Supporting Information

Rohmer *et al.* 10.1073/pnas.0805696105

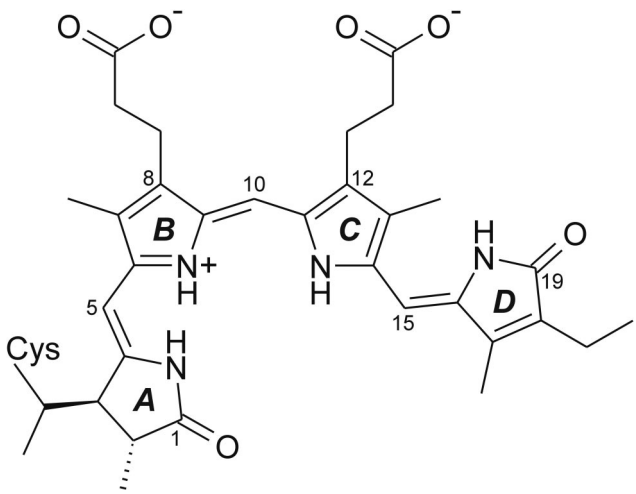

Fig. S1. Structural formula of protein-bound PCB shown in the *ZZZssa* geometry, as assumed for the Pr state.

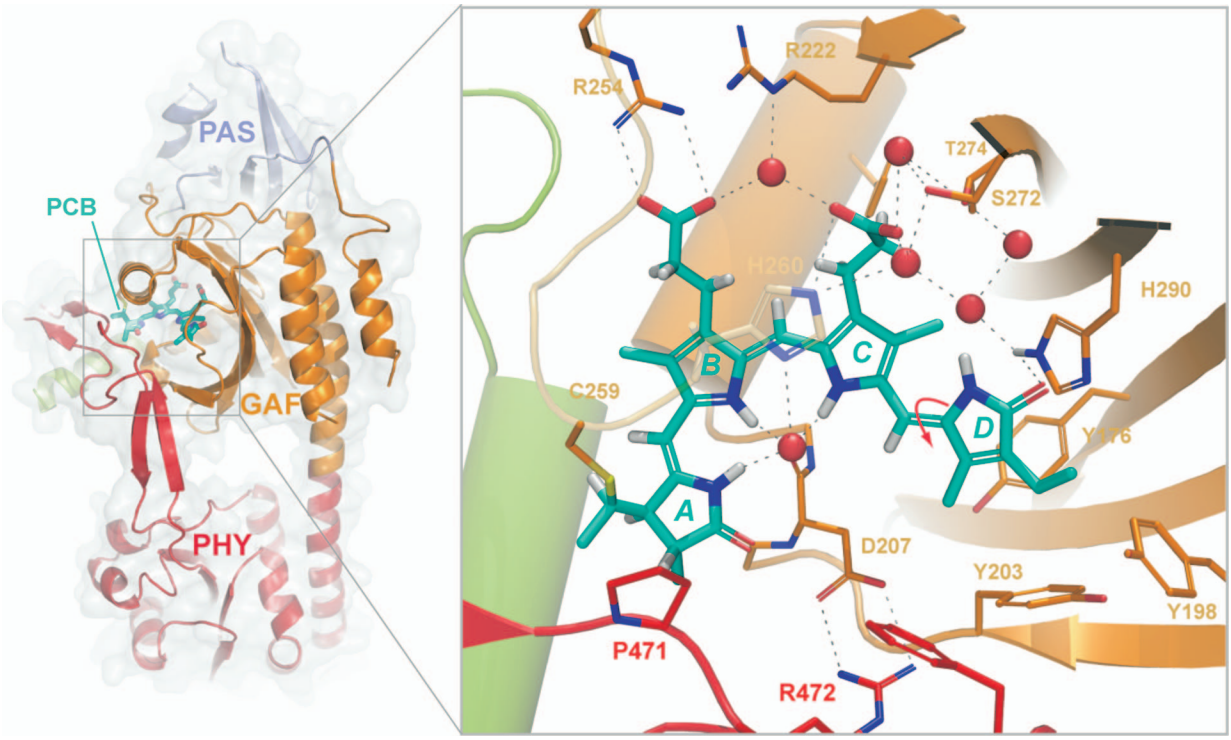

Fig. S2. Domain architecture (*Left*) and chromophore pocket (*Right*) in Cph1Δ2 (1). This figure was made by PyMol (2).

1. Essen LO, Maillet J, Hughes J (2008) The structure of a complete phytochrome sensory module in the Pr ground state. *Proc Natl Acad Sci USA* 105:14709–14714.
2. DeLano WL (2002). *The PyMOL Molecular Graphics System*. www.pymol.org (DeLano Scientific, San Carlos, CA).

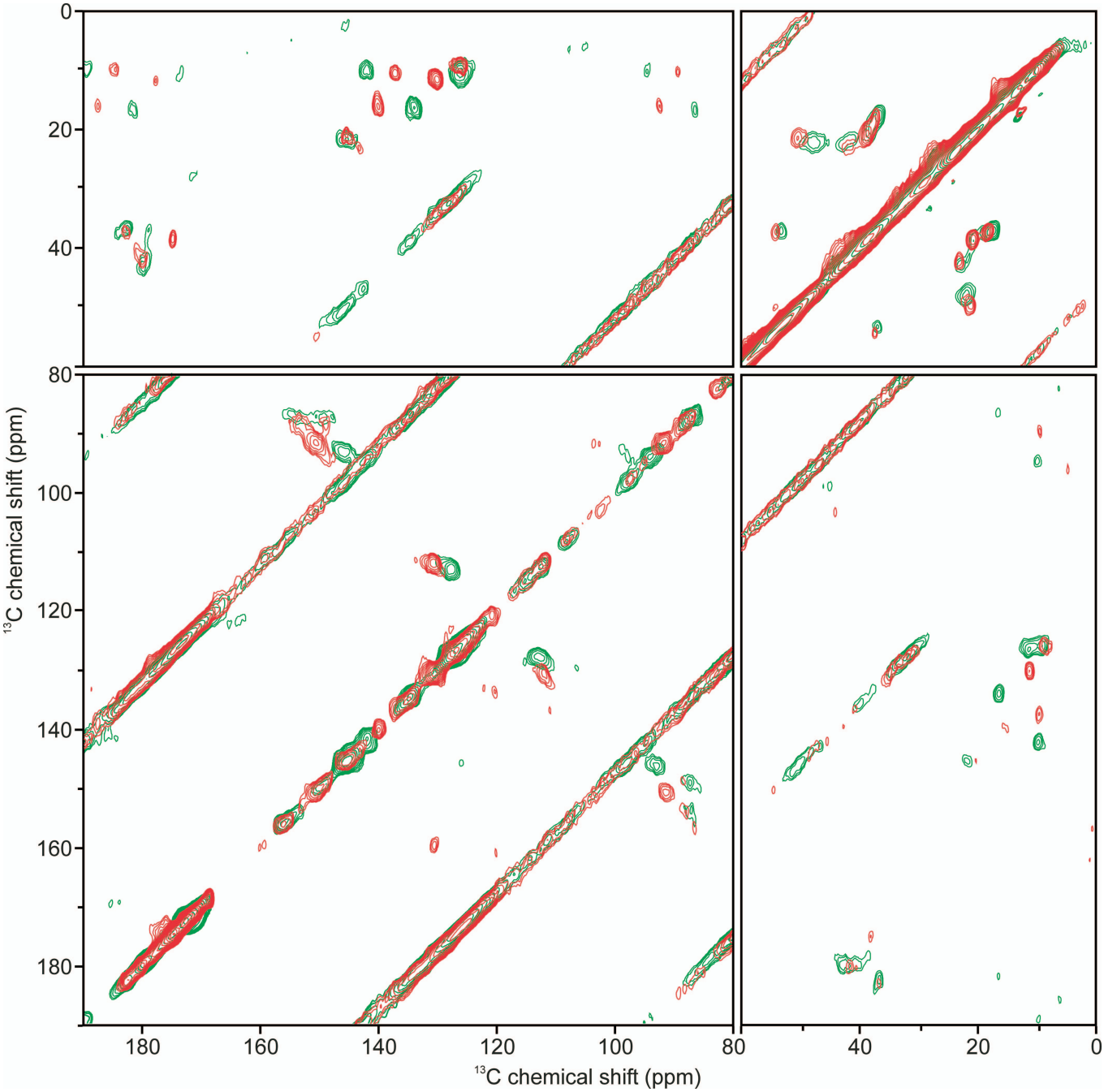

Fig. S3. Enlarged contour plot of the 2D ^{13}C-^{13}C DARR NMR spectra of u-[^{13}C, ^{15}N]-PCB-Cph1Δ2 in the Pr (green) and Pfr states (red). The spectra were recorded with a proton mixing times of 5 ms at 233 K and a spinning frequency of 9 kHz.

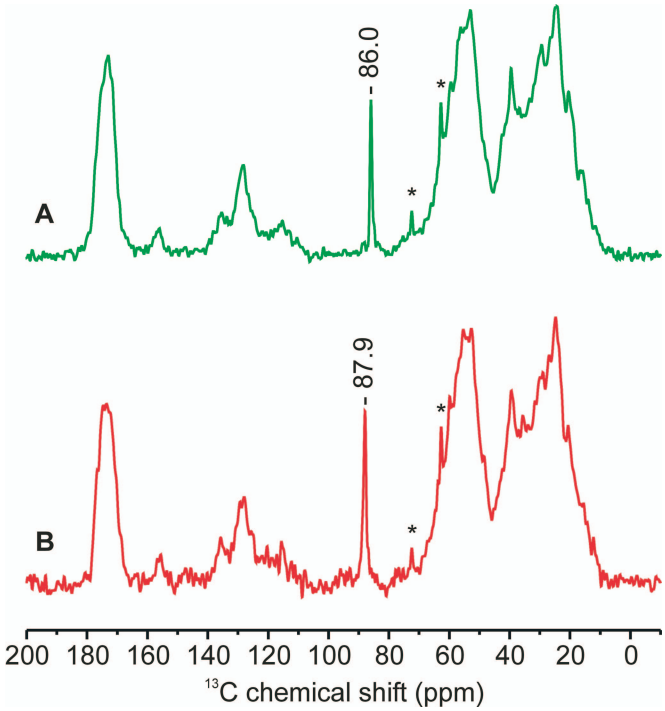

Fig. S4. The 1D ^{13}C CP/MAS NMR spectra of $^{13}C_5$-PCB-*phyA*65 in the Pr (*A*) and Pfr (*B*) states recorded at 9.4 T, 10 kHz and 243 K.

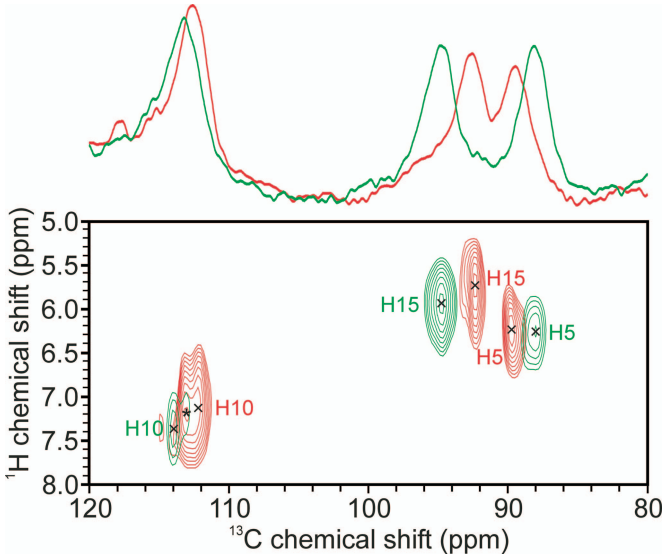

Fig. S5. Contour plot of 2D heteronuclear dipolar correlation spectra of the methine bridge region obtained from u-[^{13}C, ^{15}N]-PCB-Cph1Δ2 in the the Pr (green) and Pfr (red) states at a magnetic field of 9.4 T, 10 kHz and 243 K. The asterisks indicate the position of protein backbone signals in natural abundance.

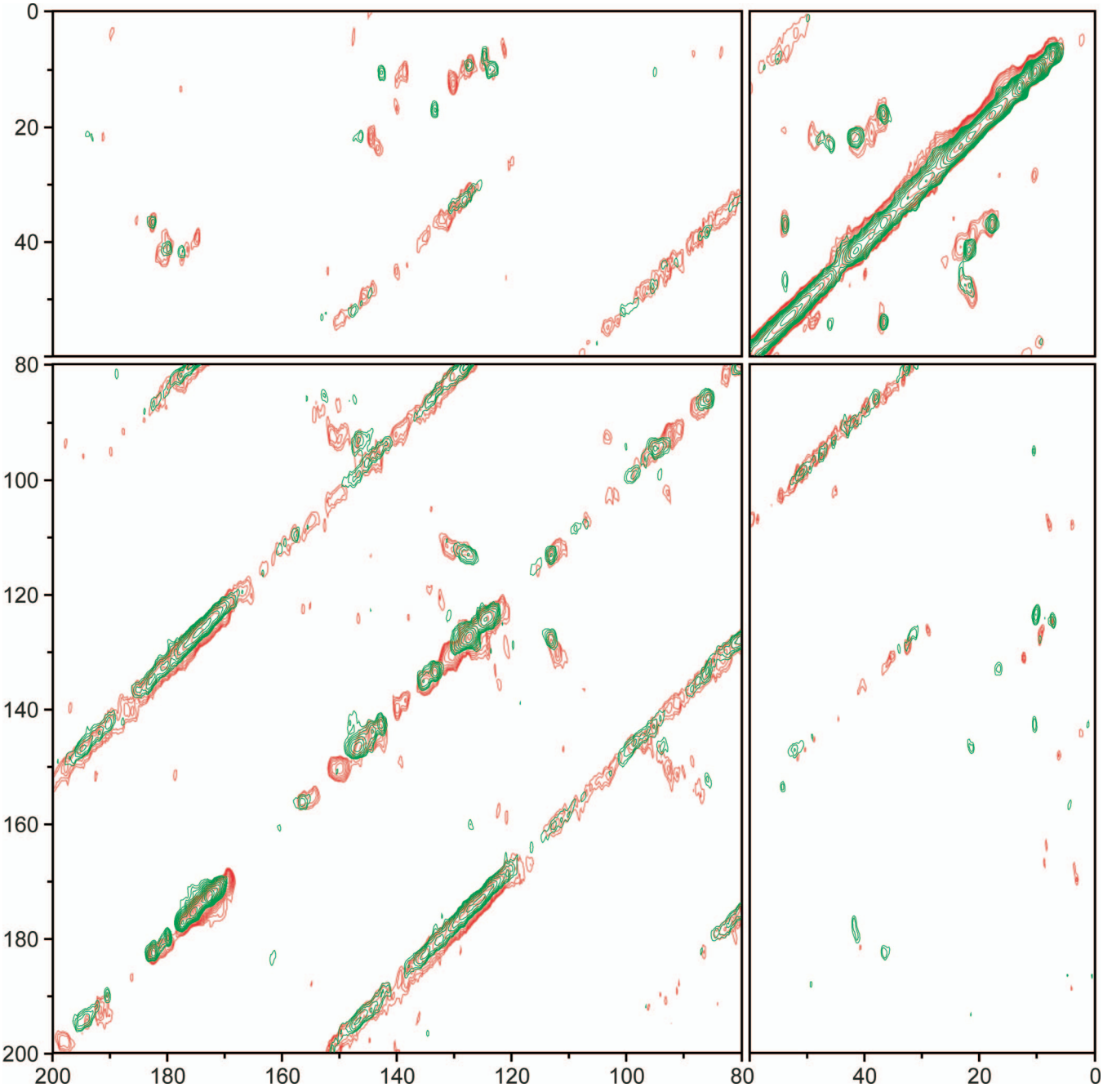

Fig. S6. Contour plot of the 2D ^{13}C-^{13}C DARR NMR spectra of u-[^{13}C, ^{15}N]-PCB-*phyA*65 in the Pr (green) and Pfr states (red). The spectra were recorded with proton mixing times of 5 ms at 233 K and a spinning frequency of 9 kHz.

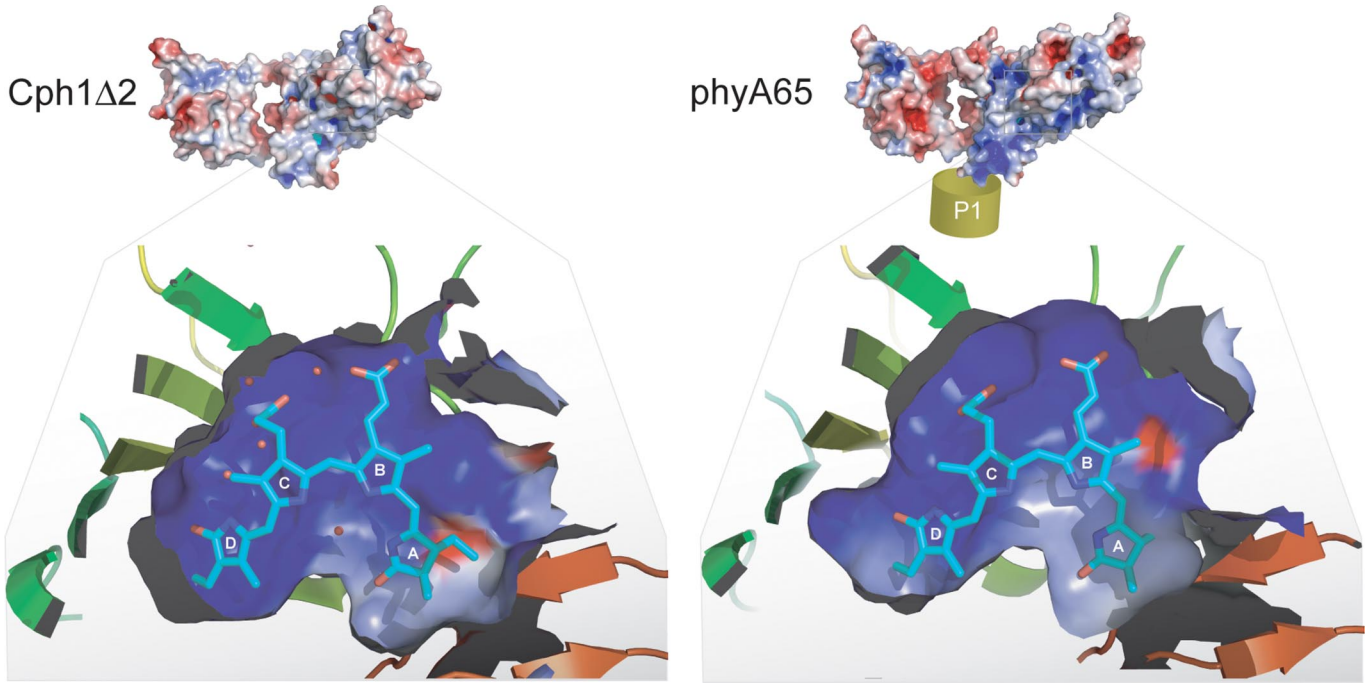

Fig. S7. Electrostatic surface properties of the photosensory modules Cph1Δ2 and *phyA*65. A homology model for *phyA*65 was generated by MODELLER version 9 (1) using the cph1Δ2 structure as template. Electrostatic surface potentials were calculated with the apoproteins structures by APBS (2) using an ionic strength of 0.1 M and mapped onto the molecular surface (top) and the PCB-harboring cavity (below; blue: +5 kcal/e, white: 0 kcal/e, red: −5 kcal/e). Of 35 residues surrounding the PCB chromophore within a distance of 5 Å, 23 are identical in Cph1Δ2 and *phyA*65. The remaining 12 residues are either from the divergent N termini (Cph1Δ2 → *phyA*65: L15T, I20H), surface exposed (Y458D), conservatively exchanged (S206T, S255A, Y257H, L264M, T274V, L469M) or have slightly larger aliphatic side chains (A256P, A288V, A457P). The P1 subdomain of *phyA*65 (light green) is a unique and structurally not yet characterized N-terminal extension of plant phytochromes. This figure was made by PyMol (3).

1. Eswar N, *et al.* (2006) Comparative protein structure modeling with MODELLER. *Curr Protocols Bioinformatics* Supplement 15:5.6.1–5.6.30.
2. Baker NA, Sept D, Joseph S, Holst MJ, McCammon JA (2001). Electrostatics of nanosystems: Application to microtubules and the ribosome. *Proc Natl Acad Sci USA* 98:10037–10041.
3. DeLano WL (2002). *The PyMOL Molecular Graphics System*. www.pymol.org (DeLano Scientific, San Carlos, CA).

Table S1. The ^{13}C chemical shift assignments obtained in the present work

	Cph1Δ2			*phyA*65		
Atom	Pr	Pfr	Pr-Pfr	Pr	Pfr	Pr-Pfr
1a	182.7	182.9	−0.2	182.6	182.5	+ 0.1
1b	184.1		+ 1.2			
2	37.1	37.3	−0.2	36.8	37.0	−0.2
2a	38.0		+ 0.7			
2^1	17.4	18.2	−0.8	17.7	17.7	0
3	53.3	54.3	−1.0	53.9	53.9	0
3^1	47.5	49.7	−2.2	47.6	49.1	−1.5
3^1a				45.8		−3.3
3^2	22.0	21.2	+ 0.8	21.7	21.3	+ 0.4
3^2b				23.0		+ 1.7
4	153.9	153.5	+ 0.4			
5	87.1	88.5	−1.4	85.8	87.1	−1.3
6	149.5	149.3	+ 0.2			
7	125.5	126.3	−0.8	124.7	124.6	+ 0.1
7^1	9.3	9.2	+ 0.1	7.2	7.5	−0.3
8	145.2	143.8	+ 1.4	146.4	143.4	+ 3.0
8^1a	22.8	22.9	−0.1	21.8	23.0	−1.2
8^1b	21.8		−1.1			
8^2a	42.9	41.8	+ 1.1	41.5	41.1	+ 0.4
8^2b	41.4		−0.4			
8^3a	180.0	180.5	−0.5	179.9	179.7	+ 0.2
8^3b	179.3		−1.2			
9	127.7	130.9	−3.2	127.7	130.6	−2.9
10	112.8	112.4	+ 0.4	113.0	111.9	+ 1.1
11	127.7	130.9	−3.2	127.7	130.6	−2.9
12	145.2	145.8	−0.6	146.4	144.5	+ 1.9
12^1	20.4	20.5	−0.1	21.8	21.0	+ 0.8
12^2	38.1	38.4	−0.3	41.5	39.0	+ 2.5
12^3	179.0	175.3	+ 3.7	177.5	174.7	+ 2.8
13	126.4	130.7	−4.3	123.7	130.1	−6.4
13^1	11.4	11.6	−0.2	10.0	12.1	−2.1
14	145.9	152.0	−6.1	146.6	150.5	−3.9
15	93.2	91.6	+ 1.6	93.3	92.3	+ 1.0
16	145.9	151.6	−6.7	146.6	150.5	−3.9
17	142.1	137.5	+ 4.6	142.6	138.6	+ 4.0
17^1	9.9	10.0	−0.1	10.3	10.3	0
18	134.1	140.5	−6.4	133.3	140.1	−6.8
18^1	16.5	15.7	+ 0.8	16.6		
18^2	13.2	13.3	−0.1			
19	172.7	169.1	+ 3.6	172.4	169.6	+ 2.8

Table S2. The ^{1}H and ^{15}N chemical shift assignments obtained in the present work

Pr			Pfr		
δ_N (ppm)	Atom	δ_H (ppm)	δ_N (ppm)	Atom	δ_H (ppm)
160.5 158.1	N22, N23	10.9, 11.7	158.6 155.8	N22, N23	11.7, 11.7
147.0	N21	10.9	142.6	N21	10.6
131.9	N24	9.9	138.0	N24	9.6