SUPPORTING INFORMATION

Solid-state NMR spectroscopy of 18.5 kDa myelin basic protein reconstituted with lipid vesicles: spectroscopic characterisation and spectral assignments of solvent-exposed protein fragments

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Table S1. Spectral assignments of rmMBP (176 residues, including a C-terminal LEH_6 tag) reconstituted with DMPC:DMPG (1:1 mass ratio) lipid vesicles, at a protein-to-lipid mass ratio of 1:1.4.

Amino acid	^{15}N	$^{13}C'$	$^{13}C^{\alpha}$	$^{13}C^{\beta}$	$^{13}C^{\gamma}$	$^{13}C^{\delta}$	$^{1}H^{\alpha}$	$^{1}H^{\beta}$	$^{1}H^{\gamma}$	$^{1}H^{\delta}$
T15		173.9	61.2	69.5						
A16	125.8	177.0	52.2	19.1			4.16	1.21		
S17	114.3	174.3	58.1	63.6			4.31	3.69		
T18	114.7	173.9	61.6	69.6	21.7		4.16	4.04	0.97	
M19	122.9	174.7	55.9	33.0						
D20	125.4	175.6	54.8	41.1	179.1		4.34	2.57		
H21	121.9	175.0	56.6	29.2						
A22	125.1	176.6	51.9	19.0						
R23	118.2	174.4	56.0							
R29		**175.8**	**56.2**	**30.4**	**27.0**	**43.3**	**4.16**	**1.66**	**1.45**	**2.99**
H30	**121.0**	**175.7**	**56.1**	**30.5**						
R31	**121.0**	**175.5**	**55.9**	**30.3**						
D32	**122.5**		**53.7**							
D46		175.7	54.1							
R47	121.6	176.4	56.7	29.9						
G48	109.0	173.3	45.1				3.74			
K51		175.7	56.6	32.4	24.7	29.0	4.15	1.60	1.22	1.48
R52	119.5	176.4	56.8	29.8						
G53	109.0	173.3	45.1				3.74			
S54	115.4	174.4	58.6	63.7			4.27	3.69		
G55	110.4		45.2				3.74			
H59		175.0	56.4							
T60	114.4	174.0	61.8	69.4	21.7		4.16	4.04	0.97	
R61	123.1	175.0	56.1	30.7	27.0	43.3	4.16	1.66	1.45	2.99
T62	114.4	174.0	61.4	69.4	21.7		4.16	4.03	0.97	

T63	115.8	173.8	61.5	69.4	21.4		4.16	4.04	0.97	
H64	122.0	175.8	55.7	30.5						
Y65	115.1	175.5	58.1	38.5						
G66	110.0	174.2	45.4							
S67	115.6		57.9	63.7			4.27	3.69		
K102		176.2	56.0	32.1	24.7	29.0	4.15	1.60	1.22	1.48
G103	109.3	173.3	45.2				3.74			
R104	120.3		55.7							
S112		172.8	57.8	63.9						
W113	125.9		58.0	30.1						
P120		176.5	63.0	31.5	27.3	50.5	4.25	2.19	1.82	3.58
G121	108.7		45.1				3.74			
Y124		175.4	57.4							
G125	109.7	174.0	45.3				3.74			
G126	108.2	173.2	44.9				3.74			
R127	116.4	175.7	56.0							
A128	126.0	176.5	51.4							
S129	114.7	173.9	58.0	63.5			4.27	3.79		
D130	125.1		54.7	41.0	179.1		4.34	2.57		
S133		**174.0**	**58.2**	**63.4**			**4.27**	**3.69**		
A134	**125.3**	**176.7**	**52.3**	**18.9**			**4.16**	**1.21**		
H135	**118.1**		**56.0**							
Y142		**175.1**	**57.7**	**38.2**						
D143	**122.4**	**176.2**	**55.1**	**42.2**			**4.21**	**2.50**		
A144	**124.2**	**177.0**	**52.1**	**19.0**			**4.16**	**1.21**		
Q145	**119.5**	**176.3**	**56.8**	**29.8**						
G146	**109.0**	**174.0**	**45.2**				**3.74**			
T147	**115.6**	**173.4**	**61.5**	**69.2**	**21.4**		**4.16**	**4.04**	**0.97**	
L148	**122.9**		**56.1**							
L154		175.2	56.0							
G155	109.7	174.0	45.2				3.74			
G156	108.2	173.2	45.1							
R157	116.4	175.5	56.0	30.3						
D158	122.5	175.5	53.7							
S161		174.4	58.3	63.7			4.27	3.69		
G162	110.4	173.4	45.2				3.74			
S163	115.4		57.9							

The spectral assignments are based on HCC, NCOCX, NCACX, CONCACX, and CAN(CO)CX experiments. Assignments with a lesser degree of certainty are given in bold font.

Table S2. Assignment statistics for membrane-associated rmMBP (176 residues, including a C-terminal LEH_6 tag).

Residue type	Number of assigned residues	Total number of residues in 18.5 kDa rmMBP
Threonine	6	10
Alanine	5	11
Serine	8	20
Methionine	1	2
Aspartate	6	9
Histidine	5	14
Arginine	9	19
Glycine	12	24
Lysine	2	12
Tyrosine	3	5
Triptophane	1	1
Proline	1	11
Leucine	2	9
Glutamine	1	8
All types	62	176

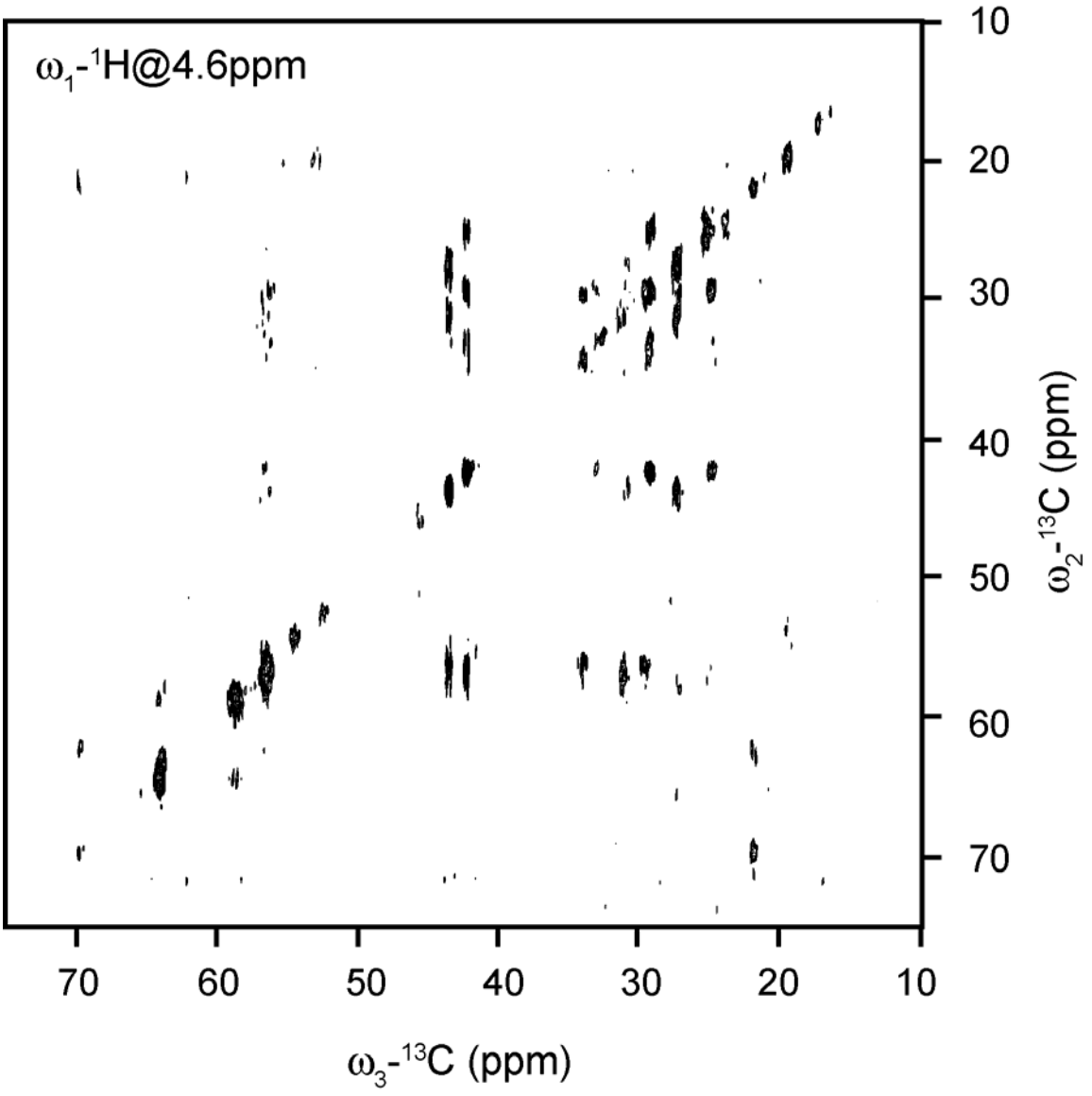

Figure S1. The two-dimensional ^{13}C-^{13}C plane taken at a proton frequency of 4.6 ppm of the full 3D HHCC experiment. The diagonal and cross-peaks identify carbon atoms that interact with water.

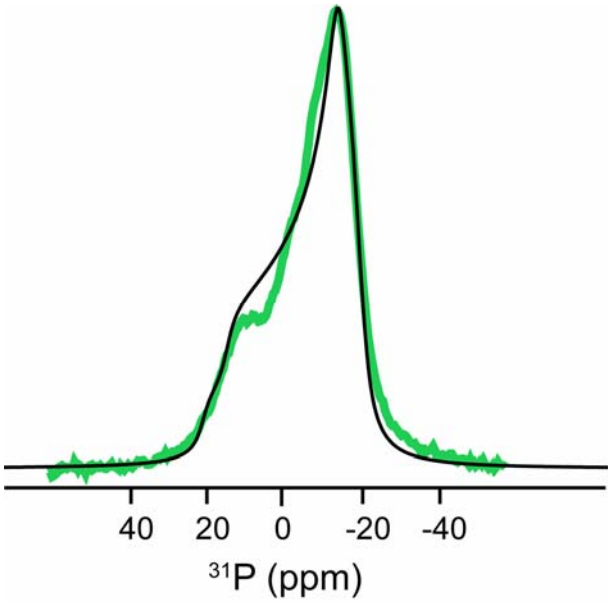

Figure S2. The static ^{31}P spectrum of rmMBP (green) reconstituted with DMPC:DMPG in a 1:1 mass ratio. The spectrum was collected on a Bruker Avance spectrometer operating at a proton Larmor frequency of 500.13 MHz at 32°C, using the Hahn Echo [1] experiment. An 83 kHz TPPM decoupling was used on the proton channel during the delay and acquisition. The CSA parameters used in a SPINEVOLUTION [2] simulation shown in black were as follows: DMPC - $\Delta\sigma$=-38.5 ppm, η=0.25; DMPG - $\Delta\sigma$=-31.1 ppm, η =0.25. The line-broadening used in processing the simulated spectrum was 0.8 kHz. The CSA values are close to those reported for lipid vesicles composed of equal molar amounts of DMPC and DMPG [3]. Slight asymmetry of the CSA tensors may be indicative of protein-lipid interactions, but is not statistically significant - similar patterns can be obtained with smaller asymmetry parameters, but with different line broadening.

[1] E.L. Hahn, Spin echoes, Phys. Rev. 80 (1950) 580-594.

[2] M. Veshtort, R.G. Griffin, SPINEVOLUTION: A powerful tool for the simulation of solid and liquid state NMR experiments, Journal of Magnetic Resonance 178 (2006) 248-282.

[3] F.M. Marassi, P.M. Macdonald, Response of the headgroup of phosphatidylglycerol to membrane surface charge as studied by deuterium and phosphorus-31 nuclear magnetic resonance, Biochemistry 30 (1991) 10558-10566.