Dataset S3. Overview of the interfacial ^{1}H contacts of the PCB chromophore. The data were obtained from *u*-[^{13}C,^{15}N]-PCB-Cph1Δ2 with an LG–CP contact time of 2.3 ms in both Pr and Pfr states. ^{13}C NMR chemical shifts of the chromophore based on the published sources (3, 4) are given in parentheses. ^{1}H NMR chemical shift differences ($\Delta\sigma^{H}$) of the chromophore contacts during Pr-to-Pfr photoconversion are listed at the right-most column as the values for Pfr minus those for Pr.

	Pr				Pfr				
Cofactor carbon	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [6]	σ^{proton} (ppm)	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [14]	σ^{proton} (ppm)	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
1	**184.1** (184.0)	Asp-207 CA	3.83	6.4	**182.9** (182.8)	Asp-207 CA	3.89	5.8	–0.6
		-	-	-		Asp-207 CB	4.46	4.0	-
		Asp-207 N	4.55	10.2		Asp-207 N	4.96	10.8	+0.6
		-	-	-		Tyr-263 CD2	4.04	9.4	-
		-	-	-		Tyr-263 CE2	4.37	8.8	-
		W1-I	3.05	7.2		-	-	-	-
		W1-II	3.05	7.7		W1	3.37	7.1	–0.6
2	**37.1** (37.1)	-	-	-	**37.3** (37.2)	Asp-207 CA	4.25	5.8	-
		-	-	-		Asp-207 CB	5.13	4.0	-
		-	-	-		Asp-207 N	4.98	10.8	-
		Leu-15 CD2	4.80	3.0		-	-	-	-
		Pro-471 CA	4.60	5.7		Pro-471 CA	-	5.3	–0.4
		-	-	-		Pro-471 CB	-	3.4	-
		Tyr-458 CB	4.47	3.7		-	-	-	-
2¹	**17.4** (17.5)	Asp-207 CA	4.65	6.4	**18.2** (18.5)	Asp-207 CA	4.78	5.8	–0.6
		-	-	-		Asp-207 N	5.20	10.8	-
		Leu-15 CD1	4.07	3.2		Leu-15 CD1	-	2.8	–0.4
		Ser-206 CB	4.31	4.8		Ser-206 CB	5.57	5.0	+0.2
		Ser-206 OG	4.25	8.0		Ser-206 OG	5.25	7.4	–0.6
		Tyr-458 CB	3.68	3.7		-	-	-	-
3	**53.3** (53.4)	-	-	-	**54.3** (54.3)	Asp-207 CA	4.71	5.8	-
		-	-	-		Asp-207 N	5.39	10.8	-
		Cys-259 CB	4.44	3.9		Cys-259 CB	-	4.5	+0.6
		His-260 N	5.61	10.2		-	-	-	-
		Leu-15 CD2	3.82	3.0		Leu-15 CD2	-	2.6	–0.4
		-	-	-		Pro-209 CG	4.36	5.1	-
3¹	**47.5** (47.6)	Cys-259 CA	4.29	5.6	**49.9** (50.0)	Cys-259 CA	-	6.2	+0.6
		Cys-259 CB	3.07	3.9		Cys-259 CB	-	4.5	+0.6
		Leu-15 CD2	4.49	3.0		Leu-15 CD2	-	2.6	–0.4
		-	-	-		Pro-209 CD	4.72	5.6	-
		-	-	-		Pro-209 CG	3.96	5.1	-
		-	-	-		Pro-209 N	5.83	11.8	-
		Pro-471 N	4.94	11.5		-	-	-	-

	Pr				Pfr				
Cofactor carbon	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [6]	σ^{proton} (ppm)	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [14]	σ^{proton} (ppm)	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
3[2]	**21.9** (21.8)	-	-	-	**21.4** (21.4)	Cys-259 CA	-	6.2	-
		Cys-259 CB	3.59	3.9		Cys-259 CB	-	4.5	+0.6
		His-470 CA	4.26	6.7		-	-	-	-
		His-470 N	3.96	10.4		His-470 N	-	9.8	–0.6
		Leu-469 CB	3.39	3.2		Leu-469 CB	-	3.4	+0.2
		-	-	-		Pro-209 CG	4.05	5.1	-
		Pro-471 CD	4.63	5.3		-	-	-	-
		Pro-471 N	4.22	11.5		Pro-471 N	-	11.4	–0.1
4	**154.0** (153.9)	Leu-15 CD2	4.39	3.0	**153.7** (153.5)	Leu-15 CD2	-	2.6	–0.4
6	**149.3** (149.5)	His-260 N	4.71	10.2	**149.3** (149.3)	-	-	-	-
		Pro-209 CD	3.49	5.7		Pro-209 CD	3.71	5.6	–0.1
		-	-	-		Pro-209 CG	4.26	5.1	-
7	**125.5** (125.7)	-	-	-	**126.3** (126.1)	Ala-212 CB	4.17	4.2	-
		-	-	-		His-260 CA	4.90	6.0	-
		His-260 CB	3.97	5.1		His-260 CB	3.65	4.8	–0.3
		His-260 CD2-II	5.49	11.4		His-260 CD2	4.89	11.0	–0.4
		His-260 CE1	6.02	10.0		His-260 CE1	5.42	10.1	+0.1
		His-260 N	4.78	10.2		-	-	-	-
		Pro-209 CD	4.12	5.7		-	-	-	-
		-	-	-		Pro-209 N	5.43	11.8	-
7[1]	**9.3** (9.2)	-	-	-	**9.2** (9.3)	Ala-212 CB	4.20	4.2	-
		-	-	-		His-260 CB	4.23	4.8	-
		His-260 N	5.05	10.2		His-260 N	5.30	10.3	+0.1
		-	-	-		Ile-20 CG2	-	2.0	-
		Leu-18 CD1	3.99	2.5		-	-	-	-
		-	-	-		Pro-209 CD	4.56	5.6	-
		Tyr-257 CB	3.47	4.5		Tyr-257 CB	-	3.6	–0.9
		Tyr-257 CD2	3.34	9.6		Tyr-257 CD2	-	9.7	+0.1

	Pr				Pfr				
Cofactor carbon	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [6]	σ^{proton} (ppm)	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [14]	σ^{proton} (ppm)	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
8	**145.2** (145.2)	Ala-212 CB	3.96	3.6	**143.6** (143.8)	Ala-212 CB	4.01	4.2	**+0.6**
		-	-	-		His-260 CA	5.30	6.0	-
		His-260 CB	3.77	5.1		His-260 CB	3.89	4.8	**–0.3**
		-	-	-		His-260 CD2	4.34	11.0	-
		His-260 CE1	5.14	10.0		His-260 CE1	4.68	10.1	**+0.1**
		His-260 ND1-I	4.44	12.3		-	-	-	-
		His-260 NE2-I	5.22	17.9		-	-	-	-
		His-260 NE2-II	5.22	14.0		His-260 NE2	4.81	13.1	**–0.9**
		-	-	-		Ile-208 CG2	5.48	3.1	-
		Pro-209 CD	4.36	5.7		-	-	-	-
		W1-II	5.18	7.7		-	-	-	-
8^1	**22.8** (21.8)	Ala-212 CB	3.87	3.6	**22.9** (23.1)	Ala-212 CB	3.83	4.2	**+0.6**
		His-260 CB	4.17	5.1		His-260 CB	4.67	4.8	**–0.3**
		His-260 CD2-I	4.39	15.4		-	-	-	-
		His-260 CD2-II	4.39	11.4		His-260 CD2	4.47	11.0	**–0.4**
		His-260 NE2-II	5.10	14.0		His-260 NE2	4.91	13.1	**–0.9**
		Ile-20 CD1	4.11	2.5		Ile-20 CD1	-	2.3	**–0.2**
		W2	4.74	7.9		W2	-	8.1	**+0.2**
8^2	**42.9** (42.9)	-	-	-	**41.8** (41.8)	Ala-256 CA	-	5.7	-
		-	-	-		Arg-222 NH1	4.62	11.6	-
		Arg-254 NH2	5.24	10.8		-	-	-	-
		His-260 CB	4.39	5.1		His-260 CB	4.20	4.8	**–0.3**
		-	-	-		His-260 CD2	3.42	11.0	-
		-	-	-		His-260 NE2	3.98	13.1	-
		Ile-20 CB	4.39	3.7		-	-	-	-
		Ile-20 CD1	3.60	2.5		Ile-20 CD1	-	2.3	**–0.2**
		Ile-20 CG2	4.16	3.0		-	-	-	-
		Tyr-257 CB	3.88	4.5		-	-	-	-
		Tyr-257 N	3.81	9.8		-	-	-	-
		W2	4.70	7.9		W2	-	8.1	**+0.2**

	Pr				Pfr				
Cofactor carbon	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [6]	σ^{proton} (ppm)	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [14]	σ^{proton} (ppm)	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
8[3]	**180.1** (180.0)	Ala-256 CA	3.90	6.6	**180.3** (180.5)	Ala-256 CA	-	5.7	**–0.9**
		Ala-256 CB	3.96	4.0		-	-	-	**-**
		-	-	-		Arg-222 CB	6.00	3.9	**-**
		-	-	-		Arg-222 CG	5.01	2.9	**-**
		-	-	-		Arg-222 NH1	3.16	11.6	**-**
		-	-	-		Arg-222 NH2	4.00	12.2	**-**
		Arg-254 NH1	3.81	8.5		-	-	-	**-**
		Arg-254 NH2	3.65	10.8		Arg-254 NH2	3.97	10.4	**–0.4**
		-	-	-		His-260 CB	5.57	4.8	**-**
		-	-	-		His-260 CD2	4.44	11.0	**-**
		Ile-20 CD1	3.53	2.5		Ile-20 CD1	-	2.3	**–0.2**
		Ile-20 CG1	4.29	3.2		-	-	-	**-**
		Tyr-257 CB	4.45	4.5		-	-	-	**-**
		Tyr-257 N	3.69	9.8		-	-	-	**-**
		W2	3.90	7.9		W2	-	8.2	**+0.3**
9	**127.9** (127.7)	-	-	-	**131.0** (129.9)	Ala-212 CB	4.75	4.2	**-**
		His-260 CB	3.76	5.1		-	-	-	**-**
		His-260 CD2-I	4.32	15.4		-	-	-	**-**
		His-260 CD2-II	4.32	11.4		His-260 CD2	4.36	11.0	**–0.4**
		His-260 CE1	4.24	10.0		His-260 CE1	4.04	10.1	**+0.1**
		His-260 ND1-I	3.61	12.3		-	-	-	**-**
		His-260 NE2-I	4.63	17.9		-	-	-	**-**
		His-260 NE2-II	4.63	14.0		His-260 NE2	4.52	13.1	**–0.9**
		-	-	-		Ile-208 CB	5.17	4.7	**-**
		Pro-209 CD	4.01	5.7		Pro-209 CD	4.72	5.6	**–0.1**
		W1-I	3.90	7.2		-	-	-	**-**
		W1-II	3.90	7.7		W1	3.88	7.1	**–0.6**
10*	**112.8** (112.8)	His-260 CD2-I	3.89	15.4	**112.4** (112.4)	-	-	-	**-**
		His-260 CD2-II	3.89	11.4		His-260 CD2	4.46	11.0	**–0.4**
		His-260 CE1	3.54	10.0		His-260 CE1	3.67	10.1	**+0.1**
		His-260 ND1-I	3.39	12.3		-	-	-	**-**
		His-260 NE2-I	3.83	17.9		-	-	-	**-**
		His-260 NE2-II	3.83	14.0		His-260 NE2	4.21	13.1	**–0.9**

*Continued on following page.

	Pr				Pfr				
Cofactor carbon	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [6]	σ^{proton} (ppm)	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [14]	σ^{proton} (ppm)	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
10	**112.8** (112.8)	-	-	-	**112.4** (112.4)	Ile-208 CB	5.02	4.7	-
		-	-	-		Ile-208 CD1	4.43	2.9	-
		Ile-208 CG2	4.72	3.5		-	-	-	-
		W1-I	4.15	7.2		-	-	-	-
		W1-II	4.15	7.7		W1	4.23	7.1	–0.6
11	**127.9** (127.7)	His-260 CD2-I	4.32	15.4	**131.0** (131.0)	-	-	-	-
		His-260 CD2-II	4.32	11.4		His-260 CD2	5.12	11.0	–0.4
		His-260 CE1	3.25	10.0		His-260 CE1	3.74	10.1	+0.1
		His-260 ND1-I	3.51	12.3		-	-	-	-
		His-260 NE2-I	3.78	17.9		-	-	-	-
		His-260 NE2-II	3.78	14.0		His-260 NE2	4.62	13.1	–0.9
		-	-	-		Ile-208 CB	4.80	4.7	-
		-	-	-		Ile-208 CD1	3.82	2.9	-
		-	-	-		Ile-208 CG1	3.78	3.3	-
		Ile-208 CG2	4.26	3.5		-	-	-	-
		W1-I	3.93	7.2		-	-	-	-
		W1-II	3.93	7.7		W1	3.78	7.1	–0.6
12	**145.2** (145.2)	His-260 CE1	3.55	10.0	**145.8** (145.8)	His-260 CE1	4.12	10.1	+0.1
		His-260 ND1-I	4.25	12.3		-	-	-	-
		His-260 NE2-I	3.75	17.9		-	-	-	-
		His-260 NE2-II	3.75	14.0		His-260 NE2	4.97	13.1	–0.9
		-	-	-		Ile-208 CB	5.22	4.7	-
		-	-	-		Ile-208 CD1	3.54	2.9	-
		-	-	-		Ile-208 CG1	3.99	3.3	-
		W1-II	5.16	7.7		W1	4.75	7.1	–0.6
		W4 (**Pr-II**)	5.25	8.9		-	-	-	-
		-	-	-		W5	-	8.4	-
		{W5+$[OH]^-_{W4}$} (**Pr-I**)	-	9.4		-	-	-	-

	Pr				Pfr				
Cofactor carbon	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [6]	σ^{proton} (ppm)	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [14]	σ^{proton} (ppm)	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
12[1]	**20.4** (20.4)	His-260 CD2-II	3.89	11.4	**20.6** (20.5)	-	-	-	-
		His-260 CE1	3.54	10.0		His-260 CE1	4.67	10.1	**+0.1**
		His-260 ND1-I	4.89	12.3		-	-	-	-
		His-260 NE2-I	3.83	17.9		-	-	-	-
		His-260 NE2-II	3.83	14.0		His-260 NE2	5.19	13.1	**–0.9**
		-	-	-		Ile-208 CD1	3.79	2.9	-
		-	-	-		Ile-208 CG1	4.68	3.3	-
		Phe-216 CE2	3.78	7.3		Phe-216 CE2	-	7.0	**–0.3**
		Phe-216 CZ	4.14	6.8		Phe-216 CZ	-	6.5	**–0.3**
		Thr-274 CG2	4.72	2.1		-	-	-	-
		W2	4.48	7.9		-	-	-	-
		-	-	-		W4	-	7.9	-
		-	-	-		W5	-	8.4	-
12[2]	**38.1** (38.1)	Arg-222 CB	4.71	4.4	**38.4** (38.4)	-	-	-	-
		His-260 CD2-II	5.00	11.4		-	-	-	-
		His-260 CE1	4.66	10.0		His-260 CE1	4.18	10.1	**+0.1**
		His-260 NE2-I	4.15	17.9		-	-	-	-
		His-260 NE2-II	4.15	14.0		His-260 NE2	4.47	13.1	**–0.9**
		Phe-216 CE2	3.73	7.3		Phe-216 CE2	-	7.0	**–0.3**
		Phe-216 CZ	3.61	6.8		Phe-216 CZ	-	6.5	**–0.3**
		-	-	-		Ser-272 OG	4.75	6.0	-
		-	-	-		Thr-274 CB	-	3.4	-
		Thr-274 CG2	3.53	2.1		Thr-274 CG2	-	2.8	**+0.7**
		Thr-274 OG1	3.14	10.7		Thr-274 OG1	-	10.6	**–0.1**
		W2	4.44	7.9		-	-	-	-
		W3	4.31	8.0		W3	-	7.5	**–0.5**
		W4 (**Pr-II**)	4.59	8.9		-	-	-	-
		{W5+$[OH]^-_{W4}$} (**Pr-I**)	-	9.4		-	-	-	-

	Pr				Pfr				
Cofactor carbon	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [6]	σ^{proton} (ppm)	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [14]	σ^{proton} (ppm)	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
12[3]	**179.0** (179.0)	Arg-222 CB	4.49	4.4	**175.3** (175.3)	-	-	-	-
		His-260 CD2-II	3.89	11.4		-	-	-	-
		His-260 CE1	3.54	10.0		-	-	-	-
		His-260 ND1-I	5.17	12.3		-	-	-	-
		His-260 NE2-I	3.83	17.9		-	-	-	-
		His-260 NE2-II	3.83	14.0		His-260 NE2	4.88	13.1	–0.9
		-	-	-		His-290 CE1	4.31	9.8	-
		-	-	-		His-290 NE2	3.55	12.3	-
		-	-	-		Phe-216 CZ	-	6.5	-
		Ser-272 OG	4.73	7.0		Ser-272 OG	4.86	6.0	–1.0
		Thr-274 CB	3.94	3.7		Thr-274 CB	-	3.4	–0.3
		Thr-274 OG1	3.14	10.7		Thr-274 OG1	-	10.6	–0.1
		-	-	-		Tyr-176 OH	3.94	9.0	-
		W2	3.59	7.9		-	-	-	-
		W3	3.10	8.0		W3	-	7.5	–0.5
		W4 (**Pr-II**)	3.50	8.9		W4	-	7.9	–1.0
		-	-	-		W5	-	8.5	-
		W6	4.92	8.4		-	-	-	-
		{W5+$[OH]^-_{W4}$} (**Pr-I**)	-	9.4		-	-	-	-
13	**126.5** (126.4)	-	-	-	**130.5** (130.7)	Asp-207 CB	5.57	4.0	-
		His-260 CE1	3.99	10.0		His-260 CE1	4.71	10.1	+0.1
		His-260 ND1-I	4.83	12.3		-	-	-	-
		His-260 NE2-I	4.47	17.9		-	-	-	-
		-	-	-		His-260 NE2	5.77	13.1	-
		Ile-208 CB	4.88	4.4		Ile-208 CB	5.42	4.7	+0.3
		Ile-208 CD1	3.76	2.8		Ile-208 CD1	3.67	2.9	+0.1
		Ile-208 CG1	4.06	3.4		Ile-208 CG1	3.99	3.3	–0.1
		-	-	-		Tyr-203 CE2	5.15	9.3	-
		-	-	-		W1	4.63	7.1	-
		W5 (**Pr-II**)	4.32	7.8		W5	-	8.5	+0.7

	Pr				Pfr				
Cofactor carbon	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [6]	σ^{proton} (ppm)	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [14]	σ^{proton} (ppm)	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
13¹	**11.4** (11.4)	-	-	-	**11.3** (11.6)	Ala-288 CB	-	3.6	-
		His-260 ND1-I	6.03	12.3		-	-	-	-
		His-260 NE2-I	5.32	17.9		-	-	-	-
		Ile-208 CD1	3.96	2.8		Ile-208 CD1	4.15	2.9	**+0.1**
		Thr-274 CB	4.87	3.7		-	-	-	-
		Thr-274 CG2	4.20	2.1		-	-	-	-
		Thr-274 OG1	4.21	10.7		-	-	-	-
		-	-	-		Tyr-176 CE1	3.47	9.3	-
		-	-	-		Tyr-203 CD2	5.18	9.8	-
		W5 (**Pr-II**)	3.73	7.8		W5	-	8.5	**+0.7**
		W6	4.53	8.4		W6	-	7.8	**–0.6**
		{W5+$[OH]^-_{W4}$} (**Pr-I**)	-	9.4		-	-	-	-
14	**146.1** (145.9)	-	-	-	**152.0** (152.0)	Asp-207 CB	4.51	4.0	-
		His-260 CE1	3.89	10.0		His-260 CE1	4.64	10.1	**+0.1**
		His-260 ND1-I	4.45	12.3		-	-	-	-
		His-260 NE2-I	4.72	17.9		-	-	-	-
		-	-	-		Ile-208 CB	5.27	4.7	-
		Ile-208 CD1	3.58	2.8		Ile-208 CD1	4.13	2.9	**+0.1**
		Ile-208 CG1	3.44	3.4		Ile-208 CG1	3.91	3.3	**–0.1**
		-	-	-		Tyr-263 CE2	5.35	8.8	-
		-	-	-		Tyr-263 OH	5.96	7.7	-
		W1-II	4.05	7.7		W1	3.51	7.1	**–0.6**
		{W5+$[OH]^-_{W4}$} (**Pr-I**)	-	9.4		-	-	-	-

	Pr				Pfr				
Cofactor carbon	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [6]	σ^{proton} (ppm)	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [14]	σ^{proton} (ppm)	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
15	**93.2** (93.2)	-	-	-	**91.5** (91.6)	Asp-207 CA	4.51	5.8	-
		-	-	-		Asp-207 CB	3.63	4.0	-
		-	-	-		Asp-207 N	5.86	10.8	-
		Ile-208 CD1	3.74	2.8		-	-	-	-
		Ile-208 CG1	3.59	3.4		Ile-208 CG1	4.61	3.3	**–0.1**
		Ile-208 N	4.95	10.3		-	-	-	-
		-	-	-		Tyr-203 CB	5.08	4.6	-
		-	-	-		Tyr-203 CD2	4.85	9.8	-
		Tyr-263 CE1	4.33	9.7		Tyr-263 CE1	5.00	9.0	**–0.7**
		-	-	-		Tyr-263 OH	4.61	7.7	-
		W1-II	4.08	7.7		W1	3.60	7.1	**–0.6**
16	**146.1** (145.9)	-	-	-	**151.1** (151.6)	Asp-207 CA	5.68	5.8	-
		-	-	-		Asp-207 CB	4.53	4.0	-
		Ile-208 CD1	4.44	2.8		-	-	-	-
		Ile-208 CG1	4.64	3.4		-	-	-	-
		-	-	-		Tyr-203 CB	4.72	4.6	-
		Tyr-263 CE1	4.29	9.7		Tyr-263 CE1	4.26	9.0	**–0.7**
		-	-	-		Tyr-263 OH	3.70	7.7	-
		-	-	-		W1	4.58	7.1	-
		{W5+[OH]$^-_{W4}$} (**Pr-I**)	-	9.4		-	-	-	-
17	**142.1** (142.1)	-	-	-	**137.7** (135.5)	Asp-207 CB	5.93	4.0	-
		His-290 CE1	5.46	10.7		-	-	-	-
		Tyr-176 CE1	4.67	8.8		-	-	-	-
		-	-	-		Tyr-203 CB	5.72	4.6	-
		-	-	-		Tyr-203 CE1	4.93	9.5	-
		Tyr-263 CE1	4.15	9.7		Tyr-263 CE1	3.95	9.0	**–0.7**
		Tyr-263 OH	3.54	8.2		Tyr-263 OH	3.92	7.7	**–0.5**

	Pr				Pfr				
Cofactor carbon	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [6]	σ^{proton} (ppm)	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [14]	σ^{proton} (ppm)	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
17[1]	**9.9** (9.9)	Arg-472 NH1	5.42	12.2	**9.9** (10.0)	-	-	-	-
		Asp-207 CB	4.05	4.2		-	-	-	-
		-	-	-		Met-174 CE	5.92	3.2	-
		-	-	-		Tyr-176 CE2	5.93	9.5	-
		Tyr-176 OH	4.55	9.1		Tyr-176 OH	4.24	9.0	**–0.1**
		Tyr-203 CB	4.22	3.7		-	-	-	-
		-	-	-		Tyr-203 CD1	5.98	10.0	-
		Tyr-203 CD2	3.67	10.0		-	-	-	-
		-	-	-		Tyr-203 OH	6.65	7.3	-
		Tyr-263 OH	2.66	8.2		-	-	-	-
		-	-	-		W4	-	7.9	-
		-	-	-		W5	-	8.4	-
		W7	5.56	7.7		-	-	-	-
18	**134.2** (134.1)	-	-	-	**140.4** (140.5)	Arg-472 NH1	-	8.5	-
		His-290 CE1	4.42	10.7		-	-	-	-
		His-290 NE2	4.60	12.7		-	-	-	-
		Met-174 CE	4.65	3.8		-	-	-	-
		Tyr-176 CE1	4.72	8.8		-	-	-	-
		-	-	-		Tyr-203 CB	5.46	4.6	-
		-	-	-		Tyr-203 CD1	4.43	10.0	-
		-	-	-		Tyr-203 CE1	4.75	9.5	-
		-	-	-		Tyr-263 CE1	4.00	9.0	-
		Tyr-263 OH	4.30	8.2		Tyr-263 OH	3.55	7.7	**–0.5**
18[1]*	**16.5** (16.5)	His-290 CE1	4.55	10.7	**15.7** (15.6)	-	-	-	-
		His-290 ND1 (**Pr-I**)	5.63	11.7		-	-	-	-
		His-290 NE2 (**Pr-II**)	5.10	12.7		-	-	-	-
		Met-174 CE	4.22	3.8		Met-174 CE	4.73	3.2	**–0.6**
		Met-267 CE	4.16	2.9		Met-267 CE	4.21	2.6	**–0.3**
		Tyr-203 CD2	4.16	10.0		-	-	-	-
		Tyr-203 CE2	3.71	9.4		-	-	-	-
		Tyr-203 OH	4.00	8.0		-	-	-	-
		-	-	-		Tyr-263 CE1	4.37	9.0	-

*Continued on following page.

	Pr				Pfr				
Cofactor carbon	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [6]	σ^{proton} (ppm)	σ^{carbon} (ppm) [3, 4]	Proton contact	XRD distance (Å) [14]	σ^{proton} (ppm)	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
18¹	**16.5** (16.5)	Tyr-263 OH	4.56	8.2	**15.7** (15.6)	Tyr-263 OH	4.26	7.7	**–0.5**
		Val-186 CG2	4.76	1.6		Val-186 CG2	6.19	1.5	**–0.1**
		-	-	-		W5	-	8.4	-
18²	**13.2** (13.2)	His-290 CE1	3.48	10.7	**13.3** (13.3)	-	-	-	-
		His-290 ND1 (**Pr-I**)	4.38	11.7		-	-	-	-
		His-290 NE2 (**Pr-II**)	4.29	12.7		-	-	-	-
		Met-174 CE	2.95	3.8		-	-	-	-
		Met-267 CE	4.25	2.9		Met-267 CE	4.58	2.6	**–0.3**
		Tyr-198 CD2	3.46	10.0		-	-	-	-
		Tyr-198 CE2	3.75	9.4		-	-	-	-
		Tyr-203 OH	4.12	8.0		-	-	-	-
		-	-	-		Tyr-263 OH	4.54	7.7	-
		-	-	-		Val-186 CG2	5.69	1.5	-
19	**172.7** (172.7)	Ala-288 CA	4.48	6.7	**169.0** (169.1)	-	-	-	-
		Ala-288 CB	5.88	3.2		-	-	-	-
		-	-	-		Arg-472 NH1	-	8.5	-
		His-290 CE1	3.87	10.7		-	-	-	-
		His-290 ND1 (**Pr-I**)	5.15	11.7		-	-	-	-
		His-290 NE2 (**Pr-II**)	3.87	12.7		-	-	-	-
		Met-174 CE	4.32	3.8		-	-	-	-
		-	-	-		Tyr-203 CA	5.54	5.2	-
		-	-	-		Tyr-203 CB	4.24	4.6	-
		-	-	-		Tyr-203 CD1	3.65	10.0	-
		-	-	-		Tyr-203 CE1	4.34	9.5	-
		-	-	-		Tyr-263 CE1	4.30	9.0	-
		-	-	-		Tyr-263 OH	3.04	7.7	-
		W5 (**Pr-II**)	3.75	7.8		-	-	-	-
		{W5+$[OH]^-_{W4}$} (**Pr-I**)	-	9.4		-	-	-	-