Supporting Information

Unraveling the Permeation of Reactive Species across Nitrated Membranes by Computer Simulations

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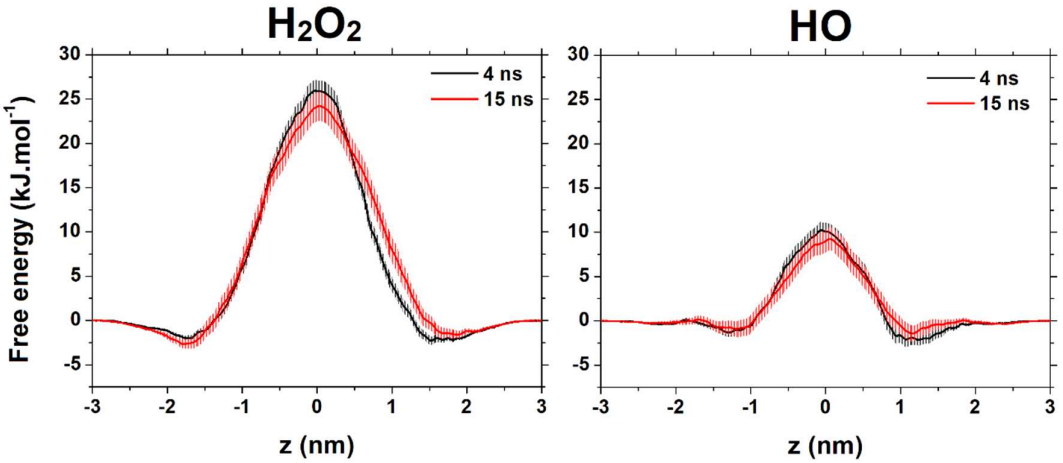

Figure S1. Comparison of the free energy profiles (FEPs) of the short US simulations (2 ns of equilibration and 4 ns of analysis) and long US simulations (15 ns of equilibration and 15 ns of analysis). The average of the ΔG values are represented as solid lines, and the uncertainties as vertical shadow lines. There are only small differences, which justifies our approach of using the shorter simulations, because of their much shorter calculation time (i.e., 5 days vs 24 days on computer time).

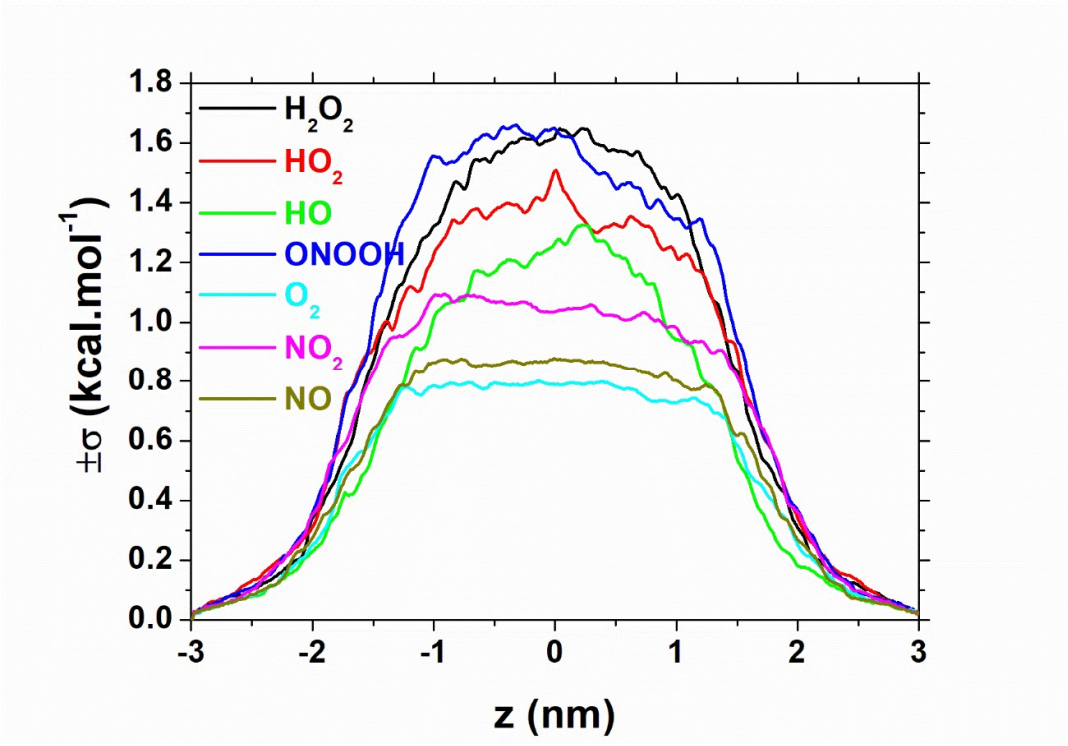

Figure S2. Calculated standard deviations of the free energy profiles (FEPs) based on the bootstrap values obtained for each five independent US simulations.

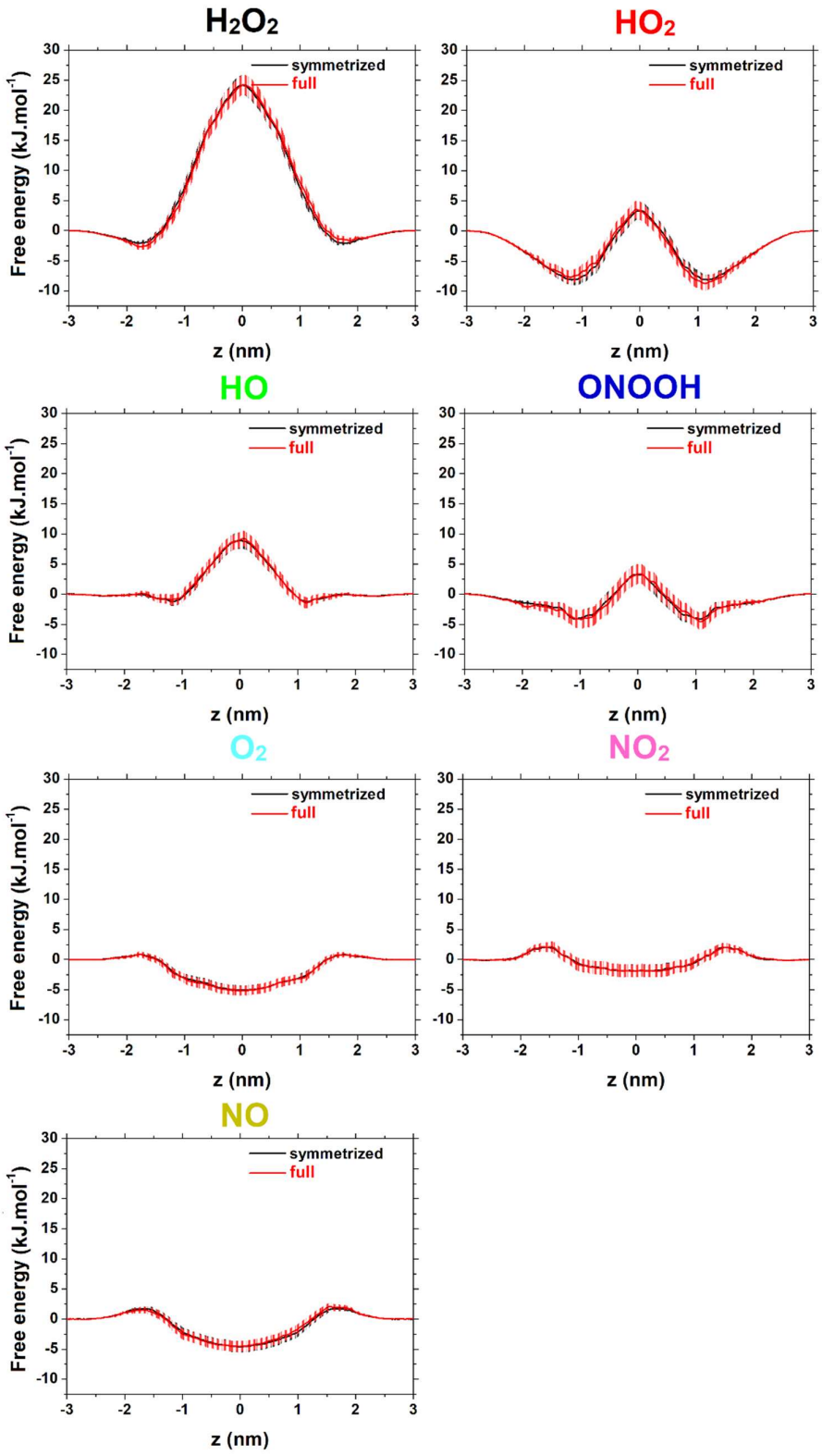

Figure S3. Comparison of the full (non-symmetrized) and symmetrized FEPs. The ΔG values were calculated from the last 4 ns of simulation of the short US simulations. The average of the ΔG values are represented as solid lines, and the uncertainties as vertical shadow lines. It is clear that the full and symmetrized FEPs are almost the same, which indicates the proper convergence of the US simulations.

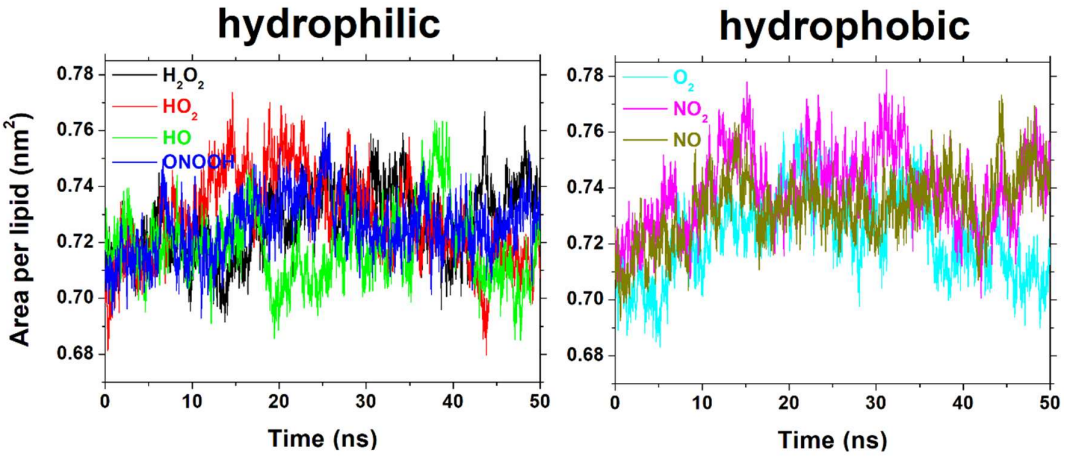

Figure S4. Temporal evolution of the area per lipid of the equilibrium simulations of the PLB with the various hydrophilic and hydrophobic RONS.

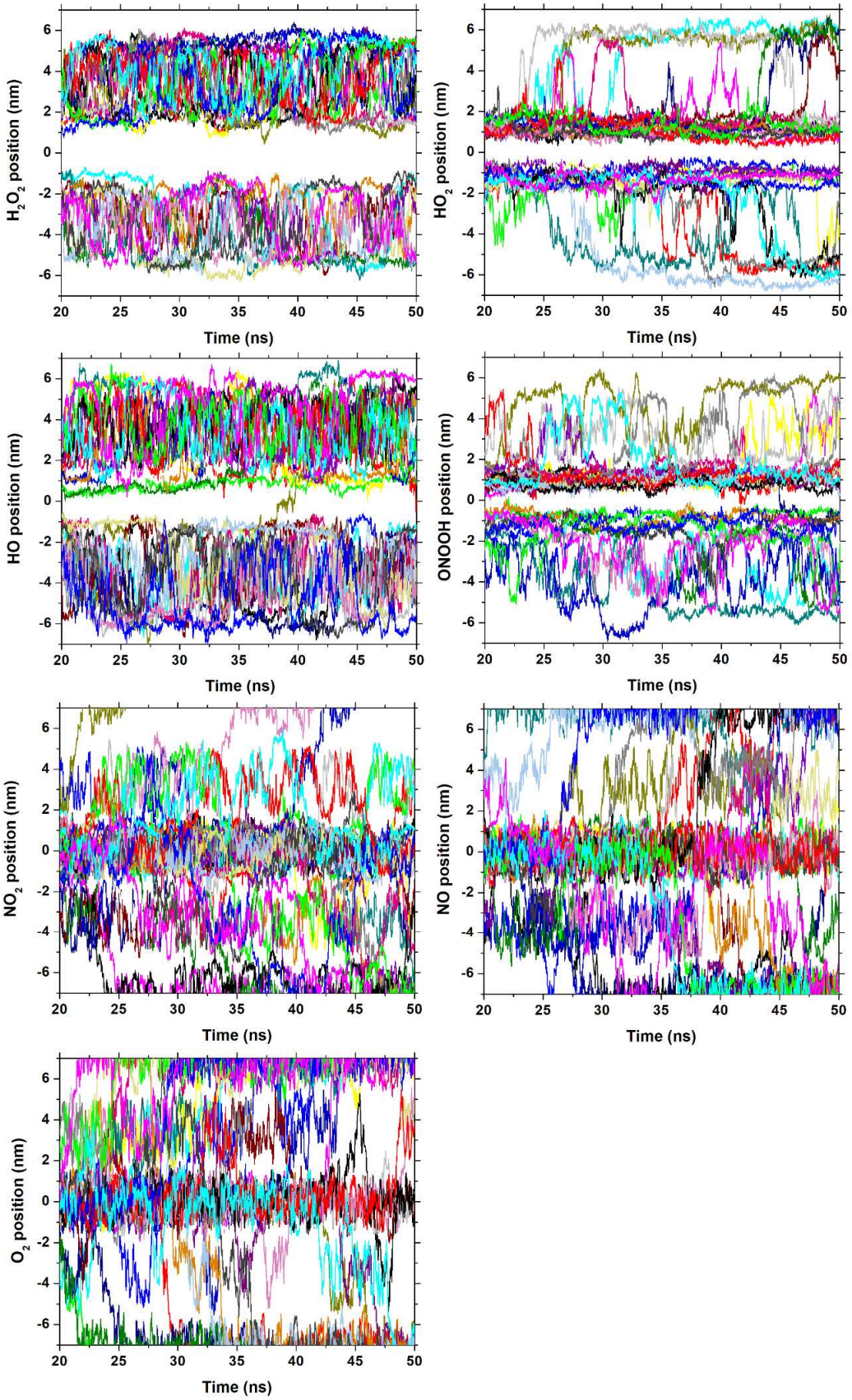

Figure S5. Time evolution of the trajectories of RONS obtained from the last 30 ns of the equilibrium simulations.