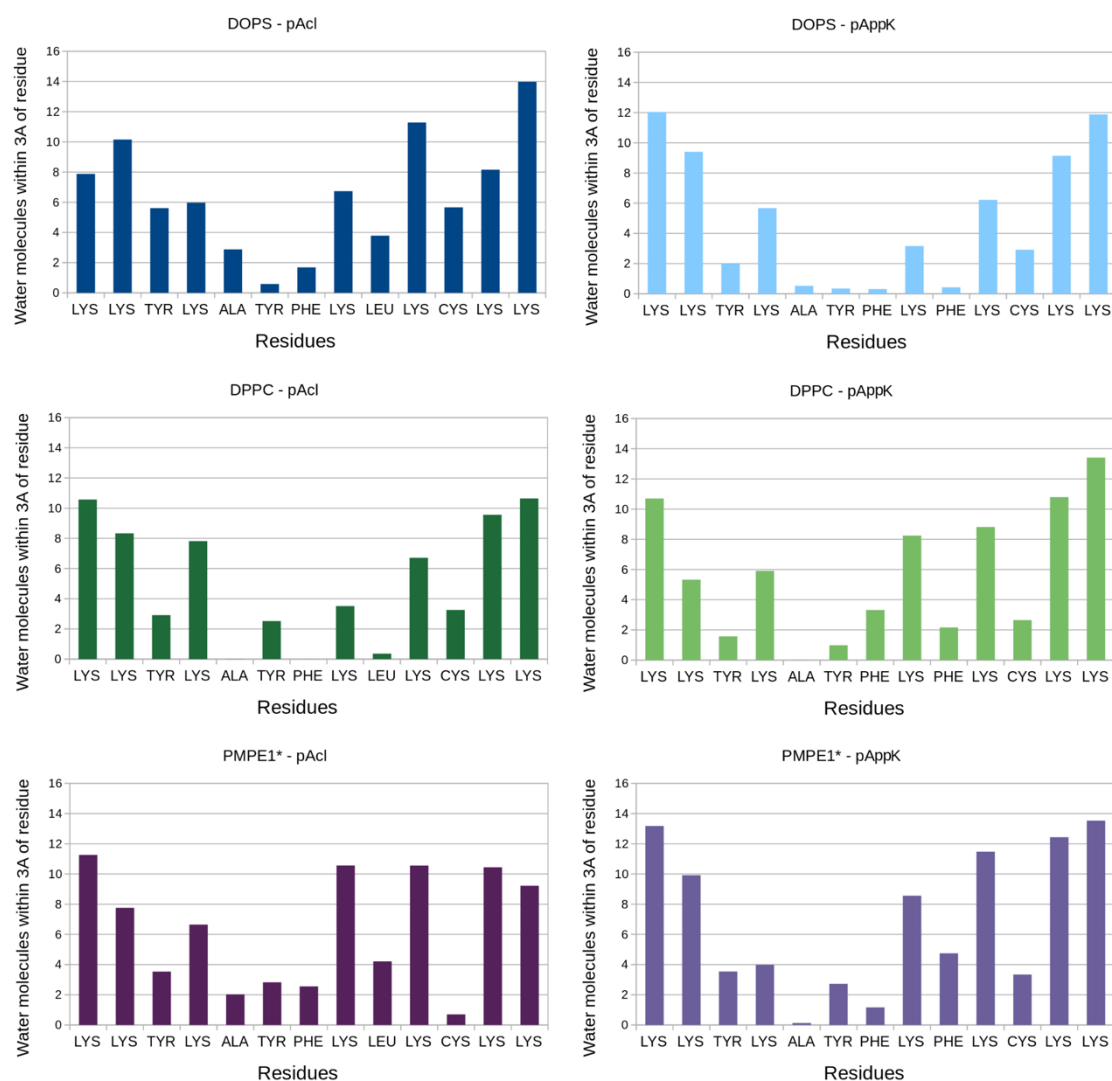
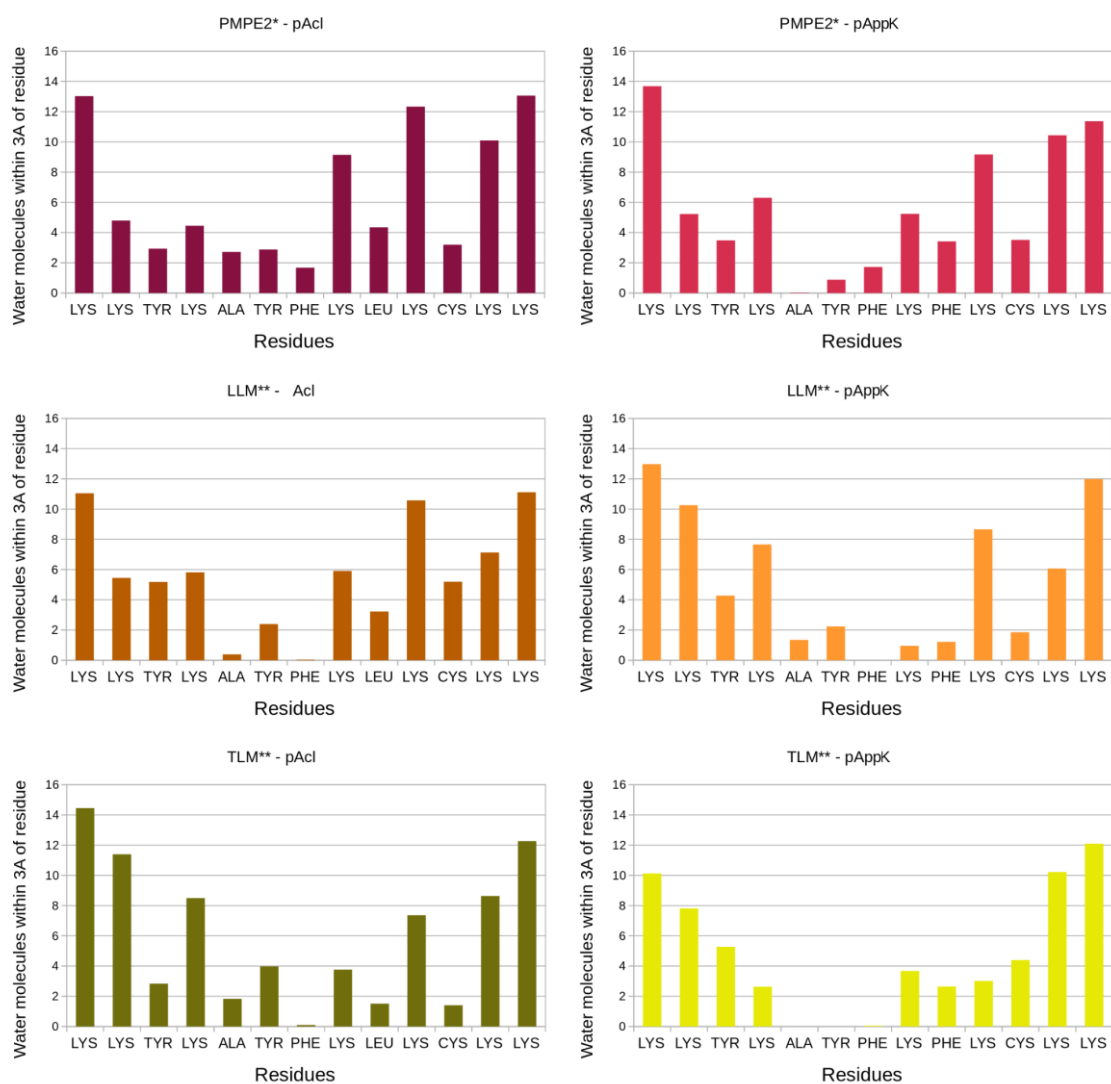


(a) (b)

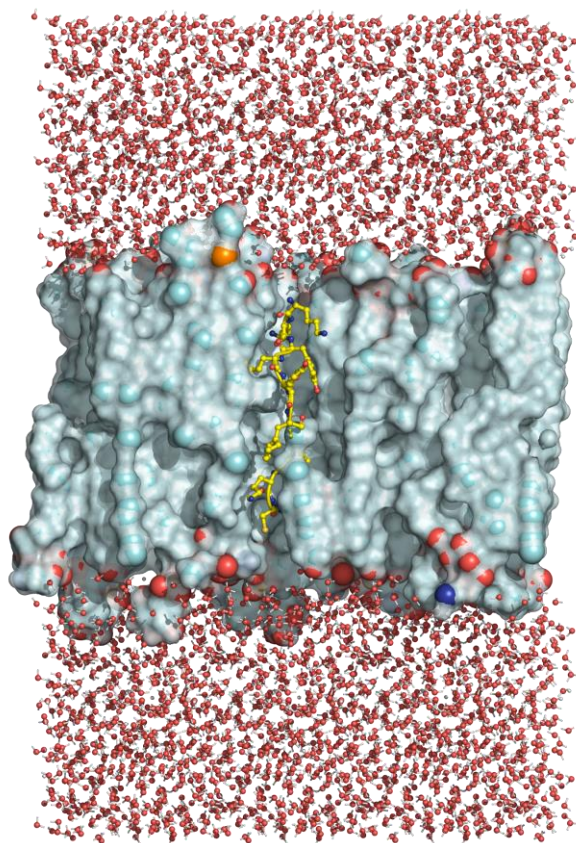
**Figure S1.** Chromatographic homogeneity and mass spectrometry analysis of the synthetic peptides. Mass spectra and chromatograms of (a) p-AppK and (b) p-Acl. The peptides show high purity degrees, and their mass was confirmed by ESI-IT MS analysis.



**Figure S2.** Number of water molecules whose oxygen atom is within 3.0 Å of any heteroatom of the p-Acl and p-AppK peptides in membrane models 1-3. PMPE (1\*) are the most dominant phospholipids in membrane 3.



**Figure S3.** Number of water molecules whose oxygen atom is within 3.0 Å of any heavy atom of the p-Acl and p-AppK peptides in membranes 4-6. The PMPE (2\*) is the most dominant phospholipid in membrane model 4. Membrane models 5 and 6 are constituted by a mixture of phospholipids, whose composition is given in tables S1 and S2; LLM\*\* Leukemia-like membrane, TLM\*\* Thymocytes-like membrane.



**Figure S4.** Representation of the DOPS model (membrane 1) used in this work with the p-Acl peptide located in the center of the bilayer (half of the membrane and water molecules were removed to visualize the peptide better).

**Table S1.** Composition of Membrane 5 (thymocytes-like membrane model). The percentage of each component is given in the first column, the name of the component in the second column and the abbreviation in the third column.

%	Name of component	Abbreviation
43%	Cholesterol	
20%	2,3-dipalmitoyl-d-glycero-1-phosphatidylcholine	DPPC
6%	2,3-distearoyl-d-glycero-1-phosphatidylcholine	DSPC
6%	2,3-dioleoyl-d-glycero-1-phosphatidylcholine	DOPC
4%	2,3-distearoyl-d-glycero-1-phosphatidylethanolamine	DSPE
4%	1,2-diarachidonyl-phosphatidylethanolamine	DAPE
e 4%	2,3-distearoyl-d-glycero-1-phosphatidylserine	DSPS
3%	2,3-dioleoyl-d-glycero-1-phosphatidylethanolamine	DOPE
3%	sphingomyelin d18;1/16;0	PSM
3%	Phosphatidylinositol	SAPI
2%	sphingomyelin d18;1/18;0	SSM
1%	2,3-dioleoyl-d-glycero-1-phosphatidylserine	DOPS
1%	2,3 dipalmitoyl-d-glycero-1-phosphatidylserine	DPPS

**Table S2.** Composition of Membrane 6 (leukemia-like membrane model). The percentage of each component is given the first column, the name of the component in the second column and the abbreviation in the third column.

%	Name of component	Abbreviation
24%	Cholesterol	
15%	2,3-dipalmitoyl-d-glycero-1-phosphatidylcholine	DPPC
10%	2,3-distearoyl-d-glycero-1-phosphatidylcholine	DSPC
9%	2,3-dilinoleoyl-d-glycero-1-phosphatidylcholine	DUPC
7%	2,3-dioleoyl-d-glycero-1-phosphatidylcholine	DOPC
7%	2,3-distearoyl-d-glycero-1-phosphatidylethanolamine	DSPE
6%	1,2-diarachidonyl-phosphatidylethanolamine	DAPE
4%	1,2-dipalmitoyl-sn-glycero-3-phosphorylethanolamine	DLiPE
4%	1-palmitoyl-2-oleoyl-inositol	POPI
3%	1-stearoyl-2-docosahexaenoyl-phosphatidylethanolamine	SDPE
3%	Phosphatidylinositol	SAPI
3%	2,3-dioleoyl-d-glycero-1-phosphatidylethanolamine	DOPE
3%	Phosphatidylinositol	SAPI
3%	2,3-distearoyl-d-glycero-1-phosphatidylserine	DSPS
1%	2,3-dioleoyl-d-glycero-1-phosphatidylserine	DOPS
1%	1-linoleoyl-2-Linolenoyl-Sn-Glycero-3-Phosphatidylserine	LLPS

**Table S3.** Molecular dynamics minimizations and equilibrations.

<b>Minimizations</b>
<pre>define = -DREST_ON -DSTEP integrator = steep emtol = 1000.0 nsteps = 5000 nstlist = 10 cutoff-scheme = Verlet rlist = 1.2 vdwtype = Cut-off vdw-modifier = Force-switch rvdw_switch = 1.0 rvdw = 1.2 coulombtype = pme rcoulomb = 1.2 ; constraints = h-bonds constraint_algorithm = LINCS</pre>
<b>Equilibrations</b>
<pre>define = -DREST_ON -DSTEP integrator = md dt = 0.002 nsteps = 50000 nstlog = 1000 nstxout = 1000 nstvout = 1000 nstfout = 1000 nstcalcenergy = 100 nstenergy = 1000 ; cutoff-scheme = Verlet nstlist = 20 rlist = 1.2 coulombtype = pme rcoulomb = 1.2 vdwtype = Cut-off vdw-modifier = Force-switch rvdw_switch = 1.0 rvdw = 1.2 ; tcoupl = berendsen tc_grps = PROT MEMB SOL_ION tau_t = 1.0 1.0 1.0 ref_t = 303.15 303.15 303.15 ;</pre>

```
pcoupl = berendsen
pcoupltype = semiisotropic
tau_p = 5.0
compressibility = 4.5e-5 4.5e-5
ref_p = 1.0 1.0
;
constraints = h-bonds
constraint_algorithm = LINCS
continuation = yes
;
nstcomm = 100
comm_mode = linear
comm_grps = PROT MEMB SOL_ION
;
refcoord_scaling = com
```