**Supplementary Text**

**Identification of core and intact polar lipids**

HPH-, PH-, DH-, MH- and C-GDGTs and C-archaeol (Suppl. Fig. 1) were identified by UHPLC-ESI-MSQ Exactive under reversed-phase conditions, and their characteristic fragment ions in MS/MS spectra were detected on samples at 120 and 140 m in KM1709\_S16 and 175 m in HOT296\_S2 (Suppl. Fig. 5 to 9). Core lipids were analyzed in both non-hydrolyzed and acid-hydrolyzed fractions. C-GDGTs with less polarity were the last eluting lipids with ammoniated [M+NH4]+, sodiated [M+Na]+ and protonated [M+H]+ molecules detected in MS spectra. Their MS/MS spectra were characterized by the protonated molecule [M+H]+ and product ions that resulted from loss of H2O, glycerol and/or biphytane moieties (Suppl. Fig. 5). C-archaeol was the first eluting compound with all three ions determined as well, the MS/MS fragmentation of which was characterized by product ion caused by loss of one phytane unit and the molecule [M+NH4]+ or [M+H]+ (Suppl. Fig. 6).

The second eluting compounds were HPH-GDGTs with ions [M+NH4]+, [M+Na]+ and [M+H]+ determined in MS spectra. The characteristic fragments in MS/MS spectra included product ions caused by loss of H2O, glycerol, hexose, the whole hexose-phosphate-hexose head group and/or biphytane units (Suppl. Fig. 7). PH-GDGTs were the third eluting compounds with only ion [M+H]+ containing SN ≥ 5 in MS spectra (Suppl. Fig. 8). The MS/MS fragmentation was conducted in PH-GDGTs enriched sample that was collected from sediment trap at 4000 m in station ALOHA. All precursors [M+NH4]+, [M+Na]+ and [M+H]+ were detected in the sediment trap sample and MS/MS fragmentation ions were characterized by the molecule [M+H]+ and product ions obtained from loss of H2O, glycerol, hexose, phosphate-hexose head group and/or biphytane units (Suppl. Fig. 8). We performed MS/MS fragmentation on the sample at 175 m of HOT296\_S2, which yielded fewer fragment ions (Suppl. Fig. 8). After the lipid cluster of PH-GDGTs, DH- and MH-GDGTs were eluted sequentially with ions [M+NH4]+ and [M+Na]+ detected in SN ≥ 5. The fragments in MS/MS spectra consisted of ions produced from loss of one (or two) hexose unit(s), H2O and/or glycerol (Suppl. Fig. 9 and 10).