Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Effects of lipid composition on membrane distribution and permeability of natural quinones

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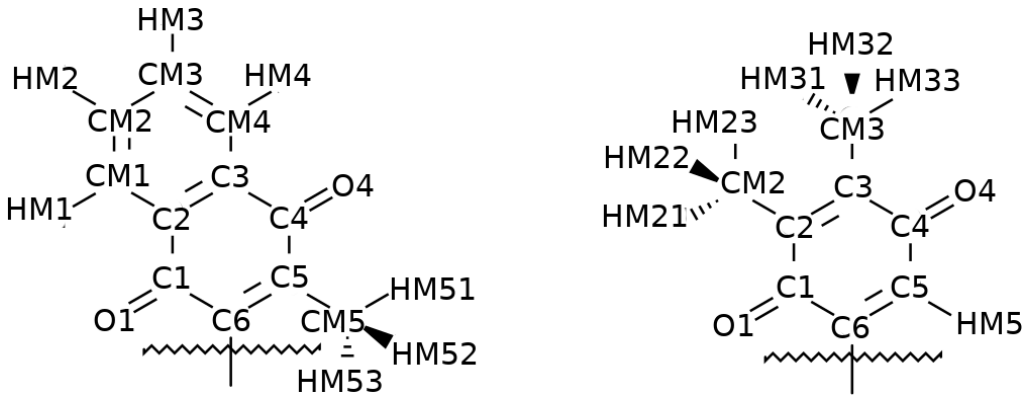

Figure S1: Atom names for PQ and MQ quinone heads.

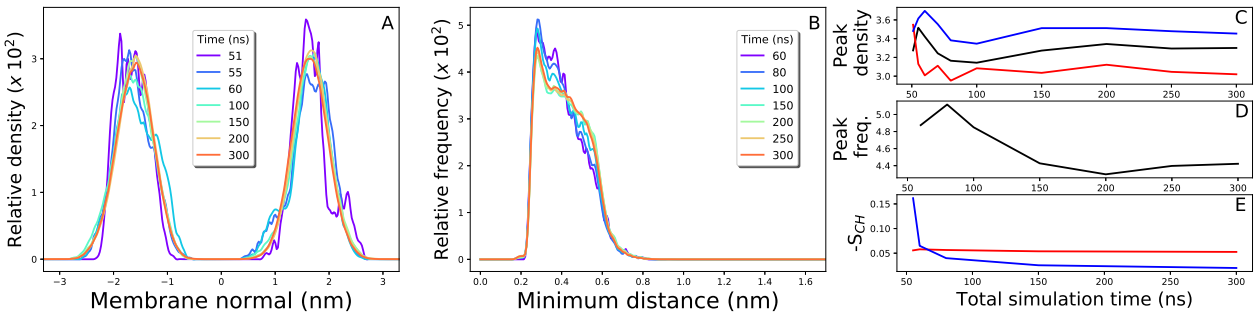

Figure S2: Convergence of calculated properties with total simulation time. Panel A shows the relative mass density of the UQ_{10} head along the membrane normal as in Fig. 2C, calculated for various simulation times as colored in the legend. Panel B shows the distribution of minimum distances between the UQ_{10} head oxygen O1 and DLPC+DLPE glycerol as in Fig. 3A for various simulation times. Panel C shows the peak of relative density ($\times 10^2$) for phosphate group of DLPC+DLPE in black, Q-head in red and Q-tail in blue. Panel D shows the peak of minimum distance ($\times 10^2$) between the UQ_{10} head oxygen O1 and DLPC+DLPE glycerol. Panel E shows the C_{10}-H bond vector order parameter for linoeoyl acyl chains (18:2, S_{CH} for C_{10}) average in red as in Fig. 5 and standard deviation in blue. The first 50 ns were discarded to allow for equilibration in the trajectories analyzed. Properties converge to within 1-2% of the longest-time values in 150 ns of simulation or less. Similar convergence behaviour was observed for other molecules and properties not shown here.

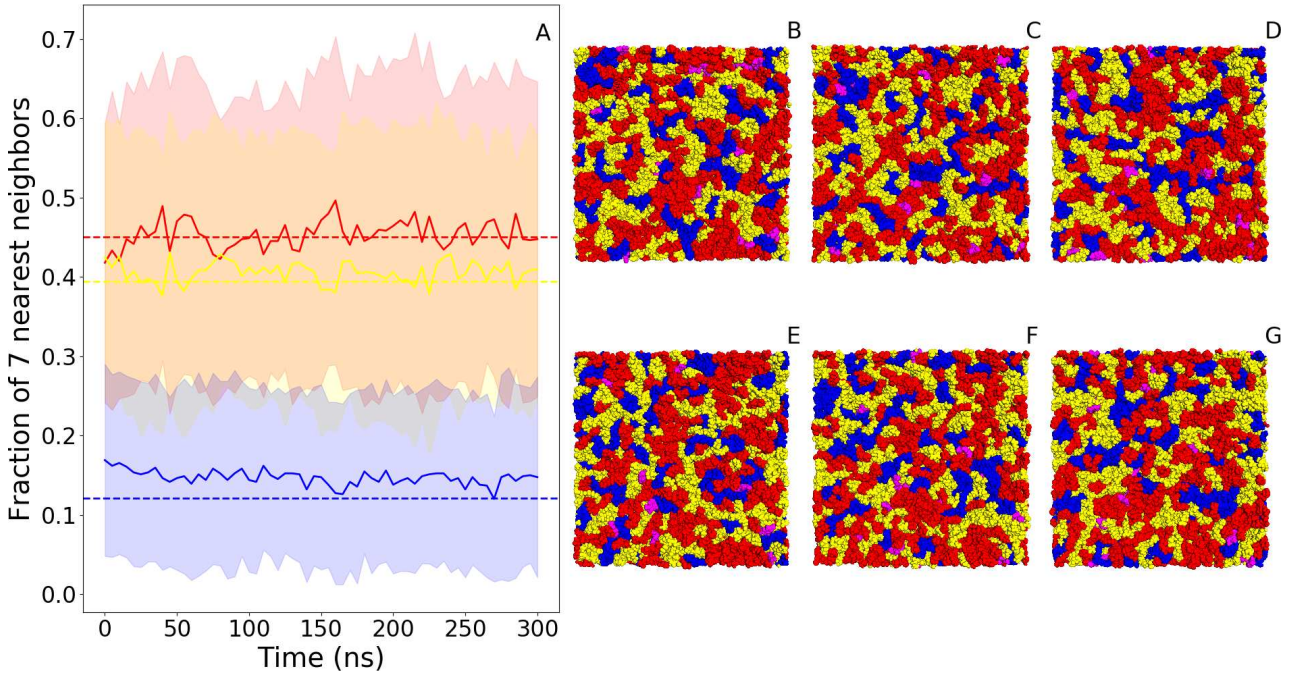

Figure S3: Multi-component membrane is well mixed. Panel A shows the average fraction of DLPC (yellow), DLPE (red) and LCL (blue) neighbors to DNPC (solid lines, with standard deviation in shadow) calculated as previously described.[76] Dashed lines show the expected fraction for an ideal mixture. Panels B-G show snapshots from 50 to 300 ns separated by 50 ns for the upper leaflet with lipids colored as in panel A plus magenta for UQ_{10}. No lipid clusters or domains are observed.

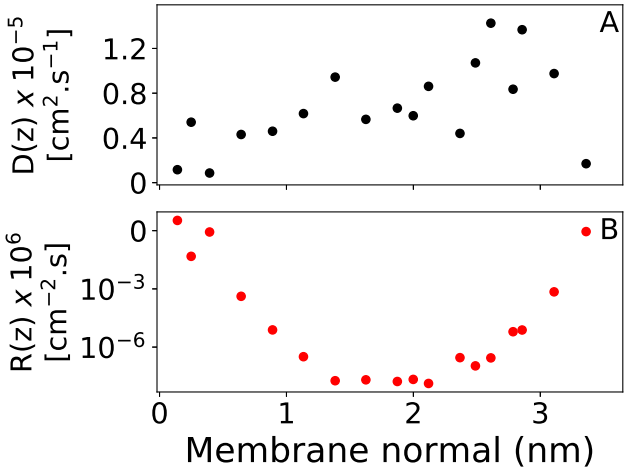

Figure S4: Coefficients of local transversal diffusion [panel A, $D(z)$] and local resistance [panel B, $R(z)$] for UQ_2 permeation along the membrane normal (z). As previously described,[60,61] coefficients were calculated by $D(z) = \frac{var(z)}{\tau}$ and $R(z) = exp[\frac{\Delta G(z)}{RT}]D(z)^{-1}$ with the variance (var) and autocorrelation characteristic time (τ) of the normal coordinate z obtained from each US simulation window and symmetrized for the two leaflets. The diffusion profile is rather noisy because of the τ values, calculated by integration of the autocorrelation function. Nevertheless, τ values have small contributions to the resistance profile, which is determined mainly by the exponential free energy contribution, $\Delta G(z)$. A permeation coefficient may be calculted as $P^{-1} = \int R(z)dz$, integrated in the membrane range z=[-3.0,3.0] nm to give P=20 cm s^{-1}. To our knowledge, there is no experimental value for Q permeation to compare with.

Table S1: Atomic types and partial charges for PQ and MQ quinone heads. See figure S1 for atom names.

PQ head		
Atom name	Atom Type	Partial Charge
C5	CA	-0.0575
C6	CA	-0.0575
C4	CA	0.57
O4	O	-0.57
C3	CA	-0.115
HM5	HP	0.115
C2	CA	-0.115
C1	CA	0.57
O1	O	-0.57
CM3	CT3	-0.155
HM31	HA3	0.09
HM32	HA3	0.09
HM33	HA3	0.09
CM2	CT3	-0.155
HM21	HA3	0.09
HM22	HA3	0.09
HM23	HA3	0.09
MQ head		
Atom name	Atom Type	Partial Charge
C5	CA	0.09
C6	CA	0.09745
C4	CA	0.57
O4	O	-0.57
C3	CA	0.00
CM4	CA	-0.115
C2	CA	0.00
CM1	CA	-0.115
C1	CA	0.57
O1	O	-0.57
CM5	CQ31	-0.45745
HM51	HA3	0.09
HM52	HA3	0.09
HM53	HA3	0.09
CM3	CA	-0.115
HM3	HP	0.115
HM4	HP	0.115
CM2	CA	-0.115
HM2	HP	0.115
HM1	HP	0.115