Supplementary Information (ESI) Soft Matter

Assessing the Extent of Structural and Dynamic Modulation of Membrane Lipids due to Pore Forming Toxins: Insights from Molecular Dynamics Simulations

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Table S1: System Details for ClyA and AHL Molecular Dynamics Simulations

	ClyA	AHL
System size (number of atoms)	526274	435739
Simulation box size - L (nm) × W (nm) × H (nm)	16.1 × 16.1 × 19.9	17.3 × 17.3 × 14.4
Number of DMPC lipid molecules	688	877
Number of water molecules	128832	99681
Run-times of simulations (ns)	500	500
Salt concentration (mM)	150	150
Number of Na^+ ions	623	449
Number of Cl^- ions	539	456
Temperature (K)	310	310
Pressure (bar, semi-isotropic)	1	1

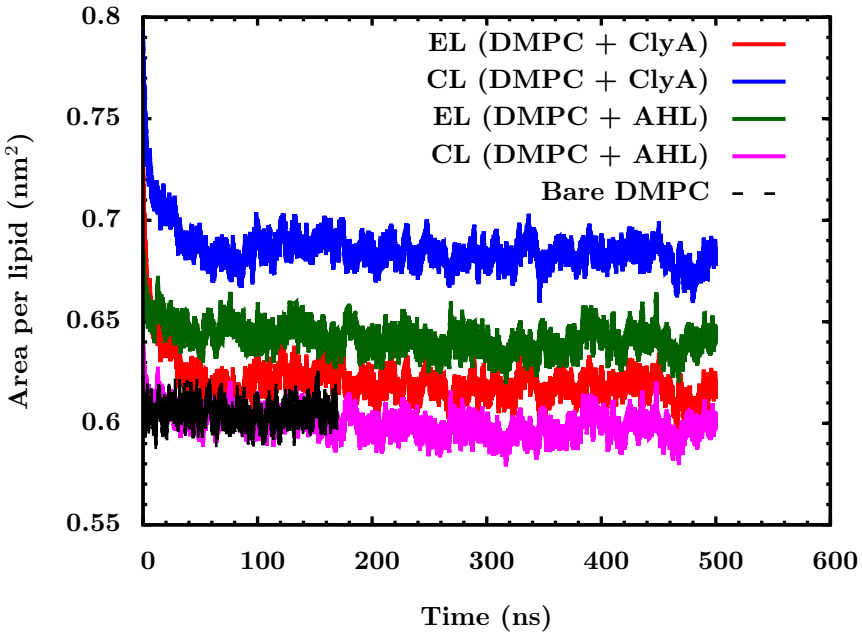

Figure S1: Area per lipid, a_l, for the PFT bound DMPC bilayer. The values of a_l indicate that areal fluctuations stabilize within the first 100 ns.

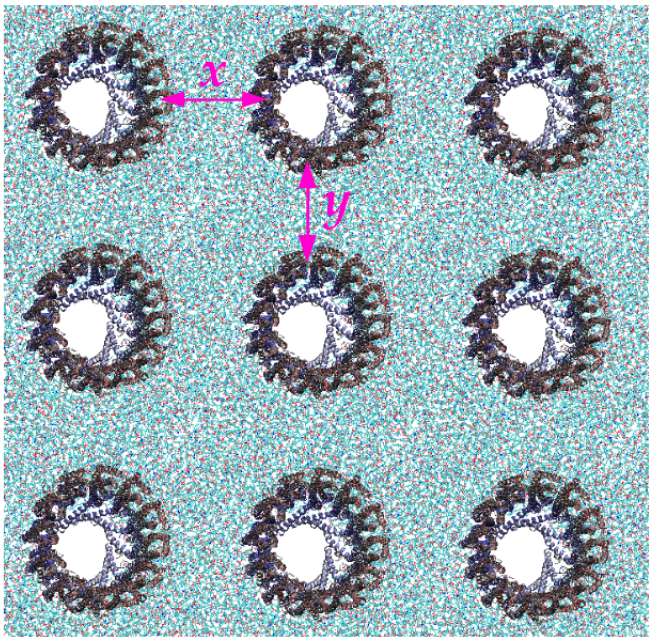

Figure S2: Periodic images of cytolysin A pores in the DMPC bilayer. The pores are separated at about 3.9 nm in the EL and 5.2 nm in the CL and are equidistant along the x and y directions.

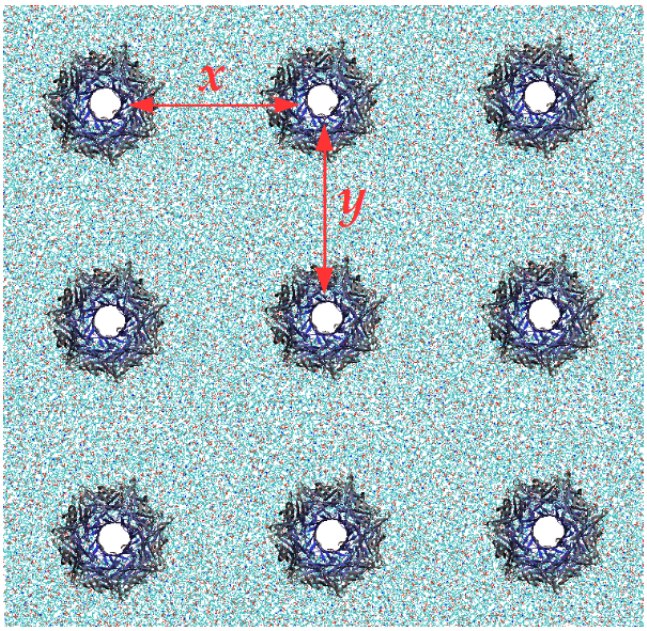

Figure S3: Periodic images of α-Hemolysin pores in the lipid bilayer. The pores are 6.4 nm away in the the EL and 6.8 nm away in the CL and are equidistant along the x and y directions.

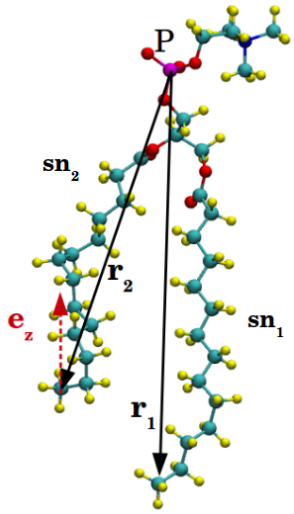

Figure S4: Illustration of the tilt angle subtended by the vector from the head group to the C-14 acyl carbon with the bilayer normal.

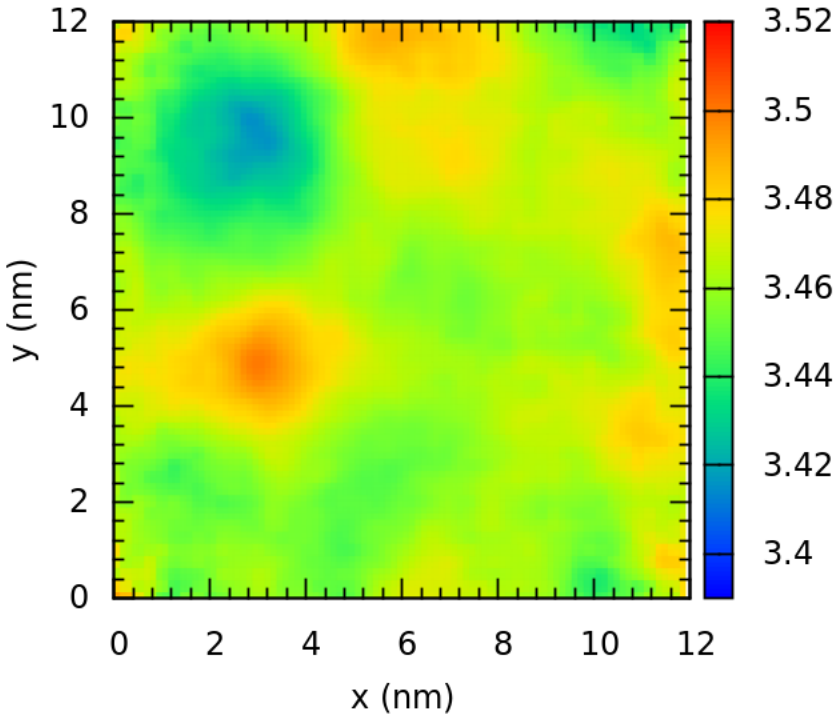

Figure S5: Thickness map of a bare DMPC bilayer at 310 K.

Table S2: Number of protein-membrane atomic contacts for the α-hemolsyin and cytolysin A pores. Values scaled to 100 with the maximum number of contacts are illustrated in Figures 11 & 13 of the main manuscript.

	AHL	ClyA
Protein-CL	25136.0 ± 999.4	85391.3 ± 2133.8
Protein-CL (headgroup)	6286.5 ± 480.1	15178.8 ± 965.6
Protein-CL (sn1)	11249.5 ± 689.9	36114.9 ± 1086.0
Protein-CL (sn2)	7600.0 ± 674.2	34097.6 ± 1520.1
Protein-EL	75643.0 ± 2055.8	75961.7 ± 1673.5
Protein-EL (headgroup)	44191.5 ± 1284.3	18828.7 ± 910.6
Protein-EL (sn1)	12667.0 ± 1047.5	25413.7 ± 1342.4
Protein-EL (sn2)	18784.4 ± 928.3	31719.3 ± 1443.6
Polar AA-CL	5170.8 ± 359.7	13310.0 ± 565.8
Polar AA-CL (headgroup)	2702.3 ± 283.1	2362.6 ± 401.8
Polar AA-CL (sn1)	1532.8 ± 228.8	6158.3 ± 350.4
Polar AA-CL (sn2)	935.7 ± 140.8	4789.1 ± 358.6
Polar AA-EL	37805.8 ± 1278.8	38686.3 ± 719.3
Polar AA-EL (headgroup)	25330.2 ± 885.2	13743.1 ± 612.8
Polar AA-EL (sn1)	4671.3 ± 523.8	10471.6 ± 612.4
Polar AA-EL (sn2)	7804.3 ± 441.3	14471.7 ± 655.9
Non-polar AA-CL	19965.2 ± 783.3	72081.3 ± 1773.6
Non-polar AA-CL (headgroup)	3584.2 ± 338.8	12816.1 ± 761.1
Non-polar AA-CL (sn1)	9716.6 ± 552.4	29956.6 ± 1024.0
Non-polar AA-CL (sn2)	6664.3 ± 574.7	29308.5 ± 1315.1
Non-polar AA-EL	37837.2 ± 976.6	37275.4 ± 1326.4
Non-polar AA-EL (headgroup)	18861.3 ± 521.3	5085.6 ± 399.8
Non-polar AA-EL (sn1)	7995.7 ± 694.7	14942.1 ± 967.9
Non-polar AA-EL (sn2)	10980.1 ± 663.1	17247.6 ± 943.0
RKWY-CL (headgroup)	828.1 ± 180.1	626.5 ± 129.9
RKWY-CL (sn1 & sn2)	76.0 ± 32.3	8258.6 ± 365.6
RKWY-EL (headgroup)	17048.5 ± 534.0	9261.4 ± 405.6
RKWY-EL (sn1 & sn2)	4697.8 ± 216.1	19612.9 ± 607.9