Dataset S4. ^{13}C PCB chromophore contacts of the protein residues. 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. ^{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				
Proton contact		σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [6]	σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [14]	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
Ala-212	**CB**	-	-	-	-	4.2	7	126.3	4.17	**+0.6**
		-	-	-	-	4.2	7^{1}	9.2	4.20	
		3.6	8	145.2	3.96	4.2	8	143.6	4.01	
		3.6	8^{1}	22.8	3.87	4.2	8^{1}	22.9	3.83	
		-	-	-	-	4.2	9	131.0	4.75	
Ala-256	**CA**	-	-	-	-	5.7	8^{2}	41.8	-	**–0.9**
		6.6	8^{3}	180.1	3.90	5.7	8^{3}	180.3	-	
	CB	4.0	8^{3}	180.1	3.96	-	-	-	-	-
Ala-288	**CA**	6.7	19	172.7	4.48	-	-	-	-	-
	CB	-	-	-	-	3.6	13^{1}	11.3	-	**+0.4**
		3.2	19	172.7	5.88	-	-	-	-	
Arg-222	**CB**	-	-	-	-	3.9	8^{3}	180.3	6.00	**–0.5**
		4.4	12^{2}	38.1	4.71	-	-	-	-	
		4.4	12^{3}	179.0	4.49	-	-	-	-	
	CG	-	-	-	-	2.9	8^{3}	180.5	5.01	-
	NH1	-	-	-	-	11.6	8^{2}	41.8	4.62	-
		-	-	-	-	11.6	8^{3}	180.3	3.16	
	NH2	-	-	-	-	12.2	8^{3}	180.3	4.00	-
Arg-254	**NH1**	8.5	8^{3}	180.1	3.81	-	-	-	-	-
	NH2	10.8	8^{2}	180.1	5.24	-	-	-	-	**–0.4**
		10.8	8^{3}	180.1	3.65	10.4	8^{3}	180.3	3.97	
Arg-472	**NH1**	12.2	17^{1}	9.9	5.42	-	-	-	-	**–3.7**
		-	-	-	-	8.5	18	140.4	-	
		-	-	-	-	8.5	19	169.0	-	
Asp-207*	**CA**	6.4	1	184.1	3.83	5.8	1	182.9	3.89	**–0.6**
		-	-	-	-	5.8	2	37.3	4.25	
		6.4	2^{1}	17.4	4.65	5.8	2^{1}	18.2	4.78	
		-	-	-	-	5.8	3	54.3	4.71	
		-	-	-	-	5.8	15	91.5	4.51	
		-	-	-	-	5.8	16	151.1	5.68	

*Continued on following page.

		Pr				Pfr				
Proton contact		σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [6]	σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [14]	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
Asp-207	**CB**	-	-	-	-	4.0	1	182.9	4.46	**–0.2**
		-	-	-	-	4.0	2	37.3	5.13	
		-	-	-	-	4.0	13	130.5	5.57	
		-	-	-	-	4.0	14	152.0	4.51	
		-	-	-	-	4.0	15	91.5	3.63	
		-	-	-	-	4.0	16	151.1	4.53	
		-	-	-	-	4.0	17	137.7	5.93	
		4.2	17[1]	9.9	4.05	-	-	-	-	
	N	10.2	1	184.1	4.55	10.8	1	182.9	4.96	**+0.6**
		-	-	-	-	10.8	2	37.3	4.98	
		-	-	-	-	10.8	2[1]	18.2	5.20	
		-	-	-	-	10.8	3	54.3	5.39	
		-	-	-	-	10.8	15	91.5	5.86	
Cys-259	**CA**	5.6	3[1]	47.5	4.29	6.2	3[1]	49.9	-	**+0.6**
		-	-	-	-	6.2	3[2]	21.4	-	
	CB	3.9	3	53.3	4.44	4.5	3	54.3	-	**+0.6**
		3.9	3[1]	47.5	3.07	4.5	3[1]	49.9	-	
		3.9	3[2]	21.9	3.59	4.5	3[2]	21.4	-	
His-260*	**CA**	-	-	-	-	6.0	7	126.3	4.90	**-**
		-	-	-	-	6.0	8	143.6	5.30	
	CB	5.1	7	125.5	3.97	4.8	7	126.3	3.65	**–0.3**
		-	-	-	-	4.8	7[1]	9.2	4.23	
		5.1	8	145.2	3.77	4.8	8	143.6	3.89	
		5.1	8[1]	22.8	4.17	4.8	8[1]	22.9	4.67	
		5.1	8[2]	42.9	4.39	4.8	8[2]	41.8	4.20	
		-	-	-	-	4.8	8[3]	180.3	5.57	
		5.1	9	127.9	3.76	-	-	-	-	
	CD2-I	15.4	8[1]	22.8	4.39	-	-	-	-	**-**
		15.4	9	127.9	4.32	-	-	-	-	
		15.4	10	112.8	3.89	-	-	-	-	
		15.4	11	127.9	4.32	-	-	-	-	

*Continued on following page.

		Pr				Pfr				
Proton contact		σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [6]	σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [14]	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
His-260*	**CD2-II**	11.4	7	125.5	5.49	11.0	7	126.3	4.89	**–0.4**
		-	-	-	-	11.0	8	143.6	4.34	
		11.4	8^{1}	22.8	4.39	11.0	8^{1}	22.9	4.47	
		-	-	-	-	11.0	8^{2}	41.8	3.42	
		-	-	-	-	11.0	8^{3}	180.3	4.44	
		11.4	9	127.9	4.32	11.0	9	131.0	4.36	
		11.4	10	112.8	3.89	11.0	10	112.4	4.46	
		11.4	11	127.9	4.32	11.0	11	131.0	5.12	
		11.4	12^{1}	20.4	3.89	-	-	-	-	
		11.4	12^{2}	38.1	5.00	-	-	-	-	
		11.4	12^{3}	179.0	3.89	-	-	-	-	
	CE1	10.0	7	125.5	6.02	10.1	7	126.3	5.42	**+0.1**
		10.0	8	145.2	5.14	10.1	8	143.6	4.68	
		10.0	9	127.9	4.24	10.1	9	131.0	4.04	
		10.0	10	112.8	3.54	10.1	10	112.4	3.67	
		10.0	11	127.9	3.25	10.1	11	131.0	3.74	
		10.0	12	145.2	3.55	10.1	12	145.8	4.12	
		10.0	12^{1}	20.4	3.54	10.1	12^{1}	20.6	4.67	
		10.0	12^{2}	38.1	4.66	10.1	12^{2}	38.4	4.18	
		10.0	12^{3}	179.0	3.54	-	-	-	-	
		10.0	13	126.5	3.99	10.1	13	130.5	4.71	
		10.0	14	146.1	3.89	10.1	14	152.0	4.64	
	N	10.2	3	53.3	5.61	-	-	-	-	**+0.1**
		10.2	6	149.3	4.71	-	-	-	-	
		10.2	7	125.5	4.78	-	-	-	-	
		10.2	7^{1}	9.3	5.05	10.3	7^{1}	9.2	5.30	
	ND1-I	12.3	8	145.2	4.44	-	-	-	-	**-**
		12.3	9	127.9	3.61	-	-	-	-	
		12.3	10	112.8	3.39	-	-	-	-	
		12.3	11	127.9	3.51	-	-	-	-	
		12.3	12	145.2	4.25	-	-	-	-	
		12.3	12^{1}	20.4	4.89	-	-	-	-	

*Continued on following page.

		Pr				Pfr				
Proton contact		σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [6]	σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [14]	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
His-260	**ND1-I**	12.3	12^{3}	179.0	5.17	-	-	-	-	-
		12.3	13	126.5	4.83	-	-	-	-	
		12.3	13^{1}	11.4	6.03	-	-	-	-	
		12.3	14	146.1	4.45	-	-	-	-	
	NE2-I	17.9	8	145.2	5.22	-	-	-	-	-
		17.9	9	127.9	4.63	-	-	-	-	
		17.9	10	112.8	3.83	-	-	-	-	
		17.9	11	127.9	3.78	-	-	-	-	
		17.9	12	145.2	3.75	-	-	-	-	
		17.9	12^{1}	20.4	3.83	-	-	-	-	
		17.9	12^{2}	38.1	4.15	-	-	-	-	
		17.9	12^{3}	179.0	3.83	-	-	-	-	
		17.9	13	126.5	4.47	-	-	-	-	
		17.9	13^{1}	11.4	5.32	-	-	-	-	
		17.9	14	146.1	4.72	-	-	-	-	
	NE2-II	14.0	8	145.2	5.22	13.1	8	143.6	4.81	**–0.9**
		14.0	8^{1}	22.8	5.10	13.1	8^{1}	22.9	4.91	
		-	-	-	-	13.1	8^{2}	41.8	3.98	
		14.0	9	127.9	4.63	13.1	9	131.0	4.52	
		14.0	10	112.8	3.83	13.1	10	112.4	4.21	
		14.0	11	127.9	3.78	13.1	11	131.0	4.62	
		14.0	12	145.2	3.75	13.1	12	145.8	4.97	
		14.0	12^{1}	20.4	3.83	13.1	12^{1}	20.6	5.19	
		14.0	12^{2}	38.1	4.15	13.1	12^{2}	38.4	4.47	
		14.0	12^{3}	179.0	3.83	13.1	12^{3}	175.3	4.88	
		-	-	-	-	13.1	13	130.5	5.77	
His-290*	**CE1**	-	-	-	-	9.8	12^{3}	175.3	4.31	**–0.9**
		10.7	17	142.1	5.46	-	-	-	-	
		10.7	18	134.2	4.42	-	-	-	-	
		10.7	18^{1}	16.5	4.55	-	-	-	-	
		10.7	18^{2}	13.2	3.48	-	-	-	-	
		10.7	19	172.7	3.87	-	-	-	-	

*Continued on following page.

		Pr				Pfr				
Proton contact		σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [6]	σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [14]	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
His-290	**ND1**	11.7	18^{1}	16.5	5.63	-	-	-	-	-
		11.7	18^{2}	13.2	4.38	-	-	-	-	
		11.7	19	172.7	5.15	-	-	-	-	
	NE2	-	-	-	-	12.3	12^{3}	175.3	3.55	**–0.4**
		12.7	18	134.2	4.60	-	-	-	-	
		12.7	18^{1}	16.5	5.10	-	-	-	-	
		12.7	18^{2}	13.2	4.29	-	-	-	-	
		12.7	19	172.7	3.68	-	-	-	-	
His-470	**CA**	6.7	3^{2}	21.9	4.26	-	-	-	-	-
	N	10.4	3^{2}	21.9	3.96	9.8	3^{2}	21.4	-	**–0.6**
Ile-20	**CB**	3.7	8^{2}	42.9	4.39	-	-	-	-	-
	CD1	2.5	8^{1}	22.8	4.11	2.3	8^{1}	22.9	-	**–0.2**
		2.5	8^{2}	42.9	3.60	2.3	8^{2}	41.8	-	
		2.5	8^{3}	180.1	3.53	2.3	8^{3}	180.3	-	
	CG1	3.2	8^{3}	180.1	4.29	-	-	-	-	-
	CG2	-	-	-	-	2.0	7^{1}	9.2	-	**–1.0**
		3.0	8^{2}	42.9	4.16	-	-	-	-	
Ile-208*	**CB**	-	-	-	-	4.7	9	131.0	5.17	**+0.3**
		-	-	-	-	4.7	10	112.4	5.02	
		-	-	-	-	4.7	11	131.0	4.80	
		-	-	-	-	4.7	12	145.8	5.22	
		4.4	13	126.5	4.88	4.7	13	130.5	5.42	
		-	-	-	-	4.7	14	152.0	5.27	
	CD1	-	-	-	-	2.9	10	112.4	4.43	**+0.1**
		-	-	-	-	2.9	11	131.0	3.82	
		-	-	-	-	2.9	12	145.8	3.54	
		-	-	-	-	2.9	12^{1}	20.6	3.79	
		2.8	13	126.5	3.76	2.9	13	130.5	3.67	
		2.8	13^{1}	11.4	3.96	2.9	13^{1}	11.3	4.15	
		2.8	14	146.1	3.58	2.9	14	152.0	4.13	
		2.8	15	93.2	3.74	-	-	-	-	
		2.8	16	146.1	4.44	-	-	-	-	

*Continued on following page.

		Pr				Pfr				
Proton contact		σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [6]	σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [14]	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
Ile-208	**CG1**	-	-	-	-	3.3	11	131.0	3.78	**–0.1**
		-	-	-	-	3.3	12	145.8	3.99	
		-	-	-	-	3.3	12^{1}	20.6	4.68	
		3.4	13	126.5	4.06	3.3	13	130.5	3.99	
		3.4	14	146.1	3.44	3.3	14	152.0	3.91	
		3.4	15	93.2	3.59	3.3	15	91.5	4.61	
		3.4	16	146.1	4.64	-	-	-	-	
	CG2	-	-	-	-	3.1	8	143.6	5.48	**–0.4**
		-	-	-	-	-	-	-	-	
		3.5	10	112.8	4.72	-	-	-	-	
		3.5	11	127.9	4.26	-	-	-	-	
	N	10.3	15	93.2	4.95	-	-	-	-	**-**
Leu-15	**CD1**	3.2	2^{1}	17.4	4.07	2.8	2^{1}	18.2	-	**–0.4**
	CD2	3.0	2	37.1	4.80	-	-	-	-	**–0.4**
		3.0	3	53.3	3.82	2.6	3	54.3	-	
		3.0	3^{1}	47.5	4.49	2.6	3^{1}	49.9	-	
		3.0	4	154.0	4.39	2.6	4	153.7	-	
Leu-18	**CD1**	2.5	7^{1}	9.3	3.99	-	-	-	-	**-**
Leu-469	**CB**	3.2	3^{2}	21.9	3.39	3.4	3^{2}	21.4	-	**+0.2**
Met-174	**CE**	-	-	-	-	3.2	17^{1}	9.9	5.92	**–0.6**
		3.8	18	134.2	4.65	-	-	-	-	
		3.8	18^{1}	16.5	4.22	3.2	18^{1}	15.7	4.73	
		3.8	18^{2}	13.2	2.95	-	-	-	-	
		3.8	19	172.7	4.32	-	-	-	-	
Met-267	**CE**	2.9	18^{1}	16.5	4.16	2.6	18^{1}	15.7	4.21	**–0.3**
		2.9	18^{2}	13.2	4.25	2.6	18^{2}	13.3	4.58	
Phe-216*	**CE2**	7.3	12^{1}	20.4	3.78	7.0	12^{1}	20.6	-	**–0.3**
		7.3	12^{2}	38.1	3.73	7.0	12^{2}	38.4	-	

*Continued on following page.

Proton contact		Pr				Pfr				$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
		σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [6]	σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [14]	
Phe-216	**CZ**	6.8	12^{1}	20.4	4.14	6.5	12^{1}	20.6	-	**–0.3**
		6.8	12^{2}	38.1	3.61	6.5	12^{2}	38.4	-	
		-	-	-	-	6.5	12^{3}	175.3	-	
Pro-209	**CD**	-	-	-	-	5.6	3^{1}	49.9	4.72	**–0.1**
		5.7	6	149.3	3.49	5.6	6	149.3	3.71	
		5.7	7	125.5	4.12	-	-	-	-	
		-	-	-	-	5.6	7^{1}	9.2	4.56	
		5.7	8	145.2	4.36	-	-	-	-	
		5.7	9	127.9	4.01	5.6	9	131.0	4.72	
	CG	-	-	-	-	5.1	3	54.3	4.36	**-**
		-	-	-	-	5.1	3^{1}	49.9	3.96	
		-	-	-	-	5.1	3^{2}	21.4	4.05	
		-	-	-	-	5.1	6	149.3	4.26	
	N	-	-	-	-	11.8	3^{1}	49.9	5.83	**-**
		-	-	-	-	11.8	7	126.3	5.43	
Pro-471	**CA**	5.7	2	37.1	4.60	5.3	2	37.3	-	**–0.4**
	CB	-	-	-	-	3.4	2	37.3	-	**-**
	CD	5.3	3^{2}	21.9	4.63	-	-	-	-	**-**
	N	11.5	3^{1}	47.5	4.94	-	-	-	-	**–0.1**
		11.5	3^{2}	21.9	4.22	11.4	3^{2}	21.4	-	
Ser-206	**CB**	4.8	2^{1}	17.4	4.31	5.0	2^{1}	18.2	5.57	**+0.2**
	OG	8.0	2^{1}	17.4	4.25	7.4	2^{1}	18.2	5.25	**–0.6**
Ser-272	**OG**	-	-	-	-	6.0	12^{2}	38.4	4.75	**–1.0**
		7.0	12^{3}	179.0	4.73	6.0	12^{3}	175.3	4.86	
Thr-274*	**CB**	-	-	-	-	3.4	12^{2}	38.4	-	**–0.3**
		3.7	12^{3}	179.0	3.94	3.4	12^{3}	175.3	-	
		3.7	13^{1}	11.4	4.87	-	-	-	-	
	CG2	2.1	12^{1}	20.4	4.72	-	-	-	-	**+0.7**
		2.1	12^{2}	38.1	3.53	2.8	12^{2}	38.4	-	
		2.1	13^{1}	11.4	4.20	-	-	-	-	

*Continued on following page.

		Pr				Pfr				
Proton contact		σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [6]	σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [14]	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
Thr-274	**OG1**	10.7	12^{2}	38.1	3.14	10.6	12^{2}	38.4	-	**–0.1**
		10.7	12^{3}	179.0	3.14	10.6	12^{3}	175.3	-	
		10.7	13^{1}	11.4	4.21	-	-	-	-	
Tyr-176	**CE1**	-	-	-	-	9.3	13^{1}	11.3	3.47	**+0.5**
		8.8	17	142.1	4.67	-	-	-	-	
		8.8	18	134.2	4.72	-	-	-	-	
	CE2	-	-	-	-	9.5	17^{1}	9.9	5.93	-
	OH	-	-	-	-	9.0	12^{3}	175.3	3.94	**–0.1**
		9.1	17^{1}	9.9	4.55	9.0	17^{1}	9.9	4.24	
Tyr-198	**CD2**	10.0	18^{2}	13.2	3.46	-	-	-	-	-
	CE2	9.4	18^{2}	13.2	3.75	-	-	-	-	-
Tyr-203*	**CA**	-	-	-	-	5.2	19	169.0	5.54	-
	CB	-	-	-	-	4.6	15	91.5	5.08	**+0.9**
		-	-	-	-	4.6	16	151.1	4.72	
		-	-	-	-	4.6	17	137.7	5.72	
		3.7	17^{1}	9.9	4.22	-	-	-	-	
		-	-	-	-	4.6	18	140.4	5.46	
		-	-	-	-	4.6	19	169.0	4.24	
	CD1	-	-	-	-	10.0	17^{1}	9.9	5.98	-
		-	-	-	-	10.0	18	140.4	4.43	
		-	-	-	-	10.0	19	169.0	3.65	
	CD2	-	-	-	-	9.8	13^{1}	11.3	5.18	**–0.2**
		-	-	-	-	9.8	15	91.5	4.85	
		10.0	17^{1}	9.9	3.67	-	-	-	-	
		10.0	18^{1}	16.5	4.16	-	-	-	-	
	CE1	-	-	-	-	9.5	17	137.7	4.93	-
		-	-	-	-	9.5	18	140.4	4.75	
		-	-	-	-	9.5	19	169.0	4.34	
	CE2	-	-	-	-	9.3	13	130.5	5.15	**–0.1**
		9.4	18^{1}	16.5	3.71	-	-	-	-	

*Continued on following page.

		Pr				Pfr				
Proton contact		σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [6]	σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [14]	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
Tyr-203	**OH**	-	-	-	-	7.3	17^{1}	9.9	6.65	**–0.7**
		8.0	18^{1}	16.5	4.00	-	-	-	-	
		8.0	18^{2}	13.2	4.12	-	-	-	-	
Tyr-257	**CB**	4.5	7^{1}	9.3	3.47	3.6	7^{1}	9.2	-	**–0.9**
		4.5	8^{2}	42.9	3.88	-	-	-	-	
		4.5	8^{3}	180.1	4.45	-	-	-	-	
	CD2	9.6	7^{1}	9.3	3.34	9.7	7^{1}	9.2	-	**+0.1**
	N	9.8	8^{2}	42.9	3.81	-	-	-	-	**-**
		9.8	8^{3}	180.1	3.69	-	-	-	-	
Tyr-263	**CD2**	-	-	-	-	9.4	1	182.9	4.04	**-**
	CE1	9.7	15	93.2	4.33	9.0	15	91.5	5.00	**–0.7**
		9.7	16	146.1	4.29	9.0	16	151.1	4.26	
		9.7	17	142.1	4.15	9.0	17	137.7	3.95	
		-	-	-	-	9.0	18	140.4	4.00	
		-	-	-	-	9.0	18^{1}	15.7	4.37	
		-	-	-	-	9.0	19	169.0	4.30	
	CE2	-	-	-	-	8.8	1	182.9	4.37	**-**
		-	-	-	-	8.8	14	152.0	5.35	
	OH	-	-	-	-	7.7	14	152.0	5.96	**–0.5**
		-	-	-	-	7.7	15	91.5	4.61	
		-	-	-	-	7.7	16	151.1	3.70	
		8.2	17	142.1	3.54	7.7	17	137.7	3.92	
		8.2	18	134.2	4.30	7.7	18	140.4	3.55	
		8.2	18^{1}	16.5	4.56	7.7	18^{1}	15.7	4.26	
		-	-	-	-	7.7	18^{2}	13.3	4.54	
		-	-	-	-	7.7	19	169.0	3.04	
Tyr-458	**CB**	3.7	2	37.1	4.47	-	-	-	-	**-**
		3.7	2^{1}	17.4	3.68	-	-	-	-	
Val-186	**CG2**	1.6	18^{1}	16.5	4.76	1.5	18^{1}	15.7	6.19	**–0.1**
		-	-	-	-	1.5	18^{2}	13.3	5.69	

		Pr				Pfr				
Proton contact		σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [6]	σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [14]	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
W1	**W1-I**	7.2	1	184.1	3.05	-	-	-	-	**-**
		7.2	9	127.9	3.90	-	-	-	-	
		7.2	10	112.8	4.15	-	-	-	-	
		7.2	11	127.9	3.93	-	-	-	-	
	W1-II	7.7	1	184.1	3.05	7.1	1	182.9	3.37	**–0.6**
		7.7	8	145.2	5.18	-	-	-	-	
		7.7	9	127.9	3.90	7.1	9	131.0	3.88	
		7.7	10	112.8	4.15	7.1	10	112.4	4.23	
		7.7	11	127.9	3.93	7.1	11	131.0	3.78	
		7.7	12	145.2	5.16	7.1	12	145.8	4.75	
		-	-	-	-	7.1	13	130.5	4.63	
		7.7	14	146.1	4.05	7.1	14	152.0	3.51	
		7.7	15	93.2	4.08	7.1	15	91.5	3.60	
		-	-	-	-	7.1	16	151.1	4.58	
W2		7.9	8^{1}	22.8	4.74	8.1	8^{1}	22.9	-	**+0.2**
		7.9	8^{2}	42.9	4.70	8.1	8^{2}	41.8	-	
		7.9	8^{3}	180.1	3.90	8.1	8^{3}	180.3	-	
		7.9	12^{1}	20.4	4.48	-	-	-	-	
		7.9	12^{2}	38.1	4.44	-	-	-	-	
		7.9	12^{3}	179.0	3.59	-	-	-	-	
W3		8.0	12^{2}	38.1	4.59	7.5	12^{2}	38.4	-	**–0.5**
		8.0	12^{3}	179.0	3.10	7.5	12^{3}	175.3	-	
W4 (-II)		9.0	12	145.2	5.25	-	-	-	-	**–1.1**
		-	-	-	-	7.9	12^{1}	20.6	-	
		8.9	12^{2}	38.1	4.59	-	-	-	-	
		8.9	12^{3}	179.0	3.50	7.9	12^{3}	175.3	-	
		-	-	-	-	7.9	17^{1}	9.9	-	

	Pr				Pfr				
Proton contact	σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [6]	σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [14]	$\Delta\sigma^{proton\ (Pfr-Pr)}$ (ppm)
W5 (-II)	-	-	-	-	8.5	12	145.8	-	**+0.7**
	-	-	-	-	8.5	12^{1}	20.6	-	
	-	-	-	-	8.5	12^{3}	175.3	-	
	7.8	13	126.5	4.32	8.5	13	130.5	-	
	7.8	13^{1}	11.4	3.73	8.5	13^{1}	11.3	-	
	-	-	-	-	8.5	17^{1}	9.9	-	
	-	-	-	-	8.5	18^{1}	15.7	-	
	7.8	19	172.7	3.75	-	-	-	-	
W6	8.4	12^{3}	179.0	4.92	-	-	-	-	**–0.6**
	8.4	13^{1}	11.4	4.53	7.8	13^{1}	11.3	-	
W7	7.7	17^{1}	9.9	5.56	-	-	-	-	**-**
{W5+$[OH]^{-}_{W4}$} (-I)	9.4	12	145.2	-	-	-	-	-	**-**
	9.4	12^{2}	38.1	-	-	-	-	-	
	9.4	12^{3}	179.0	-	-	-	-	-	
	9.4	13^{1}	11.4	-	-	-	-	-	
	9.4	14	146.1	-	-	-	-	-	
	9.4	16	146.1	-	-	-	-	-	
	9.4	19	172.7	-	-	-	-	-	