Supporting Information for "Conformational Properties of Peptides Corresponding to the Ebolavirus GP2 Membrane-Proximal External Region in the Presence of Micelle-Forming Surfactants and Lipids"

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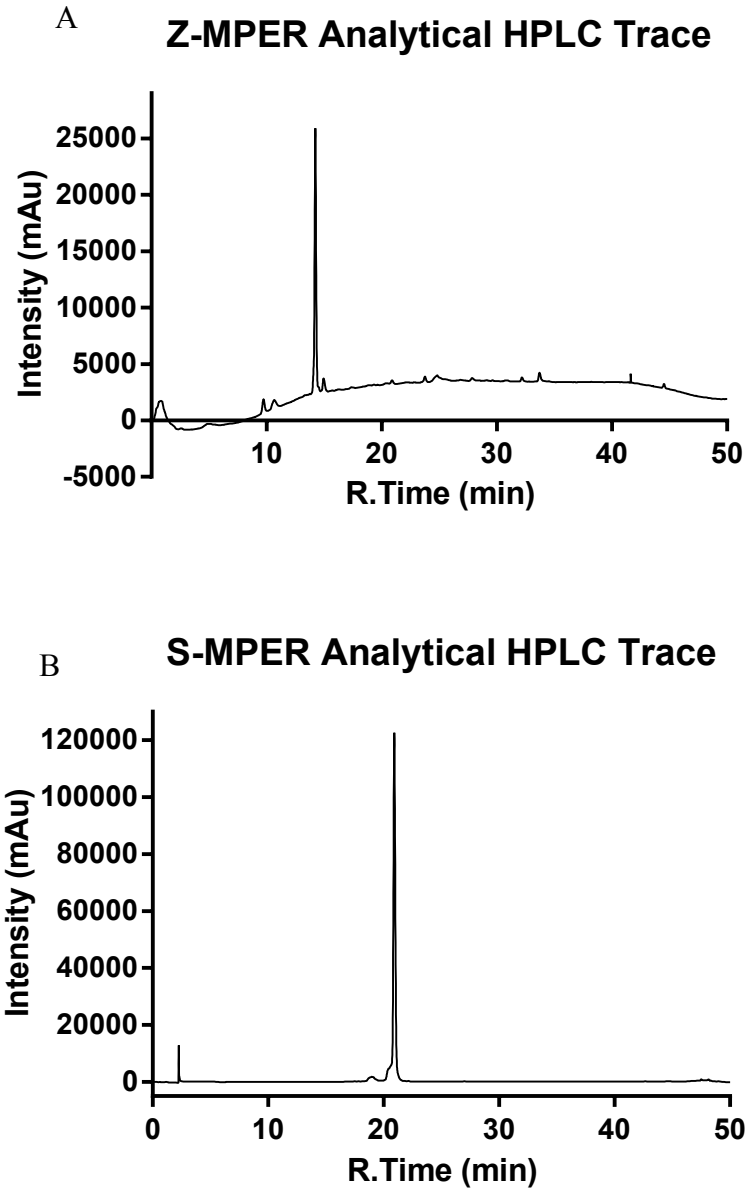

Figure S1. Analytical HPLC traces of Z-MPER (A) and S-MPER (B), monitored at 280 nm.

Table S1 – θ_{min} and θ_{max} values used for Figure 3.

Peptide	pH	Surfactant	θ_{min} (200 nm) mdeg cm^2 / dmol	θ_{max} (200 nm) mdeg cm^2 / dmol	θ_{min} (222 nm) mdeg cm^2 / dmol	θ_{max} (222 nm) mdeg cm^2 / dmol
S-MPER	4.6	SDS	-4174.181	-11720.92	-4753.148	-9128.605
S-MPER	7.1	SDS	-4796.728	-15926.3	-5118.574	-10486.04
S-MPER	4.6	DPC	-11375.48	-16330.53	-5708.096	-10586.98
S-MPER	7.1	DPC	-12576.53	-16340.72	-4842.579	-10307.1
Z-MPER	4.6	SDS	-3041.001	-11760.94	-3622.097	-6939.166
Z-MPER	7.1	SDS	-4445.712	-11566.86	-3190.531	-7922.87
Z-MPER	4.6	DPC	-7690.022	-11432.77	-3181.878	-7209.583
Z-MPER	7.1	DPC	-8030.179	-11901.48	-2960.193	-6812.805

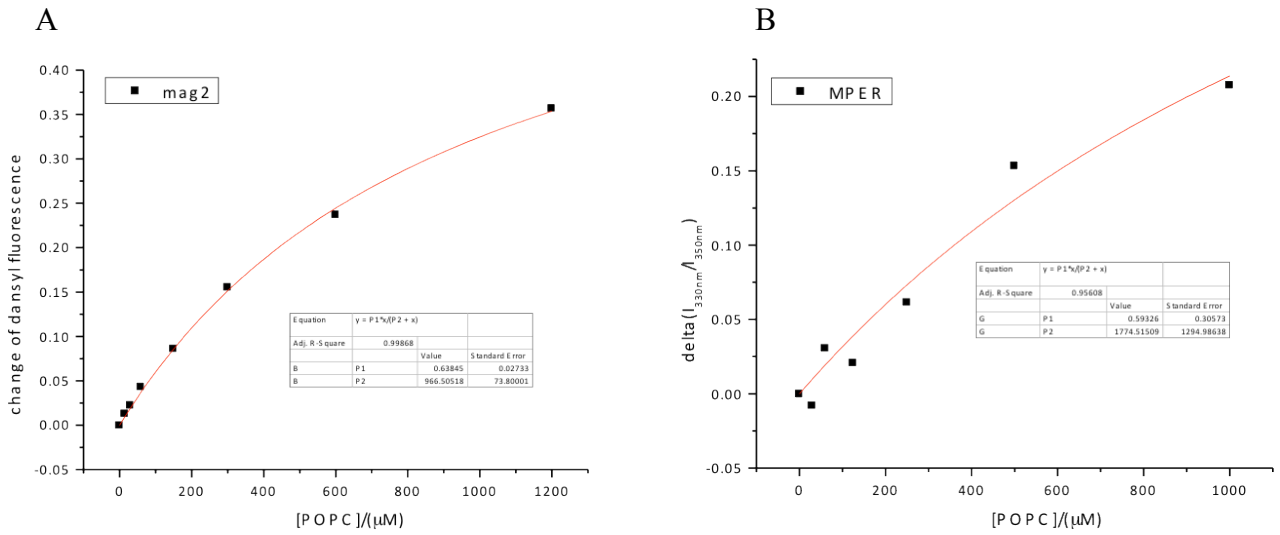

Figure S2. Binding of fY-Magainin 2 (A) and S-MPER (B) to POPC LUVs (500 μM lipids) at 10 μM peptide concentration. Binding was monitored with Trp fluorescence change, I_{330nm}/I_{350nm}. The conditions were: 10 mM TES, 100 mM sodium citrate, pH 5.0.

Table S2 – $^{1}H,^{13}C,^{15}N$ chemical shifts for S-MPER in 10mM NaOAc pH4.5

Residue	Amide		α		β		γ		δ		other	
	H	N	H	C	H	C	H	C	H	C	H	C/N
D632	8.38	124.5	4.68		2.86,2.77	38.1						
N633	8.40	120.1	4.93		2.61,2.77	38.8					6.88	113.0 δ2
											7.56	
P634			4.38	63.1	1.86,2.19	32.0	1.94	27.1	3.64,3.69	50.5		
L635	8.22	123.4	4.56	53.0	1.52,1.58	41.6	1.68	27.1	0.90	25.2		
									0.92	23.2		
P636			4.36	63.2	1.85,2.22	31.9	1.96	27.3	3.58,3.75	50.4		
N637	8.42	118.0	4.58	53.4	2.78	38.6						
Q638	8.28	120.1	4.27	56.1	1.95,2.09	29.2	2.29	33.7				
D639	8.41	119.1	4.64	53.1	2.79,2.90	37.8						
N640	8.27	118.7	4.64		2.73,2.79	38.6					6.83	112.6 δ2
											7.50	
D641	8.26	118.5	4.64		2.80,2.90	37.8						
D642	8.28	117.7	4.53	53.1	2.72	37.6						
N643	8.12	118.4	4.44	53.3	2.50	38.3					6.79	112.4 δ2
											7.36	
W644	7.73	120.4	4.45	57.7	3.10,3.18	29.1			7.06	127.3	10.04	129.7 ε1
											7.41	120.9 ε3
											7.42	114.6 ζ2
											7.01	122.1 ζ3
											7.15	124.8 η2
W645	7.48	121.0	4.50	57.5	2.93,3.01	28.9			7.00	127.2	10.03	129.9 ε1
											7.20	120.7 ε3
											7.14	114.7 ζ2
											7.00	122.2 ζ3
											7.14	124.8 η2
T646	7.76	114.7	4.12	62.4	4.09	69.4	1.05	21.4				
G647	7.52	110.0	3.70	45.4								
W648	7.69	120.8	4.37	57.7	3.12	29.1			7.14	127.2	9.98	129.3 ε1
											7.47	120.9 ε3
											7.41	114.6 ζ2
											7.07	122.1 ζ3
											7.17	124.7 η2
R649	7.68	122.4	3.91	56.0	1.29,1.41	30.6	1.06	26.5	2.79	43.1	6.83	89.6 ε
Q650	7.90	120.4	4.02	56.0	1.75,1.82	29.0	2.04	33.5				
W651	7.86	122.0	4.62	56.6	3.16,3.29	29.7			7.17	127.3	10.01	129.1 ε1
											7.60	121.1 ε3
											7.42	114.6 ζ2
											7.08	122.1 ζ3
											7.17	124.7 η2

Table S3 – $^{1}H,^{13}C,^{15}N$ chemical shifts for S-MPER in 10mM NaOAc pH4.5, 200mM DPC

Residue	Amide		α		β		γ		δ		other	
	H	N	H	C	H	C	H	C	H	C	H	C/N
D632	8.30	124.2										
N633	8.30	119.7	4.95	51.4	2.64,2.80	39.0					6.80	112.4 δ2
											7.51	
P634			4.42	63.2	1.91,2.23	32.1	1.97	27.2	3.70,3.76	50.6		
L635	8.13	122.8	4.56	53.1	1.53,1.61	41.7	1.69	27.2	0.92	25.3		
									0.95	23.4		
P636			4.40	63.4	1.89,2.27	32.0	2.01	27.4	3.62,3.80	50.5		
N637	8.37	117.9	4.60	53.5	2.80	38.8					7.53	112.7 δ2
											6.84	
Q638	8.24	120.0	4.31	56.1	1.98,2.13	29.3	2.33	33.8				
D639	8.38	119.3	4.68	53.2	2.82,2.93	38.2						
N640	8.26	19.0	4.68	52.8	2.77,2.86	38.6					6.83	112.5 δ2
											7.51	
D641	8.29	118.7	4.69	53.1								
D642	8.29	118.7	4.66	53.3	2.80,2.88	38.2						
N643	8.12	118.4	4.45	53.2	2.36,2.45	38.5					6.80	112.4 δ2
											7.42	
W644	8.04	121.1	4.34	59.0	3.20,3.31	29.1			7.41	127.8	10.62	130.8 ε1
											7.32	120.9 ε3
											7.46	114.6 ζ2
											6.86	121.7 ζ3
											7.03	124.0 η2
W645	7.16	117.2	4.50	57.9	2.69,3.11	29.1			6.98	127.2	10.48	130.8 ε1
											7.02	120.9 ε3
											7.42	114.6 ζ2
											7.00	121.9 ζ3
											7.11	124.4 η2
T646	7.47	112.6	4.05	63.7	4.10	69.2	1.05	21.8				
G647	7.96	109.8	3.75	46.2								
			3.87									
W648	7.41	120.2	3.70	58.3	3.08,3.12	28.5			7.14	127.2	10.05	129.4 ε1
											7.38	120.8 ε3
											7.38	114.4 ζ2
											6.89	121.5 ζ3
											7.08	124.0 η2
R649	7.38	118.7	3.70	58.1	1.32,1.55	29.7	0.81	27.2	2.87,2.90	43.2	7.26	85.1 ε
							0.90					
Q650	7.72	116.2*	4.20	56.2	1.92,2.09	28.8	2.21	34.0				
W651	7.72	121.6*	4.54	57.5	3.36	29.7			7.19	126.3	10.35	129.3 ε1
											7.64	121.0 ε3
											7.49	114.5 ζ2
											7.08	121.5 ζ3
											7.15	124.1 η2

* Assignments interchangeable

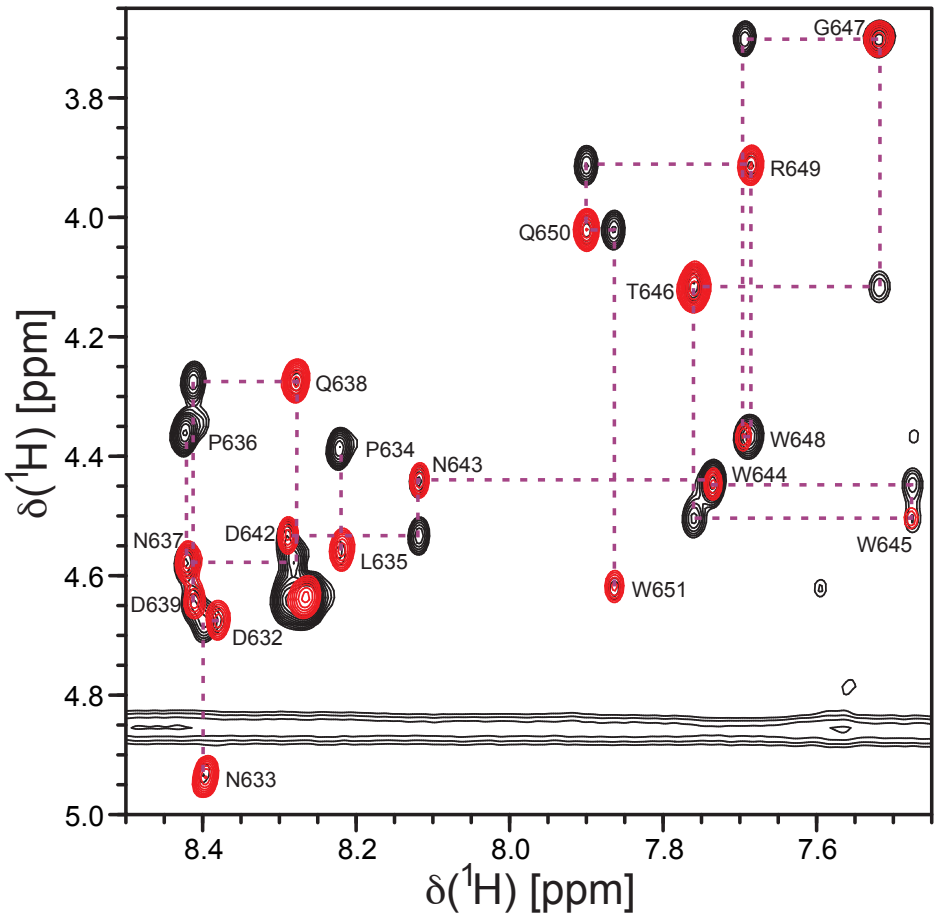

Figure S3. Overlay of the assigned HN-Hα region of the 2D NOESY and 2D TOCSY spectra of S-MPER (2mM) in 5mM NaOAc pH4.5 recorded at 298K on an 800 MHz Bruker Avance II spectrometer equipped with a cryogenically cooled probe. The mixing times were 400ms for the NOESY and 80ms for the TOCSY and water suppression was by the Excitation Sculpting approach. Dotted line represents the backbone walk for assignment of the amide HN and Hα protons.

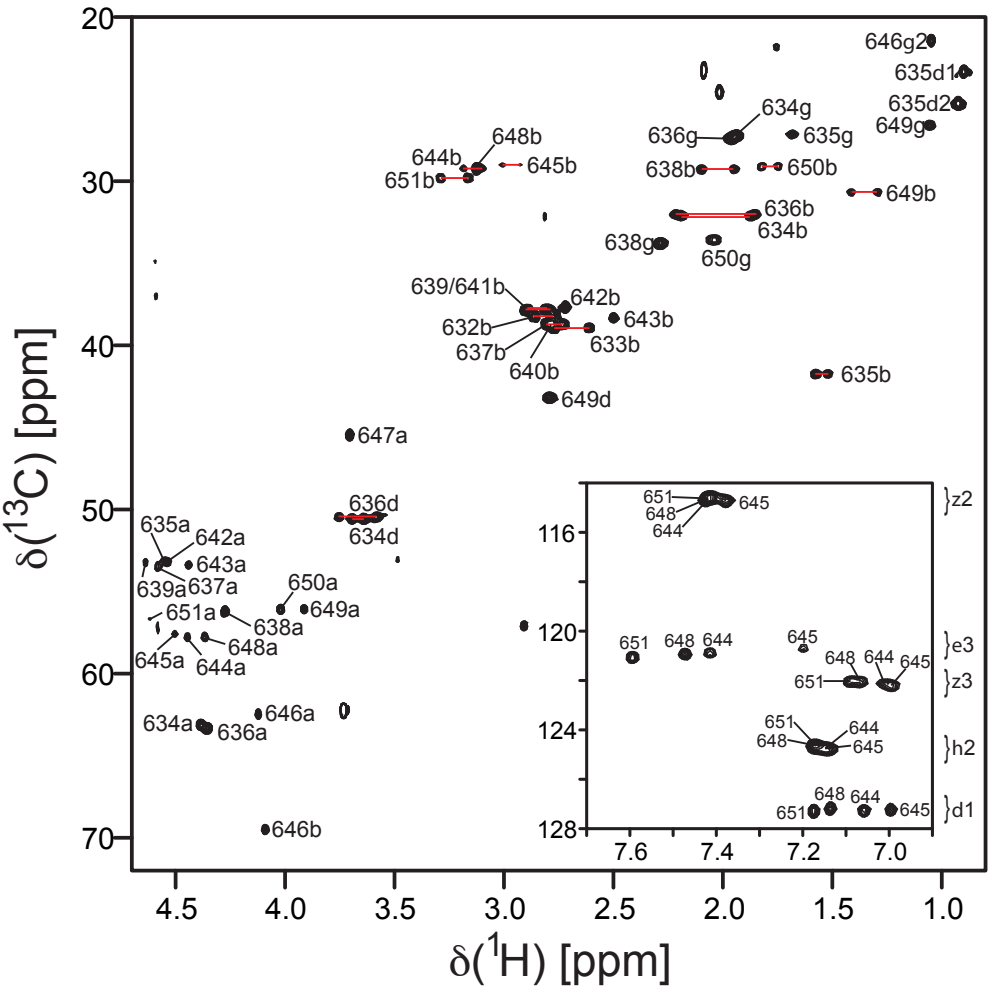

Figure S4. Assigned ^{1}H,^{13}C HSQC aliphatic and aromatic (inset) of S-MPER (2mM) in 5mM NaOAc pH4.5 recorded at 298K on a 800MHz Bruker Avance II spectrometer equipped with a cryogenically cooled probe. The spectra were acquired with the MDDNMR approach to non-uniform sampling (50% sparse data), with either 256 or 224 transients, for a total acquisition time of 13 hours (aliphatic) and 6 hours (aromatic).

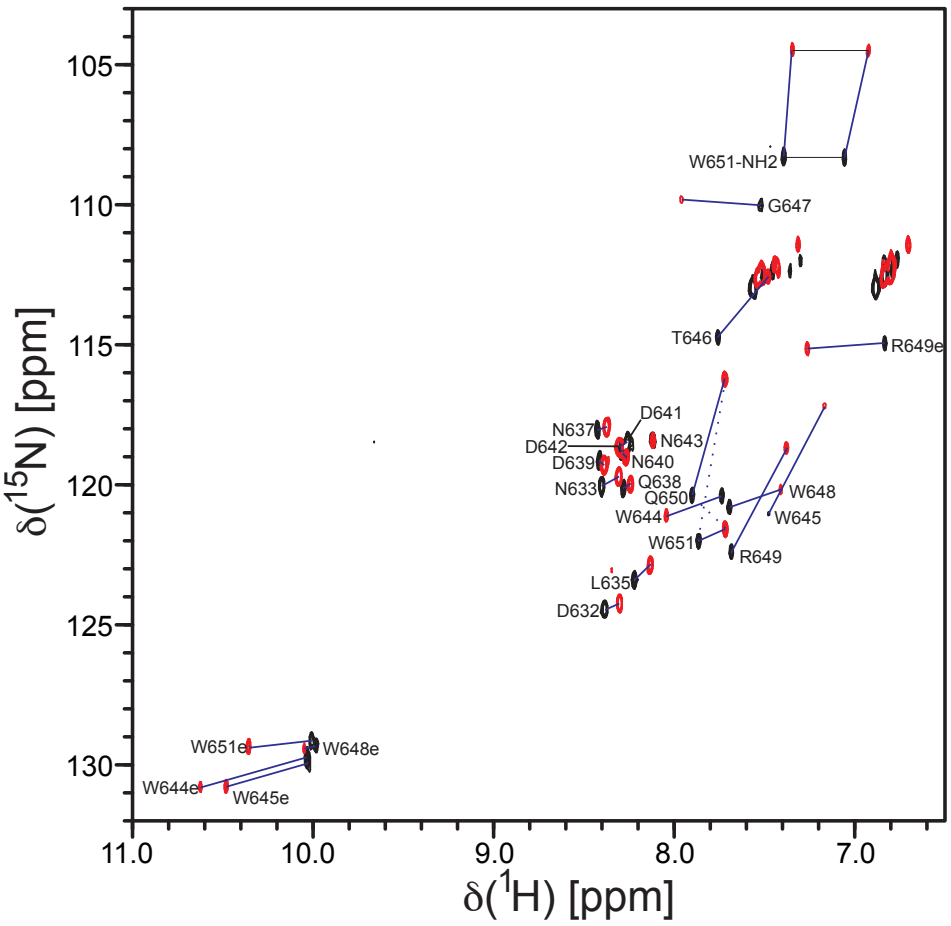

Figure S5. Overlay of the assigned ^{1}H,^{15}N HSQC spectra of S-MPER (2mM) in 5mM NaOAc pH4.5, either with 200mM DPC micelles (red) or without (black) recorded at 310K (900 MHz) or 298K (800 MHz), respectively on a Bruker Avance II spectrometer equipped with a cryogenically cooled probe. Spectra were acquired with the MDDNMR approach to non-uniform sampling (50% sparse data), with 512 transients, for a total acquisition time of 15 hours.