Molecular Simulations of Oxidised Phospholipids

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I will first provide a perspective of our prior work on oxidized lipids, which includes the first demonstration of reversal[1] and reorientation[2] of oxidized acyl chains in lipid bilayers, the pairing of cholesterol and fully oxidized lipid species in bilayers[3], and the unusual conformation of double-headed, 4-tailed Schiff base oxidized lipids[4]. In particular, I will focus on the protective property of cholesterol on oxidized membranes, and make the unusual claim that the protection arises not from the ordering effect of cholesterol, but from complementary shape factors of cholesterol and oxidized lipid species which drive them closer together, preventing membrane leakage by an excess of non-cylindrical surfactant-like polar lipids in the membrane. The simulations have consistently been complemented by biophysical experiments demonstrating a critical need for theoretical and experimental biophysicists to work together.

References:
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[3] **Khandelia, H.**, Loubet, B., Olzynska, A., Jurkiewicz, P., and Hof, M. (2014) Pairing of cholesterol with oxidized phospholipid species in lipid bilayers, *Soft Matter 10*, 639-647.
[4] Hermetter, A., Kopec, W., and **Khandelia, H.** (2013) Conformations of double-headed, triple-tailed phospholipid oxidation lipid products in model membranes, *Biochim. Biophys. Acta 1828*, 1700-1706.