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Use of molecular dynamics to assess the biophysiological role of hydroxyl groups in glycerol dyalkyl glycerol teraethers

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The cell membrane of some Archaea is constituted by lipids that span the whole membrane width and contain two alkyl chains bound by two glycerol groups (glycerol dyalkyl glycerol teraethers or GDGTs). These lipids confer stability to the membrane in mesophile to extremophile environments. Besides the more frequently studied isoprenoid archaeal lipids, both mono- and dihydroxy-GDGTs (OH-GDGT) have been recently reported to occur in marine sediments (1). OH-GDGTs contain up to two cyclopentane moieties and have been identified in both core and intact forms. In 2013, a correlation between OH-GDGTs and temperature was reported, with higher relative OH-GDGT abundances at high latitudes (2,3). The physiological function of the hydroxyl group in a GDGT is not yet known, but given the field results, it could be linked to an adaptation of the membrane to changes in temperature. For hydroxydiether lipid cores in methanogenic bacteria, it has been postulated that the hydroxyl group may alter the cell membrane properties: either extending the polar head group region or creating a hydrophilic pocket (4). It has also been suggested that the hydroxylation of the biphytany (l) moiety may result in enhanced membrane rigidity (1). To improve our understanding of the effect of the hydroxylation on physical properties of membranes, we performed molecular-dynamics simulations of GDGT membranes presenting and lacking these additional OH groups. This is an approach with a great development potential in the archaea lipid field, especially in relation to proxy validation. Our results indicate that the addition of an OH increases the membrane fluidity, thus providing an advantage in cold environments. We also observe a widening of the polar head group area, which could enhance transport.

1. Liu et al. 2012, GCA
2. Huguet et al. 2013, Org. Geochem
3. Fietz et al. 2013
4. Sprott et al. 1990. J. Biol. Chem. 265, 13735-13740.