Supplementary Information for

The Effect of Lipid Oxidation on the Water Permeability of Phospholipid Bilayers

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Figure 1S. A scheme of the considered oxidation reaction.

oxidation ratio (%)	no. water molecules	no. DOPC molecules	no. OX1PC molecules	no. nonanal molecules	Simulation time [ns]
15	4810	108	20	20	100
30	4810	88	40	40	100
50	4810	62	66	66	200
58	4810	54	74	74	100
66	4810	44	84	84	100
75	4810	32	96	96	100
90	4810	10	118	118	100
100	4810	0	128	128	100

Table 1S. Composition of the oxidized bilayers considered in MD simulations. The bilayer with 100% of oxidation is taken from our previous work.¹¹



Figure 2S. The slopes derived from data seen on Fig.2 as a function of the oxidized lipid content in the lipid bilayer are compared.



Figure 3S. The slopes derived from data from Fig.4 as a function of the oxidized lipid content in the lipid bilayer.



Figure 4S. The figure shows parameters of osmotically-induced water flux through DOPC (\bullet) and eggPC (\blacksquare) liposomes. The calculated slopes for the upper panel are: 0.0548±0.005 (DOPC) and 0.0586± 0.03 (eggPC) and for the lower panel: 7.02±0.45 (DOPC) and 6.65±0.52 (eggPC).



Figure 5S. Area per lipid for membranes with different degree of oxidation as a function of simulation time.



Figure 6S. Penetration of water through the oxidized membrane. Interactions between water molecules and the polar moieties of selected oxidized lipids are highlighted. The system with 75% oxidarion ratio is depicted.