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Heteronuclear multidimensional NMR-spectroscopy of solubilized membrane proteins: Resonance assignment of native bacteriorhodopsin

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Table S1. Chemical shift list of $^{2}H/^{13}C/^{15}N$ labeled bacteriorhodopsin at 323.5 K referenced to H_2O.[22] The ^{15}N and $^{1}H^{N}$ chemical shifts are taken from the TROSY spectra. The carbon chemical shifts have not been corrected for a deuterium isotope effect.

residue	$\delta\ ^{15}N$ [ppm]	$\delta\ ^{1}H^{N}$ [ppm]	$\delta\ ^{13}CO$ [ppm]	$\delta\ ^{13}C^{\alpha}$ [ppm]	$\delta\ ^{13}C^{\beta}$ [ppm]
E1	125.3	7.61	177.5	59.1	27.0
A2	124.1	8.12	177.5	52.1	18.4
Q3	119.7	8.29	176.4	55.6	28.7
I4	121.7	8.04	176.3	61.9	37.7
T5	113.5	7.65	174.8	61.7	68.4
G6	110.2	7.88	173.9	45.0	-
R7	120.7	7.72	175.0	53.3	30.0
V29	-	-	-	65.8	-
K30	120.4	8.31	179.6	57.8	-
G31	106.7	8.10	176.0	46.0	-
M32	119.8	7.54	177.2	57.7	-
G33	105.5	7.58	174.2	44.7	-
V34	121.7	6.97	175.3	62.3	31.9
S35	120.5	8.63	174.5	57.8	-
D36	126.1	7.24	-	52.0	43.2
F71	-	-	176.4	57.3	39.1
G72	112.9	8.48	175.0	45.8	-
G73	109.5	8.27	173.9	45.0	-
E74	119.8	7.66	175.5	54.7	30.6
Q75	120.1	8.26	175.0	55.1	29.0
N76	121.5	8.27	172.6	50.5	40.2
A103	-	-	176.2	51.7	18.8
D104	117.0	7.82	176.3	52.8	41.9
Q105	119.6	8.55	177.6	59.4	28.7
G106	107.3	8.45	-	47.3	-
F153a	-	-	177.6	61.3	-
F154a	117.5	8.59	177.1	59.7	37.7
G155a	110.9	7.83	176.8	47.1	-
F156a	121.1	8.73	178.0	57.4	34.3?
T157a	115.5	6.73	175.2	67.2	67.9
S158a	115.1	7.42	176.9	61.0	62.0
K159a	121.2	7.03	-	57.8	-
F153b	-	-	177.1	61.4	-
F154b	117.6	8.51	177.1	59.4	37.5
G155b	110.8	7.83	176.7	47.2	-
F156b	120.7	8.88	178.0	57.2	36.4?
T157b	115.7	6.72	175.2	67.2	68.0
S158b	115.3	7.53	177.0	61.0	-
K159b	121.3	7.11	-	57.9	-

A160	122.0	8.04	179.1	54.6	-
E161	113.2	7.72	177.3	57.9	-
S162	113.1	7.36	174.2	58.1	63.8
M163	122.3	7.29	174.8	54.8	33.4
R164	118.7	7.96	175.6	54.8?	28.5?
P165	-	-	178.8	65.7	-
E166	116.9	9.60	179.6	59.1	28.0
V167	121.2	7.47	176.9	65.8	-
A168	122.3	7.66	179.9	55.9	18.1
S169	111.3	8.43	177.1	61.0	62.1
T170	119.0	7.32	175.5	66.6	-
F171	120.1	8.91	175.6	62.5	-
K172	117.6	7.83	177.8	61.0	-
V173	116.8	7.07	177.6	66.2	30.7?
L174	118.9	7.57	180.0	57.1	-
R175	123.4	9.02	-	58.6	-
P200	-	-	177.7	61.5	-
L201	122.9	8.72	180.0	57.8	41.0
N202	118.8	9.33	175.6	57.8	-
I203	119.7	6.85	177.2	61.3	35.7
E204	122.8	8.45	-	59.3	-
G218	-	-	174.6	48.3	-
F219	119.6	7.05	176.2	60.7	-
G220	104.5	7.85	174.2	47.5	-
L221	122.0	8.54	178.6	57.8	-
I222	116.9	7.31	178.2	64.1	-
L223	118.0	7.58	178.6	57.8	-
L224	113.2	8.43	177.9	55.9	-
R225	116.2	7.02	176.0	55.4	-
S226	116.4	7.34	175.0	57.7	64.3
R227	120.6	8.55	178.0	55.8	28.6
A228	120.3	8.01	176.3	53.5	-
I229	104.6	6.09	173.8	61.3	-
F230	116.7	6.86	-	57.5	
G231					
E232	-	-	176.0	55.9	29.4
A233	125.1	8.17	177.5	52.0	18.5
E234	120.4	8.09	175.7	55.6	29.1
A235	126.8	8.08	175.5	49.9	-
P236	-	-	176.8	62.3	31.3
E237	122.1	8.13	174.9	53.6	28.8
P238	-	-	177.1	62.9	31.3
S239	115.9	8.12	174.5	57.8	63.3
A240	126.2	8.10	178.1	52.1	18.5
G241	108.5	8.06	174.1	44.9	-
D242	121.1	7.91	177.0	53.2	40.5
G243	109.7	8.18	174.2	45.1	-
A244	123.9	7.90	177.5	52.0	18.4
A245	124.1	-	177.5	51.9	18.3
A246	123.4	7.97	177.9	51.9	18.4
T247	113.1	7.87	174.0	61.1	69.5
S248	123.3	7.73	178.5	59.3	63.8

Table S2. Relaxation data T_1, T_2, T_1/T_2 and a coresponding τ_C of $^{2}H/^{15}N$ labeled bacteriorhodopsin at 323.5 K. The formula to estimate τ_C[25] is not valid for a correlation time < 3ns (*).

residue	T_1 [s^{-1}]	T_2 [s^{-1}]	T_1/T_2	τ_C [ns]
A2	0.492	0.231	2.13	3.14
Q3	0.483	0.102	4.74	6.06
I4	0.466	0.110	4.24	5.62
T5	0.639	0.027	23.67	15.20
G6	0.600	0.047	12.77	10.92
R7	0.586	0.080	7.33	8.00
D104	1.083	0.029	37.34	19.27
Q105	1.130	0.016	70.63	26.71
G106	1.708	0.015	113.87	34.02
F154a	0.623	0.039	15.97	12.329
F154b	0.753	0.034	22.14	14.676
F156a	0.230	0.020	11.50	10.30
M163	0.500	0.023	21.74	14.54
L201	1.796	0.018	99.77	31.82
N202	1.416	0.011	128.73	36.19
A233	0.401	0.356	1.12	*
A235	0.428	0.239	1.79	*
E237	0.431	0.395	1.09	*
S239	0.460	0.593	0.78	*
A240	0.535	0.695	0.77	*
G241	0.673	1.012	0.67	*
D242	0.682	0.756	0.90	*
G243	0.612	1.025	0.60	*
A246	0.758	1.18	0.64	*
T247	0.935	1.63	0.57	*
S248	1.094	1.16	0.95	*