Hydroxylation of glycerol dialkyl glycerol tetraethers may enhance membrane fluidity in Archaea adapted to cold environments.

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Abstract

Archaea have isoprenoid membrane lipids that span the whole membrane width and present two alkyl chains bound by two glycerol groups. These lipids are thought to confer stability and maintain the fluidity of the membrane in mesophile to extremophile environments. In addition to the traditionally studied isoprenoid archaeal lipids, mono- and dihydroxyl derivatives have been reported in recent years and their relative abundance shown to increase at lower temperatures. Therefore, even though the physiological function of the hydroxyl moiety is not yet known, it is expected to be linked to temperature. Here, we present an analysis of the properties of membranes formed by the archaea lipid acyclic glycerol dialkyl glycerol tetraether (GDGT-0) and its mono-hydroxylated variant (OH-GDGT-0). We use molecular-dynamics simulation to understand the differential physico-chemical properties conferred by this additional hydroxyl moiety to the membrane. While archaea lipids are ubiquitous, very few cultures are now available, rendering the *in silico* approach a suitable alternative to define the physico-chemical characteristics of isoprenoid lipids. We observe that the additional hydroxyl group forms hydrogen bonds mainly with the sugar moieties of adjacent lipids and with water molecules, effectively increasing the size of the polar head group. The hydroxyl addition also introduces local disorder that propagates along the alkyl chains, resulting in a membrane slightly more fluid. These changes might help maintain trans-membrane transport in cold environments, explaining why the relative abundance of hydroxylated archaea lipids increases at lower temperatures.