CORRECTION

Correction to: Atomistic Simulations Modify Interpretation of Spin-Label Oximetry Data. Part 1: Intensified Water–Lipid Interfacial Resistances

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In the print published article, Fig. 5 was published incorrectly. The correct figure is given below.

The curves in Fig. 5 panels A and C of the article should be identified as molecular dynamics (MD) simulation data from ref. 33, rather than as experimental nuclear magnetic resonance (NMR) data. In the combined experimental and simulation study of ref. 33, Prosser and colleagues found strong agreement between the MD oxygen concentration profile and O_2-induced ^{13}C paramagnetic shifts. In a follow-up 2011 study, Prosser and colleagues went on to estimate an experimental oxygen concentration profile along the bilayer depth through scaling of the paramagnetic shifts. The scaling was achieved by multiplying the paramagnetic shift values by a constant scaling factor calculated through fitting to MD simulation data for oxygen concentration and carbon atom location along the bilayer depth (M.S. Al-Abdul-Wahid, F. Evanics, R.S. Prosser. Biochemistry **50**:3975–83 (2011)). The resulting NMR-based oxygen concentration curve is compared with the MD-based curve of ref. 33 in **Corrected Fig. 5A**, below. The NMR-based curve (solid circles) shows headgroup-associated dips consistent with strong interfacial resistances (blue arrows).

Plotting the inverse curve, in **Corrected Fig. 5C**, reveals high sensitivity to the estimated scaling factor, such that the NMR-based profile is vertically "compressed" relative to the MD-based profile at the headgroup-associated peaks. Notably, however, the

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inverse-curve peaks occur in approximately the same bilayer-depth positions in both datasets, consistent with strong resistances at the water–lipid interface. In addition, these peaks occur beyond the points of maximum resistance estimated from electron paramagnetic resonance (EPR) oximetry experiments for 1-palmitoyl,2-oleoylphosphatidylcholine (POPC), indicated as blue dashed lines in **Corrected Fig. 5C**. Given the positioning of these peaks at the water–lipid interface and their increase in intensity relative to what would likely be observed by EPR oximetry, the NMR-based data presented in the corrected figure are consistent with the conclusions of the article. Specifically, the corrected figure supports the occurrence of strong, rate-limiting interfacial resistance peaks.
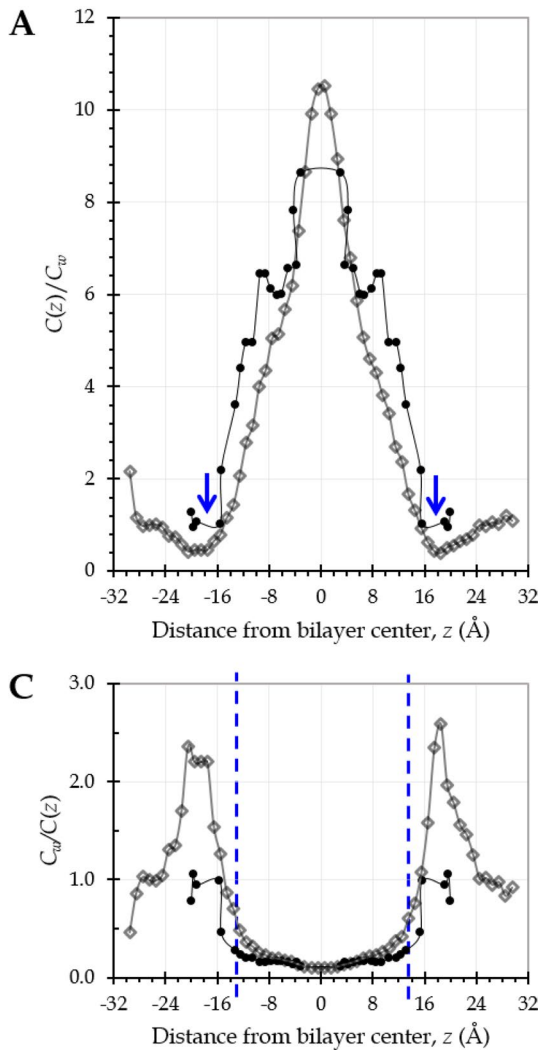
Corrected Fig. 5A, C. Experimental NMR-derived oxygen concentration profile suggests strong interfacial resistances. $C(z)$ is the oxygen concentration at each bilayer depth, z, and C_w is the average oxygen concentration in the aqueous phase. (**A**) Normalized oxygen concentration profiles, $C(z)/C_w$, equivalent to depth-dependent partition coefficient curves. Open diamonds represent the MD simulation dataset from ref. 33 originally replotted in Fig. 5 panels A and C of the article. Filled circles represent the NMR-based dataset, derived from a plot of estimated depth-dependent oxygen concentration reported in the 2011 follow-up study by Prosser and colleagues. There, experimental NMR O_2-induced paramagnetic shifts were transformed to O_2 concentrations using a fit to MD data (M.S. Al-Abdul-Wahid, F. Evanics, R.S. Prosser. Biochemistry 50:3975–83 (2011)). C_w is approximated as 23.7 mM, given an O_2 partial pressure of 30 bar in that study. Blue arrows mark headgroup-associated dips in oxygen concentration in the NMR-based curve, indicative of interfacial resistance spikes. Both curves relate to bilayers of the phospholipid 1-myristelaidoyl,2-myristoylphosphatidylcholine (MLMPC) at 318 K. (**C**) Inverse of the normalized oxygen concentration profiles shown in panel A, giving $C_w/C(z)$ profiles. $C_w/C(z)$ is equivalent to the oxygen concentration component of the resistance to permeation curve (see Eq. 5 in the article). Blue dashed lines indicate the approximate positions of peak resistance to oxygen permeation estimated in EPR studies of POPC at 298–318 K (ref. 11 of the article).