

Supplemental Information for
Phage-induced Alignment of Membrane Proteins Enables the
Measurement and Structural Analysis of Residual Dipolar Couplings
with Dipolar Waves and λ -Maps

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Protein sequences

Pf1: GVIDTSAVES AITDGQGDMK AIGGYIVGAL VILAVAGLIY SMLRKA
Vpucyto: EYRKILRQRK IDRLIDRLIE RAEDSGNESE GEISALVELG VELGHHPWD VDDL
MerFt: LIGTTLVALS SFTPVLVILL GVVGLSALTG YLDYVLLPAL AIFIGLTIYA IQRKRQADAS

NH RDCs of Pf1 coat protein

Table S1. Amide ¹H-¹⁵N residual dipolar couplings of Pf1 coat protein in 100 mM DHPC, pH 6.7 obtained from stressed polyacrylamide gel and fd bacteriophage induced alignments.

residue	aa	¹ H- ¹⁵ N RDC (Hz) ^a	
		gel	fd phage
1	G	ND ^b	ND
2	V	2.19	ND
3	I	0.90	-2.38
4	D	0.31	-2.96
5	T	-2.46	1.53
6	S	-3.68	3.45
7	A	-2.09	3.56
8	V	-3.49	2.36
9	E	-4.00	2.25
10	S	-2.88	3.69
11	A	-1.84	2.85
12	I	-3.51	2.88
13	T	-2.52	2.56
14	D	-0.05	0.26
15	G	0.12	0.85
16	Q	-0.79	-0.10
17	G	0.75	-3.52
18	D	4.19	-1.42
19	M	4.13	-6.85
20	K	0.80	-11.97
21	A	11.16	-16.00
22	I	10.77	-15.76
23	G	-0.20	-11.33
24	G	-0.76	-13.08
25	Y	14.80	-22.15
26	I	3.93	-15.36
27	V	-4.05	-10.75
28	G	5.22	-18.46
29	A	13.27	-22.02
30	L	1.27	-12.34
31	V	-1.92	-13.01
32	I	11.60	-21.84
33	L	ND	-20.29
34	A	-2.37	-11.35
35	V	1.63	-14.91
36	A	12.20	-22.36
37	G	4.84	-15.74
38	L	-5.35	-8.96
39	I	4.98	-17.78
40	Y	ND	-20.82
41	S	-4.19	-10.65
42	M	10.23	-9.04
43	L	ND	-21.03
44	R	-5.53	-7.30
45	K	3.29	2.53
46	A	4.15	ND

^aEstimated average error in the measurements is ± 0.5 Hz. ^bND: not determined.

Experimental Details

We observed 2 Hz -5 Hz splittings of the 2H NMR resonances in the sample solutions containing ca. 20 mg/ml of fd bacteriophage in 100 mM of LMPC, DPC and DHPC at pH 6.5 and 30°C. The splittings decrease somewhat at higher temperatures. We found the fd bacteriophage particles to be stable between pH 6 and 8 in the presence of 100 mM of zwitterionic detergents DHPC, DPC and LMPC; the bacteriophage particles are unstable at lower pH values; they are probably stable at higher pH values but we did not investigate above pH 8. In contrast, fd bacteriophage particles are unstable in anionic detergents such as SDS and LMPG.

Scalar product between orientations

The scalar product between orientations of the two order tensors S1 and S2 is shown below:

$$S1 \cdot S2 = \begin{bmatrix} -9.016e-01 & 2.786e-01 & 3.309e-01 \\ 3.024e-01 & 9.529e-01 & 2.172e-02 \\ -3.093e-01 & 1.196e-01 & -9.434e-01 \end{bmatrix}$$

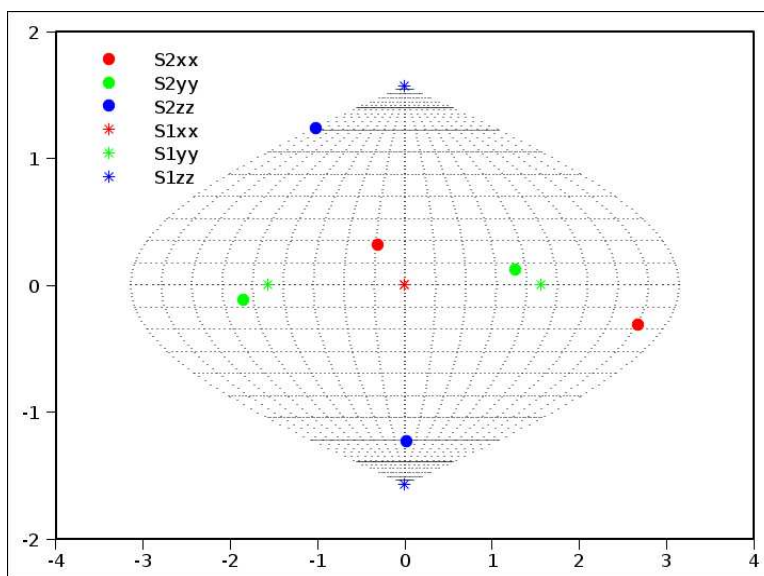


Figure S1. SF-plot visualizes the relative orientation of the two alignment tensors with respect to each other (the information reported by the scalar product matrix above). S1 and S2 refer to the two alignment media. Labels xx, yy and zz refer to the direction of the principal alignments for each of the alignment tensors.