Electronic Supplementary Material (ESI) for Soft Matter.
This journal is © The Royal Society of Chemistry 2018

Supporting Information

Antimicrobial action of the cationic peptide, Chrysophsin-3: A coarse-grained molecular dynamics study

Andrea Catte,[a] Mark R. Wilson,[b] Martin Walker [b] and Vasily S. Oganesyan[a*]

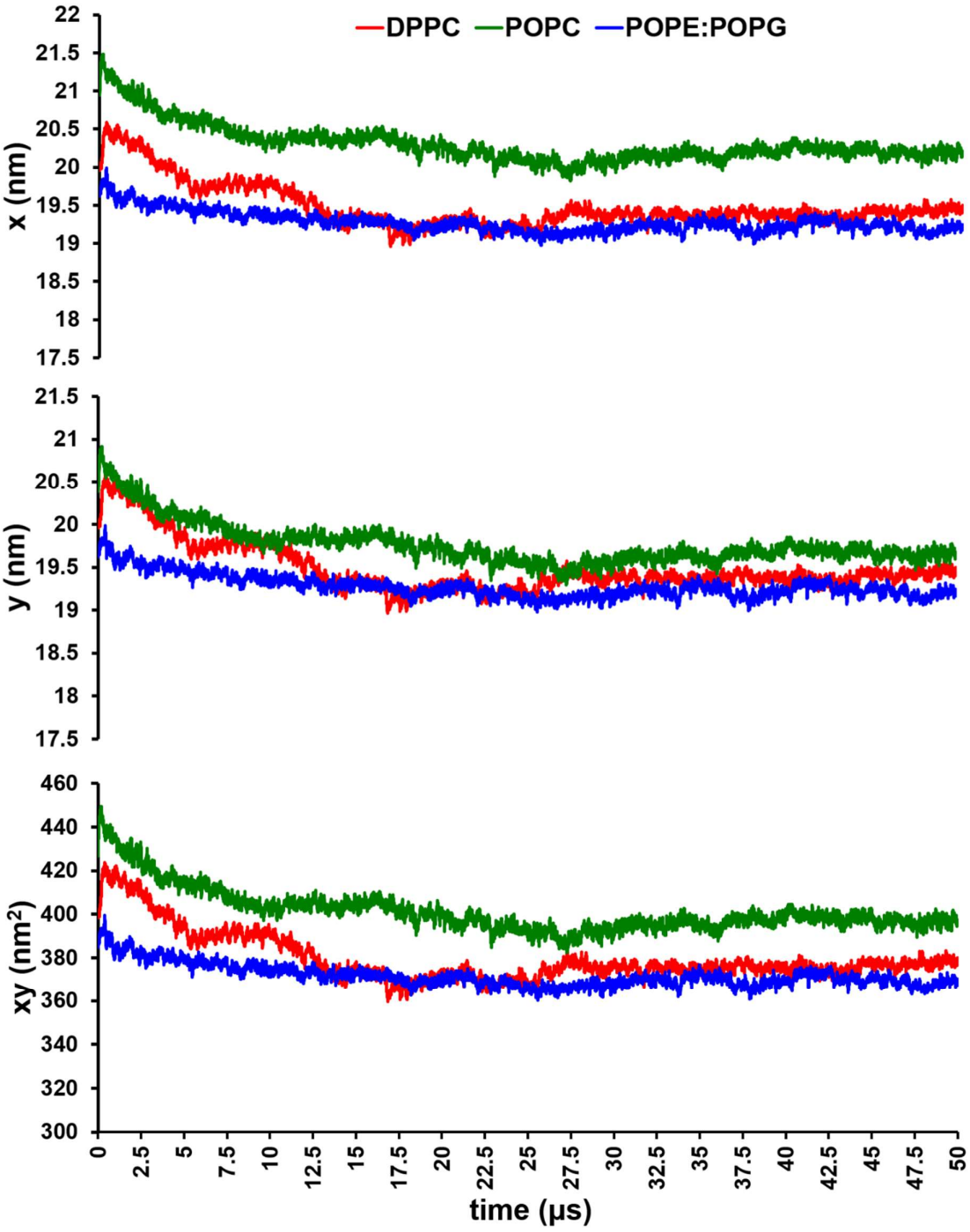


Figure S1 x, y and product of x and y box dimensions versus time of simulation from 50 μs CG MD simulations of the DPPC, POPC and POPE:POPG lipid bilayers containing 100 chrys-3 peptides and having a P:L molar ratio of 1:12. The formation of lipid protrusions is considered complete when each plot reaches a plateau.

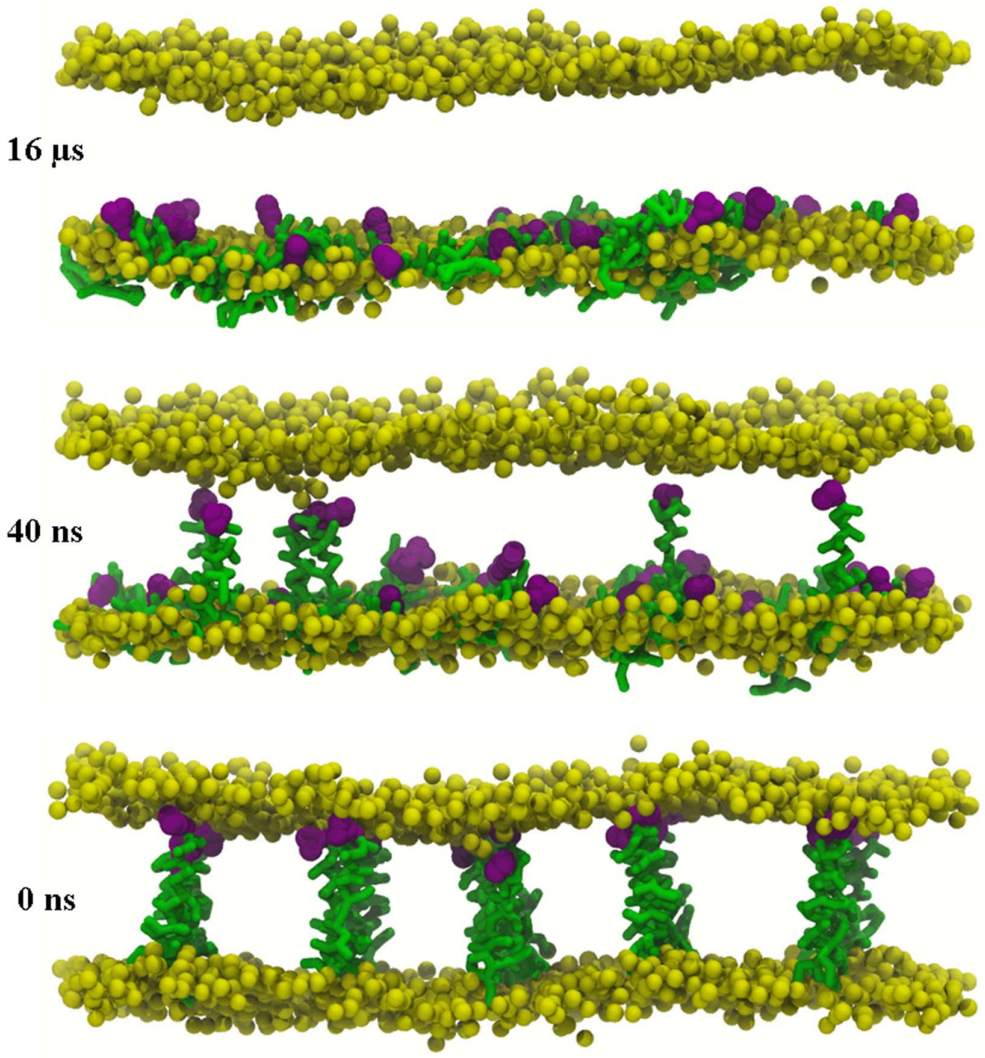


Figure S2 Snapshots of a 16 µs CG MD simulation of the POPC lipid bilayer containing 1125 lipids and 25 chrys-3 peptides in parallel orientation. Phenylalanine and the rest of chrys-3 residues are shown in purple and green representations, respectively. POPC polar head groups are shown in yellow space filling representation. POPC hydrophobic acyl chains are not shown for clarity.

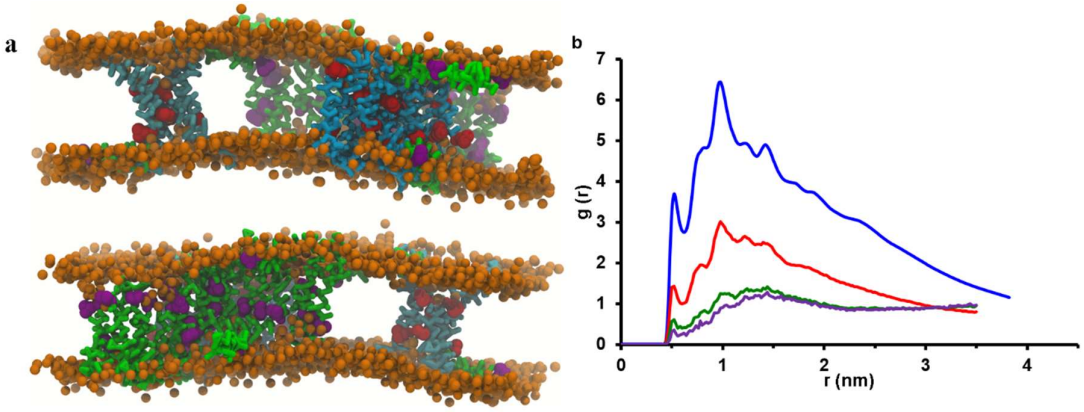


Figure S3 (a) Different views of the 50 μs CG structure of a DPPC lipid bilayer containing 1053 lipids and 50 chrys-3 peptides. Phenylalanine and the rest of the residues of surface and aggregate chrys-3 are shown in purple and green representations, respectively. Phenylalanine and the rest of the residues of pore forming chrys-3 peptides are shown in red and cyan representations, respectively. POPC polar head groups are shown in orange (b) Radial distribution functions of peptides backbone beads after 50 ns (purple), 100 ns (green), 1 μs (red) and over the last 20 μs (blue) of the simulation.

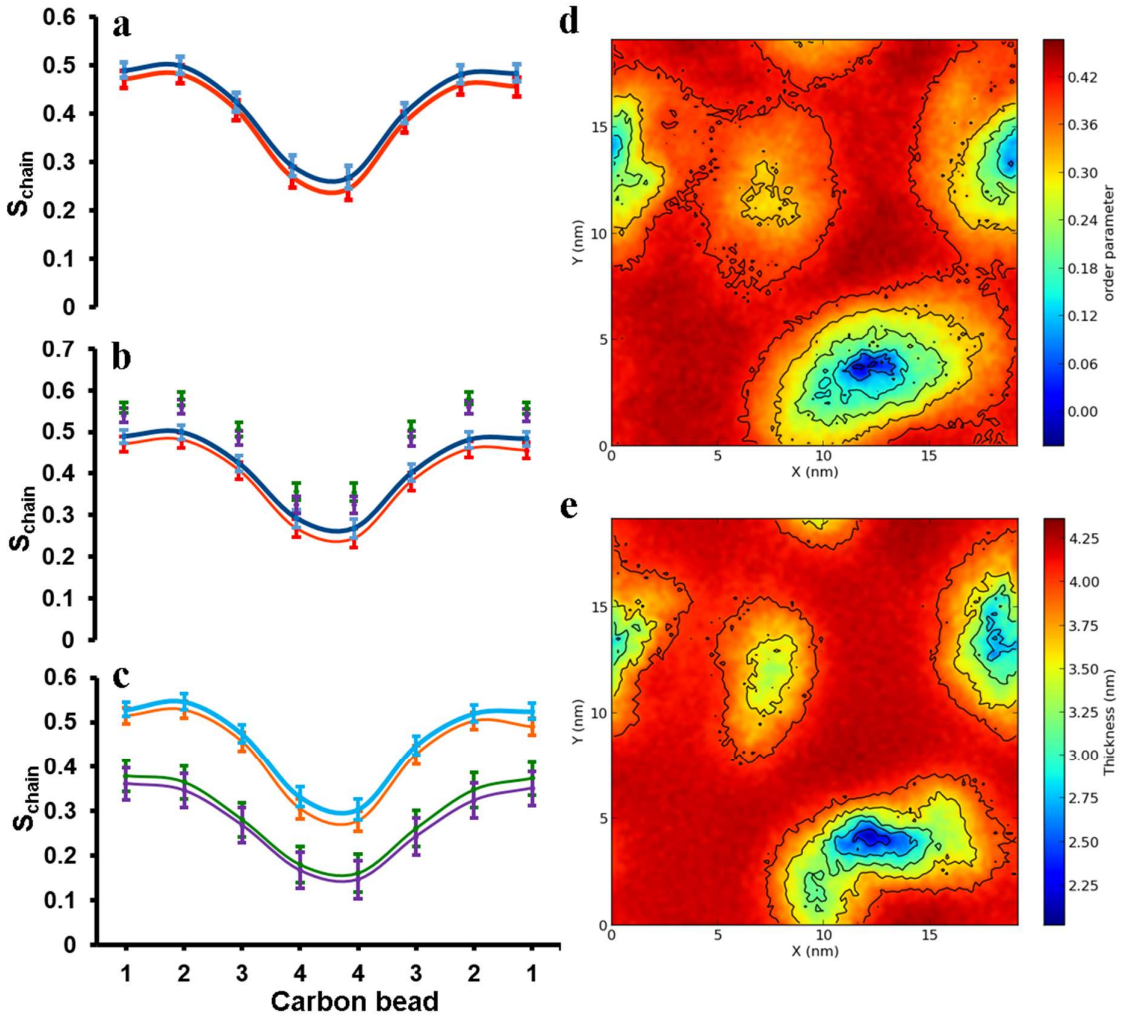


Figure S4 (a) Order parameters of DPPC sn-1 (skyblue) and sn-2 (red) acyl chains. (b) Comparison of order parameters displayed in (a) with those of sn-1 (blue) and sn-2 (green) acyl chains of a pure DPPC lipid bilayer CG MD simulated for 5 μs at 310 K and 1 atm. (c) Sn-1 (skyblue) and sn-2 (orange) acyl chains order parameters of bulk lipids are compared with correspondent sn-1 (green) and sn-2 (purple) order parameters of peptide lipids. Peptide lipids are defined as those lipids with at least one bead within 0.52 nm of any peptide bead. The order parameters of different bonds of each acyl chain belonging to upper and lower leaflets of the lipid bilayer are shown from left to right. (d) DPPC acyl chains average order parameter and (e) lipid bilayer thickness around chrys-3 peptides.

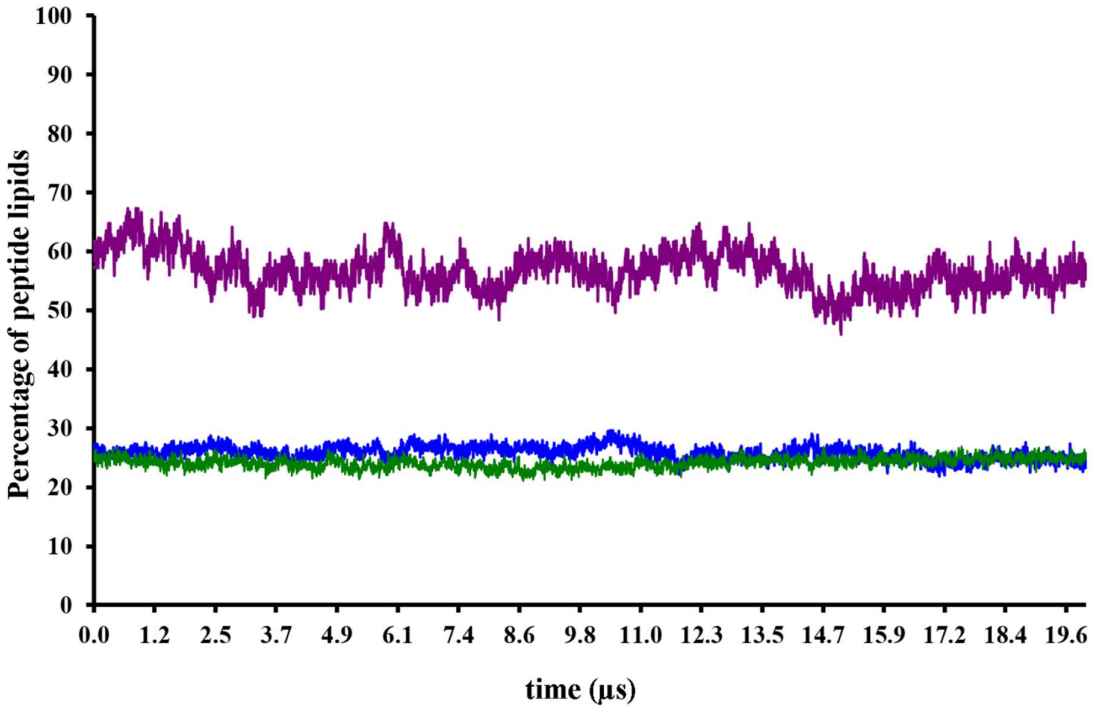
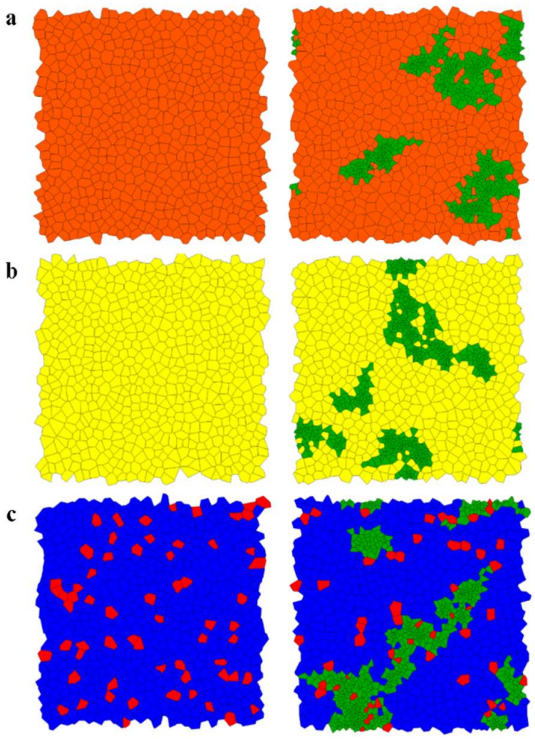


Figure S5 Percentage of peptide lipids interacting with chrysophsin-3 peptides over the last 40% of the simulation. A lipid is defined as a peptide lipid when at least one of its beads is within 0.52 nm of any chrys-3 beads. Results for POPC, POPE and POPG of peptide lipids are show in green, blue and purple, respectively.



Lipid	Area per lipid (nm^2) Outer leaflet	Inner leaflet
DPPC	0.608 ± 0.004	0.608 ± 0.004
DPPC + chrys-3	0.563 ± 0.005	0.587 ± 0.006
POPC	0.653 ± 0.002	0.651 ± 0.002
POPC + chrys-3	0.620 ± 0.005	0.625 ± 0.005
POPE	0.612 ± 0.003	0.617 ± 0.004
POPE + chrys-3	0.588 ± 0.006	0.600 ± 0.007
POPG	0.607 ± 0.018	0.615 ± 0.012
POPG + chrys-3	0.450 ± 0.020	0.465 ± 0.015

Figure S6 Voronoi diagrams from 50 μs CG MD simulations of DPPC (a), POPC (b) and POPE:POPG (c) lipid bilayers without and with 50 chrys-3 peptides. DPPC, POPC, POPE, POPG phosphates used to perform the Voronoi triangulation are shown in orange, yellow, blue and red, respectively. Chrys-3 peptides are shown in green. The areas per lipid are estimated over the last 40% of each simulation and their errors are standard deviations.

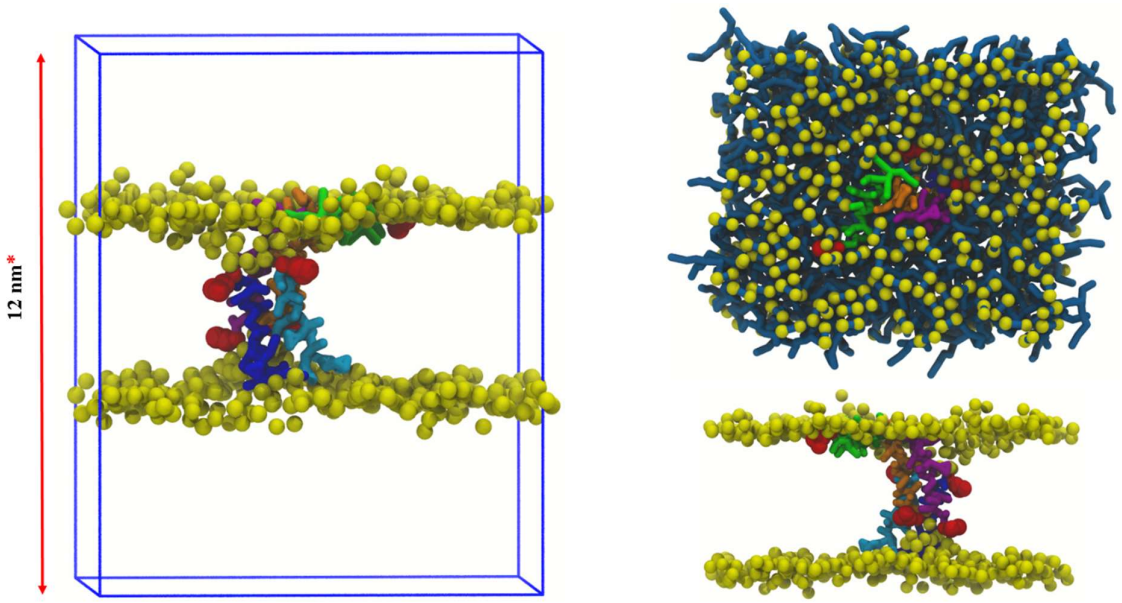


Figure S7 (Left) Size of the box used for umbrella sampling simulations. Transmembrane chrys-3 peptides forming a small disordered toroidal pore are shown in blue, cyan, purple and orange, respectively. The surface adsorbed peptide is shown in green. Phenylalanine residues are shown in red space filling representation. (Right) Top and side views of the starting system. The same colour code of Figure 1 is used for phosphate beads and acyl chains. The chrys-3 peptide shown in blue is subjected to different pulling forces in order to sample the different states of the peptide. The chrys-3 peptide shown in cyan is used as the reference peptide.

Figure S8 45 WHAM windows used for equilibration and production runs of umbrella sampling simulations, which were generated with a force constant of 2200 kJ mol^{-1} nm^{-2} and a spacing of 0.1 nm. The same colour code of Figure S6 is used.

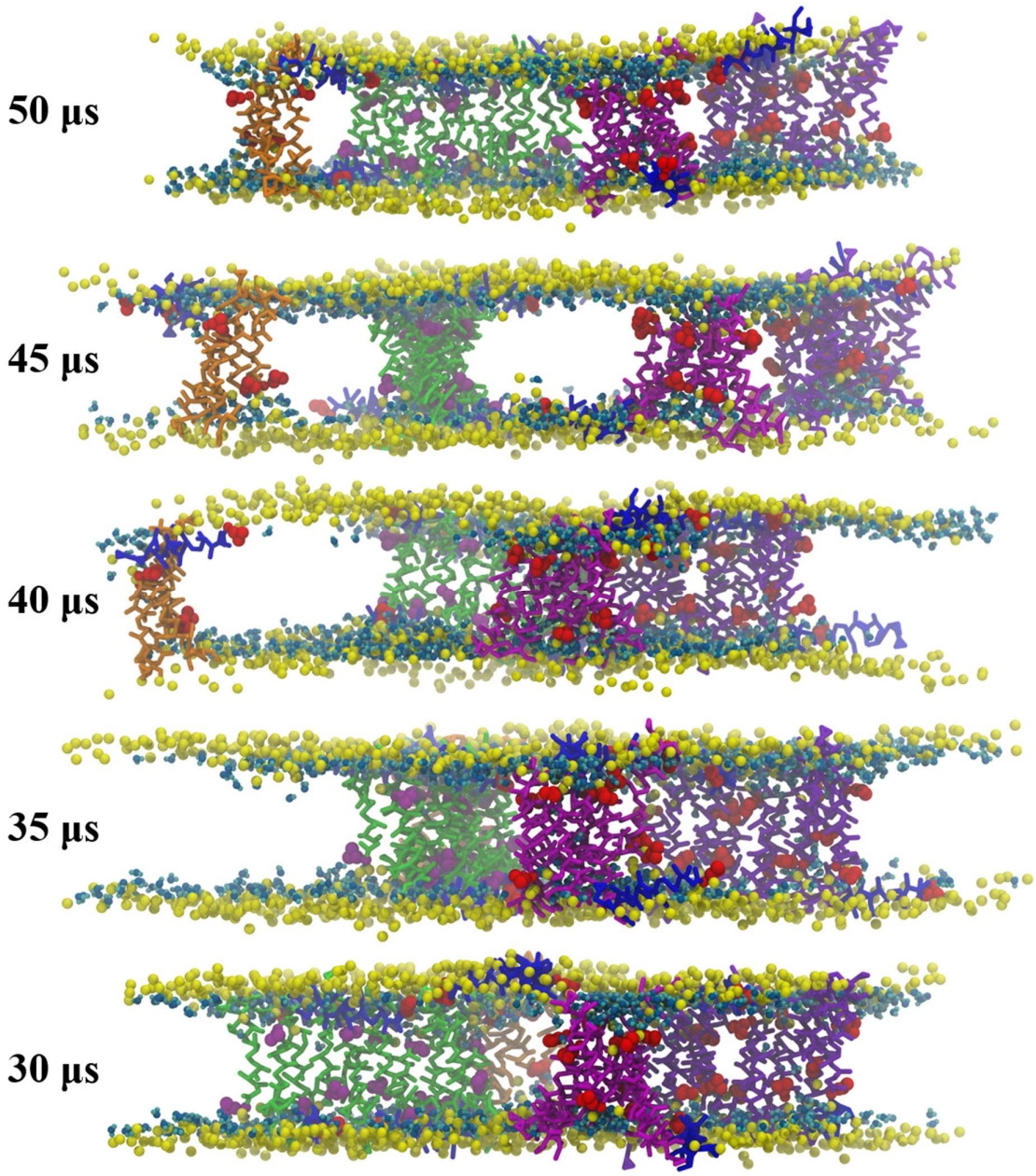


Figure S9 Snapshots from the 50 µs CG MD simulation of a POPC lipid bilayer with 50 chrys-3 peptides with polarizable CG water showing the permeation of water through the pores. The water is shown between the average positions of glycerol backbone beads GL1 and GL2 of POPC molecules in upper and lower leaflets of the lipid bilayer. W, WM and WP beads of polarizable coarse grained water molecules are shown in skyblue and cyan space filling representations, respectively. POPC phosphate beads are shown in yellow. Chrys-3 peptides belonging to the pores containing 4, 9 and 13 peptides are shown in orange, magenta and violet, respectively. Surface adsorbed chrys-3 peptides are shown in blue. Phenylalanine residues belonging to pores are in red. Chrys-3 peptides forming a peptide aggregate and their phenylalanine residues are shown in green and purple, respectively. POPC acyl chains are not shown for clarity.