Supplementary Material

The dynamic orientation of membrane-bound peptides: Bridging simulations and experiments

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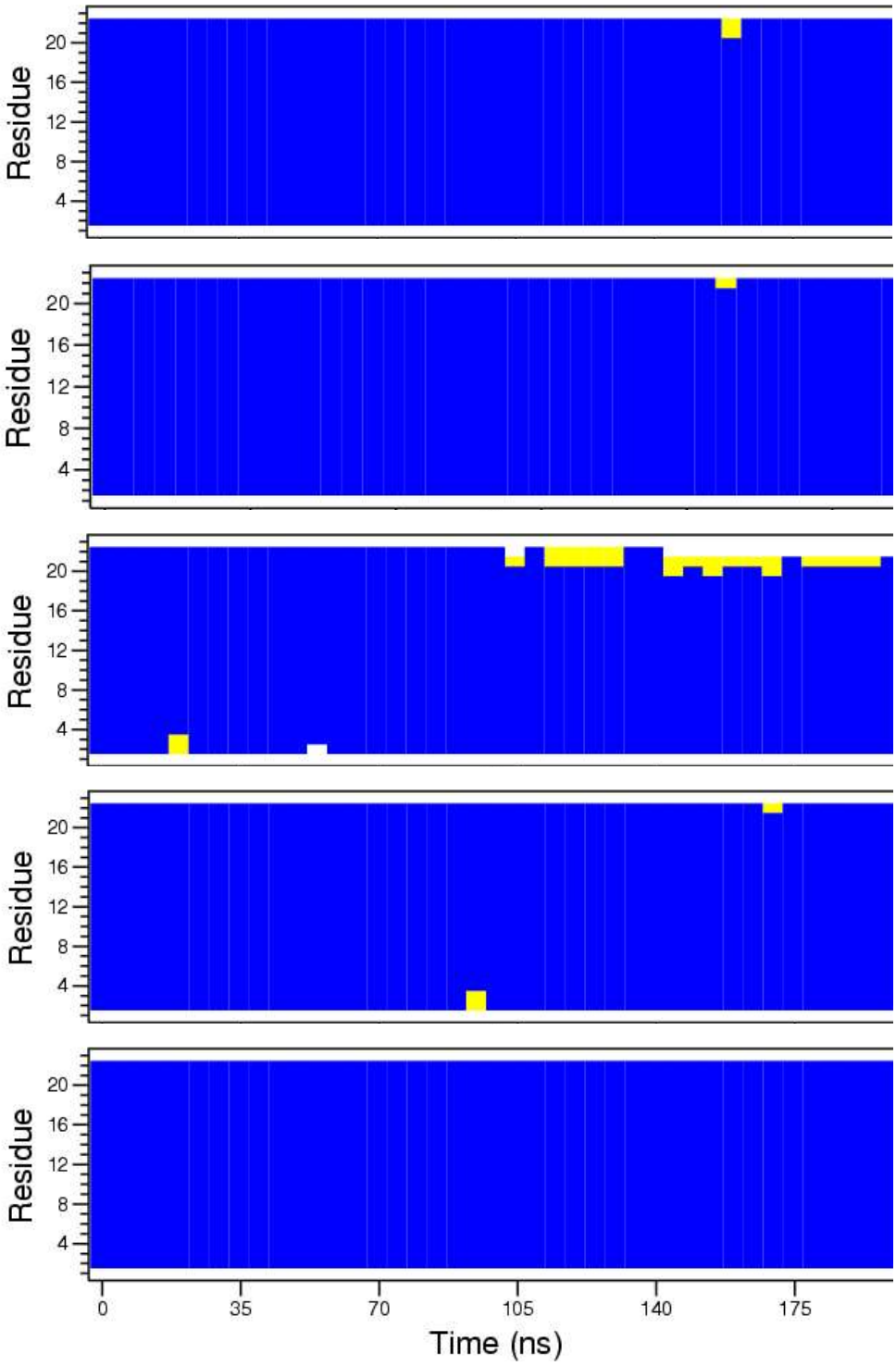
Table 1. Comparison of experimental and experiment-like ^{2}H quadrupolar splittings.

Peptide	*Simulation number*	*Experimental[¥] and calculated[§] ^{2}H quadrupolar splittings, kHz*			
		residue 11	*residue 12*	*residue 13*	*residue 14*
WLP23	1	52.7	0.7	-38.6	-9.8
	2	12.8	-15.2	-12.5	14.4
	3	43.5	13.7	-39.2	-23.8
	4	54.9	-33.8	-38.2	36.9
	5	-16.4	43.0	-14.6	-33.5
	Global	29.7	1.8	-28.8	-3.3
	Experimental	5.4	2.4	19.2	8.8
KLP23	1	-38.9	-25.0	60.3	-19.6
	2	-10.6	1.0	2.7	-13.1
	3	-0.6	13.0	-14.7	-20.9
	4	9.6	15.0	-25.1	-17.9
	Global	-9.8	1.4	5.2	-17.8
	Experimental	14.6	5.4	5.2	21.8

[¥] Taken from reference (33).

[§] Experiment-like splittings calculated using Equation 1. Absolute values were considered for comparison with experimental splittings.

A



B

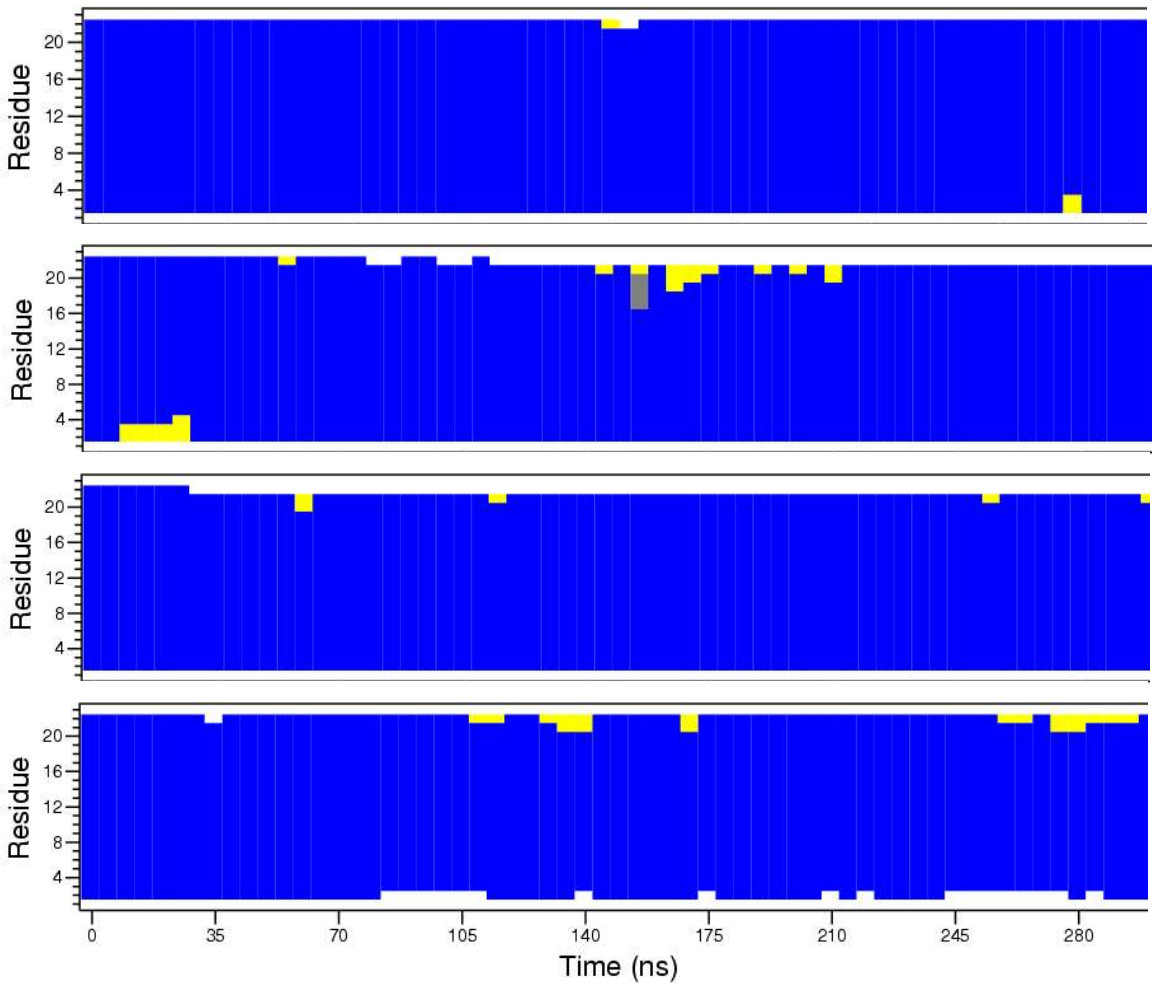


Figure 1. Secondary structure representation for the peptides WLP23 (A, simulations 1-5, from top to bottom) and KLP23 (B, simulations 1-4, from top to bottom) in DMPC bilayers. Blue colour stands for α-helix, yellow for turn and white for coil structures. The profiles were obtained with the help of standard GROMACS analysis tools, which use the DSSP algorithm (58).

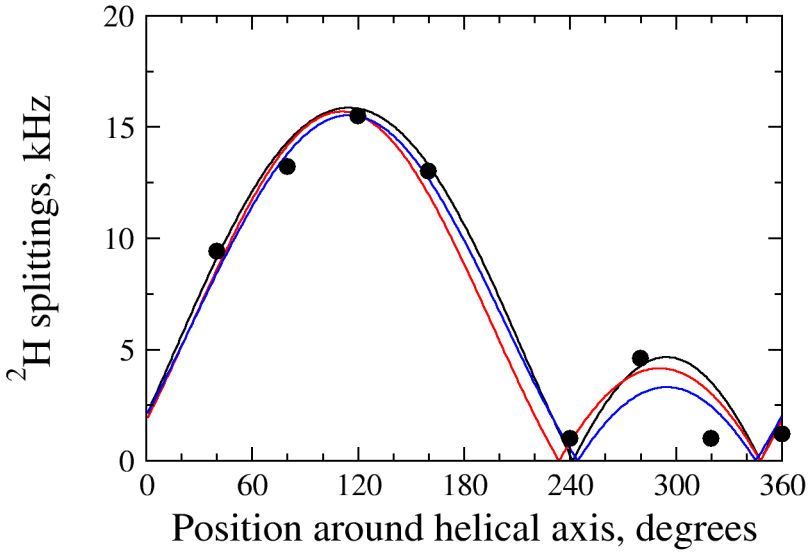


Figure 2. Best fit of theoretical quadrupolar splitting waves (Equation 2) to experimental values for WALP23 in DMPC (11). Black line: $\tau = 6°$, $\rho = 158°$, s.d.= 0.0°, error = 0.9 kHz and $\varepsilon_{\parallel} = 58.2°$. Red line: $\tau = 20°$, $\rho = 158°$, s.d.= 97°, error = 0.93 kHz and $\varepsilon_{\parallel} = 58.9°$. Blue line: $\tau = 30°$, $\rho = 158°$, s.d. = 111°, error = 0.96 kHz and $\varepsilon_{\parallel} = 59.8°$.