A)	
		pCDF-pecE-pecF	
		pCDF-pecE(W29A)-pecF	
		pCDF-pecF(R63A)-pecF	
		pCDF-pecE(C87A)-pecE	
		pCDF-pecE(C157A)-pecE	
		pCDF-pecE(W189A)-pecF	
		nCDE-necE-necE(S51A)	
		$pCDE_{pecE} pecE(057A)$	
		pCDE-pocE-pocE(D53A)	
		pCDF pacE pacE(053A)	
		pCDF-pecE-pecF(Q34A)	
		pCDF-pecE-pecF(QS/A)	
		pCDF-pecE-pecF(H8/A)	
		pCDF-pecE-pecF(C88A)	
		pCDF-pecE-pecF(C885)	
		pCDF-pecE-pecF(Q89A)	
		pCDF-nblB	

The plasmids pACYCDuet, pCDFDuet, pET28, and pET30, from Novagen, are T7 promoter expression vectors. pACYCDuet and pCDFDuet are designed to coexpress two target proteins in *E. coli*. By using the three vector derivatives together with compatible replicons and antibiotic resistance, five proteins could be coexpressed in the same cell, thereby generating the respective designed PC or PEC in *E. coli*.

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