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The D-ring, Not the A-ring, Rotates in *Synechococcus* OS-B' Phytochrome

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**Table 1.**  $^{13}\text{C}$  and  $^{15}\text{N}$  chemical shifts ( $\delta^{\text{C}}$  and  $\delta^{\text{N}}$ ) of the chromophore in Cph1(PAS-GAF-PHY) and SyB.Cph2(GAF). Data were obtained from  $u\text{-}[^{13}\text{C},^{15}\text{N}]\text{-PCB-Cph1(PAS-GAF-PHY)}$  as Pr and Pfr (2) and  $u\text{-}[^{13}\text{C},^{15}\text{N}]\text{-PCB-SyB.Cph2(GAF)}$  as P630 and P690 (Figs. 1 and 2).  $\Delta\delta^{\text{C}}$  and  $\Delta\delta^{\text{N}}$  for Cph1(PAS-GAF-PHY) (Pfr - Pr) as  $\Delta\delta^{\text{C(Pfr-Pr)}}$ , SyB.Cph2(GAF) (P690 - P630) as  $\Delta\delta^{\text{C(P690-P630)}}$ , SyB.Cph2(GAF) P630 - Cph1(PAS-GAF-PHY) Pr as  $\Delta\delta^{\text{C(P630-Pr)}}$  and SyB.Cph2(GAF) P690 - Cph1(PAS-GAF-PHY) Pfr as  $\Delta\delta^{\text{C(P690-Pfr)}}$  are listed.

chromophore carbon	Cph1(PAS-GAF-PHY)			SyB.Cph2(GAF)			SyB.Cph2(GAF) - Cph1(PAS-GAF-PHY)		
	$\delta^{\text{Pr}}$ (ppm)	$\delta^{\text{Pfr}}$ (ppm)	$\Delta\delta^{\text{C(Pfr-Pr)}}$ (ppm)	$\delta^{\text{P630}}$ (ppm)	$\delta^{\text{P690}}$ (ppm)	$\Delta\delta^{\text{C(P690-P630)}}$ (ppm)	$\Delta\delta^{\text{C(P630-Pr)}}$ (ppm)	$\Delta\delta^{\text{C(P690-Pfr)}}$ (ppm)	
<b>Ring A</b>	1	184.0	182.8	-1.2	182.0	183.3	+1.3	-2.0	+0.5
	2	37.1	37.2	+0.1	35.2	36.4	+1.2	-1.9	-0.8
	2 <sup>1</sup>	17.5	18.5	+1.0	17.2 (2 <sup>1a</sup> ) 18.1 (2 <sup>1b</sup> )	17.6 (2 <sup>1a</sup> ) 18.0 (2 <sup>1b</sup> )	+0.4 -0.1	-0.3 +0.6	-0.9 -0.5
	3	53.4	54.3	+0.9	53.3 (3 <sup>a</sup> ) 53.6 (3 <sup>b</sup> )	51.0 (3 <sup>a</sup> ) 52.7 (3 <sup>b</sup> )	-2.3 -0.9	-0.1 +0.2	-3.3 -1.6
	3 <sup>1</sup>	47.6	50.0	+2.4	47.4	48.4	+1.0	-0.2	-1.6
	3 <sup>2</sup>	21.8	21.4	-0.4	20.6	19.3	-1.3	-1.2	-2.1
	4	153.9	153.5	-0.4	156.9 (4 <sup>a</sup> ) 157.4 (4 <sup>b</sup> ) 157.9 (4 <sup>c</sup> )	156.6	-0.3 -0.8 -1.3	+3.0 +3.5 +4.0	+3.1
	<b>A-B</b>	5	87.1	88.5	+1.4	85.4 (5 <sup>a</sup> ) 86.5 (5 <sup>b</sup> )	86.1	+0.7 -0.4	-1.7 -0.6
<b>Ring B</b>	6	149.5	149.3	-0.2	151.4 (6 <sup>a</sup> ) 152.1 (6 <sup>b</sup> )	151.8	+0.4 -0.3	+1.9 +2.6	+2.5
	7	125.7	126.1	+0.4	127.4	127.2	-0.2	+1.7	+1.1
	7 <sup>1</sup>	9.2	9.3	+0.1	8.3	9.9	+1.6	-0.9	+0.6
	8	145.2	143.8	-1.4	147.5	146.7	-0.8	+2.3	+2.9
	8 <sup>1</sup>	21.8	23.1	+1.3	20.9	20.1	-0.8	-0.9	-3.0
	8 <sup>2</sup>	42.9	41.8	-1.1	38.5	39.1	+0.6	-4.4	-2.7
	8 <sup>3</sup>	180.0	180.5	+0.5	180.2	179.7	-0.5	+0.2	-0.8
	9	127.7	129.9	+2.2	126.4	126.6	+0.2	-1.3	-3.3
<b>B-C</b>	10	112.8	112.4	-0.4	112.9	113.1	+0.2	+0.1	+0.7
<b>Ring C</b>	11	127.7	131.0	+3.3	130.0	129.7	-0.3	+2.3	-1.3
	12	145.2	145.8	+0.6	138.5	138.3	-0.2	-6.7	-7.5
	12 <sup>1</sup>	20.4	20.5	+0.1	21.3	22.3	+1.0	+0.9	+1.8
	12 <sup>2</sup>	38.1	38.4	+0.3	37.3	38.2	+0.9	-0.8	-0.2
	12 <sup>3</sup>	179.0	175.3	-3.7	177.6	177.0	-0.6	-1.4	+1.7
	13	126.4	130.7	+4.3	123.6	124.3	+0.7	-2.8	-6.4
	13 <sup>1</sup>	11.4	11.6	+0.2	11.2	11.3	+0.1	-0.2	-0.3
	14	145.9	152.0	+6.1	140.4	140.3	-0.1	-5.5	-11.7
<b>C-D</b>	15	93.2	91.6	-1.6	94.7	94.6	-0.1	+1.5	+3.0
<b>Ring D</b>	16	145.9	151.6	+5.7	143.6	143.4	-0.2	-2.3	-8.2
	17	142.1	135.5	-6.6	140.9	141.3	+0.4	-1.2	+5.8
	17 <sup>1</sup>	9.9	10.0	+0.1	8.5	8.8	+0.3	-1.4	-1.2
	18	134.0	140.5	+6.5	132.7	132.6	-0.1	-1.3	-7.9
	18 <sup>1</sup>	16.5	15.6	-0.9	15.0	15.4	+0.4	-1.5	-0.2
	18 <sup>2</sup>	13.2	13.3	+0.1	11.3	12.3	+1.0	-1.9	-1.0
	19	172.7	169.1	-3.6	171.7	171.0	-0.7	-1.0	+1.9
	pyrrole nitrogen	$\delta^{\text{Pr}}$ (ppm)	$\delta^{\text{Pfr}}$ (ppm)	$\Delta\delta^{\text{N(Pfr-Pr)}}$ (ppm)	$\delta^{\text{P630}}$ (ppm)	$\delta^{\text{P690}}$ (ppm)	$\Delta\delta^{\text{N(P690-P630)}}$ (ppm)	$\Delta\delta^{\text{N(P630-Pr)}}$ (ppm)	$\Delta\delta^{\text{N(P690-Pfr)}}$ (ppm)
<b>Ring A</b>	21	158.6	158.7	+0.1	156.6	156.0	-0.6	-2.0	-2.7
<b>Ring B</b>	22	160.7	156.7	-4.0	161.7	161.5	-0.2	+1.0	+4.8
<b>Ring C</b>	23	148.0	142.2	-5.8	145.4	145.6	+0.2	-2.6	+3.4
<b>Ring D</b>	24	133.1	138.8	+5.7	131.9	132.0	+0.1	-1.2	-6.8