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 linoleoyl 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. 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 $D(z) = \frac{\text{var}(z)}{\tau}$ and $R(z) = \exp\left(\Delta G(z)\right)D(z)^{-1}$ with the variance (var) and autocorrelation characteristic time ($\tau$) 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 $\tau$ values, calculated by integration of the autocorrelation function. Nevertheless, $\tau$ 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 calculated 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     |